Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:10 pm BST

PDB ID	:	6H7H
Title	:	Crystal structure of redox-sensitive phosphoribulokinase (PRK) from Arabidopsis thaliana
Authors	:	Fermani, S.; Sparla, F.; Gurrieri, L.; Falini, G.; Trost, P.
Deposited on	:	2018-07-31
Resolution	:	2.47 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 following versions of software and data (see references ⓘ) were used in the production of this report:

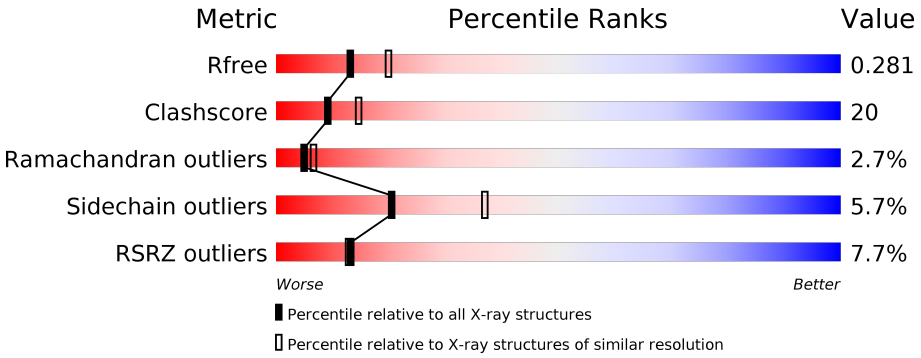
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.47 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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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 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 <=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	351	5% 61% 29% 6%
1	B	351	9% 68% 25%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5385 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 Phosphoribulokinase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2688	1716	446	515	11			
1	B	336	Total	C	N	O	S	0	0	0
			2667	1703	442	511	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	HIS	-	expression tag	UNP P25697
A	0	MET	-	expression tag	UNP P25697
B	-1	HIS	-	expression tag	UNP P25697
B	0	MET	-	expression tag	UNP P25697

- Molecule 2 is water.

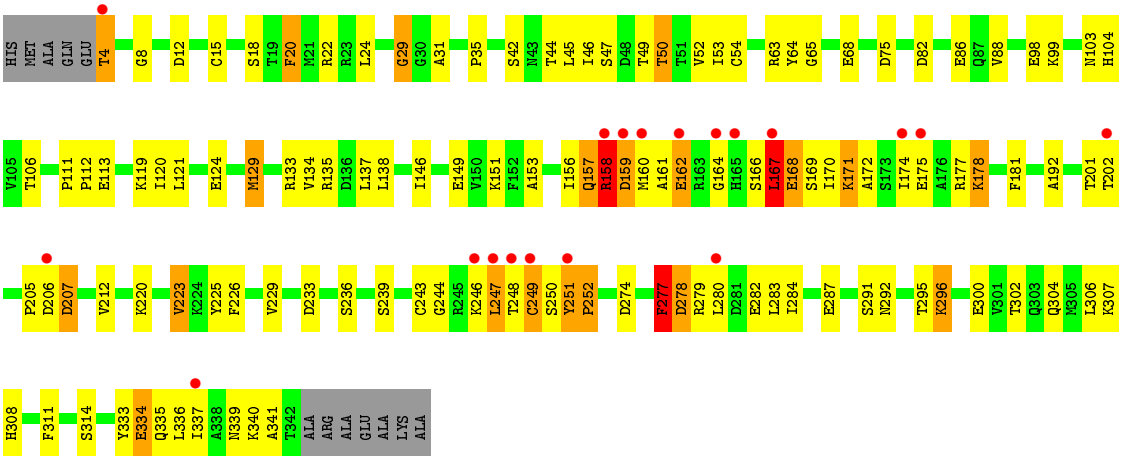
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	13	Total	O	0	0
			13	13		
2	B	17	Total	O	0	0
			17	17		

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 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.

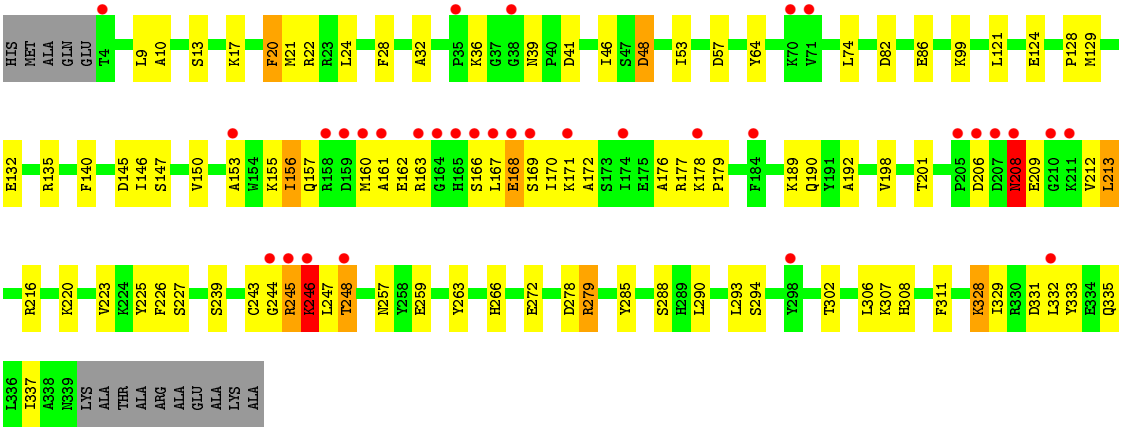
- Molecule 1: Phosphoribulokinase, chloroplastic

Chain A:



- Molecule 1: Phosphoribulokinase, chloroplastic

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α, β, γ	116.30Å 116.30Å 106.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.76 – 2.47 46.76 – 2.47	Depositor EDS
% Data completeness (in resolution range)	96.7 (46.76-2.47) 96.7 (46.76-2.47)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.226 , 0.281 0.226 , 0.281	Depositor DCC
R_{free} test set	1255 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	52.5	Xtriage
Anisotropy	0.771	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 63.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.052 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5385	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.45	1/2747 (0.0%)	0.69	2/3721 (0.1%)
1	B	0.45	2/2726 (0.1%)	0.62	2/3693 (0.1%)
All	All	0.45	3/5473 (0.1%)	0.65	4/7414 (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	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	LYS	CE-NZ	11.14	1.76	1.49
1	A	251	TYR	CE1-CZ	-6.92	1.29	1.38
1	B	246	LYS	CG-CD	-5.03	1.35	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	246	LYS	CG-CD-CE	-6.40	92.69	111.90
1	A	4	THR	CA-CB-CG2	-6.36	103.49	112.40
1	A	167	LEU	CA-CB-CG	-5.57	102.50	115.30
1	B	246	LYS	N-CA-CB	5.17	119.91	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	A	277	PHE	Peptide

5.2 Too-close contacts (i)

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	2688	0	2667	119	0
1	B	2667	0	2640	95	0
2	A	13	0	0	0	0
2	B	17	0	0	0	0
All	All	5385	0	5307	213	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 20.

All (213) 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:B:246:LYS:NZ	1:B:246:LYS:CE	1.76	1.45
1:A:247:LEU:HD22	1:A:249:CYS:HB3	1.34	1.09
1:B:13:SER:HB2	1:B:17:LYS:NZ	1.76	1.00
1:A:249:CYS:SG	1:A:250:SER:HB2	2.04	0.98
1:B:163:ARG:NE	1:B:170:ILE:HD11	1.81	0.96
1:B:13:SER:HA	1:B:17:LYS:HE2	1.51	0.91
1:B:22:ARG:HD3	1:B:311:PHE:CZ	2.10	0.87
1:B:13:SER:HB2	1:B:17:LYS:CE	2.08	0.83
1:B:13:SER:HB2	1:B:17:LYS:HZ1	1.43	0.80
1:B:302:THR:O	1:B:306:LEU:HD12	1.82	0.78
1:A:248:THR:HG23	1:A:279:ARG:NH2	1.99	0.77
1:A:157:GLN:HG2	1:A:162:GLU:HG2	1.69	0.74
1:B:13:SER:CA	1:B:17:LYS:HE2	2.17	0.73
1:B:160:MET:SD	1:B:163:ARG:NH2	2.63	0.72
1:B:82:ASP:O	1:B:86:GLU:HG3	1.89	0.72
1:A:53:ILE:HD12	1:A:121:LEU:HD11	1.73	0.71
1:A:170:ILE:O	1:A:172:ALA:N	2.22	0.71
1:A:99:LYS:NZ	1:A:113:GLU:OE1	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:SER:O	1:A:169:SER:OG	2.10	0.70
1:A:157:GLN:O	1:A:159:ASP:N	2.25	0.70
1:A:4:THR:HG21	1:A:333:TYR:CA	2.23	0.68
1:A:247:LEU:CD2	1:A:249:CYS:HB3	2.20	0.68
1:B:10:ALA:HB2	1:B:129:MET:HE1	1.76	0.68
1:B:146:ILE:HD13	1:B:198:VAL:HB	1.76	0.68
1:A:162:GLU:C	1:A:168:GLU:HB3	2.14	0.68
1:B:302:THR:HG22	1:B:306:LEU:HD11	1.74	0.67
1:A:249:CYS:HB2	1:A:278:ASP:OD1	1.94	0.67
1:A:153:ALA:O	1:A:156:ILE:HG13	1.95	0.67
1:A:164:GLY:O	1:A:168:GLU:HA	1.95	0.67
1:A:283:LEU:HD12	1:A:302:THR:HG22	1.76	0.67
1:B:153:ALA:HB2	1:B:208:ASN:HB2	1.78	0.65
1:A:280:LEU:HD22	1:A:280:LEU:H	1.61	0.65
1:B:163:ARG:CD	1:B:170:ILE:HD11	2.26	0.65
1:A:239:SER:HB2	1:B:239:SER:HB3	1.79	0.64
1:A:277:PHE:HA	1:A:278:ASP:OD1	1.96	0.64
1:A:157:GLN:HA	1:A:161:ALA:HA	1.80	0.64
1:A:129:MET:HE2	1:A:138:LEU:CD1	2.27	0.64
1:A:4:THR:HG21	1:A:333:TYR:HB2	1.80	0.63
1:B:294:SER:OG	1:B:328:LYS:NZ	2.31	0.63
1:A:4:THR:HG21	1:A:333:TYR:CB	2.29	0.62
1:A:296:LYS:NZ	1:A:334:GLU:OE2	2.32	0.62
1:A:157:GLN:H	1:A:162:GLU:CD	2.03	0.62
1:A:63:ARG:NH2	1:A:104:HIS:O	2.33	0.62
1:A:129:MET:HE2	1:A:138:LEU:HD13	1.82	0.61
1:A:4:THR:HG21	1:A:333:TYR:HA	1.83	0.61
1:B:172:ALA:O	1:B:176:ALA:HB2	2.01	0.61
1:B:155:LYS:HZ3	1:B:163:ARG:HH12	1.49	0.61
1:B:13:SER:CB	1:B:17:LYS:CE	2.78	0.61
1:B:163:ARG:NE	1:B:170:ILE:CD1	2.62	0.60
1:A:246:LYS:O	1:A:279:ARG:NH1	2.34	0.60
1:A:18:SER:O	1:A:22:ARG:HG3	2.02	0.60
1:A:15:CYS:HB3	1:A:146:ILE:HG13	1.82	0.60
1:A:82:ASP:O	1:A:86:GLU:HG2	2.00	0.60
1:B:223:VAL:HB	1:B:226:PHE:HB3	1.83	0.59
1:A:129:MET:CE	1:A:138:LEU:CD1	2.81	0.59
1:A:133:ARG:O	1:A:137:LEU:HD12	2.01	0.59
1:B:244:GLY:HA2	1:B:245:ARG:C	2.23	0.59
1:B:20:PHE:O	1:B:24:LEU:HD12	2.03	0.59
1:A:171:LYS:O	1:A:174:ILE:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:ILE:N	1:B:170:ILE:HD12	2.18	0.58
1:B:225:TYR:HB3	1:B:335:GLN:OE1	2.03	0.58
1:A:129:MET:CE	1:A:138:LEU:HD13	2.33	0.58
1:A:12:ASP:OD2	1:A:177:ARG:NH2	2.37	0.57
1:A:88:VAL:HG23	1:A:137:LEU:HD22	1.86	0.57
1:B:246:LYS:NZ	1:B:246:LYS:CD	2.65	0.57
1:B:160:MET:HB3	1:B:163:ARG:HG2	1.87	0.57
1:B:227:SER:O	1:B:328:LYS:HE2	2.05	0.57
1:A:49:THR:HG22	1:A:119:LYS:HE2	1.87	0.56
1:A:35:PRO:HG2	1:A:113:GLU:OE2	2.05	0.56
1:A:249:CYS:HB2	1:A:278:ASP:CG	2.27	0.55
1:B:10:ALA:HB2	1:B:129:MET:CE	2.37	0.55
1:A:50:THR:HB	1:A:120:ILE:HB	1.88	0.55
1:A:333:TYR:O	1:A:337:ILE:HG22	2.07	0.55
1:A:158:ARG:HD3	1:A:159:ASP:HB2	1.87	0.55
1:A:223:VAL:HG23	1:A:226:PHE:HB3	1.88	0.54
1:A:280:LEU:HG	1:A:306:LEU:HD11	1.89	0.54
1:B:302:THR:HG22	1:B:306:LEU:CD1	2.36	0.54
1:A:167:LEU:HD22	1:A:167:LEU:N	2.21	0.54
1:B:167:LEU:HD23	1:B:168:GLU:OE1	2.08	0.54
1:A:283:LEU:CD1	1:A:302:THR:HG22	2.38	0.54
1:B:333:TYR:CE1	1:B:337:ILE:HD11	2.42	0.53
1:A:64:TYR:O	1:A:68:GLU:HG3	2.08	0.53
1:B:145:ASP:OD2	1:B:189:LYS:NZ	2.37	0.53
1:B:24:LEU:HB3	1:B:28:PHE:CE2	2.43	0.53
1:A:129:MET:O	1:A:135:ARG:NH1	2.41	0.53
1:B:166:SER:HB2	1:B:167:LEU:HD12	1.90	0.53
1:B:167:LEU:HB3	1:B:168:GLU:HB3	1.89	0.53
1:B:13:SER:CB	1:B:17:LYS:HE2	2.38	0.53
1:A:42:SER:OG	1:A:113:GLU:OE2	2.18	0.53
1:A:4:THR:CG2	1:A:333:TYR:HA	2.37	0.53
1:A:133:ARG:HG3	1:A:133:ARG:HH11	1.74	0.53
1:B:160:MET:HB2	1:B:163:ARG:CZ	2.39	0.52
1:A:282:GLU:N	1:A:282:GLU:OE1	2.43	0.52
1:A:233:ASP:O	1:A:236:SER:OG	2.27	0.52
1:A:223:VAL:CG2	1:A:226:PHE:HB3	2.39	0.52
1:A:206:ASP:O	1:A:207:ASP:HB2	2.09	0.52
1:B:206:ASP:OD1	1:B:208:ASN:N	2.41	0.52
1:B:307:LYS:HG2	1:B:308:HIS:CD2	2.45	0.51
1:B:155:LYS:NZ	1:B:163:ARG:HH12	2.08	0.51
1:A:98:GLU:HG3	1:A:112:PRO:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:O	1:A:46:ILE:HD13	2.11	0.51
1:A:161:ALA:O	1:A:162:GLU:C	2.48	0.51
1:A:31:ALA:HB3	1:A:47:SER:HB3	1.93	0.51
1:A:279:ARG:HB2	1:A:282:GLU:OE1	2.11	0.51
1:B:132:GLU:HG2	1:B:135:ARG:NH2	2.26	0.51
1:A:44:THR:HG22	1:A:46:ILE:CD1	2.41	0.50
1:B:170:ILE:CG2	1:B:172:ALA:HB3	2.41	0.50
1:B:307:LYS:HG2	1:B:308:HIS:NE2	2.26	0.50
1:A:202:THR:HG22	1:A:274:ASP:OD2	2.12	0.50
1:A:248:THR:CG2	1:A:279:ARG:NH2	2.73	0.50
1:B:53:ILE:HD12	1:B:121:LEU:HD11	1.93	0.50
1:B:190:GLN:HG3	1:B:266:HIS:NE2	2.27	0.49
1:A:178:LYS:HA	1:A:181:PHE:HB3	1.95	0.49
1:B:129:MET:O	1:B:135:ARG:HD3	2.12	0.49
1:A:134:VAL:HA	1:A:137:LEU:CD1	2.43	0.49
1:A:201:THR:HG21	1:A:212:VAL:HG13	1.94	0.49
1:A:280:LEU:N	1:A:280:LEU:HD22	2.28	0.48
1:A:277:PHE:CE1	1:A:283:LEU:HD22	2.48	0.48
1:A:44:THR:HG22	1:A:46:ILE:HD11	1.95	0.48
1:A:156:ILE:HB	1:A:162:GLU:OE2	2.13	0.48
1:B:246:LYS:HD3	1:B:246:LYS:HA	1.29	0.48
1:B:278:ASP:HB3	1:B:279:ARG:HD2	1.96	0.48
1:B:128:PRO:HG2	1:B:129:MET:HE2	1.95	0.48
1:B:170:ILE:HG22	1:B:172:ALA:HB3	1.96	0.48
1:A:229:VAL:HA	1:A:292:ASN:HB2	1.95	0.48
1:A:52:VAL:HG12	1:A:124:GLU:OE1	2.14	0.47
1:A:225:TYR:CD1	1:A:335:GLN:HG2	2.49	0.47
1:B:156:ILE:O	1:B:156:ILE:HG13	2.14	0.47
1:A:20:PHE:HE1	1:A:24:LEU:HD11	1.79	0.47
1:A:103:ASN:CG	1:A:106:THR:HG22	2.35	0.47
1:B:57:ASP:OD2	1:B:99:LYS:NZ	2.47	0.47
1:A:4:THR:O	1:A:120:ILE:HG23	2.14	0.47
1:A:8:GLY:HA3	1:A:129:MET:HE1	1.96	0.47
1:A:334:GLU:HA	1:A:337:ILE:HG22	1.97	0.47
1:B:128:PRO:HG2	1:B:129:MET:CE	2.44	0.47
1:A:20:PHE:CE1	1:A:24:LEU:CD1	2.97	0.47
1:A:157:GLN:CA	1:A:161:ALA:HA	2.45	0.46
1:B:192:ALA:O	1:B:220:LYS:HE2	2.15	0.46
1:B:216:ARG:NH2	1:B:259:GLU:OE2	2.48	0.46
1:B:302:THR:CG2	1:B:306:LEU:HD11	2.45	0.46
1:B:208:ASN:O	1:B:208:ASN:ND2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:TYR:CZ	1:B:337:ILE:HD11	2.50	0.46
1:A:164:GLY:HA2	1:A:170:ILE:HG13	1.97	0.46
1:A:229:VAL:HG23	1:A:291:SER:O	2.15	0.46
1:A:334:GLU:HA	1:A:337:ILE:CG2	2.46	0.46
1:B:308:HIS:HB3	1:B:311:PHE:CD1	2.51	0.45
1:B:32:ALA:HA	1:B:46:ILE:O	2.16	0.45
1:B:163:ARG:CZ	1:B:170:ILE:CD1	2.95	0.45
1:A:284:ILE:HA	1:A:302:THR:HG21	1.98	0.45
1:B:290:LEU:HB2	1:B:293:LEU:HD11	1.98	0.45
1:B:160:MET:O	1:B:163:ARG:HG2	2.17	0.45
1:B:285:TYR:O	1:B:288:SER:OG	2.30	0.45
1:A:249:CYS:SG	1:A:250:SER:CB	2.91	0.45
1:B:246:LYS:HB2	1:B:246:LYS:HE2	1.27	0.45
1:A:307:LYS:HE3	1:A:308:HIS:CE1	2.51	0.45
1:B:189:LYS:HD2	1:B:263:TYR:OH	2.17	0.45
1:A:280:LEU:CD2	1:A:280:LEU:H	2.28	0.44
1:B:225:TYR:HB2	1:B:332:LEU:CD1	2.47	0.44
1:A:340:LYS:HB3	1:A:341:ALA:HB2	1.99	0.44
1:B:21:MET:CE	1:B:24:LEU:HD13	2.48	0.44
1:A:251:TYR:HD2	1:A:252:PRO:HD3	1.82	0.44
1:B:145:ASP:OD1	1:B:146:ILE:N	2.50	0.44
1:B:163:ARG:CZ	1:B:170:ILE:HD11	2.47	0.44
1:A:31:ALA:HB3	1:A:47:SER:CB	2.48	0.44
1:A:164:GLY:CA	1:A:170:ILE:HG13	2.47	0.44
1:A:20:PHE:CE1	1:A:24:LEU:HD11	2.52	0.44
1:B:220:LYS:HZ2	1:B:266:HIS:CD2	2.35	0.43
1:A:295:THR:OG1	1:A:300:GLU:HB3	2.18	0.43
1:A:336:LEU:O	1:A:340:LYS:NZ	2.52	0.43
1:B:9:LEU:HD22	1:B:21:MET:HE2	2.00	0.43
1:B:331:ASP:O	1:B:335:GLN:HG3	2.18	0.43
1:A:251:TYR:CD2	1:A:252:PRO:HD3	2.53	0.43
1:B:21:MET:HE2	1:B:24:LEU:HD13	2.00	0.43
1:A:304:GLN:O	1:A:308:HIS:HD2	2.02	0.43
1:B:155:LYS:HZ1	1:B:163:ARG:HH22	1.65	0.43
1:B:246:LYS:HA	1:B:246:LYS:CE	2.39	0.43
1:B:163:ARG:CD	1:B:170:ILE:CD1	2.93	0.43
1:B:243:CYS:HA	1:B:247:LEU:HB3	2.00	0.43
1:A:243:CYS:HA	1:A:244:GLY:HA3	1.43	0.43
1:B:206:ASP:OD2	1:B:209:GLU:HB2	2.18	0.43
1:B:247:LEU:O	1:B:248:THR:OG1	2.26	0.42
1:A:339:ASN:O	1:A:340:LYS:HD3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:CG1	1:B:213:LEU:HD22	2.49	0.42
1:A:174:ILE:HD12	1:A:175:GLU:N	2.35	0.42
1:A:287:GLU:OE2	1:A:302:THR:HG23	2.19	0.42
1:A:22:ARG:HB2	1:A:311:PHE:HE2	1.84	0.42
1:A:111:PRO:HA	1:A:112:PRO:HD3	1.86	0.42
1:A:134:VAL:HA	1:A:137:LEU:HD13	2.02	0.42
1:B:243:CYS:HA	1:B:244:GLY:HA3	1.77	0.42
1:A:20:PHE:HE1	1:A:24:LEU:CD1	2.32	0.42
1:A:54:CYS:HA	1:A:124:GLU:OE2	2.20	0.42
1:B:290:LEU:CB	1:B:293:LEU:HD11	2.50	0.42
1:B:168:GLU:HG2	1:B:169:SER:N	2.35	0.42
1:A:279:ARG:HD3	1:A:282:GLU:CD	2.40	0.42
1:A:29:GLY:HA3	1:A:49:THR:OG1	2.20	0.42
1:A:65:GLY:HA2	1:A:68:GLU:HG3	2.02	0.41
1:A:157:GLN:HA	1:A:162:GLU:H	1.85	0.41
1:A:157:GLN:HB3	1:A:158:ARG:H	1.59	0.41
1:A:22:ARG:HB2	1:A:311:PHE:CE2	2.56	0.41
1:B:201:THR:HG21	1:B:212:VAL:HG13	2.02	0.41
1:B:170:ILE:H	1:B:170:ILE:HD12	1.83	0.41
1:A:158:ARG:HD3	1:A:159:ASP:N	2.35	0.41
1:A:167:LEU:HA	1:A:167:LEU:HD13	1.63	0.41
1:B:163:ARG:HD3	1:B:170:ILE:HD11	2.02	0.41
1:B:48:ASP:OD1	1:B:48:ASP:N	2.52	0.41
1:B:74:LEU:N	1:B:74:LEU:HD12	2.36	0.41
1:A:192:ALA:O	1:A:220:LYS:HE3	2.21	0.41
1:B:147:SER:OG	1:B:150:VAL:HG23	2.22	0.41
1:B:216:ARG:HG2	1:B:272:GLU:HG3	2.02	0.40
1:A:157:GLN:OE1	1:A:161:ALA:HB1	2.22	0.40
1:A:311:PHE:O	1:A:314:SER:HB2	2.22	0.40
1:B:140:PHE:CE1	1:B:329:ILE:HD11	2.57	0.40
1:A:171:LYS:HD3	1:A:171:LYS:O	2.21	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	337/351 (96%)	307 (91%)	20 (6%)	10 (3%)	4 5
1	B	334/351 (95%)	306 (92%)	20 (6%)	8 (2%)	6 8
All	All	671/702 (96%)	613 (91%)	40 (6%)	18 (3%)	5 6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	162	GLU
1	A	171	LYS
1	B	161	ALA
1	B	168	GLU
1	B	208	ASN
1	B	246	LYS
1	A	252	PRO
1	B	39	ASN
1	B	248	THR
1	A	167	LEU
1	B	156	ILE
1	B	157	GLN
1	A	157	GLN
1	A	278	ASP
1	A	29	GLY
1	A	168	GLU
1	A	205	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	298/305 (98%)	282 (95%)	16 (5%)	22 40
1	B	296/305 (97%)	278 (94%)	18 (6%)	18 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	594/610 (97%)	560 (94%)	34 (6%)	20 37

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	50	THR
1	A	75	ASP
1	A	129	MET
1	A	149	GLU
1	A	151	LYS
1	A	158	ARG
1	A	159	ASP
1	A	160	MET
1	A	178	LYS
1	A	207	ASP
1	A	247	LEU
1	A	249	CYS
1	A	277	PHE
1	A	296	LYS
1	A	334	GLU
1	B	20	PHE
1	B	36	LYS
1	B	41	ASP
1	B	48	ASP
1	B	64	TYR
1	B	124	GLU
1	B	162	GLU
1	B	171	LYS
1	B	177	ARG
1	B	178	LYS
1	B	179	PRO
1	B	208	ASN
1	B	213	LEU
1	B	245	ARG
1	B	246	LYS
1	B	257	ASN
1	B	279	ARG
1	B	328	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	148	ASN
1	A	157	GLN
1	B	266	HIS

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	339/351 (96%)	0.38	19 (5%) 24 25	44, 67, 145, 192	0
1	B	336/351 (95%)	0.57	33 (9%) 7 6	52, 71, 144, 203	0
All	All	675/702 (96%)	0.48	52 (7%) 13 13	44, 69, 145, 203	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	THR	9.2
1	B	159	ASP	6.3
1	A	251	TYR	6.2
1	B	166	SER	6.2
1	B	161	ALA	6.1
1	B	164	GLY	5.5
1	B	208	ASN	5.2
1	A	247	LEU	5.1
1	A	249	CYS	4.9
1	B	168	GLU	4.6
1	B	210	GLY	4.4
1	B	245	ARG	4.3
1	B	160	MET	4.3
1	B	167	LEU	4.2
1	A	246	LYS	4.2
1	B	248	THR	4.1
1	A	206	ASP	4.0
1	A	4	THR	3.8
1	A	174	ILE	3.6
1	B	206	ASP	3.6
1	B	332	LEU	3.5
1	B	205	PRO	3.4
1	B	158	ARG	3.4
1	A	159	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	280	LEU	3.3
1	B	4	THR	3.3
1	B	207	ASP	3.3
1	B	70	LYS	3.2
1	B	244	GLY	3.2
1	B	211	LYS	3.2
1	B	163	ARG	3.1
1	B	174	ILE	3.0
1	A	165	HIS	2.9
1	A	167	LEU	2.8
1	B	169	SER	2.8
1	B	165	HIS	2.7
1	A	158	ARG	2.7
1	B	171	LYS	2.4
1	A	162	GLU	2.4
1	A	175	GLU	2.4
1	B	184	PHE	2.4
1	B	35	PRO	2.3
1	B	246	LYS	2.3
1	A	337	ILE	2.3
1	A	164	GLY	2.2
1	B	71	VAL	2.2
1	B	153	ALA	2.2
1	A	160	MET	2.1
1	B	38	GLY	2.1
1	B	298	TYR	2.1
1	A	202	THR	2.1
1	B	178	LYS	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.