



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:03 PM GMT

PDB ID : 1WAO
Title : PP5 STRUCTURE
Authors : Barford, D.
Deposited on : 2004-10-27
Resolution : 2.90 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

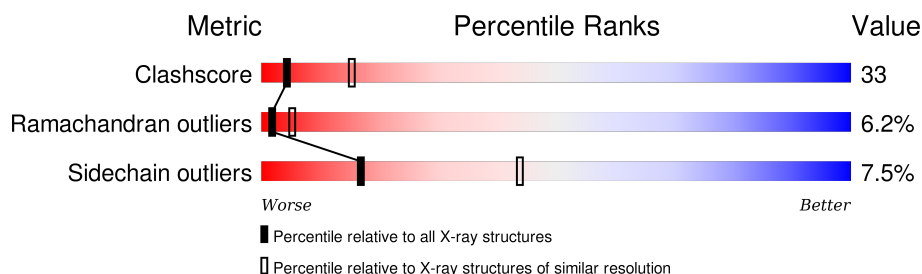
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	477	
1	2	477	
1	3	477	
1	4	477	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15082 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 SERINE/THREONINE PROTEIN PHOSPHATASE 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	471	Total	C	N	O	S	0	0	0
			3781	2407	641	712	21			
1	2	469	Total	C	N	O	S	0	0	0
			3768	2399	639	710	20			
1	3	471	Total	C	N	O	S	0	0	0
			3778	2405	641	712	20			
1	4	466	Total	C	N	O	S	0	0	0
			3747	2386	635	706	20			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	2	2	Total	Mn	0	0
			2	2		
2	1	2	Total	Mn	0	0
			2	2		
2	4	2	Total	Mn	0	0
			2	2		
2	3	2	Total	Mn	0	0
			2	2		

H463	H464	Q465	Q466	S467	D468	L469	R470	P471	Q472	T477	A478	V479	P480	H481	P482	Q483	V484	I485	P486	N487	A488	Y489	A490	I491	T492	L493	L494	GLN	LEU	GLY	MET	MET
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.74Å 117.54Å 200.41Å 90.00° 93.79° 90.00°	Depositor
Resolution (Å)	33.78 – 2.90	Depositor
% Data completeness (in resolution range)	99.0 (33.78-2.90)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.247 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15082	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	1	0.51	1/3864 (0.0%)	0.69	0/5211
1	2	0.36	0/3850	0.61	0/5191
1	3	0.35	0/3861	0.61	0/5208
1	4	0.48	0/3830	0.69	0/5166
All	All	0.43	1/15405 (0.0%)	0.65	0/20776

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	498	MET	CG-SD	5.20	1.94	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	3781	0	3714	257	0
1	2	3768	0	3702	208	0
1	3	3778	0	3707	298	0
1	4	3747	0	3681	224	0
2	1	2	0	0	0	0
2	2	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	3	2	0	0	0	0
2	4	2	0	0	0	0
All	All	15082	0	14804	987	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 33.

All (987) 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)
1:1:498:MET:CE	1:1:498:MET:SD	2.04	1.46
1:1:165:LEU:HG	1:1:168:GLU:HB2	1.21	1.18
1:4:185:LYS:HE3	1:4:185:LYS:HA	1.36	1.05
1:1:166:ASP:HA	1:1:170:MET:HG3	1.38	1.00
1:1:187:THR:HG22	1:1:189:SER:H	1.27	0.98
1:1:232:LYS:H	1:1:232:LYS:HD3	1.30	0.96
1:1:165:LEU:HG	1:1:168:GLU:CB	1.96	0.95
1:3:350:ILE:HG22	1:3:424:ILE:HB	1.47	0.95
1:4:232:LYS:H	1:4:232:LYS:HD3	1.31	0.94
1:3:89:ILE:HD12	1:3:102:ARG:HD3	1.50	0.94
1:1:217:LYS:HB2	1:1:334:VAL:HG12	1.50	0.94
1:3:68:ARG:O	1:3:72:TYR:HB2	1.68	0.93
1:1:350:ILE:HG22	1:1:424:ILE:HB	1.49	0.93
1:2:232:LYS:HD3	1:2:232:LYS:H	1.32	0.92
1:1:24:ALA:HB1	1:1:27:ARG:HB3	1.50	0.91
1:2:350:ILE:HG22	1:2:424:ILE:HB	1.53	0.90
1:3:232:LYS:HD3	1:3:232:LYS:H	1.34	0.90
1:4:217:LYS:HB2	1:4:334:VAL:HG12	1.52	0.90
1:3:116:LEU:HD22	1:3:143:VAL:HG21	1.53	0.89
1:1:171:THR:O	1:1:172:ILE:HB	1.73	0.88
1:3:217:LYS:HB2	1:3:334:VAL:HG12	1.55	0.88
1:2:171:THR:O	1:2:207:LYS:HD2	1.74	0.87
1:3:32:LYS:NZ	1:3:63:ILE:HG21	1.90	0.87
1:3:165:LEU:O	1:3:166:ASP:HB2	1.75	0.86
1:3:267:ILE:HD13	1:3:350:ILE:HD11	1.58	0.85
1:2:165:LEU:HB3	1:2:168:GLU:HG2	1.58	0.85
1:3:350:ILE:CG2	1:3:424:ILE:HB	2.07	0.84
1:4:146:LYS:NZ	1:4:311:GLN:HE22	1.75	0.84
1:1:267:ILE:HD13	1:1:350:ILE:HD11	1.59	0.84
1:4:23:GLY:C	1:4:25:LEU:H	1.79	0.84
1:3:31:LEU:HB2	1:3:54:ALA:HB2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:166:ASP:CA	1:1:170:MET:HG3	2.07	0.83
1:2:307:ASP:H	1:2:374:GLN:HE22	1.21	0.83
1:4:172:ILE:HG23	1:4:173:GLU:N	1.93	0.83
1:3:80:TYR:CE1	1:3:399:LYS:HG2	2.14	0.83
1:4:201:GLN:N	1:4:201:GLN:HE21	1.76	0.83
1:4:350:ILE:HG22	1:4:424:ILE:HB	1.60	0.83
1:1:165:LEU:CG	1:1:168:GLU:HB2	2.06	0.83
1:3:450:ASN:HD22	1:3:456:GLY:H	1.26	0.83
1:2:165:LEU:HB2	1:2:169:SER:HB3	1.61	0.82
1:3:165:LEU:HB3	1:3:168:GLU:HB2	1.61	0.82
1:2:217:LYS:HB2	1:2:334:VAL:HG12	1.59	0.82
1:1:201:GLN:N	1:1:201:GLN:HE21	1.76	0.82
1:1:350:ILE:CG2	1:1:424:ILE:HB	2.09	0.82
1:3:267:ILE:CD1	1:3:350:ILE:HD11	2.11	0.80
1:3:145:GLN:HA	1:3:148:PHE:HB2	1.64	0.79
1:1:312:ILE:O	1:1:494:LEU:HD13	1.83	0.79
1:2:350:ILE:CG2	1:2:424:ILE:HB	2.11	0.79
1:2:450:ASN:HD22	1:2:456:GLY:H	1.30	0.79
1:3:351:MET:HE2	1:3:354:GLY:HA2	1.65	0.78
1:2:351:MET:HE2	1:2:354:GLY:HA2	1.65	0.78
1:2:172:ILE:HG12	1:2:173:GLU:H	1.49	0.78
1:2:167:ILE:HD13	1:2:211:GLN:HE21	1.49	0.78
1:3:181:LEU:HG	1:3:184:GLY:HA2	1.65	0.78
1:2:187:THR:HG22	1:2:189:SER:H	1.48	0.78
1:1:126:LYS:HB3	1:1:129:ASP:HB2	1.66	0.78
1:3:55:ILE:HD11	1:3:64:TYR:HB2	1.66	0.77
1:1:356:PHE:CE1	1:1:361:VAL:HG11	2.19	0.77
1:1:137:GLN:O	1:1:141:LYS:HG3	1.84	0.77
1:3:33:THR:O	1:3:37:ASP:HB2	1.84	0.77
1:2:169:SER:O	1:2:171:THR:HG23	1.85	0.76
1:1:80:TYR:CE1	1:1:399:LYS:HG2	2.20	0.76
1:3:96:ILE:HG13	1:3:126:LYS:HE3	1.67	0.76
1:2:137:GLN:O	1:2:141:LYS:HG3	1.85	0.76
1:2:356:PHE:CE1	1:2:361:VAL:HG11	2.20	0.76
1:4:137:GLN:O	1:4:141:LYS:HG3	1.85	0.76
1:4:126:LYS:HB3	1:4:129:ASP:HB2	1.66	0.76
1:2:267:ILE:HD13	1:2:350:ILE:HD11	1.67	0.76
1:1:267:ILE:CD1	1:1:350:ILE:HD11	2.16	0.75
1:3:80:TYR:CE2	1:3:399:LYS:HA	2.21	0.75
1:1:320:LYS:HE2	1:1:325:ALA:HB1	1.69	0.75
1:3:32:LYS:HB2	1:3:64:TYR:CE2	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:283:ILE:HD11	1:4:287:PHE:CZ	2.22	0.75
1:4:172:ILE:HG23	1:4:173:GLU:H	1.52	0.74
1:3:373:ARG:HH12	1:3:376:PRO:HG3	1.52	0.74
1:4:167:ILE:CD1	1:4:211:GLN:HE21	2.00	0.74
1:2:267:ILE:CD1	1:2:350:ILE:HD11	2.17	0.74
1:1:351:MET:HE2	1:1:354:GLY:HA2	1.70	0.74
1:2:45:GLU:O	1:2:49:LYS:HG2	1.88	0.74
1:3:83:GLY:HA2	1:3:86:THR:OG1	1.88	0.73
1:3:320:LYS:HG2	1:3:325:ALA:HA	1.71	0.73
1:3:373:ARG:NH1	1:3:376:PRO:HG3	2.04	0.73
1:2:126:LYS:HB3	1:2:129:ASP:HB2	1.70	0.73
1:1:487:MET:HB2	1:1:498:MET:HE2	1.69	0.73
1:4:267:ILE:HD13	1:4:350:ILE:HD11	1.69	0.73
1:2:167:ILE:CD1	1:2:211:GLN:HE21	2.03	0.72
1:3:356:PHE:CE1	1:3:361:VAL:HG11	2.23	0.72
1:2:145:GLN:O	1:2:149:GLU:HG3	1.88	0.72
1:1:320:LYS:HG2	1:1:325:ALA:HA	1.70	0.72
1:4:318:GLU:HA	1:4:489:TYR:CD2	2.24	0.72
1:3:307:ASP:H	1:3:374:GLN:HE22	1.37	0.72
1:4:45:GLU:O	1:4:49:LYS:HG2	1.89	0.72
1:1:36:ASN:HA	1:1:51:TYR:OH	1.90	0.72
1:1:450:ASN:HD22	1:1:456:GLY:H	1.38	0.71
1:4:483:ASN:O	1:4:484:VAL:HB	1.89	0.71
1:3:35:ALA:HA	1:3:50:PHE:HB2	1.72	0.71
1:3:31:LEU:CB	1:3:54:ALA:HB2	2.20	0.71
1:3:185:LYS:O	1:3:186:VAL:HB	1.90	0.71
1:1:307:ASP:O	1:1:311:GLN:HG2	1.91	0.71
1:3:320:LYS:HE2	1:3:325:ALA:HB1	1.72	0.71
1:2:106:ASN:OD1	1:2:111:LYS:HD3	1.91	0.70
1:3:307:ASP:OD2	1:3:332:SER:HB2	1.92	0.70
1:3:97:LYS:O	1:3:101:ARG:HG3	1.92	0.70
1:3:301:ARG:NH1	1:3:336:GLU:HA	2.06	0.70
1:2:318:GLU:HA	1:2:489:TYR:CD2	2.26	0.70
1:2:483:ASN:O	1:2:484:VAL:HB	1.92	0.70
1:1:307:ASP:H	1:1:374:GLN:HE22	1.40	0.69
1:3:312:ILE:O	1:3:494:LEU:HD13	1.92	0.69
1:3:187:THR:HG22	1:3:189:SER:H	1.58	0.69
1:3:129:ASP:HB3	1:3:132:ALA:HB3	1.75	0.69
1:4:232:LYS:N	1:4:232:LYS:HD3	2.06	0.69
1:1:483:ASN:O	1:1:484:VAL:HB	1.92	0.69
1:2:24:ALA:HB1	1:2:27:ARG:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:356:PHE:CE1	1:4:361:VAL:HG11	2.27	0.69
1:1:232:LYS:HD3	1:1:232:LYS:N	2.06	0.68
1:2:306:THR:HG23	1:2:374:GLN:NE2	2.08	0.68
1:3:44:TYR:O	1:3:48:ILE:HG13	1.94	0.68
1:4:450:ASN:HD22	1:4:456:GLY:H	1.40	0.68
1:2:112:PHE:HD2	1:2:113:ARG:HG3	1.58	0.68
1:3:131:ASP:HA	1:3:134:MET:HB2	1.75	0.68
1:4:350:ILE:CG2	1:4:424:ILE:HB	2.23	0.68
1:3:340:LEU:HB3	1:3:384:LEU:HD23	1.76	0.68
1:1:318:GLU:HA	1:1:489:TYR:CD2	2.29	0.68
1:3:201:GLN:N	1:3:201:GLN:HE21	1.92	0.68
1:4:148:PHE:O	1:4:150:ARG:N	2.26	0.68
1:3:237:ILE:HA	1:3:265:PRO:HG2	1.76	0.67
1:2:172:ILE:HG12	1:2:173:GLU:N	2.08	0.67
1:4:139:CYS:O	1:4:143:VAL:HG23	1.93	0.67
1:1:172:ILE:HG23	1:1:173:GLU:N	2.07	0.67
1:4:267:ILE:CD1	1:4:350:ILE:HD11	2.23	0.67
1:2:201:GLN:HE21	1:2:201:GLN:N	1.92	0.67
1:3:165:LEU:HB3	1:3:168:GLU:CB	2.25	0.67
1:3:425:ARG:O	1:3:444:THR:HA	1.94	0.67
1:2:140:ASN:OD1	1:2:144:LYS:HE2	1.95	0.67
1:3:118:ASP:O	1:3:122:VAL:HG23	1.94	0.67
1:2:139:CYS:O	1:2:143:VAL:HG23	1.94	0.67
1:4:429:VAL:HG22	1:4:446:PHE:CZ	2.30	0.67
1:2:429:VAL:HG22	1:2:446:PHE:CZ	2.30	0.67
1:1:373:ARG:NH1	1:1:376:PRO:HG3	2.10	0.67
1:3:232:LYS:HD3	1:3:232:LYS:N	2.09	0.67
1:1:487:MET:HB2	1:1:498:MET:CE	2.24	0.66
1:1:234:THR:O	1:1:235:GLU:HB2	1.95	0.66
1:2:160:SER:HB3	1:2:333:GLU:OE2	1.95	0.66
1:3:140:ASN:C	1:3:142:ILE:H	1.99	0.66
1:1:165:LEU:CD1	1:1:168:GLU:HG3	2.26	0.66
1:3:31:LEU:HD13	1:3:53:GLN:C	2.15	0.66
1:3:147:ALA:HA	1:3:150:ARG:NH2	2.10	0.66
1:3:395:ARG:HH11	1:3:395:ARG:HG2	1.61	0.66
1:4:146:LYS:HZ2	1:4:311:GLN:HE22	1.41	0.66
1:1:87:ARG:NH2	1:1:91:LEU:HD21	2.10	0.66
1:1:45:GLU:O	1:1:49:LYS:HG2	1.96	0.66
1:4:301:ARG:NH1	1:4:336:GLU:HA	2.10	0.66
1:4:373:ARG:NH1	1:4:376:PRO:HG3	2.10	0.66
1:3:96:ILE:HG13	1:3:126:LYS:CE	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:45:GLU:O	1:3:49:LYS:HG2	1.96	0.66
1:2:148:PHE:O	1:2:150:ARG:N	2.29	0.66
1:2:29:GLU:OE2	1:2:32:LYS:HD3	1.95	0.66
1:1:166:ASP:O	1:1:170:MET:HB2	1.96	0.65
1:3:185:LYS:HA	1:3:185:LYS:HE3	1.78	0.65
1:3:399:LYS:HG3	1:3:405:GLN:NE2	2.11	0.65
1:3:27:ARG:NH2	1:3:31:LEU:HD11	2.12	0.65
1:4:307:ASP:OD2	1:4:332:SER:HB2	1.97	0.65
1:2:173:GLU:HG3	1:2:174:ASP:H	1.61	0.65
1:4:306:THR:HG23	1:4:374:GLN:NE2	2.11	0.65
1:4:244:HIS:O	1:4:276:GLY:HA3	1.96	0.65
1:3:105:SER:O	1:3:109:LEU:HG	1.97	0.65
1:1:165:LEU:HG	1:1:168:GLU:CG	2.26	0.64
1:4:307:ASP:O	1:4:311:GLN:HG2	1.97	0.64
1:4:356:PHE:HZ	1:4:366:ILE:HD11	1.62	0.64
1:4:351:MET:HE2	1:4:354:GLY:HA2	1.79	0.64
1:4:159:ARG:O	1:4:161:VAL:N	2.26	0.64
1:1:232:LYS:H	1:1:232:LYS:CD	2.07	0.64
1:2:232:LYS:HD3	1:2:232:LYS:N	2.08	0.64
1:2:373:ARG:NH1	1:2:376:PRO:HG3	2.12	0.64
1:3:140:ASN:O	1:3:142:ILE:N	2.30	0.64
1:1:85:ALA:HB1	1:1:102:ARG:HB2	1.80	0.64
1:4:232:LYS:CD	1:4:232:LYS:H	2.07	0.64
1:1:171:THR:O	1:1:172:ILE:CB	2.46	0.64
1:3:44:TYR:HA	1:3:47:ALA:HB3	1.79	0.64
1:2:275:ARG:HG3	1:2:275:ARG:HH11	1.63	0.64
1:3:165:LEU:HB3	1:3:168:GLU:HG2	1.80	0.64
1:4:167:ILE:HD13	1:4:211:GLN:HE21	1.63	0.64
1:3:32:LYS:HZ2	1:3:63:ILE:HG21	1.59	0.64
1:2:174:ASP:HB2	1:2:175:GLU:OE2	1.98	0.64
1:1:450:ASN:HD22	1:1:456:GLY:N	1.96	0.64
1:4:68:ARG:HG2	1:4:72:TYR:CE1	2.34	0.63
1:1:165:LEU:HD23	1:1:169:SER:OG	1.98	0.63
1:1:139:CYS:O	1:1:143:VAL:HG23	1.99	0.63
1:4:159:ARG:O	1:4:161:VAL:HG23	1.98	0.63
1:1:275:ARG:HH11	1:1:275:ARG:HG3	1.63	0.63
1:3:232:LYS:CD	1:3:232:LYS:H	2.09	0.63
1:3:483:ASN:O	1:3:484:VAL:HB	1.98	0.63
1:3:318:GLU:HA	1:3:489:TYR:CD2	2.34	0.63
1:1:356:PHE:CZ	1:1:366:ILE:HD11	2.34	0.63
1:1:356:PHE:HZ	1:1:366:ILE:HD11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:85:ALA:HB1	1:4:102:ARG:HB2	1.81	0.63
1:3:62:ALA:HB2	1:3:91:LEU:CB	2.28	0.63
1:3:450:ASN:HD22	1:3:456:GLY:N	1.95	0.63
1:3:210:TYR:O	1:3:214:VAL:HG23	1.98	0.63
1:4:234:THR:O	1:4:235:GLU:HB2	1.99	0.63
1:1:29:GLU:HG3	1:1:32:LYS:HD3	1.80	0.62
1:2:210:TYR:O	1:2:214:VAL:HG23	1.99	0.62
1:4:112:PHE:CD2	1:4:113:ARG:HG3	2.34	0.62
1:2:320:LYS:HG2	1:2:325:ALA:HA	1.81	0.62
1:4:491:ASN:OD1	1:4:493:LEU:HB2	1.99	0.62
1:4:351:MET:HE1	1:4:423:ILE:HD12	1.81	0.62
1:3:62:ALA:HB2	1:3:91:LEU:HB2	1.81	0.62
1:2:232:LYS:H	1:2:232:LYS:CD	2.07	0.62
1:1:26:LYS:O	1:1:30:GLU:HG3	1.99	0.62
1:2:338:LEU:O	1:2:371:ARG:HD3	2.00	0.62
1:3:429:VAL:HG22	1:3:446:PHE:CZ	2.35	0.62
1:4:275:ARG:HH11	1:4:275:ARG:HG3	1.65	0.62
1:3:88:ALA:HB1	1:3:95:TYR:CD2	2.34	0.62
1:3:129:ASP:HB3	1:3:132:ALA:CB	2.30	0.62
1:4:112:PHE:HD2	1:4:113:ARG:HG3	1.65	0.62
1:4:187:THR:HG22	1:4:189:SER:H	1.65	0.62
1:3:450:ASN:ND2	1:3:456:GLY:H	1.97	0.62
1:4:106:ASN:OD1	1:4:111:LYS:HD3	1.99	0.62
1:4:25:LEU:O	1:4:28:ALA:HB3	2.00	0.61
1:1:32:LYS:HD2	1:1:64:TYR:HE1	1.66	0.61
1:4:171:THR:O	1:4:172:ILE:HG22	2.01	0.61
1:1:237:ILE:HA	1:1:265:PRO:HG2	1.82	0.61
1:3:27:ARG:HG2	1:3:57:LEU:HD13	1.82	0.61
1:1:32:LYS:HD2	1:1:64:TYR:CE1	2.35	0.61
1:2:234:THR:O	1:2:235:GLU:HB2	1.99	0.61
1:4:373:ARG:HH12	1:4:376:PRO:HG3	1.64	0.61
1:3:234:THR:O	1:3:235:GLU:HB2	2.01	0.61
1:2:80:TYR:CE1	1:2:399:LYS:HG2	2.36	0.61
1:1:492:THR:O	1:1:496:LEU:HG	1.99	0.61
1:4:23:GLY:C	1:4:25:LEU:N	2.51	0.61
1:4:112:PHE:N	1:4:112:PHE:CD1	2.67	0.61
1:4:120:GLU:HB2	1:4:136:TYR:HE1	1.65	0.61
1:1:356:PHE:CD1	1:1:361:VAL:HG11	2.35	0.61
1:2:87:ARG:NH2	1:2:91:LEU:HD21	2.16	0.60
1:3:32:LYS:HZ1	1:3:63:ILE:HG21	1.64	0.60
1:2:165:LEU:HD12	1:2:168:GLU:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:320:LYS:HE2	1:2:325:ALA:HB1	1.83	0.60
1:2:395:ARG:HG2	1:2:395:ARG:HH11	1.67	0.60
1:1:233:GLU:HA	1:1:233:GLU:OE1	2.00	0.60
1:3:27:ARG:CZ	1:3:31:LEU:HD11	2.31	0.60
1:2:307:ASP:OD2	1:2:332:SER:HB2	2.01	0.60
1:4:126:LYS:HB3	1:4:129:ASP:CB	2.31	0.60
1:1:373:ARG:HH12	1:1:376:PRO:HG3	1.66	0.60
1:2:85:ALA:HB1	1:2:102:ARG:HB2	1.82	0.60
1:1:112:PHE:HD2	1:1:113:ARG:HG3	1.67	0.60
1:3:275:ARG:HH11	1:3:275:ARG:HG3	1.65	0.60
1:4:134:MET:O	1:4:138:GLU:HB2	2.02	0.60
1:4:483:ASN:O	1:4:484:VAL:CB	2.49	0.60
1:4:356:PHE:CZ	1:4:366:ILE:HD11	2.36	0.60
1:3:409:ASP:OD1	1:3:410:VAL:HG23	2.02	0.60
1:4:409:ASP:OD1	1:4:410:VAL:N	2.34	0.60
1:2:332:SER:O	1:2:336:GLU:HG3	2.00	0.60
1:1:126:LYS:HB3	1:1:129:ASP:CB	2.32	0.60
1:2:112:PHE:N	1:2:112:PHE:CD1	2.68	0.60
1:1:58:ASN:HD22	1:1:58:ASN:C	2.04	0.60
1:2:450:ASN:HD22	1:2:456:GLY:N	1.99	0.60
1:1:142:ILE:CG2	1:1:146:LYS:HE3	2.32	0.60
1:3:39:PHE:CE1	1:3:71:ALA:HB2	2.37	0.60
1:4:320:LYS:HE2	1:4:325:ALA:HB1	1.84	0.60
1:1:181:LEU:HB3	1:1:184:GLY:HA2	1.84	0.60
1:4:145:GLN:O	1:4:149:GLU:HG3	2.02	0.59
1:2:130:LYS:O	1:2:131:ASP:HB3	2.02	0.59
1:2:347:LYS:HD2	1:2:421:ASP:OD1	2.02	0.59
1:2:331:PHE:O	1:2:334:VAL:HG22	2.02	0.59
1:2:112:PHE:CD2	1:2:113:ARG:HG3	2.35	0.59
1:1:409:ASP:OD1	1:1:410:VAL:N	2.34	0.59
1:2:373:ARG:HH12	1:2:376:PRO:HG3	1.67	0.59
1:1:483:ASN:O	1:1:484:VAL:CB	2.50	0.59
1:2:134:MET:O	1:2:138:GLU:HB2	2.02	0.59
1:2:237:ILE:HA	1:2:265:PRO:HG2	1.84	0.59
1:3:165:LEU:HB3	1:3:168:GLU:CG	2.32	0.59
1:1:399:LYS:HG3	1:1:405:GLN:NE2	2.18	0.59
1:2:244:HIS:O	1:2:276:GLY:HA3	2.02	0.59
1:4:307:ASP:H	1:4:374:GLN:HE22	1.49	0.59
1:1:201:GLN:N	1:1:201:GLN:NE2	2.50	0.59
1:2:165:LEU:HB3	1:2:168:GLU:CG	2.30	0.59
1:4:146:LYS:HZ1	1:4:311:GLN:HE22	1.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:201:GLN:N	1:4:201:GLN:NE2	2.49	0.59
1:1:409:ASP:OD1	1:1:410:VAL:HG23	2.03	0.59
1:2:415:LEU:HD11	1:2:441:ARG:HB3	1.83	0.59
1:4:393:ASN:HB3	1:4:409:ASP:OD2	2.02	0.59
1:2:252:ASN:CG	1:2:479:VAL:HG21	2.23	0.59
1:2:26:LYS:O	1:2:30:GLU:HG3	2.02	0.59
1:3:307:ASP:O	1:3:311:GLN:HG2	2.02	0.58
1:3:86:THR:O	1:3:90:GLU:HG3	2.03	0.58
1:3:185:LYS:O	1:3:186:VAL:CB	2.51	0.58
1:1:168:GLU:O	1:1:169:SER:C	2.41	0.58
1:1:200:ASP:C	1:1:201:GLN:HE21	2.07	0.58
1:1:73:LEU:HD22	1:1:81:ALA:HB1	1.85	0.58
1:1:165:LEU:HG	1:1:168:GLU:HG3	1.84	0.58
1:3:36:ASN:HB2	1:3:51:TYR:OH	2.02	0.58
1:1:35:ALA:HB2	1:1:50:PHE:HB3	1.85	0.58
1:4:338:LEU:O	1:4:371:ARG:HD3	2.03	0.58
1:4:172:ILE:CG2	1:4:173:GLU:N	2.64	0.58
1:3:356:PHE:CZ	1:3:366:ILE:HD11	2.39	0.58
1:4:221:SER:HA	1:4:337:TRP:CE3	2.38	0.58
1:1:338:LEU:O	1:1:371:ARG:HD3	2.04	0.58
1:1:145:GLN:HA	1:1:148:PHE:HB3	1.85	0.58
1:1:130:LYS:O	1:1:131:ASP:HB3	2.04	0.58
1:3:313:TYR:HA	1:3:487:MET:HE3	1.83	0.58
1:1:185:LYS:O	1:1:186:VAL:HB	2.04	0.58
1:3:415:LEU:HD11	1:3:441:ARG:HB3	1.86	0.58
1:2:307:ASP:O	1:2:311:GLN:HG2	2.04	0.58
1:1:221:SER:HA	1:1:337:TRP:CE3	2.39	0.57
1:3:165:LEU:H	1:3:165:LEU:HD22	1.68	0.57
1:1:201:GLN:O	1:1:202:LYS:HB2	2.04	0.57
1:2:172:ILE:HG23	1:2:173:GLU:N	2.19	0.57
1:4:493:LEU:O	1:4:494:LEU:HG	2.04	0.57
1:1:106:ASN:OD1	1:1:111:LYS:HD3	2.03	0.57
1:1:31:LEU:HB2	1:1:54:ALA:HB2	1.85	0.57
1:1:142:ILE:HG22	1:1:146:LYS:HE3	1.85	0.57
1:2:356:PHE:CZ	1:2:366:ILE:HD11	2.39	0.57
1:2:181:LEU:HD11	1:2:185:LYS:H	1.68	0.57
1:4:165:LEU:HG	1:4:169:SER:HB2	1.87	0.57
1:1:134:MET:O	1:1:138:GLU:HB2	2.03	0.57
1:2:126:LYS:HB3	1:2:129:ASP:CB	2.35	0.57
1:4:450:ASN:HD22	1:4:456:GLY:N	2.02	0.57
1:1:307:ASP:OD2	1:1:332:SER:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:120:GLU:HB2	1:1:136:TYR:HE1	1.70	0.57
1:3:465:GLN:O	1:3:469:LEU:HD13	2.04	0.57
1:3:181:LEU:CG	1:3:184:GLY:HA2	2.35	0.56
1:1:33:THR:O	1:1:37:ASP:HB2	2.04	0.56
1:3:356:PHE:HZ	1:3:366:ILE:HD11	1.70	0.56
1:4:166:ASP:O	1:4:168:GLU:N	2.38	0.56
1:2:483:ASN:O	1:2:484:VAL:CB	2.53	0.56
1:3:91:LEU:O	1:3:92:ASP:HB2	2.06	0.56
1:4:120:GLU:HB2	1:4:136:TYR:CE1	2.39	0.56
1:1:150:ARG:HG3	1:1:151:ALA:H	1.70	0.56
1:1:399:LYS:HD2	1:1:405:GLN:HE22	1.70	0.56
1:3:356:PHE:CD1	1:3:361:VAL:HG11	2.41	0.56
1:3:393:ASN:HB3	1:3:409:ASP:OD2	2.05	0.56
1:3:221:SER:HA	1:3:337:TRP:CE3	2.41	0.56
1:1:331:PHE:O	1:1:334:VAL:HG22	2.06	0.56
1:3:39:PHE:HE1	1:3:71:ALA:HB2	1.71	0.56
1:1:393:ASN:HB3	1:1:409:ASP:OD2	2.05	0.56
1:4:415:LEU:HD11	1:4:441:ARG:HB3	1.86	0.56
1:1:244:HIS:O	1:1:276:GLY:HA3	2.05	0.56
1:2:173:GLU:HB3	1:2:176:TYR:HB3	1.87	0.56
1:3:42:LYS:HD3	1:3:454:GLN:O	2.06	0.56
1:3:273:VAL:O	1:3:274:ASP:HB2	2.07	0.55
1:1:51:TYR:O	1:1:55:ILE:HG12	2.05	0.55
1:1:465:GLN:O	1:1:469:LEU:HD13	2.05	0.55
1:2:169:SER:O	1:2:171:THR:N	2.39	0.55
1:2:129:ASP:OD2	1:2:132:ALA:HB2	2.06	0.55
1:3:332:SER:O	1:3:336:GLU:HG3	2.06	0.55
1:3:187:THR:HG22	1:3:188:ILE:N	2.22	0.55
1:4:181:LEU:HD11	1:4:186:VAL:N	2.21	0.55
1:3:87:ARG:NE	1:3:91:LEU:HD11	2.22	0.55
1:3:252:ASN:CG	1:3:479:VAL:HG21	2.27	0.55
1:1:187:THR:HG22	1:1:188:ILE:N	2.20	0.55
1:2:356:PHE:CZ	1:2:384:LEU:HD13	2.41	0.55
1:4:130:LYS:O	1:4:131:ASP:HB3	2.07	0.55
1:2:120:GLU:HB2	1:2:136:TYR:HE1	1.70	0.55
1:1:145:GLN:O	1:1:148:PHE:HB3	2.07	0.55
1:2:393:ASN:HB3	1:2:409:ASP:OD2	2.07	0.55
1:1:324:THR:C	1:1:326:GLN:H	2.09	0.55
1:2:356:PHE:CD1	1:2:361:VAL:HG11	2.41	0.55
1:3:188:ILE:HG12	1:3:292:LEU:HD21	1.88	0.55
1:1:112:PHE:N	1:1:112:PHE:CD1	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:39:PHE:HZ	1:3:70:LEU:HG	1.71	0.55
1:3:69:SER:O	1:3:73:LEU:HB2	2.07	0.55
1:3:113:ARG:O	1:3:116:LEU:N	2.40	0.55
1:1:112:PHE:CD2	1:1:113:ARG:HG3	2.41	0.55
1:1:140:ASN:OD1	1:1:144:LYS:HE2	2.06	0.55
1:4:320:LYS:HG2	1:4:325:ALA:HA	1.87	0.55
1:4:421:ASP:OD1	1:4:421:ASP:N	2.40	0.55
1:4:232:LYS:HE2	1:4:235:GLU:HB2	1.89	0.54
1:4:129:ASP:OD2	1:4:132:ALA:HB2	2.07	0.54
1:1:429:VAL:HG22	1:1:446:PHE:CZ	2.42	0.54
1:3:87:ARG:HE	1:3:91:LEU:HD11	1.72	0.54
1:2:58:ASN:C	1:2:58:ASN:HD22	2.10	0.54
1:1:129:ASP:OD2	1:1:132:ALA:HB2	2.07	0.54
1:4:351:MET:CE	1:4:354:GLY:HA2	2.37	0.54
1:2:185:LYS:O	1:2:186:VAL:HG23	2.06	0.54
1:3:483:ASN:O	1:3:484:VAL:CB	2.56	0.54
1:1:190:PHE:HD2	1:1:191:MET:HE2	1.73	0.54
1:2:191:MET:O	1:2:195:MET:HG3	2.06	0.54
1:3:69:SER:CB	1:3:85:ALA:HB2	2.37	0.54
1:3:233:GLU:HA	1:3:233:GLU:OE1	2.07	0.54
1:4:234:THR:O	1:4:235:GLU:CB	2.56	0.54
1:1:450:ASN:ND2	1:1:456:GLY:HA2	2.23	0.54
1:4:191:MET:O	1:4:195:MET:HG3	2.07	0.54
1:3:80:TYR:CZ	1:3:399:LYS:HA	2.43	0.54
1:3:340:LEU:HD11	1:3:381:MET:HE3	1.89	0.54
1:1:34:GLN:O	1:1:34:GLN:HG2	2.07	0.54
1:2:307:ASP:N	1:2:374:GLN:HE22	2.00	0.54
1:4:200:ASP:C	1:4:201:GLN:HE21	2.12	0.54
1:3:96:ILE:HG13	1:3:126:LYS:NZ	2.23	0.53
1:3:485:LYS:HB3	1:3:486:PRO:HD2	1.90	0.53
1:4:432:GLU:OE1	1:4:458:LYS:NZ	2.39	0.53
1:4:331:PHE:O	1:4:334:VAL:HG22	2.08	0.53
1:2:336:GLU:O	1:2:371:ARG:HG2	2.08	0.53
1:1:477:THR:HG23	1:1:478:ALA:N	2.24	0.53
1:1:486:PRO:O	1:1:498:MET:HE3	2.08	0.53
1:2:351:MET:CE	1:2:354:GLY:HA2	2.38	0.53
1:4:168:GLU:O	1:4:170:MET:N	2.40	0.53
1:4:324:THR:C	1:4:326:GLN:H	2.12	0.53
1:3:361:VAL:HA	1:3:365:ASP:OD1	2.09	0.53
1:4:140:ASN:OD1	1:4:144:LYS:HE2	2.07	0.53
1:1:347:LYS:HD2	1:1:421:ASP:OD1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:68:ARG:HG2	1:2:72:TYR:CE1	2.44	0.53
1:3:399:LYS:HG3	1:3:405:GLN:HE22	1.72	0.53
1:3:360:GLY:O	1:3:361:VAL:O	2.27	0.53
1:3:140:ASN:C	1:3:142:ILE:N	2.61	0.53
1:2:399:LYS:HG3	1:2:405:GLN:NE2	2.24	0.53
1:2:87:ARG:CZ	1:2:91:LEU:HD21	2.39	0.53
1:4:346:GLY:O	1:4:420:LEU:HD23	2.08	0.53
1:1:487:MET:SD	1:1:498:MET:HG2	2.48	0.53
1:3:112:PHE:N	1:3:112:PHE:CD1	2.76	0.53
1:1:145:GLN:O	1:1:148:PHE:N	2.41	0.53
1:2:73:LEU:HD22	1:2:81:ALA:HB1	1.89	0.53
1:4:485:LYS:HB3	1:4:486:PRO:HD2	1.90	0.53
1:4:220:LEU:HD13	1:4:338:LEU:HD23	1.91	0.53
1:2:301:ARG:NH1	1:2:336:GLU:HA	2.24	0.53
1:3:128:HIS:HA	1:3:133:LYS:HE2	1.89	0.53
1:3:123:VAL:HG21	1:3:133:LYS:HG2	1.91	0.53
1:4:233:GLU:OE1	1:4:233:GLU:HA	2.09	0.53
1:4:201:GLN:O	1:4:202:LYS:HB2	2.08	0.53
1:1:361:VAL:HA	1:1:365:ASP:OD1	2.09	0.53
1:3:88:ALA:HB1	1:3:95:TYR:CE2	2.44	0.53
1:2:307:ASP:H	1:2:374:GLN:NE2	1.98	0.53
1:4:400:ARG:NE	1:4:427:HIS:NE2	2.57	0.53
1:1:356:PHE:CD1	1:1:356:PHE:N	2.76	0.53
1:3:179:PRO:HG2	1:3:194:LEU:HA	1.89	0.53
1:2:239:VAL:HA	1:2:267:ILE:HG23	1.90	0.52
1:3:395:ARG:HH11	1:3:395:ARG:CG	2.20	0.52
1:3:400:ARG:NE	1:3:427:HIS:NE2	2.58	0.52
1:2:409:ASP:OD1	1:2:410:VAL:N	2.42	0.52
1:2:283:ILE:HD11	1:2:287:PHE:CZ	2.43	0.52
1:1:487:MET:SD	1:1:498:MET:HE2	2.49	0.52
1:2:356:PHE:HZ	1:2:366:ILE:HD11	1.72	0.52
1:2:312:ILE:HG23	1:2:494:LEU:CD1	2.38	0.52
1:1:283:ILE:HD11	1:1:287:PHE:CZ	2.44	0.52
1:1:487:MET:SD	1:1:498:MET:CE	2.98	0.52
1:3:89:ILE:O	1:3:93:LYS:HG2	2.09	0.52
1:3:27:ARG:HE	1:3:57:LEU:HD12	1.73	0.52
1:3:239:VAL:HA	1:3:267:ILE:HG23	1.91	0.52
1:4:232:LYS:O	1:4:466:GLY:HA3	2.09	0.52
1:3:306:THR:HG23	1:3:374:GLN:NE2	2.25	0.52
1:4:158:LYS:O	1:4:159:ARG:CB	2.58	0.52
1:4:390:GLN:HE22	1:4:396:SER:CB	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:54:ALA:O	1:3:58:ASN:HB3	2.10	0.52
1:2:213:LEU:HD21	1:2:331:PHE:CE1	2.44	0.52
1:3:130:LYS:O	1:3:131:ASP:HB3	2.10	0.52
1:1:234:THR:O	1:1:235:GLU:CB	2.55	0.52
1:4:200:ASP:O	1:4:202:LYS:HG3	2.10	0.52
1:3:150:ARG:HG2	1:3:150:ARG:HH11	1.75	0.52
1:1:188:ILE:HG12	1:1:292:LEU:HD21	1.91	0.52
1:2:232:LYS:HE2	1:2:235:GLU:HB2	1.92	0.52
1:2:159:ARG:O	1:2:161:VAL:N	2.41	0.52
1:3:162:VAL:HG12	1:3:162:VAL:O	2.10	0.52
1:4:58:ASN:HD22	1:4:58:ASN:C	2.13	0.52
1:1:232:LYS:HE2	1:1:235:GLU:HB2	1.92	0.52
1:3:350:ILE:HG22	1:3:424:ILE:CB	2.31	0.52
1:3:232:LYS:HE2	1:3:235:GLU:HB2	1.91	0.52
1:2:233:GLU:HA	1:2:233:GLU:OE1	2.09	0.52
1:3:72:TYR:HB3	1:3:81:ALA:HB2	1.92	0.51
1:4:159:ARG:C	1:4:161:VAL:H	2.11	0.51
1:3:244:HIS:O	1:3:276:GLY:HA3	2.10	0.51
1:4:116:LEU:HD22	1:4:143:VAL:HG21	1.92	0.51
1:1:150:ARG:O	1:1:151:ALA:HB3	2.10	0.51
1:2:221:SER:HA	1:2:337:TRP:CE3	2.45	0.51
1:3:176:TYR:CE2	1:3:205:HIS:HB2	2.46	0.51
1:4:181:LEU:HG	1:4:184:GLY:HA2	1.91	0.51
1:2:167:ILE:HD13	1:2:211:GLN:NE2	2.23	0.51
1:3:338:LEU:O	1:3:371:ARG:HD3	2.10	0.51
1:1:29:GLU:O	1:1:29:GLU:HG2	2.10	0.51
1:3:409:ASP:OD1	1:3:410:VAL:N	2.43	0.51
1:4:409:ASP:OD1	1:4:410:VAL:HG23	2.10	0.51
1:3:315:PHE:O	1:3:319:VAL:HG23	2.10	0.51
1:1:165:LEU:HB3	1:1:169:SER:HB2	1.93	0.51
1:3:72:TYR:O	1:3:77:CYS:HB2	2.10	0.51
1:4:238:THR:O	1:4:267:ILE:HG22	2.11	0.51
1:3:400:ARG:CZ	1:3:427:HIS:NE2	2.74	0.51
1:3:347:LYS:HD2	1:3:421:ASP:OD1	2.11	0.51
1:3:87:ARG:O	1:3:87:ARG:HG3	2.11	0.51
1:3:267:ILE:HD11	1:3:350:ILE:HD11	1.91	0.51
1:4:148:PHE:CD1	1:4:149:GLU:N	2.78	0.51
1:1:58:ASN:C	1:1:58:ASN:ND2	2.64	0.51
1:2:44:TYR:O	1:2:48:ILE:HG13	2.11	0.51
1:3:245:GLY:O	1:3:278:PHE:HB2	2.10	0.51
1:1:169:SER:O	1:1:170:MET:C	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:145:GLN:C	1:3:147:ALA:H	2.14	0.51
1:4:237:ILE:HA	1:4:265:PRO:HG2	1.93	0.51
1:4:340:LEU:HD11	1:4:381:MET:HE3	1.93	0.51
1:1:235:GLU:HA	1:1:235:GLU:OE1	2.10	0.50
1:1:27:ARG:HA	1:1:30:GLU:OE1	2.10	0.50
1:4:165:LEU:HD12	1:4:169:SER:N	2.27	0.50
1:4:415:LEU:HD12	1:4:441:ARG:HD2	1.93	0.50
1:1:468:ASP:OD2	1:1:470:ARG:HB2	2.12	0.50
1:2:234:THR:O	1:2:235:GLU:CB	2.58	0.50
1:3:331:PHE:O	1:3:334:VAL:HG22	2.11	0.50
1:2:176:TYR:CZ	1:2:205:HIS:HB2	2.46	0.50
1:3:72:TYR:CE1	1:3:80:TYR:HB3	2.47	0.50
1:3:57:LEU:O	1:3:58:ASN:HB2	2.11	0.50
1:3:123:VAL:CG2	1:3:133:LYS:HG2	2.41	0.50
1:4:187:THR:HG22	1:4:188:ILE:N	2.26	0.50
1:4:399:LYS:HG3	1:4:405:GLN:NE2	2.26	0.50
1:3:324:THR:C	1:3:326:GLN:H	2.13	0.50
1:1:399:LYS:HG3	1:1:405:GLN:HE22	1.76	0.50
1:4:415:LEU:CD1	1:4:441:ARG:HB3	2.41	0.50
1:3:262:GLU:HA	1:3:296:HIS:CG	2.47	0.50
1:1:393:ASN:CB	1:1:409:ASP:OD2	2.59	0.50
1:4:27:ARG:O	1:4:31:LEU:HD12	2.12	0.50
1:1:487:MET:HG3	1:1:498:MET:HE1	1.94	0.50
1:3:89:ILE:O	1:3:89:ILE:HG22	2.11	0.50
1:2:187:THR:HG22	1:2:188:ILE:N	2.26	0.50
1:3:96:ILE:HD11	1:3:125:VAL:HG11	1.93	0.50
1:2:450:ASN:ND2	1:2:456:GLY:H	2.02	0.50
1:4:166:ASP:OD1	1:4:210:TYR:HB3	2.11	0.50
1:3:72:TYR:HH	1:3:80:TYR:HD1	1.59	0.50
1:1:320:LYS:HE2	1:1:325:ALA:CB	2.41	0.49
1:2:24:ALA:O	1:2:27:ARG:HB3	2.12	0.49
1:3:283:ILE:HD11	1:3:287:PHE:CZ	2.47	0.49
1:4:91:LEU:O	1:4:92:ASP:HB2	2.11	0.49
1:2:182:GLU:O	1:2:184:GLY:N	2.43	0.49
1:3:83:GLY:O	1:3:86:THR:HB	2.12	0.49
1:2:201:GLN:NE2	1:2:201:GLN:N	2.58	0.49
1:4:393:ASN:CB	1:4:409:ASP:OD2	2.60	0.49
1:3:346:GLY:O	1:3:420:LEU:HD23	2.12	0.49
1:3:32:LYS:O	1:3:36:ASN:HB3	2.13	0.49
1:3:64:TYR:CD1	1:3:64:TYR:N	2.79	0.49
1:3:125:VAL:HG13	1:3:126:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:450:ASN:ND2	1:4:456:GLY:HA2	2.27	0.49
1:4:489:TYR:CD1	1:4:489:TYR:N	2.80	0.49
1:1:32:LYS:O	1:1:32:LYS:HG2	2.13	0.49
1:2:415:LEU:CD1	1:2:441:ARG:HB3	2.42	0.49
1:3:93:LYS:C	1:3:95:TYR:H	2.15	0.49
1:3:320:LYS:HE2	1:3:325:ALA:CB	2.42	0.49
1:3:356:PHE:N	1:3:356:PHE:CD1	2.79	0.49
1:4:158:LYS:HG3	1:4:158:LYS:O	2.13	0.49
1:1:415:LEU:HD12	1:1:441:ARG:HD2	1.95	0.49
1:1:242:ASP:OD1	1:1:426:SER:HB3	2.12	0.49
1:2:267:ILE:HD11	1:2:350:ILE:HD11	1.93	0.49
1:2:360:GLY:O	1:2:361:VAL:O	2.30	0.49
1:3:492:THR:HG22	1:3:495:GLN:OE1	2.12	0.49
1:1:403:SER:OG	1:1:404:CYS:N	2.43	0.49
1:2:172:ILE:HG23	1:2:173:GLU:H	1.77	0.49
1:1:355:LEU:CD1	1:1:411:THR:HA	2.43	0.49
1:2:340:LEU:HB3	1:2:384:LEU:HD23	1.95	0.49
1:3:60:SER:C	1:3:91:LEU:HD13	2.33	0.49
1:2:409:ASP:OD1	1:2:410:VAL:HG23	2.12	0.49
1:2:445:VAL:O	1:2:445:VAL:HG13	2.13	0.49
1:4:232:LYS:HE2	1:4:235:GLU:CB	2.43	0.49
1:1:301:ARG:NH1	1:1:336:GLU:HA	2.27	0.49
1:1:165:LEU:CG	1:1:168:GLU:HG3	2.42	0.48
1:1:87:ARG:CZ	1:1:91:LEU:HD21	2.43	0.48
1:3:35:ALA:HB2	1:3:50:PHE:HB3	1.94	0.48
1:2:48:ILE:HD13	1:2:72:TYR:CE2	2.48	0.48
1:2:485:LYS:HB3	1:2:486:PRO:HD2	1.95	0.48
1:3:35:ALA:CA	1:3:50:PHE:HB2	2.42	0.48
1:1:400:ARG:CZ	1:1:427:HIS:NE2	2.76	0.48
1:1:487:MET:CG	1:1:498:MET:HE1	2.43	0.48
1:4:23:GLY:O	1:4:25:LEU:N	2.46	0.48
1:4:283:ILE:HG23	1:4:284:LEU:N	2.28	0.48
1:1:351:MET:HE1	1:1:423:ILE:HD12	1.96	0.48
1:1:450:ASN:HD22	1:1:456:GLY:CA	2.26	0.48
1:3:415:LEU:HD12	1:3:441:ARG:HD2	1.96	0.48
1:3:213:LEU:HD21	1:3:331:PHE:CE1	2.48	0.48
1:3:181:LEU:HD23	1:3:211:GLN:OE1	2.14	0.48
1:1:274:ASP:O	1:1:276:GLY:N	2.42	0.48
1:1:400:ARG:NE	1:1:427:HIS:NE2	2.62	0.48
1:1:38:TYR:HD1	1:1:46:ASN:HB3	1.78	0.48
1:3:112:PHE:HB2	1:3:143:VAL:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:167:ILE:O	1:2:207:LYS:HE3	2.14	0.48
1:3:165:LEU:CB	1:3:168:GLU:HB2	2.37	0.48
1:4:371:ARG:O	1:4:373:ARG:N	2.47	0.48
1:4:450:ASN:HD22	1:4:456:GLY:HA2	1.77	0.48
1:1:145:GLN:O	1:1:146:LYS:C	2.51	0.48
1:2:478:ALA:O	1:2:479:VAL:HB	2.13	0.48
1:1:161:VAL:C	1:1:163:ASP:N	2.67	0.48
1:2:181:LEU:HD12	1:2:182:GLU:N	2.28	0.48
1:1:371:ARG:HA	1:1:381:MET:HE3	1.95	0.48
1:1:120:GLU:HB2	1:1:136:TYR:CE1	2.49	0.48
1:2:313:TYR:HA	1:2:487:MET:HE3	1.94	0.48
1:3:29:GLU:HA	1:3:64:TYR:OH	2.14	0.48
1:1:332:SER:O	1:1:336:GLU:HG3	2.13	0.48
1:4:87:ARG:NH2	1:4:91:LEU:HD21	2.29	0.48
1:3:95:TYR:CD2	1:3:98:GLY:HA3	2.49	0.48
1:2:200:ASP:C	1:2:201:GLN:HE21	2.17	0.48
1:3:351:MET:HE2	1:3:354:GLY:CA	2.41	0.47
1:4:361:VAL:HA	1:4:365:ASP:OD1	2.14	0.47
1:4:491:ASN:CG	1:4:493:LEU:HD12	2.34	0.47
1:1:283:ILE:HG23	1:1:284:LEU:N	2.29	0.47
1:1:182:GLU:HG2	1:1:182:GLU:O	2.14	0.47
1:4:207:LYS:O	1:4:211:GLN:HG3	2.14	0.47
1:2:395:ARG:CG	1:2:395:ARG:HH11	2.27	0.47
1:1:44:TYR:O	1:1:48:ILE:HG13	2.14	0.47
1:3:81:ALA:HA	1:3:84:ASP:HB3	1.97	0.47
1:2:181:LEU:HD11	1:2:185:LYS:N	2.28	0.47
1:3:127:PRO:O	1:3:129:ASP:N	2.45	0.47
1:4:450:ASN:HD22	1:4:456:GLY:CA	2.27	0.47
1:3:200:ASP:C	1:3:201:GLN:HE21	2.18	0.47
1:4:112:PHE:H	1:4:112:PHE:HD1	1.55	0.47
1:2:324:THR:C	1:2:326:GLN:H	2.17	0.47
1:2:306:THR:HG23	1:2:374:GLN:HE22	1.79	0.47
1:1:399:LYS:CD	1:1:405:GLN:HE22	2.27	0.47
1:3:120:GLU:O	1:3:123:VAL:HG12	2.13	0.47
1:1:35:ALA:HB2	1:1:50:PHE:CB	2.44	0.47
1:1:279:SER:O	1:1:283:ILE:HG22	2.14	0.47
1:4:395:ARG:HG2	1:4:395:ARG:HH11	1.79	0.47
1:3:234:THR:O	1:3:235:GLU:CB	2.62	0.47
1:3:42:LYS:HG2	1:3:44:TYR:OH	2.15	0.47
1:3:415:LEU:CD1	1:3:441:ARG:HB3	2.43	0.47
1:1:167:ILE:HD11	1:1:211:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:73:LEU:HD22	1:4:81:ALA:HB1	1.97	0.47
1:1:107:MET:O	1:1:110:GLY:N	2.43	0.47
1:4:146:LYS:HZ1	1:4:311:GLN:NE2	2.12	0.47
1:2:146:LYS:HE2	1:2:311:GLN:OE1	2.13	0.47
1:1:351:MET:HE2	1:1:354:GLY:CA	2.43	0.47
1:1:29:GLU:HG3	1:1:32:LYS:HB3	1.97	0.47
1:4:429:VAL:HG22	1:4:446:PHE:CE2	2.49	0.47
1:4:136:TYR:CE2	1:4:140:ASN:ND2	2.82	0.47
1:2:58:ASN:C	1:2:58:ASN:ND2	2.67	0.47
1:4:432:GLU:OE1	1:4:432:GLU:HA	2.15	0.47
1:1:38:TYR:HB3	1:1:43:ASP:HB3	1.95	0.47
1:4:306:THR:HG23	1:4:374:GLN:HE22	1.77	0.47
1:2:273:VAL:O	1:2:274:ASP:HB2	2.13	0.47
1:3:66:GLY:O	1:3:69:SER:N	2.44	0.47
1:4:171:THR:O	1:4:172:ILE:CB	2.63	0.47
1:3:44:TYR:O	1:3:47:ALA:HB3	2.15	0.47
1:1:371:ARG:O	1:1:373:ARG:N	2.48	0.47
1:2:355:LEU:CD1	1:2:411:THR:HA	2.44	0.47
1:3:185:LYS:CA	1:3:185:LYS:HE3	2.44	0.46
1:1:232:LYS:HE2	1:1:235:GLU:CB	2.45	0.46
1:3:168:GLU:O	1:3:170:MET:N	2.48	0.46
1:3:31:LEU:HB2	1:3:54:ALA:CB	2.40	0.46
1:3:35:ALA:HB2	1:3:50:PHE:CB	2.45	0.46
1:4:450:ASN:ND2	1:4:456:GLY:H	2.10	0.46
1:3:463:HIS:HB2	1:3:472:GLN:HB2	1.97	0.46
1:4:464:LEU:HD12	1:4:464:LEU:HA	1.80	0.46
1:1:187:THR:CG2	1:1:188:ILE:N	2.78	0.46
1:3:232:LYS:O	1:3:466:GLY:HA3	2.15	0.46
1:2:120:GLU:HB2	1:2:136:TYR:CE1	2.50	0.46
1:1:346:GLY:O	1:1:420:LEU:HD23	2.15	0.46
1:3:116:LEU:HD22	1:3:143:VAL:CG2	2.37	0.46
1:3:383:ASP:HA	1:3:403:SER:OG	2.15	0.46
1:1:235:GLU:CD	1:1:235:GLU:N	2.68	0.46
1:3:64:TYR:C	1:3:66:GLY:H	2.18	0.46
1:3:116:LEU:CD2	1:3:143:VAL:HG21	2.35	0.46
1:4:131:ASP:O	1:4:134:MET:N	2.48	0.46
1:4:275:ARG:NH1	1:4:275:ARG:HG3	2.31	0.46
1:3:393:ASN:CB	1:3:409:ASP:OD2	2.64	0.46
1:4:80:TYR:CE1	1:4:399:LYS:HG2	2.50	0.46
1:2:165:LEU:O	1:2:168:GLU:OE2	2.34	0.46
1:1:356:PHE:CZ	1:1:384:LEU:HD13	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:336:GLU:O	1:3:371:ARG:HG2	2.16	0.46
1:4:168:GLU:C	1:4:170:MET:H	2.19	0.46
1:4:210:TYR:O	1:4:214:VAL:HG23	2.16	0.46
1:4:356:PHE:CD1	1:4:356:PHE:N	2.83	0.46
1:4:400:ARG:CZ	1:4:427:HIS:NE2	2.79	0.46
1:4:468:ASP:OD2	1:4:470:ARG:HB2	2.16	0.46
1:4:239:VAL:HA	1:4:267:ILE:HG23	1.97	0.46
1:3:375:PRO:HA	1:3:376:PRO:HD3	1.82	0.46
1:4:211:GLN:O	1:4:215:GLN:HG3	2.15	0.46
1:2:275:ARG:HG3	1:2:275:ARG:NH1	2.30	0.46
1:1:412:LYS:HE2	1:1:416:GLU:OE1	2.16	0.46
1:4:355:LEU:CD1	1:4:411:THR:HA	2.46	0.46
1:3:436:VAL:CG1	1:3:440:GLY:HA2	2.46	0.46
1:4:201:GLN:O	1:4:202:LYS:CB	2.64	0.46
1:4:356:PHE:CD1	1:4:361:VAL:HG11	2.51	0.46
1:3:60:SER:HA	1:3:87:ARG:HH21	1.80	0.46
1:3:60:SER:O	1:3:91:LEU:HD22	2.16	0.46
1:3:176:TYR:CE1	1:3:178:GLY:HA3	2.52	0.46
1:1:450:ASN:HD22	1:1:456:GLY:HA2	1.79	0.45
1:3:103:ALA:C	1:3:105:SER:N	2.69	0.45
1:4:136:TYR:O	1:4:140:ASN:HB2	2.16	0.45
1:1:191:MET:O	1:1:195:MET:HG3	2.15	0.45
1:3:179:PRO:HB2	1:3:190:PHE:CE1	2.51	0.45
1:4:336:GLU:O	1:4:371:ARG:HG2	2.17	0.45
1:3:181:LEU:CD2	1:3:184:GLY:HA2	2.44	0.45
1:1:85:ALA:O	1:1:89:ILE:HG13	2.16	0.45
1:3:371:ARG:O	1:3:373:ARG:N	2.50	0.45
1:1:324:THR:C	1:1:326:GLN:N	2.70	0.45
1:3:112:PHE:HB2	1:3:113:ARG:H	1.53	0.45
1:2:96:ILE:HG13	1:2:126:LYS:HE3	1.97	0.45
1:1:29:GLU:HG3	1:1:32:LYS:CD	2.46	0.45
1:4:58:ASN:ND2	1:4:58:ASN:C	2.68	0.45
1:4:245:GLY:HA2	1:4:282:VAL:HG21	1.99	0.45
1:1:450:ASN:O	1:1:451:TYR:C	2.55	0.45
1:2:131:ASP:O	1:2:134:MET:N	2.50	0.45
1:1:492:THR:HG22	1:1:495:GLN:OE1	2.17	0.45
1:3:89:ILE:HD11	1:3:99:TYR:HA	1.99	0.45
1:1:138:GLU:HB3	1:1:493:LEU:HD11	1.99	0.45
1:2:279:SER:O	1:2:283:ILE:HG22	2.16	0.45
1:1:388:ASP:OD1	1:1:427:HIS:HD2	1.99	0.45
1:4:64:TYR:N	1:4:64:TYR:HD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:26:LYS:O	1:3:30:GLU:HG3	2.16	0.45
1:3:307:ASP:N	1:3:374:GLN:HE22	2.10	0.45
1:3:42:LYS:HA	1:3:44:TYR:CZ	2.51	0.45
1:3:283:ILE:HG23	1:3:284:LEU:N	2.32	0.45
1:1:292:LEU:HD23	1:1:293:TYR:CE2	2.51	0.45
1:4:336:GLU:HB3	1:4:372:ASN:HA	1.98	0.45
1:1:201:GLN:O	1:1:202:LYS:CB	2.62	0.45
1:2:188:ILE:HG12	1:2:292:LEU:HD21	1.98	0.45
1:4:64:TYR:N	1:4:64:TYR:CD1	2.83	0.45
1:3:445:VAL:O	1:3:445:VAL:HG13	2.17	0.45
1:3:73:LEU:HD13	1:3:81:ALA:HB3	1.99	0.45
1:1:96:ILE:HG13	1:1:126:LYS:HE3	1.99	0.45
1:1:130:LYS:HG3	1:1:130:LYS:H	1.59	0.45
1:4:313:TYR:HA	1:4:487:MET:HE3	1.99	0.45
1:2:340:LEU:HD11	1:2:381:MET:HE3	1.99	0.45
1:2:262:GLU:HA	1:2:296:HIS:CG	2.52	0.45
1:3:481:HIS:O	1:3:482:PRO:O	2.35	0.45
1:3:115:ALA:O	1:3:119:TYR:CD2	2.71	0.45
1:2:213:LEU:O	1:2:216:VAL:HG12	2.17	0.44
1:2:172:ILE:HD11	1:2:180:LYS:NZ	2.32	0.44
1:1:218:GLU:OE2	1:1:222:LYS:NZ	2.50	0.44
1:4:213:LEU:HD21	1:4:331:PHE:CE1	2.52	0.44
1:2:356:PHE:CD1	1:2:356:PHE:N	2.84	0.44
1:3:201:GLN:N	1:3:201:GLN:NE2	2.63	0.44
1:4:148:PHE:C	1:4:148:PHE:CD1	2.90	0.44
1:3:468:ASP:OD2	1:3:470:ARG:HB2	2.17	0.44
1:3:113:ARG:C	1:3:117:ARG:HG3	2.37	0.44
1:2:207:LYS:O	1:2:211:GLN:HG3	2.17	0.44
1:3:191:MET:O	1:3:195:MET:HG3	2.18	0.44
1:1:463:HIS:HB2	1:1:472:GLN:HB2	1.99	0.44
1:4:481:HIS:O	1:4:482:PRO:O	2.35	0.44
1:4:181:LEU:HD11	1:4:186:VAL:H	1.82	0.44
1:4:166:ASP:HB3	1:4:167:ILE:H	1.67	0.44
1:3:122:VAL:O	1:3:122:VAL:HG12	2.16	0.44
1:2:415:LEU:HD12	1:2:441:ARG:HD2	1.99	0.44
1:1:273:VAL:O	1:1:274:ASP:HB2	2.17	0.44
1:3:468:ASP:C	1:3:470:ARG:H	2.21	0.44
1:2:70:LEU:HB2	1:2:101:ARG:HE	1.83	0.44
1:2:316:GLU:HA	1:2:328:TYR:CD1	2.52	0.44
1:2:194:LEU:HD11	1:2:198:TYR:CZ	2.52	0.44
1:1:245:GLY:O	1:1:278:PHE:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:267:ILE:HD13	1:3:350:ILE:CD1	2.40	0.44
1:3:450:ASN:O	1:3:451:TYR:C	2.56	0.44
1:1:306:THR:HG23	1:1:374:GLN:NE2	2.33	0.44
1:2:399:LYS:HD2	1:2:405:GLN:HE22	1.81	0.44
1:1:136:TYR:O	1:1:140:ASN:HB2	2.17	0.44
1:2:51:TYR:O	1:2:55:ILE:HG12	2.18	0.44
1:2:481:HIS:HB2	1:2:482:PRO:HD2	1.98	0.44
1:1:165:LEU:HD11	1:1:168:GLU:HG3	1.98	0.44
1:4:307:ASP:N	1:4:374:GLN:HE22	2.14	0.44
1:3:44:TYR:HA	1:3:47:ALA:CB	2.47	0.44
1:2:32:LYS:O	1:2:36:ASN:HB2	2.17	0.44
1:3:107:MET:SD	1:3:493:LEU:HD13	2.58	0.44
1:4:181:LEU:CG	1:4:184:GLY:HA2	2.47	0.44
1:4:146:LYS:NZ	1:4:311:GLN:NE2	2.55	0.44
1:4:171:THR:O	1:4:172:ILE:CG2	2.65	0.44
1:3:147:ALA:HA	1:3:150:ARG:HH22	1.80	0.44
1:3:336:GLU:HB3	1:3:372:ASN:HA	2.00	0.44
1:3:220:LEU:HB3	1:3:337:TRP:O	2.18	0.44
1:3:107:MET:HG3	1:3:115:ALA:HB1	2.00	0.44
1:1:278:PHE:CZ	1:1:482:PRO:HG2	2.53	0.44
1:4:181:LEU:HD11	1:4:186:VAL:CA	2.48	0.44
1:3:96:ILE:HG13	1:3:126:LYS:HZ1	1.82	0.44
1:2:49:LYS:HA	1:2:49:LYS:HD3	1.78	0.44
1:3:44:TYR:CA	1:3:47:ALA:HB3	2.47	0.44
1:1:232:LYS:O	1:1:466:GLY:HA3	2.18	0.44
1:3:50:PHE:HA	1:3:53:GLN:NE2	2.32	0.44
1:3:395:ARG:CG	1:3:395:ARG:NH1	2.78	0.44
1:1:120:GLU:O	1:1:123:VAL:HG12	2.18	0.44
1:2:312:ILE:CG2	1:2:494:LEU:HD13	2.48	0.44
1:1:316:GLU:HA	1:1:328:TYR:CD1	2.53	0.44
1:3:159:ARG:O	1:3:160:SER:HB3	2.18	0.44
1:4:218:GLU:OE2	1:4:222:LYS:NZ	2.51	0.44
1:1:194:LEU:HD11	1:1:198:TYR:CZ	2.53	0.44
1:3:88:ALA:HB1	1:3:95:TYR:HD2	1.82	0.43
1:4:399:LYS:HG3	1:4:405:GLN:HE22	1.83	0.43
1:4:51:TYR:O	1:4:55:ILE:HG12	2.18	0.43
1:4:426:SER:O	1:4:428:GLU:N	2.50	0.43
1:1:313:TYR:HA	1:1:487:MET:HE3	1.99	0.43
1:1:213:LEU:HD21	1:1:331:PHE:CE1	2.53	0.43
1:2:142:ILE:HG22	1:2:146:LYS:HE3	1.99	0.43
1:1:33:THR:HA	1:1:36:ASN:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:127:PRO:HB2	1:3:128:HIS:H	1.66	0.43
1:2:150:ARG:HA	1:2:150:ARG:NE	2.33	0.43
1:3:468:ASP:OD1	1:3:470:ARG:NH1	2.51	0.43
1:2:390:GLN:N	1:2:406:PHE:O	2.51	0.43
1:2:218:GLU:OE2	1:2:222:LYS:NZ	2.51	0.43
1:4:332:SER:O	1:4:336:GLU:HG3	2.19	0.43
1:1:360:GLY:O	1:1:361:VAL:O	2.37	0.43
1:1:91:LEU:O	1:1:92:ASP:HB2	2.17	0.43
1:4:286:LEU:HB3	1:4:299:LEU:HD21	2.00	0.43
1:1:486:PRO:O	1:1:498:MET:CE	2.67	0.43
1:3:275:ARG:NH1	1:3:451:TYR:OH	2.51	0.43
1:2:357:SER:O	1:2:395:ARG:NH2	2.51	0.43
1:3:242:ASP:OD1	1:3:426:SER:HB3	2.19	0.43
1:1:464:LEU:HD12	1:1:464:LEU:HA	1.74	0.43
1:4:185:LYS:O	1:4:186:VAL:HB	2.19	0.43
1:3:351:MET:CE	1:3:354:GLY:HA2	2.42	0.43
1:2:200:ASP:O	1:2:202:LYS:HG3	2.18	0.43
1:2:249:ASP:OD1	1:2:478:ALA:O	2.36	0.43
1:3:309:MET:HE3	1:3:313:TYR:CE2	2.53	0.43
1:3:487:MET:O	1:3:495:GLN:NE2	2.50	0.43
1:1:468:ASP:OD1	1:1:470:ARG:NH1	2.52	0.43
1:3:324:THR:C	1:3:326:GLN:N	2.72	0.43
1:1:165:LEU:HA	1:1:165:LEU:HD12	1.80	0.43
1:2:375:PRO:HA	1:2:376:PRO:HD3	1.81	0.43
1:2:109:LEU:HD12	1:2:111:LYS:HD2	2.01	0.43
1:1:185:LYS:O	1:1:186:VAL:CB	2.67	0.43
1:4:179:PRO:HD3	1:4:197:TRP:CD2	2.54	0.43
1:4:181:LEU:CD2	1:4:184:GLY:HA2	2.48	0.43
1:1:32:LYS:O	1:1:36:ASN:HB2	2.18	0.43
1:1:307:ASP:N	1:1:374:GLN:HE22	2.11	0.43
1:1:489:TYR:O	1:1:490:ALA:HB3	2.17	0.43
1:2:468:ASP:C	1:2:470:ARG:H	2.22	0.43
1:3:72:TYR:HA	1:3:72:TYR:HD2	1.77	0.43
1:3:209:ALA:O	1:3:213:LEU:HG	2.18	0.43
1:3:233:GLU:O	1:3:467:SER:N	2.51	0.43
1:1:38:TYR:CD2	1:1:38:TYR:N	2.87	0.43
1:1:167:ILE:CD1	1:1:211:GLN:HE21	2.31	0.43
1:4:425:ARG:O	1:4:444:THR:HA	2.19	0.43
1:1:485:LYS:HB3	1:1:486:PRO:HD2	2.01	0.43
1:1:494:LEU:O	1:1:497:GLY:N	2.44	0.43
1:2:173:GLU:HG2	1:2:176:TYR:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:188:ILE:O	1:2:192:LYS:HG3	2.19	0.43
1:4:166:ASP:O	1:4:167:ILE:C	2.57	0.43
1:1:351:MET:CE	1:1:354:GLY:HA2	2.45	0.43
1:4:366:ILE:O	1:4:369:ILE:HG13	2.19	0.43
1:2:112:PHE:HD1	1:2:112:PHE:H	1.59	0.43
1:3:389:PRO:HD3	1:3:425:ARG:CZ	2.49	0.43
1:2:148:PHE:C	1:2:148:PHE:CD1	2.91	0.43
1:1:196:GLN:O	1:1:197:TRP:C	2.57	0.43
1:1:320:LYS:HG2	1:1:325:ALA:CA	2.45	0.43
1:1:233:GLU:O	1:1:467:SER:N	2.52	0.43
1:3:238:THR:O	1:3:267:ILE:HG22	2.19	0.42
1:4:489:TYR:O	1:4:490:ALA:HB3	2.18	0.42
1:1:64:TYR:N	1:1:64:TYR:CD1	2.87	0.42
1:3:45:GLU:C	1:3:47:ALA:H	2.21	0.42
1:3:389:PRO:HB3	1:3:442:CYS:SG	2.59	0.42
1:4:188:ILE:HG12	1:4:292:LEU:HD21	1.99	0.42
1:3:345:ASN:C	1:3:347:LYS:H	2.22	0.42
1:2:468:ASP:OD1	1:2:470:ARG:NH1	2.52	0.42
1:2:432:GLU:OE1	1:2:458:LYS:NZ	2.52	0.42
1:4:181:LEU:HD23	1:4:184:GLY:HA2	2.00	0.42
1:4:166:ASP:HA	1:4:170:MET:HG3	2.01	0.42
1:2:312:ILE:HG23	1:2:494:LEU:HD11	2.01	0.42
1:1:391:PRO:HG2	1:1:392:GLN:H	1.85	0.42
1:3:31:LEU:HD13	1:3:53:GLN:HB3	2.01	0.42
1:2:361:VAL:HA	1:2:365:ASP:OD1	2.19	0.42
1:4:27:ARG:HA	1:4:30:GLU:HG3	2.01	0.42
1:2:373:ARG:HD2	1:2:374:GLN:O	2.18	0.42
1:4:167:ILE:HD13	1:4:211:GLN:NE2	2.31	0.42
1:1:49:LYS:HA	1:1:49:LYS:HD3	1.82	0.42
1:3:432:GLU:OE1	1:3:458:LYS:NZ	2.49	0.42
1:2:224:SER:C	1:2:371:ARG:NH2	2.73	0.42
1:2:220:LEU:HD13	1:2:338:LEU:HD23	2.01	0.42
1:4:356:PHE:CZ	1:4:361:VAL:HG11	2.55	0.42
1:2:479:VAL:HA	1:2:480:PRO:HD2	1.90	0.42
1:1:323:TYR:CG	1:1:327:MET:HE2	2.54	0.42
1:1:498:MET:CE	1:1:498:MET:CG	2.98	0.42
1:3:274:ASP:O	1:3:276:GLY:N	2.42	0.42
1:4:356:PHE:CZ	1:4:384:LEU:HD13	2.54	0.42
1:3:478:ALA:O	1:3:479:VAL:HB	2.19	0.42
1:3:479:VAL:HG12	1:3:479:VAL:O	2.19	0.42
1:3:388:ASP:OD1	1:3:427:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:481:HIS:O	1:1:482:PRO:O	2.37	0.42
1:2:432:GLU:HA	1:2:432:GLU:OE1	2.20	0.42
1:2:373:ARG:CZ	1:2:376:PRO:HG3	2.50	0.42
1:3:275:ARG:HG3	1:3:275:ARG:NH1	2.31	0.42
1:3:351:MET:N	1:3:351:MET:SD	2.92	0.42
1:1:55:ILE:CD1	1:1:64:TYR:HB3	2.50	0.42
1:1:64:TYR:N	1:1:64:TYR:HD1	2.17	0.42
1:3:389:PRO:CD	1:3:425:ARG:CZ	2.98	0.42
1:3:489:TYR:CD1	1:3:489:TYR:N	2.87	0.42
1:2:190:PHE:CD2	1:2:191:MET:HE2	2.55	0.42
1:1:74:ARG:HH11	1:1:74:ARG:HG3	1.84	0.42
1:4:185:LYS:HE3	1:4:185:LYS:CA	2.23	0.42
1:3:244:HIS:CD2	1:3:451:TYR:HE2	2.38	0.42
1:1:33:THR:O	1:1:37:ASP:CB	2.67	0.42
1:1:489:TYR:CD1	1:1:489:TYR:N	2.88	0.42
1:1:345:ASN:C	1:1:347:LYS:H	2.23	0.42
1:3:279:SER:O	1:3:283:ILE:HG22	2.20	0.42
1:1:487:MET:CG	1:1:498:MET:CE	2.98	0.42
1:1:165:LEU:CD2	1:1:168:GLU:HB2	2.50	0.42
1:3:351:MET:HE1	1:3:423:ILE:HD12	2.01	0.42
1:3:184:GLY:O	1:3:215:GLN:NE2	2.53	0.42
1:2:275:ARG:NH1	1:2:451:TYR:OH	2.53	0.42
1:2:395:ARG:NH1	1:2:395:ARG:CG	2.83	0.42
1:1:181:LEU:O	1:1:183:ASP:N	2.52	0.42
1:2:248:TYR:O	1:2:479:VAL:HG11	2.20	0.42
1:2:312:ILE:O	1:2:494:LEU:HD13	2.20	0.42
1:1:211:GLN:O	1:1:215:GLN:HG3	2.20	0.42
1:1:487:MET:CB	1:1:498:MET:CE	2.96	0.42
1:4:279:SER:O	1:4:283:ILE:HG22	2.19	0.42
1:4:168:GLU:HB3	1:4:169:SER:H	1.44	0.42
1:1:421:ASP:OD1	1:1:421:ASP:N	2.53	0.42
1:4:70:LEU:O	1:4:73:LEU:HB2	2.20	0.42
1:4:248:TYR:CE1	1:4:482:PRO:HD2	2.55	0.42
1:3:464:LEU:HA	1:3:464:LEU:HD12	1.75	0.42
1:1:487:MET:CB	1:1:498:MET:HE2	2.47	0.41
1:3:87:ARG:NH2	1:3:91:LEU:HD21	2.35	0.41
1:3:411:THR:O	1:3:415:LEU:HG	2.20	0.41
1:2:393:ASN:CB	1:2:409:ASP:OD2	2.68	0.41
1:4:399:LYS:HD2	1:4:405:GLN:HE22	1.85	0.41
1:4:453:ASP:OD1	1:4:481:HIS:HE1	2.03	0.41
1:4:42:LYS:HD3	1:4:454:GLN:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:135:LYS:CE	1:3:496:LEU:HD12	2.50	0.41
1:2:489:TYR:CD1	1:2:489:TYR:N	2.87	0.41
1:4:72:TYR:HE1	1:4:84:ASP:OD2	2.03	0.41
1:1:181:LEU:HD23	1:1:184:GLY:HA2	2.02	0.41
1:3:75:THR:O	1:3:76:GLU:HB2	2.20	0.41
1:1:479:VAL:HA	1:1:480:PRO:HD2	1.88	0.41
1:3:73:LEU:HA	1:3:73:LEU:HD12	1.91	0.41
1:2:181:LEU:CD1	1:2:186:VAL:N	2.84	0.41
1:3:31:LEU:HD13	1:3:53:GLN:CB	2.49	0.41
1:3:65:TYR:CD2	1:3:87:ARG:HG2	2.55	0.41
1:1:390:GLN:N	1:1:406:PHE:O	2.53	0.41
1:2:64:TYR:CD1	1:2:64:TYR:N	2.88	0.41
1:1:487:MET:O	1:1:495:GLN:HG2	2.21	0.41
1:2:165:LEU:O	1:2:166:ASP:HB2	2.20	0.41
1:3:38:TYR:HE2	1:3:50:PHE:CZ	2.38	0.41
1:4:267:ILE:HD12	1:4:342:GLN:CD	2.41	0.41
1:1:362:THR:O	1:1:365:ASP:HB2	2.20	0.41
1:4:166:ASP:HA	1:4:170:MET:CG	2.49	0.41
1:1:280:VAL:HG23	1:1:318:GLU:OE2	2.20	0.41
1:4:493:LEU:C	1:4:494:LEU:HG	2.40	0.41
1:3:355:LEU:CD1	1:3:411:THR:HA	2.50	0.41
1:2:312:ILE:HG23	1:2:494:LEU:HD13	2.01	0.41
1:4:463:HIS:HB2	1:4:472:GLN:HB2	2.02	0.41
1:2:267:ILE:HD12	1:2:342:GLN:CD	2.40	0.41
1:4:217:LYS:HB2	1:4:334:VAL:CG1	2.37	0.41
1:2:283:ILE:HG23	1:2:284:LEU:N	2.35	0.41
1:1:161:VAL:C	1:1:163:ASP:H	2.22	0.41
1:2:70:LEU:HB2	1:2:101:ARG:NE	2.34	0.41
1:1:445:VAL:O	1:1:445:VAL:HG13	2.19	0.41
1:4:232:LYS:O	1:4:233:GLU:C	2.58	0.41
1:1:160:SER:HB3	1:1:333:GLU:OE2	2.21	0.41
1:2:106:ASN:O	1:2:111:LYS:HG3	2.20	0.41
1:2:195:MET:HE1	1:2:289:PHE:HZ	1.86	0.41
1:3:303:ASN:HB2	1:3:386:TRP:CE2	2.55	0.41
1:2:162:VAL:HG12	1:2:162:VAL:O	2.20	0.41
1:3:267:ILE:HD12	1:3:342:GLN:CD	2.41	0.41
1:3:112:PHE:O	1:3:113:ARG:C	2.59	0.41
1:4:373:ARG:CZ	1:4:376:PRO:HG3	2.50	0.41
1:3:31:LEU:HD13	1:3:54:ALA:N	2.36	0.41
1:2:216:VAL:O	1:2:220:LEU:HG	2.20	0.41
1:1:275:ARG:NH1	1:1:275:ARG:HG3	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:347:LYS:HD2	1:4:421:ASP:OD1	2.20	0.41
1:1:217:LYS:NZ	1:1:333:GLU:OE1	2.51	0.41
1:3:64:TYR:C	1:3:66:GLY:N	2.74	0.41
1:2:136:TYR:CE2	1:2:140:ASN:ND2	2.89	0.41
1:4:415:LEU:HD23	1:4:415:LEU:HA	1.93	0.41
1:3:481:HIS:HB2	1:3:482:PRO:HD2	2.02	0.41
1:2:425:ARG:O	1:2:444:THR:HA	2.21	0.41
1:1:436:VAL:CG1	1:1:440:GLY:HA2	2.51	0.41
1:4:74:ARG:HD3	1:4:74:ARG:HA	1.93	0.41
1:2:181:LEU:HD13	1:2:186:VAL:N	2.36	0.41
1:2:181:LEU:HD23	1:2:211:GLN:OE1	2.21	0.41
1:4:220:LEU:CD1	1:4:338:LEU:HD23	2.50	0.41
1:3:304:HIS:C	1:3:306:THR:H	2.24	0.41
1:1:29:GLU:OE2	1:1:32:LYS:HD3	2.21	0.41
1:3:128:HIS:HA	1:3:133:LYS:CE	2.51	0.41
1:3:425:ARG:HD3	1:3:425:ARG:C	2.41	0.41
1:2:136:TYR:O	1:2:140:ASN:HB2	2.21	0.41
1:1:112:PHE:H	1:1:112:PHE:HD1	1.55	0.41
1:4:345:ASN:C	1:4:347:LYS:H	2.24	0.41
1:3:197:TRP:CH2	1:3:202:LYS:HD3	2.56	0.41
1:4:123:VAL:HG22	1:4:123:VAL:O	2.21	0.41
1:4:267:ILE:HD11	1:4:350:ILE:HD11	2.02	0.41
1:3:181:LEU:HG	1:3:184:GLY:CA	2.44	0.41
1:1:493:LEU:HD23	1:1:493:LEU:HA	1.91	0.41
1:4:42:LYS:HZ2	1:4:454:GLN:HA	1.85	0.41
1:1:68:ARG:HG2	1:1:72:TYR:CE1	2.56	0.41
1:4:223:LEU:O	1:4:371:ARG:NH2	2.36	0.40
1:4:130:LYS:O	1:4:132:ALA:N	2.48	0.40
1:4:343:CYS:SG	1:4:346:GLY:HA2	2.62	0.40
1:4:452:CYS:C	1:4:454:GLN:N	2.74	0.40
1:1:188:ILE:O	1:1:192:LYS:HG3	2.21	0.40
1:2:232:LYS:HE2	1:2:235:GLU:CB	2.51	0.40
1:3:168:GLU:C	1:3:170:MET:H	2.24	0.40
1:1:375:PRO:HA	1:1:376:PRO:HD3	1.74	0.40
1:3:87:ARG:O	1:3:91:LEU:HD12	2.20	0.40
1:1:112:PHE:HB3	1:1:146:LYS:HD2	2.02	0.40
1:2:172:ILE:HD11	1:2:180:LYS:HZ2	1.85	0.40
1:3:96:ILE:HD11	1:3:125:VAL:CG1	2.52	0.40
1:3:306:THR:HG22	1:3:308:ASN:H	1.86	0.40
1:2:357:SER:O	1:2:395:ARG:CZ	2.70	0.40
1:1:190:PHE:CD2	1:1:191:MET:HE2	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:324:THR:C	1:4:326:GLN:N	2.74	0.40
1:3:345:ASN:O	1:3:347:LYS:N	2.54	0.40
1:3:245:GLY:HA2	1:3:282:VAL:HG21	2.03	0.40
1:3:52:SER:O	1:3:56:GLU:HB2	2.22	0.40
1:1:357:SER:O	1:1:395:ARG:NH2	2.55	0.40
1:3:80:TYR:CD2	1:3:399:LYS:HA	2.57	0.40
1:2:371:ARG:O	1:2:373:ARG:N	2.53	0.40
1:4:173:GLU:HB3	1:4:174:ASP:H	1.48	0.40
1:1:429:VAL:HG21	1:1:451:TYR:CD1	2.57	0.40
1:1:315:PHE:O	1:1:319:VAL:HG23	2.22	0.40
1:4:479:VAL:HA	1:4:480:PRO:HD2	1.87	0.40
1:1:432:GLU:O	1:1:475:GLN:NE2	2.44	0.40
1:4:316:GLU:HA	1:4:328:TYR:CD1	2.57	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	1	467/477 (98%)	390 (84%)	50 (11%)	27 (6%)	2	6
1	2	463/477 (97%)	387 (84%)	48 (10%)	28 (6%)	2	6
1	3	467/477 (98%)	358 (77%)	77 (16%)	32 (7%)	1	4
1	4	462/477 (97%)	385 (83%)	49 (11%)	28 (6%)	2	5
All	All	1859/1908 (97%)	1520 (82%)	224 (12%)	115 (6%)	2	5

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	168	GLU
1	1	169	SER

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Mol	Chain	Res	Type
1	1	172	ILE
1	1	361	VAL
1	1	372	ASN
1	1	451	TYR
1	1	478	ALA
1	2	149	GLU
1	2	168	GLU
1	2	170	MET
1	2	361	VAL
1	2	372	ASN
1	2	451	TYR
1	2	478	ALA
1	3	58	ASN
1	3	127	PRO
1	3	165	LEU
1	3	166	ASP
1	3	169	SER
1	3	181	LEU
1	3	361	VAL
1	3	372	ASN
1	3	451	TYR
1	3	478	ALA
1	4	149	GLU
1	4	160	SER
1	4	167	ILE
1	4	168	GLU
1	4	169	SER
1	4	171	THR
1	4	172	ILE
1	4	361	VAL
1	4	372	ASN
1	4	451	TYR
1	4	478	ALA
1	1	182	GLU
1	1	186	VAL
1	1	235	GLU
1	1	360	GLY
1	1	483	ASN
1	2	169	SER
1	2	202	LYS
1	2	360	GLY
1	2	484	VAL

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Mol	Chain	Res	Type
1	3	92	ASP
1	3	141	LYS
1	3	186	VAL
1	3	202	LYS
1	3	360	GLY
1	3	484	VAL
1	4	164	SER
1	4	235	GLU
1	4	427	HIS
1	4	484	VAL
1	1	92	ASP
1	1	159	ARG
1	1	160	SER
1	1	170	MET
1	1	380	PRO
1	1	427	HIS
1	1	479	VAL
1	1	490	ALA
1	2	160	SER
1	2	163	ASP
1	2	235	GLU
1	2	380	PRO
1	2	483	ASN
1	2	490	ALA
1	3	82	LEU
1	3	159	ARG
1	3	235	GLU
1	3	380	PRO
1	3	469	LEU
1	3	482	PRO
1	3	483	ASN
1	3	490	ALA
1	3	497	GLY
1	4	92	ASP
1	4	159	ARG
1	4	360	GLY
1	4	380	PRO
1	4	482	PRO
1	4	490	ALA
1	1	112	PHE
1	1	484	VAL
1	2	469	LEU

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Mol	Chain	Res	Type
1	2	479	VAL
1	2	482	PRO
1	3	113	ARG
1	3	346	GLY
1	3	479	VAL
1	4	166	ASP
1	4	479	VAL
1	4	483	ASN
1	1	202	LYS
1	1	413	ALA
1	1	469	LEU
1	1	482	PRO
1	2	112	PHE
1	2	172	ILE
1	2	184	GLY
1	2	373	ARG
1	2	413	ALA
1	3	114	ALA
1	3	164	SER
1	3	171	THR
1	4	186	VAL
1	4	202	LYS
1	2	176	TYR
1	2	267	ILE
1	4	24	ALA
1	2	162	VAL
1	3	267	ILE
1	4	346	GLY
1	1	346	GLY

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	407/413 (98%)	374 (92%)	33 (8%)	15	39
1	2	406/413 (98%)	382 (94%)	24 (6%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	406/413 (98%)	373 (92%)	33 (8%)	15	39
1	4	404/413 (98%)	372 (92%)	32 (8%)	15	41
All	All	1623/1652 (98%)	1501 (92%)	122 (8%)	17	44

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	45	GLU
1	1	58	ASN
1	1	107	MET
1	1	111	LYS
1	1	112	PHE
1	1	118	ASP
1	1	170	MET
1	1	172	ILE
1	1	183	ASP
1	1	189	SER
1	1	196	GLN
1	1	201	GLN
1	1	216	VAL
1	1	235	GLU
1	1	243	THR
1	1	246	GLN
1	1	263	THR
1	1	272	PHE
1	1	309	MET
1	1	332	SER
1	1	351	MET
1	1	356	PHE
1	1	402	VAL
1	1	421	ASP
1	1	425	ARG
1	1	450	ASN
1	1	463	HIS
1	1	464	LEU
1	1	469	LEU
1	1	470	ARG
1	1	477	THR
1	1	483	ASN
1	1	498	MET
1	2	36	ASN

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Mol	Chain	Res	Type
1	2	45	GLU
1	2	58	ASN
1	2	73	LEU
1	2	107	MET
1	2	111	LYS
1	2	112	PHE
1	2	118	ASP
1	2	196	GLN
1	2	201	GLN
1	2	235	GLU
1	2	243	THR
1	2	246	GLN
1	2	263	THR
1	2	272	PHE
1	2	351	MET
1	2	402	VAL
1	2	421	ASP
1	2	425	ARG
1	2	463	HIS
1	2	465	GLN
1	2	470	ARG
1	2	477	THR
1	2	483	ASN
1	3	51	TYR
1	3	58	ASN
1	3	64	TYR
1	3	65	TYR
1	3	72	TYR
1	3	99	TYR
1	3	112	PHE
1	3	129	ASP
1	3	148	PHE
1	3	166	ASP
1	3	175	GLU
1	3	185	LYS
1	3	196	GLN
1	3	201	GLN
1	3	216	VAL
1	3	235	GLU
1	3	242	ASP
1	3	243	THR
1	3	246	GLN

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Mol	Chain	Res	Type
1	3	263	THR
1	3	272	PHE
1	3	309	MET
1	3	351	MET
1	3	395	ARG
1	3	402	VAL
1	3	421	ASP
1	3	425	ARG
1	3	463	HIS
1	3	464	LEU
1	3	465	GLN
1	3	470	ARG
1	3	477	THR
1	3	483	ASN
1	4	32	LYS
1	4	45	GLU
1	4	58	ASN
1	4	107	MET
1	4	111	LYS
1	4	112	PHE
1	4	140	ASN
1	4	165	LEU
1	4	173	GLU
1	4	185	LYS
1	4	196	GLN
1	4	201	GLN
1	4	216	VAL
1	4	235	GLU
1	4	243	THR
1	4	246	GLN
1	4	263	THR
1	4	271	ASP
1	4	272	PHE
1	4	275	ARG
1	4	351	MET
1	4	402	VAL
1	4	421	ASP
1	4	425	ARG
1	4	450	ASN
1	4	463	HIS
1	4	464	LEU
1	4	465	GLN

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Mol	Chain	Res	Type
1	4	469	LEU
1	4	470	ARG
1	4	477	THR
1	4	483	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	36	ASN
1	1	58	ASN
1	1	137	GLN
1	1	201	GLN
1	1	246	GLN
1	1	257	ASN
1	1	296	HIS
1	1	310	ASN
1	1	374	GLN
1	1	393	ASN
1	1	405	GLN
1	1	419	ASN
1	1	450	ASN
1	1	463	HIS
1	1	481	HIS
1	2	36	ASN
1	2	58	ASN
1	2	137	GLN
1	2	201	GLN
1	2	211	GLN
1	2	296	HIS
1	2	298	HIS
1	2	310	ASN
1	2	374	GLN
1	2	405	GLN
1	2	419	ASN
1	2	450	ASN
1	2	481	HIS
1	3	46	ASN
1	3	67	ASN
1	3	137	GLN
1	3	201	GLN
1	3	257	ASN
1	3	296	HIS

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Mol	Chain	Res	Type
1	3	298	HIS
1	3	310	ASN
1	3	374	GLN
1	3	390	GLN
1	3	405	GLN
1	3	450	ASN
1	3	463	HIS
1	3	481	HIS
1	4	58	ASN
1	4	137	GLN
1	4	201	GLN
1	4	211	GLN
1	4	296	HIS
1	4	298	HIS
1	4	310	ASN
1	4	311	GLN
1	4	374	GLN
1	4	390	GLN
1	4	393	ASN
1	4	405	GLN
1	4	450	ASN
1	4	481	HIS

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 ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.