



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:37 AM GMT

PDB ID : 2RFZ  
Title : Crystal structure of cellobiohydrolase from *Melanocarpus albomyces* complexed with cellotriose  
Authors : Parkkinen, T.; Koivula, A.; Vehmaanper, J.; Rouvinen, J.  
Deposited on : 2007-10-02  
Resolution : 1.80 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

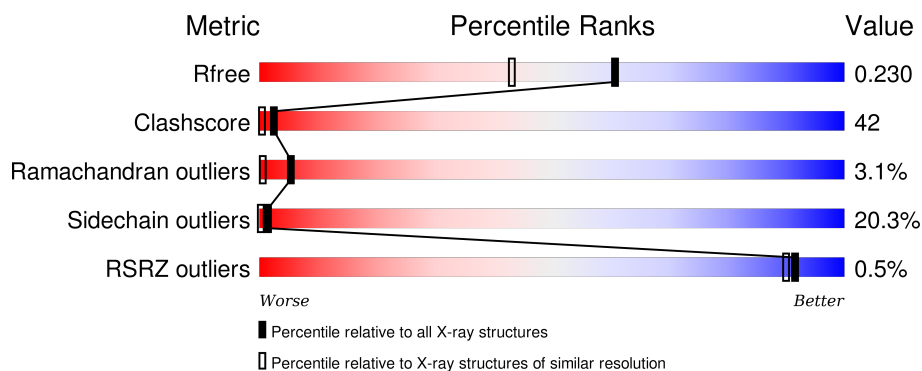
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	430	<div> <div>23%</div> <div>56%</div> <div>20%</div> <div>.</div> </div>
1	B	430	<div> <div>33%</div> <div>49%</div> <div>17%</div> <div>.</div> </div>
1	C	430	<div> <div>40%</div> <div>47%</div> <div>13%</div> <div>.</div> </div>
1	D	430	<div> <div>43%</div> <div>46%</div> <div>10%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	PCA	A	1	-	-	X	-
2	CTR	A	431	X	-	-	-
2	CTR	A	432	X	-	-	-
2	CTR	B	431	X	-	-	-
2	CTR	C	431	X	-	-	-
2	CTR	C	432	X	-	-	-
2	CTR	D	431	X	-	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14399 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.

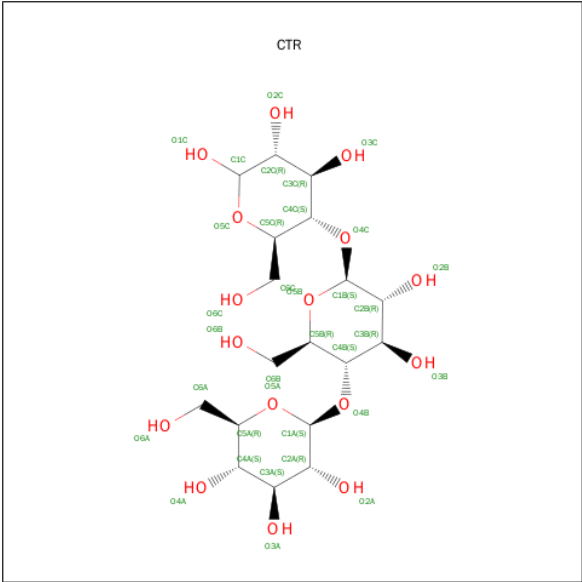
- Molecule 1 is a protein called Cellulose 1,4-beta-cellobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	B	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	C	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			
1	D	430	Total	C	N	O	S	0	0	0
			3333	2075	558	669	31			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
B	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
C	1	PCA	GLN	ENGINEERED	UNP Q8J0K6
D	1	PCA	GLN	ENGINEERED	UNP Q8J0K6

- Molecule 2 is SUGAR (CELLOTRIOSE) (three-letter code: CTR) (formula: C<sub>18</sub>H<sub>32</sub>O<sub>16</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			34	18	16		
2	A	1	Total	C	O	0	0
			34	18	16		
2	B	1	Total	C	O	0	0
			34	18	16		
2	C	1	Total	C	O	0	0
			34	18	16		
2	C	1	Total	C	O	0	0
			34	18	16		
2	D	1	Total	C	O	0	0
			34	18	16		

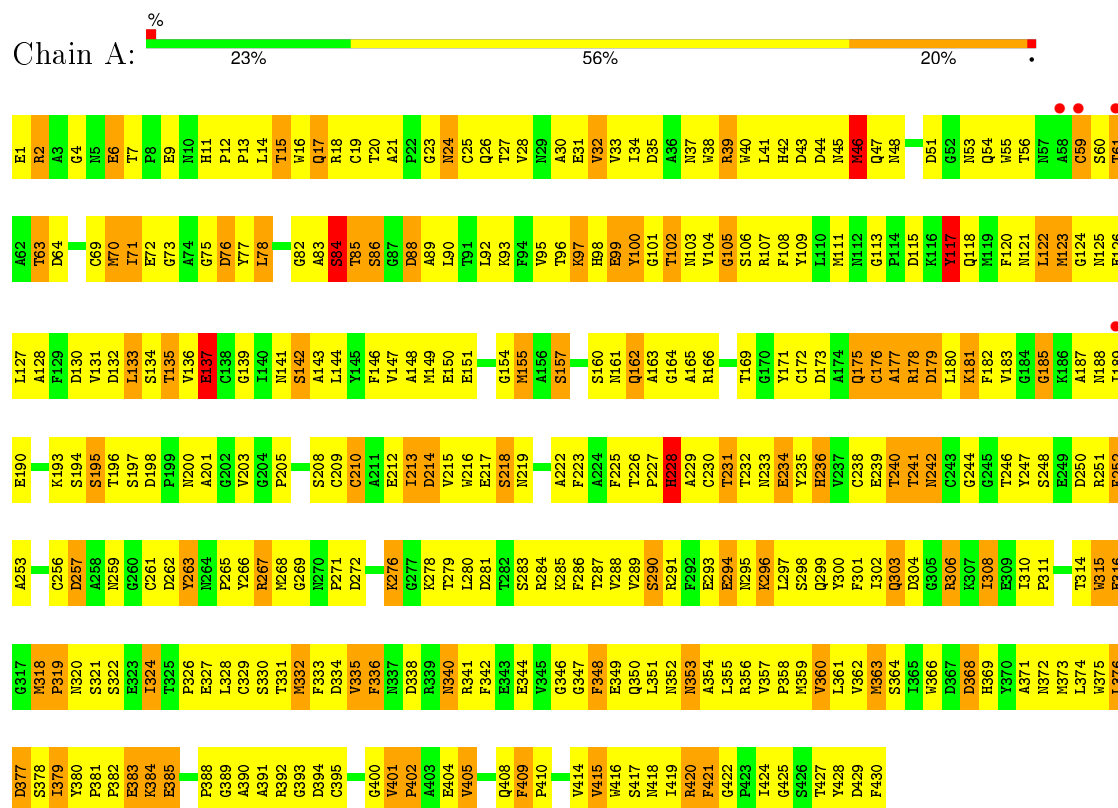
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	202	Total	O	0	0
			202	202		
3	B	191	Total	O	0	0
			191	191		
3	C	225	Total	O	0	0
			225	225		
3	D	245	Total	O	0	0
			245	245		

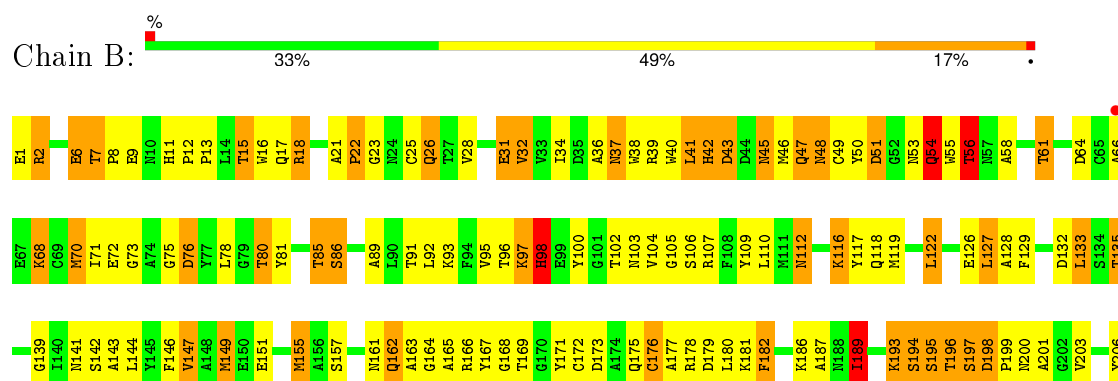
### 3 Residue-property plots

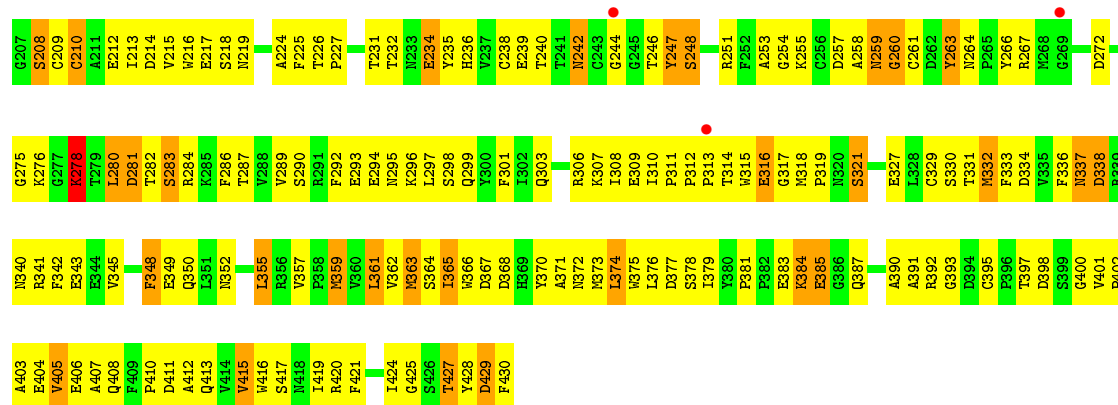
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Cellulose 1,4-beta-cellobiosidase

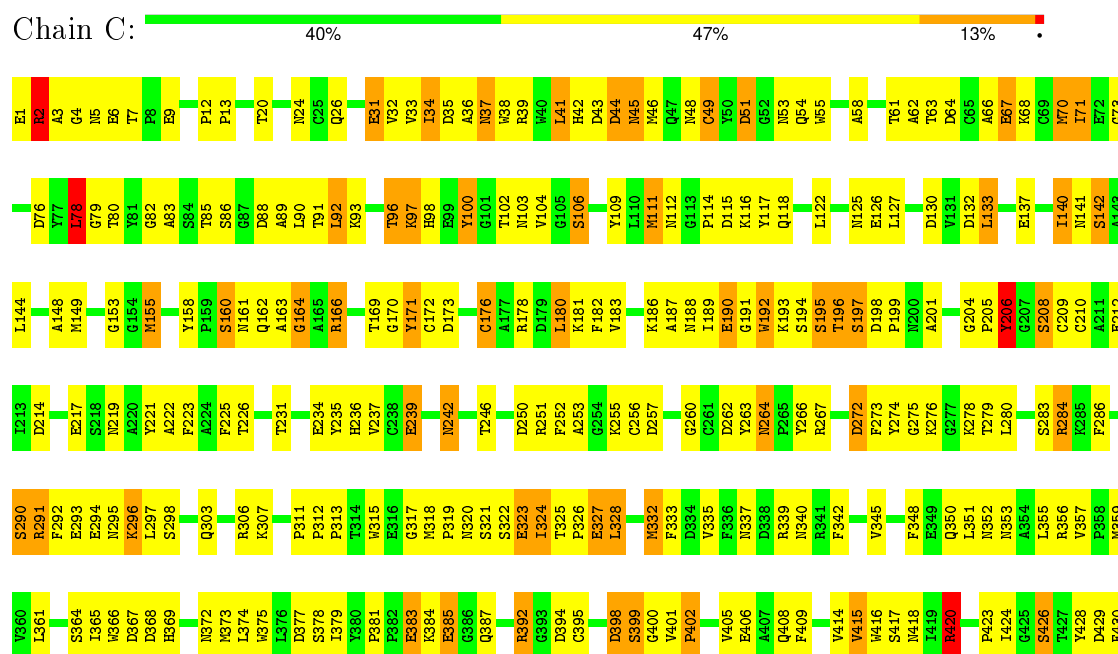


- Molecule 1: Cellulose 1,4-beta-cellobiosidase

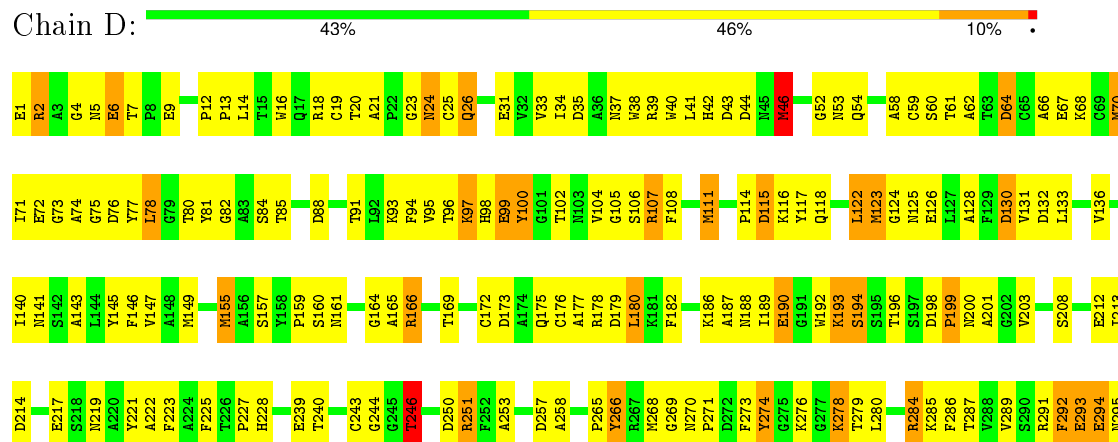




• Molecule 1: Cellulose 1,4-beta-cellobiosidase



• Molecule 1: Cellulose 1,4-beta-cellobiosidase



K296	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K400	K401	K402	K405	K406	K407	K408	K409	K410	K413	K414	K415	K418	K423	K424	K425	K426	K427	K428	K430
L297	L382	L383	L384	L385	L386	L387	L388	L389	L390	L391	L392	L393	L394	L395	L400	L401	L402	L405	L406	L407	L408	L409	L410	L413	L414	L415	L418	L423	L424	L425	L426	L427	L428	L430
S298	S383	S384	S385	S386	S387	S388	S389	S390	S391	S392	S393	S394	S395	S396	S400	S401	S402	S405	S406	S407	S408	S409	S410	S413	S414	S415	S418	S423	S424	S425	S426	S427	S428	S430
I302	I303	I304	I305	I306	I307	I308	I309	I310	I311	I312	I313	I314	I315	I322	I327	I331	I332	I333	I334	I335	I336	I337	I338	I339	I340	I341	I344	I345	I348	I349	I350	I351	I352	
D304	D305	D306	D307	D308	D309	D310	D311	D312	D313	D314	D315	D322	D327	D331	D332	D333	D334	D335	D336	D337	D338	D339	D340	D341	D344	D345	D348	D349	D350	D351	D352	D355		
F348	F349	F350	F351	F352	F355	F359	F364	F365	F366	F367	F368	F369	F370	F371	F372	F373	F374	F375	F376	F377	F378	F379	F380	F381	F382	F383	F384	F385	F386	F387	F388	F389	F390	



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.80Å 94.37Å 189.91Å 90.00° 90.19° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 24.53 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.8 (20.00-1.80) 96.6 (24.53-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.03 (at 1.80Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.261 , 0.237 0.190 , 0.230	Depositor DCC
$R_{free}$ test set	8081 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	12.8	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 70.5	EDS
Estimated twinning fraction	0.427 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	3 of 161992 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14399	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.69% 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: PCA, CTR

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	0.36	0/3416	1.09	11/4648 (0.2%)
1	B	0.36	0/3416	1.12	10/4648 (0.2%)
1	C	0.37	0/3416	1.16	10/4648 (0.2%)
1	D	0.38	0/3416	1.15	14/4648 (0.3%)
All	All	0.37	0/13664	1.13	45/18592 (0.2%)

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	58	ALA	C-N-CA	10.35	147.57	121.70
1	D	166	ARG	NE-CZ-NH1	-9.23	115.68	120.30
1	D	107	ARG	NE-CZ-NH1	-8.17	116.21	120.30
1	B	306	ARG	CD-NE-CZ	7.89	134.65	123.60
1	C	392	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	B	341	ARG	CD-NE-CZ	7.31	133.83	123.60
1	C	2	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	A	256	CYS	C-N-CA	6.80	138.70	121.70
1	A	324	ILE	C-N-CA	6.76	138.61	121.70
1	C	206	TYR	CB-CG-CD2	6.69	125.01	121.00
1	A	231	THR	C-N-CA	6.64	138.29	121.70
1	D	368	ASP	CB-CG-OD1	6.57	124.21	118.30
1	B	341	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	D	339	ARG	CD-NE-CZ	6.47	132.65	123.60
1	B	306	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	A	142	SER	C-N-CA	6.32	137.49	121.70
1	D	274	TYR	CB-CG-CD2	6.30	124.78	121.00
1	D	130	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	42	HIS	C-N-CA	6.14	137.06	121.70
1	D	284	ARG	NE-CZ-NH1	6.07	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	218	SER	C-N-CA	5.97	136.62	121.70
1	B	411	ASP	CB-CG-OD1	5.94	123.65	118.30
1	B	263	TYR	C-N-CA	5.88	136.41	121.70
1	D	274	TYR	CA-CB-CG	5.82	124.46	113.40
1	A	228	HIS	CA-CB-CG	5.78	123.43	113.60
1	C	420	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	54	GLN	C-N-CA	5.73	136.04	121.70
1	A	353	ASN	C-N-CA	5.69	135.94	121.70
1	C	160	SER	C-N-CA	5.59	135.68	121.70
1	D	173	ASP	CB-CG-OD2	5.59	123.33	118.30
1	D	266	TYR	CB-CG-CD1	5.59	124.35	121.00
1	C	171	TYR	CB-CG-CD2	5.54	124.32	121.00
1	D	284	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	A	117	TYR	CA-CB-CG	5.51	123.86	113.40
1	C	420	ARG	CD-NE-CZ	5.47	131.26	123.60
1	C	178	ARG	NE-CZ-NH2	5.31	122.96	120.30
1	B	341	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	C	290	SER	C-N-CA	5.23	134.77	121.70
1	A	263	TYR	C-N-CA	5.23	134.76	121.70
1	A	84	SER	C-N-CA	5.22	134.74	121.70
1	A	137	GLU	C-N-CA	5.18	134.65	121.70
1	D	166	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	D	111	MET	C-N-CA	5.15	134.57	121.70
1	C	206	TYR	CA-CB-CG	5.07	123.03	113.40
1	B	97	LYS	C-N-CA	5.03	134.27	121.70

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	3333	0	3028	345	0
1	B	3333	0	3028	288	0
1	C	3333	0	3028	239	0
1	D	3333	0	3027	239	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	68	0	64	15	0
2	B	34	0	32	5	0
2	C	68	0	64	9	0
2	D	34	0	32	5	0
3	A	202	0	0	18	0
3	B	191	0	0	15	0
3	C	225	0	0	19	0
3	D	245	0	0	19	0
All	All	14399	0	12303	1087	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 42.

All (1087) 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:97:LYS:HD3	1:D:6:GLU:HG3	1.38	1.01
1:A:128:ALA:HB2	1:A:289:VAL:HG13	1.44	1.00
1:D:123:MET:HE2	1:D:294:GLU:H	1.25	0.98
1:C:298:SER:HB3	1:C:323:GLU:HG3	1.49	0.95
1:C:132:ASP:HB3	1:C:415:VAL:HG13	1.49	0.93
1:B:36:ALA:HA	1:B:39:ARG:HD2	1.51	0.92
1:D:115:ASP:HA	1:D:166:ARG:HG2	1.52	0.92
1:D:95:VAL:HG22	1:D:104:VAL:HG22	1.55	0.89
1:A:175:GLN:HG3	2:A:431:CTR:H3A	1.54	0.88
1:A:373:MET:HG3	1:A:376:LEU:HD23	1.54	0.88
1:B:17:GLN:HB2	1:B:420:ARG:HG2	1.57	0.87
1:B:177:ALA:HB1	1:B:180:LEU:HG	1.57	0.86
1:B:214:ASP:HB2	1:B:226:THR:HB	1.58	0.85
1:B:374:LEU:HD13	1:B:378:SER:HB3	1.60	0.84
1:B:171:TYR:HB3	1:B:180:LEU:HD11	1.58	0.84
1:D:291:ARG:HH11	1:D:424:ILE:HG23	1.45	0.82
1:B:319:PRO:HG3	1:B:327:GLU:HG3	1.61	0.82
1:A:263:TYR:HB2	1:A:324:ILE:HD11	1.61	0.82
1:C:272:ASP:HA	1:C:278:LYS:HE2	1.61	0.82
1:A:2:ARG:HG2	1:A:162:GLN:HE21	1.45	0.81
1:C:82:GLY:HA3	1:C:93:LYS:HB2	1.62	0.81
1:A:77:TYR:HB3	1:A:83:ALA:HB3	1.60	0.81
1:C:368:ASP:HB2	1:C:373:MET:HE2	1.61	0.81
1:C:34:ILE:HG23	1:C:39:ARG:HE	1.45	0.80
1:D:147:VAL:HG23	1:D:149:MET:HG3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LEU:HD11	1:B:397:THR:HA	1.63	0.79
1:A:155:MET:HE1	1:A:166:ARG:HE	1.48	0.78
1:A:76:ASP:HB2	1:D:76:ASP:HB3	1.63	0.78
1:B:139:GLY:HA3	1:B:400:GLY:HA2	1.65	0.78
1:C:92:LEU:HD13	1:C:106:SER:OG	1.83	0.78
1:B:91:THR:HG23	1:B:415:VAL:HG13	1.64	0.77
1:A:13:PRO:HA	1:A:31:GLU:HA	1.65	0.77
1:D:295:ASN:H	1:D:352:ASN:HD21	1.32	0.77
1:A:178:ARG:HG3	1:A:247:TYR:HB2	1.67	0.77
1:A:21:ALA:HB3	1:B:116:LYS:HE2	1.66	0.77
1:B:177:ALA:HB3	1:B:208:SER:OG	1.84	0.77
1:A:6:GLU:HB2	1:A:72:GLU:OE2	1.84	0.76
1:D:122:LEU:HD23	1:D:355:LEU:HD22	1.67	0.76
1:A:78:LEU:HD12	1:D:75:GLY:HA2	1.67	0.76
1:B:76:ASP:HB3	1:C:76:ASP:OD2	1.86	0.76
1:A:269:GLY:HA3	1:A:314:THR:OG1	1.84	0.76
1:D:155:MET:HG2	1:D:161:ASN:O	1.85	0.76
1:B:231:THR:OG1	1:B:255:LYS:HB3	1.86	0.75
1:C:195:SER:HB2	1:C:201:ALA:O	1.86	0.75
1:C:67:GLU:HG3	3:C:471:HOH:O	1.87	0.75
1:B:53:ASN:HB2	1:B:201:ALA:O	1.87	0.75
1:B:98:HIS:HA	1:C:7:THR:OG1	1.86	0.75
1:D:287:THR:HB	1:D:302:ILE:HB	1.69	0.74
1:A:18:ARG:HD2	3:A:515:HOH:O	1.87	0.74
1:D:62:ALA:HA	1:D:187:ALA:HB3	1.70	0.74
1:B:379:ILE:HA	1:B:390:ALA:O	1.88	0.74
1:D:198:ASP:HB3	1:D:201:ALA:HB3	1.69	0.74
1:B:234:GLU:HG3	3:B:644:HOH:O	1.88	0.73
1:B:155:MET:HG2	1:B:161:ASN:O	1.88	0.73
1:C:384:LYS:O	1:C:387:GLN:HG3	1.88	0.73
1:C:327:GLU:HG3	3:C:615:HOH:O	1.88	0.73
1:A:177:ALA:HB3	1:A:208:SER:OG	1.88	0.73
1:C:2:ARG:HG3	1:C:70:MET:HA	1.69	0.73
1:A:124:GLY:O	1:A:424:ILE:HG13	1.89	0.73
1:B:112:ASN:ND2	1:B:116:LYS:HB2	2.04	0.72
1:C:166:ARG:HD2	3:C:581:HOH:O	1.89	0.72
1:A:238:CYS:HB2	1:A:242:ASN:O	1.89	0.72
1:B:259:ASN:HB3	2:B:431:CTR:H5C	1.70	0.72
1:A:147:VAL:HG12	1:A:212:GLU:HG3	1.72	0.72
1:B:112:ASN:HB3	1:B:118:GLN:HA	1.71	0.72
1:C:372:ASN:HB3	1:C:400:GLY:HA3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:LEU:HA	1:C:70:MET:O	1.89	0.72
1:A:401:VAL:HB	1:A:404:GLU:HG3	1.70	0.72
1:B:37:ASN:OD1	1:B:180:LEU:HD22	1.88	0.72
1:B:372:ASN:HB3	1:B:400:GLY:HA3	1.72	0.72
1:B:231:THR:HA	1:B:350:GLN:HE21	1.55	0.71
1:B:61:THR:HG23	1:B:64:ASP:OD2	1.90	0.71
1:A:318:MET:HG3	1:A:319:PRO:HD2	1.72	0.71
1:A:332:MET:O	1:A:336:PHE:HB2	1.91	0.71
1:B:16:TRP:HB3	1:B:419:ILE:HB	1.70	0.71
1:C:35:ASP:OD2	1:C:37:ASN:HB2	1.91	0.70
1:A:379:ILE:HA	1:A:390:ALA:O	1.90	0.70
1:C:173:ASP:HB2	1:C:212:GLU:OE1	1.90	0.70
1:C:418:ASN:HD21	1:C:420:ARG:HH21	1.39	0.70
1:A:155:MET:HG2	1:A:161:ASN:O	1.91	0.70
1:A:1:PCA:OE	1:A:185:GLY:HA2	1.91	0.70
1:C:122:LEU:O	1:C:292:PHE:HB2	1.92	0.70
1:D:105:GLY:HA2	1:D:365:ILE:HG23	1.74	0.70
1:C:325:THR:HB	1:C:327:GLU:OE2	1.91	0.70
1:B:372:ASN:O	1:B:400:GLY:HA3	1.93	0.69
1:A:319:PRO:HG3	1:A:328:LEU:HA	1.73	0.69
1:C:418:ASN:HD21	1:C:420:ARG:NH2	1.90	0.69
1:B:246:THR:HG23	3:B:677:HOH:O	1.92	0.69
1:C:31:GLU:HG2	3:C:518:HOH:O	1.91	0.69
1:A:143:ALA:HB3	1:A:364:SER:OG	1.92	0.69
1:A:173:ASP:HB2	1:A:212:GLU:OE1	1.93	0.69
1:A:200:ASN:HB2	3:A:535:HOH:O	1.92	0.68
1:A:319:PRO:HG2	1:A:328:LEU:HD23	1.75	0.68
1:B:8:PRO:HG2	1:C:78:LEU:HD11	1.74	0.68
1:A:334:ASP:OD2	1:A:335:VAL:HG22	1.92	0.68
1:B:209:CYS:HB2	1:B:236:HIS:NE2	2.09	0.68
1:A:226:THR:OG1	1:A:262:ASP:HB3	1.95	0.67
1:C:326:PRO:HD2	1:C:327:GLU:OE2	1.93	0.67
1:B:144:LEU:HD23	1:B:362:VAL:O	1.94	0.67
1:D:54:GLN:HG3	1:D:194:SER:OG	1.94	0.67
1:C:96:THR:O	1:C:102:THR:HA	1.95	0.67
1:B:51:ASP:HB2	1:B:56:THR:HG23	1.76	0.67
1:A:82:GLY:O	1:A:93:LYS:HD3	1.93	0.67
1:D:123:MET:HE2	1:D:294:GLU:N	2.07	0.67
1:A:379:ILE:HG13	1:A:391:ALA:HA	1.77	0.67
1:B:97:LYS:HB3	1:C:6:GLU:HG3	1.77	0.67
1:A:14:LEU:HD22	1:A:90:LEU:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASN:HB3	1:A:366:TRP:NE1	2.10	0.66
1:B:267:ARG:HA	1:B:391:ALA:O	1.96	0.66
1:C:379:ILE:HG21	1:C:385:GLU:OE2	1.96	0.66
1:B:97:LYS:HG3	1:B:102:THR:HG23	1.78	0.66
1:A:331:THR:HA	1:A:334:ASP:OD1	1.96	0.66
1:A:14:LEU:HD13	1:A:85:THR:OG1	1.96	0.66
1:B:231:THR:HA	1:B:350:GLN:NE2	2.11	0.66
1:B:96:THR:OG1	1:B:103:ASN:HB3	1.96	0.66
1:B:307:LYS:HD3	1:B:309:GLU:OE2	1.96	0.66
1:A:76:ASP:HB3	1:D:80:THR:HG23	1.76	0.66
1:A:346:GLY:HA3	1:A:350:GLN:HB2	1.78	0.65
1:B:46:MET:HE3	1:C:97:LYS:HE2	1.78	0.65
1:A:351:LEU:O	1:A:354:ALA:HB3	1.95	0.65
1:A:121:ASN:HB3	3:A:516:HOH:O	1.95	0.65
1:D:349:GLU:OE1	1:D:349:GLU:HA	1.95	0.65
1:A:7:THR:OG1	1:D:98:HIS:HA	1.96	0.65
1:C:266:TYR:HB3	1:C:392:ARG:O	1.96	0.65
1:C:2:ARG:HE	1:C:70:MET:HG2	1.62	0.65
1:D:19:CYS:HA	1:D:24:ASN:O	1.97	0.65
1:D:39:ARG:HD3	1:D:72:GLU:O	1.97	0.65
1:D:212:GLU:OE2	2:D:431:CTR:H6A1	1.97	0.65
1:B:424:ILE:HG21	3:B:640:HOH:O	1.97	0.65
1:B:58:ALA:O	1:B:68:LYS:HD3	1.97	0.65
1:C:63:THR:O	1:C:67:GLU:HG2	1.96	0.64
1:D:307:LYS:HD2	1:D:430:PHE:HB3	1.79	0.64
1:B:349:GLU:O	1:B:352:ASN:HB2	1.97	0.64
1:B:345:VAL:O	1:B:350:GLN:HG2	1.98	0.64
1:B:75:GLY:HA2	1:C:78:LEU:HD13	1.78	0.64
2:C:431:CTR:H6B1	2:C:431:CTR:O2A	1.98	0.64
1:B:143:ALA:HB2	1:B:217:GLU:HA	1.79	0.64
1:C:49:CYS:HA	1:C:58:ALA:HB3	1.80	0.64
1:D:274:TYR:CD1	1:D:280:LEU:HD12	2.33	0.64
1:D:175:GLN:HE22	1:D:258:ALA:HB1	1.61	0.64
1:A:132:ASP:HB3	1:A:415:VAL:HG13	1.78	0.64
1:A:17:GLN:HG2	1:A:419:ILE:O	1.97	0.64
1:A:259:ASN:OD1	2:A:431:CTR:H3C	1.98	0.63
1:B:48:ASN:HB3	1:B:50:TYR:O	1.98	0.63
1:B:377:ASP:O	1:B:395:CYS:HB2	1.99	0.63
1:B:293:GLU:HB2	1:B:296:LYS:O	1.99	0.63
1:A:144:LEU:HD12	1:A:363:MET:HG2	1.79	0.63
1:C:214:ASP:HB2	1:C:226:THR:HB	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:O	1:A:285:LYS:HG3	1.98	0.63
1:D:147:VAL:HG12	1:D:212:GLU:HG3	1.81	0.63
1:C:402:PRO:O	1:C:406:GLU:HG3	1.99	0.63
1:C:381:PRO:HB2	1:C:383:GLU:HG2	1.79	0.63
1:A:82:GLY:HA3	1:A:93:LYS:HB2	1.81	0.63
1:D:394:ASP:HB2	3:D:650:HOH:O	1.97	0.63
1:D:41:LEU:HA	1:D:70:MET:O	1.99	0.62
1:C:33:VAL:HG21	1:C:166:ARG:O	2.00	0.62
1:B:117:TYR:OH	1:B:168:GLY:HA2	1.98	0.62
1:C:317:GLY:HA3	3:C:542:HOH:O	1.98	0.62
1:A:231:THR:HG21	3:A:434:HOH:O	1.99	0.62
1:A:2:ARG:HG2	1:A:162:GLN:NE2	2.14	0.62
1:C:297:LEU:HB2	1:C:324:ILE:HG13	1.81	0.62
1:D:295:ASN:H	1:D:352:ASN:ND2	1.97	0.62
1:B:135:THR:OG1	1:B:412:ALA:HA	1.99	0.62
1:C:164:GLY:O	1:C:169:THR:HG23	2.00	0.62
2:B:431:CTR:O2A	2:B:431:CTR:H6B1	2.00	0.61
1:C:225:PHE:CD1	1:C:324:ILE:HD11	2.35	0.61
1:B:135:THR:HG1	1:B:413:GLN:H	1.48	0.61
1:D:35:ASP:HB3	1:D:38:TRP:CE3	2.35	0.61
1:A:188:ASN:OD1	1:A:205:PRO:HD2	2.00	0.61
1:B:110:LEU:HD22	1:B:361:LEU:HD22	1.80	0.61
1:C:225:PHE:CZ	1:C:297:LEU:HD23	2.35	0.61
1:D:91:THR:HB	3:D:876:HOH:O	2.00	0.61
1:B:253:ALA:HB1	3:B:740:HOH:O	1.99	0.61
1:B:71:ILE:HD11	1:B:163:ALA:HB1	1.82	0.61
1:D:217:GLU:OE2	2:D:431:CTR:H6A2	2.00	0.61
1:B:32:VAL:HA	1:B:109:TYR:O	2.00	0.61
1:D:64:ASP:O	1:D:68:LYS:HB2	2.00	0.61
1:D:341:ARG:HG3	1:D:341:ARG:O	1.99	0.61
1:C:295:ASN:H	1:C:352:ASN:HD21	1.49	0.61
1:B:11:HIS:HB3	1:B:32:VAL:O	2.01	0.61
1:C:12:PRO:HD2	1:C:32:VAL:O	2.01	0.61
1:A:137:GLU:HG3	1:A:409:PHE:CZ	2.36	0.61
1:D:4:GLY:HA3	1:D:72:GLU:OE2	2.01	0.61
1:B:12:PRO:HG2	1:B:32:VAL:HG23	1.82	0.61
1:C:20:THR:OG1	1:C:24:ASN:HB2	2.01	0.61
1:D:273:PHE:O	1:D:279:THR:HB	2.00	0.61
1:D:266:TYR:HA	1:D:270:ASN:O	2.01	0.61
1:C:112:ASN:HB3	3:C:644:HOH:O	2.00	0.61
1:B:264:ASN:HB3	1:B:267:ARG:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:GLY:HA2	1:A:250:ASP:O	2.02	0.60
1:B:330:SER:HB3	3:B:666:HOH:O	2.02	0.60
1:A:316:GLU:OE2	1:A:316:GLU:HA	2.00	0.60
1:B:86:SER:HA	3:B:727:HOH:O	2.01	0.60
1:D:96:THR:HG23	3:D:833:HOH:O	2.02	0.60
1:B:112:ASN:O	1:B:116:LYS:HG3	2.01	0.60
1:D:188:ASN:O	1:D:192:TRP:HB2	2.00	0.60
1:C:88:ASP:O	1:C:417:SER:HA	2.02	0.60
1:B:127:LEU:HG	1:B:128:ALA:N	2.16	0.60
1:D:309:GLU:HG2	3:D:657:HOH:O	2.02	0.60
1:A:1:PCA:OE	1:A:161:ASN:HB2	2.02	0.60
1:B:43:ASP:HB2	1:B:47:GLN:O	2.01	0.60
1:A:252:PHE:HB3	1:A:341:ARG:HD3	1.84	0.59
1:A:392:ARG:HH12	2:A:431:CTR:C6C	2.14	0.59
1:C:273:PHE:O	1:C:279:THR:HB	2.02	0.59
1:A:122:LEU:HD12	1:A:421:PHE:HZ	1.67	0.59
1:C:130:ASP:OD2	1:C:418:ASN:HB3	2.03	0.59
1:B:141:ASN:HB3	1:B:366:TRP:NE1	2.17	0.59
1:B:106:SER:O	1:B:364:SER:HB2	2.01	0.59
1:B:1:PCA:HA	1:B:66:ALA:O	2.03	0.59
1:B:92:LEU:HD22	1:B:106:SER:OG	2.01	0.59
1:C:356:ARG:HD3	3:C:442:HOH:O	2.02	0.59
1:A:210:CYS:HB3	1:A:235:TYR:HA	1.84	0.59
1:D:312:PRO:HD2	3:D:665:HOH:O	2.02	0.59
1:A:225:PHE:CE2	1:A:297:LEU:HD23	2.38	0.59
1:D:175:GLN:HG3	2:D:431:CTR:O2A	2.03	0.59
1:C:114:PRO:O	1:C:166:ARG:HD3	2.02	0.59
1:D:52:GLY:O	1:D:200:ASN:HA	2.01	0.59
1:B:401:VAL:HG12	1:B:404:GLU:H	1.66	0.59
1:A:150:GLU:OE1	1:A:154:GLY:HA2	2.03	0.59
1:B:289:VAL:O	1:B:299:GLN:HA	2.03	0.59
1:C:38:TRP:CE2	2:C:432:CTR:H5B	2.37	0.59
1:A:326:PRO:HG3	1:A:348:PHE:CG	2.38	0.59
1:D:268:MET:O	1:D:313:PRO:HA	2.03	0.59
1:A:212:GLU:OE2	2:A:431:CTR:H6A2	2.02	0.59
1:B:259:ASN:OD1	2:B:431:CTR:H3C	2.03	0.59
1:B:50:TYR:HA	1:B:55:TRP:HA	1.85	0.58
1:D:13:PRO:O	1:D:85:THR:HG21	2.03	0.58
1:A:177:ALA:O	1:A:180:LEU:HG	2.02	0.58
1:A:117:TYR:HB2	1:A:360:VAL:HG21	1.85	0.58
1:D:293:GLU:HG2	1:D:424:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:MET:SD	1:A:162:GLN:HA	2.43	0.58
1:B:146:PHE:O	1:B:147:VAL:HG13	2.03	0.58
1:C:183:VAL:HG13	1:C:208:SER:OG	2.03	0.58
1:A:250:ASP:HB3	1:A:253:ALA:HB2	1.84	0.58
1:A:127:LEU:HB2	1:A:421:PHE:CE1	2.37	0.58
1:A:48:ASN:O	1:A:56:THR:HG21	2.04	0.58
1:A:27:THR:HG22	1:A:28:VAL:H	1.68	0.58
1:D:331:THR:O	1:D:334:ASP:HB2	2.04	0.58
1:B:196:THR:HG23	3:B:709:HOH:O	2.04	0.58
1:B:179:ASP:HB3	1:B:247:TYR:CZ	2.39	0.57
1:B:384:LYS:HG2	1:B:387:GLN:OE1	2.04	0.57
1:A:341:ARG:O	1:A:344:GLU:HB2	2.05	0.57
1:C:368:ASP:HB2	1:C:373:MET:CE	2.34	0.57
1:B:12:PRO:O	1:B:31:GLU:HB2	2.04	0.57
1:D:78:LEU:HG	1:D:84:SER:HB3	1.86	0.57
1:C:208:SER:HB3	1:C:235:TYR:CZ	2.38	0.57
1:A:378:SER:O	1:A:392:ARG:HD2	2.04	0.57
1:D:175:GLN:NE2	1:D:258:ALA:HB1	2.18	0.57
1:B:96:THR:O	1:B:102:THR:HA	2.03	0.57
1:B:42:HIS:HB2	1:B:47:GLN:O	2.03	0.57
1:D:278:LYS:HD3	3:D:751:HOH:O	2.04	0.57
1:A:294:GLU:HG3	1:A:295:ASN:OD1	2.05	0.57
1:A:281:ASP:HB2	3:A:598:HOH:O	2.02	0.57
1:D:407:ALA:HA	3:D:843:HOH:O	2.05	0.57
1:C:291:ARG:HG2	1:C:424:ILE:HG12	1.86	0.57
1:A:183:VAL:HG22	1:A:208:SER:HB3	1.85	0.57
1:C:423:PRO:O	1:C:426:SER:HB3	2.04	0.57
1:C:246:THR:HA	3:C:445:HOH:O	2.04	0.57
1:D:172:CYS:HA	1:D:208:SER:HB3	1.85	0.57
1:A:1:PCA:HG3	1:A:182:PHE:CD2	2.40	0.57
1:C:195:SER:HA	3:C:450:HOH:O	2.03	0.57
1:B:401:VAL:HG11	1:B:404:GLU:OE2	2.04	0.57
1:A:130:ASP:HA	1:A:286:PHE:O	2.04	0.57
1:C:137:GLU:O	1:C:140:ILE:HG13	2.04	0.57
1:C:307:LYS:HD3	1:D:304:ASP:O	2.05	0.57
1:B:199:PRO:HB2	1:B:200:ASN:HD22	1.70	0.57
1:D:327:GLU:O	1:D:331:THR:HG23	2.05	0.57
1:A:287:THR:HB	1:A:302:ILE:HB	1.87	0.57
1:D:74:ALA:HB1	1:D:81:TYR:CE2	2.39	0.57
1:B:15:THR:HB	1:B:28:VAL:O	2.04	0.57
1:B:17:GLN:HB3	1:B:25:CYS:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:LYS:HE3	3:B:705:HOH:O	2.04	0.57
1:A:11:HIS:HB3	1:A:32:VAL:O	2.05	0.57
1:B:193:LYS:HD3	1:B:203:VAL:CG1	2.34	0.57
1:C:1:PCA:HG3	1:C:182:PHE:CG	2.40	0.56
1:D:341:ARG:HA	1:D:344:GLU:HB2	1.86	0.56
1:C:372:ASN:O	1:C:400:GLY:HA3	2.04	0.56
1:C:36:ALA:HA	1:C:39:ARG:HG3	1.87	0.56
1:D:145:TYR:HB3	1:D:214:ASP:HA	1.87	0.56
1:B:173:ASP:O	1:B:209:CYS:HA	2.04	0.56
1:A:136:VAL:O	1:A:219:ASN:HB2	2.05	0.56
1:B:224:ALA:HA	1:B:263:TYR:O	2.05	0.56
1:C:61:THR:HB	1:C:190:GLU:OE1	2.04	0.56
1:A:147:VAL:HB	1:A:172:CYS:O	2.05	0.56
1:A:103:ASN:HA	2:A:432:CTR:O2A	2.05	0.56
1:D:41:LEU:CD2	1:D:71:ILE:HG23	2.36	0.56
1:C:318:MET:HE3	1:C:332:MET:HA	1.87	0.56
1:D:18:ARG:HB2	1:D:26:GLN:HG2	1.87	0.56
1:B:163:ALA:HB1	1:B:167:TYR:HB2	1.88	0.56
1:D:157:SER:O	1:D:159:PRO:HD3	2.06	0.56
1:B:193:LYS:HD3	1:B:203:VAL:HG13	1.86	0.56
1:B:22:PRO:HB3	1:B:429:ASP:OD2	2.05	0.56
1:B:350:GLN:HA	1:B:350:GLN:OE1	2.05	0.56
1:A:368:ASP:HB3	1:A:373:MET:CE	2.36	0.56
1:D:122:LEU:HD11	1:D:146:PHE:CE1	2.41	0.56
1:C:63:THR:CB	1:C:186:LYS:HZ2	2.18	0.56
1:A:379:ILE:HG13	1:A:391:ALA:CA	2.35	0.56
1:B:47:GLN:HG3	1:B:48:ASN:N	2.21	0.56
1:A:213:ILE:HD13	1:A:227:PRO:CB	2.36	0.56
1:D:315:TRP:CZ3	1:D:388:PRO:HG3	2.41	0.56
1:D:291:ARG:HH11	1:D:424:ILE:CG2	2.17	0.56
1:A:144:LEU:HD21	1:A:361:LEU:HD11	1.88	0.56
1:A:122:LEU:HD11	1:A:146:PHE:CE2	2.41	0.56
1:D:339:ARG:HA	3:D:722:HOH:O	2.05	0.56
1:A:225:PHE:CZ	1:A:297:LEU:HD23	2.41	0.56
1:A:16:TRP:HB2	1:A:419:ILE:HB	1.86	0.55
1:A:288:VAL:HG22	1:A:301:PHE:CD2	2.40	0.55
1:B:46:MET:HG3	1:C:97:LYS:HD2	1.87	0.55
1:A:333:PHE:CE2	1:A:340:ASN:HA	2.41	0.55
1:A:37:ASN:OD1	1:A:181:LYS:HD3	2.07	0.55
1:D:291:ARG:HB3	1:D:424:ILE:HG12	1.88	0.55
1:A:78:LEU:HD12	1:D:75:GLY:CA	2.34	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:MET:HA	1:A:117:TYR:HA	1.87	0.55
1:D:410:PRO:HD3	3:D:843:HOH:O	2.06	0.55
1:A:59:CYS:HB3	1:A:189:ILE:CD1	2.37	0.55
1:D:98:HIS:HD2	1:D:100:TYR:H	1.54	0.55
1:A:225:PHE:CE1	1:A:299:GLN:HB2	2.42	0.55
1:C:176:CYS:HA	1:C:208:SER:O	2.07	0.55
1:B:126:GLU:HB2	1:B:290:SER:O	2.06	0.55
1:A:95:VAL:HG11	1:A:410:PRO:HB3	1.88	0.55
1:A:160:SER:OG	1:A:185:GLY:HA3	2.06	0.55
1:B:352:ASN:O	1:B:355:LEU:HB2	2.07	0.55
1:C:137:GLU:H	1:C:140:ILE:HD12	1.72	0.55
1:B:287:THR:O	1:B:301:PHE:HA	2.06	0.55
1:B:401:VAL:O	1:B:405:VAL:HG22	2.06	0.55
1:D:276:LYS:HB2	3:D:656:HOH:O	2.07	0.55
1:A:109:TYR:CD1	1:A:362:VAL:HG22	2.42	0.55
1:A:109:TYR:HD1	1:A:362:VAL:HG22	1.72	0.55
1:D:428:TYR:HB3	1:D:430:PHE:CD1	2.40	0.55
1:D:250:ASP:OD2	1:D:253:ALA:HB2	2.07	0.55
1:A:97:LYS:HG2	1:D:46:MET:CE	2.36	0.55
1:D:293:GLU:HG2	1:D:424:ILE:CD1	2.37	0.55
1:A:35:ASP:OD2	1:A:38:TRP:HZ3	1.90	0.55
1:B:139:GLY:O	1:B:373:MET:HE3	2.07	0.55
1:A:31:GLU:HG3	1:A:111:MET:HB2	1.89	0.55
1:A:401:VAL:HB	1:A:404:GLU:CG	2.36	0.55
1:D:175:GLN:O	1:D:176:CYS:HB2	2.07	0.54
1:C:366:TRP:CH2	2:C:431:CTR:H2A	2.41	0.54
1:C:133:LEU:HD11	1:C:286:PHE:CZ	2.42	0.54
1:D:384:LYS:HE3	1:D:385:GLU:O	2.07	0.54
1:C:205:PRO:HB2	1:C:206:TYR:HD2	1.72	0.54
1:A:155:MET:HE3	1:A:166:ARG:HH21	1.72	0.54
1:D:147:VAL:HG12	1:D:212:GLU:HB2	1.89	0.54
1:A:315:TRP:CH2	1:A:388:PRO:HA	2.42	0.54
1:D:368:ASP:HB2	1:D:373:MET:HE1	1.89	0.54
1:A:97:LYS:HG2	1:D:46:MET:HE3	1.89	0.54
1:A:132:ASP:HB3	1:A:415:VAL:CG1	2.37	0.54
1:D:266:TYR:CD2	1:D:271:PRO:HA	2.43	0.54
1:D:266:TYR:HE1	1:D:391:ALA:HB1	1.72	0.54
1:C:85:THR:HG22	3:C:505:HOH:O	2.07	0.54
1:A:41:LEU:HD21	1:A:182:PHE:HE2	1.72	0.54
1:B:198:ASP:HB3	1:B:201:ALA:HB3	1.89	0.54
1:A:16:TRP:NE1	1:A:28:VAL:HG11	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:PHE:CD2	1:C:339:ARG:HD3	2.43	0.54
1:C:9:GLU:HB2	1:C:73:GLY:HA2	1.89	0.54
1:A:276:LYS:HD2	3:A:448:HOH:O	2.06	0.54
1:D:155:MET:HG3	1:D:164:GLY:CA	2.38	0.54
1:B:178:ARG:HG2	1:B:206:TYR:O	2.08	0.54
1:A:377:ASP:HB2	1:A:395:CYS:SG	2.48	0.54
1:D:428:TYR:HB3	1:D:430:PHE:CE1	2.43	0.54
1:B:143:ALA:CB	1:B:217:GLU:HA	2.38	0.54
1:B:146:PHE:HB3	1:B:359:MET:HB3	1.90	0.54
1:D:384:LYS:HG2	1:D:387:GLN:NE2	2.23	0.54
1:C:209:CYS:HB2	1:C:236:HIS:NE2	2.23	0.54
1:A:19:CYS:HA	1:A:25:CYS:HA	1.90	0.54
1:D:95:VAL:HG13	1:D:104:VAL:HG23	1.89	0.53
1:B:110:LEU:HB2	1:B:361:LEU:HD23	1.89	0.53
1:B:143:ALA:HA	1:B:216:TRP:O	2.08	0.53
1:D:35:ASP:HB3	1:D:38:TRP:CZ3	2.43	0.53
1:A:181:LYS:HE2	3:A:472:HOH:O	2.08	0.53
1:C:209:CYS:HB2	1:C:236:HIS:CE1	2.42	0.53
1:B:177:ALA:CB	1:B:180:LEU:HG	2.34	0.53
1:C:209:CYS:HB3	1:C:256:CYS:SG	2.49	0.53
1:D:381:PRO:HB2	1:D:383:GLU:OE2	2.07	0.53
1:A:267:ARG:HE	1:A:389:GLY:HA2	1.74	0.53
1:B:91:THR:CG2	1:B:415:VAL:HG13	2.37	0.53
1:A:209:CYS:O	1:A:210:CYS:HB3	2.09	0.53
1:B:126:GLU:OE2	1:B:427:THR:HG23	2.07	0.53
1:C:250:ASP:HB3	1:C:253:ALA:HB2	1.89	0.53
1:D:34:ILE:HB	1:D:108:PHE:CE2	2.43	0.53
1:C:34:ILE:HD11	1:C:38:TRP:CD1	2.43	0.53
1:B:209:CYS:O	1:B:210:CYS:HB3	2.09	0.53
1:D:286:PHE:HA	3:D:713:HOH:O	2.08	0.53
1:A:38:TRP:CH2	2:A:432:CTR:H6C2	2.44	0.53
1:B:13:PRO:O	1:B:85:THR:HG21	2.09	0.53
1:A:357:VAL:O	1:A:359:MET:HG3	2.09	0.53
1:A:77:TYR:O	1:A:83:ALA:HB3	2.09	0.53
1:D:114:PRO:HG2	1:D:115:ASP:OD1	2.08	0.53
1:B:132:ASP:HB3	1:B:415:VAL:HG23	1.89	0.53
1:D:243:CYS:O	1:D:253:ALA:HB3	2.09	0.53
1:A:43:ASP:O	1:A:46:MET:HE3	2.09	0.53
1:A:198:ASP:HB3	1:A:201:ALA:HB3	1.91	0.53
1:B:141:ASN:O	1:B:365:ILE:HA	2.09	0.53
1:C:88:ASP:HB3	3:C:481:HOH:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:MET:HE2	1:C:332:MET:HB2	1.90	0.53
1:A:60:SER:O	1:A:61:THR:HG23	2.09	0.53
1:C:353:ASN:HA	1:C:356:ARG:HD2	1.91	0.53
1:A:133:LEU:HD12	3:A:597:HOH:O	2.08	0.53
1:B:286:PHE:HB3	1:B:303:GLN:NE2	2.23	0.53
1:B:368:ASP:OD2	1:B:371:ALA:HB3	2.09	0.52
1:D:164:GLY:O	1:D:169:THR:HG23	2.09	0.52
1:C:297:LEU:CB	1:C:324:ILE:HG13	2.39	0.52
1:C:237:VAL:HB	3:C:640:HOH:O	2.10	0.52
1:C:217:GLU:O	1:C:223:PHE:HA	2.09	0.52
1:C:418:ASN:ND2	1:C:420:ARG:HH21	2.04	0.52
1:C:31:GLU:HG3	1:C:111:MET:HG3	1.92	0.52
1:A:132:ASP:O	1:A:415:VAL:HG13	2.08	0.52
1:A:299:GLN:O	1:A:310:ILE:HD12	2.09	0.52
1:B:2:ARG:HA	1:B:162:GLN:HB2	1.90	0.52
1:B:118:GLN:HE21	1:B:119:MET:N	2.06	0.52
1:B:280:LEU:HD23	1:B:308:ILE:HD12	1.91	0.52
1:A:98:HIS:HA	1:D:40:TRP:CZ3	2.45	0.52
1:A:232:THR:HG23	1:A:234:GLU:HG2	1.91	0.52
1:A:1:PCA:HB3	1:A:182:PHE:CZ	2.45	0.52
1:B:294:GLU:HG3	1:B:295:ASN:ND2	2.25	0.52
1:D:94:PHE:HZ	1:D:367:ASP:OD2	1.92	0.52
1:A:379:ILE:HG21	1:A:385:GLU:HB2	1.91	0.52
1:A:351:LEU:HD11	1:A:355:LEU:HD21	1.91	0.52
1:A:115:ASP:O	1:A:165:ALA:HB3	2.10	0.52
1:A:375:TRP:O	1:A:392:ARG:HD3	2.08	0.52
1:D:66:ALA:HB2	1:D:182:PHE:HE1	1.74	0.52
1:B:45:ASN:O	1:B:46:MET:HB2	2.08	0.52
1:B:11:HIS:HE1	1:B:166:ARG:HG3	1.74	0.52
1:D:310:ILE:H	1:D:310:ILE:HD12	1.74	0.52
1:C:342:PHE:HD2	3:C:502:HOH:O	1.91	0.52
1:A:126:GLU:HB2	1:A:290:SER:O	2.09	0.52
1:A:155:MET:HE1	1:A:166:ARG:NE	2.20	0.52
1:B:135:THR:HG21	1:B:413:GLN:HG2	1.92	0.52
3:A:469:HOH:O	1:D:78:LEU:HD12	2.10	0.52
1:B:244:GLY:CA	1:B:254:GLY:H	2.23	0.52
1:C:115:ASP:HA	1:C:166:ARG:CD	2.40	0.52
1:A:15:THR:HG22	1:A:88:ASP:HA	1.92	0.52
1:B:317:GLY:O	1:B:331:THR:HB	2.10	0.52
1:B:281:ASP:HB2	1:B:303:GLN:OE1	2.10	0.51
1:A:147:VAL:HG23	1:A:147:VAL:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ALA:HA	1:C:71:ILE:CD1	2.41	0.51
1:D:53:ASN:ND2	1:D:194:SER:HB3	2.24	0.51
1:D:335:VAL:HG12	1:D:388:PRO:HB3	1.91	0.51
1:A:212:GLU:HG2	1:A:214:ASP:OD1	2.10	0.51
1:A:182:PHE:CE1	1:A:187:ALA:HB2	2.45	0.51
1:B:112:ASN:HB3	1:B:118:GLN:CA	2.39	0.51
1:A:89:ALA:HA	1:A:417:SER:HB3	1.93	0.51
1:A:98:HIS:NE2	1:A:101:GLY:HA3	2.26	0.51
1:C:312:PRO:HB3	1:C:321:SER:N	2.26	0.51
1:B:227:PRO:HD2	1:B:261:CYS:O	2.11	0.51
1:D:212:GLU:OE2	1:D:214:ASP:OD1	2.29	0.51
1:A:209:CYS:HB2	1:A:236:HIS:CE1	2.46	0.51
1:A:229:ALA:O	1:A:257:ASP:HB2	2.11	0.51
1:B:427:THR:HG1	1:B:428:TYR:HD1	1.59	0.51
1:A:141:ASN:HB3	1:A:366:TRP:CE2	2.45	0.51
1:C:34:ILE:HG23	1:C:39:ARG:NE	2.22	0.51
1:D:132:ASP:CB	1:D:415:VAL:HG22	2.40	0.51
1:B:372:ASN:HB3	1:B:400:GLY:CA	2.38	0.51
1:B:199:PRO:HB2	1:B:200:ASN:ND2	2.26	0.51
1:C:148:ALA:HB3	1:C:210:CYS:HB2	1.93	0.51
1:C:198:ASP:OD1	1:C:199:PRO:HD2	2.11	0.51
1:C:381:PRO:HB2	1:C:383:GLU:CG	2.41	0.51
1:D:132:ASP:HB3	1:D:415:VAL:HG22	1.93	0.51
1:B:333:PHE:HD2	1:B:338:ASP:O	1.94	0.51
1:A:6:GLU:O	1:D:97:LYS:HB3	2.12	0.50
1:B:244:GLY:HA3	1:B:254:GLY:H	1.76	0.50
1:A:92:LEU:HD21	1:A:108:PHE:CD1	2.45	0.50
1:C:372:ASN:N	1:C:372:ASN:HD22	2.09	0.50
1:C:103:ASN:OD1	2:C:432:CTR:O6B	2.29	0.50
1:C:379:ILE:HG21	1:C:385:GLU:HB3	1.94	0.50
1:A:223:PHE:HE1	1:A:299:GLN:OE1	1.94	0.50
1:A:302:ILE:O	1:A:302:ILE:HG22	2.12	0.50
1:B:193:LYS:HB2	1:B:203:VAL:CG1	2.41	0.50
1:B:2:ARG:HE	1:B:70:MET:HG2	1.75	0.50
1:B:367:ASP:OD2	1:B:406:GLU:OE2	2.28	0.50
1:A:125:ASN:HB3	1:A:422:GLY:O	2.11	0.50
1:B:373:MET:HA	1:B:375:TRP:NE1	2.26	0.50
1:A:318:MET:SD	1:A:332:MET:HA	2.51	0.50
1:C:137:GLU:HG3	1:C:409:PHE:CD1	2.47	0.50
1:C:144:LEU:CD2	1:C:361:LEU:HD11	2.42	0.50
1:B:17:GLN:HA	1:B:26:GLN:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:PRO:HG2	1:B:319:PRO:O	2.12	0.50
1:A:176:CYS:O	1:A:178:ARG:HG2	2.11	0.50
1:B:97:LYS:O	1:B:98:HIS:O	2.30	0.50
1:B:146:PHE:HB3	1:B:359:MET:CB	2.42	0.50
1:C:275:GLY:O	1:C:278:LYS:HB2	2.11	0.50
1:A:76:ASP:O	1:A:76:ASP:OD2	2.30	0.50
1:A:190:GLU:O	1:A:205:PRO:HG3	2.12	0.50
1:D:19:CYS:HA	1:D:25:CYS:HA	1.93	0.50
1:B:349:GLU:OE2	1:B:352:ASN:OD1	2.30	0.50
1:B:127:LEU:HD21	1:B:129:PHE:HD1	1.77	0.50
1:B:172:CYS:HB3	1:B:235:TYR:CE1	2.46	0.50
1:A:139:GLY:HA3	1:A:400:GLY:HA2	1.94	0.50
1:C:2:ARG:HD2	1:C:70:MET:HB3	1.93	0.50
1:A:198:ASP:HB2	1:A:369:HIS:CD2	2.47	0.50
1:D:307:LYS:HD2	1:D:430:PHE:HD2	1.77	0.50
1:D:43:ASP:OD1	1:D:68:LYS:O	2.30	0.50
1:D:228:HIS:HB3	1:D:257:ASP:O	2.12	0.50
1:D:291:ARG:CD	1:D:424:ILE:HG23	2.42	0.50
1:C:133:LEU:HD11	1:C:286:PHE:HZ	1.76	0.50
1:D:276:LYS:HG3	3:D:656:HOH:O	2.12	0.50
1:A:45:ASN:O	1:A:46:MET:O	2.30	0.50
1:A:107:ARG:HH12	2:A:432:CTR:C6C	2.25	0.50
1:B:6:GLU:HB2	1:B:72:GLU:OE2	2.11	0.50
1:A:261:CYS:HB2	1:A:342:PHE:CD1	2.46	0.50
1:D:128:ALA:CB	1:D:289:VAL:HG22	2.42	0.50
1:C:429:ASP:C	1:D:284:ARG:HH22	2.15	0.50
1:D:31:GLU:O	1:D:111:MET:HB2	2.12	0.50
1:B:163:ALA:HB3	1:B:169:THR:HG21	1.93	0.50
1:A:147:VAL:CG1	1:A:212:GLU:HG3	2.42	0.50
1:B:401:VAL:O	1:B:401:VAL:HG12	2.11	0.50
1:D:401:VAL:O	1:D:405:VAL:HG13	2.11	0.50
1:D:12:PRO:HA	3:D:739:HOH:O	2.11	0.50
1:A:147:VAL:O	1:A:149:MET:HG3	2.11	0.49
1:A:2:ARG:O	1:A:70:MET:HA	2.12	0.49
1:D:145:TYR:CB	1:D:214:ASP:HA	2.42	0.49
1:C:369:HIS:CD2	1:C:402:PRO:HG2	2.46	0.49
1:A:150:GLU:OE1	1:A:157:SER:OG	2.30	0.49
1:C:293:GLU:HG2	1:C:424:ILE:HD11	1.93	0.49
1:D:130:ASP:HA	1:D:286:PHE:O	2.12	0.49
1:A:173:ASP:OD2	2:A:431:CTR:O4A	2.29	0.49
1:D:147:VAL:HG12	1:D:212:GLU:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:CYS:SG	1:B:238:CYS:HB3	2.52	0.49
1:A:283:SER:OG	1:A:284:ARG:HG3	2.12	0.49
1:A:104:VAL:O	1:A:105:GLY:O	2.30	0.49
1:B:374:LEU:HD11	1:B:397:THR:CA	2.37	0.49
1:A:155:MET:CE	1:A:166:ARG:HE	2.22	0.49
1:C:34:ILE:HD11	1:C:38:TRP:CG	2.47	0.49
1:D:178:ARG:HB3	1:D:203:VAL:HG13	1.93	0.49
1:D:349:GLU:OE1	1:D:352:ASN:OD1	2.30	0.49
1:A:324:ILE:HG22	1:A:324:ILE:O	2.11	0.49
1:D:214:ASP:OD2	1:D:217:GLU:OE2	2.30	0.49
1:C:398:ASP:O	1:C:399:SER:O	2.29	0.49
1:D:53:ASN:HB3	1:D:200:ASN:HA	1.95	0.49
1:C:13:PRO:HD2	1:C:85:THR:HG21	1.94	0.49
1:B:206:TYR:CD2	1:B:239:GLU:HG3	2.48	0.49
1:C:345:VAL:HG23	1:C:345:VAL:O	2.11	0.49
1:A:160:SER:OG	1:A:185:GLY:O	2.30	0.49
1:C:92:LEU:HB2	1:C:414:VAL:HG12	1.93	0.49
1:B:116:LYS:HB3	1:B:151:GLU:OE1	2.12	0.49
1:D:177:ALA:HB1	1:D:180:LEU:HD23	1.94	0.49
1:C:137:GLU:HG3	1:C:409:PHE:CE1	2.47	0.49
1:D:348:PHE:CZ	1:D:351:LEU:HD23	2.48	0.49
1:A:267:ARG:HG3	1:A:392:ARG:CG	2.42	0.49
1:D:246:THR:HG23	1:D:251:ARG:HH12	1.77	0.49
1:C:272:ASP:HA	1:C:278:LYS:CE	2.38	0.49
1:A:163:ALA:O	1:A:166:ARG:HG3	2.11	0.49
1:B:307:LYS:HB2	1:B:430:PHE:CE2	2.48	0.49
1:B:32:VAL:HG12	1:B:109:TYR:O	2.12	0.49
1:D:96:THR:O	1:D:102:THR:HA	2.12	0.49
1:B:403:ALA:O	1:B:407:ALA:HB2	2.13	0.49
1:C:13:PRO:HD2	1:C:85:THR:CG2	2.43	0.49
1:C:79:GLY:O	1:C:98:HIS:HB3	2.13	0.49
1:C:333:PHE:O	1:C:337:ASN:HA	2.13	0.49
1:A:405:VAL:O	1:A:405:VAL:HG23	2.12	0.49
1:B:212:GLU:OE2	1:B:214:ASP:OD1	2.30	0.49
1:D:366:TRP:CZ2	2:D:431:CTR:H4A	2.47	0.49
1:A:35:ASP:OD1	1:A:109:TYR:OH	2.30	0.49
1:A:318:MET:CE	1:A:332:MET:HA	2.42	0.49
1:D:384:LYS:HG2	1:D:387:GLN:HE21	1.78	0.49
1:B:315:TRP:O	1:B:318:MET:HB2	2.13	0.49
1:C:239:GLU:O	1:C:242:ASN:OD1	2.29	0.49
1:C:142:SER:OG	1:C:142:SER:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASN:O	1:B:194:SER:OG	2.30	0.48
1:A:328:LEU:O	1:A:332:MET:HB2	2.12	0.48
1:B:1:PCA:HG3	1:B:182:PHE:CE2	2.48	0.48
1:D:384:LYS:O	1:D:385:GLU:HB2	2.13	0.48
1:B:295:ASN:HA	1:B:348:PHE:CE2	2.48	0.48
1:B:425:GLY:HA2	3:B:590:HOH:O	2.12	0.48
1:C:109:TYR:OH	1:C:171:TYR:HB2	2.13	0.48
1:B:379:ILE:HG21	1:B:385:GLU:CG	2.43	0.48
1:C:197:SER:OG	1:C:369:HIS:HD2	1.96	0.48
1:B:105:GLY:O	1:B:106:SER:HB3	2.13	0.48
1:C:125:ASN:HD22	1:C:423:PRO:HA	1.77	0.48
1:A:271:PRO:HD2	3:A:442:HOH:O	2.13	0.48
1:B:71:ILE:HD11	1:B:163:ALA:CB	2.43	0.48
1:A:155:MET:HG3	1:A:164:GLY:CA	2.43	0.48
1:B:217:GLU:O	1:B:218:SER:HB3	2.13	0.48
1:D:38:TRP:CZ2	1:D:106:SER:HA	2.49	0.48
1:D:82:GLY:N	1:D:96:THR:HG21	2.28	0.48
1:A:130:ASP:OD1	1:A:287:THR:OG1	2.30	0.48
1:B:104:VAL:HG21	1:B:406:GLU:OE1	2.14	0.48
1:C:63:THR:HG23	1:C:186:LYS:NZ	2.29	0.48
1:A:288:VAL:HG22	1:A:301:PHE:CE2	2.48	0.48
1:A:310:ILE:HG23	1:A:311:PRO:HD2	1.96	0.48
1:D:131:VAL:HA	1:D:415:VAL:O	2.13	0.48
1:A:86:SER:O	1:A:86:SER:OG	2.29	0.48
1:A:135:THR:OG1	1:A:135:THR:O	2.29	0.48
1:B:55:TRP:O	1:B:56:THR:O	2.31	0.48
1:B:141:ASN:HB3	1:B:366:TRP:CD1	2.48	0.48
3:C:530:HOH:O	1:D:304:ASP:HA	2.14	0.48
1:B:266:TYR:CD2	1:B:393:GLY:HA2	2.49	0.48
1:D:95:VAL:HG11	1:D:97:LYS:NZ	2.27	0.48
1:A:377:ASP:O	1:A:393:GLY:HA3	2.14	0.48
1:B:272:ASP:O	1:B:278:LYS:HG2	2.13	0.48
1:B:100:TYR:HB3	1:C:100:TYR:CD1	2.48	0.48
1:A:226:THR:HG22	1:A:228:HIS:CD2	2.48	0.48
1:A:373:MET:HB3	1:A:377:ASP:OD2	2.14	0.48
1:D:78:LEU:O	1:D:82:GLY:HA2	2.13	0.48
1:A:127:LEU:HD13	1:A:421:PHE:CD1	2.49	0.48
1:C:66:ALA:HA	1:C:182:PHE:HE1	1.78	0.48
1:B:408:GLN:O	1:B:410:PRO:HD3	2.14	0.48
1:D:369:HIS:HA	1:D:402:PRO:HG2	1.95	0.48
1:B:133:LEU:HD13	1:B:219:ASN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:THR:HG23	1:C:186:LYS:HZ2	1.78	0.48
1:C:383:GLU:O	1:C:384:LYS:HB2	2.13	0.48
1:B:54:GLN:HE21	1:B:54:GLN:HB3	1.45	0.48
1:A:14:LEU:O	1:A:30:ALA:HB3	2.14	0.48
1:A:131:VAL:C	1:A:285:LYS:HG3	2.34	0.48
1:B:280:LEU:CD2	1:B:308:ILE:HD12	2.43	0.48
1:A:374:LEU:HD13	1:A:382:PRO:HG2	1.96	0.48
1:B:307:LYS:HE3	1:B:430:PHE:HB3	1.96	0.47
1:A:39:ARG:HB2	1:A:71:ILE:HG22	1.96	0.47
1:D:239:GLU:HG3	1:D:240:THR:OG1	2.13	0.47
1:A:289:VAL:HB	1:A:300:TYR:CE2	2.49	0.47
1:C:415:VAL:HG22	1:C:415:VAL:O	2.14	0.47
1:B:119:MET:HE2	1:B:151:GLU:HB2	1.97	0.47
1:D:384:LYS:HG3	1:D:385:GLU:N	2.29	0.47
1:B:133:LEU:HD13	1:B:219:ASN:C	2.34	0.47
1:D:53:ASN:CG	1:D:194:SER:HB3	2.35	0.47
1:D:270:ASN:HA	1:D:271:PRO:HD2	1.69	0.47
1:D:303:GLN:O	1:D:306:ARG:HG3	2.15	0.47
1:B:400:GLY:O	1:B:402:PRO:HD3	2.14	0.47
1:D:213:ILE:HA	1:D:227:PRO:HA	1.95	0.47
1:D:9:GLU:OE1	1:D:77:TYR:OH	2.29	0.47
1:D:296:LYS:HE3	1:D:298:SER:OG	2.14	0.47
2:A:432:CTR:O6A	1:D:99:GLU:OE2	2.31	0.47
1:A:420:ARG:HB3	1:A:427:THR:CG2	2.43	0.47
1:D:405:VAL:HA	1:D:408:GLN:HG2	1.97	0.47
1:A:272:ASP:HA	1:A:278:LYS:HD2	1.97	0.47
1:B:292:PHE:HD2	1:B:297:LEU:HG	1.80	0.47
1:A:102:THR:HG22	1:A:102:THR:O	2.15	0.47
1:A:9:GLU:OE2	1:A:73:GLY:HA2	2.15	0.47
1:B:374:LEU:HD13	1:B:378:SER:CB	2.39	0.47
1:D:375:TRP:CE2	2:D:431:CTR:H5B	2.50	0.47
1:D:122:LEU:HG	1:D:292:PHE:CG	2.50	0.47
1:B:13:PRO:HG2	1:B:85:THR:HG21	1.97	0.47
1:D:82:GLY:HA3	1:D:96:THR:HG21	1.97	0.47
1:A:23:GLY:O	1:A:24:ASN:OD1	2.33	0.47
1:A:293:GLU:OE1	1:A:296:LYS:HD2	2.15	0.47
1:A:97:LYS:HZ2	1:D:46:MET:HE1	1.80	0.47
1:D:213:ILE:O	1:D:213:ILE:HG22	2.14	0.47
1:D:122:LEU:HG	1:D:292:PHE:CD1	2.50	0.47
1:A:336:PHE:HD1	1:A:336:PHE:HA	1.62	0.47
1:C:262:ASP:OD1	2:C:431:CTR:O6C	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ASN:OD1	1:A:354:ALA:HB2	2.14	0.47
1:A:213:ILE:HD13	1:A:227:PRO:HB3	1.97	0.47
1:C:263:TYR:CE1	1:C:322:SER:HA	2.50	0.47
1:C:155:MET:HG2	1:C:161:ASN:O	2.14	0.47
1:D:126:GLU:OE2	1:D:427:THR:OG1	2.29	0.47
1:A:319:PRO:HD3	1:A:331:THR:OG1	2.14	0.47
1:C:319:PRO:HD2	1:C:328:LEU:HD23	1.97	0.47
1:C:297:LEU:HD11	1:C:355:LEU:HD11	1.96	0.47
1:A:44:ASP:HB3	3:A:539:HOH:O	2.15	0.47
1:A:179:ASP:OD2	2:A:432:CTR:O6C	2.30	0.47
1:A:95:VAL:HB	1:A:410:PRO:O	2.15	0.47
1:C:188:ASN:CG	1:C:204:GLY:HA3	2.36	0.47
1:C:71:ILE:HD11	1:C:163:ALA:HB2	1.96	0.46
1:B:258:ALA:HB3	1:B:259:ASN:ND2	2.30	0.46
1:B:259:ASN:O	1:B:260:GLY:O	2.32	0.46
1:A:154:GLY:HA3	3:A:464:HOH:O	2.15	0.46
1:B:373:MET:HA	1:B:375:TRP:CD1	2.51	0.46
1:B:225:PHE:CZ	1:B:297:LEU:HD23	2.50	0.46
1:A:371:ALA:O	1:A:374:LEU:HB2	2.15	0.46
1:B:381:PRO:HB2	1:B:383:GLU:HG2	1.97	0.46
1:A:228:HIS:HB3	1:A:257:ASP:HB3	1.98	0.46
1:B:187:ALA:CB	1:B:189:ILE:HG22	2.46	0.46
1:B:6:GLU:OE1	1:B:46:MET:HE3	2.15	0.46
1:A:428:TYR:HB3	1:A:430:PHE:CD1	2.51	0.46
1:B:172:CYS:HB3	1:B:235:TYR:CD1	2.50	0.46
1:D:20:THR:O	1:D:21:ALA:HB2	2.16	0.46
1:D:179:ASP:O	1:D:192:TRP:HH2	1.97	0.46
1:C:104:VAL:O	2:C:432:CTR:H6B1	2.16	0.46
2:A:432:CTR:HO4A	1:D:100:TYR:HE1	1.61	0.46
1:D:345:VAL:O	1:D:350:GLN:HG2	2.16	0.46
1:B:11:HIS:CE1	1:B:166:ARG:HG3	2.51	0.46
1:A:234:GLU:HG2	1:A:234:GLU:H	1.40	0.46
1:A:63:THR:HG22	1:A:64:ASP:N	2.30	0.46
1:B:49:CYS:O	1:B:55:TRP:HE3	1.98	0.46
1:B:196:THR:O	1:B:197:SER:HB3	2.16	0.46
1:C:137:GLU:OE2	1:C:221:TYR:OH	2.30	0.46
1:D:368:ASP:OD2	1:D:371:ALA:HB3	2.15	0.46
1:C:257:ASP:CG	1:C:260:GLY:H	2.19	0.46
1:B:316:GLU:OE1	1:B:316:GLU:HA	2.15	0.46
1:C:115:ASP:HA	1:C:166:ARG:NE	2.31	0.46
1:B:43:ASP:N	1:B:47:GLN:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:LEU:HD22	1:B:49:CYS:HB2	1.98	0.46
1:C:295:ASN:O	1:C:296:LYS:HB2	2.16	0.46
1:C:125:ASN:ND2	1:C:423:PRO:HA	2.31	0.46
1:A:134:SER:HB3	1:A:283:SER:O	2.16	0.46
1:C:64:ASP:O	1:C:68:LYS:HB2	2.15	0.46
1:A:34:ILE:HB	1:A:77:TYR:HE2	1.80	0.46
1:B:97:LYS:HB3	1:C:6:GLU:CG	2.43	0.46
1:B:16:TRP:HH2	1:B:18:ARG:NH1	2.14	0.46
1:A:303:GLN:HB2	1:A:308:ILE:HD13	1.97	0.46
1:C:267:ARG:NH1	2:C:431:CTR:O6C	2.49	0.46
1:B:86:SER:O	1:B:89:ALA:HB3	2.15	0.46
1:A:107:ARG:HH12	2:A:432:CTR:H6C1	1.80	0.45
1:C:357:VAL:O	1:C:359:MET:HG2	2.15	0.45
1:D:41:LEU:O	1:D:42:HIS:HB3	2.15	0.45
1:C:296:LYS:HE3	1:C:296:LYS:HB2	1.69	0.45
1:A:286:PHE:HB3	1:A:303:GLN:HG2	1.97	0.45
1:D:225:PHE:CZ	1:D:297:LEU:HD23	2.50	0.45
1:A:222:ALA:HA	3:A:463:HOH:O	2.16	0.45
1:D:126:GLU:OE1	1:D:424:ILE:HA	2.16	0.45
1:B:9:GLU:CD	1:B:39:ARG:HH22	2.20	0.45
1:D:147:VAL:HG12	1:D:212:GLU:CG	2.45	0.45
1:C:212:GLU:OE2	1:C:214:ASP:OD1	2.35	0.45
1:B:286:PHE:HB3	1:B:303:GLN:HE21	1.82	0.45
1:A:101:GLY:O	1:A:102:THR:OG1	2.30	0.45
1:A:99:GLU:HB3	1:A:100:TYR:CD2	2.51	0.45
1:D:115:ASP:OD1	1:D:115:ASP:N	2.50	0.45
1:A:141:ASN:OD1	1:A:218:SER:N	2.50	0.45
1:A:141:ASN:HA	1:A:218:SER:O	2.17	0.45
1:D:213:ILE:HG13	1:D:227:PRO:CB	2.47	0.45
1:B:379:ILE:HG21	1:B:385:GLU:HG2	1.98	0.45
1:C:2:ARG:HG3	1:C:70:MET:CA	2.42	0.45
1:A:327:GLU:O	1:A:330:SER:OG	2.30	0.45
1:A:214:ASP:OD2	1:A:228:HIS:NE2	2.50	0.45
1:D:180:LEU:O	1:D:188:ASN:ND2	2.50	0.45
1:C:280:LEU:HD11	1:C:286:PHE:CG	2.51	0.45
1:D:40:TRP:N	3:D:702:HOH:O	2.49	0.45
1:C:80:THR:HA	1:C:98:HIS:CD2	2.52	0.45
1:C:43:ASP:OD1	1:C:44:ASP:N	2.49	0.45
1:D:16:TRP:HZ2	1:D:118:GLN:OE1	1.99	0.45
1:C:374:LEU:HB3	1:C:378:SER:HB3	1.98	0.45
1:C:34:ILE:HG13	1:C:35:ASP:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ARG:NH2	1:A:205:PRO:O	2.50	0.45
1:D:62:ALA:O	1:D:187:ALA:HB3	2.15	0.45
1:A:198:ASP:OD1	1:A:201:ALA:N	2.50	0.45
1:A:244:GLY:N	1:A:253:ALA:O	2.50	0.45
1:C:1:PCA:HG3	1:C:182:PHE:CD1	2.52	0.45
1:D:368:ASP:HB2	1:D:373:MET:CE	2.47	0.45
1:C:144:LEU:HD21	1:C:361:LEU:HD11	1.97	0.45
1:A:142:SER:HB2	1:A:414:VAL:HB	1.98	0.45
1:B:368:ASP:OD2	1:B:372:ASN:N	2.50	0.45
1:C:366:TRP:HE3	1:C:367:ASP:O	2.00	0.45
1:B:40:TRP:CE3	1:B:72:GLU:HG3	2.52	0.45
1:C:172:CYS:HB3	1:C:235:TYR:CE1	2.52	0.45
1:B:239:GLU:O	1:B:242:ASN:N	2.50	0.45
1:C:242:ASN:N	1:C:242:ASN:OD1	2.49	0.45
1:D:2:ARG:NH1	1:D:67:GLU:O	2.50	0.45
1:C:264:ASN:ND2	3:C:443:HOH:O	2.49	0.45
1:A:378:SER:OG	1:A:395:CYS:O	2.30	0.45
1:B:17:GLN:OE1	1:B:420:ARG:NE	2.50	0.45
1:C:368:ASP:O	1:C:372:ASN:ND2	2.50	0.45
1:D:155:MET:HG3	1:D:164:GLY:HA2	1.99	0.45
1:C:327:GLU:N	3:C:615:HOH:O	2.50	0.45
1:C:3:ALA:O	1:C:5:ASN:ND2	2.50	0.45
1:D:20:THR:N	1:D:24:ASN:O	2.50	0.45
1:B:11:HIS:HB2	1:B:31:GLU:HG3	1.99	0.45
1:A:294:GLU:OE2	1:A:349:GLU:OE1	2.35	0.45
1:A:240:THR:OG1	1:A:241:THR:N	2.50	0.45
1:B:276:LYS:N	1:B:282:THR:OG1	2.50	0.45
1:D:332:MET:HG2	1:D:333:PHE:N	2.31	0.45
1:C:196:THR:OG1	1:C:196:THR:O	2.29	0.45
1:B:283:SER:O	1:B:283:SER:OG	2.35	0.45
1:C:42:HIS:HA	1:C:48:ASN:HA	1.99	0.45
1:A:401:VAL:HA	1:A:402:PRO:HD2	1.62	0.45
1:B:51:ASP:O	1:B:54:GLN:O	2.34	0.45
1:A:250:ASP:CB	1:A:253:ALA:HB2	2.47	0.45
1:B:142:SER:O	1:B:416:TRP:HH2	1.99	0.45
1:A:37:ASN:O	1:A:181:LYS:NZ	2.50	0.45
1:C:205:PRO:HB2	1:C:206:TYR:CD2	2.51	0.45
1:B:244:GLY:H	1:B:254:GLY:CA	2.30	0.45
1:A:35:ASP:HB3	1:A:38:TRP:CZ3	2.52	0.45
1:B:251:ARG:NH2	2:B:431:CTR:O5B	2.50	0.45
1:B:144:LEU:HD21	1:B:361:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:PHE:CE1	1:B:187:ALA:HB2	2.51	0.45
1:B:41:LEU:O	1:B:48:ASN:ND2	2.50	0.45
1:B:296:LYS:HB2	1:B:296:LYS:HE3	1.71	0.45
1:A:223:PHE:CE2	1:A:265:PRO:HG2	2.51	0.45
1:A:302:ILE:HA	1:A:306:ARG:O	2.17	0.45
1:C:242:ASN:ND2	3:C:592:HOH:O	2.50	0.45
1:B:7:THR:HG22	1:B:73:GLY:HA3	1.99	0.45
1:D:349:GLU:HB2	3:D:641:HOH:O	2.16	0.45
1:A:117:TYR:OH	1:A:169:THR:O	2.30	0.45
1:A:85:THR:HA	1:A:89:ALA:O	2.17	0.45
1:A:123:MET:HB2	1:A:355:LEU:O	2.17	0.45
1:A:415:VAL:HG22	1:A:415:VAL:O	2.16	0.45
1:C:189:ILE:O	1:C:191:GLY:N	2.50	0.45
1:A:356:ARG:HD3	1:B:21:ALA:HB2	1.99	0.45
1:D:143:ALA:HB3	1:D:364:SER:OG	2.17	0.45
1:A:368:ASP:HB3	1:A:373:MET:HE1	1.98	0.44
1:B:313:PRO:HD2	1:B:319:PRO:O	2.17	0.44
1:A:18:ARG:O	1:A:26:GLN:N	2.50	0.44
1:D:4:GLY:O	1:D:5:ASN:ND2	2.50	0.44
1:B:413:GLN:NE2	3:B:606:HOH:O	2.49	0.44
1:A:286:PHE:HB3	1:A:303:GLN:CG	2.48	0.44
1:A:147:VAL:O	1:A:149:MET:N	2.50	0.44
1:C:180:LEU:HD23	3:C:436:HOH:O	2.17	0.44
1:A:88:ASP:OD2	1:A:418:ASN:N	2.50	0.44
1:B:314:THR:HG22	3:B:584:HOH:O	2.16	0.44
1:D:372:ASN:HB3	1:D:400:GLY:HA3	1.98	0.44
1:D:349:GLU:OE1	1:D:352:ASN:HB2	2.17	0.44
1:A:214:ASP:OD1	1:A:214:ASP:N	2.50	0.44
1:B:214:ASP:N	1:B:226:THR:O	2.49	0.44
1:A:195:SER:OG	1:A:198:ASP:N	2.50	0.44
1:B:176:CYS:O	1:B:178:ARG:N	2.50	0.44
1:A:120:PHE:N	1:A:359:MET:O	2.49	0.44
1:A:405:VAL:HG12	3:A:585:HOH:O	2.17	0.44
1:A:142:SER:OG	1:A:142:SER:O	2.33	0.44
1:B:21:ALA:O	1:B:23:GLY:N	2.50	0.44
1:A:172:CYS:HB2	1:A:208:SER:O	2.18	0.44
1:A:173:ASP:HB2	1:A:212:GLU:CD	2.36	0.44
1:D:1:PCA:HG3	1:D:182:PHE:CD1	2.52	0.44
1:D:269:GLY:O	1:D:271:PRO:HD3	2.18	0.44
1:B:416:TRP:O	1:B:417:SER:HB3	2.17	0.44
1:D:250:ASP:OD2	1:D:253:ALA:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:THR:HG22	1:A:88:ASP:CA	2.47	0.44
1:C:231:THR:OG1	1:C:255:LYS:HG2	2.17	0.44
1:A:341:ARG:HD2	1:A:344:GLU:OE1	2.18	0.44
1:D:62:ALA:CA	1:D:187:ALA:HB3	2.43	0.44
1:B:85:THR:O	1:B:86:SER:HB2	2.16	0.44
1:D:130:ASP:OD2	1:D:418:ASN:HB3	2.17	0.44
1:A:230:CYS:HB2	1:A:232:THR:O	2.18	0.44
1:C:158:TYR:O	1:C:161:ASN:HB3	2.18	0.44
1:B:312:PRO:HB3	1:B:321:SER:HA	1.99	0.44
1:A:77:TYR:HB3	1:A:83:ALA:CB	2.38	0.44
1:A:176:CYS:O	1:A:178:ARG:N	2.49	0.44
1:C:41:LEU:HD11	1:C:71:ILE:HG23	1.98	0.44
1:C:122:LEU:HD13	1:C:359:MET:HG3	1.98	0.44
1:B:38:TRP:CZ2	1:B:106:SER:HA	2.52	0.44
1:C:89:ALA:HA	1:C:416:TRP:O	2.18	0.44
1:D:125:ASN:HD22	1:D:423:PRO:HA	1.81	0.44
1:D:123:MET:HG2	1:D:293:GLU:HA	1.99	0.44
1:C:37:ASN:ND2	2:C:432:CTR:O2B	2.50	0.44
1:B:95:VAL:HA	1:B:103:ASN:O	2.18	0.44
1:C:379:ILE:O	1:C:379:ILE:HG22	2.18	0.44
1:D:21:ALA:N	1:D:426:SER:HB2	2.33	0.44
1:A:326:PRO:HG3	1:A:348:PHE:CB	2.47	0.44
1:A:281:ASP:O	1:A:303:GLN:NE2	2.50	0.44
1:C:83:ALA:HA	1:C:91:THR:O	2.18	0.44
1:A:118:GLN:O	1:A:360:VAL:HG23	2.18	0.44
1:C:63:THR:CG2	1:C:186:LYS:HZ2	2.31	0.44
1:A:26:GLN:NE2	3:A:444:HOH:O	2.50	0.44
1:A:318:MET:HE3	1:A:332:MET:HA	1.99	0.44
1:D:345:VAL:HG23	1:D:345:VAL:O	2.16	0.44
1:D:189:ILE:HG23	1:D:190:GLU:N	2.33	0.44
1:A:54:GLN:HG3	1:A:194:SER:OG	2.17	0.44
1:A:384:LYS:HD3	1:A:384:LYS:HA	1.38	0.44
1:B:36:ALA:CA	1:B:39:ARG:HD2	2.37	0.44
1:D:213:ILE:HG12	1:D:355:LEU:HD21	1.99	0.44
1:C:195:SER:HB2	1:C:201:ALA:C	2.36	0.44
1:C:38:TRP:CZ3	2:C:432:CTR:H6C1	2.52	0.43
1:A:302:ILE:HD11	1:A:430:PHE:CD1	2.53	0.43
1:C:307:LYS:HB2	1:C:430:PHE:CE2	2.53	0.43
1:A:42:HIS:O	1:A:69:CYS:HA	2.18	0.43
1:A:366:TRP:CZ3	1:A:368:ASP:HB2	2.53	0.43
1:A:404:GLU:O	1:A:408:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:GLU:OE2	1:D:74:ALA:N	2.50	0.43
1:B:329:CYS:O	1:B:333:PHE:HD1	2.01	0.43
1:D:33:VAL:HG11	1:D:111:MET:CE	2.47	0.43
1:C:428:TYR:HA	3:C:454:HOH:O	2.16	0.43
1:A:78:LEU:HD23	1:A:84:SER:HB3	1.99	0.43
1:D:1:PCA:OE	1:D:161:ASN:HB2	2.18	0.43
1:A:346:GLY:HA3	1:A:350:GLN:CB	2.46	0.43
1:B:242:ASN:N	1:B:242:ASN:OD1	2.50	0.43
1:C:377:ASP:O	1:C:395:CYS:HB2	2.19	0.43
1:A:378:SER:O	1:A:392:ARG:N	2.50	0.43
1:A:78:LEU:HA	1:A:83:ALA:O	2.17	0.43
1:B:173:ASP:OD1	1:B:175:GLN:N	2.49	0.43
1:B:55:TRP:CD1	1:B:189:ILE:HA	2.54	0.43
1:B:336:PHE:O	1:B:338:ASP:OD2	2.36	0.43
1:A:342:PHE:O	1:A:347:GLY:N	2.49	0.43
1:B:36:ALA:HB2	1:B:167:TYR:O	2.17	0.43
1:B:155:MET:HG3	1:B:164:GLY:CA	2.48	0.43
1:C:41:LEU:HG	1:C:71:ILE:HA	2.00	0.43
1:C:226:THR:HG23	1:C:262:ASP:HB3	2.00	0.43
1:A:141:ASN:HD21	1:A:217:GLU:HB3	1.83	0.43
1:B:234:GLU:H	1:B:234:GLU:HG2	1.34	0.43
1:A:200:ASN:ND2	3:A:584:HOH:O	2.50	0.43
1:A:372:ASN:HB3	1:A:400:GLY:HA3	2.01	0.43
1:A:99:GLU:HB3	1:A:100:TYR:CE2	2.53	0.43
1:C:54:GLN:HA	1:C:192:TRP:CD1	2.53	0.43
1:D:140:ILE:HG22	1:D:141:ASN:N	2.34	0.43
1:A:97:LYS:HD2	1:A:97:LYS:H	1.82	0.43
1:D:95:VAL:HG13	1:D:104:VAL:CG2	2.49	0.43
1:C:272:ASP:C	1:C:278:LYS:HD3	2.39	0.43
1:D:217:GLU:O	1:D:223:PHE:HA	2.18	0.43
1:B:122:LEU:CD2	1:B:359:MET:HG3	2.49	0.43
1:A:98:HIS:CE1	1:A:101:GLY:HA3	2.54	0.43
1:C:55:TRP:CH2	1:C:187:ALA:HB1	2.53	0.43
1:D:115:ASP:HB3	1:D:166:ARG:NE	2.33	0.43
1:A:392:ARG:HH12	2:A:431:CTR:H6C1	1.81	0.43
1:D:198:ASP:HA	1:D:199:PRO:HD2	1.68	0.43
1:A:319:PRO:HG3	1:A:328:LEU:CA	2.47	0.43
1:A:288:VAL:O	1:A:288:VAL:HG12	2.18	0.43
1:A:131:VAL:HG13	1:A:131:VAL:O	2.18	0.43
1:A:349:GLU:O	1:A:352:ASN:N	2.51	0.43
1:B:2:ARG:NE	1:B:70:MET:HG2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ASN:O	1:C:365:ILE:HA	2.18	0.43
1:D:41:LEU:HG	1:D:71:ILE:HG23	2.01	0.43
1:C:88:ASP:OD1	1:C:88:ASP:N	2.50	0.43
1:B:357:VAL:HB	1:B:359:MET:HE2	2.00	0.43
1:C:293:GLU:HG2	1:C:424:ILE:CD1	2.49	0.43
1:A:19:CYS:HA	1:A:25:CYS:CB	2.49	0.43
1:A:44:ASP:OD1	1:A:45:ASN:N	2.50	0.43
1:C:263:TYR:CZ	1:C:322:SER:HA	2.54	0.43
1:C:274:TYR:C	1:C:278:LYS:HD2	2.39	0.43
1:A:77:TYR:O	1:A:83:ALA:N	2.50	0.43
1:A:268:MET:O	1:A:314:THR:N	2.50	0.43
1:A:216:TRP:CZ3	1:A:288:VAL:HG21	2.53	0.43
1:D:136:VAL:HG12	1:D:219:ASN:HB3	1.99	0.43
1:A:41:LEU:O	1:A:48:ASN:HA	2.19	0.42
1:C:348:PHE:O	1:C:351:LEU:HB3	2.19	0.42
1:C:284:ARG:HD2	1:C:303:GLN:NE2	2.33	0.42
1:C:315:TRP:HB3	1:C:335:VAL:HG11	2.01	0.42
1:B:119:MET:HG2	1:B:151:GLU:HG3	2.00	0.42
1:B:11:HIS:CB	1:B:31:GLU:HG3	2.49	0.42
1:D:257:ASP:HA	1:D:341:ARG:HG2	1.99	0.42
1:C:80:THR:HG23	1:C:98:HIS:NE2	2.34	0.42
1:B:275:GLY:O	1:B:278:LYS:HB2	2.18	0.42
1:A:226:THR:HG22	1:A:228:HIS:HD2	1.83	0.42
1:C:251:ARG:HG2	1:C:251:ARG:O	2.18	0.42
1:B:71:ILE:CD1	1:B:167:TYR:HB3	2.49	0.42
1:A:21:ALA:HB3	1:B:116:LYS:CE	2.44	0.42
1:B:68:LYS:HE3	3:B:715:HOH:O	2.19	0.42
1:C:401:VAL:O	1:C:405:VAL:HG13	2.19	0.42
1:D:310:ILE:HD12	3:D:657:HOH:O	2.18	0.42
1:A:142:SER:HB2	1:A:414:VAL:HG21	2.01	0.42
1:A:381:PRO:O	1:A:383:GLU:N	2.49	0.42
1:D:294:GLU:O	1:D:295:ASN:HB2	2.19	0.42
1:C:383:GLU:H	1:C:383:GLU:HG2	1.37	0.42
1:B:246:THR:HG22	1:B:370:TYR:CD2	2.55	0.42
1:D:5:ASN:N	1:D:72:GLU:OE2	2.52	0.42
1:D:418:ASN:HA	3:D:677:HOH:O	2.18	0.42
1:D:221:TYR:O	1:D:222:ALA:HB2	2.19	0.42
1:D:124:GLY:N	1:D:292:PHE:O	2.50	0.42
1:A:416:TRP:O	1:A:417:SER:HB3	2.19	0.42
1:D:23:GLY:O	1:D:25:CYS:N	2.50	0.42
1:B:11:HIS:HB2	3:B:629:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ASP:CG	1:A:253:ALA:HB2	2.40	0.42
1:C:279:THR:HG22	1:C:280:LEU:N	2.34	0.42
1:A:428:TYR:HB3	1:A:430:PHE:CE1	2.55	0.42
1:A:126:GLU:CD	1:A:425:GLY:H	2.22	0.42
1:A:418:ASN:HD21	1:A:420:ARG:NH2	2.18	0.42
1:A:420:ARG:HB3	1:A:427:THR:HG22	2.01	0.42
1:D:369:HIS:CG	1:D:402:PRO:HG2	2.54	0.42
1:B:257:ASP:OD2	1:B:342:PHE:HD1	2.02	0.42
1:C:117:TYR:HE2	1:C:153:GLY:HA2	1.83	0.42
1:D:291:ARG:HD3	1:D:424:ILE:HG23	2.01	0.42
1:D:95:VAL:HG11	1:D:97:LYS:HZ1	1.85	0.42
1:A:257:ASP:HA	1:A:341:ARG:HG2	2.01	0.42
1:B:129:PHE:HZ	1:B:216:TRP:CG	2.38	0.42
1:B:141:ASN:ND2	1:B:217:GLU:OE1	2.50	0.42
1:C:66:ALA:HA	1:C:182:PHE:CE1	2.54	0.42
1:B:2:ARG:HG2	1:B:162:GLN:HE22	1.85	0.42
1:A:420:ARG:HB3	1:A:427:THR:HB	2.02	0.42
1:A:429:ASP:OD2	1:A:429:ASP:O	2.37	0.42
1:B:80:THR:HB	1:B:81:TYR:CD2	2.55	0.42
2:A:431:CTR:O2A	2:A:431:CTR:H6B2	2.20	0.42
1:B:92:LEU:HD12	1:B:416:TRP:HE1	1.84	0.42
1:C:48:ASN:ND2	1:C:51:ASP:OD2	2.50	0.42
1:D:117:TYR:CZ	1:D:165:ALA:HB1	2.55	0.42
1:A:267:ARG:HG3	1:A:392:ARG:HG2	2.02	0.42
1:B:251:ARG:NH2	2:B:431:CTR:O6B	2.50	0.42
1:C:375:TRP:O	1:C:392:ARG:HG2	2.19	0.42
1:D:4:GLY:N	1:D:71:ILE:O	2.50	0.42
1:D:9:GLU:OE2	1:D:73:GLY:HA2	2.20	0.42
1:C:318:MET:CE	1:C:332:MET:HA	2.50	0.42
1:C:250:ASP:HB3	1:C:253:ALA:CB	2.50	0.42
1:A:232:THR:CG2	1:A:234:GLU:HG2	2.49	0.42
1:B:333:PHE:O	1:B:337:ASN:HA	2.20	0.42
1:A:373:MET:CG	1:A:376:LEU:HD23	2.38	0.42
1:C:4:GLY:N	1:C:71:ILE:O	2.50	0.42
1:C:111:MET:HA	1:C:118:GLN:H	1.84	0.42
1:B:127:LEU:HB2	1:B:421:PHE:HD1	1.84	0.42
1:D:82:GLY:CA	1:D:96:THR:HG21	2.50	0.42
1:A:146:PHE:HE1	1:A:215:VAL:HG21	1.83	0.42
1:A:295:ASN:N	1:A:352:ASN:OD1	2.52	0.42
1:B:225:PHE:O	1:B:263:TYR:N	2.49	0.42
1:A:142:SER:HB2	1:A:414:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:LYS:HD3	3:B:701:HOH:O	2.19	0.42
1:A:76:ASP:CB	1:D:76:ASP:HB3	2.43	0.41
1:A:178:ARG:HD3	1:A:248:SER:OG	2.19	0.41
1:D:155:MET:O	1:D:159:PRO:HA	2.20	0.41
1:C:3:ALA:HA	1:C:71:ILE:HD12	2.01	0.41
1:C:405:VAL:HG23	1:C:406:GLU:HG3	2.02	0.41
1:D:74:ALA:HB3	1:D:77:TYR:CZ	2.55	0.41
1:A:356:ARG:HD3	1:B:21:ALA:CB	2.50	0.41
1:A:279:THR:HG22	1:A:280:LEU:N	2.34	0.41
1:A:14:LEU:HA	1:A:14:LEU:HD12	1.77	0.41
1:C:350:GLN:O	1:C:353:ASN:N	2.52	0.41
1:B:179:ASP:HB3	1:B:247:TYR:OH	2.19	0.41
1:D:244:GLY:HA2	1:D:250:ASP:O	2.20	0.41
1:B:310:ILE:HA	1:B:311:PRO:HD3	1.81	0.41
1:A:4:GLY:N	1:A:70:MET:HB2	2.35	0.41
1:C:141:ASN:HB2	1:C:373:MET:SD	2.61	0.41
1:A:329:CYS:HA	1:A:332:MET:HE2	2.02	0.41
1:B:42:HIS:CB	1:B:48:ASN:HA	2.50	0.41
1:C:402:PRO:O	1:C:405:VAL:HG22	2.20	0.41
1:B:32:VAL:HG12	1:B:109:TYR:C	2.41	0.41
1:D:310:ILE:HD12	1:D:310:ILE:N	2.35	0.41
1:C:286:PHE:HB3	1:C:303:GLN:NE2	2.36	0.41
1:A:374:LEU:HD13	1:A:382:PRO:CG	2.50	0.41
1:B:186:LYS:HA	1:B:186:LYS:HD3	1.53	0.41
1:A:251:ARG:HH22	2:A:431:CTR:H6B1	1.85	0.41
1:B:327:GLU:OE1	1:B:327:GLU:HA	2.20	0.41
1:C:91:THR:C	1:C:92:LEU:HD23	2.41	0.41
1:B:349:GLU:HA	1:B:352:ASN:HB2	2.03	0.41
1:A:380:TYR:CD1	1:A:382:PRO:HD3	2.55	0.41
1:A:366:TRP:HZ3	1:A:368:ASP:HB2	1.85	0.41
1:D:375:TRP:O	1:D:392:ARG:HD3	2.20	0.41
1:C:122:LEU:CD1	1:C:359:MET:HG3	2.50	0.41
1:C:324:ILE:HG23	1:C:328:LEU:HD12	2.03	0.41
1:B:85:THR:HG23	1:B:86:SER:N	2.35	0.41
1:A:12:PRO:O	1:A:32:VAL:N	2.53	0.41
1:C:62:ALA:N	1:C:190:GLU:OE1	2.50	0.41
1:C:313:PRO:HG2	1:C:318:MET:HB3	2.02	0.41
1:C:53:ASN:CG	1:C:194:SER:HB3	2.40	0.41
1:B:332:MET:HB2	1:B:332:MET:HE2	1.92	0.41
1:A:1:PCA:HG3	1:A:182:PHE:CG	2.55	0.41
1:B:368:ASP:HB3	1:B:373:MET:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:TYR:HD1	1:D:280:LEU:HD12	1.81	0.41
1:D:80:THR:HG22	1:D:98:HIS:CE1	2.56	0.41
1:B:251:ARG:NH1	1:B:251:ARG:HG3	2.36	0.41
1:C:324:ILE:CG2	1:C:328:LEU:HD12	2.51	0.41
1:D:278:LYS:HG3	1:D:278:LYS:HZ3	1.67	0.41
1:A:326:PRO:HG3	1:A:348:PHE:HB3	2.01	0.41
1:D:14:LEU:HD13	1:D:85:THR:OG1	2.20	0.41
1:D:34:ILE:HG13	1:D:107:ARG:O	2.20	0.41
1:A:374:LEU:HB3	1:A:380:TYR:CD1	2.56	0.41
1:D:176:CYS:HA	1:D:208:SER:O	2.20	0.41
1:D:80:THR:HA	1:D:98:HIS:CE1	2.56	0.41
1:B:368:ASP:O	1:B:372:ASN:HA	2.20	0.41
1:A:18:ARG:NH1	1:A:28:VAL:HG22	2.36	0.41
1:C:115:ASP:HA	1:C:166:ARG:HD3	2.02	0.41
1:B:175:GLN:OE1	1:B:175:GLN:HA	2.20	0.41
1:B:355:LEU:HA	1:B:355:LEU:HD22	1.85	0.41
1:B:404:GLU:O	1:B:407:ALA:HB3	2.20	0.41
1:B:280:LEU:HD11	1:B:286:PHE:CD1	2.56	0.41
1:B:337:ASN:HA	1:B:337:ASN:HD22	1.49	0.41
1:A:372:ASN:HB3	1:A:400:GLY:C	2.41	0.41
1:C:126:GLU:HA	1:C:290:SER:O	2.21	0.41
1:B:107:ARG:NH1	3:B:664:HOH:O	2.50	0.41
1:C:132:ASP:CB	1:C:415:VAL:HG13	2.36	0.41
1:B:17:GLN:HB2	1:B:420:ARG:CG	2.41	0.41
1:C:222:ALA:N	1:C:274:TYR:HE2	2.19	0.41
1:A:7:THR:HG21	1:A:75:GLY:H	1.86	0.41
1:B:231:THR:HG1	1:B:255:LYS:HB3	1.86	0.41
1:C:63:THR:OG1	1:C:186:LYS:NZ	2.50	0.41
1:D:7:THR:N	1:D:72:GLU:OE1	2.52	0.41
1:B:365:ILE:O	1:B:365:ILE:HG23	2.21	0.41
1:C:295:ASN:HA	1:C:348:PHE:CE2	2.55	0.41
1:D:265:PRO:HA	1:D:268:MET:HB2	2.01	0.41
1:A:357:VAL:HA	1:A:358:PRO:HD2	1.78	0.41
1:C:109:TYR:HH	1:C:171:TYR:HB2	1.85	0.41
1:A:142:SER:HB2	1:A:414:VAL:CB	2.51	0.41
1:D:2:ARG:HD3	1:D:2:ARG:HH11	1.74	0.41
1:D:60:SER:C	1:D:189:ILE:HD13	2.41	0.41
1:A:51:ASP:O	1:A:54:GLN:O	2.38	0.41
1:D:61:THR:OG1	1:D:64:ASP:OD2	2.30	0.41
1:D:188:ASN:HB3	1:D:192:TRP:CE3	2.56	0.41
1:B:195:SER:OG	1:B:196:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TRP:CE3	1:A:388:PRO:HB3	2.55	0.41
1:C:311:PRO:HA	1:C:312:PRO:HD3	1.95	0.41
1:D:239:GLU:C	1:D:240:THR:HG1	2.23	0.41
1:C:149:MET:HG2	1:C:170:GLY:O	2.21	0.41
1:C:276:LYS:HG2	1:C:283:SER:HB3	2.03	0.41
1:C:37:ASN:OD1	1:C:180:LEU:HA	2.21	0.40
1:A:143:ALA:HA	1:A:216:TRP:O	2.21	0.40
1:B:15:THR:HA	1:B:28:VAL:O	2.21	0.40
1:B:215:VAL:HA	1:B:225:PHE:CE2	2.56	0.40
1:A:171:TYR:OH	1:A:173:ASP:OD2	2.30	0.40
1:B:251:ARG:HH11	1:B:251:ARG:HG3	1.86	0.40
1:D:278:LYS:HB3	1:D:279:THR:H	1.61	0.40
1:A:11:HIS:CD2	1:A:33:VAL:HG23	2.57	0.40
1:A:113:GLY:HA3	3:A:477:HOH:O	2.20	0.40
1:A:103:ASN:ND2	3:A:436:HOH:O	2.55	0.40
1:A:55:TRP:CG	1:A:189:ILE:HG13	2.57	0.40
1:A:189:ILE:HG23	1:A:190:GLU:N	2.36	0.40
1:B:377:ASP:HB2	1:B:395:CYS:SG	2.62	0.40
1:C:401:VAL:O	1:C:405:VAL:HG22	2.22	0.40
1:C:208:SER:HB3	1:C:235:TYR:CE1	2.56	0.40
1:D:381:PRO:HB2	1:D:383:GLU:CD	2.42	0.40
1:A:126:GLU:OE1	1:A:291:ARG:HG2	2.21	0.40
1:A:252:PHE:HB3	1:A:341:ARG:CD	2.50	0.40
1:C:82:GLY:CA	1:C:96:THR:HG21	2.51	0.40
1:B:118:GLN:NE2	1:B:119:MET:N	2.69	0.40
1:A:198:ASP:OD1	1:A:200:ASN:N	2.50	0.40
1:B:362:VAL:HG12	1:B:363:MET:N	2.37	0.40
1:D:52:GLY:HA2	3:D:840:HOH:O	2.22	0.40
1:A:99:GLU:HG2	1:A:100:TYR:CE2	2.56	0.40
1:C:219:ASN:OD1	1:C:222:ALA:N	2.53	0.40
1:D:292:PHE:HB3	1:D:355:LEU:HD13	2.02	0.40
1:A:16:TRP:CE2	1:A:28:VAL:HG11	2.56	0.40
1:A:28:VAL:O	1:A:28:VAL:HG12	2.22	0.40
1:B:251:ARG:HG2	1:B:251:ARG:O	2.22	0.40
1:B:147:VAL:O	1:B:149:MET:N	2.54	0.40
1:D:382:PRO:O	1:D:384:LYS:N	2.54	0.40
1:D:193:LYS:NZ	3:D:712:HOH:O	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	428/430 (100%)	359 (84%)	54 (13%)	15 (4%)	4	0
1	B	428/430 (100%)	355 (83%)	56 (13%)	17 (4%)	4	0
1	C	428/430 (100%)	379 (89%)	37 (9%)	12 (3%)	6	1
1	D	428/430 (100%)	373 (87%)	46 (11%)	9 (2%)	9	1
All	All	1712/1720 (100%)	1466 (86%)	193 (11%)	53 (3%)	5	0

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	MET
1	A	47	GLN
1	A	148	ALA
1	A	240	THR
1	A	384	LYS
1	B	43	ASP
1	B	56	THR
1	B	98	HIS
1	B	232	THR
1	B	248	SER
1	B	278	LYS
1	C	44	ASP
1	C	45	ASN
1	C	164	GLY
1	C	399	SER
1	D	383	GLU
1	D	390	ALA
1	A	105	GLY
1	A	177	ALA
1	A	210	CYS
1	A	385	GLU
1	B	86	SER

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Mol	Chain	Res	Type
1	B	165	ALA
1	B	176	CYS
1	B	189	ILE
1	B	197	SER
1	B	210	CYS
1	B	260	GLY
1	D	246	THR
1	D	385	GLU
1	A	102	THR
1	A	176	CYS
1	B	240	THR
1	B	385	GLU
1	C	46	MET
1	C	176	CYS
1	C	296	LYS
1	D	46	MET
1	A	123	MET
1	A	185	GLY
1	A	402	PRO
1	B	247	TYR
1	C	31	GLU
1	D	24	ASN
1	A	24	ASN
1	B	22	PRO
1	C	78	LEU
1	C	192	TRP
1	C	190	GLU
1	C	402	PRO
1	D	388	PRO
1	D	402	PRO
1	D	199	PRO

### 5.3.2 Protein sidechains ⓘ

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	354/354 (100%)	260 (73%)	94 (27%)	0	0
1	B	354/354 (100%)	274 (77%)	80 (23%)	1	0
1	C	354/354 (100%)	292 (82%)	62 (18%)	2	0
1	D	354/354 (100%)	303 (86%)	51 (14%)	4	0
All	All	1416/1416 (100%)	1129 (80%)	287 (20%)	1	0

All (287) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	6	GLU
1	A	15	THR
1	A	17	GLN
1	A	20	THR
1	A	32	VAL
1	A	39	ARG
1	A	40	TRP
1	A	46	MET
1	A	53	ASN
1	A	59	CYS
1	A	61	THR
1	A	63	THR
1	A	70	MET
1	A	71	ILE
1	A	76	ASP
1	A	78	LEU
1	A	84	SER
1	A	85	THR
1	A	86	SER
1	A	88	ASP
1	A	96	THR
1	A	97	LYS
1	A	99	GLU
1	A	100	TYR
1	A	106	SER
1	A	117	TYR
1	A	122	LEU
1	A	133	LEU
1	A	135	THR

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Mol	Chain	Res	Type
1	A	137	GLU
1	A	151	GLU
1	A	155	MET
1	A	157	SER
1	A	162	GLN
1	A	175	GLN
1	A	178	ARG
1	A	179	ASP
1	A	181	LYS
1	A	193	LYS
1	A	195	SER
1	A	196	THR
1	A	197	SER
1	A	203	VAL
1	A	213	ILE
1	A	214	ASP
1	A	228	HIS
1	A	234	GLU
1	A	236	HIS
1	A	239	GLU
1	A	241	THR
1	A	242	ASN
1	A	246	THR
1	A	252	PHE
1	A	257	ASP
1	A	266	TYR
1	A	267	ARG
1	A	276	LYS
1	A	290	SER
1	A	294	GLU
1	A	296	LYS
1	A	298	SER
1	A	303	GLN
1	A	304	ASP
1	A	306	ARG
1	A	308	ILE
1	A	315	TRP
1	A	316	GLU
1	A	318	MET
1	A	319	PRO
1	A	320	ASN
1	A	321	SER

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Mol	Chain	Res	Type
1	A	322	SER
1	A	332	MET
1	A	335	VAL
1	A	336	PHE
1	A	338	ASP
1	A	340	ASN
1	A	348	PHE
1	A	353	ASN
1	A	360	VAL
1	A	363	MET
1	A	368	ASP
1	A	376	LEU
1	A	377	ASP
1	A	379	ILE
1	A	383	GLU
1	A	394	ASP
1	A	401	VAL
1	A	405	VAL
1	A	409	PHE
1	A	415	VAL
1	A	420	ARG
1	A	421	PHE
1	B	2	ARG
1	B	6	GLU
1	B	7	THR
1	B	15	THR
1	B	18	ARG
1	B	26	GLN
1	B	31	GLU
1	B	32	VAL
1	B	34	ILE
1	B	37	ASN
1	B	41	LEU
1	B	45	ASN
1	B	47	GLN
1	B	48	ASN
1	B	51	ASP
1	B	54	GLN
1	B	56	THR
1	B	61	THR
1	B	68	LYS
1	B	70	MET

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Mol	Chain	Res	Type
1	B	76	ASP
1	B	78	LEU
1	B	80	THR
1	B	85	THR
1	B	93	LYS
1	B	98	HIS
1	B	112	ASN
1	B	116	LYS
1	B	122	LEU
1	B	127	LEU
1	B	133	LEU
1	B	135	THR
1	B	147	VAL
1	B	149	MET
1	B	155	MET
1	B	157	SER
1	B	162	GLN
1	B	181	LYS
1	B	182	PHE
1	B	189	ILE
1	B	193	LYS
1	B	194	SER
1	B	195	SER
1	B	196	THR
1	B	198	ASP
1	B	208	SER
1	B	213	ILE
1	B	234	GLU
1	B	242	ASN
1	B	248	SER
1	B	259	ASN
1	B	278	LYS
1	B	280	LEU
1	B	281	ASP
1	B	283	SER
1	B	284	ARG
1	B	298	SER
1	B	316	GLU
1	B	321	SER
1	B	332	MET
1	B	334	ASP
1	B	337	ASN

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Mol	Chain	Res	Type
1	B	338	ASP
1	B	340	ASN
1	B	343	GLU
1	B	348	PHE
1	B	355	LEU
1	B	359	MET
1	B	361	LEU
1	B	363	MET
1	B	365	ILE
1	B	374	LEU
1	B	376	LEU
1	B	384	LYS
1	B	392	ARG
1	B	398	ASP
1	B	405	VAL
1	B	415	VAL
1	B	427	THR
1	B	429	ASP
1	C	2	ARG
1	C	26	GLN
1	C	34	ILE
1	C	37	ASN
1	C	41	LEU
1	C	45	ASN
1	C	49	CYS
1	C	51	ASP
1	C	67	GLU
1	C	70	MET
1	C	71	ILE
1	C	78	LEU
1	C	86	SER
1	C	90	LEU
1	C	92	LEU
1	C	96	THR
1	C	97	LYS
1	C	100	TYR
1	C	106	SER
1	C	111	MET
1	C	116	LYS
1	C	127	LEU
1	C	133	LEU
1	C	140	ILE

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Mol	Chain	Res	Type
1	C	142	SER
1	C	155	MET
1	C	160	SER
1	C	162	GLN
1	C	166	ARG
1	C	180	LEU
1	C	181	LYS
1	C	193	LYS
1	C	195	SER
1	C	196	THR
1	C	197	SER
1	C	206	TYR
1	C	208	SER
1	C	234	GLU
1	C	239	GLU
1	C	242	ASN
1	C	264	ASN
1	C	272	ASP
1	C	284	ARG
1	C	291	ARG
1	C	294	GLU
1	C	306	ARG
1	C	320	ASN
1	C	323	GLU
1	C	324	ILE
1	C	327	GLU
1	C	328	LEU
1	C	332	MET
1	C	340	ASN
1	C	364	SER
1	C	383	GLU
1	C	385	GLU
1	C	394	ASP
1	C	398	ASP
1	C	408	GLN
1	C	415	VAL
1	C	420	ARG
1	C	426	SER
1	D	2	ARG
1	D	6	GLU
1	D	26	GLN
1	D	37	ASN

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Mol	Chain	Res	Type
1	D	44	ASP
1	D	46	MET
1	D	59	CYS
1	D	64	ASP
1	D	70	MET
1	D	78	LEU
1	D	88	ASP
1	D	93	LYS
1	D	97	LYS
1	D	99	GLU
1	D	100	TYR
1	D	115	ASP
1	D	116	LYS
1	D	122	LEU
1	D	123	MET
1	D	133	LEU
1	D	155	MET
1	D	160	SER
1	D	180	LEU
1	D	186	LYS
1	D	190	GLU
1	D	193	LYS
1	D	194	SER
1	D	196	THR
1	D	246	THR
1	D	251	ARG
1	D	278	LYS
1	D	285	LYS
1	D	292	PHE
1	D	293	GLU
1	D	294	GLU
1	D	298	SER
1	D	306	ARG
1	D	322	SER
1	D	332	MET
1	D	337	ASN
1	D	338	ASP
1	D	348	PHE
1	D	349	GLU
1	D	359	MET
1	D	369	HIS
1	D	383	GLU

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Mol	Chain	Res	Type
1	D	388	PRO
1	D	402	PRO
1	D	413	GLN
1	D	415	VAL
1	D	430	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	24	ASN
1	A	29	ASN
1	A	48	ASN
1	A	103	ASN
1	A	162	GLN
1	A	320	ASN
1	A	353	ASN
1	A	372	ASN
1	B	24	ASN
1	B	29	ASN
1	B	48	ASN
1	B	54	GLN
1	B	118	GLN
1	B	125	ASN
1	B	162	GLN
1	B	200	ASN
1	B	337	ASN
1	B	340	ASN
1	B	352	ASN
1	B	353	ASN
1	B	369	HIS
1	B	372	ASN
1	B	408	GLN
1	B	413	GLN
1	C	5	ASN
1	C	125	ASN
1	C	162	GLN
1	C	320	ASN
1	C	337	ASN
1	C	340	ASN
1	C	352	ASN
1	C	353	ASN

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Mol	Chain	Res	Type
1	C	369	HIS
1	C	372	ASN
1	C	418	ASN
1	D	5	ASN
1	D	26	GLN
1	D	29	ASN
1	D	45	ASN
1	D	98	HIS
1	D	103	ASN
1	D	125	ASN
1	D	320	ASN
1	D	352	ASN
1	D	353	ASN
1	D	369	HIS
1	D	387	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	PCA	A	1	1	7,8,9	1.76	1 (14%)	9,10,12	1.45	2 (22%)
1	PCA	B	1	1	7,8,9	1.71	1 (14%)	9,10,12	1.50	3 (33%)
1	PCA	C	1	1	7,8,9	1.82	1 (14%)	9,10,12	1.88	2 (22%)
1	PCA	D	1	1	7,8,9	1.77	1 (14%)	9,10,12	1.70	3 (33%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	B	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	PCA	CD-N	4.16	1.47	1.33
1	B	1	PCA	CD-N	4.23	1.47	1.33
1	C	1	PCA	CD-N	4.34	1.48	1.33
1	A	1	PCA	CD-N	4.34	1.48	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	PCA	CB-CA-C	-3.32	108.22	112.76
1	D	1	PCA	OE-CD-CG	-3.29	119.46	126.81
1	C	1	PCA	OE-CD-CG	-3.27	119.51	126.81
1	B	1	PCA	OE-CD-CG	-2.87	120.40	126.81
1	A	1	PCA	O-C-CA	-2.78	118.09	125.44
1	D	1	PCA	CB-CA-C	-2.70	109.07	112.76
1	B	1	PCA	CB-CA-C	-2.19	109.76	112.76
1	B	1	PCA	O-C-CA	-2.16	119.72	125.44
1	A	1	PCA	CB-CA-C	-2.11	109.87	112.76
1	D	1	PCA	O-C-CA	-2.10	119.90	125.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	PCA	5	0
1	B	1	PCA	2	0
1	C	1	PCA	2	0
1	D	1	PCA	2	0

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

6 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	CTR	A	431	-	36,36,36	0.56	0	53,53,53	1.40	8 (15%)
2	CTR	A	432	-	36,36,36	0.46	0	53,53,53	1.43	9 (16%)
2	CTR	B	431	-	36,36,36	0.51	0	53,53,53	1.10	5 (9%)
2	CTR	C	431	-	36,36,36	0.59	0	53,53,53	1.49	6 (11%)
2	CTR	C	432	-	36,36,36	0.50	0	53,53,53	1.32	6 (11%)
2	CTR	D	431	-	36,36,36	0.55	0	53,53,53	1.34	6 (11%)

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	CTR	A	431	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	A	432	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	B	431	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	C	431	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	C	432	-	1/1/15/15	0/14/74/74	0/3/3/3
2	CTR	D	431	-	1/1/15/15	0/14/74/74	0/3/3/3

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	432	CTR	C1A-O4B-C4B	-3.77	108.16	118.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	432	CTR	C1B-O5B-C5B	-3.59	106.78	113.75
2	B	431	CTR	C1B-O5B-C5B	-3.50	106.96	113.75
2	C	431	CTR	C1B-O4C-C4C	-3.49	108.89	118.01
2	C	432	CTR	C1A-O5A-C5A	-3.48	107.00	113.75
2	A	431	CTR	C1C-O5C-C5C	-3.46	107.08	113.47
2	D	431	CTR	C1B-O4C-C4C	-3.22	109.60	118.01
2	C	431	CTR	C1A-O4B-C4B	-3.16	109.74	118.01
2	C	432	CTR	C1B-O4C-C4C	-3.07	110.00	118.01
2	B	431	CTR	C1A-O4B-C4B	-2.96	110.26	118.01
2	A	431	CTR	C1B-O5B-C5B	-2.80	108.30	113.75
2	A	432	CTR	O5A-C1A-C2A	-2.70	104.75	110.28
2	A	432	CTR	C1C-O5C-C5C	-2.61	108.64	113.47
2	C	431	CTR	C1B-O5B-C5B	-2.44	109.01	113.75
2	A	432	CTR	C1A-O5A-C5A	-2.44	109.02	113.75
2	A	432	CTR	C1A-O4B-C4B	-2.43	111.66	118.01
2	B	431	CTR	C1B-O4C-C4C	-2.23	112.18	118.01
2	A	431	CTR	C3C-C4C-C5C	-2.20	105.87	110.84
2	D	431	CTR	C3B-C4B-C5B	-2.18	105.90	110.84
2	C	431	CTR	O5B-C1B-C2B	-2.12	105.92	110.28
2	A	431	CTR	C1B-O4C-C4C	-2.12	112.48	118.01
2	A	431	CTR	O5B-C1B-C2B	-2.08	106.01	110.28
2	B	431	CTR	C6A-C5A-C4A	-2.05	107.97	113.02
2	B	431	CTR	C1A-O5A-C5A	-2.01	109.85	113.75
2	A	431	CTR	C2B-C3B-C4B	2.06	114.12	109.60
2	D	431	CTR	O5B-C5B-C4B	2.07	114.12	109.75
2	A	432	CTR	O5C-C5C-C6C	2.12	111.70	106.36
2	C	432	CTR	O5A-C5A-C6A	2.16	111.81	106.36
2	A	432	CTR	C1B-C2B-C3B	2.27	114.45	109.97
2	A	431	CTR	O5A-C5A-C6A	2.39	112.40	106.36
2	D	431	CTR	O5B-C5B-C6B	2.40	112.42	106.36
2	C	432	CTR	O2C-C2C-C1C	2.65	115.66	109.82
2	A	432	CTR	O5A-C5A-C4A	2.69	114.74	109.68
2	D	431	CTR	O5C-C5C-C4C	2.72	115.50	109.75
2	C	432	CTR	O4B-C1A-C2A	2.74	114.76	108.10
2	A	432	CTR	C2B-C3B-C4B	3.01	116.20	109.60
2	C	431	CTR	C1C-O5C-C5C	3.16	119.31	113.47
2	A	431	CTR	C1C-C2C-C3C	3.81	116.10	110.43
2	D	431	CTR	C1A-C2A-C3A	4.33	118.50	109.97
2	C	431	CTR	O5C-C5C-C4C	5.76	121.91	109.75

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	431	CTR	C1C
2	C	431	CTR	C1C
2	A	432	CTR	C1C
2	B	431	CTR	C1C
2	D	431	CTR	C1C
2	C	432	CTR	C1C

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	431	CTR	8	0
2	A	432	CTR	7	0
2	B	431	CTR	5	0
2	C	431	CTR	4	0
2	C	432	CTR	5	0
2	D	431	CTR	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	429/430 (99%)	-0.13	4 (0%) 85 83	9, 29, 48, 80	0
1	B	429/430 (99%)	-0.17	4 (0%) 85 83	11, 28, 44, 61	0
1	C	429/430 (99%)	-0.50	0 100 100	6, 22, 37, 68	0
1	D	429/430 (99%)	-0.50	0 100 100	7, 20, 36, 58	0
All	All	1716/1720 (99%)	-0.33	8 (0%) 91 90	6, 25, 42, 80	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	244	GLY	2.7
1	B	66	ALA	2.6
1	B	269	GLY	2.6
1	A	61	THR	2.3
1	A	59	CYS	2.2
1	A	189	ILE	2.2
1	B	313	PRO	2.1
1	A	58	ALA	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	PCA	D	1	8/9	0.99	0.06	-	5,17,23,43	0
1	PCA	C	1	8/9	0.94	0.12	-	14,25,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	PCA	B	1	8/9	0.95	0.09	-	17,32,40,51	0
1	PCA	A	1	8/9	0.91	0.13	-	24,29,38,39	0

### 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	CTR	C	432	34/34	0.93	0.12	1.44	7,35,60,78	0
2	CTR	D	431	34/34	0.95	0.09	1.04	14,29,53,59	0
2	CTR	A	432	34/34	0.93	0.12	0.17	15,36,57,76	0
2	CTR	B	431	34/34	0.96	0.09	-0.12	9,29,47,66	0
2	CTR	A	431	34/34	0.95	0.09	-0.51	10,30,41,43	0
2	CTR	C	431	34/34	0.98	0.06	-0.96	7,18,31,65	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.