



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:39 PM UTC

PDB ID : 1FBV / pdb_00001fbv
Title : STRUCTURE OF A CBL-UBCH7 COMPLEX: RING DOMAIN FUNCTION
IN UBIQUITIN-PROTEIN LIGASES
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Deposited on : 2000-07-17
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

<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
Mogul	:	2022.3.0, CSD as543be (2022)
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

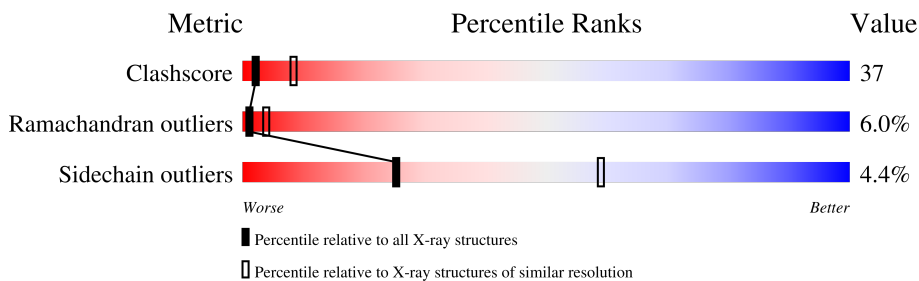
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 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	388	
2	B	9	
3	C	154	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4393 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 SIGNAL TRANSDUCTION PROTEIN CBL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3145	2020	528	572	25			

- Molecule 2 is a protein called ZAP-70 PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	P	0	0	0
			70	40	9	20	1			

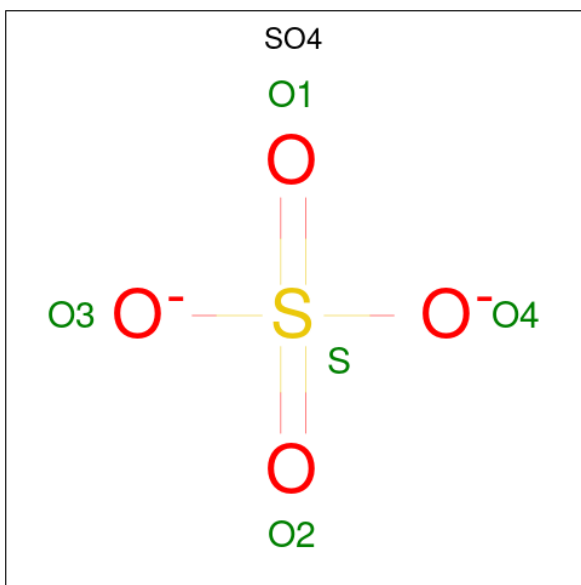
- Molecule 3 is a protein called UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCH7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	144	Total	C	N	O	S	0	0	0
			1151	743	197	206	5			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



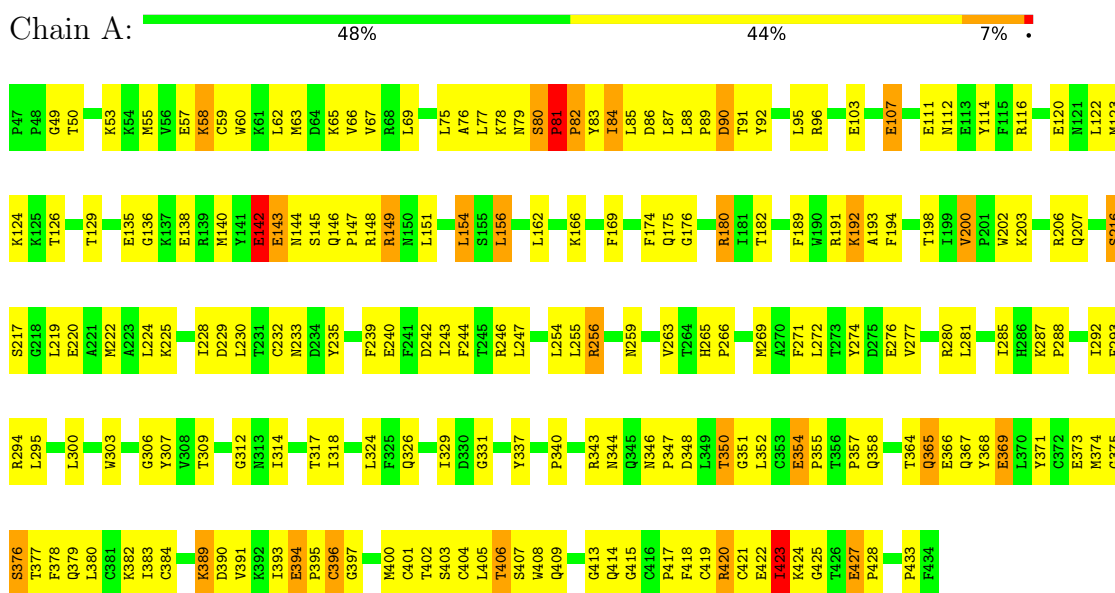
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

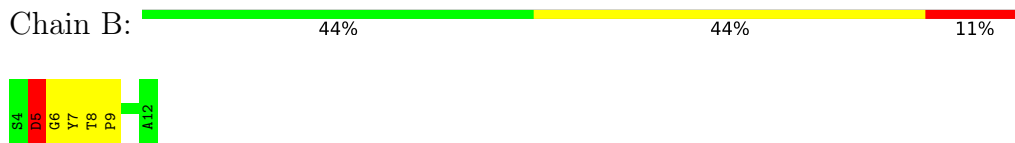
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

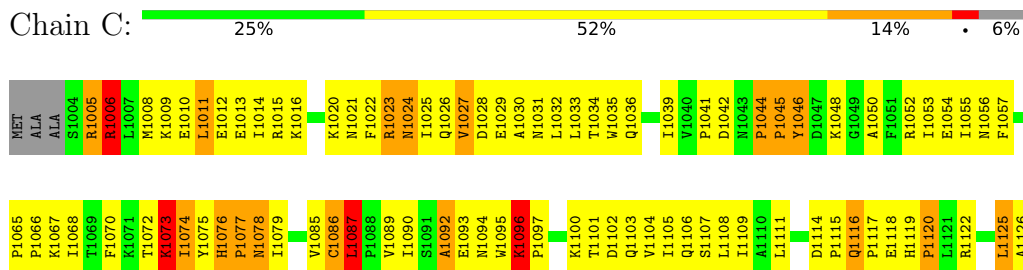
• Molecule 1: SIGNAL TRANSDUCTION PROTEIN CBL



• Molecule 2: ZAP-70 PEPTIDE



• Molecule 3: UBIQUITIN-CONJUGATING ENZYME E12-18 KDA UBCH7



R1133	K1134	C1137	K1138	N1139	A1140	E1141	E1142	F1143	T1144	K1145	K1146	Y1147	GLY	GLU	LYS	ARG	PRO	VAL	ASP
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4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	219.00Å 219.00Å 219.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4393	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, PTR, SO4

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	0.71	1/3227 (0.0%)	1.23	27/4360 (0.6%)
2	B	0.77	0/54	1.73	1/71 (1.4%)
3	C	0.53	0/1180	1.21	14/1599 (0.9%)
All	All	0.67	1/4461 (0.0%)	1.23	42/6030 (0.7%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	374	MET	SD-CE	5.15	1.92	1.79

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	LEU	N-CA-C	-12.06	95.55	111.71
1	A	136	GLY	N-CA-C	-11.61	97.17	112.14
1	A	423	ILE	N-CA-C	11.28	121.14	110.53
1	A	81	PRO	N-CA-C	10.07	122.99	110.70
1	A	80	SER	CA-C-N	9.74	130.41	120.38
1	A	80	SER	C-N-CA	9.74	130.41	120.38
1	A	394	GLU	N-CA-C	8.95	129.59	109.81
3	C	1107	SER	N-CA-C	-8.87	101.99	113.17
3	C	1087	LEU	CA-C-N	8.08	127.38	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1087	LEU	C-N-CA	8.08	127.38	118.97
1	A	58	LYS	N-CA-C	-7.72	102.56	110.97
1	A	81	PRO	CA-C-N	-7.68	110.83	119.28
1	A	81	PRO	C-N-CA	-7.68	110.83	119.28
3	C	1006	ARG	N-CA-C	-7.40	103.20	112.90
1	A	350	THR	N-CA-C	-7.21	99.61	110.28
3	C	1108	LEU	N-CA-C	-6.92	104.87	113.38
1	A	103	GLU	N-CA-C	-6.91	99.66	109.96
3	C	1005	ARG	N-CA-C	-6.88	96.16	110.80
1	A	217	SER	N-CA-C	6.71	117.49	108.23
1	A	326	GLN	N-CA-C	-6.31	104.48	111.36
1	A	394	GLU	CA-C-N	-6.07	112.25	119.84
1	A	394	GLU	C-N-CA	-6.07	112.25	119.84
1	A	389	LYS	N-CA-C	-6.04	100.89	109.96
1	A	84	ILE	N-CA-C	5.90	116.64	110.62
3	C	1142	GLU	N-CA-C	-5.82	106.22	113.55
3	C	1061	TYR	N-CA-C	-5.71	102.20	110.08
1	A	329	ILE	N-CA-C	-5.70	105.06	110.42
1	A	354	GLU	CA-C-N	5.59	125.91	119.93
1	A	354	GLU	C-N-CA	5.59	125.91	119.93
1	A	365	GLN	N-CA-C	-5.51	105.81	112.54
1	A	256	ARG	N-CA-C	-5.50	105.20	111.14
3	C	1078	ASN	N-CA-C	5.36	117.12	111.28
2	B	5	ASP	N-CA-C	5.34	122.18	110.80
1	A	180	ARG	N-CA-C	5.34	117.38	107.99
3	C	1140	ALA	N-CA-C	-5.23	107.92	114.56
1	A	182	THR	N-CA-C	5.15	116.58	110.97
3	C	1096	LYS	CA-C-N	5.13	124.85	119.82
3	C	1096	LYS	C-N-CA	5.13	124.85	119.82
1	A	82	PRO	N-CA-C	-5.11	106.76	113.65
3	C	1073	LYS	N-CA-C	5.11	121.68	110.80
1	A	427	GLU	N-CA-CB	-5.08	106.49	111.27
3	C	1086	CYS	N-CA-C	5.05	116.12	107.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	TYR	Sidechain

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	3145	0	3114	193	0
2	B	70	0	50	4	0
3	C	1151	0	1144	136	0
4	A	2	0	0	0	0
5	A	25	0	0	2	0
All	All	4393	0	4308	322	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 37.

All (322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD13	1:A:378:PHE:HZ	1.21	1.03
3:C:1009:LYS:O	3:C:1013:GLU:HG3	1.59	1.00
1:A:317:THR:HG22	2:B:8:THR:O	1.62	0.99
3:C:1014:ILE:HD12	3:C:1015:ARG:N	1.85	0.92
3:C:1039:ILE:HD13	3:C:1053:ILE:HD11	1.50	0.92
3:C:1101:THR:O	3:C:1104:VAL:HG22	1.75	0.86
1:A:154:LEU:HD13	1:A:378:PHE:CZ	2.10	0.86
1:A:402:THR:O	1:A:406:THR:HG22	1.74	0.86
3:C:1090:ILE:HD11	3:C:1104:VAL:HB	1.56	0.85
3:C:1078:ASN:HB2	3:C:1117:PRO:HB3	1.59	0.83
3:C:1044:PRO:HB2	3:C:1045:PRO:HD2	1.60	0.83
1:A:87:LEU:O	1:A:91:THR:HG23	1.79	0.83
1:A:369:GLU:HG3	3:C:1008:MET:HB3	1.60	0.82
3:C:1009:LYS:O	3:C:1013:GLU:CG	2.29	0.81
1:A:219:LEU:HD12	1:A:365:GLN:HG3	1.63	0.79
3:C:1026:GLN:HB2	3:C:1036:GLN:HB2	1.64	0.79
3:C:1076:HIS:HE1	3:C:1115:PRO:HB3	1.46	0.78
3:C:1014:ILE:HD12	3:C:1015:ARG:H	1.45	0.78
3:C:1122:ARG:HD2	3:C:1125:LEU:HB2	1.65	0.78
1:A:390:ASP:OD2	1:A:391:VAL:HG23	1.84	0.77
3:C:1046:TYR:HA	3:C:1144:THR:HG21	1.65	0.76
3:C:1089:VAL:HG13	3:C:1090:ILE:HG13	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:ILE:HD11	1:A:312:GLY:O	1.86	0.75
3:C:1143:PHE:HA	3:C:1146:LYS:HE2	1.70	0.73
1:A:194:PHE:CD1	1:A:200:VAL:HG11	2.24	0.73
1:A:224:LEU:HD11	1:A:228:ILE:HD11	1.70	0.71
1:A:377:THR:N	1:A:379:GLN:HE22	1.88	0.71
3:C:1012:GLU:HB3	3:C:1016:LYS:HE3	1.71	0.71
3:C:1074:ILE:HG12	3:C:1075:TYR:H	1.56	0.71
3:C:1111:LEU:O	3:C:1115:PRO:HG3	1.92	0.70
1:A:143:GLU:HG3	1:A:144:ASN:ND2	2.06	0.70
1:A:375:GLY:O	1:A:377:THR:HG23	1.91	0.70
3:C:1085:VAL:HG12	3:C:1086:CYS:H	1.58	0.69
1:A:92:TYR:CZ	1:A:96:ARG:HD2	2.28	0.69
1:A:192:LYS:O	1:A:192:LYS:HD3	1.93	0.69
3:C:1116:GLN:N	3:C:1117:PRO:HD3	2.09	0.68
1:A:379:GLN:HE21	1:A:380:LEU:HG	1.59	0.67
1:A:219:LEU:HB2	1:A:365:GLN:HE21	1.59	0.67
1:A:408:TRP:HZ3	1:A:415:GLY:O	1.78	0.67
3:C:1116:GLN:H	3:C:1117:PRO:HD3	1.60	0.67
3:C:1005:ARG:HH11	3:C:1005:ARG:HG2	1.58	0.67
3:C:1087:LEU:HD23	3:C:1087:LEU:H	1.57	0.67
1:A:394:GLU:HB2	1:A:425:GLY:O	1.94	0.66
3:C:1143:PHE:HA	3:C:1146:LYS:HG2	1.75	0.66
3:C:1065:PRO:HD3	3:C:1095:TRP:CD1	2.31	0.66
1:A:269:MET:HE1	1:A:280:ARG:CZ	2.25	0.66
1:A:408:TRP:CZ3	1:A:415:GLY:O	2.50	0.65
1:A:175:GLN:NE2	1:A:175:GLN:HA	2.12	0.65
1:A:364:THR:OG1	1:A:367:GLN:HG3	1.95	0.65
3:C:1085:VAL:HG12	3:C:1086:CYS:N	2.12	0.65
3:C:1075:TYR:HD1	3:C:1140:ALA:HB2	1.62	0.65
1:A:394:GLU:O	1:A:395:PRO:C	2.38	0.64
1:A:369:GLU:O	1:A:373:GLU:HG3	1.96	0.64
3:C:1133:ARG:HD3	3:C:1137:CYS:SG	2.37	0.64
1:A:219:LEU:HB2	1:A:365:GLN:NE2	2.12	0.64
1:A:228:ILE:HG12	1:A:244:PHE:CD1	2.32	0.63
1:A:191:ARG:CZ	1:A:191:ARG:HB2	2.27	0.63
1:A:277:VAL:HG13	1:A:292:ILE:HD11	1.80	0.63
1:A:154:LEU:CD1	1:A:378:PHE:HZ	2.04	0.63
1:A:354:GLU:O	1:A:357:PRO:HD3	1.99	0.63
1:A:65:LYS:HE3	1:A:69:LEU:HD21	1.79	0.63
3:C:1053:ILE:HG22	3:C:1054:GLU:N	2.13	0.63
1:A:107:GLU:O	1:A:111:GLU:HG3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1062:PRO:O	3:C:1097:PRO:HB3	1.99	0.62
1:A:66:VAL:HA	1:A:69:LEU:HD23	1.80	0.62
3:C:1118:GLU:HG3	3:C:1119:HIS:N	2.15	0.62
3:C:1023:ARG:NE	3:C:1024:ASN:H	1.98	0.62
3:C:1025:ILE:HD12	3:C:1036:GLN:O	1.98	0.62
3:C:1010:GLU:O	3:C:1013:GLU:HB2	2.00	0.62
1:A:369:GLU:CG	3:C:1008:MET:HB3	2.28	0.62
3:C:1078:ASN:HA	3:C:1120:PRO:HB3	1.81	0.62
1:A:376:SER:HB2	1:A:379:GLN:OE1	2.00	0.61
1:A:395:PRO:HG3	1:A:422:GLU:O	2.01	0.61
3:C:1055:ILE:HD11	3:C:1105:ILE:HD11	1.83	0.61
3:C:1021:ASN:O	3:C:1039:ILE:HA	2.00	0.61
1:A:203:LYS:O	1:A:207:GLN:HG3	2.00	0.61
3:C:1076:HIS:CD2	3:C:1079:ILE:HG13	2.36	0.60
1:A:293:PHE:CD2	1:A:324:LEU:HD21	2.36	0.60
1:A:122:LEU:O	1:A:126:THR:HG23	2.02	0.60
1:A:395:PRO:HD3	1:A:424:LYS:HB2	1.82	0.60
1:A:53:LYS:O	1:A:57:GLU:HG3	2.01	0.60
3:C:1055:ILE:CD1	3:C:1105:ILE:HD11	2.31	0.60
3:C:1028:ASP:OD2	3:C:1030:ALA:HB3	2.02	0.60
3:C:1096:LYS:NZ	3:C:1096:LYS:HB3	2.17	0.59
3:C:1006:ARG:HG3	3:C:1006:ARG:HH11	1.68	0.59
1:A:377:THR:H	1:A:379:GLN:HE22	1.49	0.59
3:C:1090:ILE:HG22	3:C:1090:ILE:O	2.03	0.59
1:A:91:THR:HG22	1:A:162:LEU:HB2	1.85	0.58
1:A:149:ARG:HD2	5:A:2004:SO4:O2	2.03	0.58
1:A:395:PRO:HD2	1:A:423:ILE:O	2.03	0.58
3:C:1139:ASN:O	3:C:1143:PHE:HB2	2.03	0.58
3:C:1072:THR:O	3:C:1073:LYS:O	2.20	0.58
3:C:1061:TYR:CD1	3:C:1062:PRO:HA	2.39	0.58
3:C:1044:PRO:CB	3:C:1045:PRO:HD2	2.33	0.57
1:A:203:LYS:HD3	1:A:206:ARG:NH2	2.18	0.57
3:C:1077:PRO:HB2	3:C:1117:PRO:HG2	1.87	0.57
1:A:364:THR:H	1:A:367:GLN:NE2	2.02	0.57
1:A:140:MET:HE1	1:A:151:LEU:HD22	1.86	0.57
3:C:1074:ILE:HG12	3:C:1075:TYR:N	2.19	0.57
1:A:138:GLU:CD	1:A:138:GLU:H	2.12	0.57
1:A:203:LYS:CD	1:A:206:ARG:NH2	2.68	0.57
1:A:376:SER:OG	1:A:377:THR:N	2.38	0.57
1:A:281:LEU:HD11	1:A:306:GLY:O	2.05	0.56
3:C:1053:ILE:HG22	3:C:1054:GLU:H	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:CYS:O	1:A:421:CYS:N	2.38	0.56
3:C:1076:HIS:HD2	3:C:1079:ILE:HG13	1.70	0.56
1:A:317:THR:HG21	2:B:9:PRO:O	2.05	0.56
3:C:1096:LYS:HB3	3:C:1096:LYS:HZ3	1.71	0.56
3:C:1131:LYS:O	3:C:1132:ASP:HB2	2.06	0.56
1:A:62:LEU:HD12	1:A:123:MET:HG3	1.89	0.55
1:A:340:PRO:HD3	1:A:346:ASN:HD22	1.71	0.55
3:C:1114:ASP:N	3:C:1115:PRO:HD3	2.21	0.55
1:A:224:LEU:O	1:A:228:ILE:HG13	2.06	0.55
1:A:91:THR:HG22	1:A:162:LEU:HD22	1.89	0.55
1:A:354:GLU:HB3	1:A:355:PRO:HD2	1.88	0.55
3:C:1035:TRP:O	3:C:1054:GLU:HA	2.05	0.55
3:C:1143:PHE:CA	3:C:1146:LYS:HE2	2.36	0.55
3:C:1020:LYS:C	3:C:1022:PHE:H	2.14	0.55
3:C:1076:HIS:CE1	3:C:1077:PRO:HD2	2.42	0.55
1:A:408:TRP:CE2	1:A:413:GLY:HA3	2.42	0.55
1:A:419:CYS:O	1:A:420:ARG:C	2.49	0.55
3:C:1067:LYS:O	3:C:1067:LYS:HG3	2.07	0.55
3:C:1103:GLN:O	3:C:1103:GLN:HG2	2.07	0.55
3:C:1140:ALA:O	3:C:1144:THR:HG23	2.07	0.55
1:A:364:THR:H	1:A:367:GLN:HE21	1.54	0.54
1:A:175:GLN:HA	1:A:175:GLN:HE21	1.71	0.54
1:A:65:LYS:O	1:A:69:LEU:HD22	2.06	0.54
1:A:142:GLU:O	1:A:143:GLU:HB2	2.06	0.54
3:C:1045:PRO:O	3:C:1046:TYR:O	2.25	0.54
1:A:405:LEU:HD23	1:A:405:LEU:O	2.08	0.54
1:A:243:ILE:HD13	1:A:300:LEU:HD22	1.88	0.54
3:C:1070:PHE:HE2	3:C:1079:ILE:HD13	1.73	0.53
1:A:91:THR:HG22	1:A:162:LEU:HD13	1.90	0.53
1:A:189:PHE:CD1	1:A:189:PHE:C	2.86	0.53
1:A:417:PRO:HB3	3:C:1097:PRO:HG2	1.90	0.53
3:C:1138:LYS:C	3:C:1140:ALA:H	2.16	0.53
1:A:405:LEU:HD23	1:A:405:LEU:C	2.33	0.53
1:A:143:GLU:HG3	1:A:144:ASN:HD22	1.72	0.53
1:A:191:ARG:C	1:A:193:ALA:H	2.16	0.53
3:C:1005:ARG:HG2	3:C:1005:ARG:NH1	2.24	0.53
1:A:162:LEU:HD11	1:A:166:LYS:HE3	1.90	0.53
1:A:203:LYS:HD3	1:A:206:ARG:CZ	2.38	0.53
3:C:1070:PHE:CE2	3:C:1079:ILE:HD13	2.44	0.53
3:C:1118:GLU:HG3	3:C:1119:HIS:H	1.72	0.53
1:A:63:MET:HG2	1:A:126:THR:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HG2	1:A:256:ARG:HH11	1.75	0.52
1:A:384:CYS:HB3	1:A:404:CYS:SG	2.48	0.52
3:C:1128:GLU:O	3:C:1132:ASP:HB3	2.09	0.52
3:C:1044:PRO:HB2	3:C:1045:PRO:CD	2.35	0.52
3:C:1006:ARG:HH11	3:C:1006:ARG:CG	2.23	0.52
3:C:1050:ALA:O	3:C:1072:THR:CG2	2.58	0.52
3:C:1077:PRO:O	3:C:1120:PRO:HB3	2.10	0.52
1:A:82:PRO:HG3	1:A:156:LEU:HD13	1.91	0.51
1:A:377:THR:O	1:A:380:LEU:HB2	2.10	0.51
1:A:112:ASN:O	1:A:116:ARG:HG3	2.11	0.51
3:C:1057:PHE:CD2	3:C:1066:PRO:HB3	2.45	0.51
1:A:67:VAL:HG23	1:A:88:LEU:HD12	1.92	0.51
3:C:1056:ASN:HB2	3:C:1067:LYS:CG	2.40	0.51
1:A:222:MET:HE2	3:C:1005:ARG:NH2	2.25	0.51
1:A:395:PRO:CD	1:A:423:ILE:O	2.58	0.51
3:C:1052:ARG:HB3	3:C:1072:THR:OG1	2.11	0.51
1:A:303:TRP:O	1:A:318:ILE:HG23	2.11	0.51
1:A:376:SER:HB2	1:A:379:GLN:CD	2.36	0.51
1:A:266:PRO:HG2	1:A:340:PRO:HB2	1.93	0.50
3:C:1046:TYR:HD1	3:C:1144:THR:CG2	2.23	0.50
3:C:1056:ASN:HB2	3:C:1067:LYS:HG2	1.92	0.50
3:C:1076:HIS:ND1	3:C:1077:PRO:HD2	2.26	0.50
3:C:1010:GLU:HA	3:C:1013:GLU:HG3	1.93	0.50
1:A:263:VAL:HA	1:A:371:TYR:CD1	2.46	0.50
3:C:1027:VAL:HG13	3:C:1027:VAL:O	2.10	0.50
3:C:1075:TYR:CD1	3:C:1140:ALA:HB2	2.46	0.50
1:A:366:GLU:HG3	3:C:1012:GLU:OE2	2.11	0.50
3:C:1031:ASN:ND2	3:C:1034:THR:H	2.09	0.50
1:A:340:PRO:O	1:A:343:ARG:HB2	2.12	0.50
3:C:1092:ALA:C	3:C:1094:ASN:H	2.20	0.50
1:A:293:PHE:CE2	1:A:324:LEU:HD21	2.47	0.50
3:C:1143:PHE:HA	3:C:1146:LYS:CE	2.42	0.50
1:A:408:TRP:CE3	1:A:417:PRO:HG3	2.46	0.49
1:A:427:GLU:HG2	1:A:428:PRO:HD2	1.94	0.49
1:A:81:PRO:O	1:A:83:TYR:CD2	2.65	0.49
1:A:145:SER:HB2	1:A:147:PRO:HD2	1.94	0.49
1:A:169:PHE:CE1	1:A:174:PHE:HB2	2.47	0.49
3:C:1065:PRO:HB3	3:C:1095:TRP:CD2	2.47	0.49
1:A:148:ARG:HD2	1:A:148:ARG:O	2.12	0.49
1:A:78:LYS:C	1:A:79:ASN:HD22	2.21	0.49
3:C:1011:LEU:HD23	3:C:1014:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:HG23	1:A:423:ILE:HG22	1.94	0.49
1:A:396:CYS:SG	1:A:397:GLY:N	2.85	0.49
3:C:1109:ILE:C	3:C:1111:LEU:H	2.19	0.49
1:A:420:ARG:HD3	3:C:1096:LYS:HZ3	1.77	0.49
1:A:86:ASP:O	1:A:90:ASP:HB2	2.12	0.48
3:C:1039:ILE:CD1	3:C:1053:ILE:HD11	2.33	0.48
3:C:1026:GLN:O	3:C:1027:VAL:HB	2.13	0.48
1:A:405:LEU:C	1:A:405:LEU:CD2	2.86	0.48
1:A:142:GLU:HB3	1:A:143:GLU:H	1.40	0.48
1:A:317:THR:HG22	2:B:8:THR:C	2.37	0.48
1:A:383:ILE:HD11	1:A:418:PHE:CE1	2.49	0.48
1:A:379:GLN:O	1:A:389:LYS:HG3	2.14	0.48
1:A:403:SER:O	1:A:406:THR:HG23	2.14	0.48
3:C:1028:ASP:C	3:C:1030:ALA:H	2.22	0.48
3:C:1060:GLU:CD	3:C:1060:GLU:H	2.22	0.48
1:A:228:ILE:HG12	1:A:244:PHE:CE1	2.48	0.48
1:A:216:SER:HB2	1:A:220:GLU:OE1	2.14	0.47
1:A:243:ILE:HD11	1:A:300:LEU:HD13	1.96	0.47
3:C:1122:ARG:NH1	3:C:1125:LEU:HD12	2.29	0.47
1:A:142:GLU:O	1:A:143:GLU:CB	2.62	0.47
1:A:203:LYS:NZ	1:A:206:ARG:NH2	2.62	0.47
1:A:404:CYS:O	1:A:405:LEU:C	2.57	0.47
1:A:377:THR:HA	1:A:380:LEU:HD12	1.95	0.47
3:C:1120:PRO:CG	3:C:1126:ALA:HB2	2.44	0.47
1:A:379:GLN:CD	1:A:379:GLN:H	2.23	0.47
1:A:269:MET:CE	1:A:280:ARG:CZ	2.93	0.47
3:C:1060:GLU:CG	3:C:1064:LYS:HD2	2.44	0.47
3:C:1143:PHE:HA	3:C:1146:LYS:CG	2.44	0.47
3:C:1116:GLN:HG3	3:C:1116:GLN:O	2.14	0.47
1:A:427:GLU:HG2	1:A:428:PRO:CD	2.45	0.47
3:C:1076:HIS:CE1	3:C:1115:PRO:HB3	2.38	0.47
1:A:146:GLN:O	1:A:147:PRO:C	2.56	0.47
1:A:50:THR:HA	1:A:116:ARG:HD2	1.97	0.47
1:A:307:TYR:CD1	1:A:307:TYR:N	2.82	0.47
1:A:175:GLN:HE21	1:A:175:GLN:CA	2.28	0.46
1:A:272:LEU:HD22	1:A:276:GLU:CB	2.44	0.46
1:A:256:ARG:NH2	1:A:351:GLY:O	2.48	0.46
3:C:1100:LYS:O	3:C:1101:THR:C	2.58	0.46
3:C:1020:LYS:O	3:C:1021:ASN:CB	2.63	0.46
1:A:277:VAL:HG21	1:A:294:ARG:HD3	1.97	0.46
1:A:274:TYR:CD1	1:A:274:TYR:C	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1116:GLN:H	3:C:1117:PRO:CD	2.29	0.45
1:A:176:GLY:HA3	1:A:198:THR:OG1	2.15	0.45
3:C:1116:GLN:N	3:C:1117:PRO:CD	2.79	0.45
1:A:400:MET:HE2	1:A:405:LEU:HB2	1.98	0.45
3:C:1092:ALA:O	3:C:1093:GLU:HB2	2.17	0.45
1:A:138:GLU:C	1:A:140:MET:N	2.74	0.45
1:A:149:ARG:NH2	1:A:271:PHE:O	2.45	0.45
1:A:247:LEU:HD11	1:A:295:LEU:HG	1.97	0.45
1:A:287:LYS:NZ	1:A:344:ASN:HD21	2.15	0.45
1:A:86:ASP:C	1:A:89:PRO:HD2	2.42	0.45
1:A:331:GLY:HA3	1:A:337:TYR:CD2	2.52	0.45
3:C:1010:GLU:CA	3:C:1013:GLU:HG3	2.47	0.45
3:C:1133:ARG:HA	3:C:1133:ARG:NH1	2.31	0.45
1:A:404:CYS:O	1:A:407:SER:N	2.50	0.45
1:A:303:TRP:CD2	1:A:324:LEU:HD22	2.52	0.44
1:A:84:ILE:CG2	1:A:85:LEU:N	2.81	0.44
1:A:242:ASP:O	1:A:246:ARG:HG3	2.18	0.44
3:C:1075:TYR:O	3:C:1076:HIS:O	2.36	0.44
3:C:1055:ILE:HG23	3:C:1068:ILE:HG12	1.99	0.44
1:A:80:SER:HA	1:A:81:PRO:HD2	1.78	0.44
1:A:354:GLU:CB	1:A:355:PRO:HD2	2.46	0.44
1:A:233:ASN:C	1:A:235:TYR:H	2.26	0.44
3:C:1009:LYS:C	3:C:1013:GLU:HG3	2.36	0.44
1:A:229:ASP:OD2	1:A:232:CYS:HA	2.18	0.44
1:A:417:PRO:HB3	3:C:1097:PRO:CG	2.48	0.44
1:A:191:ARG:HG3	1:A:191:ARG:HH11	1.84	0.43
1:A:272:LEU:HD22	1:A:276:GLU:HB3	2.00	0.43
1:A:285:ILE:HD13	1:A:314:ILE:HG13	2.00	0.43
3:C:1050:ALA:O	3:C:1072:THR:HG21	2.17	0.43
1:A:65:LYS:O	1:A:69:LEU:CD2	2.66	0.43
3:C:1006:ARG:CG	3:C:1006:ARG:NH1	2.79	0.43
3:C:1057:PHE:CZ	3:C:1101:THR:HG21	2.53	0.43
1:A:138:GLU:C	1:A:140:MET:H	2.26	0.43
3:C:1119:HIS:HA	3:C:1120:PRO:HD2	1.91	0.43
1:A:265:HIS:HA	1:A:266:PRO:HD2	1.91	0.43
1:A:272:LEU:HD23	1:A:272:LEU:HA	1.91	0.43
1:A:191:ARG:O	1:A:193:ALA:N	2.51	0.43
3:C:1020:LYS:O	3:C:1021:ASN:HB2	2.18	0.43
1:A:124:LYS:HB3	1:A:124:LYS:HE2	1.83	0.43
1:A:348:ASP:OD1	1:A:350:THR:OG1	2.33	0.43
3:C:1115:PRO:O	3:C:1116:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HG13	1:A:129:THR:HG21	2.01	0.43
3:C:1045:PRO:HG2	3:C:1046:TYR:H	1.83	0.43
1:A:401:CYS:SG	1:A:403:SER:HB3	2.59	0.43
3:C:1053:ILE:CG2	3:C:1054:GLU:N	2.81	0.43
3:C:1118:GLU:CG	3:C:1119:HIS:N	2.81	0.43
1:A:259:ASN:ND2	1:A:368:TYR:OH	2.52	0.42
3:C:1031:ASN:C	3:C:1033:LEU:H	2.27	0.42
1:A:60:TRP:HD1	1:A:63:MET:HE2	1.83	0.42
1:A:78:LYS:O	1:A:79:ASN:ND2	2.44	0.42
1:A:202:TRP:CZ2	1:A:225:LYS:HB2	2.54	0.42
1:A:288:PRO:HB3	1:A:309:THR:O	2.19	0.42
1:A:376:SER:HB2	1:A:379:GLN:NE2	2.34	0.42
3:C:1101:THR:O	3:C:1102:ASP:C	2.61	0.42
1:A:62:LEU:HD21	1:A:433:PRO:HD3	2.01	0.42
1:A:143:GLU:O	1:A:144:ASN:HB2	2.20	0.42
1:A:369:GLU:HG3	3:C:1008:MET:HE3	2.01	0.42
1:A:49:GLY:O	1:A:116:ARG:HD2	2.20	0.42
1:A:77:LEU:CD2	1:A:148:ARG:NH2	2.83	0.42
1:A:75:LEU:O	1:A:76:ALA:C	2.61	0.42
1:A:191:ARG:C	1:A:193:ALA:N	2.75	0.42
3:C:1050:ALA:HB1	3:C:1072:THR:HG21	2.01	0.42
3:C:1076:HIS:HD2	3:C:1079:ILE:H	1.68	0.42
1:A:378:PHE:O	1:A:389:LYS:HE3	2.19	0.41
2:B:5:ASP:HB3	2:B:6:GLY:H	1.49	0.41
3:C:1006:ARG:O	3:C:1010:GLU:HG2	2.20	0.41
1:A:379:GLN:NE2	1:A:380:LEU:HG	2.30	0.41
1:A:84:ILE:HG23	1:A:85:LEU:N	2.35	0.41
1:A:303:TRP:CE2	1:A:324:LEU:HD22	2.55	0.41
1:A:287:LYS:HZ1	1:A:344:ASN:HD21	1.68	0.41
1:A:180:ARG:HG2	1:A:180:ARG:HH11	1.86	0.41
1:A:255:LEU:O	1:A:259:ASN:OD1	2.38	0.41
1:A:277:VAL:CG2	1:A:294:ARG:HD3	2.51	0.41
1:A:414:GLN:OE1	1:A:420:ARG:HB3	2.21	0.41
3:C:1045:PRO:HB3	3:C:1141:GLU:HB2	2.02	0.41
1:A:224:LEU:CD1	1:A:228:ILE:HD11	2.45	0.41
3:C:1046:TYR:HD1	3:C:1144:THR:HG21	1.85	0.41
1:A:382:LYS:HE2	5:A:2005:SO4:O4	2.21	0.41
3:C:1096:LYS:O	3:C:1096:LYS:HG3	2.20	0.41
1:A:55:MET:O	1:A:58:LYS:HB3	2.21	0.41
1:A:59:CYS:O	1:A:63:MET:HG3	2.20	0.41
1:A:88:LEU:HB2	1:A:89:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:O	1:A:240:GLU:C	2.64	0.41
1:A:346:ASN:HA	1:A:347:PRO:HD2	1.82	0.41
1:A:402:THR:HG23	1:A:403:SER:N	2.36	0.41
1:A:77:LEU:HD21	1:A:148:ARG:CZ	2.52	0.40
1:A:293:PHE:CD1	1:A:293:PHE:N	2.89	0.40
1:A:60:TRP:HE1	1:A:95:LEU:HD12	1.85	0.40
1:A:88:LEU:N	1:A:89:PRO:CD	2.85	0.40
1:A:405:LEU:CD2	1:A:409:GLN:CD	2.95	0.40
1:A:423:ILE:H	1:A:423:ILE:HG12	1.55	0.40
3:C:1039:ILE:HD11	3:C:1070:PHE:HE1	1.87	0.40
3:C:1118:GLU:CG	3:C:1119:HIS:H	2.34	0.40
3:C:1032:LEU:N	3:C:1032:LEU:HD12	2.35	0.40
3:C:1087:LEU:HD23	3:C:1087:LEU:N	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/388 (100%)	335 (87%)	40 (10%)	11 (3%)	4	15
2	B	6/9 (67%)	4 (67%)	1 (17%)	1 (17%)	0	0
3	C	142/154 (92%)	96 (68%)	26 (18%)	20 (14%)	0	0
All	All	534/551 (97%)	435 (82%)	67 (12%)	32 (6%)	1	4

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	142	GLU
1	A	143	GLU
1	A	216	SER

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Mol	Chain	Res	Type
1	A	358	GLN
1	A	376	SER
1	A	420	ARG
2	B	5	ASP
3	C	1024	ASN
3	C	1027	VAL
3	C	1041	PRO
3	C	1046	TYR
3	C	1073	LYS
3	C	1116	GLN
3	C	1132	ASP
1	A	192	LYS
3	C	1042	ASP
3	C	1045	PRO
3	C	1048	LYS
3	C	1074	ILE
3	C	1076	HIS
3	C	1092	ALA
3	C	1120	PRO
3	C	1125	LEU
1	A	135	GLU
1	A	254	LEU
3	C	1044	PRO
3	C	1106	GLN
3	C	1134	LYS
1	A	396	CYS
3	C	1029	GLU
3	C	1077	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/349 (100%)	336 (96%)	13 (4%)	30	64
2	B	6/6 (100%)	6 (100%)	0	100	100
3	C	122/138 (88%)	114 (93%)	8 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	477/493 (97%)	456 (96%)	21 (4%)	25	59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	PRO
1	A	90	ASP
1	A	107	GLU
1	A	120	GLU
1	A	142	GLU
1	A	149	ARG
1	A	154	LEU
1	A	156	LEU
1	A	200	VAL
1	A	230	LEU
1	A	369	GLU
1	A	406	THR
1	A	423	ILE
3	C	1006	ARG
3	C	1011	LEU
3	C	1023	ARG
3	C	1060	GLU
3	C	1062	PRO
3	C	1087	LEU
3	C	1096	LYS
3	C	1147	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	128	GLN
1	A	144	ASN
1	A	146	GLN
1	A	175	GLN
1	A	259	ASN
1	A	282	GLN
1	A	344	ASN
1	A	346	ASN
1	A	365	GLN
1	A	367	GLN

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Mol	Chain	Res	Type
1	A	379	GLN
1	A	409	GLN
3	C	1026	GLN
3	C	1031	ASN
3	C	1036	GLN
3	C	1076	HIS
3	C	1106	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PTR	B	7	2	15,16,17	1.72	3 (20%)	17,22,24	0.60	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	B	7	2	-	1/10/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	PTR	P-OH	4.64	1.68	1.59
2	B	7	PTR	P-O1P	3.39	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	PTR	OH-CZ	-2.18	1.35	1.40

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	7	PTR	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	SO4	A	2003	-	4,4,4	0.37	0	6,6,6	0.21	0
5	SO4	A	2001	-	4,4,4	0.21	0	6,6,6	0.06	0
5	SO4	A	2002	-	4,4,4	0.12	0	6,6,6	0.19	0
5	SO4	A	2004	-	4,4,4	0.24	0	6,6,6	0.15	0
5	SO4	A	2005	-	4,4,4	0.43	0	6,6,6	0.15	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2004	SO4	1	0
5	A	2005	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.