Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 02:33 PM EDT

PDB ID	:	2QYG
Title	:	Crystal Structure of a RuBisCO-like Protein rlp2 from Rhodopseudomonas palustris
Authors	:	Li, H.; Chan, S.; Tabita, F.R.; Eisenberg, D.
Deposited on	:	2007-08-14
Resolution	:	3.30 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

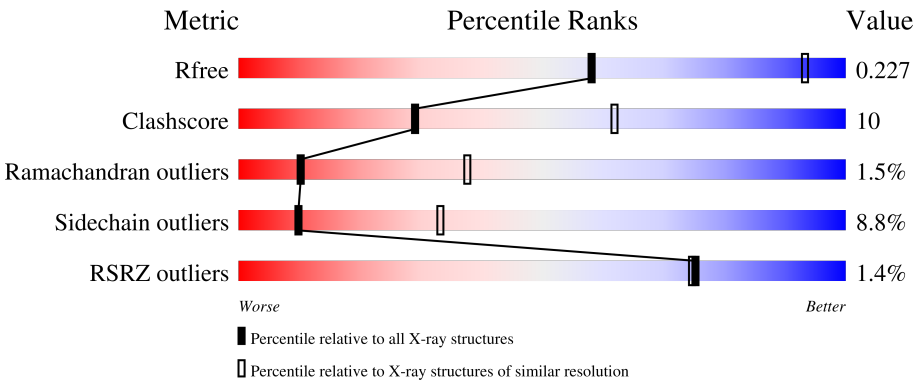
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	452	72% 21% • 5%
1	B	452	% 74% 18% • 5%
1	C	452	2% 74% 18% • 5%
1	D	452	2% 70% 22% • 5%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 13012 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 Ribulose bisphosphate carboxylase-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	429	3253	2076	575	582	20	0	0	0
1	B	429	3253	2076	575	582	20	0	0	0
1	C	429	3253	2076	575	582	20	0	0	0
1	D	429	3253	2076	575	582	20	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q6ND47
A	-18	GLY	-	expression tag	UNP Q6ND47
A	-17	SER	-	expression tag	UNP Q6ND47
A	-16	SER	-	expression tag	UNP Q6ND47
A	-15	HIS	-	expression tag	UNP Q6ND47
A	-14	HIS	-	expression tag	UNP Q6ND47
A	-13	HIS	-	expression tag	UNP Q6ND47
A	-12	HIS	-	expression tag	UNP Q6ND47
A	-11	HIS	-	expression tag	UNP Q6ND47
A	-10	HIS	-	expression tag	UNP Q6ND47
A	-9	SER	-	expression tag	UNP Q6ND47
A	-8	SER	-	expression tag	UNP Q6ND47
A	-7	GLY	-	expression tag	UNP Q6ND47
A	-6	LEU	-	expression tag	UNP Q6ND47
A	-5	VAL	-	expression tag	UNP Q6ND47
A	-4	PRO	-	expression tag	UNP Q6ND47
A	-3	ARG	-	expression tag	UNP Q6ND47
A	-2	GLY	-	expression tag	UNP Q6ND47
A	-1	SER	-	expression tag	UNP Q6ND47
A	0	HIS	-	expression tag	UNP Q6ND47
B	-19	MET	-	expression tag	UNP Q6ND47

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q6ND47
B	-17	SER	-	expression tag	UNP Q6ND47
B	-16	SER	-	expression tag	UNP Q6ND47
B	-15	HIS	-	expression tag	UNP Q6ND47
B	-14	HIS	-	expression tag	UNP Q6ND47
B	-13	HIS	-	expression tag	UNP Q6ND47
B	-12	HIS	-	expression tag	UNP Q6ND47
B	-11	HIS	-	expression tag	UNP Q6ND47
B	-10	HIS	-	expression tag	UNP Q6ND47
B	-9	SER	-	expression tag	UNP Q6ND47
B	-8	SER	-	expression tag	UNP Q6ND47
B	-7	GLY	-	expression tag	UNP Q6ND47
B	-6	LEU	-	expression tag	UNP Q6ND47
B	-5	VAL	-	expression tag	UNP Q6ND47
B	-4	PRO	-	expression tag	UNP Q6ND47
B	-3	ARG	-	expression tag	UNP Q6ND47
B	-2	GLY	-	expression tag	UNP Q6ND47
B	-1	SER	-	expression tag	UNP Q6ND47
B	0	HIS	-	expression tag	UNP Q6ND47
C	-19	MET	-	expression tag	UNP Q6ND47
C	-18	GLY	-	expression tag	UNP Q6ND47
C	-17	SER	-	expression tag	UNP Q6ND47
C	-16	SER	-	expression tag	UNP Q6ND47
C	-15	HIS	-	expression tag	UNP Q6ND47
C	-14	HIS	-	expression tag	UNP Q6ND47
C	-13	HIS	-	expression tag	UNP Q6ND47
C	-12	HIS	-	expression tag	UNP Q6ND47
C	-11	HIS	-	expression tag	UNP Q6ND47
C	-10	HIS	-	expression tag	UNP Q6ND47
C	-9	SER	-	expression tag	UNP Q6ND47
C	-8	SER	-	expression tag	UNP Q6ND47
C	-7	GLY	-	expression tag	UNP Q6ND47
C	-6	LEU	-	expression tag	UNP Q6ND47
C	-5	VAL	-	expression tag	UNP Q6ND47
C	-4	PRO	-	expression tag	UNP Q6ND47
C	-3	ARG	-	expression tag	UNP Q6ND47
C	-2	GLY	-	expression tag	UNP Q6ND47
C	-1	SER	-	expression tag	UNP Q6ND47
C	0	HIS	-	expression tag	UNP Q6ND47
D	-19	MET	-	expression tag	UNP Q6ND47
D	-18	GLY	-	expression tag	UNP Q6ND47
D	-17	SER	-	expression tag	UNP Q6ND47

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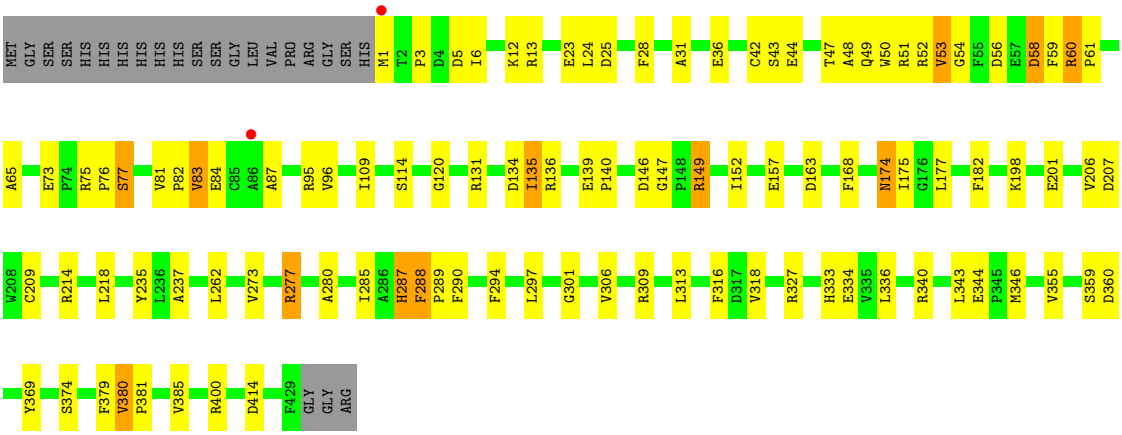
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q6ND47
D	-15	HIS	-	expression tag	UNP Q6ND47
D	-14	HIS	-	expression tag	UNP Q6ND47
D	-13	HIS	-	expression tag	UNP Q6ND47
D	-12	HIS	-	expression tag	UNP Q6ND47
D	-11	HIS	-	expression tag	UNP Q6ND47
D	-10	HIS	-	expression tag	UNP Q6ND47
D	-9	SER	-	expression tag	UNP Q6ND47
D	-8	SER	-	expression tag	UNP Q6ND47
D	-7	GLY	-	expression tag	UNP Q6ND47
D	-6	LEU	-	expression tag	UNP Q6ND47
D	-5	VAL	-	expression tag	UNP Q6ND47
D	-4	PRO	-	expression tag	UNP Q6ND47
D	-3	ARG	-	expression tag	UNP Q6ND47
D	-2	GLY	-	expression tag	UNP Q6ND47
D	-1	SER	-	expression tag	UNP Q6ND47
D	0	HIS	-	expression tag	UNP Q6ND47

3 Residue-property plots (i)

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

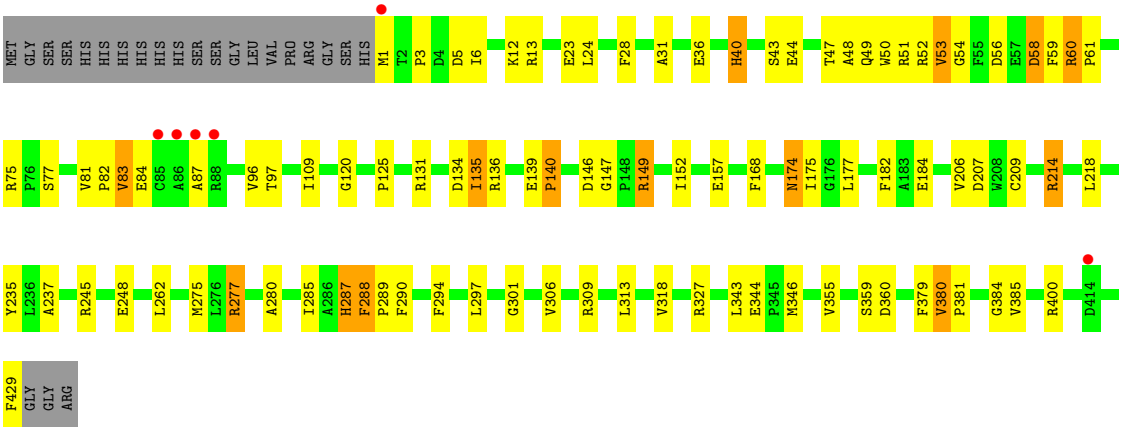
• Molecule 1: Ribulose bisphosphate carboxylase-like protein 2

Chain A: 72% 21% • 5%



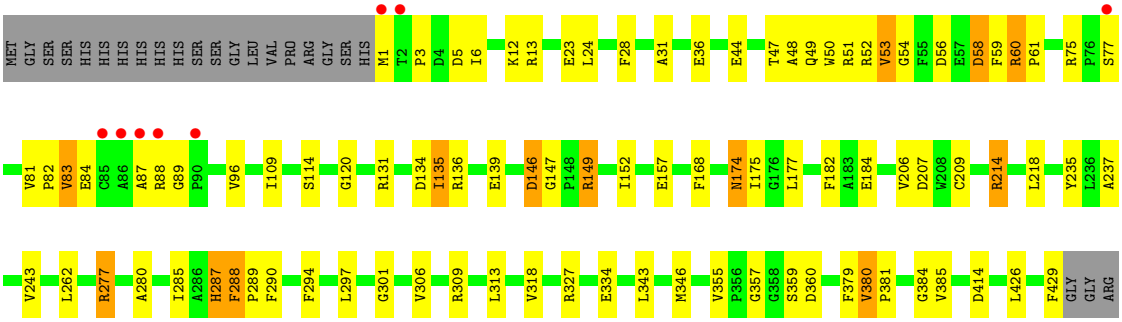
• Molecule 1: Ribulose bisphosphate carboxylase-like protein 2

Chain B: % 74% 18% • 5%



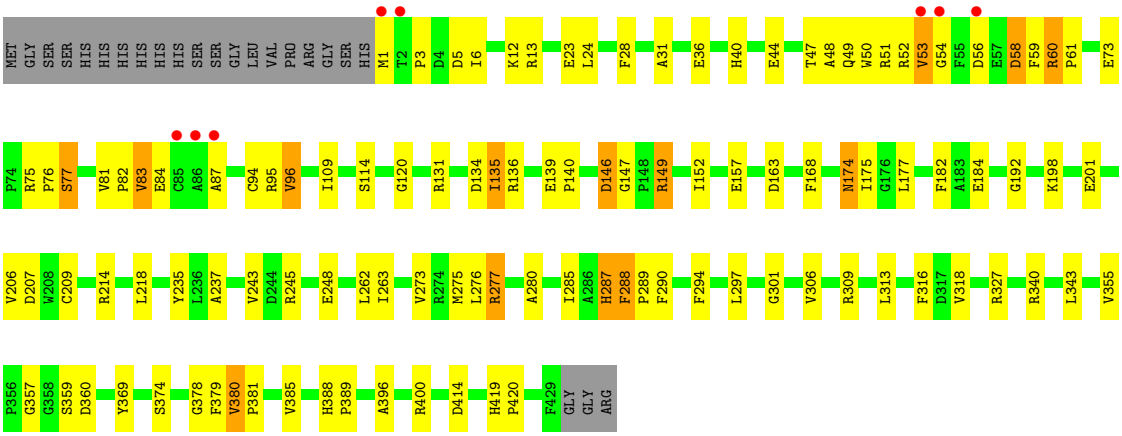
• Molecule 1: Ribulose bisphosphate carboxylase-like protein 2

Chain C: 2% 74% 18% • 5%



- Molecule 1: Ribulose bisphosphate carboxylase-like protein 2

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.66Å 119.53Å 203.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.38 – 3.30 77.38 – 3.26	Depositor EDS
% Data completeness (in resolution range)	99.7 (77.38-3.30) 98.0 (77.38-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.232 0.202 , 0.227	Depositor DCC
R_{free} test set	1336 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	43.5	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 23.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13012	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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 (i)

5.1 Standard geometry (i)

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	0.60	0/3344	0.68	0/4554
1	B	0.56	0/3344	0.67	0/4554
1	C	0.60	0/3344	0.67	0/4554
1	D	0.61	1/3344 (0.0%)	0.68	0/4554
All	All	0.59	1/13376 (0.0%)	0.68	0/18216

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	CYS	CB-SG	-5.04	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3253	0	3200	73	0
1	B	3253	0	3200	59	0
1	C	3253	0	3200	59	0
1	D	3253	0	3200	76	0
All	All	13012	0	12800	248	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 10.

All (248) 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:177:LEU:HD21	1:B:52:ARG:HD2	1.44	0.99
1:C:285:ILE:HG13	1:C:318:VAL:HB	1.55	0.89
1:C:58:ASP:OD1	1:C:60:ARG:HB2	1.73	0.88
1:A:285:ILE:HG13	1:A:318:VAL:HB	1.56	0.86
1:D:58:ASP:OD1	1:D:60:ARG:HB2	1.77	0.85
1:B:285:ILE:HG13	1:B:318:VAL:HB	1.60	0.83
1:B:58:ASP:OD1	1:B:60:ARG:HB2	1.78	0.83
1:C:52:ARG:HD2	1:D:177:LEU:HD21	1.59	0.83
1:A:58:ASP:OD1	1:A:60:ARG:HB2	1.78	0.82
1:D:149:ARG:HH11	1:D:149:ARG:HB2	1.48	0.79
1:A:77:SER:HB3	1:D:369:TYR:OH	1.82	0.79
1:D:285:ILE:HG13	1:D:318:VAL:HB	1.65	0.79
1:D:53:VAL:HG13	1:D:54:GLY:H	1.51	0.75
1:A:149:ARG:HH11	1:A:149:ARG:HB2	1.50	0.74
1:C:28:PHE:HE1	1:C:96:VAL:HG21	1.51	0.74
1:C:53:VAL:HG13	1:C:54:GLY:H	1.51	0.74
1:A:147:GLY:O	1:A:277:ARG:NH1	2.21	0.74
1:B:149:ARG:HH11	1:B:149:ARG:HB2	1.52	0.73
1:C:147:GLY:O	1:C:277:ARG:NH1	2.22	0.73
1:C:28:PHE:HE1	1:C:96:VAL:CG2	2.02	0.73
1:B:147:GLY:O	1:B:277:ARG:NH1	2.22	0.72
1:A:374:SER:CB	1:D:73:GLU:HG3	2.19	0.72
1:A:53:VAL:HG13	1:A:54:GLY:H	1.55	0.72
1:D:28:PHE:HE1	1:D:96:VAL:HG21	1.55	0.71
1:C:149:ARG:HH11	1:C:149:ARG:HB2	1.57	0.70
1:B:28:PHE:HE1	1:B:96:VAL:HG21	1.56	0.69
1:B:28:PHE:HE1	1:B:96:VAL:CG2	2.04	0.69
1:A:28:PHE:HE1	1:A:96:VAL:HG21	1.58	0.68
1:D:147:GLY:O	1:D:277:ARG:NH1	2.25	0.68
1:A:381:PRO:HB2	1:A:385:VAL:HG23	1.74	0.68
1:D:28:PHE:HE1	1:D:96:VAL:CG2	2.08	0.65
1:B:53:VAL:HG13	1:B:54:GLY:H	1.59	0.65
1:C:381:PRO:HB2	1:C:385:VAL:HG23	1.79	0.65
1:B:47:THR:O	1:B:48:ALA:HB3	1.97	0.64
1:C:177:LEU:HD21	1:D:52:ARG:HD2	1.80	0.63
1:B:381:PRO:HB2	1:B:385:VAL:HG23	1.80	0.63
1:A:52:ARG:HD2	1:B:177:LEU:HD21	1.78	0.63
1:C:262:LEU:HD11	1:C:287:HIS:HB2	1.81	0.62
1:D:24:LEU:HD23	1:D:135:ILE:HG23	1.81	0.62
1:A:135:ILE:HD11	1:A:306:VAL:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:TYR:OH	1:D:77:SER:HB3	1.99	0.61
1:D:262:LEU:HD11	1:D:287:HIS:HB2	1.82	0.61
1:A:6:ILE:HD11	1:A:36:GLU:HG2	1.83	0.60
1:A:28:PHE:HE1	1:A:96:VAL:CG2	2.15	0.59
1:A:374:SER:OG	1:D:73:GLU:HG3	2.02	0.59
1:B:131:ARG:HA	1:B:301:GLY:O	2.02	0.59
1:A:1:MET:HE1	1:A:6:ILE:HA	1.85	0.59
1:D:381:PRO:HB2	1:D:385:VAL:HG23	1.84	0.59
1:A:163:ASP:O	1:D:76:PRO:HG3	2.03	0.58
1:B:209:CYS:SG	1:B:214:ARG:HG3	2.44	0.58
1:B:309:ARG:NH2	1:B:344:GLU:OE1	2.35	0.58
1:B:262:LEU:HD11	1:B:287:HIS:HB2	1.85	0.58
1:A:47:THR:O	1:A:48:ALA:HB3	2.03	0.57
1:D:174:ASN:HD22	1:D:175:ILE:HG12	1.69	0.57
1:C:6:ILE:HD11	1:C:36:GLU:HG2	1.86	0.57
1:C:209:CYS:SG	1:C:214:ARG:HG3	2.44	0.57
1:A:73:GLU:HG3	1:D:374:SER:CB	2.35	0.56
1:D:168:PHE:O	1:D:381:PRO:HD2	2.05	0.56
1:D:83:VAL:HG12	1:D:84:GLU:H	1.71	0.56
1:C:168:PHE:O	1:C:381:PRO:HD2	2.05	0.56
1:A:134:ASP:OD2	1:A:309:ARG:NH1	2.39	0.56
1:D:135:ILE:HD11	1:D:306:VAL:HG13	1.88	0.56
1:C:149:ARG:NH2	1:C:280:ALA:O	2.37	0.55
1:B:168:PHE:O	1:B:381:PRO:HD2	2.06	0.55
1:C:174:ASN:HD22	1:C:175:ILE:HG12	1.71	0.55
1:D:6:ILE:HD11	1:D:36:GLU:HG2	1.87	0.55
1:A:235:TYR:CE2	1:A:237:ALA:HB2	2.42	0.55
1:A:294:PHE:HB3	1:B:294:PHE:HB3	1.89	0.55
1:D:53:VAL:HG13	1:D:54:GLY:N	2.21	0.55
1:D:1:MET:HE1	1:D:6:ILE:HA	1.89	0.54
1:B:24:LEU:HD23	1:B:135:ILE:HG23	1.89	0.54
1:A:168:PHE:O	1:A:381:PRO:HD2	2.06	0.54
1:B:174:ASN:HD22	1:B:175:ILE:HG12	1.72	0.54
1:B:134:ASP:OD2	1:B:309:ARG:NH1	2.42	0.53
1:A:262:LEU:HD11	1:A:287:HIS:HB2	1.90	0.53
1:C:355:VAL:HG12	1:C:380:VAL:CG2	2.39	0.53
1:C:23:GLU:HB3	1:C:136:ARG:NH1	2.24	0.53
1:D:47:THR:O	1:D:48:ALA:HB3	2.08	0.53
1:B:1:MET:HE3	1:B:5:ASP:HB2	1.91	0.53
1:C:24:LEU:HD23	1:C:135:ILE:HG23	1.91	0.53
1:C:83:VAL:HG12	1:C:84:GLU:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:GLU:HB3	1:D:120:GLY:HA2	1.91	0.53
1:B:44:GLU:HB3	1:B:120:GLY:HA2	1.90	0.53
1:D:5:ASP:HB3	1:D:50:TRP:HZ2	1.74	0.53
1:A:44:GLU:HB3	1:A:120:GLY:HA2	1.91	0.52
1:C:47:THR:O	1:C:48:ALA:HB3	2.08	0.52
1:C:134:ASP:OD2	1:C:309:ARG:NH1	2.42	0.52
1:C:294:PHE:HB3	1:D:294:PHE:HB3	1.92	0.52
1:D:134:ASP:OD2	1:D:309:ARG:NH1	2.41	0.52
1:A:23:GLU:HB3	1:A:136:ARG:NH1	2.25	0.52
1:D:139:GLU:HB2	1:D:140:PRO:CD	2.39	0.52
1:A:83:VAL:HG12	1:A:84:GLU:H	1.75	0.52
1:A:309:ARG:HD3	1:A:346:MET:HE1	1.92	0.52
1:D:131:ARG:HA	1:D:301:GLY:O	2.10	0.52
1:A:174:ASN:HD22	1:A:175:ILE:HG12	1.75	0.51
1:D:152:ILE:HD11	1:D:343:LEU:HD23	1.92	0.51
1:A:53:VAL:HG13	1:A:54:GLY:N	2.25	0.51
1:B:149:ARG:NH2	1:B:280:ALA:O	2.41	0.51
1:C:28:PHE:CE1	1:C:96:VAL:CG2	2.91	0.51
1:C:53:VAL:HG13	1:C:54:GLY:N	2.22	0.51
1:A:24:LEU:HD23	1:A:135:ILE:HG23	1.93	0.51
1:A:139:GLU:HB2	1:A:140:PRO:CD	2.41	0.51
1:C:184:GLU:OE1	1:C:184:GLU:HA	2.11	0.51
1:A:309:ARG:HD3	1:A:346:MET:CE	2.41	0.51
1:D:5:ASP:HB3	1:D:50:TRP:CZ2	2.46	0.50
1:A:209:CYS:SG	1:A:214:ARG:HG3	2.52	0.50
1:C:5:ASP:HB3	1:C:50:TRP:CZ2	2.47	0.50
1:C:288:PHE:N	1:C:289:PRO:HD2	2.27	0.50
1:A:288:PHE:N	1:A:289:PRO:HD2	2.27	0.50
1:C:44:GLU:HB3	1:C:120:GLY:HA2	1.94	0.50
1:D:288:PHE:N	1:D:289:PRO:HD2	2.27	0.49
1:D:355:VAL:HG12	1:D:380:VAL:CG2	2.42	0.49
1:A:152:ILE:HD11	1:A:343:LEU:HD23	1.93	0.49
1:B:184:GLU:OE1	1:B:184:GLU:HA	2.11	0.49
1:B:139:GLU:HB2	1:B:140:PRO:CD	2.41	0.49
1:C:309:ARG:HD3	1:C:346:MET:CE	2.42	0.49
1:B:23:GLU:HB3	1:B:136:ARG:NH1	2.27	0.49
1:D:31:ALA:HB3	1:D:87:ALA:HB3	1.95	0.48
1:A:355:VAL:HG12	1:A:380:VAL:CG2	2.42	0.48
1:B:235:TYR:CE2	1:B:237:ALA:HB2	2.47	0.48
1:A:23:GLU:HB3	1:A:136:ARG:HH11	1.79	0.48
1:C:5:ASP:HB3	1:C:50:TRP:HZ2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:LEU:CD2	1:D:135:ILE:HG23	2.43	0.48
1:B:5:ASP:HB3	1:B:50:TRP:CZ2	2.49	0.48
1:A:374:SER:HB3	1:D:73:GLU:HG3	1.92	0.48
1:B:47:THR:O	1:B:48:ALA:CB	2.62	0.48
1:A:5:ASP:HB3	1:A:50:TRP:HZ2	1.78	0.47
1:A:340:ARG:HD3	1:D:95:ARG:CZ	2.44	0.47
1:B:53:VAL:HG13	1:B:54:GLY:N	2.28	0.47
1:B:360:ASP:HB3	1:B:379:PHE:CZ	2.49	0.47
1:C:146:ASP:HB2	1:C:277:ARG:NH1	2.29	0.47
1:B:355:VAL:HG12	1:B:380:VAL:CG2	2.44	0.47
1:A:5:ASP:HB3	1:A:50:TRP:CZ2	2.49	0.47
1:D:149:ARG:HH11	1:D:149:ARG:CB	2.24	0.47
1:C:243:VAL:HG11	1:D:243:VAL:HG11	1.97	0.47
1:C:288:PHE:N	1:C:289:PRO:CD	2.78	0.47
1:B:81:VAL:HG12	1:B:82:PRO:HD2	1.97	0.46
1:C:152:ILE:HD11	1:C:343:LEU:HD23	1.96	0.46
1:D:245:ARG:HD2	1:D:248:GLU:OE1	2.16	0.46
1:D:273:VAL:HG21	1:D:316:PHE:CZ	2.50	0.46
1:A:31:ALA:HB3	1:A:87:ALA:HB3	1.96	0.46
1:A:76:PRO:HG3	1:D:163:ASP:O	2.15	0.46
1:B:23:GLU:HB3	1:B:136:ARG:HH11	1.81	0.46
1:B:288:PHE:N	1:B:289:PRO:HD2	2.30	0.46
1:A:288:PHE:N	1:A:289:PRO:CD	2.79	0.46
1:A:198:LYS:HZ1	1:A:287:HIS:CD2	2.32	0.46
1:C:360:ASP:HB3	1:C:379:PHE:CZ	2.50	0.46
1:D:209:CYS:SG	1:D:214:ARG:HG3	2.56	0.46
1:D:47:THR:C	1:D:49:GLN:H	2.19	0.46
1:D:146:ASP:HB2	1:D:277:ARG:NH1	2.31	0.46
1:D:288:PHE:N	1:D:289:PRO:CD	2.79	0.46
1:B:5:ASP:HB3	1:B:50:TRP:HZ2	1.81	0.46
1:B:24:LEU:CD2	1:B:135:ILE:HG23	2.47	0.45
1:B:6:ILE:HD11	1:B:36:GLU:HG2	1.98	0.45
1:D:23:GLU:HB3	1:D:136:ARG:NH1	2.31	0.45
1:C:1:MET:HE3	1:C:5:ASP:HB2	1.98	0.45
1:C:31:ALA:HB3	1:C:87:ALA:HB3	1.99	0.45
1:C:131:ARG:HA	1:C:301:GLY:O	2.16	0.45
1:B:31:ALA:HB3	1:B:87:ALA:HB3	1.99	0.45
1:D:184:GLU:HA	1:D:184:GLU:OE1	2.17	0.45
1:C:23:GLU:CB	1:C:136:ARG:HH11	2.30	0.45
1:C:174:ASN:ND2	1:C:175:ILE:H	2.15	0.45
1:B:81:VAL:CG1	1:B:82:PRO:HD2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:GLY:HA2	1:C:429:PHE:CE1	2.52	0.44
1:B:52:ARG:O	1:B:53:VAL:C	2.56	0.44
1:C:52:ARG:O	1:C:53:VAL:C	2.56	0.44
1:B:152:ILE:HD11	1:B:343:LEU:HD23	1.99	0.44
1:B:174:ASN:ND2	1:B:175:ILE:H	2.16	0.44
1:B:1:MET:HE1	1:B:6:ILE:HA	2.00	0.44
1:C:24:LEU:CD2	1:C:135:ILE:HG23	2.47	0.44
1:D:23:GLU:HB3	1:D:136:ARG:HH11	1.82	0.44
1:D:360:ASP:HB3	1:D:379:PHE:CZ	2.53	0.44
1:C:23:GLU:HB3	1:C:136:ARG:HH11	1.82	0.44
1:C:355:VAL:CG1	1:C:380:VAL:HG22	2.48	0.44
1:D:400:ARG:HA	1:D:400:ARG:HD2	1.73	0.44
1:B:309:ARG:HD3	1:B:346:MET:CE	2.48	0.44
1:D:1:MET:HE3	1:D:5:ASP:HB2	2.00	0.44
1:A:1:MET:O	1:A:1:MET:HG3	2.18	0.43
1:C:235:TYR:CE2	1:C:237:ALA:HB2	2.53	0.43
1:A:149:ARG:NH2	1:A:280:ALA:O	2.45	0.43
1:D:28:PHE:CE1	1:D:96:VAL:CG2	2.96	0.43
1:C:1:MET:HE1	1:C:6:ILE:HA	1.99	0.43
1:D:1:MET:HB3	1:D:40:HIS:NE2	2.32	0.43
1:A:23:GLU:CB	1:A:136:ARG:HH11	2.31	0.43
1:A:309:ARG:NH2	1:A:344:GLU:OE1	2.48	0.43
1:B:28:PHE:CE1	1:B:96:VAL:CG2	2.94	0.43
1:B:83:VAL:HG12	1:B:84:GLU:H	1.82	0.43
1:A:25:ASP:OD2	1:A:136:ARG:NH2	2.52	0.43
1:A:52:ARG:O	1:A:53:VAL:C	2.57	0.43
1:C:384:GLY:HA2	1:C:429:PHE:CZ	2.54	0.43
1:A:149:ARG:HH11	1:A:149:ARG:CB	2.23	0.43
1:C:47:THR:C	1:C:49:GLN:H	2.22	0.43
1:C:135:ILE:HD11	1:C:306:VAL:HG13	2.00	0.43
1:D:52:ARG:O	1:D:53:VAL:C	2.57	0.43
1:A:273:VAL:HG21	1:A:316:PHE:CZ	2.54	0.43
1:C:88:ARG:HB3	1:C:89:GLY:H	1.72	0.43
1:A:42:CYS:HB3	1:A:65:ALA:O	2.19	0.42
1:A:174:ASN:ND2	1:A:175:ILE:H	2.17	0.42
1:D:201:GLU:HG3	1:D:287:HIS:CD2	2.54	0.42
1:B:245:ARG:HD2	1:B:248:GLU:OE1	2.20	0.42
1:D:263:ILE:HD11	1:D:276:LEU:HD23	2.00	0.42
1:A:47:THR:C	1:A:49:GLN:H	2.23	0.42
1:A:355:VAL:CG1	1:A:380:VAL:HG22	2.49	0.42
1:B:40:HIS:CD2	1:B:125:PRO:HG2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:PHE:N	1:B:289:PRO:CD	2.82	0.42
1:A:1:MET:HE3	1:A:5:ASP:HB2	2.01	0.42
1:B:135:ILE:HD11	1:B:306:VAL:HG13	2.01	0.42
1:D:60:ARG:N	1:D:61:PRO:CD	2.83	0.42
1:D:149:ARG:NH2	1:D:280:ALA:O	2.49	0.42
1:D:355:VAL:HG13	1:D:378:GLY:HA3	2.02	0.42
1:A:201:GLU:CD	1:A:201:GLU:H	2.22	0.41
1:A:340:ARG:CZ	1:D:95:ARG:HD2	2.50	0.41
1:A:400:ARG:HA	1:A:400:ARG:HD2	1.80	0.41
1:B:47:THR:C	1:B:49:GLN:H	2.24	0.41
1:B:60:ARG:N	1:B:61:PRO:CD	2.83	0.41
1:A:360:ASP:HB3	1:A:379:PHE:CZ	2.55	0.41
1:D:192:GLY:HA3	1:D:396:ALA:HB3	2.01	0.41
1:C:177:LEU:HD23	1:C:177:LEU:HA	1.94	0.41
1:D:235:TYR:CE2	1:D:237:ALA:HB2	2.55	0.41
1:A:95:ARG:CZ	1:D:340:ARG:HD3	2.51	0.41
1:D:81:VAL:CG1	1:D:82:PRO:HD2	2.50	0.41
1:D:174:ASN:ND2	1:D:175:ILE:H	2.19	0.41
1:B:24:LEU:O	1:B:97:THR:HA	2.19	0.41
1:A:131:ARG:HA	1:A:301:GLY:O	2.20	0.41
1:B:152:ILE:HD11	1:B:343:LEU:CD2	2.51	0.41
1:C:81:VAL:HG12	1:C:82:PRO:HD2	2.03	0.41
1:D:419:HIS:HA	1:D:420:PRO:HD3	1.91	0.41
1:A:60:ARG:N	1:A:61:PRO:CD	2.84	0.41
1:B:384:GLY:HA2	1:B:429:PHE:CZ	2.56	0.41
1:D:198:LYS:HZ1	1:D:287:HIS:CD2	2.37	0.41
1:D:201:GLU:H	1:D:201:GLU:CD	2.24	0.41
1:C:60:ARG:N	1:C:61:PRO:CD	2.83	0.41
1:D:1:MET:HG3	1:D:1:MET:O	2.21	0.41
1:A:81:VAL:CG1	1:A:82:PRO:HD2	2.51	0.40
1:A:43:SER:OG	1:A:48:ALA:HA	2.21	0.40
1:A:333:HIS:HA	1:A:336:LEU:HD12	2.04	0.40
1:C:81:VAL:CG1	1:C:82:PRO:HD2	2.51	0.40
1:C:287:HIS:HD1	1:C:288:PHE:H	1.68	0.40
1:C:309:ARG:HD3	1:C:346:MET:HE2	2.03	0.40
1:D:287:HIS:HD1	1:D:288:PHE:H	1.69	0.40
1:A:81:VAL:HG12	1:A:82:PRO:HD2	2.04	0.40
1:A:287:HIS:HB3	1:A:289:PRO:HD2	2.04	0.40
1:B:400:ARG:HA	1:B:400:ARG:HD2	1.82	0.40
1:C:426:LEU:HD23	1:C:426:LEU:HA	1.92	0.40
1:D:388:HIS:HA	1:D:389:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ARG:HD2	1:D:340:ARG:NH2	2.36	0.40
1:B:23:GLU:CB	1:B:136:ARG:HH11	2.35	0.40
1:B:43:SER:OG	1:B:48:ALA:HA	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	427/452 (94%)	393 (92%)	28 (7%)	6 (1%)	11	38
1	B	427/452 (94%)	391 (92%)	30 (7%)	6 (1%)	11	38
1	C	427/452 (94%)	391 (92%)	29 (7%)	7 (2%)	9	36
1	D	427/452 (94%)	395 (92%)	25 (6%)	7 (2%)	9	36
All	All	1708/1808 (94%)	1570 (92%)	112 (7%)	26 (2%)	10	38

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
1	B	53	VAL
1	C	53	VAL
1	D	53	VAL
1	A	58	ASP
1	A	290	PHE
1	B	58	ASP
1	B	290	PHE
1	C	58	ASP
1	D	58	ASP
1	D	290	PHE
1	A	3	PRO

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Mol	Chain	Res	Type
1	B	3	PRO
1	C	3	PRO
1	C	290	PHE
1	D	3	PRO
1	B	83	VAL
1	C	357	GLY
1	D	357	GLY
1	A	83	VAL
1	C	83	VAL
1	D	83	VAL
1	A	288	PHE
1	C	288	PHE
1	D	288	PHE
1	B	288	PHE

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	331/349 (95%)	303 (92%)	28 (8%)	10 35
1	B	331/349 (95%)	302 (91%)	29 (9%)	10 33
1	C	331/349 (95%)	301 (91%)	30 (9%)	9 31
1	D	331/349 (95%)	302 (91%)	29 (9%)	10 33
All	All	1324/1396 (95%)	1208 (91%)	116 (9%)	10 33

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LYS
1	A	13	ARG
1	A	51	ARG
1	A	56	ASP
1	A	59	PHE
1	A	60	ARG
1	A	75	ARG

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Mol	Chain	Res	Type
1	A	77	SER
1	A	109	ILE
1	A	114	SER
1	A	135	ILE
1	A	146	ASP
1	A	149	ARG
1	A	157	GLU
1	A	174	ASN
1	A	182	PHE
1	A	206	VAL
1	A	207	ASP
1	A	218	LEU
1	A	277	ARG
1	A	287	HIS
1	A	297	LEU
1	A	313	LEU
1	A	327	ARG
1	A	334	GLU
1	A	359	SER
1	A	380	VAL
1	A	414	ASP
1	B	12	LYS
1	B	13	ARG
1	B	40	HIS
1	B	51	ARG
1	B	56	ASP
1	B	59	PHE
1	B	60	ARG
1	B	75	ARG
1	B	77	SER
1	B	109	ILE
1	B	135	ILE
1	B	140	PRO
1	B	146	ASP
1	B	149	ARG
1	B	157	GLU
1	B	174	ASN
1	B	182	PHE
1	B	206	VAL
1	B	207	ASP
1	B	214	ARG
1	B	218	LEU

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Mol	Chain	Res	Type
1	B	275	MET
1	B	277	ARG
1	B	287	HIS
1	B	297	LEU
1	B	313	LEU
1	B	327	ARG
1	B	359	SER
1	B	380	VAL
1	C	12	LYS
1	C	13	ARG
1	C	51	ARG
1	C	56	ASP
1	C	59	PHE
1	C	60	ARG
1	C	75	ARG
1	C	77	SER
1	C	109	ILE
1	C	114	SER
1	C	135	ILE
1	C	139	GLU
1	C	146	ASP
1	C	149	ARG
1	C	157	GLU
1	C	174	ASN
1	C	182	PHE
1	C	206	VAL
1	C	207	ASP
1	C	214	ARG
1	C	218	LEU
1	C	277	ARG
1	C	287	HIS
1	C	297	LEU
1	C	313	LEU
1	C	327	ARG
1	C	334	GLU
1	C	359	SER
1	C	380	VAL
1	C	414	ASP
1	D	12	LYS
1	D	13	ARG
1	D	51	ARG
1	D	56	ASP

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Mol	Chain	Res	Type
1	D	59	PHE
1	D	60	ARG
1	D	75	ARG
1	D	77	SER
1	D	96	VAL
1	D	109	ILE
1	D	114	SER
1	D	135	ILE
1	D	146	ASP
1	D	149	ARG
1	D	157	GLU
1	D	174	ASN
1	D	182	PHE
1	D	206	VAL
1	D	207	ASP
1	D	218	LEU
1	D	275	MET
1	D	277	ARG
1	D	287	HIS
1	D	297	LEU
1	D	313	LEU
1	D	327	ARG
1	D	359	SER
1	D	380	VAL
1	D	414	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	ASN
1	A	174	ASN
1	A	311	GLN
1	A	367	ASN
1	B	45	GLN
1	B	104	ASN
1	B	174	ASN
1	B	367	ASN
1	C	104	ASN
1	C	174	ASN
1	C	311	GLN
1	C	367	ASN
1	D	104	ASN

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Mol	Chain	Res	Type
1	D	174	ASN
1	D	367	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	429/452 (94%)	-0.15	2 (0%)	91	91	22, 33, 50, 68	0
1	B	429/452 (94%)	0.10	6 (1%)	75	75	22, 33, 50, 68	0
1	C	429/452 (94%)	0.01	8 (1%)	66	65	21, 33, 50, 68	0
1	D	429/452 (94%)	-0.06	8 (1%)	66	65	22, 33, 50, 68	0
All	All	1716/1808 (94%)	-0.03	24 (1%)	75	75	21, 33, 50, 68	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	87	ALA	5.6
1	D	1	MET	4.9
1	B	86	ALA	4.7
1	C	86	ALA	4.5
1	C	1	MET	4.0
1	B	87	ALA	3.6
1	D	86	ALA	3.5
1	C	85	CYS	3.3
1	B	85	CYS	3.2
1	D	54	GLY	3.0
1	B	1	MET	3.0
1	C	88	ARG	2.9
1	D	85	CYS	2.7
1	A	86	ALA	2.6
1	D	53	VAL	2.5
1	D	56	ASP	2.5
1	B	88	ARG	2.3
1	B	414	ASP	2.2
1	A	1	MET	2.2
1	D	2	THR	2.1
1	D	87	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	2	THR	2.1
1	C	77	SER	2.1
1	C	90	PRO	2.0

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 monosaccharides 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.