



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2017 – 05:52 AM EDT

PDB ID : 1FBV
Title : STRUCTURE OF A CBL-UBCH7 COMPLEX: RING DOMAIN FUNCTION
IN UBIQUITIN-PROTEIN LIGASES
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Deposited on : unknown
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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

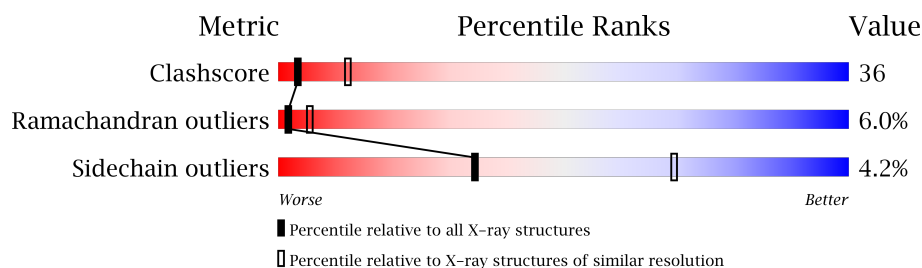
1 Overall quality at a glance

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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (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	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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



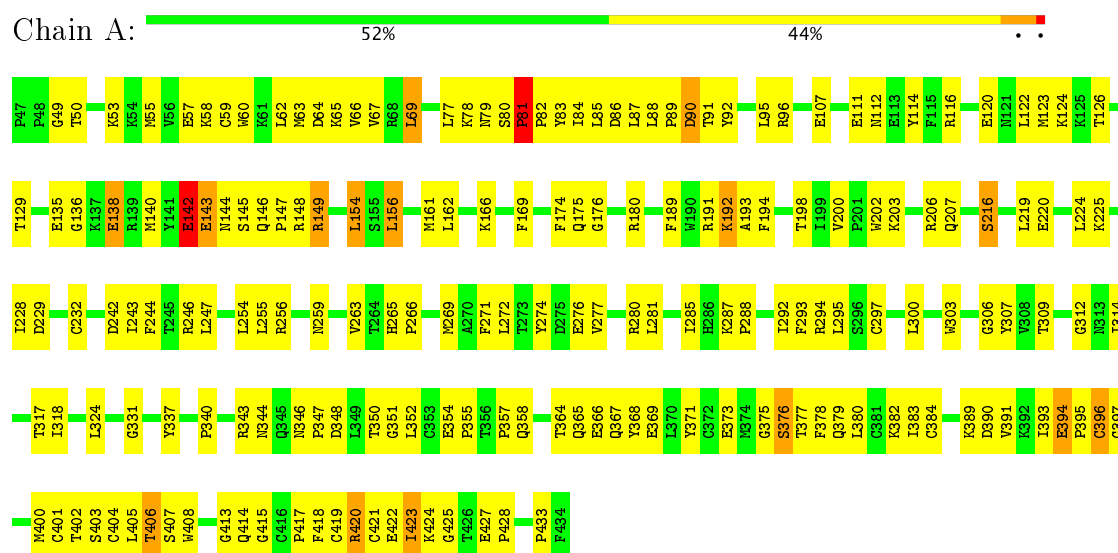
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

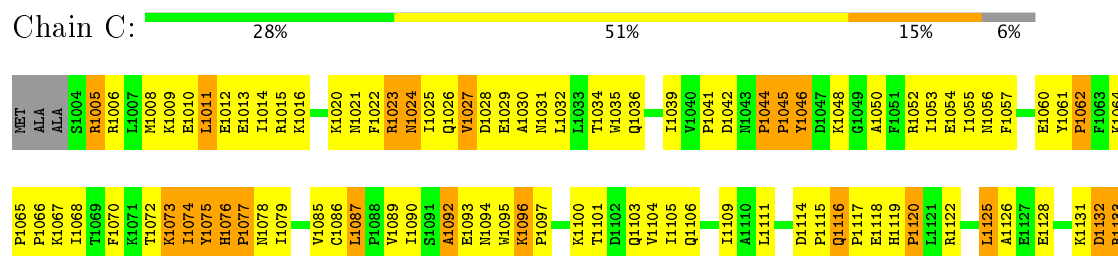
• Molecule 1: SIGNAL TRANSDUCTION PROTEIN CBL



• Molecule 2: ZAP-70 PEPTIDE



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



K1134	
C1137	
K1138	
N1139	
A1140	
E1141	
E1142	
F1143	
T1144	
K1145	
K1146	
Y1147	
GLY	
GLU	
LYS	
ARG	
PRO	
VAL	
ASP	

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	219.00 Å 219.00 Å 219.00 Å 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, SO4, PTR

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	0.56	1/3227 (0.0%)	0.82	4/4360 (0.1%)
2	B	0.67	0/54	1.14	0/71
3	C	0.47	0/1180	0.77	1/1599 (0.1%)
All	All	0.54	1/4461 (0.0%)	0.81	5/6030 (0.1%)

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	297	CYS	CB-SG	-5.44	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	394	GLU	N-CA-C	6.88	129.59	111.00
1	A	136	GLY	N-CA-C	-6.37	97.17	113.10
1	A	69	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	352	LEU	N-CA-C	-5.72	95.55	111.00
3	C	1005	ARG	N-CA-C	-5.50	96.16	111.00

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	183	0
2	B	70	0	50	3	0
3	C	1151	0	1144	131	0
4	A	2	0	0	0	0
5	A	25	0	0	2	0
All	All	4393	0	4308	309	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 (309) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:192:LYS:HD3	1:A:192:LYS:O	1.93	0.69
1:A:92:TYR:CZ	1:A:96:ARG:HD2	2.28	0.69
1:A:269:MET:HE1	1:A:280:ARG:CZ	2.23	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:408:TRP:CZ3	1:A:415:GLY:O	2.50	0.65
1:A:175:GLN:HA	1:A:175:GLN:NE2	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: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:354:GLU:O	1:A:357:PRO:HD3	1.99	0.63
1:A:154:LEU:CD1	1:A:378:PHE:HZ	2.04	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:394:GLU:O	1:A:395:PRO:C	2.38	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:149:ARG:HD2	5:A:2004:SO4:O2	2.03	0.58
1:A:91:THR:HG22	1:A:162:LEU:HB2	1.85	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
3:C:1074:ILE:HG12	3:C:1075:TYR:N	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:354:GLU:HB3	1:A:355:PRO:HD2	1.88	0.55
1:A:91:THR:HG22	1:A:162:LEU:HD22	1.89	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: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
3:C:1067:LYS:HG3	3:C:1067:LYS:O	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:O	1:A:405:LEU:HD23	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:417:PRO:HB3	3:C:1097:PRO:HG2	1.90	0.53
1:A:91:THR:HG22	1:A:162:LEU:HD13	1.90	0.53
1:A:138:GLU:H	1:A:138:GLU:CD	2.12	0.53
1:A:143:GLU:HG3	1:A:144:ASN:HD22	1.72	0.53
1:A:400:MET:HE1	1:A:405:LEU:HA	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CG	3:C:1006:ARG:HH11	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: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:266:PRO:HG2	1:A:340:PRO:HB2	1.93	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:1046:TYR:HD1	3:C:1144:THR:CG2	2.23	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:O	3:C:1027:VAL:HG13	2.10	0.50
3:C:1020:LYS:C	3:C:1022:PHE:H	2.14	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
1:A:419:CYS:O	1:A:420:ARG:C	2.49	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: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
1:A:81:PRO:O	1:A:83:TYR:CD2	2.65	0.49
3:C:1065:PRO:HB3	3:C:1095:TRP:CD2	2.47	0.49
1:A:148:ARG:O	1:A:148:ARG:HD2	2.12	0.49
1:A:191:ARG:C	1:A:193:ALA:H	2.16	0.49
3:C:1011:LEU:HD23	3:C:1014:ILE:HD11	1.93	0.49
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
1:A:420:ARG:HD3	3:C:1096:LYS:HZ3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PHE:C	1:A:189:PHE:CD1	2.86	0.49
3:C:1138:LYS:C	3:C:1140:ALA:H	2.16	0.49
1:A:405:LEU:C	1:A:405:LEU:HD23	2.33	0.48
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:142:GLU:HB3	1:A:143:GLU:H	1.40	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
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: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: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:O	3:C:1116:GLN:HG3	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:307:TYR:CD1	1:A:307:TYR:N	2.82	0.47
1:A:50:THR:HA	1:A:116:ARG:HD2	1.97	0.47
1:A:175:GLN:CA	1:A:175:GLN:HE21	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: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:376:SER:HB2	1:A:379:GLN:CD	2.36	0.46
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:1092:ALA:C	3:C:1094:ASN:H	2.20	0.45
3:C:1116:GLN:N	3:C:1117:PRO:CD	2.79	0.45
1:A:400:MET:HE1	1:A:405:LEU:CA	2.46	0.45
3:C:1092:ALA:O	3:C:1093:GLU:HB2	2.17	0.45
1:A:247:LEU:HD11	1:A:295:LEU:HG	1.97	0.45
1:A:149:ARG:NH2	1:A:271:PHE:O	2.45	0.45
1:A:287:LYS:NZ	1:A:344:ASN:HD21	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NH1	3:C:1133:ARG:HA	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
3:C:1109:ILE:C	3:C:1111:LEU:H	2.19	0.44
1:A:78:LYS:C	1:A:79:ASN:HD22	2.21	0.44
1:A:242:ASP:O	1:A:246:ARG:HG3	2.18	0.44
1:A:84:ILE:CG2	1:A:85:LEU:N	2.81	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:354:GLU:CB	1:A:355:PRO:HD2	2.46	0.44
1:A:80:SER:HA	1:A:81:PRO:HD2	1.78	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:HH11	1:A:191:ARG:HG3	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
1:A:405:LEU:C	1:A:405:LEU:CD2	2.86	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
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:HA	1:A:272:LEU:HD23	1.91	0.43
3:C:1028:ASP:C	3:C:1030:ALA:H	2.22	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
3:C:1060:GLU:H	3:C:1060:GLU:CD	2.22	0.43
1:A:124:LYS:HE2	1:A:124:LYS:HB3	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
1:A:66:VAL:HG13	1:A:129:THR:HG21	2.01	0.43
1:A:404:CYS:O	1:A:405:LEU:C	2.57	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
1:A:379:GLN:CD	1:A:379:GLN:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:LEU:HA	1:A:161:MET:HE1	2.01	0.42
1:A:376:SER:HB2	1:A:379:GLN:NE2	2.34	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:146:GLN:O	1:A:147:PRO:C	2.56	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
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
3:C:1096:LYS:O	3:C:1096:LYS:HG3	2.20	0.41
1:A:303:TRP:CE2	1:A:324:LEU:HD22	2.55	0.41
1:A:84:ILE:HG23	1:A:85:LEU:N	2.35	0.41
3:C:1100:LYS:O	3:C:1101:THR:C	2.58	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:274:TYR:CD1	1:A:274:TYR:C	2.93	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:140:MET:HE3	1:A:140:MET:HB3	1.92	0.41
1:A:382:LYS:HE2	5:A:2005:SO4:O4	2.21	0.41
1:A:402:THR:HG23	1:A:403:SER:N	2.36	0.41
1:A:55:MET:O	1:A:58:LYS:HB3	2.21	0.41
1:A:346:ASN:HA	1:A:347:PRO:HD2	1.82	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
1:A:77:LEU:HD21	1:A:148:ARG:CZ	2.52	0.40
1:A:293:PHE:N	1:A:293:PHE:CD1	2.89	0.40
1:A:138:GLU:C	1:A:140:MET:N	2.74	0.40
1:A:60:TRP:HE1	1:A:95:LEU:HD12	1.85	0.40
1:A:423:ILE:HG12	1:A:423:ILE:H	1.55	0.40
1:A:88:LEU:N	1:A:89:PRO:CD	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	3:C:1087:LEU:HD23	2.29	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	386/388 (100%)	335 (87%)	40 (10%)	11 (3%)	6	22
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%)	2	5

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
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

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Mol	Chain	Res	Type
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%)	338 (97%)	11 (3%)	44	78
2	B	6/6 (100%)	6 (100%)	0	100	100
3	C	122/138 (88%)	113 (93%)	9 (7%)	16	42
All	All	477/493 (97%)	457 (96%)	20 (4%)	34	69

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	A	81	PRO
1	A	90	ASP

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Mol	Chain	Res	Type
1	A	120	GLU
1	A	138	GLU
1	A	142	GLU
1	A	149	ARG
1	A	154	LEU
1	A	156	LEU
1	A	406	THR
1	A	423	ILE
3	C	1011	LEU
3	C	1023	ARG
3	C	1062	PRO
3	C	1075	TYR
3	C	1087	LEU
3	C	1096	LYS
3	C	1133	ARG
3	C	1143	PHE
3	C	1147	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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
1	A	379	GLN
1	A	409	GLN
3	C	1026	GLN
3	C	1031	ASN
3	C	1036	GLN
3	C	1076	HIS

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	1.12	2 (13%)	19,22,24	0.66	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	-	0/9/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	PTR	OH-CZ	-2.10	1.35	1.40
2	B	7	PTR	P-O1P	3.02	1.61	1.50

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.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	2001	-	4,4,4	0.11	0	6,6,6	0.08	0
5	SO4	A	2002	-	4,4,4	0.07	0	6,6,6	0.19	0
5	SO4	A	2003	-	4,4,4	0.29	0	6,6,6	0.17	0
5	SO4	A	2004	-	4,4,4	0.16	0	6,6,6	0.11	0
5	SO4	A	2005	-	4,4,4	0.41	0	6,6,6	0.17	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
5	SO4	A	2001	-	-	0/0/0/0	0/0/0/0
5	SO4	A	2002	-	-	0/0/0/0	0/0/0/0
5	SO4	A	2003	-	-	0/0/0/0	0/0/0/0
5	SO4	A	2004	-	-	0/0/0/0	0/0/0/0
5	SO4	A	2005	-	-	0/0/0/0	0/0/0/0

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.