



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

PDB ID : 1JYW  
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH PNPG  
Authors : Juers, D.H.; Matthews, B.W.  
Deposited on : 2001-09-13  
Resolution : 1.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

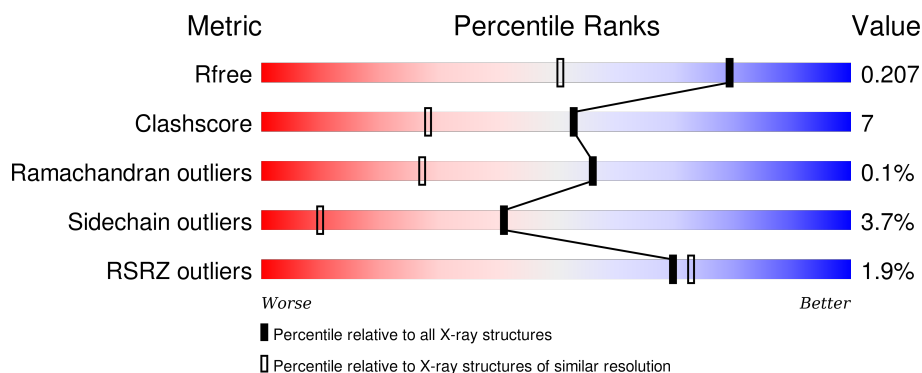
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1665 (1.58-1.54)
Clashscore	102246	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)
RSRZ outliers	91569	1668 (1.58-1.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	<div> <div>2%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
1	B	1023	<div> <div>%</div> <div>74%</div> <div>21%</div> <div>• •</div> </div>
1	C	1023	<div> <div>2%</div> <div>74%</div> <div>22%</div> <div>• • •</div> </div>
1	D	1023	<div> <div>3%</div> <div>73%</div> <div>21%</div> <div>• •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	A	8402	-	-	-	X
5	DMS	A	8404	-	-	-	X
5	DMS	A	8405	-	-	-	X
5	DMS	A	8406	-	-	-	X
5	DMS	A	8407	-	-	-	X
5	DMS	A	8412	-	-	-	X
5	DMS	A	8413	-	X	-	-
5	DMS	A	8415	-	X	-	-
5	DMS	A	8417	-	-	-	X
5	DMS	A	8419	-	-	-	X
5	DMS	A	8420	-	-	-	X
5	DMS	A	8423	-	-	-	X
5	DMS	A	8502	-	X	-	-
5	DMS	B	8402	-	X	-	-
5	DMS	B	8403	-	-	-	X
5	DMS	B	8404	-	-	-	X
5	DMS	B	8406	-	-	-	X
5	DMS	B	8407	-	-	-	X
5	DMS	B	8408	-	-	-	X
5	DMS	B	8415	-	X	-	-
5	DMS	B	8417	-	-	-	X
5	DMS	B	8420	-	-	-	X
5	DMS	B	8423	-	-	-	X
5	DMS	B	8502	-	-	-	X
5	DMS	B	8506	-	-	-	X
5	DMS	B	8508	-	-	-	X
5	DMS	C	8402	-	-	X	X
5	DMS	C	8404	-	-	-	X
5	DMS	C	8405	-	-	-	X
5	DMS	C	8406	-	-	-	X
5	DMS	C	8407	-	-	-	X
5	DMS	C	8412	-	-	-	X
5	DMS	C	8417	-	-	-	X
5	DMS	C	8419	-	-	-	X
5	DMS	C	8420	-	-	-	X
5	DMS	C	8423	-	-	-	X
5	DMS	C	8501	-	-	-	X
5	DMS	C	8506	-	-	-	X
5	DMS	C	8602	-	-	-	X
5	DMS	D	8404	-	-	-	X
5	DMS	D	8406	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	D	8407	-	X	-	X
5	DMS	D	8416	-	-	X	-
5	DMS	D	8417	-	-	-	X
5	DMS	D	8419	-	-	-	X
5	DMS	D	8423	-	-	-	X
5	DMS	D	8425	-	-	-	X
5	DMS	D	8501	-	-	-	X
5	DMS	D	8508	-	-	-	X
5	DMS	D	8705	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37524 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	2	0
			8127	5139	1441	1509	38			
1	B	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	C	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	D	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

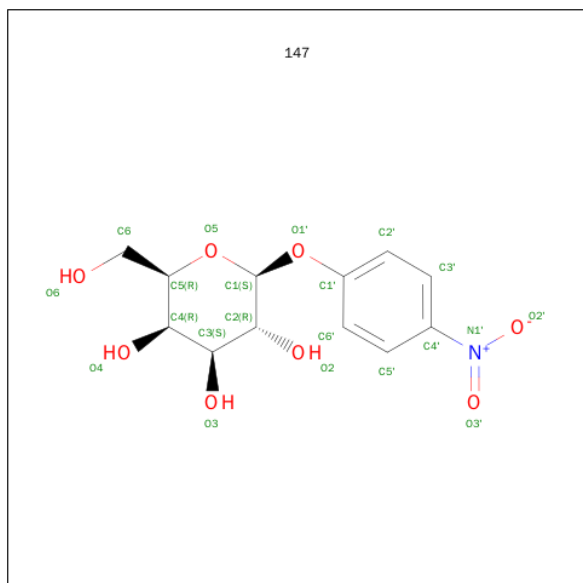
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	CLONING ARTIFACT	? P00722
A	2	SER	MET	CLONING ARTIFACT	? P00722
A	3	HIS	ILE	CLONING ARTIFACT	? P00722
A	4	MET	THR	CLONING ARTIFACT	? P00722
A	5	LEU	ASP	CLONING ARTIFACT	? P00722
A	6	GLU	SER	CLONING ARTIFACT	? P00722
A	7	ASP	LEU	CLONING ARTIFACT	? P00722
A	8	PRO	ALA	CLONING ARTIFACT	? P00722
A	537	GLN	GLU	ENGINEERED	? P00722
B	1	GLY	THR	CLONING ARTIFACT	? P00722
B	2	SER	MET	CLONING ARTIFACT	? P00722
B	3	HIS	ILE	CLONING ARTIFACT	? P00722
B	4	MET	THR	CLONING ARTIFACT	? P00722
B	5	LEU	ASP	CLONING ARTIFACT	? P00722
B	6	GLU	SER	CLONING ARTIFACT	? P00722
B	7	ASP	LEU	CLONING ARTIFACT	? P00722
B	8	PRO	ALA	CLONING ARTIFACT	? P00722
B	537	GLN	GLU	ENGINEERED	? P00722
C	1	GLY	THR	CLONING ARTIFACT	? P00722
C	2	SER	MET	CLONING ARTIFACT	? P00722
C	3	HIS	ILE	CLONING ARTIFACT	? P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	THR	CLONING ARTIFACT	? P00722
C	5	LEU	ASP	CLONING ARTIFACT	? P00722
C	6	GLU	SER	CLONING ARTIFACT	? P00722
C	7	ASP	LEU	CLONING ARTIFACT	? P00722
C	8	PRO	ALA	CLONING ARTIFACT	? P00722
C	537	GLN	GLU	ENGINEERED	? P00722
D	1	GLY	THR	CLONING ARTIFACT	? P00722
D	2	SER	MET	CLONING ARTIFACT	? P00722
D	3	HIS	ILE	CLONING ARTIFACT	? P00722
D	4	MET	THR	CLONING ARTIFACT	? P00722
D	5	LEU	ASP	CLONING ARTIFACT	? P00722
D	6	GLU	SER	CLONING ARTIFACT	? P00722
D	7	ASP	LEU	CLONING ARTIFACT	? P00722
D	8	PRO	ALA	CLONING ARTIFACT	? P00722
D	537	GLN	GLU	ENGINEERED	? P00722

- Molecule 2 is SUGAR (1-O-[P-NITROPHENYL]-BETA-D-GALACTOPYRANOSE) (three-letter code: 147) (formula: C<sub>12</sub>H<sub>15</sub>NO<sub>8</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	12	1	8		
2	B	1	Total	C	N	O	0	0
			21	12	1	8		
2	C	1	Total	C	N	O	0	0
			21	12	1	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			21	12	1	8		

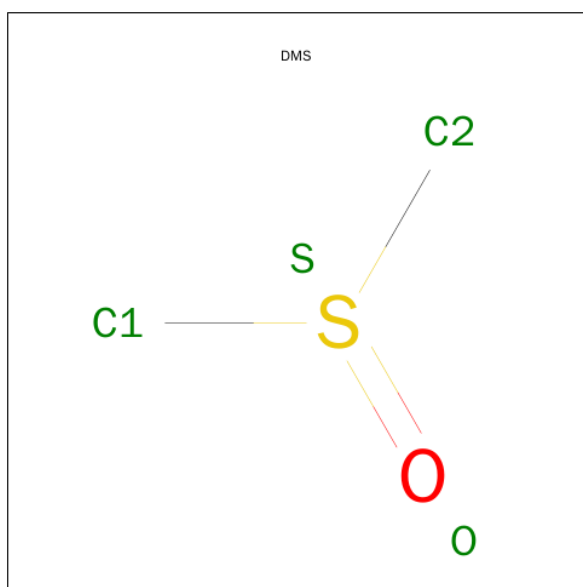
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	A	4	Total	Mg	0	0
			4	4		
3	D	4	Total	Mg	0	0
			4	4		
3	C	4	Total	Mg	0	0
			4	4		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Na	0	0
			4	4		
4	A	4	Total	Na	0	0
			4	4		
4	D	4	Total	Na	0	0
			4	4		
4	C	4	Total	Na	0	0
			4	4		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0

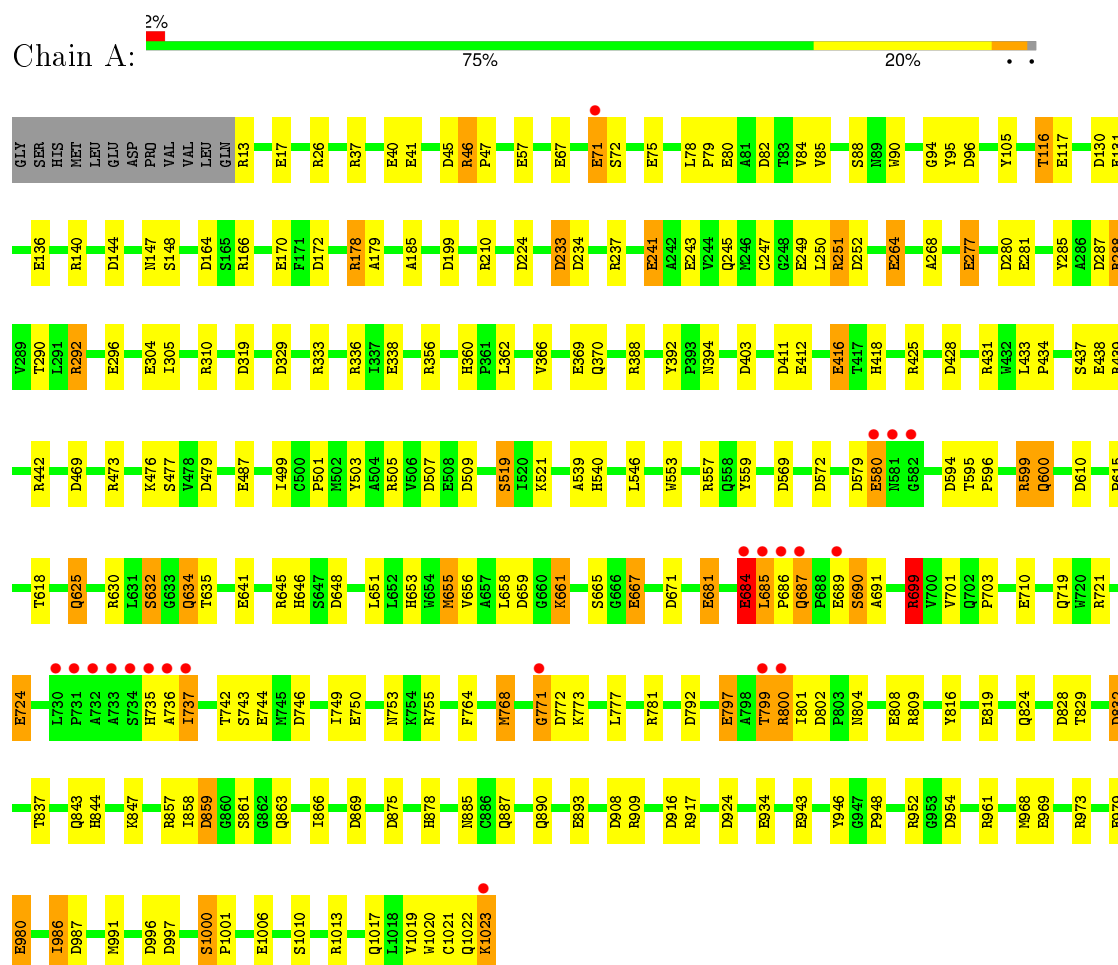
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1112	Total 1112	O 1112	0	0
6	B	1128	Total 1128	O 1128	0	0
6	C	1104	Total 1104	O 1104	0	0
6	D	1118	Total 1118	O 1118	0	0

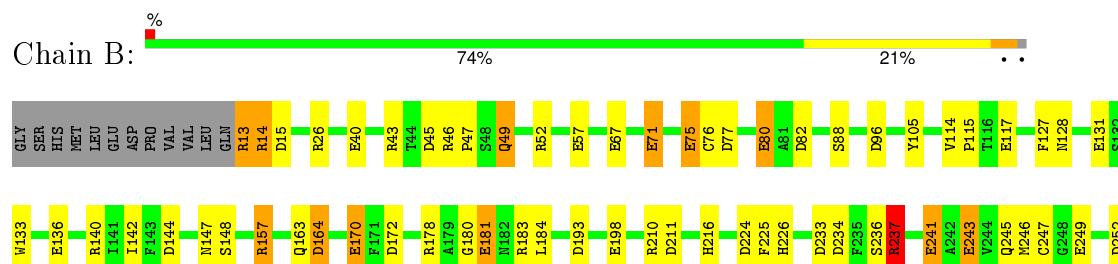
### 3 Residue-property plots

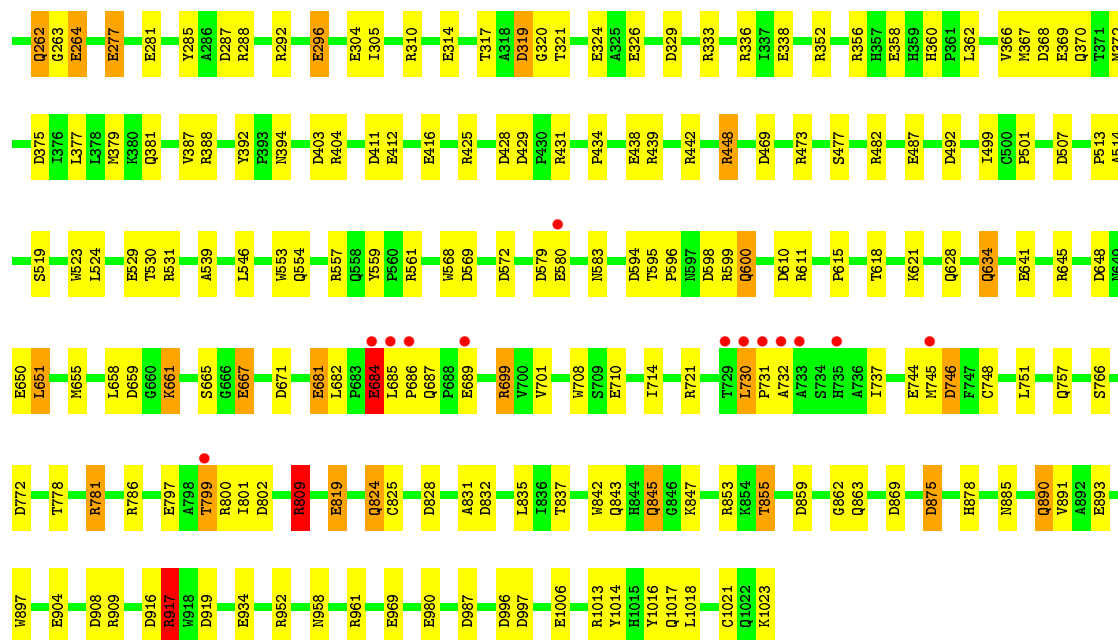
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Beta-Galactosidase

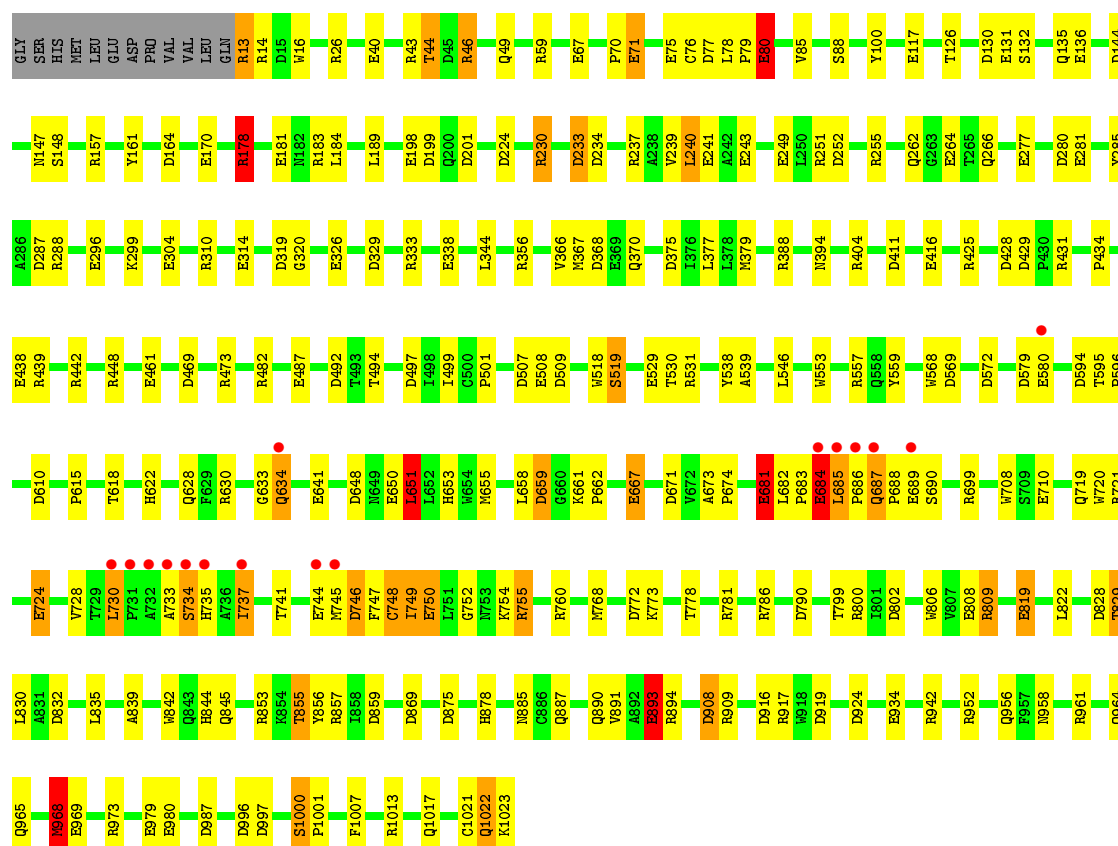


#### • Molecule 1: Beta-Galactosidase

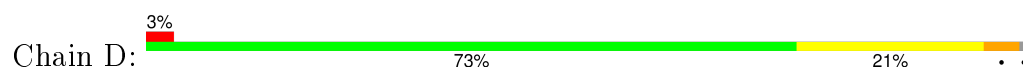




• Molecule 1: Beta-Galactosidase



• Molecule 1: Beta-Galactosidase



Q135	Q136	Q137	Q138	Q139	Q140	Q141	Q142	Q143	Q144	Q145	Q146	Q147	Q148	Q149	Q150	Q151	Q152	Q153	Q154	Q155	Q156	Q157	Q158	Q159	Q160	Q161	Q162	Q163	Q164	Q165	Q166	Q167	Q168	Q169	Q170	Q171	Q172	Q173	Q174	Q175	Q176	Q177	Q178	Q179	Q180	Q181	Q182	Q183	Q184	Q185	Q186	Q187	Q188	Q189	Q190	Q191	Q192	Q193	Q194	Q195	Q196	Q197	Q198	Q199	Q200	Q201	Q202	Q203	Q204	Q205	Q206	Q207	Q208	Q209	Q210	Q211	Q212	Q213	Q214	Q215	Q216	Q217	Q218	Q219	Q220	Q221	Q222	Q223	Q224	Q225	Q226	Q227	Q228	Q229	Q230	Q231	Q232	Q233	Q234	Q235	Q236	Q237	Q238	Q239	Q240	Q241	Q242	Q243	Q244	Q245	Q246	Q247	Q248	Q249	Q250	Q251	Q252	Q253	Q254	Q255	Q256	Q257	Q258	Q259	Q260	Q261	Q262	Q263	Q264	Q265	Q266	Q267	Q268	Q269	Q270	Q271	Q272	Q273	Q274	Q275	Q276	Q277	Q278	Q279	Q280	Q281	Q282	Q283	Q284	Q285	Q286	Q287	Q288	Q289	Q290	Q291	Q292	Q293	Q294	Q295	Q296	Q297	Q298	Q299	Q300	Q301	Q302	Q303	Q304	Q305	Q306	Q307	Q308	Q309	Q310	Q311	Q312	Q313	Q314	Q315	Q316	Q317	Q318	Q319	Q320	Q321	Q322	Q323	Q324	Q325	Q326	Q327	Q328	Q329	Q330	Q331	Q332	Q333	Q334	Q335	Q336	Q337	Q338	Q339	Q340	Q341	Q342	Q343	Q344	Q345	Q346	Q347	Q348	Q349	Q350	Q351	Q352	Q353	Q354	Q355	Q356	Q357	Q358	Q359	Q360	Q361	Q362	Q363	Q364	Q365	Q366	Q367	Q368	Q369	Q370	Q371	Q372	Q373	Q374	Q375	Q376	Q377	Q378	Q379	Q380	Q381	Q382	Q383	Q384	Q385	Q386	Q387	Q388	Q389	Q390	Q391	Q392	Q393	Q394	Q395	Q396	Q397	Q398	Q399	Q400	Q401	Q402	Q403	Q404	Q405	Q406	Q407	Q408	Q409	Q410	Q411	Q412	Q413	Q414	Q415	Q416	Q417	Q418	Q419	Q420	Q421	Q422	Q423	Q424	Q425	Q426	Q427	Q428	Q429	Q430	Q431	Q432	Q433	Q434	Q435	Q436	Q437	Q438	Q439	Q440	Q441	Q442	Q443	Q444	Q445	Q446	Q447	Q448	Q449	Q450	Q451	Q452	Q453	Q454	Q455	Q456	Q457	Q458	Q459	Q460	Q461	Q462	Q463	Q464	Q465	Q466	Q467	Q468	Q469	Q470	Q471	Q472	Q473	Q474	Q475	Q476	Q477	Q478	Q479	Q480	Q481	Q482	Q483	Q484	Q485	Q486	Q487	Q488	Q489	Q490	Q491	Q492	Q493	Q494	Q495	Q496	Q497	Q498	Q499	Q500	Q501	Q502	Q503	Q504	Q505	Q506	Q507	Q508	Q509	Q510	Q511	Q512	Q513	Q514	Q515	Q516	Q517	Q518	Q519	Q520	Q521	Q522	Q523	Q524	Q525	Q526	Q527	Q528	Q529	Q530	Q531	Q532	Q533	Q534	Q535	Q536	Q537	Q538	Q539	Q540	Q541	Q542	Q543	Q544	Q545	Q546	Q547	Q548	Q549	Q550	Q551	Q552	Q553	Q554	Q555	Q556	Q557	Q558	Q559	Q560	Q561	Q562	Q563	Q564	Q565	Q566	Q567	Q568	Q569	Q570	Q571	Q572	Q573	Q574	Q575	Q576	Q577	Q578	Q579	Q580	Q581	Q582	Q583	Q584	Q585	Q586	Q587	Q588	Q589	Q590	Q591	Q592	Q593	Q594	Q595	Q596	Q597	Q598	Q599	Q600	Q601	Q602	Q603	Q604	Q605	Q606	Q607	Q608	Q609	Q610	Q611	Q612	Q613	Q614	Q615	Q616	Q617	Q618	Q619	Q620	Q621	Q622	Q623	Q624	Q625	Q626	Q627	Q628	Q629	Q630	Q631	Q632	Q633	Q634	Q635	Q636	Q637	Q638	Q639	Q640	Q641	Q642	Q643	Q644	Q645	Q646	Q647	Q648	Q649	Q650	Q651	Q652	Q653	Q654	Q655	Q656	Q657	Q658	Q659	Q660	Q661	Q662	Q663	Q664	Q665	Q666	Q667	Q668	Q669	Q670	Q671	Q672	Q673	Q674	Q675	Q676	Q677	Q678	Q679	Q680	Q681	Q682	Q683	Q684	Q685	Q686	Q687	Q688	Q689	Q690	Q691	Q692	Q693	Q694	Q695	Q696	Q697	Q698	Q699	Q700	Q701	Q702	Q703	Q704	Q705	Q706	Q707	Q708	Q709	Q710	Q711	Q712	Q713	Q714	Q715	Q716	Q717	Q718	Q719	Q720	Q721	Q722	Q723	Q724	Q725	Q726	Q727	Q728	Q729	Q730	Q731	Q732	Q733	Q734	Q735	Q736	Q737	Q738	Q739	Q740	Q741	Q742	Q743	Q744	Q745	Q746	Q747	Q748	Q749	Q750	Q751	Q752	Q753	Q754	Q755	Q756	Q757	Q758	Q759	Q760	Q761	Q762	Q763	Q764	Q765	Q766	Q767	Q768	Q769	Q770	Q771	Q772	Q773	Q774	Q775	Q776	Q777	Q778	Q779	Q780	Q781	Q782	Q783	Q784	Q785	Q786	Q787	Q788	Q789	Q790	Q791	Q792	Q793	Q794	Q795	Q796	Q797	Q798	Q799	Q800	Q801	Q802	Q803	Q804	Q805	Q806	Q807	Q808	Q809	Q810	Q811	Q812	Q813	Q814	Q815	Q816	Q817	Q818	Q819	Q820	Q821	Q822	Q823	Q824	Q825	Q826	Q827	Q828	Q829	Q830	Q831	Q832	Q833	Q834	Q835	Q836	Q837	Q838	Q839	Q840	Q841	Q842	Q843	Q844	Q845	Q846	Q847	Q848	Q849	Q850	Q851	Q852	Q853	Q854	Q855	Q856	Q857	Q858	Q859	Q860	Q861	Q862	Q863	Q864	Q865	Q866	Q867	Q868	Q869	Q870	Q871	Q872	Q873	Q874	Q875	Q876	Q877	Q878	Q879	Q880	Q881	Q882	Q883	Q884	Q885	Q886	Q887	Q888	Q889	Q890	Q891	Q892	Q893	Q894	Q895	Q896	Q897	Q898	Q899	Q900	Q901	Q902	Q903	Q904	Q905	Q906	Q907	Q908	Q909	Q910	Q911	Q912	Q913	Q914	Q915	Q916	Q917	Q918	Q919	Q920	Q921	Q922	Q923	Q924	Q925	Q926	Q927	Q928	Q929	Q930	Q931	Q932	Q933	Q934	Q935	Q936	Q937	Q938	Q939	Q940	Q941	Q942	Q943	Q944	Q945	Q946	Q947	Q948	Q949	Q950	Q951	Q952	Q953	Q954	Q955	Q956	Q957	Q958	Q959	Q960	Q961	Q962	Q963	Q964	Q965	Q966	Q967	Q968	Q969	Q970	Q971	Q972	Q973	Q974	Q975	Q976	Q977	Q978	Q979	Q980	Q981	Q982	Q983	Q984	Q985	Q986	Q987	Q988	Q989	Q990	Q991	Q992	Q993	Q994	Q995	Q996	Q997	Q998	Q999	Q1000	Q1001	Q1002	Q1003	Q1004	Q1005	Q1006	Q1007	Q1008	Q1009	Q1010	Q1011	Q1012	Q1013	Q1014	Q1015	Q1016	Q1017	Q1018	Q1019	Q1020	Q1021	Q1022	Q1023	Q1024	Q1025	Q1026	Q1027	Q1028	Q1029	Q1030	Q1031	Q1032	Q1033	Q1034	Q1035	Q1036	Q1037	Q1038	Q1039	Q1040	Q1041	Q1042	Q1043	Q1044	Q1045	Q1046	Q1047	Q1048	Q1049	Q1050	Q1051	Q1052	Q1053	Q1054	Q1055	Q1056	Q1057	Q1058	Q1059	Q1060	Q1061	Q1062	Q1063	Q1064	Q1065	Q1066	Q1067	Q1068	Q1069	Q1070	Q1071	Q1072	Q1073	Q1074	Q1075	Q1076	Q1077	Q1078	Q1079	Q1080	Q1081	Q1082	Q1083	Q1084	Q1085	Q1086	Q1087	Q1088	Q1089	Q1090	Q1091	Q1092	Q1093	Q1094	Q1095	Q1096	Q1097	Q1098	Q1099	Q1100	Q1101	Q1102	Q1103	Q1104	Q1105	Q1106	Q1107	Q1108	Q1109	Q1110	Q1111	Q1112	Q1113	Q1114	Q1115	Q1116	Q1117	Q1118	Q1119	Q1120	Q1121	Q1122	Q1123	Q1124	Q1125	Q1126	Q1127	Q1128	Q1129	Q1130	Q1131	Q1132	Q1133	Q1134	Q1135	Q1136	Q1137	Q1138	Q1139	Q1140	Q1141	Q1142	Q1143	Q1144	Q1145	Q1146	Q1147	Q1148	Q1149	Q1150	Q1151	Q1152	Q1153	Q1154	Q1155	Q1156	Q1157	Q1158	Q1159	Q1160	Q1161	Q1162	Q1163	Q1164	Q1165	Q1166	Q1167	Q1168	Q1169	Q1170	Q1171	Q1172	Q1173	Q1174	Q1175	Q1176	Q1177	Q1178	Q1179	Q1180	Q1181	Q1182	Q1183	Q1184	Q1185	Q1186	Q1187	Q1188	Q1189	Q1190	Q1191	Q1192	Q1193	Q1194	Q1195	Q1196	Q1197	Q1198	Q1199	Q1200	Q1201	Q1202	Q1203	Q1204	Q1205	Q1206	Q1207	Q1208	Q1209	Q1210	Q1211	Q1212	Q1213	Q1214	Q1215	Q1216	Q1217	Q1218	Q1219	Q1220	Q1221	Q1222	Q1223	Q1224	Q1225	Q1226	Q1227	Q1228	Q1229	Q1230	Q1231	Q1232	Q1233	Q1234	Q1235	Q1236	Q1237	Q1238	Q1239	Q1240	Q1241	Q1242	Q1243	Q1244	Q1245	Q1246	Q1247	Q1248	Q1249	Q1250	Q1251	Q1252	Q1253	Q1254	Q1255	Q1256	Q1257	Q1258	Q1259	Q1260	Q1261	Q1262	Q1263	Q1264	Q1265	Q1266	Q1267	Q1268	Q1269	Q1270	Q1271	Q1272	Q1273	Q1274	Q1275	Q1276	Q1277	Q1278	Q1279	Q1280	Q1281	Q1282	Q1283	Q1284	Q1285	Q1286	Q1287	Q1288	Q1289	Q1290	Q1291	Q1292	Q1293	Q1294	Q1295	Q1296	Q1297	Q1298	Q1299	Q1300	Q1301	Q1302	Q1303	Q1304	Q1305	Q1306	Q1307	Q1308	Q1309	Q1310	Q1311	Q1312	Q1313	Q1314	Q1315	Q1316	Q1317	Q1318	Q1319	Q1320	Q1321	Q1322	Q1323	Q1324	Q1325	Q1326	Q1327	Q1328	Q1329	Q1330	Q1331	Q1332	Q1333	Q1334	Q1335	Q1336	Q1337	Q1338	Q1339	Q1340	Q1341	Q1342	Q1343	Q1344	Q1345	Q1346	Q1347	Q1348	Q1349	Q1350	Q1351	Q1352	Q1353	Q1354	Q1355	Q1356	Q1357	Q1358	Q1359	Q1360	Q1361	Q1362	Q1363	Q1364	Q1365	Q1366	Q1367	Q1368	Q1369	Q1370	Q1371	Q1372	Q1373	Q1374	Q1375	Q1376	Q1377	Q1378	Q1379	Q1380	Q1381	Q1382	Q1383	Q1384	Q1385	Q1386	Q1387	Q1388	Q1389	Q1390	Q1391	Q1392	Q1393	Q1394	Q1395	Q1396	Q1397	Q1398	Q1399	Q1400	Q1401	Q1402	Q1403	Q1404	Q1405	Q1406	Q1407	Q1408	Q1409	Q1410	Q1411	Q1412	Q1413	Q1414	Q1415	Q1416	Q1417	Q1418	Q1419	Q1420	Q1421	Q1422	Q1423	Q1424	Q1425	Q1426	Q1427	Q1428	Q1429	Q1430	Q1431	Q1432	Q1433	Q1434	Q1435	Q1436	Q1437	Q1438	Q1439	Q1440	Q1441	Q1442	Q1443	Q1444	Q1445	Q
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.68Å 168.60Å 201.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.80 – 1.55 28.75 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.3 (28.80-1.55) 91.2 (28.75-1.55)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.69 (at 1.54Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.180 , 0.229 0.164 , 0.207	Depositor DCC
$R_{free}$ test set	10423 reflections (1.59%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 84.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 715525 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	37524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.91 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.4252e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 147, MG, DMS, NA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.21	49/8382 (0.6%)	1.67	163/11435 (1.4%)
1	B	1.23	51/8383 (0.6%)	1.65	169/11437 (1.5%)
1	C	1.21	46/8383 (0.5%)	1.71	180/11437 (1.6%)
1	D	1.22	47/8383 (0.6%)	1.61	161/11437 (1.4%)
All	All	1.22	193/33531 (0.6%)	1.66	673/45746 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1006	GLU	CD-OE2	10.08	1.36	1.25
1	D	681	GLU	CD-OE2	9.79	1.36	1.25
1	D	893	GLU	CD-OE2	9.79	1.36	1.25
1	B	71	GLU	CD-OE2	9.33	1.35	1.25
1	B	689	GLU	CD-OE2	9.25	1.35	1.25
1	B	1006	GLU	CD-OE2	8.94	1.35	1.25
1	B	650	GLU	CD-OE2	8.87	1.35	1.25
1	C	243	GLU	CD-OE2	8.81	1.35	1.25
1	D	650	GLU	CD-OE2	8.72	1.35	1.25
1	A	243	GLU	CD-OE2	8.56	1.35	1.25
1	C	80	GLU	CD-OE2	8.56	1.35	1.25
1	C	684	GLU	CD-OE2	8.40	1.34	1.25
1	C	304	GLU	CD-OE2	8.27	1.34	1.25
1	A	170	GLU	CD-OE2	8.21	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	667	GLU	CD-OE2	8.20	1.34	1.25
1	C	71	GLU	CD-OE2	8.18	1.34	1.25
1	A	80	GLU	CD-OE2	8.10	1.34	1.25
1	D	170	GLU	CD-OE2	8.05	1.34	1.25
1	A	580	GLU	CD-OE2	8.04	1.34	1.25
1	C	689	GLU	CD-OE2	8.05	1.34	1.25
1	D	75	GLU	CD-OE2	7.93	1.34	1.25
1	C	338	GLU	CD-OE2	7.86	1.34	1.25
1	A	241	GLU	CD-OE2	7.85	1.34	1.25
1	A	249	GLU	CD-OE2	7.83	1.34	1.25
1	B	819	GLU	CD-OE2	7.78	1.34	1.25
1	D	17	GLU	CD-OE2	7.76	1.34	1.25
1	C	75	GLU	CD-OE2	7.76	1.34	1.25
1	B	667	GLU	CD-OE2	7.75	1.34	1.25
1	C	281	GLU	CD-OE2	7.68	1.34	1.25
1	D	689	GLU	CD-OE2	7.68	1.34	1.25
1	C	819	GLU	CD-OE2	7.67	1.34	1.25
1	A	681	GLU	CD-OE2	7.59	1.33	1.25
1	B	296	GLU	CD-OE2	7.59	1.33	1.25
1	A	281	GLU	CD-OE2	7.57	1.33	1.25
1	C	934	GLU	CD-OE2	7.52	1.33	1.25
1	A	979	GLU	CD-OE2	7.50	1.33	1.25
1	D	580	GLU	CD-OE2	7.50	1.33	1.25
1	A	487	GLU	CD-OE2	7.50	1.33	1.25
1	A	969	GLU	CD-OE2	7.43	1.33	1.25
1	D	326	GLU	CD-OE2	7.41	1.33	1.25
1	C	131	GLU	CD-OE2	7.39	1.33	1.25
1	B	684	GLU	CD-OE2	7.39	1.33	1.25
1	D	281	GLU	CD-OE2	7.38	1.33	1.25
1	C	67	GLU	CD-OE2	7.38	1.33	1.25
1	D	243	GLU	CD-OE2	7.37	1.33	1.25
1	D	296	GLU	CD-OE2	7.34	1.33	1.25
1	B	249	GLU	CD-OE2	7.33	1.33	1.25
1	A	980	GLU	CD-OE2	7.32	1.33	1.25
1	D	819	GLU	CD-OE2	7.30	1.33	1.25
1	B	40	GLU	CD-OE2	7.29	1.33	1.25
1	A	438	GLU	CD-OE2	7.28	1.33	1.25
1	B	980	GLU	CD-OE2	7.28	1.33	1.25
1	B	338	GLU	CD-OE2	7.19	1.33	1.25
1	C	241	GLU	CD-OE2	7.19	1.33	1.25
1	B	314	GLU	CD-OE2	7.18	1.33	1.25
1	C	264	GLU	CD-OE2	7.17	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	744	GLU	CD-OE2	7.16	1.33	1.25
1	A	689	GLU	CD-OE2	7.14	1.33	1.25
1	C	170	GLU	CD-OE2	7.12	1.33	1.25
1	A	684	GLU	CD-OE2	7.11	1.33	1.25
1	D	80	GLU	CD-OE2	7.10	1.33	1.25
1	C	198	GLU	CD-OE2	7.10	1.33	1.25
1	B	580	GLU	CD-OE2	7.08	1.33	1.25
1	D	241	GLU	CD-OE2	6.99	1.33	1.25
1	B	487	GLU	CD-OE2	6.94	1.33	1.25
1	D	684	GLU	CD-OE2	6.91	1.33	1.25
1	A	71	GLU	CD-OE2	6.90	1.33	1.25
1	D	136	GLU	CD-OE2	6.88	1.33	1.25
1	A	296	GLU	CD-OE2	6.85	1.33	1.25
1	D	277	GLU	CD-OE2	6.83	1.33	1.25
1	D	637	GLU	CD-OE2	6.83	1.33	1.25
1	C	326	GLU	CD-OE2	6.82	1.33	1.25
1	B	281	GLU	CD-OE2	6.78	1.33	1.25
1	D	338	GLU	CD-OE2	6.75	1.33	1.25
1	B	529	GLU	CD-OE2	6.74	1.33	1.25
1	D	724	GLU	CD-OE2	6.74	1.33	1.25
1	B	934	GLU	CD-OE2	6.72	1.33	1.25
1	D	71	GLU	CD-OE2	6.71	1.33	1.25
1	C	893	GLU	CD-OE2	6.71	1.33	1.25
1	A	943	GLU	CD-OE2	6.68	1.32	1.25
1	A	277	GLU	CD-OE2	6.61	1.32	1.25
1	C	529	GLU	CD-OE2	6.61	1.32	1.25
1	C	136	GLU	CD-OE2	6.58	1.32	1.25
1	C	969	GLU	CD-OE2	6.52	1.32	1.25
1	B	117	GLU	CD-OE2	6.51	1.32	1.25
1	C	277	GLU	CD-OE2	6.49	1.32	1.25
1	C	710	GLU	CD-OE2	6.47	1.32	1.25
1	C	979	GLU	CD-OE2	6.46	1.32	1.25
1	D	979	GLU	CD-OE2	6.46	1.32	1.25
1	A	136	GLU	CD-OE2	6.43	1.32	1.25
1	A	710	GLU	CD-OE2	6.43	1.32	1.25
1	A	744	GLU	CD-OE2	6.42	1.32	1.25
1	C	750	GLU	CD-OE2	6.40	1.32	1.25
1	A	117	GLU	CD-OE2	6.39	1.32	1.25
1	D	67	GLU	CD-OE2	6.39	1.32	1.25
1	D	334	GLU	CD-OE2	6.38	1.32	1.25
1	D	264	GLU	CD-OE2	6.37	1.32	1.25
1	B	243	GLU	CD-OE2	6.34	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	GLU	CD-OE2	6.34	1.32	1.25
1	C	117	GLU	CD-OE2	6.33	1.32	1.25
1	D	943	GLU	CD-OE2	6.30	1.32	1.25
1	B	710	GLU	CD-OE2	6.30	1.32	1.25
1	C	808	GLU	CD-OE2	6.28	1.32	1.25
1	D	710	GLU	CD-OE2	6.28	1.32	1.25
1	A	57	GLU	CD-OE1	-6.26	1.18	1.25
1	C	980	GLU	CD-OE2	6.25	1.32	1.25
1	D	117	GLU	CD-OE2	6.23	1.32	1.25
1	A	75	GLU	CD-OE2	6.22	1.32	1.25
1	A	797	GLU	CD-OE1	-6.22	1.18	1.25
1	C	681	GLU	CD-OE2	6.20	1.32	1.25
1	B	744	GLU	CD-OE2	6.20	1.32	1.25
1	D	750	GLU	CD-OE2	6.19	1.32	1.25
1	C	296	GLU	CD-OE2	6.19	1.32	1.25
1	A	667	GLU	CD-OE2	6.16	1.32	1.25
1	C	487	GLU	CD-OE2	6.16	1.32	1.25
1	A	369	GLU	CD-OE2	6.15	1.32	1.25
1	A	338	GLU	CD-OE2	6.14	1.32	1.25
1	B	416	GLU	CD-OE2	6.11	1.32	1.25
1	B	681	GLU	CD-OE2	6.11	1.32	1.25
1	D	667	GLU	CD-OE2	6.09	1.32	1.25
1	B	136	GLU	CD-OE2	6.09	1.32	1.25
1	B	75	GLU	CD-OE2	6.03	1.32	1.25
1	B	181	GLU	CD-OE2	6.03	1.32	1.25
1	B	893	GLU	CD-OE2	6.01	1.32	1.25
1	D	41	GLU	CD-OE2	6.01	1.32	1.25
1	A	131	GLU	CD-OE2	6.00	1.32	1.25
1	D	131	GLU	CD-OE2	6.00	1.32	1.25
1	B	277	GLU	CD-OE2	5.99	1.32	1.25
1	B	170	GLU	CD-OE2	5.99	1.32	1.25
1	B	241	GLU	CD-OE2	5.94	1.32	1.25
1	A	724	GLU	CD-OE2	5.91	1.32	1.25
1	B	243	GLU	CD-OE1	-5.89	1.19	1.25
1	B	969	GLU	CD-OE1	-5.88	1.19	1.25
1	D	461	GLU	CD-OE2	5.87	1.32	1.25
1	B	80	GLU	CD-OE2	5.86	1.32	1.25
1	D	808	GLU	CD-OE2	5.82	1.32	1.25
1	A	819	GLU	CD-OE2	5.80	1.32	1.25
1	A	505	ARG	CZ-NH2	5.80	1.40	1.33
1	C	416	GLU	CD-OE2	5.80	1.32	1.25
1	B	442	ARG	CZ-NH1	5.78	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	GLU	CD-OE2	5.77	1.31	1.25
1	A	412	GLU	CD-OE2	5.76	1.31	1.25
1	D	304	GLU	CD-OE2	5.75	1.31	1.25
1	B	369	GLU	CD-OE2	5.71	1.31	1.25
1	B	641	GLU	CD-OE1	-5.71	1.19	1.25
1	B	198	GLU	CD-OE2	5.68	1.31	1.25
1	C	230	ARG	NE-CZ	5.68	1.40	1.33
1	C	249	GLU	CD-OE2	5.66	1.31	1.25
1	A	264	GLU	CD-OE2	5.65	1.31	1.25
1	D	249	GLU	CD-OE2	5.63	1.31	1.25
1	D	181	GLU	CD-OE2	5.62	1.31	1.25
1	A	893	GLU	CD-OE2	5.62	1.31	1.25
1	C	580	GLU	CD-OE2	5.62	1.31	1.25
1	A	934	GLU	CD-OE2	5.61	1.31	1.25
1	B	264	GLU	CD-OE2	5.61	1.31	1.25
1	D	487	GLU	CD-OE2	5.61	1.31	1.25
1	C	461	GLU	CD-OE2	5.57	1.31	1.25
1	B	131	GLU	CD-OE2	5.57	1.31	1.25
1	B	969	GLU	CD-OE2	5.56	1.31	1.25
1	C	650	GLU	CD-OE2	5.49	1.31	1.25
1	C	508	GLU	CD-OE2	5.48	1.31	1.25
1	C	641	GLU	CD-OE1	-5.47	1.19	1.25
1	B	412	GLU	CD-OE2	5.42	1.31	1.25
1	B	904	GLU	CD-OE1	-5.41	1.19	1.25
1	D	508	GLU	CD-OE2	5.40	1.31	1.25
1	D	314	GLU	CD-OE2	5.38	1.31	1.25
1	A	41	GLU	CD-OE2	5.33	1.31	1.25
1	B	641	GLU	CD-OE2	5.31	1.31	1.25
1	C	314	GLU	CD-OE2	5.30	1.31	1.25
1	A	67	GLU	CD-OE2	5.26	1.31	1.25
1	C	482	ARG	CZ-NH1	5.25	1.39	1.33
1	D	619	GLU	CD-OE2	5.24	1.31	1.25
1	A	750	GLU	CD-OE2	5.22	1.31	1.25
1	D	980	GLU	CD-OE2	5.22	1.31	1.25
1	B	326	GLU	CD-OE2	5.20	1.31	1.25
1	A	808	GLU	CD-OE2	5.19	1.31	1.25
1	B	324	GLU	CD-OE1	-5.18	1.20	1.25
1	C	492	ASP	CG-OD2	5.17	1.37	1.25
1	D	425	ARG	NE-CZ	5.15	1.39	1.33
1	A	243	GLU	CD-OE1	-5.11	1.20	1.25
1	D	641	GLU	CD-OE2	5.08	1.31	1.25
1	A	17	GLU	CD-OE2	5.08	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	324	GLU	CD-OE1	-5.07	1.20	1.25
1	A	437	SER	CB-OG	-5.07	1.35	1.42
1	C	724	GLU	CD-OE2	5.06	1.31	1.25
1	B	57	GLU	CD-OE2	5.06	1.31	1.25
1	B	897	TRP	CD2-CE2	5.06	1.47	1.41
1	A	416	GLU	CD-OE2	5.04	1.31	1.25
1	B	781	ARG	CZ-NH2	5.03	1.39	1.33
1	A	310	ARG	CZ-NH2	5.02	1.39	1.33
1	A	641	GLU	CD-OE1	-5.01	1.20	1.25
1	B	67	GLU	CD-OE2	5.01	1.31	1.25
1	D	717	TRP	CD2-CE2	5.01	1.47	1.41

All (673) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	ARG	NE-CZ-NH1	33.80	137.20	120.30
1	C	630	ARG	NE-CZ-NH2	-20.87	109.87	120.30
1	C	721	ARG	NE-CZ-NH1	19.65	130.13	120.30
1	A	755	ARG	NE-CZ-NH1	17.36	128.98	120.30
1	A	431	ARG	NE-CZ-NH2	-16.56	112.02	120.30
1	C	442	ARG	NE-CZ-NH2	-16.22	112.19	120.30
1	C	630	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	A	755	ARG	NE-CZ-NH2	-14.84	112.88	120.30
1	C	230	ARG	CD-NE-CZ	14.15	143.41	123.60
1	A	233	ASP	CB-CG-OD1	14.14	131.03	118.30
1	B	46	ARG	NE-CZ-NH2	-13.96	113.32	120.30
1	C	230	ARG	NE-CZ-NH2	-13.72	113.44	120.30
1	B	442	ARG	NE-CZ-NH1	13.57	127.08	120.30
1	A	431	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	A	233	ASP	CB-CG-OD2	-13.27	106.35	118.30
1	B	786	ARG	NE-CZ-NH2	-13.17	113.71	120.30
1	C	579	ASP	CB-CG-OD2	-13.13	106.48	118.30
1	B	425	ARG	NE-CZ-NH2	-12.95	113.82	120.30
1	A	800	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	C	224	ASP	CB-CG-OD1	12.15	129.24	118.30
1	A	166	ARG	NE-CZ-NH2	-11.99	114.31	120.30
1	A	251	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	D	172	ASP	CB-CG-OD2	-11.72	107.75	118.30
1	B	46	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	C	809	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	C	832	ASP	CB-CG-OD1	11.61	128.75	118.30
1	C	832	ASP	CB-CG-OD2	-11.54	107.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	579	ASP	CB-CG-OD1	11.54	128.69	118.30
1	B	832	ASP	CB-CG-OD1	11.39	128.55	118.30
1	C	178	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	D	630	ARG	NE-CZ-NH1	11.27	125.93	120.30
1	D	13	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	B	832	ASP	CB-CG-OD2	-11.01	108.40	118.30
1	A	610	ASP	CB-CG-OD1	10.96	128.16	118.30
1	D	446	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	A	224	ASP	CB-CG-OD1	10.91	128.12	118.30
1	A	336	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	D	446	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	D	183	ARG	NE-CZ-NH1	-10.59	115.00	120.30
1	A	599	ARG	NE-CZ-NH1	-10.43	115.09	120.30
1	B	853	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	B	233	ASP	CB-CG-OD1	10.14	127.43	118.30
1	C	996	ASP	CB-CG-OD2	-10.14	109.17	118.30
1	C	473	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	B	482	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	D	233	ASP	CB-CG-OD1	10.00	127.30	118.30
1	B	442	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	D	832	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	A	411	ASP	CB-CG-OD2	-9.69	109.58	118.30
1	A	442	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	C	234	ASP	CB-CG-OD1	9.61	126.95	118.30
1	A	909	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	D	233	ASP	CB-CG-OD2	-9.57	109.69	118.30
1	D	429	ASP	CB-CG-OD2	-9.55	109.71	118.30
1	D	996	ASP	CB-CG-OD1	9.50	126.85	118.30
1	B	234	ASP	CB-CG-OD1	9.48	126.83	118.30
1	A	144	ASP	CB-CG-OD1	9.44	126.80	118.30
1	D	594	ASP	CB-CG-OD1	9.43	126.78	118.30
1	D	996	ASP	CB-CG-OD2	-9.38	109.86	118.30
1	D	659	ASP	CB-CG-OD1	9.32	126.69	118.30
1	C	659	ASP	CB-CG-OD1	9.31	126.68	118.30
1	B	13	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	B	336	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	C	43	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	D	429	ASP	CB-CG-OD1	9.24	126.62	118.30
1	C	199	ASP	CB-CG-OD1	9.21	126.59	118.30
1	D	45	ASP	CB-CG-OD1	9.21	126.59	118.30
1	B	952	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	C	961	ARG	NE-CZ-NH1	9.19	124.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ASP	CB-CG-OD1	9.16	126.54	118.30
1	C	230	ARG	NH1-CZ-NH2	-9.16	109.33	119.40
1	A	26	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	A	172	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	A	356	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	B	919	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	B	425	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	C	875	ASP	CB-CG-OD1	9.04	126.44	118.30
1	C	961	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	800	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	C	46	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	B	252	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	D	15	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	A	802	ASP	CB-CG-OD1	8.98	126.39	118.30
1	B	909	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	45	ASP	CB-CG-OD1	8.94	126.34	118.30
1	A	594	ASP	CB-CG-OD1	8.93	126.33	118.30
1	A	924	ASP	CB-CG-OD1	8.89	126.30	118.30
1	D	144	ASP	CB-CG-OD1	8.88	126.29	118.30
1	B	448	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	329	ASP	CB-CG-OD2	-8.85	110.34	118.30
1	B	648	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	C	428	ASP	CB-CG-OD1	8.81	126.22	118.30
1	C	509	ASP	CB-CG-OD1	8.78	126.20	118.30
1	B	77	ASP	CB-CG-OD1	8.77	126.19	118.30
1	D	746	ASP	CB-CG-OD2	-8.76	110.42	118.30
1	A	610	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	699	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	96	ASP	CB-CG-OD1	8.68	126.11	118.30
1	A	411	ASP	CB-CG-OD1	8.67	126.10	118.30
1	D	507	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	C	786	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	46	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	C	233	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	C	13	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	D	368	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	B	352	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	A	632	SER	N-CA-CB	8.59	123.38	110.50
1	C	178	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	746	ASP	CB-CG-OD2	-8.56	110.60	118.30
1	B	233	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	C	234	ASP	CB-CG-OD2	-8.54	110.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	507	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	C	473	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	D	869	ASP	CB-CG-OD1	8.51	125.96	118.30
1	D	224	ASP	CB-CG-OD1	8.51	125.96	118.30
1	B	388	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	C	859	ASP	CB-CG-OD1	8.46	125.91	118.30
1	A	917	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	C	721	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	D	755	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	C	869	ASP	CB-CG-OD1	8.38	125.84	118.30
1	D	425	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	539[A]	ALA	CB-CA-C	-8.35	97.57	110.10
1	B	539[B]	ALA	CB-CA-C	-8.35	97.57	110.10
1	A	559	TYR	CB-CG-CD2	-8.33	116.00	121.00
1	C	659	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	B	802	ASP	CB-CG-OD1	8.33	125.80	118.30
1	A	509	ASP	CB-CG-OD1	8.31	125.78	118.30
1	D	172	ASP	CB-CG-OD1	8.27	125.74	118.30
1	A	832	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	D	439	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	B	77	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	B	492	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	234	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	D	166	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	B	368	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	A	816	TYR	CB-CG-CD1	-8.16	116.10	121.00
1	D	909	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	428	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	924	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	D	193	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	A	572	ASP	CB-CG-OD1	8.14	125.63	118.30
1	D	403	ASP	CB-CG-OD1	8.14	125.62	118.30
1	D	909	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	B	572	ASP	CB-CG-OD1	8.07	125.56	118.30
1	C	233	ASP	CB-CG-OD1	8.06	125.55	118.30
1	D	916	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	329	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	B	594	ASP	CB-CG-OD1	8.01	125.51	118.30
1	D	809	ARG	CD-NE-CZ	7.99	134.79	123.60
1	B	183	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	B	411	ASP	CB-CG-OD2	-7.98	111.11	118.30
1	C	853	ARG	NE-CZ-NH2	-7.96	116.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	B	875	ASP	CB-CG-OD1	7.95	125.46	118.30
1	A	954	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	C	908	ASP	CB-CG-OD1	7.93	125.44	118.30
1	D	193	ASP	CB-CG-OD1	7.93	125.44	118.30
1	D	578	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	B	611	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	859	ASP	CB-CG-OD1	7.89	125.40	118.30
1	D	319	ASP	CB-CG-OD1	7.86	125.37	118.30
1	A	909	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	C	594	ASP	CB-CG-OD1	7.83	125.34	118.30
1	A	973	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	172	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	961	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	C	630	ARG	CD-NE-CZ	7.75	134.45	123.60
1	C	996	ASP	CB-CG-OD1	7.74	125.26	118.30
1	C	610	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	178	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	431	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	329	ASP	CB-CG-OD1	7.70	125.23	118.30
1	D	428	ASP	CB-CG-OD1	7.69	125.22	118.30
1	B	746	ASP	CB-CG-OD1	7.68	125.21	118.30
1	B	671	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	671	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	C	319	ASP	CB-CG-OD2	-7.63	111.44	118.30
1	A	946	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	D	924	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	285	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	D	579	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	431	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	329	ASP	CB-CG-OD1	7.60	125.14	118.30
1	B	439	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	B	659	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	B	908	ASP	CB-CG-OD1	7.57	125.11	118.30
1	D	942	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	D	492	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	A	442	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	C	13	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	D	559	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	D	578	TYR	CB-CG-CD1	7.51	125.51	121.00
1	B	853	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	C	255	ARG	NE-CZ-NH1	7.48	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	659	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	D	411	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	A	439	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	D	469	ASP	CB-CG-OD1	7.45	125.01	118.30
1	A	559	TYR	CG-CD2-CE2	-7.44	115.35	121.30
1	A	425	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	746	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	C	492	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	A	659	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	D	539[A]	ALA	CB-CA-C	-7.40	99.00	110.10
1	D	539[B]	ALA	CB-CA-C	-7.40	99.00	110.10
1	D	980	GLU	C-N-CA	-7.40	106.77	122.30
1	C	183	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	D	431	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	116	THR	CA-CB-CG2	-7.39	102.06	112.40
1	C	507	ASP	CB-CG-OD1	7.36	124.92	118.30
1	B	473	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	D	482	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	428	ASP	CB-CG-OD1	7.34	124.90	118.30
1	A	859	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	B	594	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	C	917	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	D	15	ASP	CB-CG-OD1	7.33	124.89	118.30
1	D	329	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	C	733	ALA	N-CA-CB	7.29	120.31	110.10
1	D	509	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	287	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	183	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	C	368	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	D	116	THR	CA-CB-CG2	-7.23	102.28	112.40
1	B	319	ASP	CB-CG-OD1	7.23	124.80	118.30
1	A	869	ASP	CB-CG-OD1	7.22	124.80	118.30
1	D	987	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	448	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	234	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	539[A]	ALA	CB-CA-C	-7.19	99.32	110.10
1	A	539[B]	ALA	CB-CA-C	-7.19	99.32	110.10
1	A	292	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	C	733	ALA	CB-CA-C	7.18	120.88	110.10
1	A	130	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	869	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	392	TYR	CG-CD1-CE1	-7.16	115.58	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	224	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	B	43	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	77	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	832	ASP	CB-CG-OD1	7.12	124.70	118.30
1	B	611	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	234	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	76	CYS	CA-CB-SG	-7.10	101.22	114.00
1	D	859	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	368	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	802	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	C	539[A]	ALA	CB-CA-C	-7.07	99.50	110.10
1	C	539[B]	ALA	CB-CA-C	-7.07	99.50	110.10
1	D	356	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	C	439	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	610	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	828	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	952	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	D	579	ASP	CB-CG-OD1	7.01	124.61	118.30
1	D	845	GLN	C-N-CA	-7.01	107.58	122.30
1	D	924	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	772	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	C	425	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	531	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	D	352	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	14	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	699	ARG	NE-CZ-NH2	6.95	123.77	120.30
1	C	859	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	D	319	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	772	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	954	ASP	CB-CG-OD1	6.91	124.52	118.30
1	D	632	SER	N-CA-CB	6.89	120.84	110.50
1	B	869	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	610	ASP	CB-CG-OD1	6.89	124.50	118.30
1	C	958	ASN	N-CA-CB	6.89	122.99	110.60
1	B	319	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	D	287	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	572	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	579	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	D	561	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	572	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	C	85	VAL	CA-CB-CG2	-6.83	100.66	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	916	ASP	CB-CG-OD1	6.82	124.43	118.30
1	C	438	GLU	CG-CD-OE2	-6.82	104.67	118.30
1	D	252	ASP	CB-CG-OD1	6.82	124.43	118.30
1	A	987	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	368	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	771	GLY	N-CA-C	-6.78	96.14	113.10
1	C	987	ASP	CB-CG-OD1	6.77	124.39	118.30
1	B	569	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	721	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	1018	LEU	CB-CA-C	-6.76	97.36	110.20
1	C	594	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	C	802	ASP	CB-CG-OD1	6.74	124.36	118.30
1	D	368	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	507	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	A	987	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	411	ASP	CB-CG-OD1	6.72	124.35	118.30
1	C	136	GLU	CB-CA-C	-6.71	96.98	110.40
1	B	561	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	C	144	ASP	CB-CG-OD1	6.71	124.34	118.30
1	D	287	ASP	CB-CG-OD2	-6.71	112.27	118.30
1	D	781	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	952	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	356	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	D	507	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	356	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	599	ARG	NE-CZ-NH2	6.65	123.62	120.30
1	C	809	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	916	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	288	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	C	659	ASP	CB-CA-C	6.63	123.66	110.40
1	D	130	ASP	CB-CG-OD1	6.63	124.27	118.30
1	C	44	THR	CA-CB-CG2	-6.63	103.12	112.40
1	D	952	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	D	919	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	809	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	519	SER	N-CA-CB	-6.60	100.59	110.50
1	B	140	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	772	ASP	CB-CG-OD1	6.59	124.24	118.30
1	A	144	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	B	507	ASP	CB-CG-OD1	6.56	124.20	118.30
1	D	144	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	A	579	ASP	CB-CG-OD2	-6.54	112.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	224	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	B	15	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	B	919	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	95	TYR	CG-CD2-CE2	-6.52	116.08	121.30
1	B	310	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	C	507	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	D	403	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	82	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	917	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	C	329	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	D	832	ASP	CB-CG-OD1	6.47	124.13	118.30
1	A	540[A]	HIS	N-CA-CB	-6.47	98.95	110.60
1	A	540[B]	HIS	N-CA-CB	-6.47	98.95	110.60
1	C	748	CYS	CA-CB-SG	-6.47	102.35	114.00
1	B	987	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	916	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	952	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	859	ASP	CB-CG-OD1	6.46	124.12	118.30
1	B	211	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	1019	VAL	CA-CB-CG2	-6.45	101.22	110.90
1	D	746	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	477	SER	N-CA-CB	6.43	120.14	110.50
1	C	280	ASP	CB-CG-OD1	6.43	124.09	118.30
1	D	800	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	B	828	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	492	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	755	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	D	329	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	952	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	D	479	ASP	CB-CG-OD1	6.38	124.05	118.30
1	B	287	ASP	CB-CG-OD1	6.38	124.04	118.30
1	D	255	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	280	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	14	ARG	N-CA-CB	6.35	122.04	110.60
1	B	557	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	996	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	B	659	ASP	CB-CG-OD1	6.33	123.99	118.30
1	B	786	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	842	TRP	CH2-CZ2-CE2	-6.32	111.08	117.40
1	D	1018	LEU	CB-CA-C	-6.32	98.20	110.20
1	B	144	ASP	CB-CG-OD1	6.32	123.98	118.30
1	C	924	ASP	CB-CG-OD1	6.31	123.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	338	GLU	CG-CD-OE2	-6.29	105.72	118.30
1	D	845	GLN	CB-CA-C	-6.27	97.85	110.40
1	D	267	VAL	CG1-CB-CG2	-6.26	100.88	110.90
1	D	802	ASP	CB-CG-OD1	6.26	123.93	118.30
1	D	625	GLN	CG-CD-OE1	-6.25	109.09	121.60
1	A	319	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	D	439	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	1021	CYS	CA-CB-SG	-6.25	102.75	114.00
1	C	799	THR	CA-CB-CG2	-6.24	103.66	112.40
1	C	610	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	D	252	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	D	919	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	958	ASN	N-CA-CB	6.22	121.81	110.60
1	D	973	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	C	404	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	438	GLU	CG-CD-OE2	-6.20	105.91	118.30
1	A	968	MET	CA-CB-CG	6.19	123.82	113.30
1	B	224	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	519	SER	N-CA-CB	-6.18	101.23	110.50
1	C	559	TYR	CD1-CE1-CZ	-6.18	114.24	119.80
1	D	770	ILE	N-CA-C	-6.18	94.33	111.00
1	B	429	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	625	GLN	CG-CD-OE1	-6.16	109.28	121.60
1	D	719	GLN	CB-CA-C	-6.16	98.08	110.40
1	D	809	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	469	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	482	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	792	ASP	CB-CG-OD1	6.15	123.84	118.30
1	C	280	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	859	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	D	448	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	747	PHE	CB-CG-CD2	6.12	125.09	120.80
1	B	247	CYS	CA-CB-SG	-6.11	103.00	114.00
1	D	492	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	568	TRP	CA-CB-CG	-6.11	102.09	113.70
1	B	855	THR	N-CA-CB	6.10	121.88	110.30
1	C	469	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	234	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	829	THR	CA-CB-CG2	-6.09	103.88	112.40
1	C	857	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	D	681	GLU	CB-CA-C	6.09	122.57	110.40
1	D	130	ASP	CB-CG-OD2	-6.08	112.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	442	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	292	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	D	594	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	859	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	828	ASP	CB-CG-OD1	6.05	123.74	118.30
1	C	404	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	792	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	388	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	B	439	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	832	ASP	N-CA-CB	-6.03	99.75	110.60
1	D	572	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	D	416	GLU	CG-CD-OE1	6.03	130.36	118.30
1	C	310	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	509	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	C	439	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	255	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	D	324	GLU	N-CA-CB	6.01	121.42	110.60
1	A	288	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	164	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	49	GLN	CB-CG-CD	6.00	127.20	111.60
1	D	588	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	D	472	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	C	411	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	D	746	ASP	CB-CA-C	-5.95	98.49	110.40
1	A	285	TYR	CD1-CE1-CZ	-5.95	114.45	119.80
1	B	917	ARG	CD-NE-CZ	-5.94	115.28	123.60
1	C	252	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	997	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	C	917	ARG	CD-NE-CZ	-5.93	115.30	123.60
1	C	572	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	13	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	237	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	179	ALA	N-CA-CB	5.89	118.35	110.10
1	B	157	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	B	157	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	D	85	VAL	CA-CB-CG2	-5.88	102.08	110.90
1	C	494	THR	CA-CB-CG2	-5.87	104.19	112.40
1	A	252	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	D	442	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	875	ASP	CB-CG-OD1	5.85	123.56	118.30
1	C	239	VAL	CA-CB-CG2	-5.83	102.15	110.90
1	A	237	ARG	NE-CZ-NH1	5.83	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	916	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	45	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	37	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	598	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	857	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	D	251	ARG	CG-CD-NE	-5.81	99.60	111.80
1	C	319	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	572	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	721	ARG	CD-NE-CZ	5.80	131.72	123.60
1	C	648	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	991	MET	CG-SD-CE	5.80	109.48	100.20
1	B	579	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	1014	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	B	997	ASP	N-CA-CB	5.77	120.99	110.60
1	B	52	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	829	THR	CA-CB-CG2	-5.76	104.33	112.40
1	B	105	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	D	482	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	746	ASP	CB-CA-C	-5.76	98.89	110.40
1	C	199	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	288	ARG	NH1-CZ-NH2	5.74	125.71	119.40
1	B	819	GLU	CB-CA-C	5.74	121.88	110.40
1	D	253	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	A	13	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	14	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	D	958	ASN	N-CA-CB	5.73	120.91	110.60
1	A	746	ASP	CB-CG-OD1	5.73	123.45	118.30
1	D	395	HIS	N-CA-CB	-5.72	100.30	110.60
1	B	721	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	845	GLN	C-N-CA	-5.72	110.29	122.30
1	D	96	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	748	CYS	CA-CB-SG	-5.71	103.72	114.00
1	B	996	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	569	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	164	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	C	750	GLU	N-CA-CB	5.68	120.82	110.60
1	D	255	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	319	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	746	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	26	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	D	610	ASP	CB-CG-OD1	5.66	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	B	172	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	C	164	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	D	908	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	772	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	482	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	648	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	691	ALA	CB-CA-C	-5.64	101.64	110.10
1	D	178	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	246	MET	CG-SD-CE	-5.61	91.22	100.20
1	C	856	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	B	559	TYR	CD1-CE1-CZ	-5.59	114.76	119.80
1	C	919	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	559	TYR	CD1-CE1-CZ	-5.58	114.78	119.80
1	B	469	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	843	GLN	O-C-N	5.57	131.62	122.70
1	A	1000	SER	N-CA-CB	5.57	118.86	110.50
1	C	157	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	648	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	559	TYR	CG-CD2-CE2	-5.57	116.85	121.30
1	C	438	GLU	CG-CD-OE1	5.56	129.43	118.30
1	C	497	ASP	CB-CG-OD1	5.56	123.30	118.30
1	C	557	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	800	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	372	MET	CG-SD-CE	5.54	109.06	100.20
1	A	996	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	130	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	95	TYR	CD1-CE1-CZ	-5.52	114.83	119.80
1	B	553	TRP	CA-CB-CG	-5.51	103.22	113.70
1	D	140	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	280	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	699	ARG	CD-NE-CZ	5.51	131.31	123.60
1	C	924	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	689	GLU	C-N-CA	5.49	135.43	121.70
1	A	671	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	288	ARG	CG-CD-NE	-5.48	100.28	111.80
1	A	746	ASP	CB-CA-C	-5.48	99.44	110.40
1	D	682	LEU	CB-CA-C	-5.48	99.79	110.20
1	A	503	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	C	839	ALA	N-CA-CB	5.48	117.77	110.10
1	D	469	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	591	ASP	CB-CG-OD1	5.47	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	GLU	OE1-CD-OE2	5.46	129.86	123.30
1	C	699	ARG	CD-NE-CZ	-5.46	115.96	123.60
1	A	719	GLN	CB-CA-C	-5.46	99.49	110.40
1	C	569	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	251	ARG	CD-NE-CZ	5.45	131.23	123.60
1	C	59	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	379	MET	CG-SD-CE	5.43	108.89	100.20
1	C	429	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	828	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	367	MET	CG-SD-CE	5.41	108.86	100.20
1	C	741	THR	CA-CB-CG2	-5.41	104.82	112.40
1	D	760	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	C	719	GLN	CB-CA-C	-5.40	99.59	110.40
1	D	878	HIS	CA-CB-CG	-5.40	104.41	113.60
1	C	909	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	86	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	D	538	TYR	CB-CG-CD2	5.40	124.24	121.00
1	D	850	PHE	CB-CA-C	-5.40	99.61	110.40
1	C	790	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	768	MET	CG-SD-CE	5.39	108.82	100.20
1	D	916	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	96	ASP	N-CA-CB	5.38	120.28	110.60
1	B	819	GLU	N-CA-CB	-5.37	100.93	110.60
1	B	96	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	388	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	942	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	553	TRP	CA-CB-CG	-5.34	103.55	113.70
1	C	752	GLY	O-C-N	5.34	131.25	122.70
1	A	507	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	687	GLN	N-CA-CB	5.34	120.21	110.60
1	C	240	LEU	CA-CB-CG	-5.34	103.02	115.30
1	C	388	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	842	TRP	CH2-CZ2-CE2	-5.34	112.06	117.40
1	A	247	CYS	CA-CB-SG	-5.34	104.39	114.00
1	B	523	TRP	CG-CD2-CE3	-5.33	129.10	133.90
1	C	100	TYR	CG-CD2-CE2	-5.33	117.03	121.30
1	A	800	ARG	CD-NE-CZ	5.32	131.05	123.60
1	B	82	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	77	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	1016	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	C	184	LEU	CB-CA-C	-5.31	100.10	110.20
1	C	285	TYR	CB-CG-CD2	-5.31	117.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	404	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	D	781	ARG	CD-NE-CZ	5.30	131.02	123.60
1	C	126	THR	CA-CB-CG2	-5.30	104.98	112.40
1	C	26	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	D	926	TYR	CB-CG-CD1	5.29	124.18	121.00
1	B	477	SER	N-CA-CB	-5.29	102.56	110.50
1	A	961	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	52	ARG	CB-CA-C	-5.29	99.82	110.40
1	D	46	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	D	164	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	249	GLU	CG-CD-OE2	-5.28	107.75	118.30
1	D	917	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	D	809	ARG	CG-CD-NE	-5.27	100.73	111.80
1	C	857	ARG	CD-NE-CZ	-5.27	116.23	123.60
1	A	439	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	802	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	594	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	252	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	690	SER	N-CA-CB	-5.24	102.64	110.50
1	A	185	ALA	N-CA-CB	5.24	117.44	110.10
1	A	1000	SER	CA-CB-OG	-5.24	97.05	111.20
1	C	973	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	136	GLU	N-CA-CB	-5.24	101.17	110.60
1	B	288	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	857	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	82	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	164	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	832	ASP	N-CA-CB	-5.21	101.22	110.60
1	A	908	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	77	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	671	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	1000	SER	N-CA-CB	5.20	118.30	110.50
1	C	633	GLY	C-N-CA	5.20	134.69	121.70
1	C	856	TYR	CG-CD2-CE2	-5.20	117.14	121.30
1	C	553	TRP	CA-CB-CG	-5.18	103.85	113.70
1	C	875	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	969	GLU	CA-CB-CG	-5.17	102.02	113.40
1	B	524	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	A	140	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	C	968	MET	CG-SD-CE	-5.17	91.94	100.20
1	A	569	ASP	CB-CG-OD1	5.16	122.95	118.30
1	C	519	SER	N-CA-CB	-5.16	102.77	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	822	LEU	CB-CG-CD2	-5.16	102.24	111.00
1	C	997	ASP	N-CA-CB	5.15	119.86	110.60
1	C	919	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	599	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	144	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	C	538	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	B	164	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	358	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	C	161	TYR	N-CA-CB	-5.12	101.38	110.60
1	D	817	GLN	CB-CG-CD	-5.12	98.29	111.60
1	B	193	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	746	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	855	THR	N-CA-CB	5.11	120.00	110.30
1	A	403	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	568	TRP	CA-CB-CG	-5.10	104.01	113.70
1	D	961	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	721	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	B	699	ARG	CB-CG-CD	5.09	124.84	111.60
1	C	651	LEU	N-CA-CB	5.09	120.58	110.40
1	A	630	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	479	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	280	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	375	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	557	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	210	ARG	N-CA-CB	5.08	119.74	110.60
1	C	917	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	210	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	559	TYR	CB-CG-CD1	5.07	124.05	121.00
1	C	40	GLU	CG-CD-OE1	5.07	128.44	118.30
1	C	181	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	D	840	HIS	CB-CA-C	-5.07	100.27	110.40
1	A	428	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	A	648	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	D	37	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	755	ARG	CD-NE-CZ	5.05	130.68	123.60
1	B	163	GLN	N-CA-CB	5.05	119.70	110.60
1	B	1013	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	C	518	TRP	CE3-CZ3-CH2	-5.05	115.64	121.20
1	C	531	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	778	THR	CA-CB-CG2	-5.05	105.33	112.40
1	B	778	THR	CA-CB-CG2	-5.04	105.34	112.40
1	B	546	LEU	N-CA-CB	5.04	120.48	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	375	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	403	ASP	CB-CG-OD1	5.04	122.84	118.30
1	D	634	GLN	N-CA-CB	5.04	119.67	110.60
1	A	277	GLU	CG-CD-OE1	5.03	128.36	118.30
1	C	842	TRP	CB-CA-C	-5.03	100.34	110.40
1	C	287	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	A	40	GLU	CG-CD-OE1	5.03	128.36	118.30
1	C	43	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	C	819	GLU	N-CA-CB	-5.03	101.55	110.60
1	D	954	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	201	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	D	997	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	D	699	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	C	411	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	392	TYR	CD1-CG-CD2	5.01	123.41	117.90
1	C	894	ARG	CB-CA-C	-5.00	100.39	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	733	ALA	CA

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8127	0	7711	104	0
1	B	8128	0	7712	89	0
1	C	8128	0	7712	93	0
1	D	8128	0	7712	120	0
2	A	21	0	14	0	0
2	B	21	0	14	0	0
2	C	21	0	14	0	0
2	D	21	0	14	0	0
3	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	108	0	162	17	0
5	B	108	0	162	14	0
5	C	112	0	168	14	0
5	D	108	0	162	19	0
6	A	1112	0	0	16	3
6	B	1128	0	0	15	0
6	C	1104	0	0	16	3
6	D	1118	0	0	27	0
All	All	37524	0	31557	427	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (427) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:8415:DMS:C1	5:D:8415:DMS:S	2.01	1.48
5:B:8508:DMS:C1	5:B:8508:DMS:S	2.02	1.47
5:A:8403:DMS:S	5:A:8403:DMS:C2	2.03	1.46
5:B:8415:DMS:C2	5:B:8415:DMS:S	2.04	1.45
5:C:8402:DMS:C2	5:C:8402:DMS:S	2.04	1.44
1:C:634:GLN:H	1:C:634:GLN:NE2	1.33	1.25
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.39	1.20
1:B:730:LEU:HD12	1:B:730:LEU:H	1.21	1.01
1:A:634:GLN:HE21	1:A:634:GLN:HA	1.27	0.99
1:B:655:MET:HE2	1:B:665:SER:HB3	1.42	0.99
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.45	0.98
1:C:634:GLN:H	1:C:634:GLN:HE21	1.11	0.97
1:A:685:LEU:HD12	1:A:686:PRO:HD3	1.42	0.96
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.29	0.95
1:C:634:GLN:N	1:C:634:GLN:NE2	2.15	0.94
1:B:634:GLN:HG2	1:B:682:LEU:O	1.67	0.93
1:A:699:ARG:HH11	1:A:699:ARG:HG3	1.36	0.91
1:A:655:MET:HE2	1:A:656:VAL:N	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:GLN:H	1:B:600:GLN:HE21	1.18	0.89
1:D:629:PHE:O	1:D:630:ARG:HD3	1.72	0.89
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.04	0.88
1:A:264:GLU:HG3	6:A:9484:HOH:O	1.73	0.88
1:A:600:GLN:H	1:A:600:GLN:HE21	1.22	0.87
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.54	0.87
1:A:268:ALA:HA	5:A:8602:DMS:H22	1.59	0.84
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.40	0.84
1:A:655:MET:HB3	1:A:699:ARG:HH22	1.40	0.84
1:C:964:GLN:O	1:C:968:MET:HG2	1.77	0.83
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.24	0.83
1:D:658:LEU:O	1:D:661:LYS:HG3	1.79	0.83
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.60	0.82
1:D:681:GLU:HG2	6:D:9469:HOH:O	1.79	0.81
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.45	0.81
1:D:634:GLN:HB2	1:D:682:LEU:HB2	1.60	0.81
1:B:655:MET:CE	1:B:665:SER:HB3	2.12	0.80
1:A:290:THR:HB	5:A:8412:DMS:C2	2.12	0.80
1:C:530:THR:HG22	6:D:8752:HOH:O	1.82	0.80
1:D:131:GLU:OE2	1:D:135:GLN:HG3	1.83	0.79
1:A:797:GLU:O	1:A:801:ILE:HD13	1.83	0.78
1:A:685:LEU:HD12	1:A:686:PRO:CD	2.14	0.78
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.48	0.77
1:D:134:LEU:HA	5:D:8705:DMS:H22	1.65	0.77
1:B:890:GLN:HG2	1:B:891:VAL:N	1.94	0.77
1:A:658:LEU:O	1:A:661:LYS:HG3	1.84	0.77
1:C:658:LEU:O	1:C:661:LYS:HE3	1.86	0.75
1:B:658:LEU:O	1:B:661:LYS:HG3	1.85	0.75
1:C:748:CYS:C	1:C:749:ILE:HD12	2.06	0.75
1:B:890:GLN:HG3	6:B:9636:HOH:O	1.86	0.75
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.49	0.75
1:D:653:HIS:HD2	1:D:667:GLU:HB3	1.51	0.74
1:B:157:ARG:HD3	6:B:9466:HOH:O	1.86	0.74
1:C:730:LEU:HD23	1:C:730:LEU:H	1.52	0.74
1:B:651:LEU:O	1:B:651:LEU:HD23	1.87	0.74
1:A:687:GLN:NE2	6:A:9446:HOH:O	2.20	0.73
5:D:8417:DMS:H12	6:D:9774:HOH:O	1.87	0.73
6:A:9690:HOH:O	1:B:530:THR:HG22	1.86	0.73
1:D:685:LEU:HB3	1:D:686:PRO:CD	2.19	0.72
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.01	0.72
1:D:773:LYS:HD2	1:D:774:LYS:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LEU:O	5:D:8705:DMS:H21	1.90	0.72
1:B:845:GLN:OE1	1:B:845:GLN:HA	1.89	0.72
1:D:473:ARG:NH1	1:D:476:LYS:HB2	2.03	0.72
1:A:887:GLN:NE2	1:A:980:GLU:O	2.21	0.71
1:B:878:HIS:HD2	6:B:8697:HOH:O	1.73	0.71
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.72	0.71
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.04	0.71
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.72	0.71
1:D:804:ASN:HA	1:D:809:ARG:HH21	1.54	0.71
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.06	0.70
1:B:1017:GLN:HB2	6:B:9559:HOH:O	1.91	0.70
1:A:290:THR:HB	5:A:8412:DMS:H22	1.74	0.70
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.07	0.70
1:D:581:ASN:HD22	1:D:583:ASN:HD22	1.40	0.69
1:D:292:ARG:HH12	5:D:8412:DMS:H22	1.58	0.69
1:C:367:MET:HE1	6:C:9644:HOH:O	1.92	0.68
1:D:887:GLN:NE2	1:D:980:GLU:O	2.25	0.68
5:B:8411:DMS:H21	6:B:9633:HOH:O	1.94	0.68
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.20	0.68
5:D:8416:DMS:H22	6:D:9410:HOH:O	1.93	0.68
1:B:730:LEU:H	1:B:730:LEU:CD1	1.99	0.68
1:A:233:ASP:HA	5:A:8417:DMS:C1	2.24	0.68
1:B:655:MET:HE2	1:B:665:SER:CB	2.21	0.67
5:A:8420:DMS:H21	6:D:9524:HOH:O	1.94	0.67
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.24	0.67
1:D:797:GLU:O	1:D:801:ILE:HD13	1.95	0.67
1:D:804:ASN:HD22	1:D:809:ARG:HH21	1.41	0.67
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.75	0.67
1:D:134:LEU:HA	5:D:8705:DMS:C2	2.25	0.66
1:C:878:HIS:HD2	6:C:8704:HOH:O	1.77	0.66
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.78	0.66
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.28	0.66
1:A:634:GLN:NE2	1:A:634:GLN:HA	2.06	0.66
1:D:237:ARG:NH1	6:D:9286:HOH:O	2.25	0.66
1:D:634:GLN:NE2	1:D:682:LEU:O	2.29	0.66
1:C:730:LEU:HD23	1:C:730:LEU:N	2.09	0.66
1:B:245:GLN:NE2	6:B:9680:HOH:O	2.28	0.66
1:B:181:GLU:OE2	6:B:9502:HOH:O	2.13	0.66
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.77	0.66
1:A:878:HIS:HD2	6:A:8674:HOH:O	1.79	0.66
1:A:655:MET:HE2	1:A:656:VAL:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:8406:DMS:O	6:D:9684:HOH:O	2.12	0.65
1:A:861:SER:OG	1:A:863:GLN:HG3	1.95	0.65
1:A:646:HIS:ND1	6:A:9438:HOH:O	2.22	0.65
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.11	0.64
1:A:290:THR:HB	5:A:8412:DMS:H21	1.79	0.64
1:C:730:LEU:CD2	1:C:730:LEU:H	2.06	0.64
1:D:128:ASN:HB3	1:D:180:GLY:O	1.97	0.64
1:B:319:ASP:OD1	1:B:321:THR:N	2.29	0.64
1:C:634:GLN:N	1:C:634:GLN:HE21	1.87	0.64
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.79	0.64
1:C:687:GLN:HE21	1:C:687:GLN:HA	1.61	0.64
1:D:878:HIS:HD2	6:D:8825:HOH:O	1.80	0.63
1:D:595:THR:HA	1:D:596:PRO:C	2.17	0.63
1:C:745:MET:HG2	6:C:9471:HOH:O	1.99	0.63
1:B:13:ARG:NH1	6:B:9618:HOH:O	2.29	0.62
1:A:890:GLN:OE1	1:A:948:PRO:HD3	1.98	0.62
1:D:844:HIS:HD2	6:D:9787:HOH:O	1.81	0.62
1:B:730:LEU:HD12	1:B:730:LEU:N	2.05	0.62
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.34	0.62
1:B:75:GLU:OE1	1:B:75:GLU:HA	2.00	0.62
1:D:1022:GLN:O	1:D:1022:GLN:HG3	1.99	0.62
1:A:737:ILE:HD11	6:A:9651:HOH:O	1.98	0.62
1:C:965:GLN:HA	1:C:968:MET:SD	2.39	0.61
1:D:135:GLN:O	1:D:136:GLU:HG2	2.00	0.61
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.82	0.61
1:C:356:ARG:HD2	1:C:379:MET:CE	2.29	0.61
1:A:277:GLU:H	1:A:277:GLU:CD	2.03	0.61
1:A:84:VAL:HB	5:A:8414:DMS:O	2.01	0.61
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.83	0.61
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.16	0.61
1:D:581:ASN:HD22	1:D:583:ASN:ND2	1.98	0.61
1:C:46:ARG:HG2	6:C:9538:HOH:O	2.00	0.60
1:A:800:ARG:HG2	6:A:9380:HOH:O	2.02	0.60
1:C:178:ARG:HD3	6:C:9502:HOH:O	2.02	0.60
1:D:773:LYS:HG3	1:D:775:GLN:HE21	1.66	0.60
1:A:724:GLU:O	1:B:847:LYS:NZ	2.30	0.60
1:C:749:ILE:HD12	1:C:749:ILE:N	2.16	0.60
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.01	0.60
1:D:844:HIS:CD2	6:D:9787:HOH:O	2.54	0.60
1:C:687:GLN:NE2	1:C:687:GLN:HA	2.15	0.59
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.83	0.59
1:D:739:HIS:ND1	6:D:8745:HOH:O	2.31	0.59
5:C:8427:DMS:H21	6:C:9067:HOH:O	2.03	0.59
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.85	0.59
5:D:8409:DMS:O	6:D:9258:HOH:O	2.16	0.59
1:D:363:HIS:HD2	6:D:9334:HOH:O	1.86	0.58
1:B:178:ARG:HG3	1:B:178:ARG:O	2.03	0.58
1:B:600:GLN:N	1:B:600:GLN:HE21	1.97	0.58
1:B:824:GLN:HG2	1:B:825:CYS:N	2.18	0.58
5:C:8406:DMS:H13	6:C:9698:HOH:O	2.03	0.58
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.11	0.58
1:A:233:ASP:HA	5:A:8417:DMS:H12	1.86	0.58
1:A:737:ILE:HD13	1:A:737:ILE:C	2.24	0.58
1:D:847:LYS:HG3	1:D:848:THR:N	2.19	0.58
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.34	0.57
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.86	0.57
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.38	0.57
1:D:230:ARG:HD3	6:D:9706:HOH:O	2.02	0.57
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.86	0.57
1:C:79:PRO:HD2	1:C:80:GLU:OE2	2.05	0.57
1:B:236:SER:C	1:B:237:ARG:HG2	2.25	0.57
5:D:8427:DMS:H12	6:D:9169:HOH:O	2.05	0.56
5:D:8406:DMS:H21	6:D:9684:HOH:O	2.05	0.56
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.85	0.56
1:A:655:MET:CB	1:A:699:ARG:HH22	2.17	0.56
1:A:241:GLU:CD	1:A:292:ARG:HE	2.08	0.56
1:C:720:TRP:HA	5:C:8427:DMS:C1	2.36	0.56
1:B:651:LEU:C	1:B:651:LEU:HD23	2.25	0.55
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.74	0.55
1:A:245:GLN:CD	1:A:288:ARG:HE	2.10	0.55
1:C:595:THR:HA	1:C:596:PRO:C	2.26	0.55
1:D:237:ARG:NH1	1:D:237:ARG:HB3	2.19	0.55
1:A:824:GLN:NE2	1:A:837:THR:HG22	2.21	0.55
1:D:804:ASN:HA	1:D:809:ARG:HE	1.72	0.55
1:C:724:GLU:O	1:D:847:LYS:NZ	2.39	0.55
1:A:595:THR:HA	1:A:596:PRO:C	2.27	0.55
1:C:634:GLN:CA	1:C:634:GLN:NE2	2.71	0.54
1:D:754:LYS:HE2	1:D:1022:GLN:HG2	1.90	0.54
1:C:240:LEU:HD23	1:C:240:LEU:C	2.28	0.54
1:A:88:SER:HA	1:A:366:VAL:HG21	1.88	0.54
1:B:890:GLN:HB3	6:B:9568:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:MET:CE	1:C:662:PRO:HB3	2.38	0.54
1:A:94:GLY:HA3	5:A:8421:DMS:H23	1.90	0.54
1:B:685:LEU:HB3	1:B:686:PRO:HD2	1.89	0.54
1:B:292:ARG:HH12	5:B:8412:DMS:C2	2.20	0.54
1:A:653:HIS:CD2	1:A:701:VAL:HG21	2.42	0.54
1:B:699:ARG:HH21	5:B:8415:DMS:C1	2.20	0.54
1:A:749:ILE:HD13	1:A:858:ILE:HD12	1.89	0.54
1:B:226:HIS:CE1	1:B:448:ARG:NH1	2.75	0.54
1:A:699:ARG:NH1	1:A:699:ARG:HG3	2.13	0.54
1:D:131:GLU:OE2	1:D:131:GLU:O	2.25	0.53
1:C:320:GLY:HA2	5:C:8406:DMS:O	2.07	0.53
1:B:360:HIS:HE1	1:B:362:LEU:HD12	1.73	0.53
1:C:367:MET:HA	1:C:367:MET:HE3	1.90	0.53
1:D:80:GLU:OE1	1:D:80:GLU:N	2.36	0.53
1:C:728:VAL:O	1:C:730:LEU:HD23	2.09	0.53
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.89	0.53
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.42	0.53
1:B:835:LEU:HD11	1:B:855:THR:HB	1.90	0.53
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.29	0.53
1:D:781:ARG:NH1	6:D:9479:HOH:O	2.23	0.53
1:A:288:ARG:NH1	6:A:9036:HOH:O	2.28	0.53
1:D:804:ASN:HD22	1:D:809:ARG:CZ	2.15	0.52
1:A:832:ASP:N	1:A:832:ASP:OD1	2.42	0.52
1:A:684:GLU:O	1:A:685:LEU:HD13	2.09	0.52
1:B:634:GLN:HB3	1:B:681:GLU:OE2	2.10	0.52
1:D:577:LYS:O	1:D:584:PRO:HA	2.09	0.52
1:A:844:HIS:HD2	6:A:9436:HOH:O	1.91	0.52
1:D:157:ARG:HG2	1:D:176:PHE:HE2	1.74	0.52
1:D:240:LEU:HD23	1:D:240:LEU:C	2.29	0.52
1:B:797:GLU:HG2	1:B:799:THR:HG23	1.92	0.52
1:D:675:GLN:HG3	6:D:9580:HOH:O	2.10	0.52
1:D:618:THR:HG23	6:D:9081:HOH:O	2.09	0.52
1:D:754:LYS:C	1:D:755:ARG:HG2	2.30	0.52
1:B:595:THR:HA	1:B:596:PRO:C	2.30	0.52
1:D:618:THR:HG21	6:D:9065:HOH:O	2.09	0.52
1:D:651:LEU:HD12	1:D:701:VAL:HB	1.92	0.51
1:A:735:HIS:O	1:A:736:ALA:HB2	2.10	0.51
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.28	0.51
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.38	0.51
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.38	0.51
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:O	1:A:737:ILE:HD13	2.11	0.51
1:B:133:TRP:CD1	5:B:8504:DMS:C1	2.94	0.51
1:A:651:LEU:CD2	1:A:703:PRO:HG3	2.41	0.51
1:C:835:LEU:HD11	1:C:855:THR:HB	1.92	0.51
1:C:288:ARG:NH1	6:C:9069:HOH:O	2.27	0.51
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.94	0.51
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.25	0.51
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.41	0.51
1:B:628:GLN:HE22	5:B:8402:DMS:C2	2.24	0.51
1:A:615:PRO:O	1:A:618:THR:HG22	2.11	0.50
1:A:600:GLN:N	1:A:600:GLN:HE21	2.02	0.50
1:A:245:GLN:OE1	1:A:288:ARG:NE	2.43	0.50
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.93	0.50
1:C:628:GLN:NE2	5:C:8402:DMS:O	2.43	0.50
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.46	0.50
1:C:651:LEU:HD11	1:C:653:HIS:HE1	1.77	0.50
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.41	0.50
1:B:320:GLY:O	5:B:8406:DMS:O	2.30	0.50
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.92	0.50
1:C:890:GLN:HG3	1:C:891:VAL:N	2.27	0.50
1:D:367:MET:HB3	1:D:372:MET:HE2	1.94	0.50
1:A:85:VAL:N	5:A:8414:DMS:O	2.42	0.50
1:D:734:SER:OG	1:D:860:GLY:HA3	2.12	0.50
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.93	0.50
5:A:8403:DMS:C1	5:A:8403:DMS:C2	2.90	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.93	0.50
5:B:8417:DMS:H23	6:D:9785:HOH:O	2.12	0.50
1:A:685:LEU:O	1:A:687:GLN:OE1	2.29	0.49
1:D:250:LEU:O	5:D:8416:DMS:H21	2.12	0.49
1:C:44:THR:OG1	1:C:46:ARG:HD3	2.13	0.49
1:D:80:GLU:HG3	6:D:9758:HOH:O	2.11	0.49
1:B:684:GLU:HG2	1:B:685:LEU:N	2.24	0.49
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.95	0.49
5:C:8506:DMS:H21	6:C:9496:HOH:O	2.12	0.49
1:D:630:ARG:NH1	6:D:9312:HOH:O	2.44	0.49
1:D:829:THR:O	1:D:830:LEU:HD23	2.13	0.49
1:A:625:GLN:NE2	6:A:8800:HOH:O	2.34	0.49
1:A:147:ASN:HA	1:A:148:SER:HA	1.59	0.49
1:C:829:THR:HG22	1:C:830:LEU:N	2.27	0.49
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.27	0.49
1:D:843:GLN:HA	1:D:847:LYS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.48	0.48
1:D:373:VAL:O	1:D:377:LEU:HG	2.14	0.48
1:D:804:ASN:HA	1:D:809:ARG:NH2	2.26	0.48
1:B:615:PRO:O	1:B:618:THR:HG22	2.13	0.48
1:D:625:GLN:NE2	6:D:8952:HOH:O	2.39	0.48
1:D:738:PRO:HG3	1:D:751:LEU:HD13	1.95	0.48
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.48	0.48
1:C:147:ASN:HA	1:C:148:SER:HA	1.64	0.48
1:D:135:GLN:C	1:D:136:GLU:HG2	2.34	0.48
5:D:8427:DMS:H11	6:D:8960:HOH:O	2.14	0.48
1:A:768:MET:HE3	1:A:1020:TRP:CZ2	2.48	0.48
1:D:737:ILE:HD12	1:D:832:ASP:HA	1.95	0.48
1:B:699:ARG:HE	1:B:714:ILE:HD13	1.79	0.48
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.74	0.48
1:B:600:GLN:H	1:B:600:GLN:NE2	2.00	0.48
1:C:615:PRO:O	1:C:618:THR:HG22	2.14	0.48
5:D:8415:DMS:C1	5:D:8415:DMS:C2	2.92	0.47
5:C:8506:DMS:C2	6:C:9496:HOH:O	2.62	0.47
1:A:600:GLN:NE2	1:A:600:GLN:H	2.03	0.47
1:D:251:ARG:HA	5:D:8416:DMS:H22	1.95	0.47
1:A:251:ARG:HH11	5:A:8416:DMS:C2	2.27	0.47
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.48	0.47
1:D:659:ASP:HA	6:D:9797:HOH:O	2.14	0.47
1:C:622:HIS:CE1	5:C:8402:DMS:C1	2.97	0.47
1:B:847:LYS:HE2	1:B:875:ASP:OD1	2.15	0.47
1:C:634:GLN:OE1	1:C:681:GLU:HG2	2.14	0.47
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.98	0.47
1:B:147:ASN:HA	1:B:148:SER:HA	1.57	0.47
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.97	0.47
1:D:737:ILE:HD13	1:D:831:ALA:O	2.15	0.47
1:D:749:ILE:CD1	1:D:858:ILE:HD12	2.45	0.47
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.50	0.47
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.96	0.47
1:C:965:GLN:O	1:C:968:MET:HG3	2.14	0.47
1:C:653:HIS:CE1	1:C:667:GLU:CG	2.98	0.47
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.97	0.47
1:C:690:SER:HB2	6:C:9380:HOH:O	2.15	0.47
1:B:681:GLU:OE1	1:B:681:GLU:HA	2.15	0.46
1:C:653:HIS:ND1	1:C:667:GLU:CG	2.79	0.46
1:B:387:VAL:HG22	6:B:9693:HOH:O	2.14	0.46
1:D:804:ASN:ND2	1:D:809:ARG:CZ	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LYS:HE2	6:A:9025:HOH:O	2.15	0.46
1:D:986:ILE:HD12	1:D:986:ILE:HG21	1.63	0.46
1:B:809:ARG:NH1	1:B:809:ARG:HG2	2.15	0.46
1:A:742:THR:HG22	1:A:743:SER:N	2.30	0.46
1:D:88:SER:HA	1:D:366:VAL:HG21	1.98	0.46
1:B:88:SER:HA	1:B:366:VAL:HG21	1.98	0.46
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.98	0.46
1:C:634:GLN:HB2	1:C:682:LEU:HB2	1.98	0.46
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.27	0.46
1:B:13:ARG:O	1:B:14:ARG:C	2.55	0.46
1:B:699:ARG:NH2	5:B:8415:DMS:C1	2.79	0.45
1:B:781:ARG:HD3	6:B:9687:HOH:O	2.16	0.45
1:B:890:GLN:CG	1:B:891:VAL:N	2.73	0.45
1:C:13:ARG:O	1:C:14:ARG:C	2.54	0.45
1:D:367:MET:HB3	1:D:372:MET:CE	2.46	0.45
1:C:952:ARG:NH2	1:C:1021:CYS:SG	2.88	0.45
1:A:781:ARG:NH1	6:A:9332:HOH:O	2.50	0.45
1:C:49:GLN:HG2	6:C:9326:HOH:O	2.16	0.45
1:A:655:MET:HE3	1:A:665:SER:HB3	1.97	0.45
1:D:962:TYR:CE1	5:D:8508:DMS:H12	2.52	0.45
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.99	0.45
1:A:685:LEU:HD13	1:A:685:LEU:HA	1.62	0.45
1:C:893:GLU:HG2	6:C:9145:HOH:O	2.17	0.45
1:D:360:HIS:HE1	1:D:362:LEU:HD12	1.82	0.45
1:A:651:LEU:CD1	1:A:653:HIS:CE1	2.99	0.45
1:B:262:GLN:NE2	1:B:263:GLY:N	2.65	0.45
6:B:9393:HOH:O	5:C:8420:DMS:H21	2.17	0.44
5:B:8421:DMS:H22	6:B:9134:HOH:O	2.16	0.44
1:C:266:GLN:NE2	5:C:8602:DMS:S	2.91	0.44
1:C:1000:SER:O	1:C:1001:PRO:C	2.56	0.44
1:C:16:TRP:CG	1:C:189:LEU:HD13	2.52	0.44
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.00	0.44
1:D:251:ARG:HA	5:D:8416:DMS:C2	2.47	0.44
1:C:233:ASP:HA	5:C:8417:DMS:S	2.57	0.44
1:D:890:GLN:HE21	1:D:892:ALA:HB2	1.83	0.44
1:C:673:ALA:HB1	1:C:674:PRO:HD2	2.00	0.44
1:C:684:GLU:HG2	1:C:685:LEU:N	2.13	0.44
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.18	0.44
5:A:8419:DMS:H23	6:A:9367:HOH:O	2.18	0.44
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.82	0.44
1:A:71:GLU:HG3	1:A:72:SER:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:688:PRO:C	1:D:690:SER:H	2.21	0.43
1:D:130:ASP:OD2	5:D:8703:DMS:H22	2.19	0.43
1:B:47:PRO:O	6:B:9658:HOH:O	2.21	0.43
5:C:8402:DMS:C2	5:C:8402:DMS:C1	2.94	0.43
1:D:651:LEU:HD12	1:D:651:LEU:O	2.18	0.43
1:B:797:GLU:O	1:B:801:ILE:HD13	2.18	0.43
1:B:381:GLN:O	1:B:621:LYS:HE3	2.19	0.43
1:B:237:ARG:HD2	1:B:296:GLU:OE1	2.18	0.43
1:C:829:THR:HG22	1:C:830:LEU:O	2.18	0.43
1:B:128:ASN:HA	1:B:180:GLY:O	2.18	0.43
1:C:749:ILE:N	1:C:749:ILE:CD1	2.82	0.43
1:C:768:MET:HB2	1:C:768:MET:HE3	1.80	0.43
1:C:844:HIS:HD2	6:C:9477:HOH:O	2.00	0.43
1:D:659:ASP:O	6:D:9319:HOH:O	2.21	0.43
1:A:178:ARG:CD	6:A:9467:HOH:O	2.66	0.43
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.19	0.43
1:D:111:PRO:HA	1:D:112:PRO:HA	1.80	0.43
1:C:781:ARG:NH1	6:C:9371:HOH:O	2.52	0.43
1:B:917:ARG:HD3	1:B:917:ARG:HH11	1.55	0.43
1:A:416:GLU:OE2	1:A:418:HIS:HB2	2.19	0.43
1:D:473:ARG:NH1	1:D:476:LYS:CB	2.79	0.43
1:C:132:SER:HB2	5:C:8504:DMS:H11	2.01	0.43
1:C:356:ARG:NH2	6:C:9644:HOH:O	2.24	0.42
1:B:133:TRP:CZ3	1:B:216:HIS:HB2	2.54	0.42
1:D:863:GLN:HG2	1:D:1021:CYS:CB	2.48	0.42
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.99	0.42
1:B:824:GLN:OE1	1:B:837:THR:HG22	2.19	0.42
1:D:893:GLU:HG3	1:D:893:GLU:O	2.19	0.42
1:A:866:ILE:O	1:A:1017:GLN:HG2	2.19	0.42
1:A:233:ASP:HA	5:A:8417:DMS:H13	1.96	0.42
1:A:433:LEU:N	1:A:434:PRO:CD	2.82	0.42
1:D:768:MET:HE2	1:D:1020:TRP:CZ2	2.54	0.42
1:C:806:TRP:HA	1:C:809:ARG:HE	1.84	0.42
1:C:595:THR:HG23	1:C:595:THR:O	2.19	0.42
1:D:1022:GLN:HE21	1:D:1022:GLN:C	2.23	0.42
1:A:753:ASN:HB2	1:A:771:GLY:HA2	2.02	0.42
1:C:237:ARG:HB3	1:C:237:ARG:NH1	2.34	0.42
1:B:133:TRP:CD1	5:B:8504:DMS:H11	2.54	0.42
1:D:639:THR:OG1	1:D:677:LYS:HE2	2.20	0.42
1:C:737:ILE:HG13	1:C:737:ILE:O	2.14	0.42
1:A:986:ILE:HD13	1:A:986:ILE:HG23	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ARG:NH1	1:D:237:ARG:CG	2.80	0.42
1:D:433:LEU:N	1:D:434:PRO:CD	2.83	0.42
1:C:237:ARG:CB	1:C:237:ARG:HH11	2.32	0.42
1:B:737:ILE:HD13	1:B:831:ALA:O	2.19	0.42
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.18	0.41
1:A:251:ARG:HH11	5:A:8416:DMS:H23	1.84	0.41
1:D:661:LYS:H	1:D:661:LYS:HG3	1.57	0.41
1:D:538:TYR:C	1:D:539[B]:ALA:O	2.57	0.41
1:C:750:GLU:HG2	1:C:755:ARG:HG3	2.01	0.41
1:B:225:PHE:HA	1:B:243:GLU:O	2.21	0.41
1:D:681:GLU:HG2	1:D:681:GLU:H	1.65	0.41
1:A:1000:SER:O	1:A:1001:PRO:C	2.57	0.41
1:B:114:VAL:HB	1:B:115:PRO:HD2	2.02	0.41
1:D:147:ASN:HA	1:D:148:SER:HA	1.69	0.41
1:A:655:MET:C	1:A:655:MET:HE2	2.38	0.41
1:A:473:ARG:NH1	1:A:476:LYS:CB	2.81	0.41
1:D:112:PRO:HD2	1:D:113:PHE:CE1	2.55	0.41
1:B:305:ILE:HD11	1:B:645:ARG:HB3	2.02	0.41
1:B:49:GLN:HG2	6:B:9314:HOH:O	2.21	0.41
1:C:684:GLU:CG	1:C:685:LEU:N	2.80	0.41
1:A:859:ASP:OD1	1:A:861:SER:OG	2.26	0.41
5:A:8409:DMS:O	6:A:9105:HOH:O	2.22	0.41
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.03	0.41
1:A:370:GLN:HG3	6:A:9074:HOH:O	2.20	0.41
1:B:751:LEU:HD23	1:B:862:GLY:HA2	2.01	0.41
1:D:340:GLY:O	1:D:561:ARG:HG2	2.21	0.41
1:A:78:LEU:HA	1:A:79:PRO:HD3	1.73	0.41
1:D:651:LEU:C	1:D:651:LEU:CD1	2.90	0.40
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.56	0.40
1:B:513:PRO:O	1:B:514:ALA:HB3	2.20	0.40
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.56	0.40
1:D:893:GLU:HG2	1:D:894:ARG:HG2	2.03	0.40
1:C:70:PRO:HG2	1:C:78:LEU:HD21	2.03	0.40
1:B:320:GLY:HA2	5:B:8406:DMS:O	2.22	0.40
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.03	0.40
1:D:513:PRO:O	1:D:514:ALA:HB3	2.22	0.40
1:C:965:GLN:HA	1:C:968:MET:CG	2.51	0.40
1:C:968:MET:HE2	1:C:968:MET:HB2	1.66	0.40
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.57	0.40
1:A:843:GLN:HA	1:A:847:LYS:O	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:9652:HOH:O	6:C:9432:HOH:O[3_544]	2.15	0.05
6:A:9694:HOH:O	6:C:9467:HOH:O[3_544]	2.16	0.04
6:A:9697:HOH:O	6:C:9628:HOH:O[2_554]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1011/1023 (99%)	974 (96%)	37 (4%)	0	100	100
1	B	1011/1023 (99%)	978 (97%)	30 (3%)	3 (0%)	46	20
1	C	1011/1023 (99%)	974 (96%)	36 (4%)	1 (0%)	56	27
1	D	1011/1023 (99%)	971 (96%)	38 (4%)	2 (0%)	52	25
All	All	4044/4092 (99%)	3897 (96%)	141 (4%)	6 (0%)	56	27

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	731	PRO
1	B	732	ALA
1	C	734	SER
1	D	688	PRO
1	B	164	ASP
1	D	164	ASP

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	839 (97%)	25 (3%)	50	17
1	B	865/875 (99%)	834 (96%)	31 (4%)	42	11
1	C	865/875 (99%)	827 (96%)	38 (4%)	35	6
1	D	865/875 (99%)	831 (96%)	34 (4%)	39	9
All	All	3459/3500 (99%)	3331 (96%)	128 (4%)	41	10

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	TRP
1	A	116	THR
1	A	250	LEU
1	A	333	ARG
1	A	394	ASN
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	600	GLN
1	A	632	SER
1	A	634	GLN
1	A	655	MET
1	A	661	LYS
1	A	667	GLU
1	A	684	GLU
1	A	685	LEU
1	A	690	SER
1	A	699	ARG
1	A	737	ILE
1	A	773	LYS
1	A	799	THR
1	A	885	ASN
1	A	986	ILE
1	A	1013	ARG
1	A	1023	LYS
1	B	71	GLU
1	B	80	GLU
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	277	GLU

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Mol	Chain	Res	Type
1	B	333	ARG
1	B	370	GLN
1	B	392	TYR
1	B	394	ASN
1	B	554	GLN
1	B	583	ASN
1	B	600	GLN
1	B	634	GLN
1	B	651	LEU
1	B	661	LYS
1	B	667	GLU
1	B	684	GLU
1	B	687	GLN
1	B	730	LEU
1	B	745	MET
1	B	766	SER
1	B	799	THR
1	B	809	ARG
1	B	819	GLU
1	B	824	GLN
1	B	845	GLN
1	B	885	ASN
1	B	890	GLN
1	B	917	ARG
1	B	1023	LYS
1	C	71	GLU
1	C	76	CYS
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG
1	C	230	ARG
1	C	251	ARG
1	C	262	GLN
1	C	299	LYS
1	C	333	ARG
1	C	344	LEU
1	C	370	GLN
1	C	394	ASN
1	C	519	SER
1	C	546	LEU
1	C	634	GLN
1	C	651	LEU

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Mol	Chain	Res	Type
1	C	659	ASP
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	749	ILE
1	C	773	LYS
1	C	800	ARG
1	C	819	GLU
1	C	885	ASN
1	C	893	GLU
1	C	956	GLN
1	C	968	MET
1	C	1013	ARG
1	C	1017	GLN
1	C	1022	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	112	PRO
1	D	237	ARG
1	D	277	GLU
1	D	319	ASP
1	D	333	ARG
1	D	344	LEU
1	D	370	GLN
1	D	394	ASN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	632	SER
1	D	651	LEU
1	D	661	LYS
1	D	667	GLU
1	D	681	GLU
1	D	684	GLU
1	D	687	GLN
1	D	730	LEU

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Mol	Chain	Res	Type
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	772	ASP
1	D	797	GLU
1	D	799	THR
1	D	885	ASN
1	D	893	GLU
1	D	910	LEU
1	D	986	ILE
1	D	1022	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	GLN
1	A	614	HIS
1	A	624	GLN
1	A	634	GLN
1	A	653	HIS
1	A	675	GLN
1	A	824	GLN
1	A	844	HIS
1	A	878	HIS
1	B	262	GLN
1	B	363	HIS
1	B	510	GLN
1	B	583	ASN
1	B	600	GLN
1	B	614	HIS
1	B	624	GLN
1	B	628	GLN
1	B	878	HIS
1	B	890	GLN
1	B	1017	GLN
1	C	363	HIS
1	C	624	GLN
1	C	634	GLN
1	C	687	GLN
1	C	824	GLN

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Mol	Chain	Res	Type
1	C	878	HIS
1	C	977	HIS
1	D	135	GLN
1	D	363	HIS
1	D	583	ASN
1	D	624	GLN
1	D	628	GLN
1	D	634	GLN
1	D	653	HIS
1	D	704	ASN
1	D	804	ASN
1	D	878	HIS
1	D	903	GLN
1	D	977	HIS
1	D	1022	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 31 are monoatomic - leaving 113 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	147	A	2001	4	20,22,22	0.73	0	29,31,31	1.54	4 (13%)
5	DMS	A	8401	-	3,3,3	0.92	0	3,3,3	0.26	0
5	DMS	A	8402	-	3,3,3	2.15	1 (33%)	3,3,3	0.33	0
5	DMS	A	8403	-	3,3,3	2.32	1 (33%)	3,3,3	0.38	0
5	DMS	A	8404	-	3,3,3	1.63	1 (33%)	3,3,3	0.35	0
5	DMS	A	8405	-	3,3,3	1.35	1 (33%)	3,3,3	0.72	0
5	DMS	A	8406	3	3,3,3	0.43	0	3,3,3	0.24	0
5	DMS	A	8407	-	3,3,3	3.20	2 (66%)	3,3,3	0.45	0
5	DMS	A	8408	-	3,3,3	1.08	0	3,3,3	1.13	0
5	DMS	A	8409	-	3,3,3	2.35	1 (33%)	3,3,3	0.62	0
5	DMS	A	8410	-	3,3,3	0.76	0	3,3,3	0.94	0
5	DMS	A	8411	-	3,3,3	0.79	0	3,3,3	0.26	0
5	DMS	A	8412	-	3,3,3	2.15	1 (33%)	3,3,3	0.27	0
5	DMS	A	8413	-	3,3,3	2.91	3 (100%)	3,3,3	0.74	0
5	DMS	A	8414	-	3,3,3	0.91	0	3,3,3	0.21	0
5	DMS	A	8415	-	3,3,3	2.62	3 (100%)	3,3,3	0.27	0
5	DMS	A	8416	-	3,3,3	1.09	0	3,3,3	0.41	0
5	DMS	A	8417	-	3,3,3	0.95	0	3,3,3	0.55	0
5	DMS	A	8419	-	3,3,3	0.66	0	3,3,3	0.62	0
5	DMS	A	8420	-	3,3,3	1.57	0	3,3,3	0.57	0
5	DMS	A	8421	-	3,3,3	0.73	0	3,3,3	0.27	0
5	DMS	A	8423	-	3,3,3	1.45	0	3,3,3	0.22	0
5	DMS	A	8425	4	3,3,3	2.08	2 (66%)	3,3,3	0.72	0
5	DMS	A	8427	-	3,3,3	0.77	0	3,3,3	0.15	0
5	DMS	A	8501	-	3,3,3	1.62	1 (33%)	3,3,3	0.36	0
5	DMS	A	8502	-	3,3,3	2.11	2 (66%)	3,3,3	1.69	1 (33%)
5	DMS	A	8504	-	3,3,3	0.26	0	3,3,3	0.51	0
5	DMS	A	8602	-	3,3,3	1.29	0	3,3,3	0.65	0
2	147	B	2001	4	20,22,22	0.80	1 (5%)	29,31,31	1.64	7 (24%)
5	DMS	B	8401	-	3,3,3	0.86	0	3,3,3	0.53	0
5	DMS	B	8402	-	3,3,3	2.50	3 (100%)	3,3,3	0.82	0
5	DMS	B	8403	-	3,3,3	1.82	2 (66%)	3,3,3	0.55	0
5	DMS	B	8404	-	3,3,3	1.49	1 (33%)	3,3,3	0.15	0
5	DMS	B	8405	-	3,3,3	1.35	1 (33%)	3,3,3	0.98	0
5	DMS	B	8406	-	3,3,3	1.16	0	3,3,3	0.88	0
5	DMS	B	8407	-	3,3,3	2.18	1 (33%)	3,3,3	0.45	0
5	DMS	B	8408	-	3,3,3	1.20	0	3,3,3	0.14	0
5	DMS	B	8409	-	3,3,3	2.79	2 (66%)	3,3,3	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	B	8410	-	3,3,3	1.68	1 (33%)	3,3,3	0.39	0
5	DMS	B	8411	-	3,3,3	1.57	0	3,3,3	0.53	0
5	DMS	B	8412	-	3,3,3	0.90	0	3,3,3	0.18	0
5	DMS	B	8413	-	3,3,3	2.13	1 (33%)	3,3,3	0.99	0
5	DMS	B	8414	-	3,3,3	0.56	0	3,3,3	1.39	1 (33%)
5	DMS	B	8415	-	3,3,3	2.83	2 (66%)	3,3,3	1.85	1 (33%)
5	DMS	B	8416	-	3,3,3	1.18	0	3,3,3	0.55	0
5	DMS	B	8417	-	3,3,3	1.44	1 (33%)	3,3,3	0.57	0
5	DMS	B	8420	-	3,3,3	1.45	1 (33%)	3,3,3	0.17	0
5	DMS	B	8421	-	3,3,3	0.76	0	3,3,3	1.07	0
5	DMS	B	8423	-	3,3,3	0.77	0	3,3,3	0.89	0
5	DMS	B	8425	4	3,3,3	1.71	1 (33%)	3,3,3	0.31	0
5	DMS	B	8427	-	3,3,3	0.63	0	3,3,3	0.27	0
5	DMS	B	8502	-	3,3,3	1.39	0	3,3,3	1.94	1 (33%)
5	DMS	B	8504	-	3,3,3	0.97	0	3,3,3	0.57	0
5	DMS	B	8506	-	3,3,3	1.85	1 (33%)	3,3,3	0.55	0
5	DMS	B	8508	-	3,3,3	2.58	2 (66%)	3,3,3	0.29	0
5	DMS	B	8601	-	3,3,3	1.81	1 (33%)	3,3,3	0.67	0
2	147	C	2001	4	20,22,22	0.83	0	29,31,31	1.25	1 (3%)
5	DMS	C	8401	-	3,3,3	0.77	0	3,3,3	0.20	0
5	DMS	C	8402	-	3,3,3	2.41	1 (33%)	3,3,3	0.37	0
5	DMS	C	8403	-	3,3,3	1.90	1 (33%)	3,3,3	0.33	0
5	DMS	C	8404	-	3,3,3	1.27	0	3,3,3	0.65	0
5	DMS	C	8405	-	3,3,3	1.95	1 (33%)	3,3,3	0.32	0
5	DMS	C	8406	-	3,3,3	1.64	0	3,3,3	0.39	0
5	DMS	C	8407	-	3,3,3	1.57	1 (33%)	3,3,3	0.14	0
5	DMS	C	8408	-	3,3,3	1.30	0	3,3,3	0.80	0
5	DMS	C	8409	-	3,3,3	2.35	1 (33%)	3,3,3	0.86	0
5	DMS	C	8410	-	3,3,3	1.16	0	3,3,3	0.38	0
5	DMS	C	8411	-	3,3,3	1.33	0	3,3,3	0.28	0
5	DMS	C	8412	-	3,3,3	1.65	1 (33%)	3,3,3	0.28	0
5	DMS	C	8413	-	3,3,3	2.27	1 (33%)	3,3,3	0.59	0
5	DMS	C	8414	-	3,3,3	1.82	2 (66%)	3,3,3	0.82	0
5	DMS	C	8415	-	3,3,3	1.64	0	3,3,3	0.46	0
5	DMS	C	8416	-	3,3,3	1.71	1 (33%)	3,3,3	0.33	0
5	DMS	C	8417	-	3,3,3	0.80	0	3,3,3	1.04	0
5	DMS	C	8419	-	3,3,3	1.10	0	3,3,3	0.26	0
5	DMS	C	8420	-	3,3,3	2.32	1 (33%)	3,3,3	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	DMS	C	8421	-	3,3,3	0.78	0	3,3,3	1.08	0
5	DMS	C	8423	-	3,3,3	0.82	0	3,3,3	0.26	0
5	DMS	C	8425	4	3,3,3	1.59	1 (33%)	3,3,3	0.52	0
5	DMS	C	8427	-	3,3,3	0.91	0	3,3,3	0.61	0
5	DMS	C	8501	-	3,3,3	1.09	0	3,3,3	0.77	0
5	DMS	C	8504	-	3,3,3	0.77	0	3,3,3	0.49	0
5	DMS	C	8506	-	3,3,3	2.21	1 (33%)	3,3,3	0.23	0
5	DMS	C	8601	-	3,3,3	1.36	1 (33%)	3,3,3	0.62	0
5	DMS	C	8602	-	3,3,3	0.25	0	3,3,3	0.59	0
2	147	D	2001	4	20,22,22	0.84	1 (5%)	29,31,31	1.34	2 (6%)
5	DMS	D	8401	-	3,3,3	1.20	0	3,3,3	0.94	0
5	DMS	D	8402	-	3,3,3	2.00	1 (33%)	3,3,3	0.60	0
5	DMS	D	8403	-	3,3,3	1.32	0	3,3,3	0.78	0
5	DMS	D	8404	-	3,3,3	1.84	1 (33%)	3,3,3	0.46	0
5	DMS	D	8405	-	3,3,3	1.26	0	3,3,3	0.48	0
5	DMS	D	8406	-	3,3,3	0.67	0	3,3,3	0.36	0
5	DMS	D	8407	-	3,3,3	2.09	3 (100%)	3,3,3	0.50	0
5	DMS	D	8408	-	3,3,3	1.25	0	3,3,3	0.31	0
5	DMS	D	8409	-	3,3,3	2.18	1 (33%)	3,3,3	1.03	0
5	DMS	D	8410	-	3,3,3	1.36	1 (33%)	3,3,3	0.45	0
5	DMS	D	8411	-	3,3,3	0.75	0	3,3,3	0.21	0
5	DMS	D	8412	-	3,3,3	1.42	0	3,3,3	0.76	0
5	DMS	D	8413	-	3,3,3	1.38	1 (33%)	3,3,3	0.45	0
5	DMS	D	8414	-	3,3,3	0.53	0	3,3,3	0.46	0
5	DMS	D	8415	-	3,3,3	3.09	2 (66%)	3,3,3	0.20	0
5	DMS	D	8416	-	3,3,3	0.73	0	3,3,3	0.60	0
5	DMS	D	8417	-	3,3,3	0.80	0	3,3,3	0.13	0
5	DMS	D	8419	-	3,3,3	0.44	0	3,3,3	0.46	0
5	DMS	D	8421	-	3,3,3	0.46	0	3,3,3	0.34	0
5	DMS	D	8423	-	3,3,3	1.59	1 (33%)	3,3,3	0.41	0
5	DMS	D	8425	4	3,3,3	0.94	0	3,3,3	0.90	0
5	DMS	D	8427	-	3,3,3	1.05	0	3,3,3	0.20	0
5	DMS	D	8501	-	3,3,3	1.17	0	3,3,3	0.41	0
5	DMS	D	8508	-	3,3,3	1.66	1 (33%)	3,3,3	0.41	0
5	DMS	D	8701	-	3,3,3	2.65	2 (66%)	3,3,3	0.48	0
5	DMS	D	8703	-	3,3,3	0.98	0	3,3,3	0.55	0
5	DMS	D	8705	-	3,3,3	1.19	0	3,3,3	0.14	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	147	A	2001	4	-	0/10/30/30	0/2/2/2
5	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8406	3	-	0/0/0/0	0/0/0/0
5	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	A	8427	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8602	-	-	0/0/0/0	0/0/0/0
2	147	B	2001	4	-	0/10/30/30	0/2/2/2
5	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8412	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	B	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	B	8427	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
2	147	C	2001	4	-	0/10/30/30	0/2/2/2
5	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	C	8427	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8506	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
2	147	D	2001	4	-	0/10/30/30	0/2/2/2
5	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	D	8427	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8705	-	-	0/0/0/0	0/0/0/0

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	147	C5'-C4'	-2.32	1.34	1.38
5	C	8414	DMS	C1-S	-2.27	1.58	1.75
5	B	8402	DMS	C1-S	-2.08	1.59	1.75
5	D	8407	DMS	O-S	2.00	1.63	1.50
5	C	8403	DMS	O-S	2.01	1.63	1.50
5	B	8403	DMS	C2-S	2.01	1.91	1.75
5	B	8508	DMS	O-S	2.02	1.64	1.50
5	D	8410	DMS	C1-S	2.02	1.91	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	8423	DMS	C1-S	2.02	1.91	1.75
5	C	8414	DMS	C2-S	2.06	1.91	1.75
5	A	8405	DMS	O-S	2.06	1.64	1.50
5	B	8402	DMS	O-S	2.11	1.64	1.50
5	B	8405	DMS	O-S	2.12	1.64	1.50
5	A	8425	DMS	C2-S	2.13	1.92	1.75
5	D	8407	DMS	C2-S	2.13	1.92	1.75
5	D	8407	DMS	C1-S	2.14	1.92	1.75
2	D	2001	147	O3-C3	2.14	1.48	1.43
5	A	8404	DMS	O-S	2.17	1.65	1.50
5	C	8407	DMS	O-S	2.18	1.65	1.50
5	C	8601	DMS	C2-S	2.24	1.93	1.75
5	A	8415	DMS	C1-S	2.24	1.93	1.75
5	A	8502	DMS	C2-S	2.25	1.93	1.75
5	B	8403	DMS	C1-S	2.26	1.93	1.75
5	B	8404	DMS	C2-S	2.27	1.93	1.75
5	B	8409	DMS	C1-S	2.27	1.93	1.75
5	A	8425	DMS	C1-S	2.30	1.93	1.75
5	D	8413	DMS	O-S	2.31	1.66	1.50
5	A	8407	DMS	C2-S	2.32	1.93	1.75
5	B	8417	DMS	O-S	2.35	1.66	1.50
5	C	8412	DMS	O-S	2.41	1.66	1.50
5	B	8601	DMS	C2-S	2.42	1.94	1.75
5	B	8420	DMS	C2-S	2.44	1.94	1.75
5	C	8416	DMS	C2-S	2.48	1.94	1.75
5	C	8425	DMS	O-S	2.51	1.67	1.50
5	A	8501	DMS	O-S	2.54	1.67	1.50
5	A	8415	DMS	C2-S	2.57	1.95	1.75
5	B	8415	DMS	O-S	2.57	1.67	1.50
5	B	8425	DMS	O-S	2.65	1.68	1.50
5	A	8413	DMS	O-S	2.65	1.68	1.50
5	D	8508	DMS	O-S	2.67	1.68	1.50
5	A	8413	DMS	C1-S	2.71	1.96	1.75
5	D	8402	DMS	C2-S	2.72	1.96	1.75
5	B	8410	DMS	C1-S	2.74	1.96	1.75
5	D	8701	DMS	C2-S	2.74	1.96	1.75
5	A	8502	DMS	C1-S	2.84	1.97	1.75
5	B	8506	DMS	C2-S	2.84	1.97	1.75
5	C	8506	DMS	C1-S	2.84	1.97	1.75
5	D	8404	DMS	C2-S	2.85	1.97	1.75
5	B	8413	DMS	O-S	2.96	1.70	1.50
5	A	8415	DMS	O-S	2.98	1.70	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8405	DMS	O-S	3.00	1.70	1.50
5	B	8407	DMS	C2-S	3.12	1.99	1.75
5	B	8402	DMS	C2-S	3.16	2.00	1.75
5	A	8412	DMS	C1-S	3.18	2.00	1.75
5	A	8402	DMS	C2-S	3.22	2.00	1.75
5	C	8413	DMS	O-S	3.27	1.72	1.50
5	A	8413	DMS	C2-S	3.33	2.01	1.75
5	D	8415	DMS	C1-S	3.37	2.01	1.75
5	D	8409	DMS	O-S	3.40	1.73	1.50
5	B	8508	DMS	C1-S	3.46	2.02	1.75
5	D	8701	DMS	O-S	3.50	1.74	1.50
5	A	8403	DMS	C2-S	3.60	2.03	1.75
5	C	8402	DMS	C2-S	3.68	2.04	1.75
5	C	8420	DMS	O-S	3.73	1.75	1.50
5	B	8415	DMS	C2-S	3.76	2.04	1.75
5	D	8415	DMS	O-S	3.80	1.76	1.50
5	A	8409	DMS	O-S	3.83	1.76	1.50
5	C	8409	DMS	O-S	3.98	1.77	1.50
5	B	8409	DMS	O-S	4.07	1.78	1.50
5	A	8407	DMS	O-S	4.80	1.83	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	147	C3'-C4'-N1'	-4.38	115.95	119.48
2	B	2001	147	C5'-C4'-N1'	-3.68	116.52	119.48
2	D	2001	147	C5'-C4'-N1'	-3.64	116.55	119.48
2	B	2001	147	C6'-C5'-C4'	-3.31	115.51	120.15
2	C	2001	147	O1'-C1-C2	-3.10	102.08	107.12
2	A	2001	147	C3-C4-C5	-2.70	105.48	110.20
2	B	2001	147	O2-C2-C1	-2.30	104.98	110.02
2	B	2001	147	C3'-C2'-C1'	-2.28	116.87	119.74
2	D	2001	147	O2-C2-C1	-2.01	105.62	110.02
2	B	2001	147	C6-C5-C4	2.07	118.13	113.02
2	B	2001	147	C1'-O1'-C1	2.14	121.07	117.87
2	B	2001	147	C5'-C6'-C1'	2.31	122.66	119.74
5	B	8414	DMS	C2-S-C1	2.33	110.49	98.46
2	A	2001	147	C1-C2-C3	2.60	115.10	109.97
5	A	8502	DMS	C2-S-C1	2.89	113.41	98.46
2	A	2001	147	C5'-C4'-C3'	2.90	124.84	119.83
5	B	8415	DMS	C2-S-C1	2.92	113.57	98.46
5	B	8502	DMS	C2-S-C1	3.35	115.76	98.46



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

37 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8403	DMS	2	0
5	A	8409	DMS	1	0
5	A	8412	DMS	3	0
5	A	8414	DMS	2	0
5	A	8416	DMS	2	0
5	A	8417	DMS	3	0
5	A	8419	DMS	1	0
5	A	8420	DMS	1	0
5	A	8421	DMS	1	0
5	A	8602	DMS	1	0
5	B	8402	DMS	1	0
5	B	8406	DMS	2	0
5	B	8411	DMS	1	0
5	B	8412	DMS	1	0
5	B	8415	DMS	3	0
5	B	8417	DMS	1	0
5	B	8421	DMS	1	0
5	B	8504	DMS	3	0
5	B	8508	DMS	1	0
5	C	8402	DMS	4	0
5	C	8406	DMS	2	0
5	C	8417	DMS	1	0
5	C	8420	DMS	1	0
5	C	8427	DMS	2	0
5	C	8504	DMS	1	0
5	C	8506	DMS	2	0
5	C	8602	DMS	1	0
5	D	8406	DMS	2	0
5	D	8409	DMS	1	0
5	D	8412	DMS	2	0
5	D	8415	DMS	2	0
5	D	8416	DMS	4	0
5	D	8417	DMS	1	0
5	D	8427	DMS	2	0
5	D	8508	DMS	1	0
5	D	8703	DMS	1	0
5	D	8705	DMS	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1011/1023 (98%)	-0.51	21 (2%) 67 70	8, 15, 45, 100	0
1	B	1011/1023 (98%)	-0.51	13 (1%) 79 82	8, 15, 43, 94	0
1	C	1011/1023 (98%)	-0.50	16 (1%) 74 77	8, 15, 47, 100	0
1	D	1011/1023 (98%)	-0.49	26 (2%) 59 63	9, 16, 46, 95	0
All	All	4044/4092 (98%)	-0.50	76 (1%) 70 73	8, 15, 46, 100	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	10.9
1	D	735	HIS	9.9
1	A	735	HIS	9.2
1	B	730	LEU	8.0
1	C	732	ALA	8.0
1	C	730	LEU	8.0
1	B	731	PRO	7.2
1	D	732	ALA	6.8
1	C	731	PRO	6.7
1	C	733	ALA	6.3
1	B	732	ALA	5.8
1	D	689	GLU	5.8
1	A	733	ALA	5.7
1	A	687	GLN	5.6
1	D	734	SER	5.5
1	D	686	PRO	5.4
1	B	733	ALA	5.3
1	C	735	HIS	5.3
1	A	730	LEU	5.2
1	A	731	PRO	5.2
1	D	730	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	733	ALA	5.0
1	A	580	GLU	4.8
1	D	731	PRO	4.4
1	A	689	GLU	4.3
1	D	581	ASN	4.0
1	D	580	GLU	3.9
1	A	737	ILE	3.8
1	B	689	GLU	3.8
1	B	580	GLU	3.5
1	B	684	GLU	3.4
1	A	732	ALA	3.3
1	D	687	GLN	3.3
1	D	684	GLU	3.3
1	B	735	HIS	3.3
1	A	581	ASN	3.2
1	B	685	LEU	3.1
1	C	745	MET	2.9
1	C	634	GLN	2.9
1	B	799	THR	2.8
1	D	1023	LYS	2.8
1	A	71	GLU	2.7
1	C	687	GLN	2.7
1	A	684	GLU	2.7
1	C	689	GLU	2.7
1	D	688	PRO	2.7
1	D	634	GLN	2.7
1	C	685	LEU	2.6
1	C	686	PRO	2.6
1	D	845	GLN	2.6
1	A	1023	LYS	2.6
1	D	683	PRO	2.5
1	A	734	SER	2.5
1	A	685	LEU	2.5
1	B	729	THR	2.5
1	D	737	ILE	2.5
1	D	582	GLY	2.4
1	A	582	GLY	2.4
1	A	771	GLY	2.4
1	C	734	SER	2.4
1	B	686	PRO	2.4
1	C	580	GLU	2.3
1	A	799	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	772	ASP	2.2
1	D	771	GLY	2.2
1	C	684	GLU	2.2
1	C	737	ILE	2.2
1	D	736	ALA	2.2
1	C	744	GLU	2.1
1	B	745	MET	2.1
1	D	800	ARG	2.1
1	D	663	LEU	2.1
1	D	799	THR	2.0
1	A	800	ARG	2.0
1	A	736	ALA	2.0
1	D	798	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	DMS	C	8602	4/4	0.89	0.20	22.08	21,74,91,100	0
5	DMS	D	8423	4/4	0.86	0.17	18.04	38,53,100,100	0
5	DMS	B	8407	4/4	0.93	0.12	16.58	28,32,33,38	0
5	DMS	D	8407	4/4	0.87	0.16	12.92	29,47,53,100	0
5	DMS	A	8406	4/4	0.91	0.20	12.36	13,59,73,100	0
5	DMS	D	8404	4/4	0.94	0.12	11.37	20,23,41,63	0
5	DMS	D	8508	4/4	0.94	0.11	10.47	36,52,53,53	0
5	DMS	C	8420	4/4	0.93	0.14	9.73	35,55,58,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	C	8407	4/4	0.95	0.14	8.76	27,30,40,42	0
5	DMS	B	8406	4/4	0.90	0.16	8.56	35,52,87,100	0
5	DMS	C	8419	4/4	0.80	0.20	8.27	41,46,50,67	0
5	DMS	A	8417	4/4	0.91	0.18	8.26	23,27,96,100	0
5	DMS	B	8420	4/4	0.89	0.16	8.11	41,60,65,69	0
5	DMS	A	8407	4/4	0.91	0.10	7.60	23,32,33,45	0
5	DMS	A	8404	4/4	0.96	0.08	7.29	18,30,31,39	0
5	DMS	D	8501	4/4	0.93	0.09	6.99	24,30,34,48	0
5	DMS	A	8420	4/4	0.94	0.10	6.00	39,45,45,47	0
5	DMS	A	8412	4/4	0.95	0.19	5.50	38,46,51,100	0
5	DMS	B	8508	4/4	0.93	0.11	5.03	27,35,48,62	0
5	DMS	C	8506	4/4	0.95	0.11	4.97	26,40,47,52	0
5	DMS	C	8423	4/4	0.93	0.13	4.72	28,64,100,100	0
5	DMS	D	8417	4/4	0.89	0.16	4.38	26,31,47,100	0
5	DMS	C	8406	4/4	0.91	0.16	4.10	37,38,46,94	0
5	DMS	B	8502	4/4	0.95	0.10	4.05	28,30,43,49	0
5	DMS	B	8423	4/4	0.94	0.09	3.72	33,34,66,100	0
5	DMS	C	8501	4/4	0.95	0.08	3.52	20,29,37,51	0
5	DMS	B	8403	4/4	0.98	0.09	3.36	21,22,28,30	0
5	DMS	A	8423	4/4	0.93	0.12	3.34	30,46,74,100	0
5	DMS	C	8412	4/4	0.96	0.11	3.25	28,31,36,100	0
5	DMS	B	8408	4/4	0.97	0.09	3.21	31,34,38,100	0
5	DMS	C	8404	4/4	0.98	0.07	3.21	18,19,26,29	0
5	DMS	D	8705	4/4	0.87	0.15	2.97	20,47,58,71	0
5	DMS	A	8405	4/4	0.99	0.09	2.75	21,24,25,32	0
5	DMS	A	8419	4/4	0.93	0.10	2.58	33,46,49,50	0
5	DMS	D	8406	4/4	0.95	0.10	2.56	26,26,28,41	0
5	DMS	C	8417	4/4	0.89	0.13	2.40	24,30,54,74	0
5	DMS	C	8405	4/4	0.98	0.09	2.36	27,27,28,32	0
5	DMS	B	8417	4/4	0.93	0.15	2.32	25,28,70,73	0
5	DMS	D	8419	4/4	0.97	0.09	2.28	33,43,46,48	0
5	DMS	A	8402	4/4	0.98	0.07	2.27	15,29,30,47	0
5	DMS	B	8506	4/4	0.98	0.07	2.26	27,34,43,44	0
5	DMS	C	8402	4/4	0.97	0.08	2.20	19,29,34,51	0
5	DMS	B	8404	4/4	0.97	0.07	2.19	18,20,31,37	0
5	DMS	D	8425	4/4	0.94	0.14	2.08	16,19,24,24	4
5	DMS	A	8504	4/4	0.97	0.09	1.95	22,43,50,100	0
5	DMS	A	8502	4/4	0.94	0.09	1.94	22,26,54,58	0
5	DMS	A	8501	4/4	0.95	0.10	1.92	17,27,37,39	0
5	DMS	C	8408	4/4	0.98	0.06	1.84	18,29,30,31	0
5	DMS	C	8411	4/4	0.99	0.10	1.76	22,23,23,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	B	8405	4/4	0.98	0.10	1.76	27,30,30,34	0
5	DMS	D	8405	4/4	0.99	0.07	1.56	24,30,30,34	0
5	DMS	D	8403	4/4	0.98	0.07	1.51	18,26,28,29	0
4	NA	A	3104	1/1	0.98	0.09	1.38	23,23,23,23	0
5	DMS	D	8701	4/4	0.98	0.09	1.27	16,17,22,44	0
5	DMS	A	8408	4/4	0.97	0.08	1.16	22,34,35,36	0
5	DMS	D	8402	4/4	0.97	0.07	1.05	17,28,31,33	0
5	DMS	C	8425	4/4	0.98	0.09	0.99	27,29,29,100	0
5	DMS	B	8402	4/4	0.97	0.07	0.94	19,19,28,33	0
5	DMS	D	8408	4/4	0.98	0.08	0.92	18,31,36,39	0
5	DMS	A	8403	4/4	0.98	0.07	0.88	23,23,25,31	0
5	DMS	B	8504	4/4	0.91	0.10	0.59	35,40,58,63	0
5	DMS	A	8401	4/4	0.99	0.06	0.56	11,13,14,15	0
5	DMS	D	8412	4/4	0.98	0.08	0.52	27,27,33,100	0
4	NA	C	3104	1/1	0.97	0.08	0.51	21,21,21,21	0
2	147	D	2001	21/21	0.97	0.06	0.51	11,13,27,32	0
5	DMS	A	8425	4/4	0.96	0.10	0.49	33,38,38,44	0
2	147	A	2001	21/21	0.97	0.06	0.33	10,13,21,30	0
5	DMS	B	8412	4/4	0.97	0.08	0.32	27,37,37,43	0
5	DMS	C	8403	4/4	0.99	0.06	0.23	22,24,25,26	0
4	NA	D	3103	1/1	0.97	0.06	0.15	27,27,27,27	0
5	DMS	B	8425	4/4	0.98	0.07	0.11	19,25,27,29	0
5	DMS	B	8401	4/4	0.99	0.05	-0.11	14,17,18,18	0
4	NA	D	3104	1/1	0.98	0.06	-0.17	28,28,28,28	0
5	DMS	B	8411	4/4	0.99	0.06	-0.22	21,23,25,33	0
2	147	C	2001	21/21	0.97	0.06	-0.23	10,12,25,50	0
4	NA	B	3104	1/1	0.98	0.06	-0.30	20,20,20,20	0
5	DMS	D	8401	4/4	0.99	0.05	-0.46	13,15,17,20	0
2	147	B	2001	21/21	0.97	0.05	-0.49	9,11,20,35	0
5	DMS	D	8411	4/4	0.99	0.05	-0.60	19,24,26,71	0
4	NA	A	3103	1/1	0.98	0.06	-0.77	23,23,23,23	0
5	DMS	A	8411	4/4	0.98	0.05	-0.86	22,26,26,43	0
5	DMS	C	8401	4/4	0.99	0.04	-1.17	14,15,18,18	0
4	NA	D	3102	1/1	1.00	0.04	-1.28	11,11,11,11	0
4	NA	C	3102	1/1	0.99	0.03	-1.49	12,12,12,12	0
4	NA	B	3102	1/1	1.00	0.03	-1.81	11,11,11,11	0
4	NA	B	3103	1/1	0.99	0.03	-1.97	19,19,19,19	0
4	NA	C	3103	1/1	0.99	0.04	-2.36	21,21,21,21	0
3	MG	B	3002	1/1	1.00	0.03	-2.36	14,14,14,14	0
4	NA	A	3101	1/1	0.99	0.04	-2.37	13,13,13,13	0
4	NA	A	3102	1/1	1.00	0.02	-2.84	12,12,12,12	0
3	MG	A	3002	1/1	0.99	0.04	-2.86	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	D	3002	1/1	0.99	0.03	-3.04	14,14,14,14	0
3	MG	C	3002	1/1	1.00	0.02	-3.04	13,13,13,13	0
4	NA	B	3101	1/1	0.99	0.03	-3.30	12,12,12,12	0
4	NA	D	3101	1/1	1.00	0.04	-3.47	13,13,13,13	0
3	MG	C	3001	1/1	1.00	0.03	-3.78	10,10,10,10	0
3	MG	A	3001	1/1	0.99	0.03	-3.92	11,11,11,11	0
3	MG	B	3001	1/1	1.00	0.02	-3.97	10,10,10,10	0
4	NA	C	3101	1/1	1.00	0.03	-4.90	11,11,11,11	0
3	MG	D	3001	1/1	1.00	0.03	-6.09	12,12,12,12	0
3	MG	C	3006	1/1	0.97	0.12	-	20,20,20,20	1
5	DMS	B	8416	4/4	0.95	0.14	-	34,36,47,90	0
5	DMS	D	8703	4/4	0.78	0.26	-	47,73,77,81	0
5	DMS	B	8427	4/4	0.87	0.14	-	35,40,68,100	0
5	DMS	D	8409	4/4	0.96	0.11	-	29,30,31,34	0
5	DMS	B	8413	4/4	0.96	0.14	-	27,31,35,39	0
5	DMS	C	8410	4/4	0.98	0.09	-	22,24,33,34	0
5	DMS	B	8601	4/4	0.96	0.09	-	30,37,41,45	0
5	DMS	B	8414	4/4	0.96	0.12	-	30,39,41,100	0
5	DMS	A	8415	4/4	0.98	0.08	-	19,36,37,46	0
5	DMS	B	8421	4/4	0.95	0.09	-	31,35,46,73	0
5	DMS	A	8409	4/4	0.96	0.09	-	26,31,34,40	0
5	DMS	A	8602	4/4	0.96	0.19	-	38,53,74,100	0
5	DMS	D	8413	4/4	0.98	0.11	-	28,31,31,100	0
5	DMS	D	8427	4/4	0.81	0.16	-	47,51,59,75	0
3	MG	A	3105	1/1	0.92	0.11	-	21,21,21,21	1
5	DMS	A	8427	4/4	0.84	0.14	-	41,54,55,100	0
3	MG	A	3005	1/1	0.95	0.06	-	33,33,33,33	0
5	DMS	C	8414	4/4	0.97	0.08	-	22,39,41,49	0
5	DMS	B	8410	4/4	0.97	0.09	-	19,28,32,38	0
5	DMS	A	8413	4/4	0.97	0.10	-	30,33,34,35	0
5	DMS	C	8421	4/4	0.94	0.10	-	32,46,55,57	0
5	DMS	C	8416	4/4	0.94	0.20	-	38,50,52,100	0
5	DMS	C	8415	4/4	0.98	0.06	-	21,26,32,45	0
5	DMS	A	8416	4/4	0.96	0.20	-	22,38,73,100	0
5	DMS	D	8414	4/4	0.97	0.09	-	24,40,87,100	0
5	DMS	C	8409	4/4	0.98	0.07	-	24,31,33,34	0
5	DMS	D	8410	4/4	0.99	0.07	-	20,29,30,34	0
5	DMS	D	8421	4/4	0.97	0.12	-	49,51,52,52	0
3	MG	B	3105	1/1	0.98	0.07	-	18,18,18,18	1
5	DMS	B	8409	4/4	0.96	0.09	-	25,26,33,34	0
3	MG	C	3105	1/1	0.93	0.12	-	19,19,19,19	1
5	DMS	C	8504	4/4	0.92	0.10	-	35,54,63,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMS	A	8414	4/4	0.95	0.12	-	24,43,84,100	0
5	DMS	B	8415	4/4	0.95	0.10	-	21,29,32,37	0
5	DMS	A	8421	4/4	0.93	0.21	-	55,56,68,100	0
3	MG	D	3105	1/1	0.93	0.11	-	24,24,24,24	1
5	DMS	C	8413	4/4	0.98	0.14	-	31,33,34,36	0
5	DMS	D	8415	4/4	0.96	0.10	-	20,37,42,100	0
5	DMS	A	8410	4/4	0.98	0.10	-	22,31,40,44	0
5	DMS	C	8427	4/4	0.91	0.12	-	49,51,56,65	0
5	DMS	C	8601	4/4	0.97	0.09	-	35,40,42,57	0
5	DMS	D	8416	4/4	0.92	0.19	-	29,53,77,80	0
3	MG	D	3005	1/1	0.97	0.07	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.