Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:09 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 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 ①) were used in the production of this report:

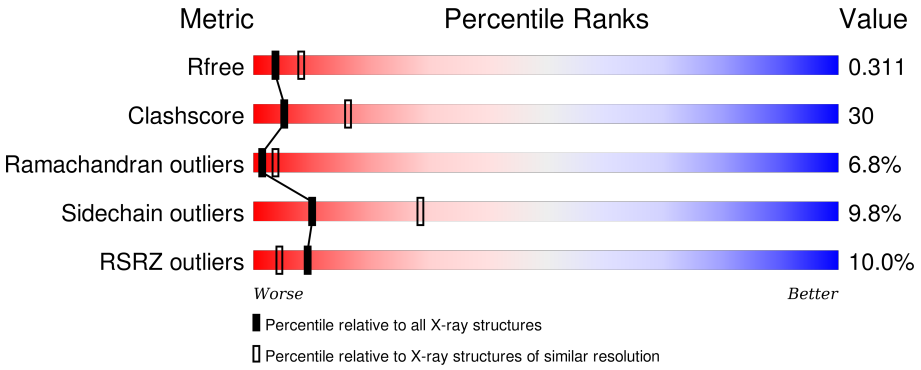
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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. 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 <=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.

Mol	Chain	Length	Quality of chain
1	A	149	11% 50% 34% 9%
2	B	312	8% 53% 25% 9% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3425 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 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.

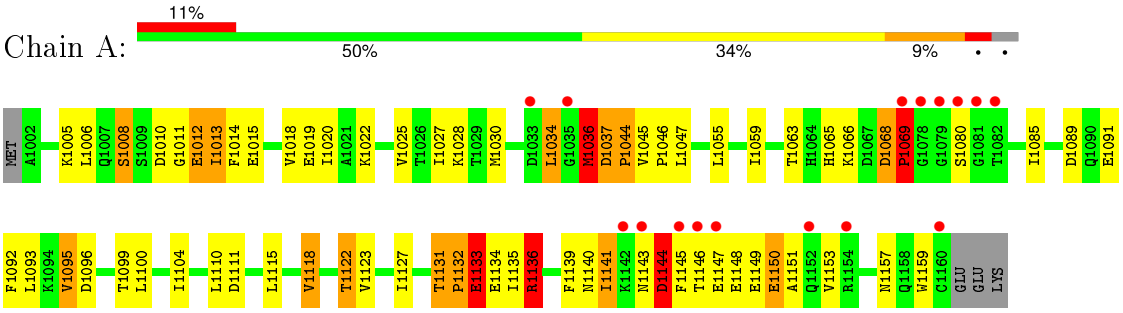
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	56	Total	O	0	0
			56	56		

3 Residue-property plots (i)

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.

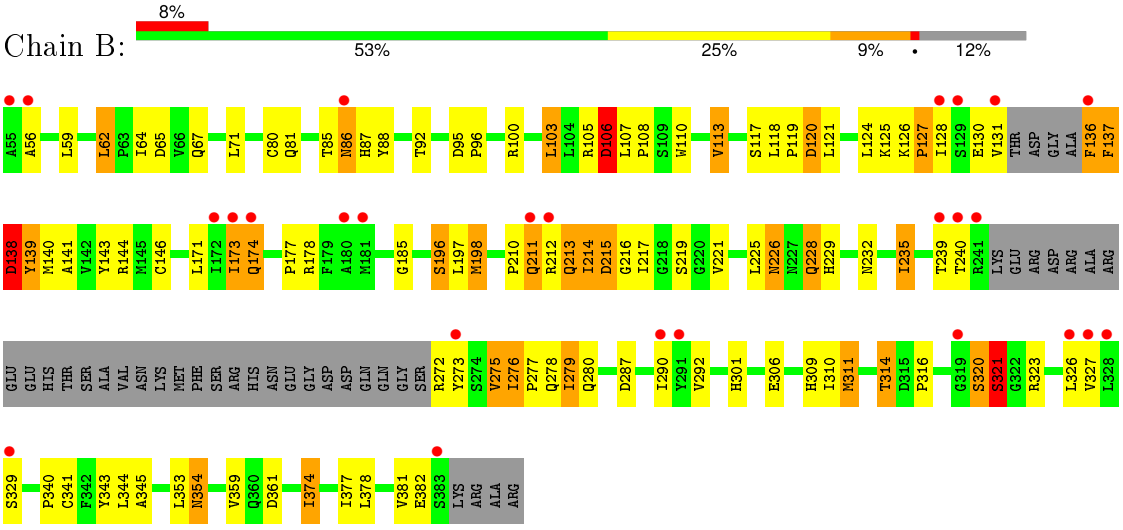
- Molecule 1: S-phase kinase-associated protein 1

Chain A:



- Molecule 2: F-box only protein 4

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.87 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.249 , 0.295 0.267 , 0.311	Depositor DCC
R_{free} test set	915 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	77.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 79.7	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	0 of 18392 reflections	Xtriage
F_o,F_c correlation	0.93	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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(^{o})	Ideal(^{o})
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 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	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

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 30.

All (201) 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: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
2:B:138:ASP:O	2:B:141:ALA:N	2.18	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:TRP:HB2	2:B:80:CYS:SG	2.53	0.48
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	143/149 (96%)	111 (78%)	17 (12%)	15 (10%)	1 1
2	B	268/312 (86%)	231 (86%)	24 (9%)	13 (5%)	3 8
All	All	411/461 (89%)	342 (83%)	41 (10%)	28 (7%)	1 4

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

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Mol	Chain	Res	Type
2	B	273	TYR
2	B	86	ASN
2	B	321	SER
1	A	1014	PHE
1	A	1069	PRO
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 (i)

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%)	11 32
2	B	247/280 (88%)	222 (90%)	25 (10%)	9 27
All	All	376/413 (91%)	339 (90%)	37 (10%)	10 28

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

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Mol	Chain	Res	Type
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
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

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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} 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%)	0.34	16 (11%)	7	3	30, 43, 69, 72	0
2	B	274/312 (87%)	0.43	26 (9%)	10	5	33, 45, 54, 63	0
All	All	419/461 (90%)	0.40	42 (10%)	9	4	30, 45, 61, 72	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1078	GLY	6.6
2	B	273	TYR	6.1
2	B	172	ILE	5.7
2	B	55	ALA	5.4
1	A	1079	GLY	5.4
2	B	136	PHE	5.2
2	B	128	ILE	3.8
1	A	1069	PRO	3.8
1	A	1142	LYS	3.7
2	B	180	ALA	3.6
1	A	1082	THR	3.5
1	A	1035	GLY	3.5
2	B	173	ILE	3.4
1	A	1145	PHE	3.3
2	B	383	SER	3.3
1	A	1152	GLN	3.3
2	B	241	ARG	3.2
1	A	1033	ASP	3.2
1	A	1081	GLY	3.2
1	A	1160	CYS	3.2
2	B	211	GLN	3.1
1	A	1154	ARG	3.0
2	B	212	ARG	2.9
2	B	290	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	326	LEU	2.9
2	B	327	VAL	2.9
2	B	329	SER	2.8
2	B	328	LEU	2.7
2	B	56	ALA	2.7
2	B	174	GLN	2.7
2	B	240	THR	2.5
2	B	239	THR	2.5
2	B	129	SER	2.5
1	A	1146	THR	2.5
2	B	181	MET	2.4
2	B	291	TYR	2.4
1	A	1080	SER	2.2
1	A	1143	ASN	2.2
2	B	131	VAL	2.2
2	B	319	GLY	2.1
1	A	1147	GLU	2.1
2	B	86	ASN	2.1

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.