Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:11 pm BST

PDB ID	:	1TQJ
Title	:	Crystal structure of D-ribulose 5-phosphate 3-epimerase from Synechocystis to 1.6 angstrom resolution
Authors	:	Wise, E.L.; Akana, J.; Gerlt, J.A.; Rayment, I.
Deposited on	:	2004-06-17
Resolution	:	1.60 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:

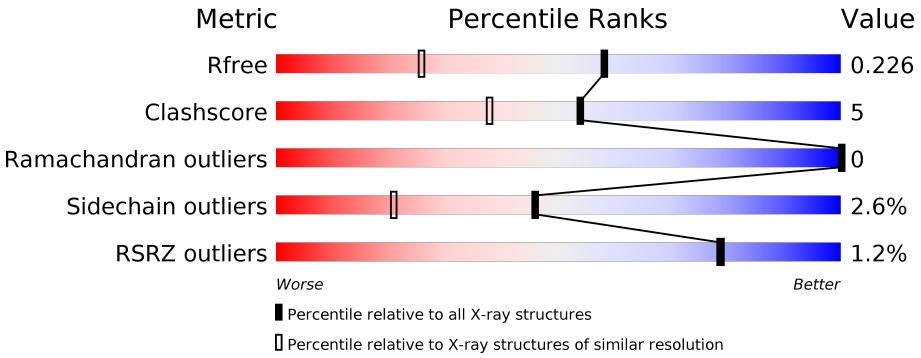
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	230	83% 10% 6%
1	B	230	87% 5% 7%
1	C	230	85% 9% • 5%
1	D	230	82% 10% • 6%
1	E	230	83% 8% • 7%
1	F	230	82% 11% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11308 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-phosphate 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	1	0
			1641	1051	281	302	7			
1	B	214	Total	C	N	O	S	0	2	0
			1639	1043	285	304	7			
1	C	218	Total	C	N	O	S	0	2	0
			1655	1055	282	311	7			
1	D	216	Total	C	N	O	S	0	0	0
			1643	1050	283	303	7			
1	E	215	Total	C	N	O	S	0	2	0
			1647	1051	286	303	7			
1	F	217	Total	C	N	O	S	0	1	0
			1644	1051	282	304	7			

- Molecule 2 is water.

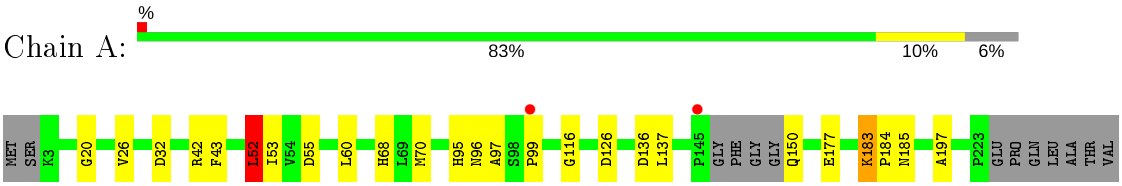
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	280	Total	O	0	0
			280	280		
2	B	264	Total	O	0	0
			264	264		
2	C	252	Total	O	0	0
			252	252		
2	D	229	Total	O	0	0
			229	229		
2	E	219	Total	O	0	0
			219	219		
2	F	195	Total	O	0	0
			195	195		

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.

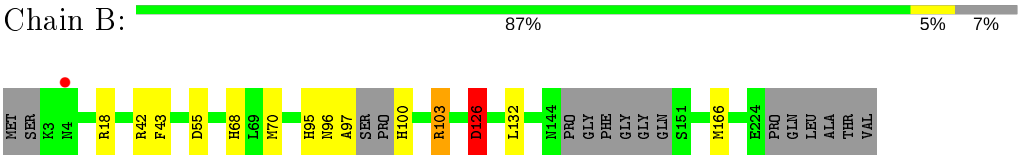
- Molecule 1: Ribulose-phosphate 3-epimerase

Chain A:



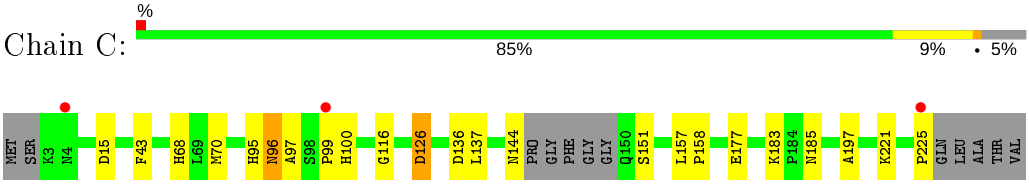
- Molecule 1: Ribulose-phosphate 3-epimerase

Chain B:



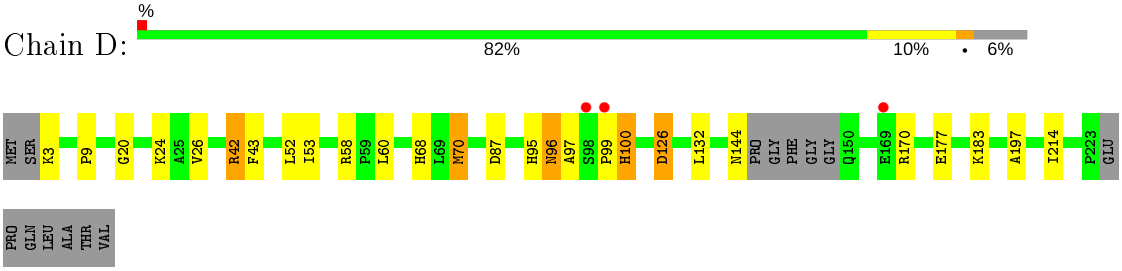
- Molecule 1: Ribulose-phosphate 3-epimerase

Chain C:



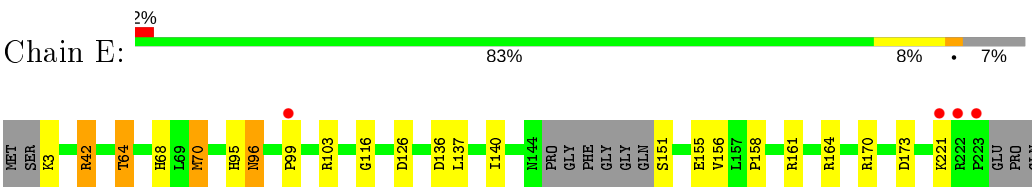
- Molecule 1: Ribulose-phosphate 3-epimerase

Chain D:



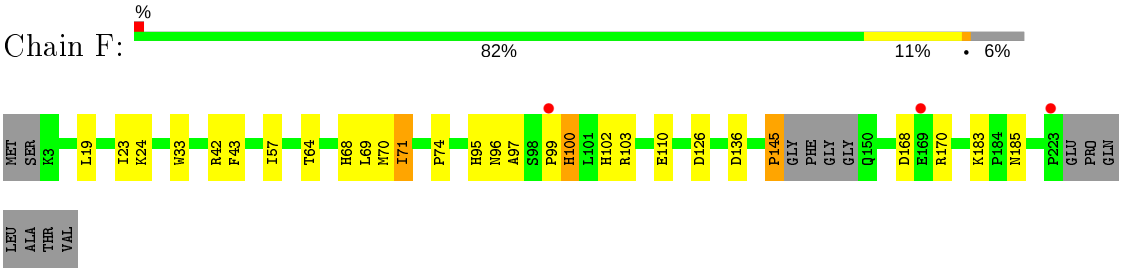
- Molecule 1: Ribulose-phosphate 3-epimerase

Chain E:



• Molecule 1: Ribulose-phosphate 3-epimerase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.56Å 87.78Å 97.82Å 90.00° 114.58° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 28.09 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.9 (50.00-1.60) 94.0 (28.09-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.170 , 0.220 0.183 , 0.226	Depositor DCC
R_{free} test set	7861 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.9	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11308	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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	0.77	0/1683	0.89	4/2299 (0.2%)
1	B	0.80	1/1683 (0.1%)	1.03	8/2292 (0.3%)
1	C	0.71	0/1699	0.90	7/2320 (0.3%)
1	D	0.68	0/1677	0.89	7/2288 (0.3%)
1	E	0.70	0/1695	0.89	3/2311 (0.1%)
1	F	0.68	0/1685	0.84	4/2299 (0.2%)
All	All	0.73	1/10122 (0.0%)	0.91	33/13809 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	MET	SD-CE	-6.09	1.43	1.77

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	126[A]	ASP	CB-CG-OD2	16.16	132.84	118.30
1	B	126[B]	ASP	CB-CG-OD2	16.16	132.84	118.30
1	C	126[A]	ASP	CB-CG-OD2	10.03	127.33	118.30
1	C	126[B]	ASP	CB-CG-OD2	10.03	127.33	118.30
1	B	42	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	B	42	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	F	136	ASP	CB-CG-OD2	7.84	125.36	118.30
1	A	126	ASP	CB-CG-OD2	7.73	125.25	118.30
1	D	170	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	B	126[A]	ASP	CB-CG-OD1	-7.14	111.88	118.30
1	B	126[B]	ASP	CB-CG-OD1	-7.14	111.88	118.30
1	E	126	ASP	CB-CG-OD2	6.77	124.39	118.30
1	D	126	ASP	CB-CG-OD2	6.63	124.27	118.30
1	D	42	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	F	126	ASP	CB-CG-OD2	6.21	123.88	118.30
1	D	87	ASP	CB-CG-OD2	6.17	123.86	118.30
1	D	58	ARG	NE-CZ-NH1	6.05	123.33	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	126[A]	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	C	126[B]	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	D	42	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	F	145	PRO	N-CA-CB	5.70	110.14	103.30
1	E	42	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	F	168	ASP	CB-CG-OD2	5.58	123.32	118.30
1	C	136	ASP	CB-CG-OD2	5.46	123.22	118.30
1	C	15	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	225	PRO	N-CA-CB	5.41	109.79	103.30
1	B	18	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	A	52	LEU	CA-CB-CG	5.26	127.39	115.30
1	D	58	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	55	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	32	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	136	ASP	CB-CG-OD2	5.04	122.83	118.30
1	E	136	ASP	CB-CG-OD2	5.02	122.82	118.30

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	1641	0	1643	27	0
1	B	1639	0	1637	12	0
1	C	1655	0	1641	18	0
1	D	1643	0	1652	22	0
1	E	1647	0	1656	25	0
1	F	1644	0	1643	26	0
2	A	280	0	0	5	0
2	B	264	0	0	3	0
2	C	252	0	0	2	0
2	D	229	0	0	3	4
2	E	219	0	0	6	4
2	F	195	0	0	2	0
All	All	11308	0	9872	105	4

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 5.

All (105) 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:C:96:ASN:H	1:C:96:ASN:HD22	1.24	0.84
1:B:96:ASN:HD21	1:D:99:PRO:HB3	1.41	0.84
1:A:99:PRO:HB3	1:E:96:ASN:HD21	1.43	0.82
1:F:110:GLU:OE1	2:F:423:HOH:O	1.98	0.82
1:F:69:LEU:HB3	1:F:71:ILE:HD12	1.67	0.75
1:D:99:PRO:O	2:D:459:HOH:O	2.07	0.73
1:F:69:LEU:HB3	1:F:71:ILE:CD1	2.20	0.72
1:F:43:PHE:CE1	1:F:97:ALA:HB2	2.24	0.72
1:A:99:PRO:CB	1:E:96:ASN:HD21	2.05	0.69
1:B:95:HIS:H	1:D:95:HIS:HD2	1.41	0.69
1:E:161[A]:ARG:NH2	2:E:448:HOH:O	2.25	0.68
1:B:96:ASN:ND2	1:D:99:PRO:HB3	2.09	0.67
1:A:68:HIS:CE1	1:A:70:MET:HE2	2.29	0.67
1:C:144:ASN:ND2	2:C:482:HOH:O	1.78	0.66
1:E:68:HIS:CE1	1:E:70:MET:HE2	2.30	0.66
1:A:95:HIS:HD2	1:E:95:HIS:H	1.44	0.66
1:F:24:LYS:HE2	2:F:265:HOH:O	1.95	0.65
1:C:68:HIS:CE1	1:C:70:MET:HE2	2.34	0.62
1:A:99:PRO:HD2	2:A:298:HOH:O	2.00	0.62
1:A:55:ASP:HB2	2:A:425:HOH:O	2.00	0.61
1:B:126[A]:ASP:OD1	1:D:126:ASP:OD1	2.18	0.61
1:B:95:HIS:H	1:D:95:HIS:CD2	2.19	0.61
1:E:3:LYS:HE3	1:E:173:ASP:O	2.00	0.61
1:A:99:PRO:HB3	1:E:96:ASN:ND2	2.14	0.60
1:A:95:HIS:CD2	1:E:95:HIS:H	2.19	0.60
1:D:96:ASN:H	1:D:96:ASN:HD22	1.49	0.59
1:B:100:HIS:HE1	1:F:43:PHE:O	1.87	0.58
1:A:95:HIS:H	1:C:95:HIS:HD2	1.51	0.58
1:A:99:PRO:CG	1:E:96:ASN:HD21	2.17	0.57
1:D:95:HIS:H	1:F:95:HIS:HD2	1.53	0.57
1:B:95:HIS:HD2	1:F:95:HIS:H	1.54	0.56
1:F:96:ASN:H	1:F:96:ASN:HD22	1.53	0.56
1:A:95:HIS:H	1:C:95:HIS:CD2	2.24	0.55
1:C:183:LYS:HG3	1:C:185:ASN:OD1	2.08	0.54
1:B:95:HIS:CD2	1:F:95:HIS:H	2.26	0.53
1:C:96:ASN:H	1:C:96:ASN:ND2	2.01	0.53
1:F:23:ILE:HG13	1:F:57[A]:ILE:HD12	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:GLU:O	1:E:158:PRO:HD2	2.10	0.52
1:C:96:ASN:N	1:C:96:ASN:HD22	2.02	0.52
1:E:99:PRO:HD2	2:E:275:HOH:O	2.09	0.52
1:D:43:PHE:CE1	1:D:97:ALA:HB2	2.46	0.51
1:F:19:LEU:HG	1:F:57[A]:ILE:HD11	1.92	0.50
1:D:95:HIS:H	1:F:95:HIS:CD2	2.29	0.50
2:A:272:HOH:O	1:C:95:HIS:HE1	1.95	0.50
1:C:43:PHE:CE1	1:C:97:ALA:HB2	2.47	0.50
1:F:68:HIS:CE1	1:F:70:MET:HE2	2.47	0.50
1:A:52:LEU:HD13	1:A:53:ILE:HD13	1.93	0.50
1:A:43:PHE:CE1	1:A:96:ASN:OD1	2.65	0.50
1:B:103:ARG:NH2	2:B:493:HOH:O	2.44	0.49
1:D:9:PRO:HG3	1:D:214:ILE:HD11	1.94	0.49
1:D:53:ILE:N	1:D:53:ILE:HD12	2.27	0.49
1:C:95:HIS:H	1:E:95:HIS:CD2	2.31	0.49
1:E:64:THR:CG2	2:E:323:HOH:O	2.61	0.48
1:C:99:PRO:HG2	1:C:100:HIS:CE1	2.48	0.48
1:E:140:ILE:CG2	1:E:156:VAL:HG11	2.43	0.48
1:E:140:ILE:CG2	1:E:156:VAL:CG1	2.91	0.48
1:B:68:HIS:CE1	1:B:70:MET:HE2	2.48	0.48
1:C:95:HIS:H	1:E:95:HIS:HD2	1.60	0.47
2:B:323:HOH:O	1:D:99:PRO:HG3	2.15	0.47
1:B:95:HIS:HE1	2:B:293:HOH:O	1.98	0.47
1:D:20:GLY:HA2	1:D:60:LEU:HD13	1.97	0.46
1:A:43:PHE:CE1	1:A:97:ALA:HB2	2.50	0.46
1:B:43:PHE:CE1	1:B:97:ALA:HB2	2.51	0.46
1:A:43:PHE:HE1	1:A:96:ASN:OD1	1.99	0.46
1:D:52:LEU:HG	1:D:53:ILE:HD12	1.99	0.45
1:A:99:PRO:HD3	1:E:96:ASN:HD21	1.81	0.45
1:A:177:GLU:HA	1:A:197:ALA:O	2.17	0.45
1:F:96:ASN:H	1:F:96:ASN:ND2	2.13	0.45
2:D:305:HOH:O	1:F:103:ARG:HD2	2.16	0.44
1:F:19:LEU:CD2	1:F:57[A]:ILE:HD11	2.47	0.44
1:A:99:PRO:CD	1:E:96:ASN:HD21	2.30	0.44
1:F:33:TRP:CD1	1:F:64:THR:HB	2.53	0.44
1:E:140:ILE:HG22	1:E:156:VAL:HG11	2.00	0.43
1:F:70:MET:HB2	1:F:70:MET:HE2	1.47	0.43
1:F:99:PRO:HB2	1:F:100:HIS:ND1	2.33	0.43
1:E:70:MET:HB2	1:E:70:MET:HE2	1.73	0.43
1:C:96:ASN:ND2	1:E:99:PRO:HB3	2.33	0.43
1:E:42:ARG:HD3	2:E:330:HOH:O	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:MET:SD	1:F:145:PRO:CB	3.07	0.43
1:F:68:HIS:CE1	1:F:70:MET:CE	3.01	0.43
1:A:99:PRO:C	2:A:338:HOH:O	2.56	0.43
1:A:70:MET:HB2	1:A:70:MET:HE2	1.76	0.43
1:A:20:GLY:HA2	1:A:60:LEU:HD13	2.02	0.42
1:C:177:GLU:HA	1:C:197:ALA:O	2.17	0.42
1:D:68:HIS:CE1	1:D:70:MET:HE2	2.54	0.42
1:D:99:PRO:HB2	1:D:100:HIS:CE1	2.55	0.42
1:A:183:LYS:HB2	1:A:184:PRO:CD	2.50	0.42
1:C:116:GLY:HA2	1:C:137:LEU:O	2.19	0.42
1:D:177:GLU:HA	1:D:197:ALA:O	2.20	0.42
1:A:150:GLN:N	2:A:325:HOH:O	2.52	0.41
1:E:116:GLY:HA2	1:E:137:LEU:O	2.21	0.41
1:D:70:MET:HE2	1:D:70:MET:HB2	1.65	0.41
1:A:42:ARG:HG3	1:F:42:ARG:HG3	2.02	0.41
1:C:70:MET:HE2	1:C:70:MET:HB2	1.87	0.41
1:D:24:LYS:CE	2:D:365:HOH:O	2.69	0.41
1:E:151:SER:N	2:E:318:HOH:O	2.53	0.41
1:F:19:LEU:CG	1:F:57[A]:ILE:HD11	2.50	0.41
2:C:320:HOH:O	1:D:42:ARG:HD3	2.20	0.41
1:F:71:ILE:HD11	1:F:74:PRO:HB3	2.02	0.41
1:A:116:GLY:HA2	1:A:137:LEU:O	2.21	0.41
1:A:68:HIS:CE1	1:A:70:MET:CE	3.02	0.41
1:C:157:LEU:HB2	1:C:158:PRO:HD3	2.03	0.40
1:E:164:ARG:NH1	2:E:449:HOH:O	2.54	0.40
1:A:183:LYS:HG3	1:A:185:ASN:OD1	2.22	0.40
1:D:144:ASN:HD21	1:F:102:HIS:HB3	1.86	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:303:HOH:O	2:E:447:HOH:O[2_646]	1.99	0.21
2:D:300:HOH:O	2:E:447:HOH:O[2_646]	2.06	0.14
2:D:257:HOH:O	2:E:447:HOH:O[2_646]	2.08	0.12
2:D:458:HOH:O	2:E:265:HOH:O[2_646]	2.18	0.02

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	214/230 (93%)	206 (96%)	8 (4%)	0	100	100
1	B	210/230 (91%)	204 (97%)	6 (3%)	0	100	100
1	C	216/230 (94%)	209 (97%)	7 (3%)	0	100	100
1	D	212/230 (92%)	204 (96%)	8 (4%)	0	100	100
1	E	213/230 (93%)	206 (97%)	7 (3%)	0	100	100
1	F	214/230 (93%)	206 (96%)	8 (4%)	0	100	100
All	All	1279/1380 (93%)	1235 (97%)	44 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	177/191 (93%)	174 (98%)	3 (2%)	60	38
1	B	177/191 (93%)	173 (98%)	4 (2%)	50	25
1	C	178/191 (93%)	173 (97%)	5 (3%)	43	18
1	D	177/191 (93%)	170 (96%)	7 (4%)	31	10
1	E	180/191 (94%)	174 (97%)	6 (3%)	38	14
1	F	177/191 (93%)	172 (97%)	5 (3%)	43	18
All	All	1066/1146 (93%)	1036 (97%)	30 (3%)	46	18

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	52	LEU
1	A	183	LYS
1	B	103	ARG
1	B	126[A]	ASP
1	B	126[B]	ASP
1	B	132	LEU
1	C	96	ASN
1	C	126[A]	ASP
1	C	126[B]	ASP
1	C	151	SER
1	C	221	LYS
1	D	3	LYS
1	D	26	VAL
1	D	70	MET
1	D	96	ASN
1	D	100	HIS
1	D	132	LEU
1	D	183	LYS
1	E	64	THR
1	E	70	MET
1	E	96	ASN
1	E	103	ARG
1	E	170	ARG
1	E	221	LYS
1	F	71	ILE
1	F	100	HIS
1	F	170	ARG
1	F	183	LYS
1	F	185	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	144	ASN
1	A	189	GLN
1	B	95	HIS
1	B	100	HIS
1	C	95	HIS
1	C	96	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	102	HIS
1	D	95	HIS
1	D	96	ASN
1	D	144	ASN
1	D	189	GLN
1	E	95	HIS
1	E	96	ASN
1	E	165	GLN
1	E	189	GLN
1	F	95	HIS
1	F	96	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	217/230 (94%)	-0.32	2 (0%)	84	84	14, 20, 31, 40	0
1	B	214/230 (93%)	-0.35	1 (0%)	91	90	15, 21, 30, 44	0
1	C	218/230 (94%)	-0.28	3 (1%)	75	75	15, 22, 33, 45	0
1	D	216/230 (93%)	-0.17	3 (1%)	75	75	18, 24, 38, 49	0
1	E	215/230 (93%)	-0.16	4 (1%)	66	65	16, 23, 37, 46	0
1	F	217/230 (94%)	-0.08	3 (1%)	75	75	17, 24, 40, 50	0
All	All	1297/1380 (93%)	-0.23	16 (1%)	79	78	14, 23, 36, 50	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	99	PRO	4.9
1	E	223	PRO	4.6
1	F	99	PRO	4.1
1	C	225	PRO	3.4
1	C	99	PRO	3.1
1	F	169	GLU	2.9
1	D	169	GLU	2.7
1	D	98	SER	2.7
1	F	223	PRO	2.6
1	B	4	ASN	2.6
1	E	221	LYS	2.6
1	A	145	PRO	2.6
1	A	99	PRO	2.3
1	E	222	ARG	2.2
1	E	99	PRO	2.1
1	C	4	ASN	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.