



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:18 AM UTC

PDB ID : 2AYN / pdb_00002ayn
Title : Structure of USP14, a proteasome-associated deubiquitinating enzyme
Authors : Hu, M.; Li, P.; Jeffrey, P.D.; Shi, Y.
Deposited on : 2005-09-07
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

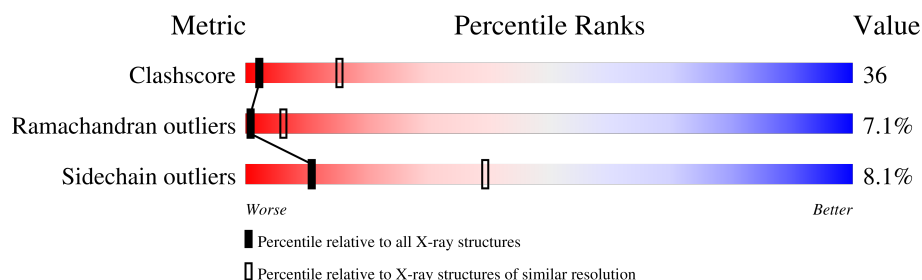
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	404	34% 40% 9% • 17%
1	B	404	32% 41% 10% • 17%
1	C	404	31% 42% 9% • 17%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8163 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 Ubiquitin carboxyl-terminal hydrolase 14.

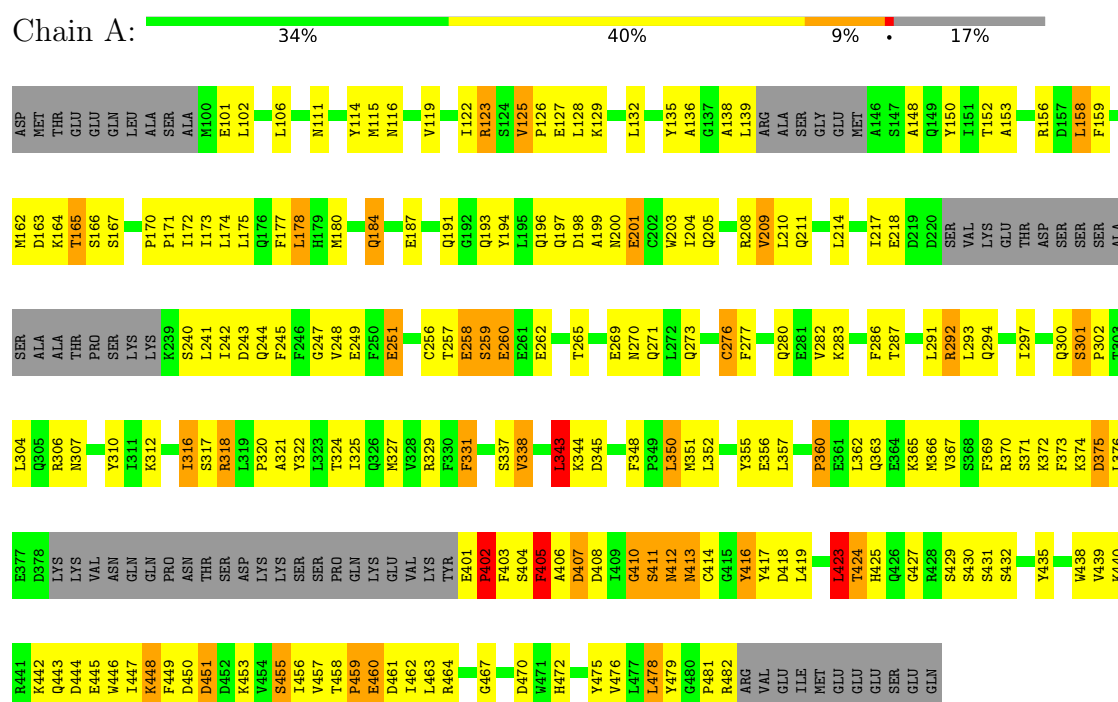
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	337	Total	C	N	O	S	0	0	0
			2721	1734	447	521	19			
1	B	337	Total	C	N	O	S	0	0	0
			2721	1734	447	521	19			
1	C	337	Total	C	N	O	S	0	0	0
			2721	1734	447	521	19			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 14



- Molecule 1: Ubiquitin carboxyl-terminal hydrolase 14



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.28Å 121.58Å 166.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (99.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.322	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8163	wwPDB-VP
Average B, all atoms (Å ²)	123.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.65	0/2772	1.15	23/3732 (0.6%)
1	B	0.70	0/2772	1.19	29/3732 (0.8%)
1	C	0.62	1/2772 (0.0%)	1.11	20/3732 (0.5%)
All	All	0.66	1/8316 (0.0%)	1.15	72/11196 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	THR	CA-CB	-5.07	1.46	1.53

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	VAL	N-CA-C	8.88	115.64	107.56
1	A	125	VAL	N-CA-C	8.75	116.21	107.55
1	C	316	ILE	N-CA-C	8.69	120.45	107.15
1	A	301	SER	CA-C-N	8.66	128.88	119.87
1	A	301	SER	C-N-CA	8.66	128.88	119.87
1	A	316	ILE	N-CA-C	8.41	119.66	106.88
1	B	448	LYS	N-CA-C	-8.31	99.33	110.55
1	B	301	SER	CA-C-N	7.83	128.82	120.12
1	B	301	SER	C-N-CA	7.83	128.82	120.12
1	B	201	GLU	N-CA-C	-7.78	102.75	111.07
1	B	350	LEU	N-CA-C	-7.74	104.07	113.97
1	B	470	ASP	N-CA-C	-7.71	103.59	113.16
1	C	448	LYS	N-CA-C	-7.65	100.44	110.53
1	B	439	VAL	N-CA-C	7.58	118.72	108.11
1	B	316	ILE	N-CA-C	7.56	119.52	107.73
1	B	407	ASP	N-CA-C	-7.46	99.98	110.50
1	C	470	ASP	N-CA-C	-7.34	104.21	113.02
1	A	448	LYS	N-CA-C	-7.31	101.41	110.41
1	A	407	ASP	N-CA-C	-7.27	100.91	110.43
1	C	350	LEU	N-CA-C	-7.11	104.87	113.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	PRO	N-CA-C	-6.92	103.92	113.53
1	B	480	GLY	CA-C-N	6.78	128.31	119.84
1	B	480	GLY	C-N-CA	6.78	128.31	119.84
1	A	470	ASP	N-CA-C	-6.72	104.71	113.17
1	A	350	LEU	N-CA-C	-6.71	105.38	113.97
1	C	125	VAL	N-CA-C	6.71	113.67	107.56
1	A	194	TYR	N-CA-C	-6.61	101.18	110.50
1	C	178	LEU	N-CA-C	-6.51	104.19	111.28
1	B	319	LEU	CA-C-N	6.51	127.75	120.66
1	B	319	LEU	C-N-CA	6.51	127.75	120.66
1	B	178	LEU	N-CA-C	-6.50	104.20	111.28
1	A	423	LEU	N-CA-C	-6.44	99.52	109.76
1	B	252	THR	N-CA-C	6.43	119.00	108.52
1	A	170	PRO	N-CA-C	-6.39	102.91	110.70
1	A	430	SER	N-CA-C	-6.36	105.00	112.89
1	A	251	GLU	N-CA-C	-6.34	98.87	109.07
1	C	407	ASP	N-CA-C	-6.32	102.15	110.43
1	C	439	VAL	N-CA-C	6.24	117.10	108.12
1	B	348	PHE	CA-C-N	6.23	126.19	120.21
1	B	348	PHE	C-N-CA	6.23	126.19	120.21
1	B	219	ASP	N-CA-C	6.23	118.24	108.96
1	C	152	THR	N-CA-C	-6.18	104.45	111.07
1	A	439	VAL	N-CA-C	6.11	116.66	108.11
1	A	297	ILE	N-CA-C	6.05	117.39	109.58
1	C	427	GLY	N-CA-C	5.89	118.81	110.74
1	B	170	PRO	N-CA-C	-5.81	103.61	110.70
1	B	475	TYR	N-CA-C	-5.79	106.77	113.88
1	A	152	THR	N-CA-C	-5.76	104.91	111.07
1	C	424	THR	N-CA-C	5.75	117.75	107.80
1	B	423	LEU	N-CA-C	-5.68	101.23	110.20
1	B	301	SER	N-CA-C	5.66	117.20	110.07
1	A	424	THR	N-CA-C	5.61	117.57	108.26
1	A	427	GLY	N-CA-C	5.57	119.83	111.42
1	A	343	LEU	N-CA-C	5.56	119.64	112.41
1	C	343	LEU	N-CA-C	5.54	119.83	112.30
1	C	423	LEU	N-CA-C	-5.54	102.09	110.28
1	A	178	LEU	N-CA-C	-5.52	105.26	111.28
1	C	301	SER	N-CA-C	5.51	116.60	109.72
1	C	194	TYR	N-CA-C	-5.49	102.76	110.50
1	A	301	SER	N-CA-C	5.48	116.57	109.72
1	C	170	PRO	N-CA-C	-5.48	104.02	110.70
1	B	343	LEU	N-CA-C	5.45	121.14	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	PRO	N-CA-C	-5.44	105.65	113.75
1	C	122	ILE	CB-CA-C	-5.39	104.98	111.88
1	C	360	PRO	N-CA-C	-5.32	106.14	113.53
1	B	147	SER	N-CA-C	-5.20	105.61	111.28
1	A	111	ASN	N-CA-C	-5.20	104.83	110.91
1	C	244	GLN	N-CA-C	5.17	118.06	111.69
1	B	122	ILE	CB-CA-C	-5.17	105.27	112.04
1	B	111	ASN	N-CA-C	-5.16	104.57	111.02
1	C	475	TYR	N-CA-C	-5.11	107.70	114.04
1	B	424	THR	N-CA-C	5.11	116.73	108.26

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	2721	0	2696	183	0
1	B	2721	0	2696	223	0
1	C	2721	0	2696	201	0
All	All	8163	0	8088	592	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 36.

All (592) 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:C:184:GLN:HE21	1:C:184:GLN:N	1.45	1.14
1:C:184:GLN:H	1:C:184:GLN:NE2	1.44	1.13
1:B:184:GLN:H	1:B:184:GLN:NE2	1.50	1.08
1:A:184:GLN:H	1:A:184:GLN:NE2	1.50	1.08
1:B:172:ILE:HD11	1:C:109:LEU:HB3	1.34	1.06
1:A:350:LEU:HD11	1:A:463:LEU:HD21	1.37	1.05
1:B:184:GLN:HE21	1:B:184:GLN:N	1.54	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:GLN:HE21	1:A:184:GLN:N	1.56	1.04
1:B:350:LEU:HD11	1:B:463:LEU:HD21	1.41	1.01
1:B:260:GLU:HG2	1:B:304:LEU:HD11	1.43	0.99
1:B:457:VAL:HG22	1:B:458:THR:H	1.29	0.96
1:A:115:MET:HE3	1:A:178:LEU:HD22	1.49	0.94
1:C:260:GLU:HG2	1:C:304:LEU:HD11	1.50	0.92
1:A:260:GLU:HG2	1:A:304:LEU:HD11	1.51	0.92
1:B:351:MET:HE1	1:B:482:ARG:HG3	1.50	0.92
1:C:350:LEU:HD11	1:C:463:LEU:HD21	1.51	0.91
1:B:109:LEU:HB3	1:C:172:ILE:HD11	1.55	0.89
1:B:300:GLN:HA	1:B:307:ASN:HA	1.55	0.88
1:A:457:VAL:HG22	1:A:458:THR:H	1.38	0.88
1:B:172:ILE:CD1	1:C:109:LEU:HB3	2.05	0.87
1:B:115:MET:HE1	1:B:175:LEU:HA	1.53	0.86
1:C:351:MET:HE1	1:C:482:ARG:HG3	1.55	0.86
1:C:187:GLU:HG3	1:C:195:LEU:HD12	1.58	0.84
1:C:343:LEU:HD12	1:C:343:LEU:N	1.93	0.83
1:A:460:GLU:CD	1:A:460:GLU:H	1.86	0.83
1:C:150:TYR:HB3	1:C:177:PHE:CD2	2.14	0.82
1:B:362:LEU:HD22	1:B:366:MET:HE2	1.62	0.81
1:C:457:VAL:HG22	1:C:458:THR:H	1.45	0.81
1:A:462:ILE:HD12	1:A:462:ILE:H	1.45	0.81
1:B:462:ILE:HD12	1:B:462:ILE:H	1.46	0.81
1:C:448:LYS:HB3	1:C:455:SER:HB3	1.60	0.81
1:B:109:LEU:HB3	1:C:172:ILE:CD1	2.11	0.81
1:A:351:MET:HE1	1:A:482:ARG:HG3	1.62	0.80
1:C:300:GLN:HA	1:C:307:ASN:HA	1.64	0.80
1:A:424:THR:HG21	1:A:472:HIS:HB3	1.65	0.79
1:C:304:LEU:N	1:C:304:LEU:HD12	1.98	0.79
1:C:424:THR:HG21	1:C:472:HIS:HB3	1.65	0.78
1:A:191:GLN:C	1:A:193:GLN:H	1.92	0.78
1:B:172:ILE:HD11	1:C:109:LEU:CB	2.14	0.78
1:C:115:MET:O	1:C:119:VAL:HG23	1.83	0.78
1:C:417:TYR:HB3	1:C:479:TYR:HB3	1.66	0.78
1:B:457:VAL:HG22	1:B:458:THR:N	1.96	0.77
1:A:300:GLN:HA	1:A:307:ASN:HA	1.66	0.77
1:A:343:LEU:HD12	1:A:343:LEU:H	1.51	0.76
1:B:258:GLU:O	1:B:260:GLU:N	2.18	0.76
1:C:153:ALA:O	1:C:156:ARG:HG3	1.84	0.76
1:B:350:LEU:HD12	1:B:350:LEU:N	2.02	0.75
1:A:459:PRO:HA	1:A:462:ILE:HD13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:PHE:HB2	1:B:292:ARG:NH1	2.03	0.74
1:A:205:GLN:HA	1:A:205:GLN:NE2	2.03	0.73
1:A:350:LEU:CD1	1:A:463:LEU:HD21	2.18	0.73
1:A:153:ALA:O	1:A:156:ARG:HG3	1.88	0.73
1:C:158:LEU:O	1:C:162:MET:HG3	1.88	0.73
1:C:460:GLU:CD	1:C:460:GLU:H	1.96	0.73
1:A:304:LEU:N	1:A:304:LEU:HD12	2.03	0.72
1:B:460:GLU:H	1:B:460:GLU:CD	1.95	0.72
1:C:115:MET:HE3	1:C:178:LEU:HD22	1.70	0.72
1:B:150:TYR:HB3	1:B:177:PHE:CD2	2.24	0.72
1:A:172:ILE:HD13	1:B:164:LYS:O	1.90	0.72
1:C:150:TYR:HB3	1:C:177:PHE:HD2	1.53	0.72
1:C:334:GLU:OE2	1:C:335:LYS:HG3	1.90	0.72
1:C:363:GLN:O	1:C:367:VAL:HG23	1.90	0.72
1:B:270:ASN:O	1:B:271:GLN:HG3	1.90	0.71
1:B:459:PRO:HA	1:B:462:ILE:HD13	1.72	0.71
1:C:405:PHE:CZ	1:C:481:PRO:HG3	2.26	0.71
1:C:457:VAL:HG22	1:C:461:ASP:OD2	1.90	0.71
1:A:457:VAL:HG22	1:A:461:ASP:OD2	1.91	0.71
1:A:283:LYS:HA	1:A:283:LYS:HE2	1.73	0.71
1:A:210:LEU:HD22	1:A:214:LEU:HD11	1.72	0.70
1:A:164:LYS:O	1:A:166:SER:N	2.24	0.70
1:B:241:LEU:O	1:B:244:GLN:HB2	1.90	0.70
1:C:262:GLU:OE1	1:C:302:PRO:HG2	1.92	0.70
1:B:424:THR:HG21	1:B:472:HIS:HB3	1.74	0.70
1:B:115:MET:HE3	1:B:178:LEU:HD22	1.73	0.69
1:B:208:ARG:O	1:B:211:GLN:HB3	1.92	0.69
1:B:417:TYR:HB3	1:B:479:TYR:HB3	1.73	0.69
1:A:150:TYR:HB3	1:A:177:PHE:CD2	2.27	0.69
1:B:165:THR:HG22	1:B:167:SER:OG	1.92	0.69
1:C:343:LEU:HD12	1:C:343:LEU:H	1.58	0.69
1:B:351:MET:CE	1:B:482:ARG:HG3	2.23	0.69
1:B:164:LYS:O	1:B:166:SER:N	2.24	0.69
1:A:248:VAL:HG22	1:A:320:PRO:HD3	1.74	0.68
1:B:262:GLU:OE1	1:B:302:PRO:HD2	1.93	0.68
1:C:277:PHE:HB2	1:C:292:ARG:NH1	2.08	0.68
1:A:407:ASP:OD1	1:A:414:CYS:HB3	1.94	0.68
1:C:448:LYS:CB	1:C:455:SER:HB3	2.23	0.68
1:A:417:TYR:HB3	1:A:479:TYR:HB3	1.75	0.68
1:B:260:GLU:HG2	1:B:304:LEU:CD1	2.21	0.68
1:C:350:LEU:N	1:C:350:LEU:HD12	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:CYS:HB2	1:B:310:TYR:CE2	2.29	0.68
1:A:457:VAL:HG22	1:A:458:THR:N	2.10	0.67
1:C:240:SER:HB2	1:C:243:ASP:OD2	1.94	0.67
1:C:258:GLU:O	1:C:260:GLU:N	2.28	0.67
1:A:196:GLN:HB3	1:A:431:SER:O	1.95	0.67
1:A:258:GLU:O	1:A:260:GLU:N	2.27	0.67
1:C:198:ASP:HB3	1:C:201:GLU:HB2	1.76	0.67
1:B:253:THR:HG22	1:B:266:LYS:HD3	1.77	0.67
1:C:459:PRO:HA	1:C:462:ILE:HD13	1.75	0.67
1:B:248:VAL:HG22	1:B:320:PRO:HD3	1.76	0.66
1:B:330:PHE:CD1	1:B:341:LYS:HB2	2.30	0.66
1:C:205:GLN:O	1:C:209:VAL:HG23	1.95	0.66
1:C:210:LEU:HD22	1:C:214:LEU:HD11	1.78	0.66
1:B:342:VAL:C	1:B:343:LEU:HD12	2.21	0.66
1:B:109:LEU:CB	1:C:172:ILE:HD11	2.24	0.66
1:B:150:TYR:HB3	1:B:177:PHE:CE2	2.31	0.66
1:B:211:GLN:HA	1:B:242:ILE:HG13	1.77	0.66
1:B:127:GLU:HG2	1:B:245:PHE:CE2	2.31	0.66
1:B:283:LYS:HE2	1:B:283:LYS:HA	1.78	0.66
1:C:114:TYR:CD1	1:C:197:GLN:HB2	2.30	0.65
1:C:283:LYS:HE2	1:C:283:LYS:HA	1.77	0.65
1:C:462:ILE:HD12	1:C:462:ILE:H	1.61	0.65
1:B:148:ALA:HB1	1:B:209:VAL:HG13	1.78	0.65
1:C:164:LYS:O	1:C:166:SER:N	2.30	0.65
1:C:196:GLN:HB3	1:C:431:SER:O	1.97	0.64
1:C:407:ASP:OD1	1:C:414:CYS:HB3	1.96	0.64
1:A:115:MET:HE1	1:A:175:LEU:HA	1.80	0.64
1:B:457:VAL:HG22	1:B:461:ASP:OD2	1.96	0.64
1:B:200:ASN:O	1:B:204:ILE:HG13	1.98	0.64
1:A:424:THR:CG2	1:A:472:HIS:HB3	2.27	0.64
1:A:247:GLY:O	1:A:320:PRO:HB3	1.98	0.64
1:C:304:LEU:N	1:C:304:LEU:CD1	2.61	0.64
1:C:165:THR:HG22	1:C:167:SER:OG	1.99	0.63
1:B:205:GLN:HA	1:B:205:GLN:NE2	2.12	0.63
1:C:423:LEU:HB3	1:C:476:VAL:HB	1.80	0.63
1:A:241:LEU:O	1:A:244:GLN:HB2	2.00	0.62
1:B:304:LEU:HD12	1:B:304:LEU:N	2.13	0.62
1:C:270:ASN:O	1:C:271:GLN:HG3	1.99	0.62
1:A:269:GLU:OE1	1:A:312:LYS:NZ	2.26	0.62
1:A:343:LEU:HD12	1:A:343:LEU:N	2.14	0.62
1:A:256:CYS:HB2	1:A:310:TYR:CE2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:SER:HB3	1:A:432:SER:HB3	1.81	0.62
1:A:270:ASN:O	1:A:271:GLN:HG3	2.00	0.61
1:C:352:LEU:O	1:C:416:TYR:HB3	1.99	0.61
1:A:405:PHE:CZ	1:A:481:PRO:HG3	2.35	0.61
1:C:256:CYS:HB2	1:C:310:TYR:CE2	2.35	0.61
1:C:446:TRP:CG	1:C:462:ILE:HD11	2.35	0.61
1:B:138:ALA:H	1:B:149:GLN:HE22	1.48	0.61
1:B:405:PHE:CZ	1:B:481:PRO:HG2	2.35	0.61
1:A:127:GLU:HG2	1:A:245:PHE:CE2	2.36	0.61
1:C:150:TYR:HB3	1:C:177:PHE:CE2	2.36	0.61
1:C:260:GLU:HG2	1:C:304:LEU:CD1	2.28	0.60
1:A:217:ILE:HG22	1:A:218:GLU:N	2.16	0.60
1:A:205:GLN:O	1:A:209:VAL:HG23	2.02	0.60
1:A:208:ARG:O	1:A:211:GLN:HB3	2.00	0.60
1:B:153:ALA:O	1:B:156:ARG:HG3	2.01	0.60
1:B:362:LEU:CD2	1:B:366:MET:HE2	2.31	0.60
1:B:424:THR:CG2	1:B:472:HIS:HB3	2.32	0.60
1:B:240:SER:HB2	1:B:243:ASP:OD2	2.02	0.60
1:C:180:MET:HA	1:C:180:MET:HE2	1.83	0.60
1:C:248:VAL:HG22	1:C:320:PRO:HD3	1.83	0.60
1:C:253:THR:HG22	1:C:266:LYS:HD3	1.84	0.60
1:B:126:PRO:O	1:B:128:LEU:N	2.35	0.59
1:B:249:GLU:HG2	1:B:270:ASN:OD1	2.02	0.59
1:C:260:GLU:HG3	1:C:262:GLU:HG3	1.84	0.59
1:C:341:LYS:O	1:C:343:LEU:HD11	2.03	0.59
1:B:418:ASP:N	1:B:480:GLY:O	2.25	0.59
1:C:424:THR:CG2	1:C:472:HIS:HB3	2.30	0.59
1:A:249:GLU:HG2	1:A:270:ASN:OD1	2.03	0.59
1:A:350:LEU:N	1:A:350:LEU:HD12	2.17	0.58
1:B:350:LEU:CD1	1:B:463:LEU:HD21	2.26	0.58
1:C:211:GLN:HA	1:C:242:ILE:HG13	1.85	0.58
1:C:355:TYR:C	1:C:357:LEU:H	2.10	0.58
1:A:251:GLU:HG3	1:A:317:SER:HB2	1.84	0.58
1:B:458:THR:O	1:B:461:ASP:HB2	2.02	0.58
1:B:345:ASP:HA	1:B:467:GLY:HA3	1.84	0.58
1:C:303:THR:HB	1:C:304:LEU:HD12	1.86	0.58
1:A:148:ALA:HB1	1:A:209:VAL:HG13	1.84	0.58
1:A:351:MET:CE	1:A:482:ARG:HG3	2.31	0.58
1:B:363:GLN:O	1:B:367:VAL:HG23	2.03	0.58
1:C:158:LEU:HD23	1:C:162:MET:HG3	1.86	0.58
1:B:163:ASP:O	1:B:164:LYS:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:HG21	1:C:337:SER:HB2	1.86	0.58
1:A:423:LEU:HB3	1:A:476:VAL:HB	1.86	0.58
1:C:115:MET:HE1	1:C:175:LEU:HA	1.86	0.58
1:A:165:THR:HG22	1:A:167:SER:OG	2.03	0.57
1:B:128:LEU:O	1:B:129:LYS:C	2.47	0.57
1:A:262:GLU:OE1	1:A:302:PRO:HD2	2.04	0.57
1:B:118:THR:HG22	1:B:122:ILE:HD11	1.86	0.57
1:A:150:TYR:HB3	1:A:177:PHE:HD2	1.70	0.57
1:A:277:PHE:HB2	1:A:292:ARG:NH1	2.20	0.57
1:A:122:ILE:O	1:A:128:LEU:HD23	2.04	0.57
1:A:240:SER:HB2	1:A:243:ASP:OD2	2.05	0.57
1:B:115:MET:O	1:B:119:VAL:HG23	2.04	0.57
1:B:462:ILE:HD12	1:B:462:ILE:N	2.17	0.57
1:C:283:LYS:NZ	1:C:344:LYS:HE2	2.20	0.57
1:B:138:ALA:H	1:B:149:GLN:NE2	2.03	0.57
1:C:122:ILE:O	1:C:128:LEU:HD23	2.05	0.57
1:B:196:GLN:HB3	1:B:431:SER:O	2.05	0.57
1:B:407:ASP:OD1	1:B:414:CYS:HB3	2.05	0.57
1:A:260:GLU:HG2	1:A:304:LEU:CD1	2.30	0.56
1:A:425:HIS:HB2	1:A:435:TYR:CD2	2.40	0.56
1:C:331:PHE:H	1:C:331:PHE:HD2	1.51	0.56
1:A:205:GLN:HA	1:A:205:GLN:HE21	1.70	0.56
1:A:114:TYR:CD1	1:A:197:GLN:HB2	2.41	0.56
1:C:158:LEU:CD2	1:C:162:MET:HG3	2.35	0.56
1:C:316:ILE:O	1:C:362:LEU:HD12	2.05	0.56
1:C:425:HIS:HB2	1:C:435:TYR:CE2	2.41	0.56
1:A:115:MET:O	1:A:116:ASN:C	2.47	0.56
1:C:148:ALA:HB1	1:C:209:VAL:HG13	1.87	0.56
1:B:355:TYR:O	1:B:357:LEU:N	2.39	0.55
1:B:457:VAL:CG2	1:B:458:THR:H	2.09	0.55
1:C:350:LEU:CD1	1:C:463:LEU:HD21	2.31	0.55
1:A:304:LEU:N	1:A:304:LEU:CD1	2.68	0.55
1:C:217:ILE:HG22	1:C:218:GLU:N	2.20	0.55
1:B:205:GLN:O	1:B:209:VAL:HG23	2.07	0.55
1:B:217:ILE:HG22	1:B:218:GLU:N	2.22	0.55
1:C:182:PHE:C	1:C:184:GLN:NE2	2.63	0.55
1:B:198:ASP:HB3	1:B:201:GLU:HB2	1.88	0.55
1:B:198:ASP:O	1:B:199:ALA:C	2.48	0.55
1:A:360:PRO:HA	1:A:363:GLN:OE1	2.07	0.55
1:A:211:GLN:HA	1:A:242:ILE:HG13	1.88	0.55
1:B:147:SER:HB3	1:B:181:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:LYS:HB3	1:B:455:SER:HB3	1.88	0.55
1:A:286:PHE:O	1:A:287:THR:C	2.49	0.55
1:B:277:PHE:HB2	1:B:292:ARG:HH11	1.70	0.55
1:B:360:PRO:HA	1:B:363:GLN:OE1	2.05	0.55
1:A:150:TYR:HB3	1:A:177:PHE:CE2	2.41	0.55
1:B:199:ALA:HB2	1:B:435:TYR:CD2	2.42	0.55
1:B:247:GLY:O	1:B:320:PRO:HB3	2.06	0.55
1:B:371:SER:C	1:B:373:PHE:H	2.15	0.55
1:B:112:THR:O	1:B:115:MET:N	2.35	0.55
1:B:260:GLU:HG3	1:B:262:GLU:HG3	1.88	0.54
1:C:457:VAL:HG22	1:C:458:THR:N	2.18	0.54
1:A:184:GLN:H	1:A:184:GLN:HE21	0.71	0.54
1:A:345:ASP:HA	1:A:467:GLY:HA3	1.90	0.54
1:C:351:MET:CE	1:C:482:ARG:HG3	2.33	0.54
1:A:106:LEU:HD22	1:A:171:PRO:HG3	1.88	0.54
1:B:352:LEU:O	1:B:416:TYR:HB3	2.07	0.54
1:A:371:SER:C	1:A:373:PHE:H	2.16	0.54
1:C:355:TYR:O	1:C:357:LEU:N	2.40	0.53
1:A:158:LEU:HD22	1:A:162:MET:SD	2.48	0.53
1:A:198:ASP:HB3	1:A:201:GLU:HB2	1.90	0.53
1:B:126:PRO:C	1:B:128:LEU:N	2.65	0.53
1:B:341:LYS:HG2	1:B:343:LEU:HD11	1.89	0.53
1:B:191:GLN:C	1:B:193:GLN:H	2.16	0.53
1:C:360:PRO:HA	1:C:363:GLN:OE1	2.09	0.53
1:A:260:GLU:OE1	1:A:262:GLU:HG2	2.08	0.53
1:B:274:LEU:O	1:B:325:ILE:HA	2.08	0.53
1:B:341:LYS:HG2	1:B:343:LEU:CD1	2.39	0.53
1:A:457:VAL:CG2	1:A:461:ASP:CG	2.82	0.53
1:A:172:ILE:HD13	1:B:164:LYS:HA	1.90	0.53
1:A:198:ASP:OD1	1:A:198:ASP:C	2.48	0.53
1:A:352:LEU:O	1:A:416:TYR:HB3	2.08	0.53
1:A:355:TYR:C	1:A:357:LEU:H	2.17	0.53
1:C:200:ASN:O	1:C:203:TRP:HB3	2.09	0.53
1:C:401:GLU:N	1:C:402:PRO:CD	2.72	0.53
1:B:163:ASP:C	1:B:164:LYS:HG3	2.34	0.53
1:C:401:GLU:N	1:C:402:PRO:HD2	2.23	0.52
1:A:316:ILE:O	1:A:362:LEU:HD12	2.09	0.52
1:B:401:GLU:O	1:B:402:PRO:C	2.51	0.52
1:B:462:ILE:H	1:B:462:ILE:CD1	2.20	0.52
1:C:202:CYS:O	1:C:206:MET:HG3	2.09	0.52
1:A:329:ARG:HH21	1:A:343:LEU:C	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:VAL:HG22	1:A:461:ASP:CG	2.35	0.52
1:C:274:LEU:O	1:C:325:ILE:HA	2.10	0.52
1:B:304:LEU:CD1	1:B:304:LEU:N	2.72	0.52
1:B:425:HIS:HB2	1:B:435:TYR:CE2	2.45	0.52
1:C:374:LYS:C	1:C:376:LEU:H	2.17	0.52
1:B:330:PHE:CE1	1:B:341:LYS:HD2	2.45	0.52
1:C:200:ASN:HD21	1:C:273:GLN:NE2	2.08	0.52
1:C:329:ARG:NH2	1:C:344:LYS:O	2.41	0.52
1:B:374:LYS:C	1:B:376:LEU:H	2.18	0.51
1:B:423:LEU:HB3	1:B:476:VAL:HB	1.92	0.51
1:A:329:ARG:HH21	1:A:343:LEU:HA	1.75	0.51
1:C:362:LEU:HD22	1:C:366:MET:HE2	1.92	0.51
1:B:172:ILE:HD11	1:C:109:LEU:HD22	1.91	0.51
1:A:401:GLU:O	1:A:402:PRO:C	2.52	0.51
1:B:270:ASN:C	1:B:271:GLN:HG3	2.35	0.51
1:B:416:TYR:CD1	1:B:416:TYR:N	2.78	0.51
1:B:425:HIS:HB2	1:B:435:TYR:CD2	2.46	0.51
1:B:459:PRO:C	1:B:461:ASP:N	2.65	0.51
1:C:200:ASN:O	1:C:204:ILE:HG13	2.10	0.51
1:B:355:TYR:C	1:B:357:LEU:H	2.17	0.51
1:B:429:SER:HB3	1:B:432:SER:HB3	1.92	0.51
1:C:401:GLU:O	1:C:402:PRO:C	2.54	0.51
1:A:209:VAL:O	1:A:210:LEU:C	2.52	0.51
1:A:401:GLU:N	1:A:402:PRO:HD2	2.26	0.51
1:A:410:GLY:O	1:A:411:SER:CB	2.59	0.51
1:C:205:GLN:HA	1:C:205:GLN:NE2	2.26	0.51
1:A:446:TRP:CG	1:A:462:ILE:HD11	2.46	0.51
1:A:205:GLN:HE21	1:A:205:GLN:CA	2.23	0.51
1:B:401:GLU:N	1:B:402:PRO:HD2	2.25	0.50
1:C:259:SER:O	1:C:260:GLU:C	2.54	0.50
1:A:200:ASN:HB2	1:A:475:TYR:CE2	2.46	0.50
1:A:460:GLU:CD	1:A:460:GLU:N	2.63	0.50
1:C:106:LEU:O	1:C:451:ASP:C	2.55	0.50
1:C:120:GLN:O	1:C:123:ARG:HG2	2.12	0.50
1:B:242:ILE:C	1:B:244:GLN:N	2.67	0.50
1:B:401:GLU:N	1:B:402:PRO:CD	2.75	0.50
1:A:374:LYS:C	1:A:376:LEU:H	2.20	0.50
1:B:449:PHE:O	1:B:451:ASP:N	2.42	0.50
1:C:209:VAL:O	1:C:210:LEU:C	2.55	0.50
1:C:424:THR:HB	1:C:438:TRP:HE1	1.76	0.50
1:A:200:ASN:O	1:A:204:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:THR:HB	1:A:438:TRP:HE1	1.77	0.50
1:C:208:ARG:O	1:C:211:GLN:HB3	2.12	0.50
1:B:211:GLN:CA	1:B:242:ILE:HG13	2.41	0.49
1:A:363:GLN:O	1:A:367:VAL:HG23	2.11	0.49
1:B:211:GLN:HA	1:B:242:ILE:CG1	2.41	0.49
1:C:277:PHE:HB2	1:C:292:ARG:HH11	1.74	0.49
1:B:109:LEU:HD22	1:C:172:ILE:HD11	1.93	0.49
1:B:350:LEU:N	1:B:350:LEU:CD1	2.74	0.49
1:C:331:PHE:CD2	1:C:331:PHE:N	2.78	0.49
1:C:425:HIS:HB2	1:C:435:TYR:CD2	2.47	0.49
1:A:200:ASN:HD21	1:A:273:GLN:NE2	2.11	0.49
1:A:211:GLN:HA	1:A:242:ILE:CG1	2.42	0.49
1:B:159:PHE:O	1:B:162:MET:HB2	2.12	0.49
1:C:163:ASP:O	1:C:164:LYS:HG3	2.12	0.49
1:B:457:VAL:CG2	1:B:461:ASP:CG	2.86	0.49
1:B:366:MET:O	1:B:370:ARG:HB2	2.13	0.49
1:A:129:LYS:O	1:A:132:LEU:HB2	2.12	0.49
1:B:122:ILE:O	1:B:128:LEU:HD23	2.12	0.49
1:C:187:GLU:HG3	1:C:195:LEU:CD1	2.38	0.49
1:C:345:ASP:HA	1:C:467:GLY:HA3	1.94	0.49
1:B:150:TYR:HB3	1:B:177:PHE:HD2	1.73	0.49
1:B:242:ILE:C	1:B:244:GLN:H	2.21	0.49
1:A:401:GLU:N	1:A:402:PRO:CD	2.76	0.49
1:A:460:GLU:O	1:A:464:ARG:HG3	2.12	0.49
1:A:461:ASP:O	1:A:462:ILE:C	2.56	0.49
1:B:448:LYS:CB	1:B:455:SER:HB3	2.43	0.48
1:B:459:PRO:C	1:B:461:ASP:H	2.21	0.48
1:A:260:GLU:HG3	1:A:260:GLU:O	2.12	0.48
1:A:355:TYR:O	1:A:357:LEU:N	2.46	0.48
1:A:447:ILE:HG22	1:A:448:LYS:O	2.13	0.48
1:A:127:GLU:H	1:A:127:GLU:CD	2.21	0.48
1:C:304:LEU:CD1	1:C:304:LEU:H	2.27	0.48
1:C:429:SER:HB3	1:C:432:SER:CB	2.43	0.48
1:A:180:MET:HA	1:A:180:MET:HE2	1.95	0.48
1:B:203:TRP:CD1	1:B:203:TRP:C	2.92	0.48
1:B:210:LEU:HD22	1:B:214:LEU:HD11	1.95	0.48
1:B:158:LEU:HD22	1:B:162:MET:SD	2.53	0.48
1:C:158:LEU:HD22	1:C:162:MET:SD	2.54	0.48
1:C:331:PHE:HD2	1:C:331:PHE:N	2.10	0.48
1:C:159:PHE:O	1:C:162:MET:HB2	2.13	0.48
1:C:442:LYS:HB3	1:C:445:GLU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:O	1:B:122:ILE:HG13	2.13	0.48
1:B:440:LYS:HB2	1:B:446:TRP:CE2	2.49	0.48
1:C:416:TYR:CD1	1:C:416:TYR:N	2.82	0.48
1:A:162:MET:C	1:A:164:LYS:H	2.22	0.48
1:B:278:ILE:HD12	1:B:329:ARG:HG2	1.95	0.48
1:C:114:TYR:CG	1:C:197:GLN:HB2	2.48	0.48
1:C:125:VAL:CG1	1:C:128:LEU:HB2	2.43	0.48
1:C:163:ASP:C	1:C:164:LYS:HG3	2.39	0.48
1:C:303:THR:HB	1:C:304:LEU:CD1	2.44	0.48
1:A:164:LYS:O	1:A:165:THR:C	2.57	0.48
1:A:448:LYS:HB3	1:A:455:SER:HB3	1.96	0.48
1:B:248:VAL:HG22	1:B:320:PRO:CD	2.43	0.48
1:B:257:THR:N	1:B:309:LEU:O	2.46	0.48
1:B:114:TYR:CD1	1:B:197:GLN:HB2	2.49	0.47
1:B:126:PRO:O	1:B:127:GLU:C	2.57	0.47
1:B:139:LEU:O	1:B:139:LEU:HD23	2.14	0.47
1:B:252:THR:N	1:B:267:GLY:O	2.43	0.47
1:B:334:GLU:C	1:B:336:GLU:H	2.21	0.47
1:C:270:ASN:C	1:C:271:GLN:HG3	2.39	0.47
1:A:270:ASN:C	1:A:271:GLN:HG3	2.39	0.47
1:C:217:ILE:HG22	1:C:218:GLU:H	1.79	0.47
1:C:251:GLU:HG3	1:C:317:SER:HB2	1.95	0.47
1:B:180:MET:HE2	1:B:180:MET:HA	1.96	0.47
1:C:158:LEU:O	1:C:158:LEU:HD23	2.13	0.47
1:A:191:GLN:C	1:A:193:GLN:N	2.63	0.47
1:C:297:ILE:O	1:C:309:LEU:HD23	2.14	0.47
1:C:371:SER:C	1:C:373:PHE:H	2.22	0.47
1:C:457:VAL:HG22	1:C:461:ASP:CG	2.39	0.47
1:A:106:LEU:O	1:A:451:ASP:C	2.57	0.47
1:C:106:LEU:HD22	1:C:171:PRO:HG3	1.96	0.47
1:B:248:VAL:HG12	1:B:249:GLU:N	2.30	0.47
1:B:410:GLY:N	1:B:412:ASN:HD21	2.12	0.47
1:B:410:GLY:O	1:B:411:SER:CB	2.63	0.47
1:A:172:ILE:CD1	1:B:164:LYS:HA	2.45	0.47
1:B:260:GLU:OE1	1:B:262:GLU:HG2	2.15	0.47
1:B:204:ILE:HG13	1:B:204:ILE:H	1.50	0.47
1:C:325:ILE:HG22	1:C:327:MET:CE	2.45	0.47
1:C:429:SER:H	1:C:432:SER:HB3	1.80	0.47
1:A:203:TRP:CD1	1:A:203:TRP:C	2.94	0.46
1:B:164:LYS:O	1:B:165:THR:C	2.57	0.46
1:B:179:HIS:O	1:B:180:MET:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:LYS:HB3	1:B:445:GLU:HB3	1.97	0.46
1:C:114:TYR:CE1	1:C:197:GLN:HB2	2.51	0.46
1:C:118:THR:HG22	1:C:122:ILE:HD11	1.97	0.46
1:A:416:TYR:CD1	1:A:416:TYR:N	2.83	0.46
1:A:455:SER:OG	1:A:456:ILE:N	2.46	0.46
1:B:405:PHE:HB3	1:B:406:ALA:H	1.42	0.46
1:A:277:PHE:HB2	1:A:292:ARG:HH11	1.81	0.46
1:A:458:THR:O	1:A:461:ASP:HB2	2.16	0.46
1:B:158:LEU:HD22	1:B:162:MET:HG3	1.98	0.46
1:A:164:LYS:C	1:A:166:SER:N	2.73	0.46
1:B:198:ASP:C	1:B:198:ASP:OD1	2.58	0.46
1:C:450:ASP:HB3	1:C:453:LYS:HB2	1.98	0.46
1:A:478:LEU:C	1:A:478:LEU:CD2	2.89	0.46
1:C:164:LYS:O	1:C:165:THR:C	2.57	0.46
1:A:101:GLU:O	1:A:102:LEU:HG	2.15	0.46
1:A:200:ASN:O	1:A:203:TRP:HB3	2.16	0.46
1:B:475:TYR:O	1:B:475:TYR:CD1	2.68	0.46
1:A:442:LYS:HB3	1:A:445:GLU:HB3	1.98	0.46
1:B:199:ALA:CB	1:B:435:TYR:CE2	2.99	0.46
1:C:211:GLN:CA	1:C:242:ILE:HG13	2.46	0.46
1:B:461:ASP:O	1:B:462:ILE:C	2.58	0.45
1:C:241:LEU:O	1:C:244:GLN:HB2	2.15	0.45
1:C:429:SER:HB3	1:C:432:SER:HB3	1.97	0.45
1:A:187:GLU:OE1	1:C:428:ARG:HG2	2.16	0.45
1:A:125:VAL:O	1:A:128:LEU:HB3	2.17	0.45
1:B:344:LYS:HA	1:B:344:LYS:HD3	1.68	0.45
1:A:405:PHE:HB3	1:A:406:ALA:H	1.47	0.45
1:B:460:GLU:O	1:B:464:ARG:HG3	2.15	0.45
1:C:457:VAL:CG2	1:C:461:ASP:CG	2.89	0.45
1:A:159:PHE:O	1:A:162:MET:HB2	2.16	0.45
1:A:462:ILE:H	1:A:462:ILE:CD1	2.23	0.45
1:C:127:GLU:HG2	1:C:245:PHE:CE2	2.52	0.45
1:C:203:TRP:HE1	1:C:207:MET:HE2	1.81	0.45
1:C:458:THR:O	1:C:461:ASP:HB2	2.17	0.45
1:A:123:ARG:O	1:A:129:LYS:HE3	2.17	0.45
1:A:158:LEU:O	1:A:162:MET:HG3	2.16	0.45
1:A:184:GLN:NE2	1:A:184:GLN:N	2.35	0.45
1:A:348:PHE:O	1:A:348:PHE:CD1	2.69	0.45
1:B:424:THR:HB	1:B:438:TRP:HE1	1.81	0.45
1:C:270:ASN:O	1:C:271:GLN:CG	2.63	0.45
1:C:405:PHE:HB3	1:C:406:ALA:H	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:LYS:O	1:C:443:GLN:C	2.60	0.45
1:A:425:HIS:HB2	1:A:435:TYR:CE2	2.52	0.45
1:B:283:LYS:O	1:B:346:VAL:HA	2.16	0.45
1:C:249:GLU:HG2	1:C:270:ASN:OD1	2.17	0.45
1:C:118:THR:O	1:C:122:ILE:HG13	2.17	0.45
1:C:203:TRP:CD1	1:C:203:TRP:C	2.95	0.45
1:A:401:GLU:O	1:A:403:PHE:N	2.50	0.45
1:A:459:PRO:C	1:A:461:ASP:N	2.75	0.45
1:B:260:GLU:HG3	1:B:260:GLU:O	2.17	0.45
1:B:109:LEU:HD12	1:B:175:LEU:HD22	1.99	0.44
1:A:344:LYS:HD3	1:A:344:LYS:HA	1.79	0.44
1:B:112:THR:C	1:B:114:TYR:N	2.75	0.44
1:C:126:PRO:C	1:C:128:LEU:N	2.73	0.44
1:C:126:PRO:O	1:C:128:LEU:N	2.50	0.44
1:C:199:ALA:HB2	1:C:435:TYR:CD2	2.52	0.44
1:C:418:ASP:N	1:C:480:GLY:O	2.40	0.44
1:C:125:VAL:O	1:C:128:LEU:HB3	2.17	0.44
1:C:211:GLN:HA	1:C:242:ILE:CG1	2.46	0.44
1:A:429:SER:HB3	1:A:432:SER:CB	2.47	0.44
1:B:135:TYR:CG	1:B:136:ALA:N	2.85	0.44
1:B:352:LEU:HD21	1:B:354:MET:SD	2.57	0.44
1:A:135:TYR:CG	1:A:136:ALA:N	2.85	0.44
1:A:260:GLU:HG3	1:A:262:GLU:HG3	2.00	0.44
1:B:211:GLN:O	1:B:240:SER:HB3	2.17	0.44
1:A:440:LYS:HB2	1:A:446:TRP:CE2	2.53	0.44
1:A:443:GLN:O	1:A:444:ASP:CG	2.61	0.44
1:A:449:PHE:O	1:A:451:ASP:N	2.48	0.44
1:C:240:SER:O	1:C:243:ASP:HB2	2.17	0.44
1:C:423:LEU:CB	1:C:476:VAL:HB	2.45	0.44
1:C:125:VAL:HG12	1:C:128:LEU:H	1.83	0.44
1:A:114:TYR:CG	1:A:197:GLN:HB2	2.52	0.43
1:A:259:SER:O	1:A:260:GLU:C	2.61	0.43
1:B:174:LEU:O	1:B:175:LEU:C	2.58	0.43
1:B:259:SER:O	1:B:260:GLU:C	2.61	0.43
1:B:278:ILE:O	1:B:278:ILE:HG22	2.17	0.43
1:B:292:ARG:NH1	1:B:292:ARG:HG2	2.33	0.43
1:C:200:ASN:HD21	1:C:273:GLN:HE22	1.65	0.43
1:C:406:ALA:HB1	1:C:412:ASN:C	2.43	0.43
1:A:429:SER:H	1:A:432:SER:HB3	1.83	0.43
1:B:125:VAL:O	1:B:128:LEU:HB3	2.18	0.43
1:B:172:ILE:O	1:B:173:ILE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:HG22	1:B:327:MET:CE	2.47	0.43
1:B:424:THR:O	1:B:424:THR:HG22	2.18	0.43
1:B:362:LEU:C	1:B:362:LEU:HD23	2.43	0.43
1:A:173:ILE:H	1:A:173:ILE:HG13	1.60	0.43
1:A:321:ALA:HA	1:A:413:ASN:HB2	1.99	0.43
1:B:158:LEU:CD2	1:B:162:MET:HG3	2.49	0.43
1:B:369:PHE:O	1:B:373:PHE:CD2	2.71	0.43
1:B:148:ALA:CB	1:B:209:VAL:HG13	2.47	0.43
1:C:204:ILE:HG13	1:C:204:ILE:H	1.51	0.43
1:C:446:TRP:CD2	1:C:462:ILE:HD11	2.53	0.43
1:A:139:LEU:HD23	1:A:139:LEU:O	2.18	0.43
1:B:184:GLN:NE2	1:B:184:GLN:N	2.34	0.43
1:B:401:GLU:O	1:B:403:PHE:N	2.51	0.43
1:A:248:VAL:HG22	1:A:320:PRO:CD	2.47	0.43
1:B:184:GLN:H	1:B:184:GLN:HE21	0.69	0.43
1:C:193:GLN:O	1:C:193:GLN:CG	2.66	0.43
1:B:109:LEU:HB2	1:B:112:THR:HG21	2.00	0.43
1:B:126:PRO:C	1:B:128:LEU:H	2.26	0.43
1:B:257:THR:CB	1:B:309:LEU:O	2.67	0.43
1:B:303:THR:HB	1:B:304:LEU:HD12	2.01	0.43
1:B:435:TYR:C	1:B:436:VAL:HG23	2.44	0.43
1:B:442:LYS:O	1:B:443:GLN:C	2.61	0.43
1:A:217:ILE:HG22	1:A:218:GLU:H	1.82	0.43
1:C:369:PHE:O	1:C:370:ARG:C	2.62	0.43
1:A:172:ILE:HG21	1:B:164:LYS:O	2.18	0.43
1:A:276:CYS:O	1:A:276:CYS:SG	2.75	0.43
1:A:325:ILE:HG22	1:A:327:MET:HE2	2.00	0.43
1:A:115:MET:O	1:A:119:VAL:HG23	2.19	0.42
1:B:158:LEU:O	1:B:159:PHE:C	2.61	0.42
1:C:148:ALA:CB	1:C:209:VAL:HG13	2.48	0.42
1:B:199:ALA:HB3	1:B:435:TYR:CE2	2.55	0.42
1:B:371:SER:C	1:B:373:PHE:N	2.77	0.42
1:B:443:GLN:C	1:B:445:GLU:H	2.28	0.42
1:C:124:SER:O	1:C:126:PRO:HD3	2.19	0.42
1:A:163:ASP:O	1:A:164:LYS:HG3	2.19	0.42
1:A:362:LEU:O	1:A:363:GLN:C	2.60	0.42
1:C:116:ASN:O	1:C:117:ALA:C	2.62	0.42
1:C:422:VAL:O	1:C:438:TRP:HD1	2.03	0.42
1:C:443:GLN:O	1:C:444:ASP:CG	2.63	0.42
1:A:362:LEU:O	1:A:365:LYS:N	2.53	0.42
1:B:171:PRO:O	1:B:172:ILE:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:O	1:B:342:VAL:N	2.36	0.42
1:C:199:ALA:CB	1:C:435:TYR:CD2	3.03	0.42
1:C:260:GLU:OE1	1:C:262:GLU:HG2	2.20	0.42
1:C:424:THR:O	1:C:424:THR:HG22	2.16	0.42
1:C:478:LEU:C	1:C:478:LEU:CD2	2.92	0.42
1:A:211:GLN:CA	1:A:242:ILE:HG13	2.48	0.42
1:A:217:ILE:CG2	1:A:218:GLU:N	2.83	0.42
1:B:106:LEU:HD22	1:B:171:PRO:HG3	2.02	0.42
1:B:300:GLN:HB2	1:B:307:ASN:OD1	2.20	0.42
1:C:286:PHE:O	1:C:287:THR:C	2.61	0.42
1:A:163:ASP:C	1:A:164:LYS:HG3	2.45	0.42
1:C:210:LEU:HD22	1:C:214:LEU:CD1	2.48	0.42
1:C:410:GLY:O	1:C:411:SER:CB	2.67	0.42
1:C:460:GLU:O	1:C:464:ARG:HG3	2.19	0.42
1:A:193:GLN:O	1:A:193:GLN:CG	2.67	0.42
1:A:199:ALA:HB2	1:A:435:TYR:CD2	2.54	0.42
1:C:138:ALA:H	1:C:149:GLN:HE22	1.67	0.42
1:B:151:ILE:HD11	1:B:178:LEU:HA	2.00	0.42
1:B:270:ASN:O	1:B:271:GLN:CG	2.65	0.42
1:B:362:LEU:HD22	1:B:366:MET:CE	2.40	0.42
1:C:327:MET:O	1:C:329:ARG:HG3	2.19	0.42
1:A:174:LEU:O	1:A:175:LEU:C	2.63	0.41
1:A:198:ASP:O	1:A:199:ALA:C	2.63	0.41
1:B:300:GLN:HG3	1:B:306:ARG:C	2.45	0.41
1:B:478:LEU:C	1:B:478:LEU:CD2	2.93	0.41
1:C:125:VAL:HG12	1:C:128:LEU:HB2	2.02	0.41
1:C:292:ARG:HA	1:C:292:ARG:HD3	1.85	0.41
1:C:306:ARG:HD2	1:C:306:ARG:O	2.20	0.41
1:B:205:GLN:NE2	1:B:205:GLN:CA	2.75	0.41
1:B:209:VAL:O	1:B:210:LEU:C	2.62	0.41
1:B:286:PHE:O	1:B:287:THR:C	2.62	0.41
1:B:450:ASP:HB3	1:B:453:LYS:HB2	2.02	0.41
1:C:202:CYS:O	1:C:203:TRP:C	2.62	0.41
1:A:211:GLN:O	1:A:240:SER:HB3	2.20	0.41
1:B:106:LEU:O	1:B:451:ASP:C	2.64	0.41
1:B:321:ALA:O	1:B:481:PRO:HD3	2.19	0.41
1:C:446:TRP:CE2	1:C:462:ILE:HG12	2.56	0.41
1:A:301:SER:HA	1:A:302:PRO:HD3	1.59	0.41
1:A:355:TYR:OH	1:A:363:GLN:HB3	2.20	0.41
1:B:330:PHE:HD1	1:B:341:LYS:HB2	1.82	0.41
1:B:457:VAL:HG22	1:B:461:ASP:CG	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:LEU:HB3	1:C:214:LEU:HD12	2.01	0.41
1:B:199:ALA:CB	1:B:435:TYR:CD2	3.03	0.41
1:C:461:ASP:O	1:C:462:ILE:C	2.63	0.41
1:A:362:LEU:HD22	1:A:366:MET:HE2	2.02	0.41
1:A:406:ALA:HB1	1:A:412:ASN:C	2.45	0.41
1:B:205:GLN:CA	1:B:205:GLN:HE21	2.32	0.41
1:B:345:ASP:CG	1:B:347:LYS:HZ3	2.28	0.41
1:B:462:ILE:O	1:B:463:LEU:C	2.64	0.41
1:A:245:PHE:HB3	1:A:322:TYR:HD1	1.86	0.41
1:A:293:LEU:O	1:A:294:GLN:NE2	2.54	0.41
1:A:329:ARG:NH2	1:A:344:LYS:O	2.51	0.41
1:A:331:PHE:CD2	1:A:331:PHE:O	2.74	0.41
1:B:128:LEU:HD12	1:B:128:LEU:HA	1.92	0.41
1:C:256:CYS:HA	1:C:310:TYR:CD2	2.56	0.41
1:A:345:ASP:OD1	1:A:345:ASP:C	2.64	0.41
1:B:158:LEU:O	1:B:162:MET:HG3	2.21	0.41
1:B:170:PRO:HG2	1:C:108:ASN:O	2.20	0.41
1:B:112:THR:O	1:B:113:CYS:C	2.62	0.41
1:B:217:ILE:HG22	1:B:218:GLU:H	1.86	0.41
1:B:334:GLU:C	1:B:336:GLU:N	2.79	0.41
1:C:128:LEU:O	1:C:131:ALA:HB3	2.21	0.41
1:C:129:LYS:O	1:C:132:LEU:HB2	2.21	0.41
1:C:164:LYS:C	1:C:166:SER:N	2.78	0.41
1:C:412:ASN:HB2	1:C:413:ASN:H	1.66	0.41
1:C:459:PRO:C	1:C:461:ASP:N	2.77	0.41
1:A:260:GLU:O	1:A:260:GLU:CG	2.69	0.41
1:A:325:ILE:HG22	1:A:327:MET:CE	2.51	0.41
1:A:442:LYS:O	1:A:443:GLN:C	2.61	0.41
1:A:450:ASP:HB3	1:A:453:LYS:HB2	2.03	0.41
1:B:251:GLU:HG3	1:B:317:SER:HB2	2.02	0.41
1:B:342:VAL:HG12	1:B:343:LEU:N	2.36	0.41
1:C:110:GLY:O	1:C:111:ASN:HB2	2.21	0.41
1:C:139:LEU:O	1:C:139:LEU:HD23	2.21	0.41
1:B:164:LYS:C	1:B:166:SER:N	2.80	0.40
1:B:320:PRO:O	1:B:417:TYR:HE2	2.04	0.40
1:C:115:MET:O	1:C:118:THR:HB	2.20	0.40
1:C:181:ALA:O	1:C:182:PHE:CD2	2.74	0.40
1:C:208:ARG:O	1:C:212:GLN:HG2	2.21	0.40
1:A:282:VAL:HG13	1:A:287:THR:HB	2.03	0.40
1:A:300:GLN:HG3	1:A:306:ARG:C	2.46	0.40
1:C:419:LEU:HD13	1:C:479:TYR:CZ	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:TRP:CH2	1:C:448:LYS:HE3	2.57	0.40
1:B:127:GLU:H	1:B:127:GLU:CD	2.24	0.40
1:B:438:TRP:CH2	1:B:448:LYS:HE3	2.56	0.40
1:B:446:TRP:CG	1:B:462:ILE:HD11	2.57	0.40
1:A:316:ILE:HG13	1:A:357:LEU:O	2.21	0.40
1:A:318:ARG:C	1:A:318:ARG:HD2	2.47	0.40
1:A:371:SER:C	1:A:373:PHE:N	2.80	0.40
1:B:115:MET:O	1:B:118:THR:HB	2.21	0.40
1:C:135:TYR:CG	1:C:136:ALA:N	2.89	0.40
1:C:184:GLN:HG2	1:C:185:PHE:N	2.36	0.40
1:C:455:SER:OG	1:C:456:ILE:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	329/404 (81%)	231 (70%)	74 (22%)	24 (7%)	1	6
1	B	329/404 (81%)	233 (71%)	73 (22%)	23 (7%)	1	6
1	C	329/404 (81%)	232 (70%)	74 (22%)	23 (7%)	1	6
All	All	987/1212 (81%)	696 (70%)	221 (22%)	70 (7%)	1	6

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	THR
1	A	259	SER
1	A	337	SER
1	A	369	PHE
1	A	370	ARG
1	A	402	PRO

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Mol	Chain	Res	Type
1	A	405	PHE
1	B	165	THR
1	B	259	SER
1	B	280	GLN
1	B	337	SER
1	B	370	ARG
1	B	402	PRO
1	B	405	PHE
1	C	165	THR
1	C	259	SER
1	C	337	SER
1	C	356	GLU
1	C	370	ARG
1	C	402	PRO
1	C	405	PHE
1	A	260	GLU
1	A	280	GLN
1	A	356	GLU
1	A	372	LYS
1	A	411	SER
1	A	419	LEU
1	B	127	GLU
1	B	260	GLU
1	B	356	GLU
1	B	411	SER
1	C	110	GLY
1	C	260	GLU
1	C	280	GLN
1	C	419	LEU
1	A	451	ASP
1	A	455	SER
1	B	126	PRO
1	B	369	PHE
1	B	372	LYS
1	B	375	ASP
1	B	419	LEU
1	B	455	SER
1	C	126	PRO
1	C	328	VAL
1	C	369	PHE
1	C	411	SER
1	A	257	THR

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Mol	Chain	Res	Type
1	A	258	GLU
1	A	375	ASP
1	B	138	ALA
1	B	444	ASP
1	B	451	ASP
1	C	372	LYS
1	C	375	ASP
1	C	413	ASN
1	C	451	ASP
1	A	138	ALA
1	A	410	GLY
1	A	413	ASN
1	B	110	GLY
1	C	127	GLU
1	C	138	ALA
1	B	410	GLY
1	C	410	GLY
1	B	338	VAL
1	A	126	PRO
1	A	209	VAL
1	C	338	VAL
1	A	338	VAL

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	A	303/363 (84%)	279 (92%)	24 (8%)	11	40
1	B	303/363 (84%)	279 (92%)	24 (8%)	11	40
1	C	303/363 (84%)	277 (91%)	26 (9%)	10	36
All	All	909/1089 (84%)	835 (92%)	74 (8%)	11	39

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	158	LEU
1	A	184	GLN
1	A	201	GLU
1	A	265	THR
1	A	276	CYS
1	A	291	LEU
1	A	292	ARG
1	A	318	ARG
1	A	324	THR
1	A	331	PHE
1	A	343	LEU
1	A	375	ASP
1	A	402	PRO
1	A	404	SER
1	A	405	PHE
1	A	408	ASP
1	A	412	ASN
1	A	416	TYR
1	A	418	ASP
1	A	423	LEU
1	A	459	PRO
1	A	460	GLU
1	A	478	LEU
1	B	158	LEU
1	B	172	ILE
1	B	184	GLN
1	B	201	GLU
1	B	265	THR
1	B	276	CYS
1	B	291	LEU
1	B	292	ARG
1	B	318	ARG
1	B	320	PRO
1	B	324	THR
1	B	331	PHE
1	B	344	LYS
1	B	375	ASP
1	B	402	PRO
1	B	405	PHE
1	B	408	ASP
1	B	412	ASN
1	B	416	TYR

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Mol	Chain	Res	Type
1	B	418	ASP
1	B	423	LEU
1	B	439	VAL
1	B	460	GLU
1	B	478	LEU
1	C	158	LEU
1	C	184	GLN
1	C	265	THR
1	C	276	CYS
1	C	291	LEU
1	C	292	ARG
1	C	318	ARG
1	C	320	PRO
1	C	324	THR
1	C	331	PHE
1	C	332	TYR
1	C	334	GLU
1	C	336	GLU
1	C	343	LEU
1	C	375	ASP
1	C	402	PRO
1	C	404	SER
1	C	405	PHE
1	C	408	ASP
1	C	411	SER
1	C	412	ASN
1	C	416	TYR
1	C	418	ASP
1	C	423	LEU
1	C	460	GLU
1	C	478	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	176	GLN
1	A	184	GLN
1	A	200	ASN
1	A	205	GLN
1	A	273	GLN
1	A	326	GLN

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Mol	Chain	Res	Type
1	A	412	ASN
1	A	472	HIS
1	B	149	GLN
1	B	176	GLN
1	B	184	GLN
1	B	200	ASN
1	B	205	GLN
1	B	294	GLN
1	B	326	GLN
1	B	412	ASN
1	B	420	GLN
1	C	120	GLN
1	C	149	GLN
1	C	176	GLN
1	C	184	GLN
1	C	200	ASN
1	C	205	GLN
1	C	273	GLN
1	C	294	GLN
1	C	326	GLN
1	C	412	ASN
1	C	420	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.