



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:17 AM GMT

PDB ID : 3L2O
Title : Structure-Based Mechanism of Dimerization-Dependent Ubiquitination by the SCFFbx4 Ubiquitin Ligase
Authors : Li, Y.; Hao, B.
Deposited on : 2009-12-15
Resolution : 2.80 Å (reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

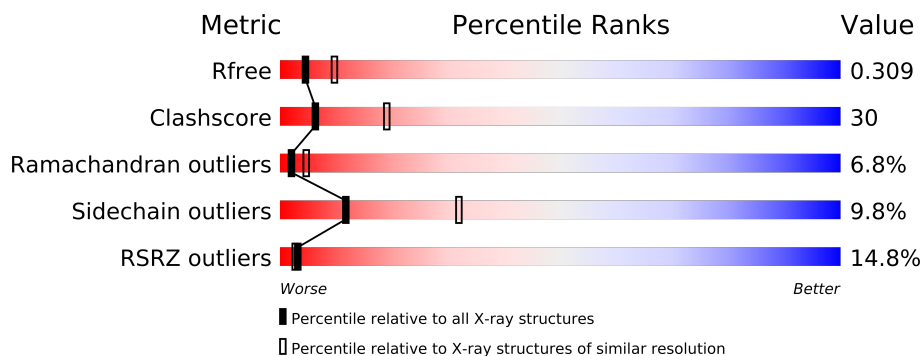
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance



The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	149	
2	B	312	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3425 atoms, of which 0 are hydrogen and 0 are deuterium.

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 S-phase kinase-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	145	Total	C	N	O	S	0	0	0
			1142	723	186	227	6			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1002	ALA	PRO	ENGINEERED	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	GLU	DELETION	UNP P63208
A	?	-	GLY	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	PRO	DELETION	UNP P63208
A	?	-	PRO	DELETION	UNP P63208
A	?	-	PRO	DELETION	UNP P63208
A	?	-	GLU	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	ASP	DELETION	UNP P63208
A	?	-	GLU	DELETION	UNP P63208
A	?	-	ASN	DELETION	UNP P63208
A	?	-	LYS	DELETION	UNP P63208
A	?	-	GLU	DELETION	UNP P63208
A	?	-	LYS	DELETION	UNP P63208
A	?	-	ARG	DELETION	UNP P63208
A	1078	GLY	-	INSERTION	UNP P63208
A	1079	GLY	-	INSERTION	UNP P63208
A	1080	SER	-	INSERTION	UNP P63208
A	1081	GLY	-	INSERTION	UNP P63208

- Molecule 2 is a protein called F-box only protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	274	Total	C	N	O	S	0	0	0
			2207	1423	364	406	14			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	THR	DELETION	UNP Q9UKT5
B	?	-	ARG	DELETION	UNP Q9UKT5
B	?	-	ARG	DELETION	UNP Q9UKT5
B	?	-	ALA	DELETION	UNP Q9UKT5
B	?	-	SER	DELETION	UNP Q9UKT5
B	?	-	LYS	DELETION	UNP Q9UKT5
B	?	-	SER	DELETION	UNP Q9UKT5
B	?	-	SER	DELETION	UNP Q9UKT5
B	?	-	ARG	DELETION	UNP Q9UKT5
B	?	-	PRO	DELETION	UNP Q9UKT5
B	?	-	MET	DELETION	UNP Q9UKT5
B	?	-	TYR	DELETION	UNP Q9UKT5
B	?	-	GLY	DELETION	UNP Q9UKT5
B	?	-	ALA	DELETION	UNP Q9UKT5
B	?	-	VAL	DELETION	UNP Q9UKT5
B	?	-	THR	DELETION	UNP Q9UKT5
B	?	-	SER	DELETION	UNP Q9UKT5
B	?	-	PHE	DELETION	UNP Q9UKT5
B	?	-	LEU	DELETION	UNP Q9UKT5
B	?	-	HIS	DELETION	UNP Q9UKT5
B	?	-	SER	DELETION	UNP Q9UKT5

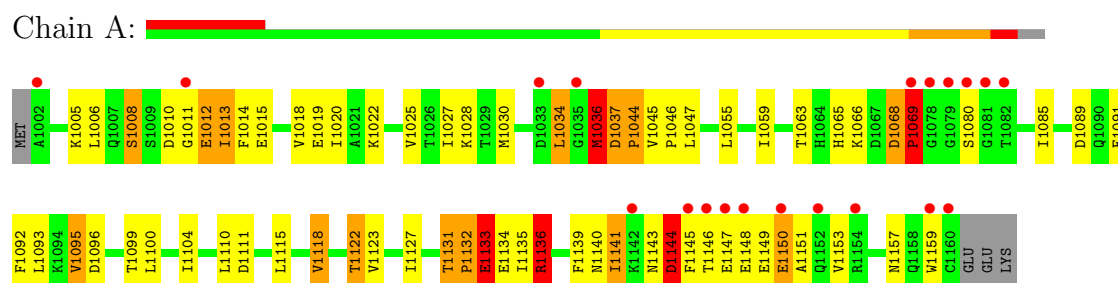
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	56	Total	O	0	0
			56	56		

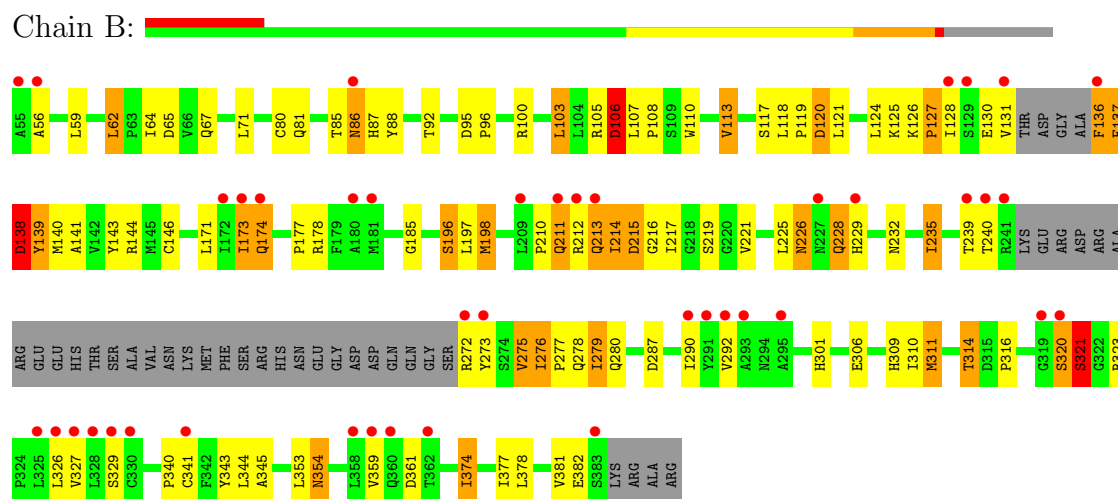
3 Residue-property plots

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

- Molecule 1: S-phase kinase-associated protein 1



- Molecule 2: F-box only protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.19Å 92.19Å 148.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 27.14 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.80) 99.7 (27.14-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.249 , 0.295 0.269 , 0.309	Depositor DCC
R_{free} test set	914 reflections (4.97%)	DCC
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 11.6	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 18392 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3425	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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	0.78	0/1161	1.05	7/1572 (0.4%)
2	B	0.81	0/2266	0.96	6/3087 (0.2%)
All	All	0.80	0/3427	0.99	13/4659 (0.3%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1144	ASP	CB-CA-C	-10.26	89.88	110.40
1	A	1133	GLU	CB-CA-C	-9.82	90.75	110.40
2	B	106	ASP	CB-CA-C	-8.57	93.27	110.40
1	A	1136	ARG	NE-CZ-NH1	8.28	124.44	120.30
2	B	106	ASP	CB-CG-OD2	7.34	124.90	118.30
1	A	1036	MET	CB-CA-C	-7.06	96.29	110.40
1	A	1144	ASP	N-CA-C	6.68	129.05	111.00
2	B	138	ASP	N-CA-C	-5.91	95.05	111.00
1	A	1131	THR	N-CA-C	5.73	126.48	111.00
1	A	1015	GLU	N-CA-C	-5.57	95.97	111.00
2	B	106	ASP	CB-CG-OD1	-5.18	113.64	118.30
2	B	113	VAL	CB-CA-C	-5.01	101.87	111.40
2	B	100	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1142	0	1139	85	0
2	B	2207	0	2148	122	0
3	A	20	0	0	1	0
3	B	56	0	0	1	0
All	All	3425	0	3287	201	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (201) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1136:ARG:HA	1:A:1141:ILE:HD11	1.26	1.13
1:A:1132:PRO:O	1:A:1134:GLU:N	1.84	1.10
2:B:198:MET:CE	2:B:221:VAL:HG21	1.81	1.09
1:A:1136:ARG:CA	1:A:1141:ILE:HD11	1.85	1.06
2:B:198:MET:HE1	2:B:221:VAL:HG21	1.05	1.05
1:A:1141:ILE:H	1:A:1141:ILE:HD12	1.22	0.99
2:B:198:MET:HE1	2:B:221:VAL:CG2	1.96	0.96
1:A:1036:MET:O	1:A:1044:PRO:O	1.85	0.95
1:A:1144:ASP:O	1:A:1144:ASP:OD2	1.88	0.90
2:B:107:LEU:HB3	2:B:108:PRO:HD3	1.56	0.87
2:B:228:GLN:HE21	2:B:228:GLN:HA	1.42	0.85
1:A:1136:ARG:HA	1:A:1141:ILE:CD1	2.07	0.83
2:B:136:PHE:HD2	2:B:137:PHE:N	1.76	0.82
1:A:1136:ARG:HH11	1:A:1136:ARG:HG3	1.43	0.82
2:B:59:LEU:HA	2:B:62:LEU:HD11	1.62	0.81
2:B:178:ARG:HE	2:B:232:ASN:HD22	1.28	0.81
2:B:137:PHE:HB3	2:B:138:ASP:HA	1.64	0.80
1:A:1139:PHE:CD2	2:B:59:LEU:HD22	2.17	0.79
1:A:1036:MET:O	1:A:1037:ASP:C	2.21	0.78
2:B:213:GLN:O	2:B:219:SER:HA	1.84	0.78
2:B:137:PHE:CB	2:B:138:ASP:HA	2.14	0.77
2:B:276:ILE:HG23	2:B:277:PRO:HD2	1.67	0.77
2:B:137:PHE:N	2:B:137:PHE:HD1	1.82	0.77
1:A:1037:ASP:CB	1:A:1044:PRO:HD2	2.15	0.77
2:B:137:PHE:N	2:B:137:PHE:CD1	2.52	0.77
1:A:1141:ILE:N	1:A:1141:ILE:HD12	1.97	0.76
2:B:85:THR:O	2:B:87:HIS:CE1	2.39	0.76
1:A:1136:ARG:HD2	1:A:1141:ILE:HD13	1.67	0.76
2:B:136:PHE:CD2	2:B:137:PHE:N	2.53	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:138:ASP:O	2:B:141:ALA:N	2.18	0.76
1:A:1144:ASP:OD1	2:B:87:HIS:HB3	1.85	0.75
2:B:137:PHE:HA	2:B:139:TYR:H	1.51	0.75
2:B:239:THR:HG23	2:B:240:THR:HG23	1.69	0.74
2:B:120:ASP:O	2:B:121:LEU:C	2.24	0.73
2:B:119:PRO:HG3	2:B:146:CYS:SG	2.29	0.72
2:B:275:VAL:HG23	2:B:280:GLN:HE21	1.56	0.71
2:B:144:ARG:HB3	2:B:173:ILE:HG22	1.73	0.71
1:A:1025:VAL:HG22	1:A:1111:ASP:HB3	1.72	0.70
2:B:217:ILE:HD11	2:B:278:GLN:HB3	1.73	0.70
2:B:171:LEU:O	3:B:31:HOH:O	2.10	0.70
2:B:381:VAL:O	2:B:382:GLU:OE1	2.10	0.69
2:B:311:MET:HA	2:B:314:THR:HG23	1.74	0.68
1:A:1145:PHE:CE1	1:A:1150:GLU:HB3	2.30	0.67
1:A:1037:ASP:HB3	1:A:1044:PRO:HD2	1.77	0.66
2:B:59:LEU:HA	2:B:62:LEU:CD1	2.25	0.66
2:B:185:GLY:HA3	2:B:292:VAL:HG12	1.79	0.65
2:B:381:VAL:HG23	2:B:381:VAL:O	1.95	0.64
1:A:1034:LEU:HD11	1:A:1036:MET:HE3	1.80	0.64
2:B:62:LEU:H	2:B:62:LEU:HD12	1.63	0.64
1:A:1010:ASP:OD2	3:A:8:HOH:O	2.15	0.63
1:A:1008:SER:N	1:A:1011:GLY:O	2.30	0.63
2:B:310:ILE:O	2:B:314:THR:HG22	1.97	0.62
2:B:137:PHE:CB	2:B:138:ASP:CA	2.78	0.61
1:A:1145:PHE:HB2	1:A:1149:GLU:HB2	1.82	0.61
1:A:1136:ARG:C	1:A:1141:ILE:HD11	2.21	0.60
1:A:1037:ASP:HB2	1:A:1044:PRO:HD2	1.82	0.60
1:A:1085:ILE:CD1	1:A:1122:THR:HG23	2.31	0.60
2:B:103:LEU:O	2:B:107:LEU:HB2	2.01	0.60
1:A:1095:VAL:HG13	1:A:1099:THR:HB	1.82	0.60
2:B:210:PRO:O	2:B:212:ARG:O	2.20	0.60
1:A:1036:MET:SD	1:A:1046:PRO:HD3	2.42	0.59
2:B:105:ARG:O	2:B:106:ASP:HB2	2.02	0.59
2:B:329:SER:OG	2:B:344:LEU:HD13	2.01	0.59
2:B:276:ILE:O	2:B:279:ILE:HG22	2.03	0.59
2:B:276:ILE:HG22	2:B:279:ILE:HB	1.85	0.59
1:A:1104:ILE:HD11	1:A:1123:VAL:HG21	1.84	0.59
2:B:86:ASN:O	2:B:87:HIS:CD2	2.56	0.59
2:B:228:GLN:NE2	2:B:228:GLN:HA	2.15	0.58
1:A:1141:ILE:H	1:A:1141:ILE:CD1	2.03	0.57
2:B:136:PHE:HD2	2:B:137:PHE:O	1.88	0.57
1:A:1036:MET:HE2	1:A:1036:MET:HA	1.87	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:239:THR:HG21	2:B:309:HIS:NE2	2.20	0.56
1:A:1018:VAL:HG22	1:A:1022:LYS:HD3	1.87	0.56
2:B:124:LEU:O	2:B:127:PRO:HD3	2.06	0.56
1:A:1141:ILE:O	1:A:1141:ILE:CD1	2.54	0.56
2:B:311:MET:HA	2:B:314:THR:CG2	2.35	0.56
2:B:177:PRO:HA	2:B:287:ASP:OD1	2.06	0.56
1:A:1095:VAL:HG13	1:A:1096:ASP:N	2.21	0.56
2:B:137:PHE:CA	2:B:139:TYR:H	2.20	0.55
1:A:1085:ILE:HG23	1:A:1118:VAL:CG2	2.36	0.55
1:A:1036:MET:O	1:A:1037:ASP:O	2.24	0.55
2:B:137:PHE:HA	2:B:139:TYR:CD1	2.42	0.55
2:B:326:LEU:HB2	2:B:377:ILE:HD13	1.89	0.55
2:B:86:ASN:C	2:B:87:HIS:CG	2.79	0.55
1:A:1093:LEU:HD11	1:A:1118:VAL:HG13	1.89	0.55
1:A:1006:LEU:O	1:A:1013:ILE:O	2.25	0.55
1:A:1037:ASP:CB	1:A:1044:PRO:CD	2.85	0.55
2:B:198:MET:CE	2:B:221:VAL:CG2	2.69	0.55
1:A:1065:HIS:O	1:A:1069:PRO:HD3	2.07	0.54
2:B:178:ARG:NE	2:B:232:ASN:HD22	2.00	0.54
2:B:125:LYS:C	2:B:127:PRO:HD3	2.27	0.54
2:B:374:ILE:O	2:B:377:ILE:HG22	2.08	0.54
2:B:173:ILE:C	2:B:173:ILE:HD12	2.27	0.54
2:B:67:GLN:O	2:B:71:LEU:HG	2.07	0.54
2:B:138:ASP:O	2:B:140:MET:N	2.41	0.53
2:B:216:GLY:C	2:B:217:ILE:HD13	2.29	0.53
1:A:1145:PHE:CD1	1:A:1150:GLU:HB3	2.43	0.52
2:B:174:GLN:CA	2:B:174:GLN:HE21	2.22	0.52
2:B:59:LEU:O	2:B:62:LEU:HD13	2.09	0.52
2:B:136:PHE:CD2	2:B:137:PHE:O	2.63	0.51
1:A:1047:LEU:HD13	1:A:1110:LEU:HD21	1.92	0.51
1:A:1136:ARG:O	1:A:1141:ILE:HD11	2.10	0.51
1:A:1136:ARG:CB	1:A:1141:ILE:HD11	2.40	0.51
2:B:327:VAL:CG1	2:B:359:VAL:HG22	2.40	0.50
2:B:173:ILE:HD12	2:B:174:GLN:N	2.27	0.50
1:A:1136:ARG:HD2	1:A:1141:ILE:CD1	2.40	0.50
1:A:1091:GLU:O	1:A:1092:PHE:C	2.49	0.50
2:B:119:PRO:O	2:B:120:ASP:O	2.30	0.50
2:B:217:ILE:HD11	2:B:278:GLN:CB	2.42	0.49
1:A:1068:ASP:H	1:A:1069:PRO:CD	2.26	0.49
2:B:88:TYR:CE2	2:B:92:THR:HG21	2.48	0.49
2:B:86:ASN:O	2:B:87:HIS:CG	2.65	0.49
1:A:1159:TRP:HB2	2:B:80:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1145:PHE:HB3	2:B:86:ASN:CG	2.34	0.48
2:B:353:LEU:O	2:B:354:ASN:C	2.52	0.48
1:A:1146:THR:OG1	1:A:1149:GLU:HG2	2.12	0.48
1:A:1127:ILE:O	1:A:1127:ILE:HG22	2.13	0.48
1:A:1034:LEU:HD13	1:A:1036:MET:HE2	1.95	0.48
2:B:103:LEU:HD11	2:B:107:LEU:HD13	1.96	0.48
2:B:174:GLN:HA	2:B:174:GLN:HE21	1.79	0.48
2:B:212:ARG:C	2:B:214:ILE:H	2.18	0.48
1:A:1104:ILE:CD1	1:A:1123:VAL:HG21	2.43	0.47
1:A:1059:ILE:O	1:A:1063:THR:HG23	2.15	0.47
1:A:1131:THR:HB	1:A:1133:GLU:HB2	1.96	0.47
1:A:1141:ILE:O	1:A:1141:ILE:HD12	2.13	0.47
1:A:1136:ARG:NH2	1:A:1143:ASN:ND2	2.63	0.47
2:B:341:CYS:HB3	2:B:361:ASP:OD2	2.15	0.47
1:A:1095:VAL:HG11	1:A:1099:THR:HG22	1.96	0.47
2:B:216:GLY:O	2:B:217:ILE:HD13	2.15	0.47
2:B:378:LEU:O	2:B:381:VAL:HG22	2.14	0.47
1:A:1034:LEU:CD1	1:A:1036:MET:CE	2.93	0.47
2:B:235:ILE:O	2:B:235:ILE:HD13	2.15	0.47
1:A:1136:ARG:HG3	1:A:1136:ARG:NH1	2.16	0.46
2:B:327:VAL:HG13	2:B:359:VAL:HA	1.97	0.46
2:B:103:LEU:O	2:B:103:LEU:HD13	2.15	0.46
2:B:381:VAL:O	2:B:381:VAL:CG2	2.63	0.46
1:A:1136:ARG:NH2	1:A:1143:ASN:HD22	2.13	0.46
1:A:1132:PRO:HB2	1:A:1136:ARG:HG2	1.98	0.46
1:A:1085:ILE:HG23	1:A:1118:VAL:HG22	1.97	0.46
1:A:1020:ILE:HD11	1:A:1066:LYS:HD3	1.96	0.46
2:B:321:SER:HB3	2:B:323:ARG:CD	2.46	0.46
1:A:1104:ILE:HD11	1:A:1123:VAL:CG2	2.45	0.46
2:B:117:SER:O	2:B:119:PRO:HD3	2.16	0.45
2:B:374:ILE:HD13	2:B:374:ILE:HA	1.89	0.45
1:A:1134:GLU:O	1:A:1135:ILE:C	2.55	0.45
1:A:1146:THR:H	1:A:1149:GLU:HG3	1.80	0.45
1:A:1065:HIS:HE1	1:A:1089:ASP:OD2	2.00	0.45
2:B:59:LEU:O	2:B:62:LEU:CD1	2.65	0.45
2:B:214:ILE:CG2	2:B:215:ASP:N	2.79	0.45
2:B:95:ASP:HA	2:B:96:PRO:HD2	1.85	0.45
2:B:327:VAL:HG13	2:B:359:VAL:HG22	1.99	0.45
1:A:1157:ASN:O	2:B:80:CYS:HB3	2.17	0.44
2:B:106:ASP:OD1	2:B:143:TYR:OH	2.24	0.44
2:B:211:GLN:O	2:B:212:ARG:C	2.54	0.44
2:B:235:ILE:O	2:B:235:ILE:CG1	2.66	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:136:PHE:O	2:B:137:PHE:C	2.56	0.44
2:B:174:GLN:NE2	2:B:174:GLN:HA	2.33	0.44
1:A:1100:LEU:HD21	1:A:1123:VAL:HG22	2.00	0.43
1:A:1027:ILE:O	1:A:1030:MET:N	2.51	0.43
2:B:103:LEU:CD2	2:B:143:TYR:HA	2.49	0.43
1:A:1139:PHE:CE2	2:B:59:LEU:HD22	2.51	0.43
1:A:1095:VAL:CG1	1:A:1096:ASP:N	2.82	0.43
2:B:316:PRO:O	2:B:320:SER:OG	2.28	0.43
1:A:1141:ILE:O	1:A:1141:ILE:HD13	2.18	0.43
2:B:178:ARG:HA	2:B:232:ASN:O	2.19	0.43
2:B:321:SER:HB3	2:B:323:ARG:HD3	2.00	0.43
1:A:1005:LYS:O	1:A:1045:VAL:HG23	2.18	0.43
2:B:301:HIS:HD2	2:B:306:GLU:OE2	2.01	0.43
2:B:105:ARG:O	2:B:106:ASP:CB	2.66	0.43
2:B:212:ARG:HA	2:B:212:ARG:HD3	1.79	0.43
2:B:290:ILE:HA	2:B:326:LEU:O	2.19	0.43
1:A:1027:ILE:O	1:A:1028:LYS:C	2.57	0.43
1:A:1132:PRO:C	1:A:1134:GLU:N	2.62	0.43
1:A:1085:ILE:HD13	1:A:1122:THR:HG23	2.01	0.42
2:B:340:PRO:HG2	2:B:343:TYR:CD2	2.54	0.42
1:A:1036:MET:SD	1:A:1044:PRO:O	2.78	0.42
2:B:178:ARG:HE	2:B:232:ASN:ND2	2.07	0.42
2:B:239:THR:CG2	2:B:309:HIS:NE2	2.82	0.42
2:B:311:MET:CE	2:B:311:MET:HA	2.50	0.42
2:B:214:ILE:C	2:B:215:ASP:OD1	2.57	0.42
2:B:103:LEU:CD1	2:B:107:LEU:HD13	2.49	0.42
1:A:1010:ASP:OD1	1:A:1010:ASP:N	2.52	0.42
1:A:1018:VAL:HG13	1:A:1019:GLU:N	2.35	0.42
1:A:1025:VAL:HG22	1:A:1111:ASP:CB	2.44	0.42
1:A:1134:GLU:O	1:A:1136:ARG:N	2.53	0.41
2:B:276:ILE:O	2:B:280:GLN:HG3	2.20	0.41
2:B:136:PHE:C	2:B:136:PHE:CD2	2.93	0.41
2:B:107:LEU:N	2:B:108:PRO:CD	2.83	0.41
2:B:64:ILE:HG23	2:B:65:ASP:N	2.34	0.41
2:B:118:LEU:HD12	2:B:119:PRO:HD2	2.02	0.41
2:B:212:ARG:O	2:B:214:ILE:N	2.53	0.41
1:A:1136:ARG:HH21	1:A:1143:ASN:ND2	2.19	0.41
2:B:126:LYS:N	2:B:127:PRO:HD3	2.36	0.41
1:A:1150:GLU:O	1:A:1153:VAL:HG22	2.21	0.40
2:B:225:LEU:O	2:B:226:ASN:C	2.59	0.40
2:B:196:SER:O	2:B:197:LEU:C	2.57	0.40
2:B:107:LEU:HA	2:B:110:TRP:CE3	2.57	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:128:ILE:HD12	2:B:131:VAL:HG12	2.03	0.40
1:A:1150:GLU:CG	1:A:1151:ALA:H	2.34	0.40
1:A:1091:GLU:O	1:A:1093:LEU:N	2.54	0.40
2:B:345:ALA:HB2	2:B:359:VAL:HG21	2.03	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	143/149 (96%)	111 (78%)	17 (12%)	15 (10%)	1	1
2	B	268/312 (86%)	231 (86%)	24 (9%)	13 (5%)	3	10
All	All	411/461 (89%)	342 (83%)	41 (10%)	28 (7%)	2	5

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1012	GLU
1	A	1013	ILE
1	A	1037	ASP
1	A	1068	ASP
1	A	1080	SER
1	A	1132	PRO
1	A	1133	GLU
1	A	1144	ASP
2	B	120	ASP
2	B	127	PRO
2	B	139	TYR
2	B	273	TYR
2	B	86	ASN
2	B	321	SER
1	A	1014	PHE
1	A	1069	PRO

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Mol	Chain	Res	Type
2	B	56	ALA
2	B	226	ASN
1	A	1008	SER
2	B	211	GLN
2	B	354	ASN
1	A	1140	ASN
1	A	1147	GLU
2	B	213	GLN
2	B	320	SER
1	A	1150	GLU
2	B	106	ASP
1	A	1044	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	129/133 (97%)	117 (91%)	12 (9%)	13	35
2	B	247/280 (88%)	222 (90%)	25 (10%)	11	30
All	All	376/413 (91%)	339 (90%)	37 (10%)	12	32

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1012	GLU
1	A	1034	LEU
1	A	1036	MET
1	A	1055	LEU
1	A	1069	PRO
1	A	1095	VAL
1	A	1115	LEU
1	A	1118	VAL
1	A	1122	THR
1	A	1136	ARG
1	A	1141	ILE
1	A	1148	GLU
2	B	62	LEU

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Mol	Chain	Res	Type
2	B	81	GLN
2	B	103	LEU
2	B	113	VAL
2	B	130	GLU
2	B	136	PHE
2	B	137	PHE
2	B	138	ASP
2	B	173	ILE
2	B	174	GLN
2	B	196	SER
2	B	198	MET
2	B	214	ILE
2	B	215	ASP
2	B	228	GLN
2	B	229	HIS
2	B	235	ILE
2	B	272	ARG
2	B	275	VAL
2	B	276	ILE
2	B	279	ILE
2	B	311	MET
2	B	314	THR
2	B	321	SER
2	B	374	ILE

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	1023	GLN
1	A	1060	GLN
1	A	1065	HIS
1	A	1090	GLN
1	A	1108	ASN
1	A	1143	ASN
2	B	81	GLN
2	B	86	ASN
2	B	87	HIS
2	B	174	GLN
2	B	228	GLN
2	B	229	HIS
2	B	232	ASN
2	B	278	GLN

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Mol	Chain	Res	Type
2	B	280	GLN
2	B	301	HIS
2	B	372	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	145/149 (97%)	0.84	20 (13%) 4 3	30, 43, 69, 72	0
2	B	274/312 (87%)	0.88	42 (15%) 3 2	33, 45, 54, 63	0
All	All	419/461 (90%)	0.87	62 (14%) 3 3	30, 45, 61, 72	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1078	GLY	7.7
2	B	273	TYR	7.4
2	B	55	ALA	6.8
2	B	172	ILE	6.2
1	A	1079	GLY	5.9
2	B	383	SER	5.8
1	A	1081	GLY	5.5
2	B	329	SER	4.9
2	B	136	PHE	4.8
1	A	1160	CYS	4.8
1	A	1142	LYS	4.6
2	B	327	VAL	4.6
2	B	180	ALA	4.5
2	B	128	ILE	4.4
2	B	326	LEU	4.4
2	B	328	LEU	4.1
1	A	1154	ARG	4.1
2	B	292	VAL	4.0
1	A	1145	PHE	4.0
2	B	212	ARG	3.9
2	B	293	ALA	3.9
2	B	241	ARG	3.9
2	B	174	GLN	3.9
1	A	1033	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	173	ILE	3.6
2	B	290	ILE	3.6
2	B	239	THR	3.6
1	A	1152	GLN	3.6
1	A	1035	GLY	3.5
1	A	1069	PRO	3.5
2	B	291	TYR	3.5
2	B	330	CYS	3.5
2	B	319	GLY	3.5
2	B	56	ALA	3.5
2	B	240	THR	3.4
1	A	1002	ALA	3.3
2	B	341	CYS	3.3
2	B	181	MET	3.3
2	B	211	GLN	3.2
1	A	1082	THR	3.1
2	B	131	VAL	2.9
2	B	129	SER	2.9
1	A	1011	GLY	2.8
1	A	1146	THR	2.8
1	A	1147	GLU	2.8
1	A	1080	SER	2.7
2	B	86	ASN	2.6
2	B	359	VAL	2.6
2	B	209	LEU	2.6
2	B	320	SER	2.5
2	B	227	ASN	2.5
2	B	358	LEU	2.5
1	A	1148	GLU	2.4
2	B	213	GLN	2.4
1	A	1159	TRP	2.4
2	B	229	HIS	2.4
2	B	360	GLN	2.4
2	B	272	ARG	2.3
1	A	1150	GLU	2.3
2	B	362	THR	2.2
2	B	295	ALA	2.1
2	B	325	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.