



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:35 PM GMT

PDB ID : 1XSK  
Title : Structure of a Family 31 alpha glycosidase glycosyl-enzyme intermediate  
Authors : Lovering, A.L.; Lee, S.S.; Kim, Y.W.; Withers, S.G.; Strynadka, N.C.  
Deposited on : 2004-10-19  
Resolution : 2.20 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

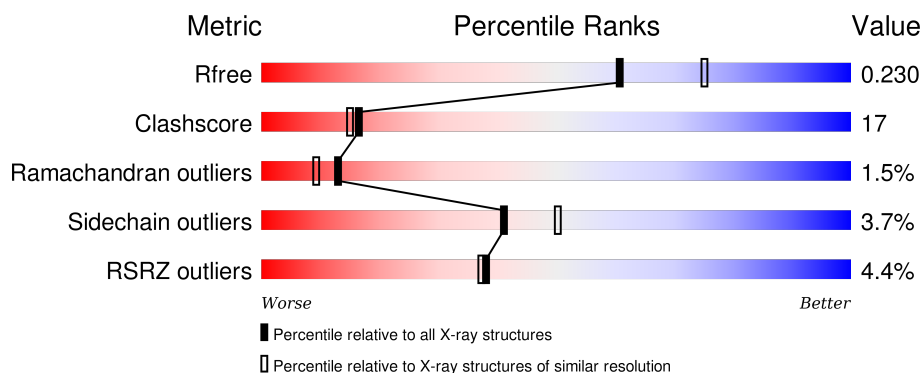
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	778	<div> <div>2%</div> <div>70% 26% ..</div> </div>
1	B	778	<div> <div>7%</div> <div>67% 30% ..</div> </div>
1	C	778	<div> <div>2%</div> <div>68% 29% ..</div> </div>
1	D	778	<div> <div>7%</div> <div>66% 30% ..</div> </div>
1	E	778	<div> <div>4%</div> <div>66% 30% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	778	

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
2	SO4	F	3001	-	-	-	X
2	SO4	F	3005	-	-	X	-
3	XYF	C	803	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 38360 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 Putative family 31 glucosidase yicI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	B	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	C	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	D	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	E	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			
1	F	773	Total	C	N	O	S	0	0	0
			6226	3978	1069	1147	32			

There are 36 discrepancies between the modelled and reference sequences:

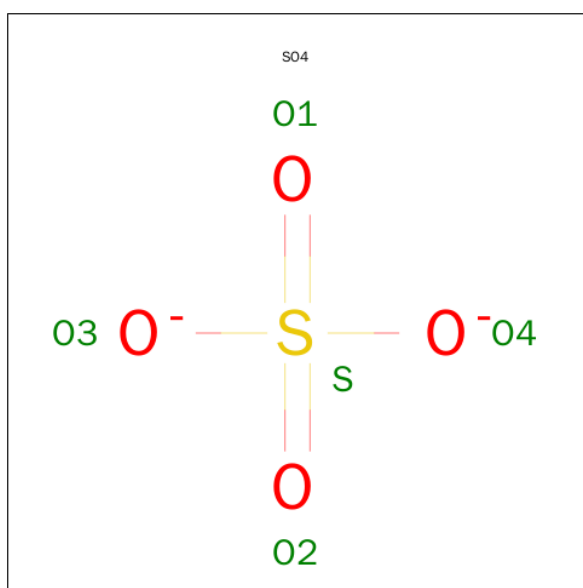
Chain	Residue	Modelled	Actual	Comment	Reference
A	773	HIS	-	EXPRESSION TAG	UNP P31434
A	774	HIS	-	EXPRESSION TAG	UNP P31434
A	775	HIS	-	EXPRESSION TAG	UNP P31434
A	776	HIS	-	EXPRESSION TAG	UNP P31434
A	777	HIS	-	EXPRESSION TAG	UNP P31434
A	778	HIS	-	EXPRESSION TAG	UNP P31434
B	773	HIS	-	EXPRESSION TAG	UNP P31434
B	774	HIS	-	EXPRESSION TAG	UNP P31434
B	775	HIS	-	EXPRESSION TAG	UNP P31434
B	776	HIS	-	EXPRESSION TAG	UNP P31434
B	777	HIS	-	EXPRESSION TAG	UNP P31434
B	778	HIS	-	EXPRESSION TAG	UNP P31434
C	773	HIS	-	EXPRESSION TAG	UNP P31434
C	774	HIS	-	EXPRESSION TAG	UNP P31434
C	775	HIS	-	EXPRESSION TAG	UNP P31434
C	776	HIS	-	EXPRESSION TAG	UNP P31434
C	777	HIS	-	EXPRESSION TAG	UNP P31434

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Chain	Residue	Modelled	Actual	Comment	Reference
C	778	HIS	-	EXPRESSION TAG	UNP P31434
D	773	HIS	-	EXPRESSION TAG	UNP P31434
D	774	HIS	-	EXPRESSION TAG	UNP P31434
D	775	HIS	-	EXPRESSION TAG	UNP P31434
D	776	HIS	-	EXPRESSION TAG	UNP P31434
D	777	HIS	-	EXPRESSION TAG	UNP P31434
D	778	HIS	-	EXPRESSION TAG	UNP P31434
E	773	HIS	-	EXPRESSION TAG	UNP P31434
E	774	HIS	-	EXPRESSION TAG	UNP P31434
E	775	HIS	-	EXPRESSION TAG	UNP P31434
E	776	HIS	-	EXPRESSION TAG	UNP P31434
E	777	HIS	-	EXPRESSION TAG	UNP P31434
E	778	HIS	-	EXPRESSION TAG	UNP P31434
F	773	HIS	-	EXPRESSION TAG	UNP P31434
F	774	HIS	-	EXPRESSION TAG	UNP P31434
F	775	HIS	-	EXPRESSION TAG	UNP P31434
F	776	HIS	-	EXPRESSION TAG	UNP P31434
F	777	HIS	-	EXPRESSION TAG	UNP P31434
F	778	HIS	-	EXPRESSION TAG	UNP P31434

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



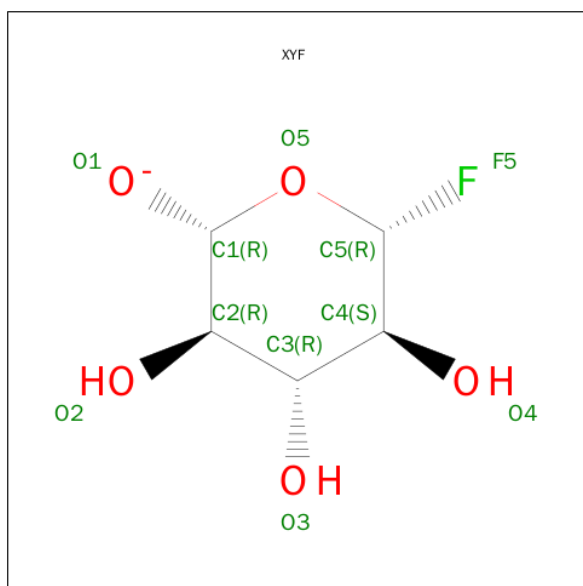
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

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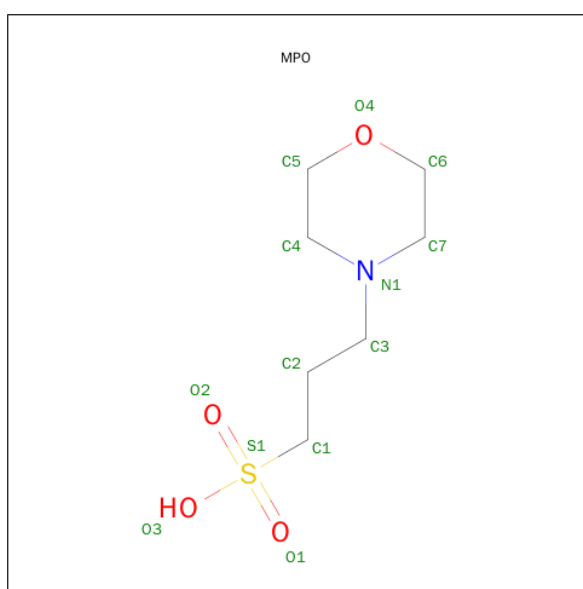
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

- Molecule 3 is 5(R)-5-FLUORO-BETA-D-XYLOPYRANOSYL-ENZYME INTERMEDIATE (three-letter code: XYF) (formula: C<sub>5</sub>H<sub>8</sub>FO<sub>5</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	F	O	0	0
			10	5	1	4		
3	B	1	Total	C	F	O	0	0
			10	5	1	4		
3	C	1	Total	C	F	O	0	0
			10	5	1	4		
3	E	1	Total	C	F	O	0	0
			10	5	1	4		

- Molecule 4 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	C	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
4	E	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	168	Total	O	0	0
			168	168		

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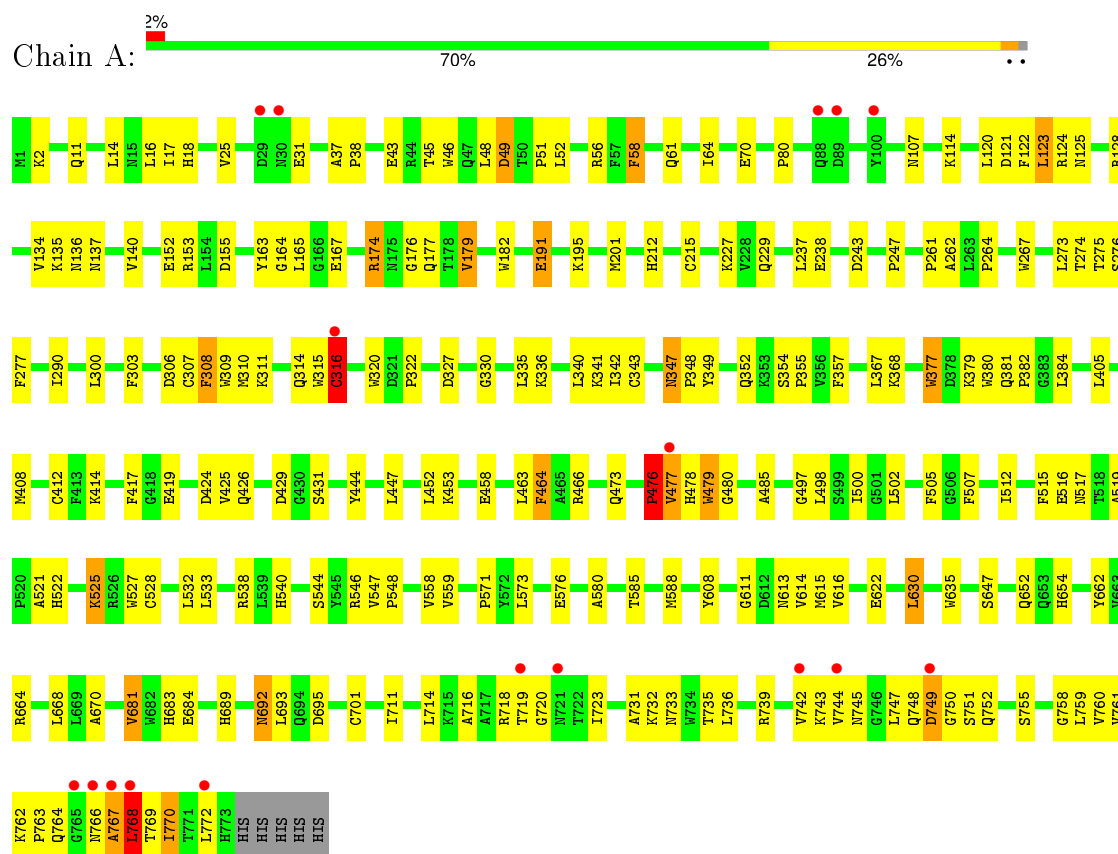
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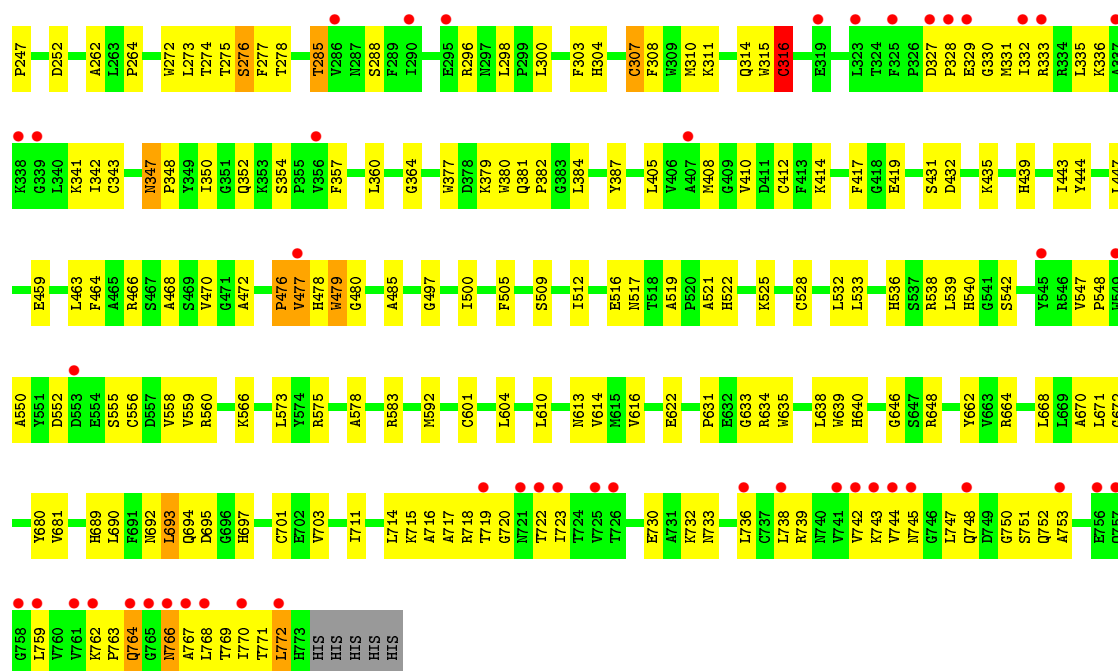
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	114	Total 114	O 114	0	0
5	C	167	Total 167	O 167	0	0
5	D	145	Total 145	O 145	0	0
5	E	122	Total 122	O 122	0	0
5	F	131	Total 131	O 131	0	0

### 3 Residue-property plots

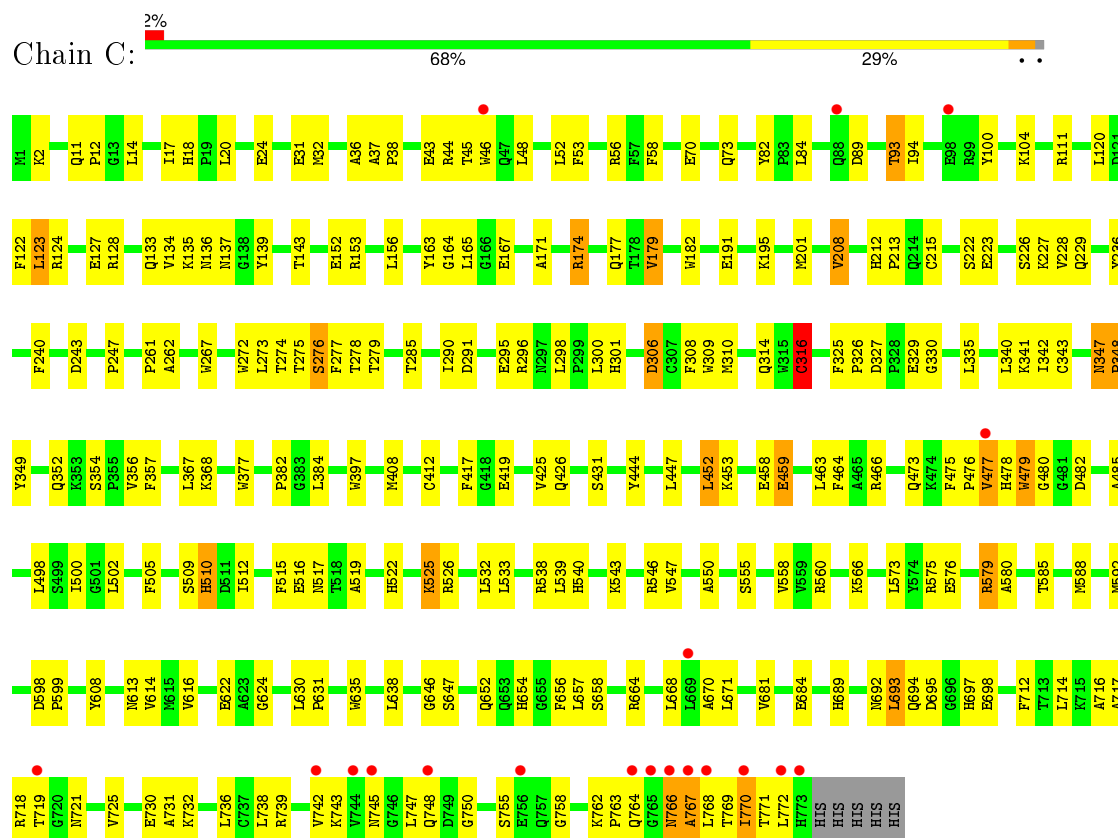
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ( $\text{RSRZ} > 2$ ). 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: Putative family 31 glucosidase yicI



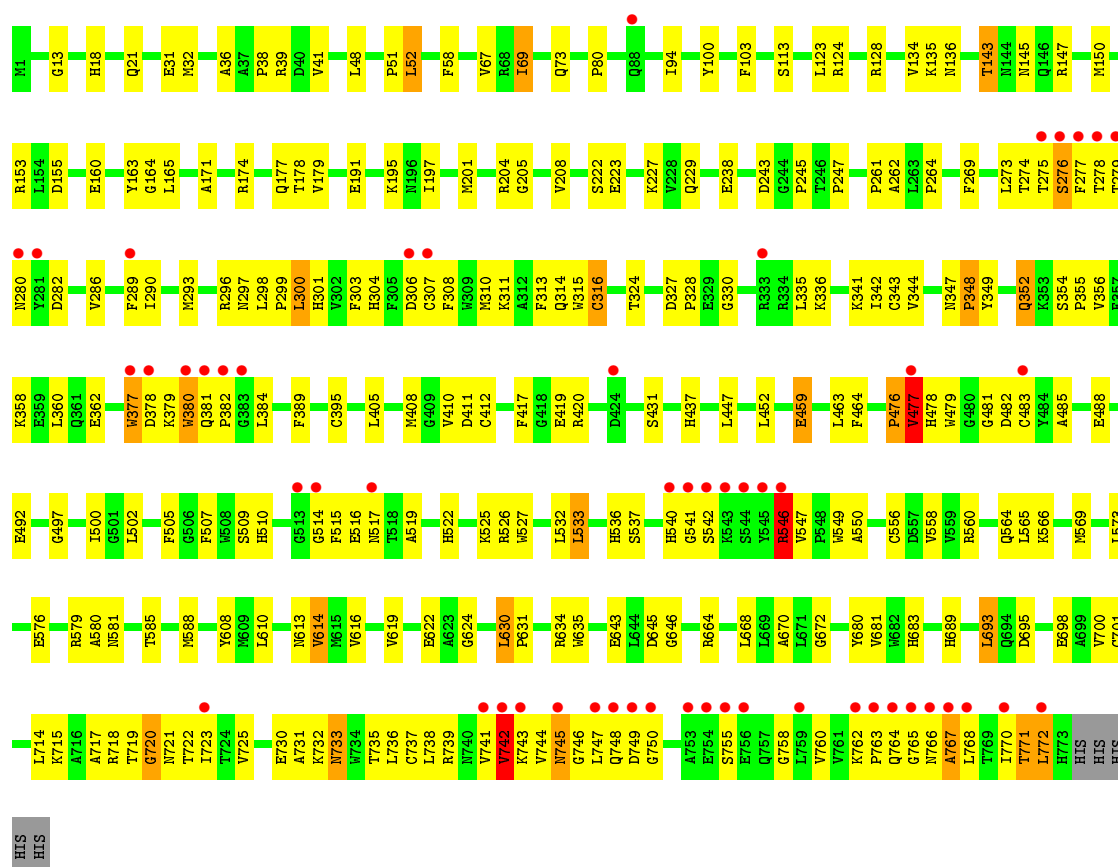


- Molecule 1: Putative family 31 glucosidase yici

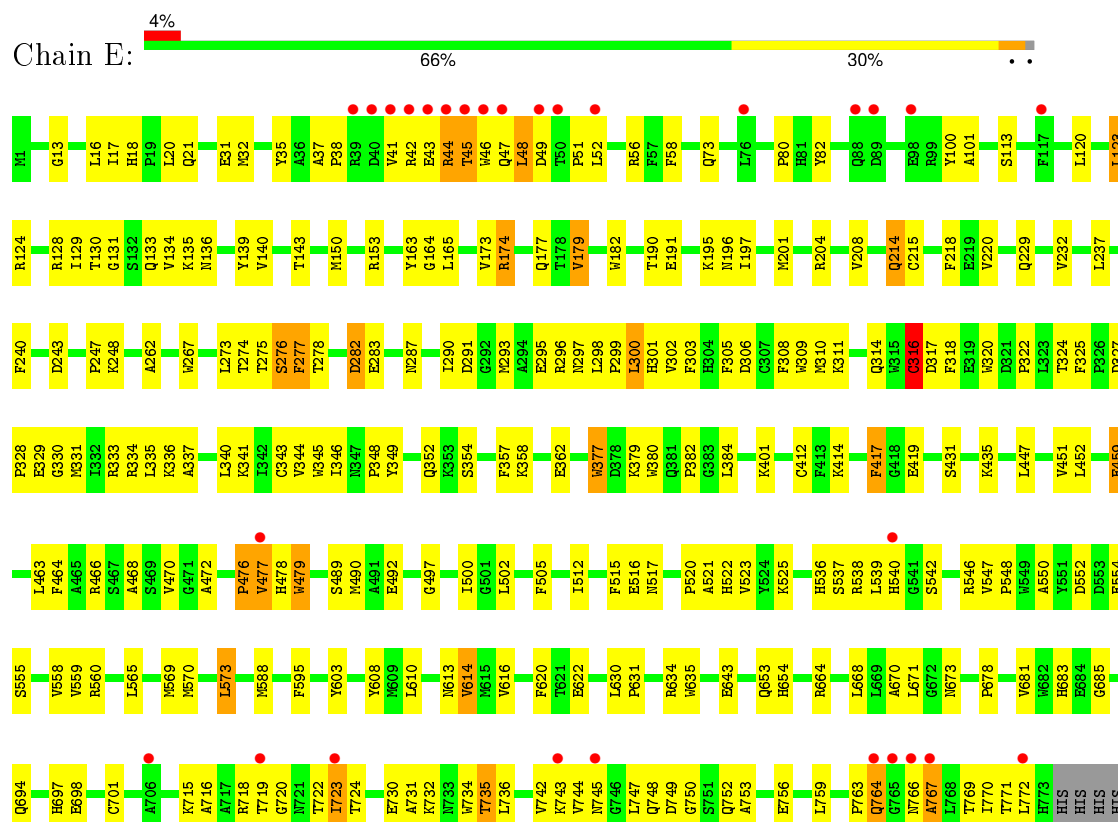


- Molecule 1: Putative family 31 glucosidase yici





- Molecule 1: Putative family 31 glucosidase yicI



L738	E643	A521	G383	I290	R153	H1
V742	G646	H522	L384	M293	L154	G13
K743		K525	V406		D155	
V744	Q652	R526	K414	R296	L156	I17
I745	Q653	L533	F417	R297	G157	H18
G746	H654	H636	G418	L298	G164	D29
L747	Q655	S337	E419	P299	L165	N30
Q748	F656	R538		L300	R174	E31
D749		L539	S431	F303	Q177	M32
G750	L659	H540		H304	I177	A37
A753	F660	V661	K435	F305	I178	P38
E754	W661	S542	D435	D306	S189	T45
S755			N438	G307		W46
E756	H664	Y545		F309	K195	
L759	L668	R546	Y444	M310	M201	F53
V760	L669	V547	L447	K311	R204	R56
V761	A670	P548		Q314	H212	F57
K762		W549	L452	H315	P213	F58
P763	P678	Y551	T455	G316	Q214	S59
Q764		D552		D327	P60	Q61
G765	W681	S553	E459	P328	E219	V67
M766	A687	E554	L463	E329	V220	E70
A767	F688	D557	F464	G330	Q221	
L768	H689	V558	V559	M331	S222	
T769	L690	P691	R560	I332	E223	
I770	P691			R333		
T771	M692	L693	V470	R334	K227	M77
L772	L693	L683	G471	L335	V228	P80
H773	D694	M569	A472	K336	Q229	H81
HIS	D695	M570	P476	L340	Y236	Y82
HIS	G696	L573	V477	K341	L237	P83
HIS	H697	Y574	W479	I342	E238	L84
HIS	C701	R575				Q88
	A705	R579	A485	M347	D243	D89
	I711	R583	E488	P348	P247	
	L714	F595	G497	I350	D252	A101
	K715		I500	G351	A262	L108
	A716	N613	F505	K352	W267	L123
	T719	V616	S509	K353	L273	V134
	G720	V619	H510	F357	T274	K135
	I723		D511	K358	T275	N136
	T724	E622	I512	L360	S276	M137
		A623		K363	F277	G138
	A731	G624	F515	W377	D278	Y139
	K732	L630	E516	D378	T279	
	W733	P631	N517	K379	W380	T143
	H734		T518	W381	N280	
	T735	L736	F519	D381	P382	P452
	W736	H634	R520	P382		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.14Å 175.47Å 210.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.20 69.48 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (29.88-2.20) 97.6 (69.48-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.21 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.235 , 0.272 0.232 , 0.230	Depositor DCC
$R_{free}$ test set	14985 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.633	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 37.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 296995 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	38360	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: MPO, SO4, XYF

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	0.41	0/6409	0.67	4/8711 (0.0%)
1	B	0.36	0/6409	0.62	1/8711 (0.0%)
1	C	0.41	0/6409	0.67	2/8711 (0.0%)
1	D	0.40	0/6409	0.65	1/8711 (0.0%)
1	E	0.40	0/6409	0.64	1/8711 (0.0%)
1	F	0.40	0/6409	0.65	2/8711 (0.0%)
All	All	0.40	0/38454	0.65	11/52266 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	316	CYS	CA-CB-SG	-6.24	102.77	114.00
1	C	316	CYS	CA-CB-SG	-6.16	102.92	114.00
1	E	613	ASN	N-CA-C	5.82	126.70	111.00
1	A	613	ASN	N-CA-C	5.81	126.67	111.00
1	D	613	ASN	N-CA-C	5.66	126.28	111.00
1	C	613	ASN	N-CA-C	5.56	126.01	111.00
1	F	613	ASN	N-CA-C	5.37	125.51	111.00
1	A	316	CYS	CA-CB-SG	-5.33	104.41	114.00
1	B	613	ASN	N-CA-C	5.12	124.84	111.00
1	A	464	PHE	N-CA-C	-5.06	97.34	111.00
1	A	476	PRO	N-CA-C	5.01	125.12	112.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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	6226	0	5934	195	0
1	B	6226	0	5934	199	0
1	C	6226	0	5934	213	0
1	D	6226	0	5934	214	0
1	E	6226	0	5934	224	0
1	F	6226	0	5934	191	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	25	0	0	2	0
3	A	10	0	7	2	0
3	B	10	0	7	1	0
3	C	10	0	7	2	0
3	E	10	0	7	2	0
4	B	13	0	15	0	0
4	C	13	0	15	0	0
4	D	13	0	15	0	0
4	E	13	0	15	0	0
5	A	168	0	0	3	0
5	B	114	0	0	6	0
5	C	167	0	0	5	0
5	D	145	0	0	5	0
5	E	122	0	0	4	0
5	F	131	0	0	6	0
All	All	38360	0	35692	1212	0

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 17.

All (1212) 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)
1:A:274:THR:HG22	1:A:276:SER:H	1.14	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:274:THR:HG22	1:E:276:SER:H	1.00	1.09
1:A:668:LEU:HD21	1:A:714:LEU:HD12	1.39	1.04
1:C:579:ARG:HB2	1:C:579:ARG:HH11	1.21	1.04
1:C:32:MET:HE2	1:C:94:ILE:HG23	1.39	1.04
1:D:485:ALA:HB1	1:D:519:ALA:HB2	1.40	1.03
1:C:93:THR:HG22	1:C:104:LYS:HB3	1.40	1.02
1:B:719:THR:HG23	1:B:720:GLY:H	1.23	1.02
1:D:668:LEU:HD21	1:D:714:LEU:HD12	1.39	1.01
1:B:157:GLY:HA3	1:B:204:ARG:HH22	1.25	1.01
1:B:668:LEU:HD21	1:B:714:LEU:HD12	1.40	1.01
1:E:694:GLN:HB2	1:E:697:HIS:HD2	1.27	0.99
1:F:485:ALA:HB1	1:F:519:ALA:HB2	1.41	0.98
1:B:274:THR:HG22	1:B:276:SER:H	1.23	0.97
1:F:463:LEU:O	1:F:477:VAL:HG13	1.65	0.96
1:C:668:LEU:HD21	1:C:714:LEU:HD12	1.46	0.96
1:C:485:ALA:HB1	1:C:519:ALA:HB2	1.46	0.95
1:F:298:LEU:HD23	1:F:560:ARG:HG3	1.48	0.94
1:E:274:THR:HG21	1:E:540:HIS:ND1	1.81	0.94
1:F:274:THR:HG22	1:F:276:SER:H	1.29	0.94
1:A:485:ALA:HB1	1:A:519:ALA:HB2	1.50	0.94
1:E:463:LEU:O	1:E:477:VAL:HG13	1.68	0.93
1:D:381:GLN:HB2	1:D:384:LEU:HD12	1.52	0.91
1:E:274:THR:HG22	1:E:276:SER:N	1.84	0.91
1:B:694:GLN:HB2	1:B:697:HIS:HD2	1.36	0.90
1:C:274:THR:HG21	1:C:540:HIS:ND1	1.86	0.90
1:D:313:PHE:HA	1:D:381:GLN:HE22	1.38	0.89
1:F:668:LEU:HD21	1:F:714:LEU:HD13	1.53	0.88
1:D:280:ASN:HA	1:E:44:ARG:HH21	1.37	0.87
1:D:547:VAL:HG23	1:D:550:ALA:HB2	1.55	0.87
1:E:45:THR:HG23	1:E:46:TRP:HD1	1.39	0.87
1:C:579:ARG:CB	1:C:579:ARG:HH11	1.88	0.87
1:B:463:LEU:O	1:B:477:VAL:HG13	1.74	0.87
1:E:165:LEU:HD13	1:E:179:VAL:HG11	1.57	0.86
1:A:367:LEU:HG	1:A:425:VAL:HG21	1.59	0.85
1:D:273:LEU:HB2	1:D:300:LEU:HD21	1.59	0.84
1:C:425:VAL:HG22	1:C:426:GLN:N	1.91	0.83
1:C:368:LYS:O	1:C:425:VAL:HG23	1.79	0.83
1:F:694:GLN:HB2	1:F:697:HIS:HD2	1.42	0.83
1:E:214:GLN:HG3	1:E:435:LYS:HG2	1.61	0.82
1:F:634:ARG:HH21	1:F:643:GLU:HB3	1.45	0.82
1:D:766:ASN:C	1:D:768:LEU:H	1.82	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:LYS:O	1:A:425:VAL:HG23	1.79	0.82
1:C:329:GLU:HG3	1:C:408:MET:HG3	1.62	0.81
1:A:463:LEU:O	1:A:477:VAL:HG22	1.81	0.81
1:C:525:LYS:HG3	1:C:558:VAL:HG21	1.62	0.81
1:C:32:MET:CE	1:C:94:ILE:HG23	2.12	0.80
1:A:525:LYS:HG3	1:A:558:VAL:HG21	1.64	0.79
1:E:179:VAL:HG13	1:E:218:PHE:HB2	1.64	0.79
1:E:382:PRO:HG2	5:E:3048:HOH:O	1.82	0.79
1:F:274:THR:HG21	1:F:540:HIS:ND1	1.97	0.79
1:B:136:ASN:HD21	1:B:227:LYS:HE3	1.47	0.79
1:B:747:LEU:HD23	1:B:748:GLN:N	1.98	0.78
1:A:107:ASN:HD22	1:A:125:ASN:HD21	1.31	0.78
1:B:44:ARG:HA	1:B:47:GLN:HG3	1.65	0.78
1:E:525:LYS:HG2	1:E:558:VAL:HG21	1.64	0.78
1:A:723:ILE:HG12	1:A:770:ILE:HG13	1.65	0.77
1:A:195:LYS:HE2	1:A:478:HIS:HB3	1.66	0.77
1:F:13:GLY:O	1:F:143:THR:HB	1.85	0.77
1:B:719:THR:HG23	1:B:720:GLY:N	1.98	0.76
1:D:280:ASN:HA	1:E:44:ARG:NH2	2.00	0.76
1:D:725:VAL:HB	1:D:768:LEU:HD12	1.67	0.76
1:C:201:MET:HE1	1:C:247:PRO:HB3	1.66	0.76
1:A:274:THR:HG22	1:A:276:SER:N	1.95	0.76
1:C:762:LYS:HD2	1:C:763:PRO:HD2	1.68	0.76
1:D:541:GLY:HA3	1:D:546:ARG:HH21	1.50	0.75
1:E:723:ILE:HG13	1:E:770:ILE:HB	1.68	0.75
1:E:476:PRO:O	1:E:477:VAL:HG12	1.86	0.75
1:E:44:ARG:HG2	1:E:47:GLN:NE2	2.01	0.75
1:E:565:LEU:HG	1:E:569:MET:CE	2.17	0.75
1:D:540:HIS:C	1:D:546:ARG:HE	1.90	0.75
1:A:761:VAL:HG11	1:A:768:LEU:HD21	1.69	0.75
1:F:273:LEU:HB2	1:F:300:LEU:HD21	1.69	0.75
1:F:300:LEU:HD12	1:F:340:LEU:HD21	1.68	0.75
1:A:522:HIS:CE1	1:A:622:GLU:HG3	2.22	0.74
1:F:347:ASN:HD22	1:F:347:ASN:C	1.91	0.74
1:E:673:ASN:HD22	1:E:685:GLY:HA3	1.52	0.74
1:B:157:GLY:HA3	1:B:204:ARG:NH2	2.01	0.74
1:B:332:ILE:HD12	1:B:333:ARG:N	2.01	0.74
1:A:635:TRP:CH2	1:A:664:ARG:HG2	2.23	0.74
1:C:579:ARG:NH1	1:C:579:ARG:HB2	2.00	0.74
1:E:694:GLN:HB2	1:E:697:HIS:CD2	2.19	0.73
1:D:13:GLY:O	1:D:143:THR:HB	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:174:ARG:O	1:E:177:GLN:HG2	1.87	0.73
1:B:689:HIS:ND1	1:B:739:ARG:NH1	2.36	0.73
1:C:274:THR:CG2	1:C:540:HIS:HA	2.18	0.73
1:B:32:MET:HE2	1:B:94:ILE:HG23	1.70	0.73
1:A:174:ARG:O	1:A:177:GLN:HG2	1.89	0.73
1:C:755:SER:HB3	1:C:758:GLY:O	1.88	0.73
1:C:352:GLN:NE2	1:D:73:GLN:HG3	2.04	0.73
1:A:750:GLY:HA2	1:A:764:GLN:HG2	1.71	0.72
1:A:762:LYS:HD2	1:A:763:PRO:HD2	1.72	0.72
1:A:367:LEU:CG	1:A:425:VAL:HG21	2.19	0.71
1:E:275:THR:O	1:E:276:SER:HB2	1.90	0.71
1:E:274:THR:CG2	1:E:276:SER:H	1.92	0.71
1:C:731:ALA:O	1:C:732:LYS:HD2	1.90	0.71
1:B:694:GLN:HB2	1:B:697:HIS:CD2	2.23	0.71
1:B:275:THR:O	1:B:276:SER:HB2	1.89	0.71
1:D:755:SER:HB3	1:D:758:GLY:O	1.90	0.71
1:D:377:TRP:HH2	1:D:420:ARG:HD3	1.54	0.71
1:C:174:ARG:O	1:C:177:GLN:HG2	1.90	0.71
1:B:274:THR:HG21	1:B:540:HIS:ND1	2.05	0.71
1:D:730:GLU:HG3	1:D:732:LYS:NZ	2.05	0.71
1:C:425:VAL:CG2	1:C:426:GLN:N	2.54	0.70
1:F:731:ALA:C	1:F:732:LYS:HD2	2.11	0.70
1:B:343:CYS:HB2	1:B:412:CYS:SG	2.31	0.70
1:F:694:GLN:HB2	1:F:697:HIS:CD2	2.25	0.70
1:F:635:TRP:CH2	1:F:664:ARG:HG2	2.27	0.70
1:D:522:HIS:CG	1:D:622:GLU:HG3	2.27	0.70
1:D:762:LYS:HD2	1:D:763:PRO:HD2	1.74	0.69
1:A:107:ASN:HD22	1:A:125:ASN:ND2	1.90	0.69
1:A:684:GLU:HG2	1:A:732:LYS:HB2	1.74	0.69
1:A:755:SER:HB3	1:A:758:GLY:O	1.91	0.69
1:D:485:ALA:HB1	1:D:519:ALA:CB	2.20	0.69
1:F:512:ILE:HB	1:F:539:LEU:HD23	1.74	0.69
1:D:32:MET:CE	1:D:94:ILE:HG23	2.23	0.69
1:C:367:LEU:HD11	1:C:425:VAL:HG21	1.74	0.69
1:C:725:VAL:HB	1:C:768:LEU:HB3	1.75	0.69
1:F:382:PRO:HG2	5:F:3046:HOH:O	1.91	0.69
1:A:742:VAL:HG23	1:A:743:LYS:H	1.57	0.69
1:B:522:HIS:CG	1:B:622:GLU:HG3	2.27	0.69
1:E:287:ASN:HD21	1:E:334:ARG:NH2	1.90	0.69
1:B:136:ASN:ND2	1:B:227:LYS:HE3	2.08	0.69
1:B:693:LEU:HD11	1:B:716:ALA:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:VAL:HG23	1:B:743:LYS:H	1.58	0.68
1:A:352:GLN:NE2	1:B:73:GLN:HG3	2.07	0.68
1:F:311:LYS:HE3	1:F:314:GLN:OE1	1.93	0.68
1:E:165:LEU:CD1	1:E:179:VAL:HG11	2.23	0.68
1:A:548:PRO:HG3	1:A:559:VAL:HG21	1.76	0.67
1:C:367:LEU:CD1	1:C:425:VAL:HG21	2.24	0.67
1:E:673:ASN:ND2	1:E:685:GLY:HA3	2.08	0.67
1:A:165:LEU:HD13	1:A:179:VAL:HG11	1.75	0.67
1:C:731:ALA:C	1:C:732:LYS:HD2	2.15	0.67
1:D:742:VAL:HG23	1:D:743:LYS:H	1.59	0.67
1:F:347:ASN:ND2	1:F:349:TYR:H	1.93	0.67
1:C:133:GLN:HB2	1:C:136:ASN:HD22	1.59	0.67
1:D:36:ALA:O	1:D:52:LEU:HD23	1.95	0.67
1:D:541:GLY:HA3	1:D:546:ARG:NH2	2.09	0.67
1:A:274:THR:HG21	1:A:540:HIS:ND1	2.09	0.66
1:E:13:GLY:O	1:E:143:THR:HB	1.95	0.66
1:C:274:THR:HG22	1:C:540:HIS:HA	1.77	0.66
1:D:731:ALA:C	1:D:732:LYS:HD2	2.16	0.66
1:B:174:ARG:O	1:B:177:GLN:HG2	1.95	0.66
1:B:195:LYS:HE2	1:B:478:HIS:HB3	1.78	0.66
1:C:532:LEU:O	1:C:566:LYS:HD2	1.94	0.66
1:D:343:CYS:HB2	1:D:412:CYS:SG	2.36	0.66
1:D:730:GLU:HG3	1:D:732:LYS:HZ2	1.61	0.66
1:F:763:PRO:HB3	1:F:768:LEU:HD22	1.78	0.66
1:D:262:ALA:HB3	1:D:476:PRO:HG3	1.79	0.65
1:C:512:ILE:HB	1:C:539:LEU:HD23	1.77	0.65
1:A:165:LEU:HD12	1:A:174:ARG:HG2	1.78	0.65
1:B:719:THR:CG2	1:B:720:GLY:H	2.05	0.65
1:F:705:ALA:HB2	1:F:711:ILE:HB	1.78	0.65
1:A:347:ASN:HD22	1:A:347:ASN:C	1.99	0.65
1:D:380:TRP:HA	1:E:49:ASP:OD1	1.97	0.65
1:D:747:LEU:HD23	1:D:748:GLN:N	2.12	0.65
1:F:174:ARG:O	1:F:177:GLN:HG2	1.96	0.65
1:A:500:ILE:HG12	1:A:505:PHE:HB2	1.78	0.65
1:E:377:TRP:CZ3	1:E:379:LYS:HD2	2.31	0.65
1:D:136:ASN:HB3	1:D:153:ARG:HB2	1.79	0.65
1:D:276:SER:HB2	1:D:279:THR:HG23	1.78	0.65
1:B:123:LEU:N	1:B:123:LEU:HD22	2.11	0.65
1:A:16:LEU:HD22	1:A:140:VAL:HG22	1.79	0.65
1:D:485:ALA:CB	1:D:519:ALA:HB2	2.23	0.65
1:C:692:ASN:H	1:C:692:ASN:HD22	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:329:GLU:O	1:E:333:ARG:HG2	1.97	0.65
1:D:540:HIS:CG	1:D:541:GLY:H	2.14	0.65
1:C:638:LEU:O	1:C:739:ARG:NH2	2.30	0.65
1:E:417:PHE:HA	1:E:419:GLU:OE2	1.97	0.64
1:C:165:LEU:HD12	1:C:174:ARG:HG2	1.79	0.64
1:F:417:PHE:HA	1:F:419:GLU:OE2	1.97	0.64
1:C:730:GLU:HG3	1:C:732:LYS:NZ	2.13	0.64
1:A:201:MET:HE1	1:A:247:PRO:HA	1.78	0.64
1:E:476:PRO:O	1:E:477:VAL:CG1	2.45	0.64
1:C:300:LEU:HD13	1:C:301:HIS:N	2.13	0.64
1:C:367:LEU:CG	1:C:425:VAL:HG21	2.27	0.64
1:E:565:LEU:HG	1:E:569:MET:HE2	1.78	0.64
1:D:417:PHE:HA	1:D:419:GLU:OE2	1.97	0.64
1:B:32:MET:CE	1:B:94:ILE:HG23	2.27	0.64
1:D:32:MET:HE2	1:D:94:ILE:HG23	1.79	0.64
1:F:692:ASN:H	1:F:692:ASN:HD22	1.46	0.64
1:A:274:THR:HG22	1:A:275:THR:N	2.13	0.64
1:B:329:GLU:O	1:B:332:ILE:HG13	1.98	0.64
1:D:565:LEU:HG	1:D:569:MET:HE2	1.80	0.64
1:B:681:VAL:O	1:B:681:VAL:HG13	1.97	0.64
1:B:485:ALA:HB1	1:B:519:ALA:HB2	1.78	0.64
1:B:748:GLN:HB2	1:B:769:THR:H	1.62	0.63
1:A:382:PRO:HG2	5:A:3018:HOH:O	1.97	0.63
1:F:274:THR:HG23	1:F:304:HIS:HD2	1.63	0.63
1:C:692:ASN:N	1:C:692:ASN:HD22	1.96	0.63
1:C:31:GLU:OE1	1:C:56:ARG:HD3	1.99	0.63
1:C:367:LEU:HG	1:C:425:VAL:HG21	1.81	0.63
1:C:153:ARG:HG2	1:C:229:GLN:HB2	1.80	0.63
1:C:698:GLU:HG3	1:C:717:ALA:HB2	1.81	0.63
1:D:746:GLY:H	1:D:771:THR:HG23	1.63	0.63
1:F:476:PRO:O	1:F:477:VAL:HG12	1.99	0.63
1:B:476:PRO:O	1:B:477:VAL:HG12	1.99	0.63
1:B:459:GLU:CD	1:B:459:GLU:H	2.00	0.63
1:C:768:LEU:HD13	1:C:769:THR:N	2.14	0.63
1:F:31:GLU:HG2	1:F:58:PHE:HB3	1.82	0.62
1:A:747:LEU:HD22	1:A:750:GLY:O	1.98	0.62
1:B:752:GLN:HB2	1:B:759:LEU:HD11	1.80	0.62
1:A:212:HIS:CE1	1:A:238:GLU:H	2.18	0.62
1:C:82:TYR:HB2	1:C:84:LEU:HD21	1.81	0.62
1:E:16:LEU:HD22	1:E:140:VAL:HG22	1.80	0.62
1:E:262:ALA:HB3	1:E:476:PRO:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:634:ARG:NH2	1:F:643:GLU:HB3	2.14	0.62
1:D:565:LEU:HG	1:D:569:MET:CE	2.29	0.62
1:D:532:LEU:O	1:D:566:LYS:HD2	2.00	0.62
1:B:347:ASN:C	1:B:347:ASN:HD22	2.03	0.62
1:D:540:HIS:CG	1:D:541:GLY:N	2.67	0.62
1:A:341:LYS:C	1:A:342:ILE:HD12	2.20	0.62
1:B:521:ALA:HB3	5:B:3120:HOH:O	1.99	0.62
1:F:681:VAL:HG13	1:F:681:VAL:O	2.00	0.62
1:B:274:THR:HG22	1:B:275:THR:N	2.15	0.61
1:C:693:LEU:HD11	1:C:716:ALA:O	2.00	0.61
1:C:382:PRO:HG2	5:C:3013:HOH:O	2.00	0.61
1:D:546:ARG:HA	1:D:546:ARG:HH11	1.66	0.61
1:E:320:TRP:O	1:E:322:PRO:HD3	1.99	0.61
1:A:273:LEU:HD13	1:A:274:THR:N	2.15	0.61
1:C:579:ARG:CG	1:C:579:ARG:HH11	2.13	0.61
1:C:425:VAL:CG2	1:C:426:GLN:H	2.13	0.61
1:E:753:ALA:O	1:E:759:LEU:HD12	2.00	0.61
1:E:18:HIS:O	1:E:38:PRO:HA	2.00	0.61
1:C:275:THR:O	1:C:276:SER:HB2	2.01	0.61
1:B:307:CYS:HB3	1:B:315:TRP:CZ2	2.36	0.61
1:D:744:VAL:HG21	1:D:770:ILE:HG23	1.83	0.61
1:A:425:VAL:HG22	1:A:426:GLN:N	2.14	0.61
1:F:195:LYS:HE2	1:F:478:HIS:HB3	1.83	0.61
1:B:766:ASN:O	1:B:767:ALA:HB3	2.00	0.61
1:D:379:LYS:O	1:D:380:TRP:HB3	2.01	0.61
1:C:689:HIS:ND1	1:C:739:ARG:NH1	2.48	0.61
1:D:195:LYS:HE2	1:D:478:HIS:HB3	1.81	0.61
1:E:100:TYR:HD2	1:E:113:SER:HA	1.66	0.61
1:F:275:THR:O	1:F:276:SER:HB2	2.01	0.61
1:C:300:LEU:HD12	1:C:340:LEU:CD2	2.30	0.61
1:B:212:HIS:HE1	1:B:238:GLU:H	1.49	0.60
1:C:347:ASN:HD22	1:C:347:ASN:C	2.04	0.60
1:F:631:PRO:HD2	1:F:635:TRP:CZ2	2.35	0.60
1:B:690:LEU:HD21	1:B:693:LEU:HD12	1.83	0.60
1:C:522:HIS:CG	1:C:622:GLU:HG3	2.37	0.60
1:D:766:ASN:C	1:D:768:LEU:N	2.53	0.60
1:A:2:LYS:HE3	1:D:191:GLU:OE2	2.01	0.60
1:A:414:LYS:HZ2	1:A:538:ARG:HH12	1.49	0.60
1:E:273:LEU:HB2	1:E:300:LEU:HD21	1.82	0.60
1:F:579:ARG:HG3	1:F:579:ARG:HH11	1.65	0.60
1:E:21:GLN:NE2	1:E:42:ARG:HG3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:PHE:HA	1:C:419:GLU:OE2	2.02	0.60
1:E:772:LEU:HD22	1:E:772:LEU:H	1.65	0.60
1:E:565:LEU:HG	1:E:569:MET:HE1	1.84	0.60
1:B:742:VAL:HG23	1:B:743:LYS:N	2.15	0.60
1:C:547:VAL:HG23	1:C:550:ALA:HB2	1.83	0.60
1:F:296:ARG:O	1:F:560:ARG:NH1	2.35	0.60
1:F:540:HIS:C	1:F:546:ARG:HG3	2.22	0.60
1:A:290:ILE:CD1	1:A:335:LEU:HD22	2.32	0.60
1:E:274:THR:HG21	1:E:540:HIS:CE1	2.36	0.59
1:A:368:LYS:O	1:A:425:VAL:CG2	2.50	0.59
1:D:731:ALA:O	1:D:732:LYS:HD2	2.02	0.59
1:B:547:VAL:HG23	1:B:550:ALA:HB2	1.82	0.59
1:F:347:ASN:C	1:F:347:ASN:ND2	2.55	0.59
1:D:463:LEU:O	1:D:477:VAL:HG13	2.01	0.59
1:F:750:GLY:HA2	1:F:764:GLN:HG2	1.84	0.59
1:B:311:LYS:HE3	1:B:314:GLN:OE1	2.02	0.59
1:C:300:LEU:HD12	1:C:340:LEU:HD22	1.83	0.59
1:D:546:ARG:CA	1:D:546:ARG:HH11	2.15	0.59
1:C:684:GLU:HG2	1:C:732:LYS:HB2	1.85	0.59
1:C:463:LEU:O	1:C:477:VAL:HB	2.02	0.59
1:F:681:VAL:HG12	2:F:3005:SO4:O3	2.02	0.59
1:E:31:GLU:OE1	1:E:56:ARG:HD3	2.02	0.59
1:B:671:LEU:HD12	1:B:671:LEU:N	2.18	0.59
1:A:163:TYR:HB3	1:A:502:LEU:HD13	1.85	0.59
1:B:123:LEU:HA	1:B:127:GLU:O	2.03	0.59
1:A:342:ILE:HD12	1:A:342:ILE:N	2.18	0.59
1:F:352:GLN:HA	1:F:357:PHE:CD2	2.37	0.59
1:B:748:GLN:CG	1:B:769:THR:HB	2.32	0.59
1:B:31:GLU:OE1	1:B:56:ARG:HD3	2.02	0.59
1:D:476:PRO:O	1:D:477:VAL:HG13	2.03	0.58
1:A:212:HIS:HE1	1:A:238:GLU:H	1.49	0.58
1:E:635:TRP:CH2	1:E:664:ARG:HG2	2.38	0.58
1:C:343:CYS:HB2	1:C:412:CYS:SG	2.42	0.58
1:D:124:ARG:NH2	1:D:243:ASP:OD1	2.34	0.58
1:B:695:ASP:HA	1:B:718:ARG:HD3	1.85	0.58
1:E:515:PHE:HD1	1:E:516:GLU:HG2	1.68	0.58
1:E:123:LEU:HD22	1:E:123:LEU:N	2.18	0.58
1:C:273:LEU:HD13	1:C:274:THR:N	2.19	0.58
1:C:274:THR:HG21	1:C:540:HIS:HA	1.85	0.58
1:E:520:PRO:O	1:E:521:ALA:HB3	2.03	0.58
1:F:123:LEU:HD22	1:F:123:LEU:N	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:GLU:HG2	1:C:58:PHE:HB3	1.85	0.58
1:C:631:PRO:O	1:C:646:GLY:HA3	2.03	0.58
1:F:300:LEU:HD12	1:F:340:LEU:CD2	2.34	0.58
1:D:747:LEU:HD22	1:D:750:GLY:O	2.04	0.58
1:D:352:GLN:OE1	1:E:73:GLN:N	2.33	0.58
1:F:310:MET:SD	1:F:316:CYS:HA	2.44	0.58
1:E:536:HIS:HA	5:E:3025:HOH:O	2.04	0.58
1:E:214:GLN:HE22	1:E:232:VAL:CG2	2.17	0.58
1:F:747:LEU:HD22	1:F:750:GLY:O	2.04	0.58
1:E:516:GLU:O	1:E:517:ASN:HB2	2.03	0.58
1:A:347:ASN:ND2	1:A:347:ASN:C	2.58	0.57
1:A:516:GLU:O	1:A:517:ASN:HB2	2.04	0.57
1:A:134:VAL:O	1:A:135:LYS:HB2	2.04	0.57
1:B:714:LEU:HD13	1:B:715:LYS:N	2.20	0.57
1:F:595:PHE:CE1	1:F:631:PRO:HG2	2.39	0.57
1:B:348:PRO:O	1:B:387:TYR:HD1	1.87	0.57
1:B:719:THR:HG22	1:B:722:THR:O	2.03	0.57
1:A:736:LEU:HD13	1:A:736:LEU:C	2.25	0.57
1:D:525:LYS:HG2	1:D:558:VAL:HG21	1.86	0.57
1:F:733:ASN:OD1	1:F:733:ASN:O	2.21	0.57
1:E:547:VAL:HG23	1:E:550:ALA:HB2	1.86	0.57
1:F:719:THR:HG23	1:F:720:GLY:N	2.20	0.57
1:D:695:ASP:HA	1:D:718:ARG:HD3	1.86	0.57
1:F:447:LEU:C	1:F:447:LEU:HD23	2.24	0.57
1:F:548:PRO:HG3	1:F:559:VAL:HG21	1.86	0.57
1:C:165:LEU:HD13	1:C:179:VAL:HG21	1.87	0.57
1:C:123:LEU:HD22	1:C:123:LEU:N	2.20	0.57
1:E:35:TYR:HB3	1:E:52:LEU:HD11	1.87	0.57
1:B:28:GLN:NE2	1:B:33:VAL:HG21	2.19	0.57
1:A:580:ALA:HA	1:A:585:THR:O	2.04	0.57
1:D:298:LEU:CD2	1:D:560:ARG:HB2	2.35	0.57
1:A:123:LEU:HD13	1:A:128:ARG:HA	1.85	0.57
1:B:512:ILE:HB	1:B:539:LEU:HD23	1.87	0.56
1:E:201:MET:HE1	1:E:247:PRO:HA	1.87	0.56
1:B:278:THR:HG21	1:F:45:THR:HA	1.86	0.56
1:D:349:TYR:HB3	1:D:384:LEU:HD21	1.87	0.56
1:D:377:TRP:CZ3	1:D:379:LYS:HD2	2.40	0.56
1:A:742:VAL:HG23	1:A:743:LYS:N	2.21	0.56
1:C:384:LEU:HD23	1:C:384:LEU:C	2.25	0.56
1:D:631:PRO:O	1:D:646:GLY:HA3	2.05	0.56
1:E:204:ARG:HH11	1:E:204:ARG:HG2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:ARG:HG2	1:F:204:ARG:O	2.05	0.56
1:A:153:ARG:HG2	1:A:229:GLN:HB2	1.87	0.56
1:E:522:HIS:CG	1:E:622:GLU:HG3	2.40	0.56
1:A:377:TRP:CZ3	1:A:379:LYS:HD2	2.41	0.56
1:B:314:GLN:HB3	1:B:354:SER:HB2	1.86	0.56
1:D:174:ARG:O	1:D:177:GLN:HG2	2.04	0.56
1:C:195:LYS:HE2	1:C:478:HIS:HB3	1.87	0.56
1:C:93:THR:CG2	1:C:104:LYS:HB3	2.25	0.56
1:E:174:ARG:HB3	1:E:220:VAL:HG11	1.87	0.56
1:C:134:VAL:O	1:C:135:LYS:HB2	2.06	0.56
1:E:539:LEU:HB3	1:E:546:ARG:HB3	1.88	0.56
1:C:296:ARG:O	1:C:560:ARG:NH1	2.39	0.56
1:A:275:THR:O	1:A:276:SER:HB2	2.04	0.56
1:F:485:ALA:HB1	1:F:519:ALA:CB	2.25	0.56
1:C:516:GLU:O	1:C:517:ASN:HB2	2.06	0.56
1:B:350:ILE:HD13	1:B:360:LEU:HD12	1.87	0.56
1:F:137:ASN:HB3	1:F:152:GLU:OE1	2.05	0.56
1:E:311:LYS:HE3	1:E:314:GLN:OE1	2.06	0.56
1:C:290:ILE:CD1	1:C:335:LEU:HD22	2.36	0.56
1:B:476:PRO:O	1:B:477:VAL:CG1	2.53	0.56
1:F:348:PRO:HG2	1:F:349:TYR:CE1	2.40	0.56
1:B:347:ASN:ND2	1:B:347:ASN:C	2.59	0.56
1:F:155:ASP:OD1	1:F:227:LYS:HE3	2.06	0.56
1:A:212:HIS:HE1	1:A:237:LEU:HD12	1.70	0.55
1:B:164:GLY:O	1:B:165:LEU:HB2	2.06	0.55
1:A:48:LEU:HD12	1:A:49:ASP:HB2	1.88	0.55
1:F:476:PRO:O	1:F:477:VAL:CG1	2.54	0.55
1:F:165:LEU:HD12	1:F:174:ARG:HG2	1.88	0.55
1:C:18:HIS:O	1:C:38:PRO:HA	2.06	0.55
1:A:692:ASN:HD22	1:A:692:ASN:H	1.52	0.55
1:F:746:GLY:N	1:F:771:THR:HG23	2.21	0.55
1:C:525:LYS:CG	1:C:558:VAL:HG21	2.33	0.55
1:C:124:ARG:NH2	1:C:243:ASP:OD1	2.38	0.55
1:D:459:GLU:CD	1:D:459:GLU:H	2.06	0.55
1:B:695:ASP:OD1	1:B:720:GLY:HA2	2.07	0.55
1:D:482:ASP:HB3	1:D:516:GLU:OE1	2.07	0.55
1:D:18:HIS:O	1:D:38:PRO:HA	2.07	0.55
1:E:44:ARG:HG2	1:E:47:GLN:HE22	1.71	0.55
1:A:770:ILE:HD12	1:A:770:ILE:C	2.27	0.55
1:A:43:GLU:HB2	1:A:46:TRP:HD1	1.71	0.55
1:C:459:GLU:H	1:C:459:GLU:CD	2.02	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:742:VAL:HG23	1:E:743:LYS:N	2.22	0.55
1:B:762:LYS:HD2	1:B:763:PRO:HD2	1.88	0.55
1:E:195:LYS:HE2	1:E:478:HIS:HB3	1.87	0.55
1:D:672:GLY:HA3	1:D:680:TYR:OH	2.07	0.55
1:B:500:ILE:HG12	1:B:505:PHE:HB2	1.88	0.55
1:D:735:THR:CG2	1:D:736:LEU:N	2.70	0.55
1:B:744:VAL:HG22	1:B:771:THR:O	2.06	0.55
1:D:631:PRO:HD2	1:D:635:TRP:CZ2	2.41	0.55
1:C:348:PRO:HG2	1:C:349:TYR:CE1	2.42	0.55
1:B:285:THR:O	1:B:288:SER:HB3	2.07	0.55
1:A:447:LEU:C	1:A:447:LEU:HD23	2.27	0.55
1:F:274:THR:HG21	1:F:540:HIS:CE1	2.42	0.54
1:B:730:GLU:HG3	1:B:732:LYS:NZ	2.22	0.54
1:B:722:THR:HG23	1:B:769:THR:HG23	1.89	0.54
1:E:718:ARG:HB2	1:E:723:ILE:HG22	1.89	0.54
1:D:136:ASN:ND2	1:D:227:LYS:HE2	2.22	0.54
1:E:447:LEU:C	1:E:447:LEU:HD23	2.28	0.54
1:B:648:ARG:HD3	5:C:3115:HOH:O	2.06	0.54
1:C:347:ASN:ND2	1:C:347:ASN:C	2.61	0.54
1:E:479:TRP:CZ2	3:E:804:XYF:H2	2.42	0.54
1:F:744:VAL:HG22	1:F:745:ASN:N	2.22	0.54
1:C:261:PRO:HA	1:C:473:GLN:O	2.08	0.54
1:E:500:ILE:HG12	1:E:505:PHE:HB2	1.89	0.54
1:E:133:GLN:HB2	1:E:136:ASN:HD22	1.72	0.54
1:B:671:LEU:HD13	1:B:689:HIS:CD2	2.43	0.54
1:F:273:LEU:HD13	1:F:274:THR:N	2.22	0.54
1:B:382:PRO:HG2	5:B:3011:HOH:O	2.08	0.54
1:F:331:MET:O	1:F:335:LEU:HG	2.08	0.54
1:E:744:VAL:HG22	1:E:745:ASN:N	2.23	0.54
1:F:350:ILE:HD13	1:F:360:LEU:HD12	1.88	0.54
1:A:571:PRO:HB2	1:A:670:ALA:O	2.06	0.54
1:D:700:VAL:HG22	1:D:715:LYS:HG2	1.90	0.54
1:F:575:ARG:NH2	1:F:579:ARG:HH12	2.05	0.54
1:F:526:ARG:HD2	1:F:619:VAL:HB	1.90	0.54
1:B:13:GLY:O	1:B:143:THR:HB	2.07	0.54
1:E:681:VAL:HG23	1:E:683:HIS:CE1	2.43	0.54
1:C:575:ARG:NH1	1:C:579:ARG:HH12	2.05	0.54
1:E:522:HIS:CE1	1:E:523:VAL:HG23	2.42	0.54
1:D:735:THR:CG2	1:D:760:VAL:HG13	2.38	0.54
1:C:277:PHE:CD2	1:C:278:THR:HG23	2.42	0.54
1:B:201:MET:CE	1:B:247:PRO:HB3	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASN:HB3	1:C:153:ARG:HB2	1.89	0.54
1:C:20:LEU:HD22	1:C:134:VAL:CG2	2.38	0.54
1:C:695:ASP:OD1	1:C:719:THR:O	2.25	0.54
1:E:128:ARG:HH22	1:E:131:GLY:HA3	1.72	0.54
1:B:479:TRP:HZ2	3:B:802:XYF:H2	1.73	0.54
1:C:291:ASP:O	1:C:295:GLU:HG3	2.08	0.54
1:F:336:LYS:HG2	1:F:342:ILE:CD1	2.37	0.54
1:F:17:ILE:HG12	1:F:139:TYR:HB3	1.90	0.54
1:A:479:TRP:HZ2	3:A:801:XYF:H2	1.73	0.54
1:F:384:LEU:HD23	1:F:384:LEU:C	2.28	0.54
1:E:352:GLN:HA	1:E:357:PHE:CD2	2.43	0.54
1:C:681:VAL:O	1:C:681:VAL:HG23	2.07	0.53
1:A:336:LYS:HG2	1:A:342:ILE:HD13	1.90	0.53
1:D:483:CYS:SG	1:D:514:GLY:HA2	2.48	0.53
1:C:327:ASP:OD2	1:C:330:GLY:HA3	2.06	0.53
1:A:766:ASN:O	1:A:767:ALA:HB2	2.08	0.53
1:F:735:THR:HG22	1:F:736:LEU:N	2.23	0.53
1:D:772:LEU:H	1:D:772:LEU:HD22	1.72	0.53
1:E:735:THR:CG2	1:E:736:LEU:N	2.72	0.53
1:D:336:LYS:HE3	1:D:411:ASP:OD2	2.09	0.53
1:E:459:GLU:H	1:E:459:GLU:CD	2.12	0.53
1:A:311:LYS:HE3	1:A:314:GLN:OE1	2.08	0.53
1:F:497:GLY:O	1:F:500:ILE:HG22	2.09	0.53
1:F:267:TRP:CE3	1:F:341:LYS:HG3	2.44	0.53
1:B:310:MET:SD	1:B:316:CYS:HA	2.49	0.53
1:F:668:LEU:O	1:F:701:CYS:HB2	2.09	0.53
1:E:745:ASN:HB3	1:E:771:THR:O	2.09	0.53
1:A:136:ASN:HB3	1:A:153:ARG:HB2	1.90	0.53
1:F:70:GLU:HB3	1:F:236:TYR:HB2	1.90	0.53
1:C:447:LEU:C	1:C:447:LEU:HD23	2.28	0.53
1:B:315:TRP:HB2	1:B:381:GLN:OE1	2.09	0.53
1:B:352:GLN:HA	1:B:357:PHE:CD2	2.43	0.53
1:A:17:ILE:O	1:A:17:ILE:HG13	2.07	0.53
1:B:668:LEU:HD13	1:B:690:LEU:HD13	1.91	0.53
1:E:333:ARG:HH11	1:E:336:LYS:HE3	1.73	0.53
1:D:282:ASP:O	1:D:286:VAL:HG23	2.09	0.53
1:E:552:ASP:OD1	1:E:555:SER:N	2.38	0.53
1:C:694:GLN:HB2	1:C:697:HIS:CD2	2.44	0.53
1:F:472:ALA:HB1	5:F:3084:HOH:O	2.08	0.53
1:D:310:MET:SD	1:D:316:CYS:HA	2.48	0.53
1:F:277:PHE:CD2	1:F:278:THR:HG23	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:547:VAL:CG2	1:D:550:ALA:HB2	2.34	0.53
1:B:16:LEU:HD22	1:B:140:VAL:HG22	1.90	0.53
1:E:749:ASP:C	1:E:764:GLN:HE22	2.13	0.53
1:D:509:SER:HB3	1:D:536:HIS:HB2	1.91	0.53
1:C:742:VAL:HG23	1:C:743:LYS:N	2.24	0.53
1:F:153:ARG:HG2	1:F:229:GLN:HB2	1.91	0.53
1:F:274:THR:HG22	1:F:275:THR:N	2.25	0.52
1:E:681:VAL:HG13	1:E:681:VAL:O	2.09	0.52
1:A:343:CYS:HB2	1:A:412:CYS:SG	2.49	0.52
1:B:262:ALA:HB3	1:B:476:PRO:HG3	1.90	0.52
1:E:744:VAL:HG21	1:E:770:ILE:CG2	2.39	0.52
1:E:742:VAL:HG23	1:E:743:LYS:H	1.74	0.52
1:B:61:GLN:NE2	1:B:87:LEU:HG	2.23	0.52
1:C:273:LEU:HB2	1:C:300:LEU:HD21	1.91	0.52
1:D:735:THR:HG22	1:D:736:LEU:N	2.24	0.52
1:D:155:ASP:OD1	1:D:227:LYS:HE3	2.09	0.52
1:E:595:PHE:CE1	1:E:631:PRO:HG2	2.43	0.52
1:C:453:LYS:HD2	1:C:458:GLU:OE1	2.09	0.52
1:B:298:LEU:CD2	1:B:560:ARG:HB2	2.39	0.52
1:D:766:ASN:O	1:D:768:LEU:N	2.42	0.52
1:F:174:ARG:HB3	1:F:220:VAL:HG11	1.92	0.52
1:F:719:THR:HG23	1:F:720:GLY:H	1.73	0.52
1:C:515:PHE:HD1	1:C:516:GLU:HG2	1.74	0.52
1:D:736:LEU:C	1:D:736:LEU:HD13	2.29	0.52
1:F:327:ASP:OD2	1:F:330:GLY:HA3	2.08	0.52
1:E:267:TRP:CE3	1:E:341:LYS:HG3	2.44	0.52
1:E:43:GLU:C	1:E:45:THR:H	2.13	0.52
1:C:201:MET:CE	1:C:247:PRO:HB3	2.38	0.52
1:B:479:TRP:HA	1:B:509:SER:O	2.10	0.52
1:E:468:ALA:HB1	1:E:472:ALA:HB3	1.91	0.52
1:A:588:MET:HE3	5:A:3065:HOH:O	2.08	0.52
1:A:212:HIS:CE1	1:A:237:LEU:HD12	2.45	0.52
1:A:43:GLU:HB3	1:A:45:THR:HG22	1.90	0.52
1:E:290:ILE:CD1	1:E:335:LEU:HD22	2.39	0.52
1:F:557:ASP:OD1	1:F:560:ARG:NH2	2.43	0.52
1:B:384:LEU:HD23	1:B:384:LEU:C	2.31	0.52
1:A:80:PRO:HD3	1:A:431:SER:HB3	1.91	0.52
1:A:719:THR:HG23	1:A:720:GLY:H	1.75	0.52
1:E:479:TRP:CH2	3:E:804:XYF:H2	2.45	0.52
1:F:290:ILE:CD1	1:F:335:LEU:HD22	2.39	0.52
1:D:719:THR:HG22	1:D:722:THR:HB	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:476:PRO:C	1:E:477:VAL:HG12	2.29	0.52
1:E:744:VAL:HG22	1:E:771:THR:O	2.10	0.52
1:D:681:VAL:HG13	1:D:681:VAL:O	2.09	0.52
1:D:80:PRO:HD3	1:D:431:SER:HB3	1.91	0.52
1:F:516:GLU:O	1:F:517:ASN:HB2	2.09	0.52
1:D:274:THR:O	1:D:546:ARG:HG3	2.10	0.51
1:D:721:ASN:O	1:D:771:THR:HA	2.10	0.51
1:A:466:ARG:HB2	1:A:479:TRP:CH2	2.44	0.51
1:D:134:VAL:O	1:D:135:LYS:HB2	2.10	0.51
1:A:347:ASN:HA	1:A:444:TYR:OH	2.11	0.51
1:E:377:TRP:HE1	1:E:384:LEU:HD22	1.75	0.51
1:C:18:HIS:HB2	1:C:20:LEU:HD21	1.91	0.51
1:D:31:GLU:HG2	1:D:58:PHE:HB3	1.92	0.51
1:B:638:LEU:O	1:B:739:ARG:NH2	2.44	0.51
1:C:352:GLN:HA	1:C:357:PHE:CD2	2.46	0.51
1:E:282:ASP:HA	1:E:324:THR:CG2	2.40	0.51
1:C:306:ASP:O	1:C:309:TRP:HD1	1.94	0.51
1:A:31:GLU:OE1	1:A:56:ARG:HD3	2.10	0.51
1:E:698:GLU:OE1	1:E:715:LYS:HD3	2.09	0.51
1:B:747:LEU:HD22	1:B:750:GLY:O	2.11	0.51
1:E:463:LEU:O	1:E:477:VAL:CG1	2.52	0.51
1:D:689:HIS:ND1	1:D:739:ARG:NE	2.53	0.51
1:A:18:HIS:O	1:A:38:PRO:HA	2.10	0.51
1:E:306:ASP:O	1:E:309:TRP:HD1	1.93	0.51
1:B:744:VAL:HG23	1:B:772:LEU:HA	1.93	0.51
1:B:31:GLU:HG2	1:B:58:PHE:HB3	1.91	0.51
1:A:122:PHE:C	1:A:123:LEU:HD22	2.31	0.51
1:B:17:ILE:HG13	1:B:53:PHE:HZ	1.75	0.51
1:A:630:LEU:O	1:A:647:SER:N	2.43	0.51
1:A:748:GLN:HB2	1:A:769:THR:HG22	1.91	0.51
1:A:635:TRP:CZ3	1:A:664:ARG:HG2	2.46	0.51
1:E:497:GLY:O	1:E:500:ILE:HG22	2.11	0.51
1:F:521:ALA:HB3	5:F:3055:HOH:O	2.10	0.51
1:F:652:GLN:NE2	1:F:654:HIS:NE2	2.59	0.51
1:F:134:VAL:O	1:F:135:LYS:HB2	2.11	0.51
1:E:150:MET:HB3	1:E:237:LEU:HB2	1.92	0.51
1:F:276:SER:HB2	1:F:279:THR:OG1	2.10	0.51
1:D:547:VAL:HG23	1:D:550:ALA:CB	2.33	0.51
1:B:274:THR:HG23	1:B:304:HIS:HD2	1.76	0.51
1:E:20:LEU:HD12	1:E:38:PRO:O	2.11	0.51
1:C:515:PHE:CD1	1:C:516:GLU:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:GLN:HG3	1:F:435:LYS:HG2	1.93	0.51
1:E:134:VAL:O	1:E:135:LYS:HB2	2.11	0.51
1:A:310:MET:SD	1:A:316:CYS:HA	2.51	0.51
1:D:293:MET:CE	1:D:300:LEU:HD23	2.41	0.50
1:A:723:ILE:O	1:A:723:ILE:HG13	2.11	0.50
1:F:767:ALA:O	1:F:768:LEU:C	2.49	0.50
1:E:343:CYS:HB2	1:E:412:CYS:SG	2.52	0.50
1:B:274:THR:CG2	1:B:275:THR:N	2.75	0.50
1:E:287:ASN:HD21	1:E:334:ARG:HH21	1.59	0.50
1:A:201:MET:HE1	1:A:247:PRO:CA	2.39	0.50
1:E:293:MET:HE2	1:E:300:LEU:HD23	1.94	0.50
1:D:165:LEU:HA	1:D:197:ILE:O	2.11	0.50
1:E:767:ALA:O	1:E:769:THR:HG23	2.12	0.50
1:D:380:TRP:H	1:E:49:ASP:HA	1.75	0.50
1:D:476:PRO:O	1:D:477:VAL:CG1	2.60	0.50
1:D:123:LEU:HD23	1:D:128:ARG:HA	1.94	0.50
1:D:296:ARG:HD2	1:D:549:TRP:CE3	2.45	0.50
1:D:670:ALA:HB2	1:D:701:CYS:SG	2.51	0.50
1:A:274:THR:CG2	1:A:275:THR:N	2.74	0.50
1:D:630:LEU:HG	1:D:635:TRP:CD1	2.46	0.50
1:D:201:MET:CE	1:D:247:PRO:HB3	2.42	0.50
1:D:765:GLY:C	1:D:767:ALA:H	2.13	0.50
1:E:668:LEU:O	1:E:701:CYS:HB2	2.12	0.50
1:B:723:ILE:O	1:B:723:ILE:HG13	2.10	0.50
1:B:671:LEU:HD13	1:B:689:HIS:HD2	1.77	0.50
1:D:378:ASP:HA	1:D:381:GLN:O	2.11	0.50
1:A:735:THR:CG2	1:A:760:VAL:HG13	2.41	0.50
1:B:332:ILE:HG12	1:B:408:MET:O	2.12	0.50
1:D:32:MET:HE1	1:D:94:ILE:HG23	1.91	0.50
1:C:133:GLN:HB2	1:C:136:ASN:ND2	2.26	0.50
1:B:379:LYS:O	1:B:380:TRP:HB3	2.11	0.50
1:A:380:TRP:CD1	1:A:381:GLN:HG2	2.47	0.50
1:C:725:VAL:CG2	1:C:768:LEU:HD12	2.42	0.50
1:F:748:GLN:O	1:F:768:LEU:HA	2.12	0.50
1:B:20:LEU:HD12	1:B:38:PRO:O	2.11	0.50
1:B:736:LEU:C	1:B:736:LEU:HD13	2.32	0.50
1:A:273:LEU:HD12	1:A:303:PHE:CE1	2.47	0.50
1:B:417:PHE:HA	1:B:419:GLU:OE2	2.12	0.50
1:B:548:PRO:HG3	1:B:559:VAL:HG21	1.94	0.50
1:A:61:GLN:HB2	1:A:64:ILE:HD12	1.94	0.50
1:C:654:HIS:ND1	1:C:658:SER:OG	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:214:GLN:NE2	1:E:232:VAL:CG2	2.75	0.50
1:F:692:ASN:N	1:F:692:ASN:HD22	2.06	0.50
1:F:554:GLU:O	1:F:558:VAL:HG23	2.12	0.50
1:D:500:ILE:HG12	1:D:505:PHE:HB2	1.94	0.50
1:B:45:THR:HG23	1:B:46:TRP:CD1	2.47	0.50
1:A:16:LEU:CD2	1:A:140:VAL:HG22	2.40	0.49
1:E:38:PRO:HG2	1:E:51:PRO:HB2	1.94	0.49
1:E:293:MET:CE	1:E:300:LEU:HD23	2.42	0.49
1:D:693:LEU:HD13	1:D:718:ARG:HB2	1.94	0.49
1:A:695:ASP:OD1	1:A:719:THR:O	2.29	0.49
1:C:17:ILE:HG13	1:C:53:PHE:HZ	1.76	0.49
1:D:546:ARG:N	1:D:546:ARG:HH11	2.09	0.49
1:C:747:LEU:HD22	1:C:750:GLY:O	2.12	0.49
1:F:17:ILE:CG1	1:F:139:TYR:HB3	2.42	0.49
1:D:588:MET:HE3	5:D:3075:HOH:O	2.12	0.49
1:E:489:SER:O	1:E:492:GLU:HG2	2.12	0.49
1:D:733:ASN:OD1	1:D:733:ASN:O	2.29	0.49
1:D:770:ILE:N	1:D:770:ILE:HD12	2.28	0.49
1:C:347:ASN:HA	1:C:444:TYR:OH	2.12	0.49
1:F:579:ARG:NH1	1:F:579:ARG:HG3	2.27	0.49
1:A:182:TRP:CE3	1:A:215:CYS:HB2	2.48	0.49
1:D:160:GLU:HG3	1:D:204:ARG:HG2	1.94	0.49
1:C:163:TYR:HB3	1:C:502:LEU:HD13	1.94	0.49
1:C:70:GLU:HG2	5:C:3100:HOH:O	2.11	0.49
1:C:274:THR:HG21	1:C:540:HIS:CG	2.48	0.49
1:B:525:LYS:HG2	1:B:558:VAL:HG21	1.94	0.49
1:C:123:LEU:HD13	1:C:128:ARG:HA	1.94	0.49
1:C:298:LEU:HD23	1:C:560:ARG:HG3	1.93	0.49
1:F:219:GLU:HB2	1:F:229:GLN:HB3	1.93	0.49
1:E:748:GLN:HB2	1:E:769:THR:OG1	2.13	0.49
1:D:749:ASP:OD2	1:D:767:ALA:HB3	2.12	0.49
1:D:738:LEU:HB2	1:D:741:VAL:HB	1.94	0.49
1:D:382:PRO:HG2	5:D:3059:HOH:O	2.11	0.49
1:D:576:GLU:O	1:D:579:ARG:HB2	2.13	0.49
1:E:305:PHE:HB2	1:E:344:VAL:HG12	1.95	0.49
1:C:479:TRP:CZ2	3:C:803:XYF:H2	2.48	0.49
1:B:747:LEU:HD23	1:B:748:GLN:H	1.76	0.49
1:B:723:ILE:CG1	1:B:770:ILE:HB	2.42	0.49
1:F:414:LYS:NZ	1:F:538:ARG:HH22	2.10	0.49
1:E:763:PRO:O	1:E:764:GLN:HB3	2.12	0.49
1:E:548:PRO:HG3	1:E:559:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:HIS:O	1:F:38:PRO:HA	2.13	0.49
1:B:447:LEU:C	1:B:447:LEU:HD23	2.33	0.49
1:A:107:ASN:ND2	1:A:125:ASN:HD21	2.05	0.49
1:A:124:ARG:NH2	1:A:243:ASP:OD1	2.43	0.49
1:A:290:ILE:HD12	1:A:335:LEU:HD22	1.95	0.49
1:E:772:LEU:N	1:E:772:LEU:HD22	2.28	0.49
1:F:438:ASN:HB3	5:F:3119:HOH:O	2.12	0.49
1:A:576:GLU:HG3	1:A:611:GLY:HA3	1.93	0.49
1:B:273:LEU:HD12	1:B:303:PHE:HE1	1.78	0.49
1:B:152:GLU:HB3	1:B:230:PHE:CE1	2.48	0.49
1:E:747:LEU:HD22	1:E:750:GLY:O	2.13	0.49
1:E:124:ARG:NH2	1:E:243:ASP:OD1	2.46	0.49
1:A:262:ALA:HB3	1:A:476:PRO:HG3	1.94	0.49
1:B:332:ILE:O	1:B:336:LYS:HG3	2.13	0.49
1:D:698:GLU:OE1	1:D:715:LYS:HD3	2.13	0.49
1:F:134:VAL:HG22	1:F:135:LYS:HG3	1.95	0.49
1:A:417:PHE:HA	1:A:419:GLU:OE2	2.12	0.49
1:C:670:ALA:C	1:C:671:LEU:HD12	2.33	0.49
1:C:668:LEU:CD2	1:C:714:LEU:HD12	2.32	0.49
1:E:736:LEU:HD13	1:E:736:LEU:C	2.33	0.49
1:A:453:LYS:HG3	1:A:458:GLU:HG3	1.93	0.49
1:F:82:TYR:HB3	1:F:84:LEU:HD13	1.95	0.49
1:F:719:THR:HG22	5:F:3140:HOH:O	2.13	0.48
1:A:58:PHE:N	1:A:58:PHE:CD1	2.81	0.48
1:C:652:GLN:NE2	1:C:654:HIS:NE2	2.60	0.48
1:C:356:VAL:HG11	1:C:397:TRP:CH2	2.48	0.48
1:D:145:ASN:OD1	1:D:147:ARG:HB2	2.13	0.48
1:B:204:ARG:HD2	1:B:206:TYR:HE2	1.79	0.48
1:E:723:ILE:CG1	1:E:770:ILE:HB	2.41	0.48
1:C:82:TYR:HB2	1:C:84:LEU:CD2	2.42	0.48
1:A:498:LEU:HD21	1:A:608:TYR:HB3	1.95	0.48
1:B:748:GLN:HG3	1:B:769:THR:HB	1.94	0.48
1:D:273:LEU:C	1:D:273:LEU:HD13	2.33	0.48
1:D:273:LEU:HD12	1:D:303:PHE:HD1	1.77	0.48
1:A:749:ASP:HB3	1:A:764:GLN:O	2.13	0.48
1:D:723:ILE:CG1	1:D:770:ILE:HB	2.43	0.48
1:B:16:LEU:CD2	1:B:140:VAL:HG22	2.43	0.48
1:E:277:PHE:CD2	1:E:278:THR:HG23	2.48	0.48
1:E:201:MET:CE	1:E:247:PRO:HA	2.43	0.48
1:B:134:VAL:O	1:B:135:LYS:HB2	2.13	0.48
1:B:432:ASP:OD2	1:B:435:LYS:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASN:HA	1:B:444:TYR:OH	2.14	0.48
1:F:336:LYS:HG2	1:F:342:ILE:HD13	1.94	0.48
1:E:634:ARG:NH2	1:E:634:ARG:HG3	2.28	0.48
1:C:208:VAL:HA	1:C:240:PHE:O	2.13	0.48
1:C:2:LYS:HA	1:C:223:GLU:OE1	2.13	0.48
1:F:280:ASN:HB3	5:F:3086:HOH:O	2.13	0.48
1:C:692:ASN:ND2	1:C:692:ASN:N	2.61	0.48
1:D:719:THR:CG2	1:D:722:THR:HB	2.44	0.48
1:F:522:HIS:CB	1:F:622:GLU:HG3	2.44	0.48
1:C:500:ILE:HG12	1:C:505:PHE:HB2	1.95	0.48
1:E:208:VAL:HA	1:E:240:PHE:O	2.13	0.48
1:D:515:PHE:CD1	1:D:542:SER:HB2	2.49	0.48
1:D:315:TRP:CE3	1:D:381:GLN:NE2	2.82	0.48
1:D:274:THR:OG1	1:D:304:HIS:HB3	2.14	0.48
1:B:332:ILE:HD12	1:B:332:ILE:C	2.34	0.48
1:E:300:LEU:HD13	1:E:301:HIS:N	2.28	0.48
1:F:136:ASN:HB3	1:F:153:ARG:HB2	1.96	0.48
1:E:282:ASP:HB3	1:E:324:THR:HG23	1.94	0.48
1:D:580:ALA:HA	1:D:585:THR:O	2.14	0.48
1:C:11:GLN:HB2	1:C:14:LEU:HD12	1.96	0.48
1:B:296:ARG:HD3	1:B:556:CYS:SG	2.53	0.48
1:A:405:LEU:O	1:A:408:MET:HB3	2.14	0.48
1:B:672:GLY:HA3	1:B:680:TYR:OH	2.13	0.48
1:E:274:THR:CG2	1:E:275:THR:N	2.77	0.48
1:F:515:PHE:CD1	1:F:542:SER:HB2	2.49	0.48
1:C:540:HIS:C	1:C:546:ARG:HG3	2.34	0.48
1:D:540:HIS:C	1:D:546:ARG:NE	2.63	0.48
1:D:725:VAL:CB	1:D:768:LEU:HD12	2.40	0.48
1:A:121:ASP:OD1	1:A:128:ARG:HD2	2.14	0.48
1:F:332:ILE:O	1:F:336:LYS:HG3	2.13	0.48
1:D:164:GLY:O	1:D:165:LEU:HB2	2.14	0.48
1:D:327:ASP:OD2	1:D:330:GLY:HA3	2.14	0.48
1:F:333:ARG:HH11	1:F:333:ARG:HG2	1.78	0.48
1:B:670:ALA:HB2	1:B:701:CYS:SG	2.54	0.48
1:F:277:PHE:HB3	1:F:542:SER:O	2.14	0.48
1:D:136:ASN:HD21	1:D:227:LYS:HE2	1.77	0.48
1:E:466:ARG:HB2	1:E:479:TRP:CZ3	2.48	0.48
1:A:31:GLU:HG2	1:A:58:PHE:HB3	1.94	0.48
1:C:272:TRP:CB	1:C:538:ARG:HG3	2.44	0.48
1:C:272:TRP:HB2	1:C:538:ARG:HG3	1.94	0.48
1:F:262:ALA:HB3	1:F:476:PRO:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:TYR:CD2	1:E:113:SER:HA	2.49	0.48
1:D:698:GLU:HG3	1:D:717:ALA:HB2	1.95	0.48
1:C:579:ARG:NH1	1:C:579:ARG:CG	2.76	0.47
1:B:693:LEU:HD21	1:B:697:HIS:O	2.14	0.47
1:D:273:LEU:HD12	1:D:303:PHE:CD1	2.49	0.47
1:D:748:GLN:O	1:D:768:LEU:HA	2.14	0.47
1:B:521:ALA:O	1:B:525:LYS:HD3	2.13	0.47
1:F:290:ILE:HD11	1:F:335:LEU:HD22	1.96	0.47
1:E:588:MET:HG3	1:E:608:TYR:CD1	2.48	0.47
1:C:772:LEU:N	1:C:772:LEU:HD22	2.29	0.47
1:B:766:ASN:O	1:B:767:ALA:CB	2.62	0.47
1:E:283:GLU:OE2	1:E:331:MET:HB2	2.14	0.47
1:B:476:PRO:C	1:B:477:VAL:HG12	2.34	0.47
1:A:167:GLU:OE2	1:A:195:LYS:NZ	2.45	0.47
1:A:267:TRP:CE3	1:A:341:LYS:HG3	2.49	0.47
1:E:43:GLU:HB3	1:E:45:THR:HG22	1.96	0.47
1:B:753:ALA:O	1:B:759:LEU:HD12	2.13	0.47
1:E:133:GLN:HB2	1:E:136:ASN:ND2	2.29	0.47
1:C:274:THR:HG23	1:C:276:SER:H	1.79	0.47
1:F:17:ILE:HG13	1:F:53:PHE:HZ	1.80	0.47
1:E:731:ALA:O	1:E:732:LYS:HD2	2.15	0.47
1:F:515:PHE:HE2	1:F:540:HIS:HE2	1.63	0.47
1:B:273:LEU:HB2	1:B:300:LEU:HD11	1.95	0.47
1:A:191:GLU:HB3	1:D:222:SER:O	2.15	0.47
1:D:746:GLY:N	1:D:771:THR:HG23	2.30	0.47
1:B:277:PHE:HB3	1:B:542:SER:O	2.15	0.47
1:C:20:LEU:HD22	1:C:134:VAL:HG22	1.97	0.47
1:A:692:ASN:HD22	1:A:692:ASN:N	2.10	0.47
1:A:479:TRP:CZ2	3:A:801:XYF:H2	2.48	0.47
1:F:735:THR:CG2	1:F:760:VAL:HG13	2.45	0.47
1:E:298:LEU:HD13	1:E:548:PRO:HG2	1.96	0.47
1:A:261:PRO:HA	1:A:473:GLN:O	2.14	0.47
1:D:405:LEU:O	1:D:408:MET:HB3	2.15	0.47
1:F:659:LEU:O	1:F:661:VAL:HG23	2.14	0.47
1:D:437:HIS:HB3	5:D:3049:HOH:O	2.13	0.47
1:A:201:MET:CE	1:A:247:PRO:HA	2.45	0.47
1:B:509:SER:HB2	1:B:536:HIS:HB2	1.97	0.47
1:A:512:ILE:HA	1:A:527:TRP:CD1	2.50	0.47
1:E:191:GLU:HB3	1:F:222:SER:O	2.14	0.47
1:B:274:THR:HG21	1:B:540:HIS:CE1	2.49	0.47
1:A:497:GLY:O	1:A:500:ILE:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:ASN:H	1:A:692:ASN:ND2	2.13	0.47
1:D:772:LEU:N	1:D:772:LEU:HD22	2.30	0.47
1:C:267:TRP:CE3	1:C:341:LYS:HG3	2.49	0.47
1:D:356:VAL:HG12	1:D:360:LEU:HG	1.96	0.47
1:E:80:PRO:HD3	1:E:431:SER:HB3	1.96	0.47
1:E:290:ILE:HD12	1:E:335:LEU:HD22	1.96	0.47
1:B:273:LEU:HD12	1:B:303:PHE:CE1	2.50	0.47
1:C:772:LEU:HD22	1:C:772:LEU:H	1.80	0.47
1:C:747:LEU:HD23	1:C:748:GLN:N	2.29	0.46
1:B:64:ILE:HG12	1:B:242:ILE:HG23	1.97	0.46
1:C:510:HIS:CD2	1:C:510:HIS:N	2.82	0.46
1:F:687:ALA:O	1:F:689:HIS:HD2	1.98	0.46
1:D:634:ARG:HH21	1:D:634:ARG:HG3	1.80	0.46
1:A:749:ASP:C	1:A:764:GLN:HB2	2.36	0.46
1:D:560:ARG:O	1:D:564:GLN:HG3	2.16	0.46
1:A:123:LEU:HD22	1:A:123:LEU:N	2.31	0.46
1:E:634:ARG:HH21	1:E:634:ARG:HG3	1.79	0.46
1:F:32:MET:HE2	1:F:101:ALA:HB1	1.96	0.46
1:E:296:ARG:HG3	1:E:296:ARG:HH11	1.80	0.46
1:B:364:GLY:HA2	5:B:3104:HOH:O	2.15	0.46
1:A:352:GLN:HA	1:A:357:PHE:CD2	2.50	0.46
1:E:300:LEU:HD12	1:E:340:LEU:HD22	1.97	0.46
1:E:472:ALA:HB1	5:E:3063:HOH:O	2.15	0.46
1:B:610:LEU:O	1:B:614:VAL:HG13	2.15	0.46
1:C:745:ASN:HB3	1:C:771:THR:O	2.16	0.46
1:B:44:ARG:HA	1:B:47:GLN:CG	2.42	0.46
1:A:761:VAL:CG1	1:A:768:LEU:HD21	2.43	0.46
1:F:735:THR:CG2	1:F:736:LEU:N	2.78	0.46
1:C:766:ASN:O	1:C:767:ALA:HB2	2.15	0.46
1:D:389:PHE:O	1:D:395:CYS:SG	2.73	0.46
1:A:70:GLU:HG3	5:A:3171:HOH:O	2.16	0.46
1:F:747:LEU:HD23	1:F:748:GLN:N	2.31	0.46
1:C:17:ILE:O	1:C:17:ILE:HG13	2.14	0.46
1:F:275:THR:O	1:F:276:SER:CB	2.62	0.46
1:D:278:THR:CG2	1:E:45:THR:HA	2.45	0.46
1:B:525:LYS:O	1:B:528:CYS:HB2	2.16	0.46
1:B:341:LYS:O	1:B:342:ILE:HD12	2.15	0.46
1:A:273:LEU:C	1:A:273:LEU:HD13	2.36	0.46
1:B:82:TYR:CD1	1:B:470:VAL:HB	2.50	0.46
1:D:479:TRP:CZ3	1:D:481:GLY:HA2	2.51	0.46
1:A:693:LEU:HD22	1:A:718:ARG:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:HD13	1:A:340:LEU:CD1	2.46	0.46
1:E:41:VAL:C	1:E:43:GLU:H	2.18	0.46
1:D:738:LEU:CB	1:D:741:VAL:HB	2.46	0.46
1:F:525:LYS:HD3	1:F:656:PHE:CG	2.51	0.46
1:C:452:LEU:HA	1:C:452:LEU:HD12	1.76	0.46
1:C:693:LEU:HD13	1:C:718:ARG:HB2	1.98	0.46
1:E:129:ILE:O	1:E:130:THR:HB	2.15	0.46
1:C:44:ARG:HB3	1:E:308:PHE:CZ	2.51	0.46
1:F:201:MET:HE3	1:F:247:PRO:HB3	1.98	0.46
1:E:287:ASN:ND2	1:E:334:ARG:HH21	2.14	0.45
1:C:84:LEU:N	1:C:84:LEU:HD22	2.31	0.45
1:C:167:GLU:OE2	1:C:195:LYS:NZ	2.43	0.45
1:B:137:ASN:HB3	1:B:152:GLU:OE1	2.15	0.45
1:B:331:MET:O	1:B:335:LEU:HG	2.16	0.45
1:F:569:MET:CB	1:F:573:LEU:HD22	2.46	0.45
1:E:248:LYS:HB2	2:E:3006:SO4:O4	2.16	0.45
1:C:262:ALA:HB3	1:C:476:PRO:HG3	1.97	0.45
1:B:717:ALA:O	1:B:723:ILE:HA	2.15	0.45
1:B:304:HIS:HA	1:B:343:CYS:O	2.17	0.45
1:E:48:LEU:HD12	1:E:49:ASP:OD2	2.16	0.45
1:D:269:PHE:O	1:D:566:LYS:HE2	2.15	0.45
1:F:289:PHE:CD1	1:F:547:VAL:HG11	2.51	0.45
1:E:129:ILE:HG22	1:E:204:ARG:NH1	2.30	0.45
1:A:719:THR:HG23	1:A:720:GLY:N	2.31	0.45
1:D:297:ASN:O	1:D:299:PRO:HD3	2.16	0.45
1:C:588:MET:HE3	5:C:3030:HOH:O	2.17	0.45
1:E:32:MET:HE1	1:E:101:ALA:HB1	1.97	0.45
1:E:348:PRO:HG2	1:E:349:TYR:CE1	2.51	0.45
1:C:425:VAL:HG22	1:C:426:GLN:H	1.68	0.45
1:A:176:GLY:O	1:D:177:GLN:HB3	2.16	0.45
1:F:746:GLY:H	1:F:771:THR:HG23	1.82	0.45
1:E:136:ASN:HB3	1:E:153:ARG:HB2	1.98	0.45
1:F:500:ILE:HG12	1:F:505:PHE:HB2	1.98	0.45
1:D:719:THR:HG23	1:D:720:GLY:N	2.32	0.45
1:F:201:MET:CE	1:F:247:PRO:HB3	2.47	0.45
1:D:205:GLY:HA3	1:D:245:PRO:O	2.15	0.45
1:E:165:LEU:HD13	1:E:179:VAL:CG1	2.38	0.45
1:C:525:LYS:HD2	1:C:555:SER:HA	1.99	0.45
1:F:732:LYS:N	1:F:732:LYS:HD2	2.30	0.45
1:D:262:ALA:HB3	1:D:476:PRO:CG	2.44	0.45
1:D:153:ARG:HG2	1:D:229:GLN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:TRP:CD2	1:A:341:LYS:HG3	2.51	0.45
1:E:282:ASP:HA	1:E:324:THR:HG23	1.98	0.45
1:C:48:LEU:HD23	1:C:48:LEU:N	2.31	0.45
1:C:267:TRP:CD2	1:C:341:LYS:HG3	2.52	0.45
1:C:736:LEU:C	1:C:736:LEU:HD13	2.37	0.45
1:A:735:THR:HG23	1:A:760:VAL:HG13	1.97	0.45
1:C:277:PHE:CZ	1:D:48:LEU:HD22	2.52	0.45
1:D:549:TRP:HB3	1:D:556:CYS:SG	2.56	0.45
1:E:291:ASP:O	1:E:295:GLU:HG3	2.17	0.45
1:C:137:ASN:HB3	1:C:152:GLU:OE1	2.17	0.45
1:A:681:VAL:HG22	1:A:681:VAL:O	2.17	0.45
1:F:60:PRO:O	1:F:61:GLN:HG3	2.16	0.45
1:F:570:MET:HG3	1:F:678:PRO:HA	1.97	0.45
1:D:447:LEU:C	1:D:447:LEU:HD23	2.37	0.45
1:E:654:HIS:N	1:E:654:HIS:CD2	2.85	0.45
1:F:476:PRO:C	1:F:477:VAL:HG12	2.37	0.45
1:A:425:VAL:CG2	1:A:426:GLN:N	2.79	0.45
1:A:767:ALA:O	1:A:768:LEU:C	2.54	0.45
1:C:730:GLU:HG3	1:C:732:LYS:HZ3	1.79	0.45
1:A:123:LEU:HD13	1:A:128:ARG:CA	2.47	0.45
1:C:671:LEU:N	1:C:671:LEU:HD12	2.32	0.45
1:B:327:ASP:OD2	1:B:330:GLY:HA3	2.17	0.45
1:A:274:THR:CG2	1:A:276:SER:H	2.05	0.45
1:B:671:LEU:CD1	1:B:671:LEU:N	2.80	0.45
1:E:45:THR:HG23	1:E:46:TRP:CD1	2.32	0.45
1:E:196:ASN:C	1:E:197:ILE:HG12	2.37	0.45
1:A:723:ILE:O	1:A:723:ILE:CG1	2.65	0.45
1:A:731:ALA:C	1:A:732:LYS:HD2	2.37	0.45
1:E:752:GLN:HB2	1:E:759:LEU:HD11	1.98	0.45
1:D:736:LEU:HD13	1:D:737:CYS:N	2.31	0.45
1:E:190:THR:HA	1:F:223:GLU:O	2.16	0.45
1:A:264:PRO:HD3	1:A:507:PHE:CE2	2.52	0.45
1:F:379:LYS:O	1:F:380:TRP:HB3	2.16	0.45
1:D:163:TYR:HB3	1:D:502:LEU:HD13	1.98	0.45
1:F:329:GLU:H	1:F:329:GLU:CD	2.20	0.45
1:A:155:ASP:OD1	1:A:227:LYS:HE3	2.16	0.45
1:B:466:ARG:HB2	1:B:479:TRP:CH2	2.52	0.45
1:A:689:HIS:CE1	1:A:739:ARG:HH21	2.35	0.45
1:F:510:HIS:CD2	1:F:510:HIS:N	2.83	0.45
1:F:538:ARG:NH2	1:F:540:HIS:CD2	2.85	0.45
1:E:718:ARG:HB2	1:E:723:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:692:ASN:ND2	1:F:692:ASN:N	2.64	0.45
1:B:277:PHE:CD2	1:B:278:THR:HG23	2.52	0.45
1:A:693:LEU:HD11	1:A:716:ALA:O	2.17	0.45
1:A:290:ILE:HD13	1:A:340:LEU:HD11	1.98	0.45
1:C:273:LEU:HD13	1:C:273:LEU:C	2.37	0.45
1:C:692:ASN:ND2	5:C:3050:HOH:O	2.48	0.45
1:C:347:ASN:ND2	1:C:349:TYR:H	2.14	0.45
1:C:466:ARG:HB2	1:C:479:TRP:CH2	2.52	0.45
1:F:690:LEU:HD21	1:F:693:LEU:HD12	1.99	0.45
1:E:297:ASN:O	1:E:299:PRO:HD3	2.16	0.45
1:B:703:VAL:O	1:B:711:ILE:HG22	2.17	0.45
1:F:634:ARG:NH2	1:F:643:GLU:CB	2.80	0.44
1:A:476:PRO:O	1:A:477:VAL:HG13	2.17	0.44
1:D:276:SER:HB2	1:D:279:THR:CG2	2.47	0.44
1:D:38:PRO:HG2	1:D:51:PRO:HD2	1.98	0.44
1:D:201:MET:HE1	1:D:247:PRO:HB3	1.99	0.44
1:F:82:TYR:CD1	1:F:470:VAL:HB	2.52	0.44
1:E:731:ALA:C	1:E:732:LYS:HD2	2.37	0.44
1:C:630:LEU:O	1:C:647:SER:N	2.50	0.44
1:E:262:ALA:HB3	1:E:476:PRO:CG	2.47	0.44
1:D:278:THR:HG21	1:E:45:THR:HA	1.98	0.44
1:C:277:PHE:HZ	1:D:48:LEU:HD22	1.81	0.44
1:B:272:TRP:HB2	1:B:538:ARG:HA	1.98	0.44
1:B:247:PRO:HD2	5:B:3046:HOH:O	2.16	0.44
1:C:498:LEU:HD21	1:C:608:TYR:HB3	1.99	0.44
1:C:24:GLU:HA	2:C:3011:SO4:O1	2.17	0.44
1:C:279:THR:HG22	1:C:543:LYS:O	2.17	0.44
1:F:89:ASP:N	1:F:89:ASP:OD1	2.49	0.44
1:C:482:ASP:OD1	3:C:803:XYF:O2	2.33	0.44
1:D:100:TYR:HE2	1:D:113:SER:HG	1.64	0.44
1:B:631:PRO:HD2	1:B:635:TRP:CZ2	2.52	0.44
1:D:275:THR:HG23	1:D:275:THR:O	2.17	0.44
1:C:576:GLU:O	1:C:579:ARG:HB3	2.16	0.44
1:D:635:TRP:CH2	1:D:664:ARG:HG2	2.52	0.44
1:F:619:VAL:HG11	1:F:624:GLY:HA2	1.99	0.44
1:F:342:ILE:HD12	1:F:342:ILE:N	2.33	0.44
1:B:635:TRP:CZ3	1:B:664:ARG:HG2	2.53	0.44
1:B:191:GLU:HB3	1:C:222:SER:O	2.17	0.44
1:F:551:TYR:O	1:F:552:ASP:HB3	2.18	0.44
1:F:252:ASP:HA	1:F:583:ARG:O	2.17	0.44
1:F:353:LYS:HG2	1:F:353:LYS:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:PRO:HG2	1:D:349:TYR:CE1	2.53	0.44
1:A:748:GLN:O	1:A:749:ASP:HB2	2.17	0.44
1:F:692:ASN:H	1:F:692:ASN:ND2	2.12	0.44
1:D:744:VAL:HG21	1:D:770:ILE:CG2	2.47	0.44
1:F:45:THR:HG23	1:F:46:TRP:CD1	2.53	0.44
1:D:749:ASP:CG	1:D:767:ALA:HB3	2.38	0.44
1:D:341:LYS:C	1:D:342:ILE:HD12	2.38	0.44
1:C:100:TYR:CD1	1:C:111:ARG:HD2	2.53	0.44
1:B:668:LEU:O	1:B:701:CYS:HB2	2.18	0.44
1:B:751:SER:OG	1:B:762:LYS:HB3	2.18	0.44
1:A:38:PRO:HG2	1:A:51:PRO:HD2	1.99	0.44
1:D:488:GLU:O	1:D:492:GLU:HG3	2.16	0.44
1:A:137:ASN:HB3	1:A:152:GLU:OE1	2.17	0.44
1:F:347:ASN:HA	1:F:444:TYR:OH	2.18	0.44
1:A:11:GLN:HB2	1:A:14:LEU:HD12	2.00	0.44
1:D:610:LEU:O	1:D:614:VAL:HG13	2.17	0.44
1:B:2:LYS:HA	1:B:223:GLU:OE1	2.18	0.44
1:D:452:LEU:HD12	1:D:452:LEU:N	2.33	0.44
1:A:711:ILE:O	1:A:711:ILE:HG12	2.17	0.44
1:A:290:ILE:HD12	1:A:335:LEU:CD2	2.48	0.44
1:D:300:LEU:HD13	1:D:301:HIS:H	1.82	0.44
1:E:744:VAL:HG23	1:E:772:LEU:HA	2.00	0.44
1:B:201:MET:HE3	1:B:247:PRO:HB3	2.00	0.44
1:E:489:SER:HA	1:E:492:GLU:CD	2.38	0.44
1:C:156:LEU:HD11	1:C:228:VAL:HG23	1.98	0.44
1:E:490:MET:HE3	1:E:620:PHE:CD1	2.53	0.44
1:D:69:ILE:HG12	1:D:150:MET:HE1	1.99	0.44
1:B:98:GLU:H	1:B:98:GLU:CD	2.21	0.44
1:B:380:TRP:CD1	1:B:381:GLN:HG2	2.53	0.43
1:E:631:PRO:HD2	1:E:635:TRP:CZ2	2.53	0.43
1:A:273:LEU:HB2	1:A:300:LEU:HD21	2.00	0.43
1:C:122:PHE:C	1:C:123:LEU:HD22	2.39	0.43
1:D:735:THR:HG21	1:D:760:VAL:HG13	1.99	0.43
1:E:734:TRP:CH2	1:E:763:PRO:HG3	2.53	0.43
1:F:214:GLN:HG3	1:F:435:LYS:CG	2.48	0.43
1:B:635:TRP:CH2	1:B:664:ARG:HG2	2.53	0.43
1:A:744:VAL:HG22	1:A:745:ASN:N	2.32	0.43
1:B:25:VAL:HG21	1:B:114:LYS:HE2	2.00	0.43
1:E:554:GLU:O	1:E:558:VAL:HG23	2.17	0.43
1:A:763:PRO:HB3	1:A:768:LEU:HD12	1.99	0.43
1:F:82:TYR:CB	1:F:84:LEU:HD13	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:GLN:HB2	1:C:14:LEU:CD1	2.48	0.43
1:C:325:PHE:N	1:C:326:PRO:HD3	2.33	0.43
1:E:163:TYR:HB3	1:E:502:LEU:HD13	2.01	0.43
1:A:327:ASP:OD2	1:A:330:GLY:HA3	2.19	0.43
1:F:359:GLU:OE2	1:F:363:LYS:NZ	2.49	0.43
1:B:532:LEU:O	1:B:566:LYS:HD2	2.18	0.43
1:A:25:VAL:HG21	1:A:114:LYS:HE2	2.00	0.43
1:A:300:LEU:HD12	1:A:340:LEU:CD2	2.48	0.43
1:C:165:LEU:HD13	1:C:179:VAL:CG2	2.48	0.43
1:D:522:HIS:CD2	1:D:622:GLU:HG3	2.53	0.43
1:A:347:ASN:ND2	1:A:349:TYR:H	2.16	0.43
1:B:575:ARG:O	1:B:578:ALA:HB3	2.18	0.43
1:C:89:ASP:N	1:C:89:ASP:OD1	2.51	0.43
1:A:425:VAL:HG22	1:A:426:GLN:H	1.81	0.43
1:D:311:LYS:HE3	1:D:314:GLN:OE1	2.18	0.43
1:E:17:ILE:HG13	1:E:17:ILE:O	2.19	0.43
1:C:575:ARG:CZ	1:C:579:ARG:HH12	2.31	0.43
1:E:165:LEU:HA	1:E:197:ILE:O	2.18	0.43
1:E:128:ARG:HH22	1:E:131:GLY:CA	2.31	0.43
1:D:290:ILE:CD1	1:D:335:LEU:HD22	2.49	0.43
1:F:509:SER:HB2	1:F:536:HIS:HB2	2.00	0.43
1:B:516:GLU:O	1:B:517:ASN:HB2	2.19	0.43
1:F:275:THR:HG22	1:F:303:PHE:HZ	1.83	0.43
1:A:262:ALA:HB3	1:A:476:PRO:CD	2.49	0.43
1:A:525:LYS:CG	1:A:558:VAL:HG21	2.42	0.43
1:A:751:SER:OG	1:A:762:LYS:HB3	2.19	0.43
1:D:32:MET:HB2	1:D:32:MET:HE2	1.71	0.43
1:A:547:VAL:HA	1:A:548:PRO:HD3	1.91	0.43
1:F:164:GLY:O	1:F:165:LEU:HB2	2.18	0.43
1:A:429:ASP:OD1	1:A:431:SER:OG	2.30	0.43
1:C:70:GLU:HB3	1:C:236:TYR:HB2	2.01	0.43
1:C:48:LEU:HD13	1:E:277:PHE:HZ	1.83	0.43
1:E:588:MET:HE3	5:E:3008:HOH:O	2.19	0.43
1:F:488:GLU:H	1:F:488:GLU:CD	2.22	0.43
1:F:479:TRP:HE1	1:F:511:ASP:CG	2.22	0.43
1:E:164:GLY:O	1:E:165:LEU:HB2	2.18	0.43
1:E:287:ASN:ND2	1:E:334:ARG:NH2	2.64	0.43
1:E:302:VAL:HG22	1:E:341:LYS:HB2	2.00	0.43
1:C:226:SER:O	1:C:227:LYS:HG3	2.19	0.43
1:B:738:LEU:HD11	1:B:770:ILE:HD13	2.01	0.43
1:C:290:ILE:HD13	1:C:340:LEU:CD1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:PRO:C	1:A:477:VAL:HG13	2.39	0.43
1:C:525:LYS:HB3	1:C:656:PHE:CD1	2.54	0.43
1:A:515:PHE:HD1	1:A:516:GLU:HG2	1.84	0.43
1:A:670:ALA:HB2	1:A:701:CYS:SG	2.59	0.43
1:D:765:GLY:O	1:D:767:ALA:N	2.50	0.43
1:D:576:GLU:OE2	1:D:579:ARG:NH1	2.52	0.43
1:C:314:GLN:HB3	1:C:354:SER:HB2	2.00	0.43
1:E:310:MET:SD	1:E:316:CYS:HA	2.59	0.43
1:A:384:LEU:C	1:A:384:LEU:HD23	2.38	0.43
1:B:262:ALA:O	1:B:264:PRO:HD3	2.19	0.42
1:D:191:GLU:N	1:D:191:GLU:OE1	2.48	0.42
1:F:723:ILE:N	1:F:723:ILE:HD12	2.34	0.42
1:D:358:LYS:HE2	1:D:362:GLU:OE2	2.19	0.42
1:F:681:VAL:HG12	2:F:3005:SO4:S	2.60	0.42
1:C:70:GLU:OE1	1:C:73:GLN:HG2	2.18	0.42
1:C:45:THR:HG23	1:C:46:TRP:CD1	2.53	0.42
1:D:354:SER:HA	1:D:355:PRO:HD3	1.91	0.42
1:E:318:PHE:HB2	1:E:401:LYS:HD2	2.00	0.42
1:A:652:GLN:NE2	1:A:654:HIS:NE2	2.66	0.42
1:F:406:VAL:HG11	1:F:455:THR:HB	2.01	0.42
1:F:98:GLU:HG3	1:F:98:GLU:O	2.19	0.42
1:D:264:PRO:HD3	1:D:507:PHE:CE2	2.54	0.42
1:C:274:THR:HG23	1:C:276:SER:N	2.34	0.42
1:D:273:LEU:HD13	1:D:274:THR:N	2.34	0.42
1:C:31:GLU:HG2	1:C:58:PHE:CB	2.49	0.42
1:E:204:ARG:NH1	1:E:204:ARG:HG2	2.33	0.42
1:F:157:GLY:HA3	1:F:204:ARG:NH2	2.33	0.42
1:A:692:ASN:ND2	1:A:692:ASN:N	2.67	0.42
1:B:341:LYS:C	1:B:342:ILE:HD12	2.38	0.42
1:A:300:LEU:HD12	1:A:340:LEU:HD21	2.02	0.42
1:F:273:LEU:HD22	1:F:274:THR:H	1.83	0.42
1:A:367:LEU:CD1	1:A:425:VAL:HG21	2.49	0.42
1:D:540:HIS:CA	1:D:546:ARG:HD2	2.50	0.42
1:C:748:GLN:HB2	1:C:769:THR:HB	2.01	0.42
1:E:379:LYS:O	1:E:380:TRP:HB3	2.19	0.42
1:F:691:PHE:O	1:F:692:ASN:C	2.57	0.42
1:A:414:LYS:NZ	1:A:538:ARG:HH12	2.15	0.42
1:C:123:LEU:HA	1:C:127:GLU:O	2.19	0.42
1:E:683:HIS:HD2	1:E:730:GLU:HG2	1.84	0.42
1:B:201:MET:HE1	1:B:247:PRO:HB3	2.02	0.42
1:C:342:ILE:N	1:C:342:ILE:HD12	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:PHE:HA	1:C:476:PRO:HD2	1.86	0.42
1:E:358:LYS:HG2	1:E:362:GLU:OE2	2.19	0.42
1:C:212:HIS:HA	1:C:213:PRO:HD3	1.88	0.42
1:A:544:SER:O	1:A:546:ARG:NH1	2.53	0.42
1:F:293:MET:CE	1:F:300:LEU:HD23	2.50	0.42
1:C:356:VAL:HG11	1:C:397:TRP:HH2	1.85	0.42
1:C:341:LYS:C	1:C:342:ILE:HD12	2.40	0.42
1:D:526:ARG:HD2	1:D:619:VAL:HB	2.00	0.42
1:D:476:PRO:C	1:D:477:VAL:CG1	2.88	0.42
1:E:320:TRP:CE2	1:E:328:PRO:HB3	2.55	0.42
1:E:520:PRO:O	1:E:521:ALA:CB	2.67	0.42
1:A:37:ALA:HA	1:A:38:PRO:HD3	1.79	0.42
1:F:693:LEU:HD11	1:F:716:ALA:O	2.18	0.42
1:C:43:GLU:HB3	1:C:45:THR:HG22	2.01	0.42
1:A:354:SER:HA	1:A:355:PRO:HD3	1.89	0.42
1:C:635:TRP:CH2	1:C:664:ARG:HB3	2.55	0.42
1:B:668:LEU:CD2	1:B:714:LEU:HD12	2.29	0.42
1:F:273:LEU:C	1:F:273:LEU:HD13	2.40	0.42
1:F:668:LEU:HD21	1:F:714:LEU:CD1	2.36	0.42
1:C:164:GLY:O	1:C:165:LEU:HB2	2.20	0.42
1:B:123:LEU:CD2	1:B:123:LEU:N	2.82	0.42
1:E:735:THR:HG23	1:E:736:LEU:N	2.34	0.42
1:E:764:GLN:NE2	1:E:764:GLN:O	2.53	0.42
1:D:58:PHE:N	1:D:58:PHE:CD1	2.88	0.42
1:D:69:ILE:HG12	1:D:150:MET:CE	2.50	0.42
1:D:619:VAL:HG11	1:D:624:GLY:HA2	2.01	0.42
1:A:320:TRP:O	1:A:322:PRO:HD3	2.20	0.42
1:A:528:CYS:O	1:A:532:LEU:HD23	2.19	0.42
1:F:753:ALA:O	1:F:759:LEU:HD12	2.20	0.42
1:E:58:PHE:CD1	1:E:58:PHE:N	2.88	0.42
1:B:744:VAL:CG2	1:B:772:LEU:HA	2.50	0.42
1:A:164:GLY:O	1:A:165:LEU:HB2	2.20	0.42
1:A:735:THR:CG2	1:A:736:LEU:N	2.81	0.42
1:D:497:GLY:O	1:D:500:ILE:HG22	2.20	0.42
1:A:424:ASP:N	1:A:424:ASP:OD2	2.50	0.42
1:F:311:LYS:HE3	1:F:314:GLN:CD	2.40	0.42
1:C:736:LEU:CD1	1:C:738:LEU:HD23	2.50	0.42
1:F:80:PRO:HD3	1:F:431:SER:HB3	2.01	0.42
1:E:670:ALA:C	1:E:671:LEU:HD12	2.40	0.42
1:E:565:LEU:O	1:E:569:MET:HG3	2.19	0.42
1:C:730:GLU:HG3	1:C:732:LYS:HZ2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:334:ARG:O	1:E:337:ALA:HB3	2.20	0.42
1:B:497:GLY:O	1:B:500:ILE:HG22	2.20	0.42
1:D:588:MET:HG3	1:D:608:TYR:CD1	2.54	0.42
1:B:414:LYS:HZ2	1:B:538:ARG:HH12	1.68	0.42
1:E:17:ILE:HG12	1:E:139:TYR:HB3	2.02	0.42
1:C:182:TRP:CE3	1:C:215:CYS:HB2	2.55	0.42
1:D:344:VAL:HG22	1:D:410:VAL:HG11	2.02	0.42
1:C:770:ILE:HD12	1:C:770:ILE:C	2.40	0.42
1:E:214:GLN:HE22	1:E:232:VAL:HG21	1.85	0.41
1:F:634:ARG:HH21	1:F:643:GLU:CB	2.24	0.41
1:A:747:LEU:HD23	1:A:747:LEU:C	2.40	0.41
1:C:171:ALA:O	1:C:174:ARG:NH2	2.39	0.41
1:B:195:LYS:HB3	1:B:468:ALA:HB3	2.00	0.41
1:D:262:ALA:HB3	1:D:476:PRO:CD	2.50	0.41
1:B:485:ALA:HB1	1:B:519:ALA:CB	2.48	0.41
1:E:37:ALA:HA	1:E:38:PRO:HD3	1.87	0.41
1:E:314:GLN:HB3	1:E:317:ASP:OD2	2.19	0.41
1:B:730:GLU:HG3	1:B:732:LYS:HZ2	1.85	0.41
1:D:634:ARG:CZ	1:D:645:ASP:OD1	2.67	0.41
1:B:405:LEU:O	1:B:410:VAL:HG23	2.20	0.41
1:B:145:ASN:OD1	1:B:147:ARG:HB2	2.19	0.41
1:A:752:GLN:OE1	1:A:759:LEU:HD21	2.20	0.41
1:A:300:LEU:CD1	1:A:340:LEU:HD22	2.51	0.41
1:C:367:LEU:HD11	1:C:425:VAL:CG2	2.46	0.41
1:F:419:GLU:H	1:F:419:GLU:CD	2.23	0.41
1:A:191:GLU:OE1	1:D:223:GLU:HA	2.21	0.41
1:B:182:TRP:CE3	1:B:215:CYS:HB2	2.55	0.41
1:C:580:ALA:HA	1:C:585:THR:O	2.19	0.41
1:B:764:GLN:HG3	1:B:764:GLN:O	2.20	0.41
1:B:768:LEU:HD23	1:B:768:LEU:C	2.41	0.41
1:F:273:LEU:HD12	1:F:303:PHE:HE1	1.85	0.41
1:F:749:ASP:CG	1:F:767:ALA:HB3	2.41	0.41
1:C:17:ILE:HG12	1:C:139:TYR:HB3	2.02	0.41
1:F:522:HIS:CG	1:F:622:GLU:HG3	2.56	0.41
1:E:17:ILE:CG1	1:E:139:TYR:HB3	2.51	0.41
1:D:21:GLN:HE22	1:D:41:VAL:H	1.68	0.41
1:B:634:ARG:HG2	1:B:692:ASN:OD1	2.20	0.41
1:B:208:VAL:HA	1:B:240:PHE:O	2.20	0.41
1:B:592:MET:C	1:B:592:MET:SD	2.98	0.41
1:F:108:LEU:HD22	1:F:243:ASP:HB2	2.02	0.41
1:C:36:ALA:O	1:C:52:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:MET:HE3	1:D:300:LEU:HD23	2.01	0.41
1:D:293:MET:HE2	1:D:300:LEU:HD23	2.02	0.41
1:E:569:MET:CB	1:E:573:LEU:HD22	2.50	0.41
1:E:547:VAL:CG2	1:E:550:ALA:HB2	2.50	0.41
1:E:634:ARG:HH21	1:E:643:GLU:HB3	1.86	0.41
1:B:190:THR:HA	1:C:223:GLU:O	2.21	0.41
1:E:296:ARG:O	1:E:560:ARG:NH1	2.54	0.41
1:D:39:ARG:HD2	5:D:3056:HOH:O	2.20	0.41
1:A:273:LEU:HD12	1:A:303:PHE:HE1	1.85	0.41
1:A:308:PHE:CZ	1:B:44:ARG:HB3	2.55	0.41
1:A:731:ALA:O	1:A:732:LYS:HD2	2.20	0.41
1:D:745:ASN:HB3	1:D:771:THR:O	2.20	0.41
1:B:200:TYR:CE2	1:B:208:VAL:HG22	2.55	0.41
1:B:222:SER:O	1:C:191:GLU:HB3	2.19	0.41
1:A:307:CYS:HB3	1:A:315:TRP:CZ2	2.56	0.41
1:C:526:ARG:NH2	1:C:624:GLY:HA2	2.35	0.41
1:E:82:TYR:CD1	1:E:470:VAL:HB	2.55	0.41
1:E:173:VAL:HG21	1:E:603:TYR:CD1	2.56	0.41
1:A:770:ILE:HD11	1:A:772:LEU:CD2	2.50	0.41
1:E:333:ARG:NH1	1:E:336:LYS:HE3	2.36	0.41
1:A:336:LYS:CG	1:A:342:ILE:HD13	2.50	0.41
1:C:453:LYS:HG3	1:C:458:GLU:HA	2.02	0.41
1:A:681:VAL:HG23	1:A:683:HIS:CE1	2.56	0.41
1:C:635:TRP:CZ3	1:C:664:ARG:HB3	2.55	0.41
1:E:182:TRP:CE3	1:E:215:CYS:HB2	2.56	0.41
1:E:345:TRP:O	1:E:346:ILE:CG2	2.69	0.41
1:B:552:ASP:OD1	1:B:555:SER:N	2.38	0.41
1:B:472:ALA:HB1	5:B:3074:HOH:O	2.21	0.41
1:C:143:THR:O	1:C:143:THR:HG22	2.20	0.41
1:E:80:PRO:HD2	1:E:435:LYS:HB2	2.01	0.41
1:A:548:PRO:CG	1:A:559:VAL:HG21	2.48	0.41
1:E:277:PHE:HB3	1:E:542:SER:HA	2.02	0.41
1:B:635:TRP:HB3	1:B:662:TYR:HB3	2.03	0.41
1:B:439:HIS:NE2	1:B:443:ILE:HD11	2.34	0.41
1:F:770:ILE:HD11	1:F:772:LEU:HD23	2.02	0.41
1:B:252:ASP:HA	1:B:583:ARG:O	2.21	0.41
1:E:275:THR:HG22	1:E:303:PHE:HZ	1.86	0.41
1:B:718:ARG:CB	1:B:723:ILE:HG22	2.51	0.41
1:B:670:ALA:C	1:B:671:LEU:HD12	2.41	0.41
1:F:485:ALA:CB	1:F:519:ALA:HB2	2.31	0.41
1:D:171:ALA:O	1:D:174:ARG:NH2	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:ARG:HD3	5:B:3057:HOH:O	2.19	0.41
1:D:67:VAL:O	1:D:238:GLU:HA	2.21	0.41
1:B:639:TRP:HE1	1:B:640:HIS:CE1	2.38	0.41
1:D:533:LEU:HD12	1:D:533:LEU:HA	1.94	0.41
1:A:521:ALA:O	1:A:525:LYS:HE3	2.20	0.41
1:F:631:PRO:O	1:F:646:GLY:HA3	2.20	0.41
1:F:547:VAL:HA	1:F:548:PRO:HD3	1.96	0.41
1:E:314:GLN:HB3	1:E:354:SER:HB2	2.01	0.41
1:F:37:ALA:HA	1:F:38:PRO:HD3	1.81	0.41
1:F:82:TYR:CE1	1:F:470:VAL:HB	2.56	0.41
1:C:11:GLN:HA	1:C:12:PRO:HD3	1.97	0.41
1:E:414:LYS:HZ2	1:E:538:ARG:HH12	1.69	0.41
1:E:570:MET:HG3	1:E:678:PRO:HA	2.03	0.41
1:F:212:HIS:HA	1:F:213:PRO:HD3	1.90	0.41
1:D:155:ASP:HB3	5:D:3094:HOH:O	2.21	0.41
1:C:37:ALA:HA	1:C:38:PRO:HD3	1.78	0.41
1:E:447:LEU:O	1:E:451:VAL:HG23	2.20	0.41
1:E:153:ARG:HG2	1:E:229:GLN:HB2	2.02	0.41
1:C:509:SER:OG	1:C:510:HIS:N	2.54	0.41
1:A:306:ASP:O	1:A:309:TRP:HD1	2.04	0.41
1:B:633:GLY:O	1:B:646:GLY:N	2.53	0.41
1:E:327:ASP:OD2	1:E:330:GLY:HA3	2.20	0.41
1:A:615:MET:SD	1:A:615:MET:C	3.00	0.41
1:E:716:ALA:HA	1:E:724:THR:O	2.21	0.41
1:C:712:PHE:CG	1:C:731:ALA:HB2	2.55	0.40
1:D:32:MET:HE3	1:D:103:PHE:HB2	2.03	0.40
1:D:681:VAL:HG23	1:D:683:HIS:CE1	2.56	0.40
1:A:11:GLN:HB2	1:A:14:LEU:CD1	2.51	0.40
1:B:120:LEU:HD23	1:B:121:ASP:N	2.36	0.40
1:D:261:PRO:O	1:D:581:ASN:HA	2.21	0.40
1:D:308:PHE:CE1	1:D:315:TRP:HZ2	2.40	0.40
1:D:277:PHE:CD2	1:D:278:THR:HG23	2.56	0.40
1:F:635:TRP:CZ3	1:F:664:ARG:HG2	2.56	0.40
1:F:761:VAL:HG11	1:F:768:LEU:HD11	2.03	0.40
1:C:349:TYR:HB3	1:C:384:LEU:HD21	2.03	0.40
1:E:273:LEU:CB	1:E:300:LEU:HD21	2.48	0.40
1:E:516:GLU:O	1:E:517:ASN:CB	2.68	0.40
1:E:719:THR:HG22	1:E:722:THR:O	2.22	0.40
1:E:610:LEU:O	1:E:614:VAL:HG13	2.20	0.40
1:B:601:CYS:HA	1:B:604:LEU:HG	2.03	0.40
1:B:122:PHE:CE1	1:B:241:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:67:VAL:O	1:F:238:GLU:HA	2.21	0.40
1:B:718:ARG:HH21	1:B:772:LEU:HD12	1.86	0.40
1:B:690:LEU:O	1:B:739:ARG:HB2	2.21	0.40
1:A:747:LEU:HD11	1:A:761:VAL:HG13	2.02	0.40
1:E:300:LEU:HD12	1:E:340:LEU:CD2	2.52	0.40
1:C:18:HIS:HB2	1:C:20:LEU:CD2	2.51	0.40
1:E:512:ILE:HB	1:E:539:LEU:HD23	2.02	0.40
1:D:772:LEU:CD2	1:D:772:LEU:H	2.34	0.40
1:C:310:MET:SD	1:C:316:CYS:HA	2.61	0.40
1:C:274:THR:HG22	1:C:539:LEU:O	2.21	0.40
1:F:670:ALA:HB2	1:F:701:CYS:SG	2.61	0.40
1:B:381:GLN:O	1:B:384:LEU:HB2	2.21	0.40
1:D:282:ASP:HA	1:D:324:THR:HG23	2.04	0.40
1:F:533:LEU:HD23	1:F:659:LEU:HD11	2.03	0.40
1:D:634:ARG:NH2	1:D:634:ARG:HG3	2.35	0.40
1:C:598:ASP:HA	1:C:599:PRO:HD2	1.94	0.40
1:F:273:LEU:CB	1:F:300:LEU:HD21	2.45	0.40
1:A:635:TRP:HB3	1:A:662:TYR:HB3	2.03	0.40
1:F:31:GLU:OE1	1:F:56:ARG:HD3	2.22	0.40
1:C:84:LEU:H	1:C:84:LEU:HD22	1.84	0.40
1:D:635:TRP:O	1:D:643:GLU:HA	2.22	0.40
1:E:324:THR:HG22	1:E:325:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

## 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	771/778 (99%)	716 (93%)	45 (6%)	10 (1%)	15	11
1	B	771/778 (99%)	712 (92%)	44 (6%)	15 (2%)	10	6
1	C	771/778 (99%)	716 (93%)	47 (6%)	8 (1%)	19	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	771/778 (99%)	709 (92%)	47 (6%)	15 (2%)	10	6
1	E	771/778 (99%)	709 (92%)	52 (7%)	10 (1%)	15	11
1	F	771/778 (99%)	709 (92%)	51 (7%)	11 (1%)	14	10
All	All	4626/4668 (99%)	4271 (92%)	286 (6%)	69 (2%)	13	9

All (69) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	767	ALA
1	B	764	GLN
1	B	766	ASN
1	C	766	ASN
1	C	767	ALA
1	D	517	ASN
1	D	764	GLN
1	A	480	GLY
1	A	681	VAL
1	B	276	SER
1	B	307	CYS
1	B	308	PHE
1	B	733	ASN
1	B	772	LEU
1	C	480	GLY
1	D	276	SER
1	D	546	ARG
1	D	720	GLY
1	D	772	LEU
1	E	720	GLY
1	E	764	GLN
1	E	767	ALA
1	F	77	ASN
1	F	767	ALA
1	F	768	LEU
1	A	692	ASN
1	A	768	LEU
1	B	476	PRO
1	C	431	SER
1	D	307	CYS
1	D	476	PRO
1	D	733	ASN
1	D	767	ALA

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Mol	Chain	Res	Type
1	E	44	ARG
1	E	316	CYS
1	F	308	PHE
1	F	552	ASP
1	A	277	PHE
1	A	476	PRO
1	B	214	GLN
1	B	316	CYS
1	B	431	SER
1	B	745	ASN
1	C	316	CYS
1	C	477	VAL
1	C	764	GLN
1	D	745	ASN
1	F	276	SER
1	F	692	ASN
1	A	308	PHE
1	A	316	CYS
1	A	477	VAL
1	B	477	VAL
1	B	480	GLY
1	C	308	PHE
1	D	380	TRP
1	D	477	VAL
1	E	417	PHE
1	E	477	VAL
1	E	766	ASN
1	F	316	CYS
1	E	277	PHE
1	F	476	PRO
1	F	477	VAL
1	D	328	PRO
1	F	720	GLY
1	D	742	VAL
1	E	476	PRO
1	B	328	PRO

### 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	659/665 (99%)	634 (96%)	25 (4%)	40	49
1	B	659/665 (99%)	643 (98%)	16 (2%)	57	69
1	C	659/665 (99%)	630 (96%)	29 (4%)	35	42
1	D	659/665 (99%)	630 (96%)	29 (4%)	35	42
1	E	659/665 (99%)	634 (96%)	25 (4%)	40	49
1	F	659/665 (99%)	635 (96%)	24 (4%)	42	52
All	All	3954/3990 (99%)	3806 (96%)	148 (4%)	41	50

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ASP
1	A	52	LEU
1	A	58	PHE
1	A	120	LEU
1	A	123	LEU
1	A	174	ARG
1	A	179	VAL
1	A	191	GLU
1	A	316	CYS
1	A	347	ASN
1	A	348	PRO
1	A	377	TRP
1	A	452	LEU
1	A	464	PHE
1	A	479	TRP
1	A	525	LYS
1	A	533	LEU
1	A	573	LEU
1	A	614	VAL
1	A	616	VAL
1	A	630	LEU
1	A	733	ASN
1	A	749	ASP
1	A	768	LEU
1	A	770	ILE
1	B	84	LEU
1	B	123	LEU

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Mol	Chain	Res	Type
1	B	146	GLN
1	B	179	VAL
1	B	208	VAL
1	B	227	LYS
1	B	285	THR
1	B	316	CYS
1	B	347	ASN
1	B	377	TRP
1	B	464	PHE
1	B	479	TRP
1	B	533	LEU
1	B	573	LEU
1	B	616	VAL
1	B	693	LEU
1	C	93	THR
1	C	120	LEU
1	C	123	LEU
1	C	174	ARG
1	C	179	VAL
1	C	208	VAL
1	C	276	SER
1	C	285	THR
1	C	306	ASP
1	C	316	CYS
1	C	347	ASN
1	C	348	PRO
1	C	377	TRP
1	C	452	LEU
1	C	459	GLU
1	C	464	PHE
1	C	479	TRP
1	C	510	HIS
1	C	525	LYS
1	C	533	LEU
1	C	573	LEU
1	C	579	ARG
1	C	592	MET
1	C	614	VAL
1	C	616	VAL
1	C	657	LEU
1	C	693	LEU
1	C	721	ASN

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Mol	Chain	Res	Type
1	C	770	ILE
1	D	52	LEU
1	D	69	ILE
1	D	143	THR
1	D	178	THR
1	D	179	VAL
1	D	208	VAL
1	D	289	PHE
1	D	300	LEU
1	D	306	ASP
1	D	316	CYS
1	D	347	ASN
1	D	348	PRO
1	D	352	GLN
1	D	377	TRP
1	D	459	GLU
1	D	464	PHE
1	D	477	VAL
1	D	510	HIS
1	D	527	TRP
1	D	533	LEU
1	D	537	SER
1	D	546	ARG
1	D	573	LEU
1	D	614	VAL
1	D	616	VAL
1	D	630	LEU
1	D	693	LEU
1	D	742	VAL
1	D	771	THR
1	E	45	THR
1	E	48	LEU
1	E	120	LEU
1	E	123	LEU
1	E	174	ARG
1	E	179	VAL
1	E	214	GLN
1	E	276	SER
1	E	282	ASP
1	E	300	LEU
1	E	316	CYS
1	E	377	TRP

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Mol	Chain	Res	Type
1	E	452	LEU
1	E	459	GLU
1	E	464	PHE
1	E	479	TRP
1	E	537	SER
1	E	573	LEU
1	E	614	VAL
1	E	616	VAL
1	E	630	LEU
1	E	653	GLN
1	E	723	ILE
1	E	735	THR
1	E	756	GLU
1	F	123	LEU
1	F	143	THR
1	F	174	ARG
1	F	178	THR
1	F	189	SER
1	F	214	GLN
1	F	306	ASP
1	F	316	CYS
1	F	347	ASN
1	F	348	PRO
1	F	377	TRP
1	F	452	LEU
1	F	459	GLU
1	F	464	PHE
1	F	533	LEU
1	F	537	SER
1	F	573	LEU
1	F	579	ARG
1	F	616	VAL
1	F	630	LEU
1	F	693	LEU
1	F	714	LEU
1	F	770	ILE
1	F	771	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS

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Mol	Chain	Res	Type
1	A	27	GLN
1	A	73	GLN
1	A	77	ASN
1	A	88	GLN
1	A	107	ASN
1	A	125	ASN
1	A	133	GLN
1	A	212	HIS
1	A	287	ASN
1	A	347	ASN
1	A	564	GLN
1	A	652	GLN
1	A	692	ASN
1	A	697	HIS
1	B	27	GLN
1	B	28	GLN
1	B	61	GLN
1	B	141	GLN
1	B	146	GLN
1	B	177	GLN
1	B	212	HIS
1	B	347	ASN
1	B	564	GLN
1	B	652	GLN
1	B	692	ASN
1	B	697	HIS
1	B	733	ASN
1	B	745	ASN
1	B	764	GLN
1	C	21	GLN
1	C	27	GLN
1	C	77	ASN
1	C	107	ASN
1	C	133	GLN
1	C	146	GLN
1	C	177	GLN
1	C	347	ASN
1	C	361	GLN
1	C	517	ASN
1	C	564	GLN
1	C	652	GLN
1	C	692	ASN

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Mol	Chain	Res	Type
1	C	697	HIS
1	C	721	ASN
1	C	733	ASN
1	D	7	ASN
1	D	21	GLN
1	D	27	GLN
1	D	107	ASN
1	D	133	GLN
1	D	146	GLN
1	D	381	GLN
1	D	652	GLN
1	D	697	HIS
1	D	733	ASN
1	E	11	GLN
1	E	21	GLN
1	E	27	GLN
1	E	47	GLN
1	E	73	GLN
1	E	77	ASN
1	E	107	ASN
1	E	146	GLN
1	E	192	GLN
1	E	280	ASN
1	E	652	GLN
1	E	697	HIS
1	E	733	ASN
1	E	745	ASN
1	E	764	GLN
1	F	27	GLN
1	F	73	GLN
1	F	77	ASN
1	F	107	ASN
1	F	177	GLN
1	F	280	ASN
1	F	347	ASN
1	F	652	GLN
1	F	653	GLN
1	F	692	ASN
1	F	697	HIS
1	F	733	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

21 ligands are modelled in this entry.

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	SO4	A	3012	-	4,4,4	3.26	2 (50%)	6,6,6	0.97	0
2	SO4	A	3013	-	4,4,4	3.30	2 (50%)	6,6,6	0.95	0
3	XYF	A	801	1	10,10,11	1.69	3 (30%)	14,14,16	0.69	0
4	MPO	B	2001	-	12,13,13	1.21	1 (8%)	15,17,17	2.37	5 (33%)
2	SO4	B	3008	-	4,4,4	3.25	2 (50%)	6,6,6	0.97	0
2	SO4	B	3010	-	4,4,4	3.30	2 (50%)	6,6,6	0.98	0
3	XYF	B	802	1	10,10,11	1.65	3 (30%)	14,14,16	0.71	0
4	MPO	C	2002	-	12,13,13	1.22	1 (8%)	15,17,17	2.32	5 (33%)
2	SO4	C	3007	-	4,4,4	3.24	2 (50%)	6,6,6	0.98	0
2	SO4	C	3011	-	4,4,4	3.21	2 (50%)	6,6,6	1.00	0
3	XYF	C	803	1	10,10,11	1.67	3 (30%)	14,14,16	0.74	0
4	MPO	D	2003	-	12,13,13	1.20	1 (8%)	15,17,17	2.27	5 (33%)
2	SO4	D	3004	-	4,4,4	3.36	2 (50%)	6,6,6	0.94	0
4	MPO	E	2004	-	12,13,13	1.23	1 (8%)	15,17,17	2.29	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	E	3006	-	4,4,4	3.30	2 (50%)	6,6,6	0.94	0
3	XYF	E	804	1	10,10,11	1.66	3 (30%)	14,14,16	0.66	0
2	SO4	F	3001	-	4,4,4	3.25	2 (50%)	6,6,6	0.96	0
2	SO4	F	3002	-	4,4,4	3.26	2 (50%)	6,6,6	0.98	0
2	SO4	F	3003	-	4,4,4	3.33	2 (50%)	6,6,6	0.99	0
2	SO4	F	3005	-	4,4,4	3.26	2 (50%)	6,6,6	0.93	0
2	SO4	F	3009	-	4,4,4	3.29	2 (50%)	6,6,6	0.98	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	SO4	A	3012	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3013	-	-	0/0/0/0	0/0/0/0
3	XYF	A	801	1	-	0/0/17/20	0/1/1/1
4	MPO	B	2001	-	-	0/7/15/15	0/1/1/1
2	SO4	B	3008	-	-	0/0/0/0	0/0/0/0
2	SO4	B	3010	-	-	0/0/0/0	0/0/0/0
3	XYF	B	802	1	-	0/0/17/20	0/1/1/1
4	MPO	C	2002	-	-	0/7/15/15	0/1/1/1
2	SO4	C	3007	-	-	0/0/0/0	0/0/0/0
2	SO4	C	3011	-	-	0/0/0/0	0/0/0/0
3	XYF	C	803	1	-	0/0/17/20	0/1/1/1
4	MPO	D	2003	-	-	0/7/15/15	0/1/1/1
2	SO4	D	3004	-	-	0/0/0/0	0/0/0/0
4	MPO	E	2004	-	-	0/7/15/15	0/1/1/1
2	SO4	E	3006	-	-	0/0/0/0	0/0/0/0
3	XYF	E	804	1	-	0/0/17/20	0/1/1/1
2	SO4	F	3001	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3002	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3003	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3005	-	-	0/0/0/0	0/0/0/0
2	SO4	F	3009	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3003	SO4	O3-S	-4.71	1.30	1.47
2	D	3004	SO4	O3-S	-4.67	1.30	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3006	SO4	O3-S	-4.61	1.30	1.47
2	B	3010	SO4	O3-S	-4.60	1.30	1.47
2	A	3013	SO4	O3-S	-4.58	1.30	1.47
2	F	3005	SO4	O3-S	-4.58	1.30	1.47
2	F	3009	SO4	O3-S	-4.57	1.31	1.47
2	F	3001	SO4	O3-S	-4.55	1.31	1.47
2	F	3002	SO4	O3-S	-4.55	1.31	1.47
2	C	3007	SO4	O3-S	-4.55	1.31	1.47
2	A	3012	SO4	O3-S	-4.53	1.31	1.47
2	C	3011	SO4	O3-S	-4.53	1.31	1.47
2	B	3008	SO4	O3-S	-4.48	1.31	1.47
3	E	804	XYF	F5-C5	-3.08	1.35	1.39
3	C	803	XYF	F5-C5	-3.05	1.35	1.39
3	A	801	XYF	F5-C5	-3.04	1.35	1.39
3	B	802	XYF	F5-C5	-3.03	1.35	1.39
4	D	2003	MPO	C4-N1	2.15	1.52	1.46
4	C	2002	MPO	C4-N1	2.26	1.53	1.46
4	E	2004	MPO	C4-N1	2.26	1.53	1.46
3	B	802	XYF	C4-C5	2.27	1.53	1.52
4	B	2001	MPO	C4-N1	2.30	1.53	1.46
3	E	804	XYF	C4-C5	2.34	1.53	1.52
3	C	803	XYF	C4-C5	2.40	1.53	1.52
3	A	801	XYF	C4-C5	2.54	1.53	1.52
3	E	804	XYF	O5-C5	3.35	1.44	1.39
3	A	801	XYF	O5-C5	3.37	1.44	1.39
3	C	803	XYF	O5-C5	3.40	1.44	1.39
3	B	802	XYF	O5-C5	3.41	1.44	1.39
2	C	3011	SO4	O1-S	4.44	1.62	1.47
2	C	3007	SO4	O1-S	4.51	1.62	1.47
2	F	3005	SO4	O1-S	4.56	1.62	1.47
2	F	3001	SO4	O1-S	4.56	1.62	1.47
2	F	3002	SO4	O1-S	4.58	1.62	1.47
2	B	3008	SO4	O1-S	4.59	1.62	1.47
2	E	3006	SO4	O1-S	4.60	1.62	1.47
2	A	3012	SO4	O1-S	4.61	1.62	1.47
2	F	3003	SO4	O1-S	4.62	1.63	1.47
2	B	3010	SO4	O1-S	4.64	1.63	1.47
2	F	3009	SO4	O1-S	4.64	1.63	1.47
2	A	3013	SO4	O1-S	4.65	1.63	1.47
2	D	3004	SO4	O1-S	4.70	1.63	1.47

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	MPO	C3-C2-C1	-4.62	104.76	112.37
4	E	2004	MPO	C3-C2-C1	-4.50	104.96	112.37
4	D	2003	MPO	C3-C2-C1	-4.44	105.06	112.37
4	C	2002	MPO	C3-C2-C1	-4.37	105.17	112.37
4	D	2003	MPO	C5-C4-N1	-2.39	106.51	110.12
4	C	2002	MPO	C5-C4-N1	-2.34	106.57	110.12
4	E	2004	MPO	C2-C3-N1	-2.33	108.04	113.89
4	D	2003	MPO	C2-C3-N1	-2.32	108.06	113.89
4	B	2001	MPO	C2-C3-N1	-2.31	108.08	113.89
4	C	2002	MPO	C2-C3-N1	-2.24	108.27	113.89
4	B	2001	MPO	C5-C4-N1	-2.21	106.78	110.12
4	E	2004	MPO	C5-C4-N1	-2.20	106.78	110.12
4	D	2003	MPO	O2-S1-C1	3.88	110.22	106.91
4	B	2001	MPO	O2-S1-C1	3.97	110.29	106.91
4	C	2002	MPO	O2-S1-C1	4.05	110.36	106.91
4	E	2004	MPO	O2-S1-C1	4.07	110.38	106.91
4	D	2003	MPO	O1-S1-C1	4.41	110.67	106.91
4	E	2004	MPO	O1-S1-C1	4.50	110.75	106.91
4	C	2002	MPO	O1-S1-C1	4.81	111.01	106.91
4	B	2001	MPO	O1-S1-C1	5.03	111.19	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	XYF	2	0
3	B	802	XYF	1	0
2	C	3011	SO4	1	0
3	C	803	XYF	2	0
2	E	3006	SO4	1	0
3	E	804	XYF	2	0
2	F	3005	SO4	2	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	773/778 (99%)	-0.04	17 (2%) 65 64	16, 28, 48, 76	0
1	B	773/778 (99%)	0.25	53 (6%) 20 19	20, 36, 61, 82	0
1	C	773/778 (99%)	-0.01	19 (2%) 61 60	17, 29, 50, 72	0
1	D	773/778 (99%)	0.21	54 (6%) 19 19	17, 31, 63, 84	0
1	E	773/778 (99%)	0.04	29 (3%) 44 43	18, 32, 55, 90	0
1	F	773/778 (99%)	0.17	34 (4%) 38 37	19, 30, 55, 77	0
All	All	4638/4668 (99%)	0.10	206 (4%) 38 37	16, 31, 56, 90	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	719	THR	9.1
1	B	767	ALA	9.0
1	E	46	TRP	8.1
1	B	766	ASN	7.8
1	D	382	PRO	7.5
1	F	766	ASN	7.4
1	C	766	ASN	7.2
1	D	277	PHE	7.1
1	E	43	GLU	7.0
1	E	766	ASN	7.0
1	B	765	GLY	6.5
1	D	278	THR	6.5
1	D	540	HIS	6.2
1	D	545	TYR	6.2
1	D	766	ASN	6.2
1	D	279	THR	6.1
1	E	42	ARG	5.8
1	D	765	GLY	5.4
1	E	765	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	541	GLY	5.2
1	F	765	GLY	5.1
1	A	766	ASN	5.1
1	C	765	GLY	5.1
1	D	546	ARG	5.0
1	F	748	GLN	5.0
1	D	281	TYR	4.9
1	C	767	ALA	4.8
1	B	719	THR	4.7
1	D	747	LEU	4.7
1	E	47	GLN	4.6
1	A	765	GLY	4.5
1	D	380	TRP	4.5
1	F	749	ASP	4.4
1	D	767	ALA	4.3
1	F	768	LEU	4.3
1	A	719	THR	4.3
1	F	770	ILE	4.3
1	C	748	GLN	4.2
1	A	768	LEU	4.2
1	D	748	GLN	4.2
1	B	768	LEU	4.1
1	F	772	LEU	4.1
1	B	753	ALA	4.0
1	F	767	ALA	4.0
1	D	764	GLN	4.0
1	E	49	ASP	4.0
1	C	770	ILE	4.0
1	E	767	ALA	3.9
1	D	477	VAL	3.9
1	B	744	VAL	3.8
1	B	407	ALA	3.8
1	B	722	THR	3.7
1	B	323	LEU	3.7
1	D	768	LEU	3.6
1	B	29	ASP	3.6
1	D	275	THR	3.6
1	D	381	GLN	3.6
1	D	276	SER	3.6
1	D	743	LYS	3.6
1	D	383	GLY	3.6
1	B	764	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	88	GLN	3.5
1	D	763	PRO	3.5
1	D	750	GLY	3.4
1	A	477	VAL	3.3
1	C	719	THR	3.3
1	D	280	ASN	3.3
1	F	724	THR	3.3
1	B	742	VAL	3.3
1	E	117	PHE	3.3
1	E	44	ARG	3.3
1	F	545	TYR	3.3
1	B	756	GLU	3.3
1	B	745	ASN	3.2
1	D	542	SER	3.2
1	B	338	LYS	3.2
1	B	738	LEU	3.2
1	A	88	GLN	3.2
1	D	762	LYS	3.1
1	B	736	LEU	3.1
1	F	88	GLN	3.1
1	B	477	VAL	3.1
1	D	753	ALA	3.1
1	D	742	VAL	3.1
1	B	88	GLN	3.0
1	B	325	PHE	3.0
1	B	295	GLU	3.0
1	E	477	VAL	3.0
1	E	41	VAL	3.0
1	E	40	ASP	2.9
1	B	545	TYR	2.9
1	D	543	LYS	2.9
1	D	745	ASN	2.9
1	F	695	ASP	2.9
1	E	45	THR	2.9
1	B	772	LEU	2.9
1	F	745	ASN	2.9
1	B	337	ALA	2.8
1	E	764	GLN	2.8
1	B	723	ILE	2.8
1	B	549	TRP	2.8
1	B	327	ASP	2.8
1	F	756	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	745	ASN	2.8
1	C	744	VAL	2.8
1	E	745	ASN	2.7
1	B	748	GLN	2.7
1	B	770	ILE	2.7
1	D	289	PHE	2.7
1	D	723	ILE	2.7
1	A	767	ALA	2.7
1	A	744	VAL	2.7
1	C	772	LEU	2.6
1	E	89	ASP	2.6
1	B	743	LYS	2.6
1	D	517	ASN	2.6
1	B	761	VAL	2.6
1	C	773	HIS	2.6
1	F	747	LEU	2.6
1	D	306	ASP	2.6
1	E	719	THR	2.6
1	C	46	TRP	2.6
1	F	762	LYS	2.6
1	D	749	ASP	2.6
1	E	706	ALA	2.6
1	B	759	LEU	2.6
1	E	772	LEU	2.5
1	F	754	GLU	2.5
1	E	723	ILE	2.5
1	F	29	ASP	2.5
1	B	333	ARG	2.5
1	C	756	GLU	2.5
1	C	768	LEU	2.5
1	F	771	THR	2.5
1	C	477	VAL	2.5
1	E	98	GLU	2.5
1	A	721	ASN	2.5
1	D	759	LEU	2.5
1	D	307	CYS	2.5
1	D	772	LEU	2.5
1	F	759	LEU	2.5
1	E	540	HIS	2.4
1	D	378	ASP	2.4
1	B	726	THR	2.4
1	D	756	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	290	ILE	2.4
1	B	757	GLN	2.4
1	F	550	ALA	2.4
1	E	39	ARG	2.4
1	A	29	ASP	2.4
1	D	544	SER	2.4
1	F	547	VAL	2.4
1	D	88	GLN	2.4
1	D	513	GLY	2.3
1	C	742	VAL	2.3
1	B	30	ASN	2.3
1	C	88	GLN	2.3
1	F	723	ILE	2.3
1	F	746	GLY	2.3
1	D	514	GLY	2.3
1	F	738	LEU	2.3
1	D	483	CYS	2.3
1	A	742	VAL	2.3
1	F	277	PHE	2.3
1	F	515	PHE	2.3
1	A	772	LEU	2.3
1	E	743	LYS	2.3
1	B	758	GLY	2.2
1	B	741	VAL	2.2
1	D	741	VAL	2.2
1	D	377	TRP	2.2
1	B	286	VAL	2.2
1	B	91	LYS	2.2
1	A	749	ASP	2.2
1	D	333	ARG	2.2
1	B	762	LYS	2.2
1	F	742	VAL	2.2
1	B	339	GLY	2.2
1	D	755	SER	2.2
1	F	764	GLN	2.2
1	B	721	ASN	2.2
1	E	50	THR	2.2
1	D	770	ILE	2.1
1	E	76	LEU	2.1
1	B	332	ILE	2.1
1	C	764	GLN	2.1
1	F	750	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	316	CYS	2.1
1	F	733	ASN	2.1
1	B	725	VAL	2.1
1	B	204	ARG	2.1
1	C	98	GLU	2.1
1	A	30	ASN	2.1
1	B	329	GLU	2.1
1	A	100	TYR	2.1
1	B	553	ASP	2.1
1	B	356	VAL	2.1
1	B	319	GLU	2.1
1	D	754	GLU	2.1
1	E	52	LEU	2.1
1	D	424	ASP	2.1
1	B	328	PRO	2.1
1	C	669	LEU	2.0
1	F	743	LYS	2.0
1	A	89	ASP	2.0
1	F	540	HIS	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( $\text{\AA}^2$ )	Q<0.9
2	SO4	F	3001	5/5	0.77	0.20	5.85	91,91,91,92	0
3	XYF	C	803	10/11	0.85	0.19	2.75	33,36,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	XYF	E	804	10/11	0.88	0.25	1.94	25,26,27,29	10
4	MPO	E	2004	13/13	0.91	0.16	1.93	53,55,57,58	0
4	MPO	D	2003	13/13	0.95	0.20	0.96	53,57,63,63	0
4	MPO	B	2001	13/13	0.88	0.17	0.88	68,68,69,69	0
2	SO4	F	3005	5/5	0.92	0.15	0.82	58,58,59,59	0
4	MPO	C	2002	13/13	0.92	0.14	0.51	52,57,61,62	0
3	XYF	B	802	10/11	0.85	0.15	0.41	37,41,43,45	0
3	XYF	A	801	10/11	0.93	0.10	-1.07	35,36,38,39	0
2	SO4	C	3007	5/5	0.96	0.21	-	75,76,76,77	0
2	SO4	D	3004	5/5	0.94	0.18	-	75,75,75,75	0
2	SO4	B	3010	5/5	0.86	0.20	-	88,89,89,90	0
2	SO4	A	3012	5/5	0.76	0.17	-	87,87,88,88	0
2	SO4	F	3003	5/5	0.93	0.19	-	67,68,69,69	0
2	SO4	C	3011	5/5	0.78	0.29	-	105,106,106,106	0
2	SO4	A	3013	5/5	0.94	0.12	-	77,77,78,78	0
2	SO4	F	3009	5/5	0.84	0.23	-	91,91,92,92	0
2	SO4	B	3008	5/5	0.95	0.15	-	72,72,72,73	0
2	SO4	E	3006	5/5	0.93	0.17	-	84,84,85,85	0
2	SO4	F	3002	5/5	0.94	0.16	-	76,77,77,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.