Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 09:52 PM EDT

PDB ID	:	3C3J
Title	:	Crystal structure of tagatose-6-phosphate ketose/aldose isomerase from Escherichia coli
Authors	:	Zhang, R.; Skarina, T.; Egorova, O.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2008-01-28
Resolution	:	1.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

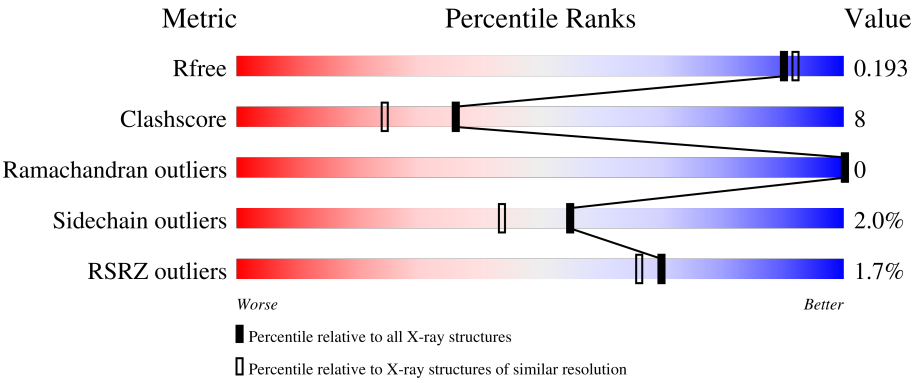
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.80 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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 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	384	3% 87% 9%
1	B	384	% 87% 9%
1	C	384	% 83% 12%
1	D	384	% 83% 11%
1	E	384	3% 80% 14%

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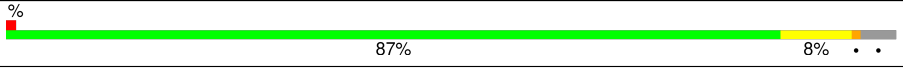
Mol	Chain	Length	Quality of chain
1	F	384	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 19285 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 Putative tagatose-6-phosphate ketose/aldose isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	370	Total	C	N	O	S	Se	0	0	0
			2840	1807	486	533	5	9			
1	B	369	Total	C	N	O	S	Se	0	0	0
			2832	1803	484	531	5	9			
1	C	367	Total	C	N	O	S	Se	0	0	0
			2820	1795	482	529	5	9			
1	D	369	Total	C	N	O	S	Se	0	0	0
			2832	1803	484	531	5	9			
1	E	369	Total	C	N	O	S	Se	0	0	0
			2835	1804	485	532	5	9			
1	F	369	Total	C	N	O	S	Se	0	0	0
			2832	1803	484	531	5	9			

- Molecule 2 is water.

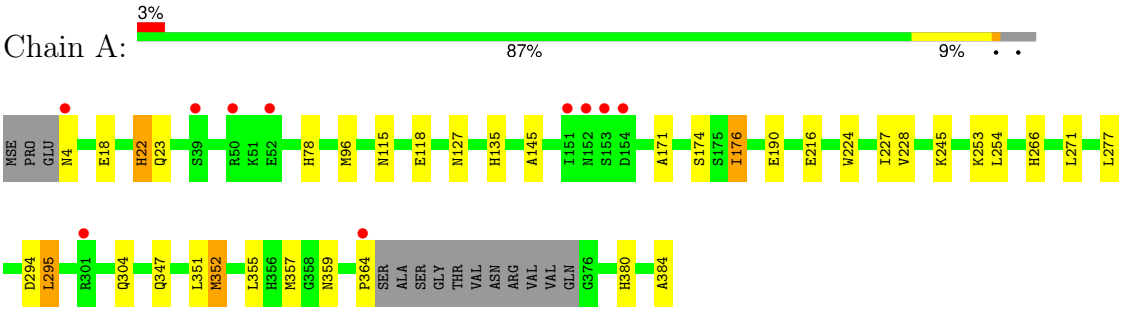
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	382	Total	O	0	0
			382	382		
2	B	386	Total	O	0	0
			386	386		
2	C	375	Total	O	0	0
			375	375		
2	D	375	Total	O	0	0
			375	375		
2	E	391	Total	O	0	0
			391	391		
2	F	385	Total	O	0	0
			385	385		

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.

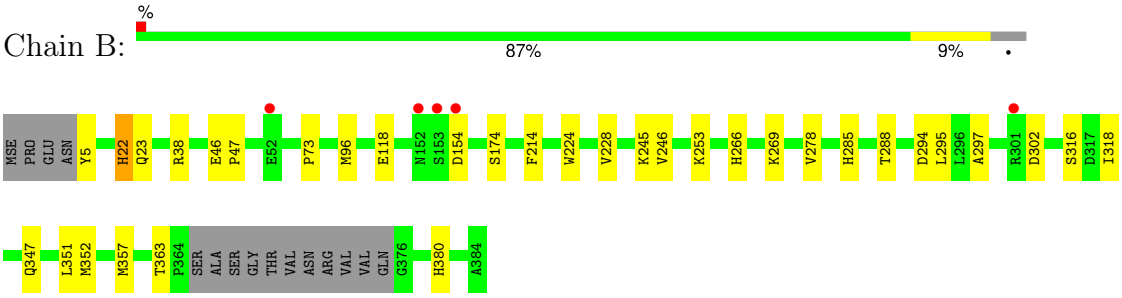
• Molecule 1: Putative tagatose-6-phosphate ketose/aldose isomerase

Chain A:



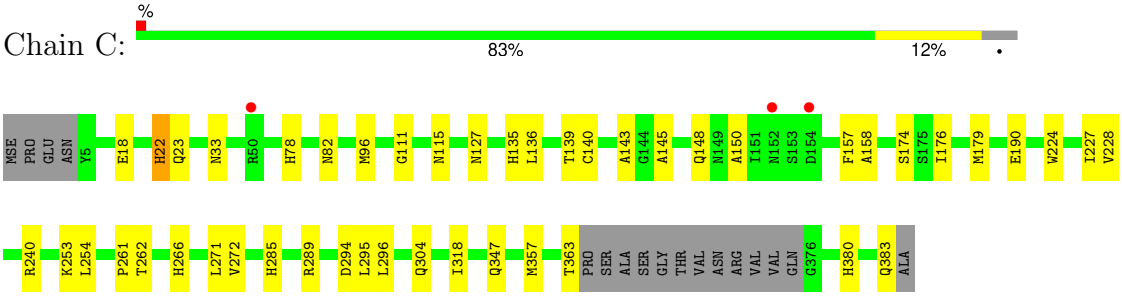
• Molecule 1: Putative tagatose-6-phosphate ketose/aldose isomerase

Chain B:



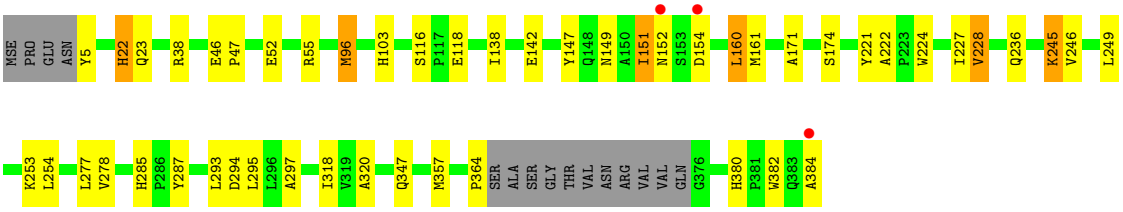
• Molecule 1: Putative tagatose-6-phosphate ketose/aldose isomerase

Chain C:

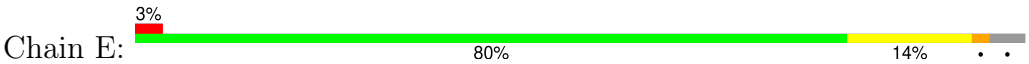


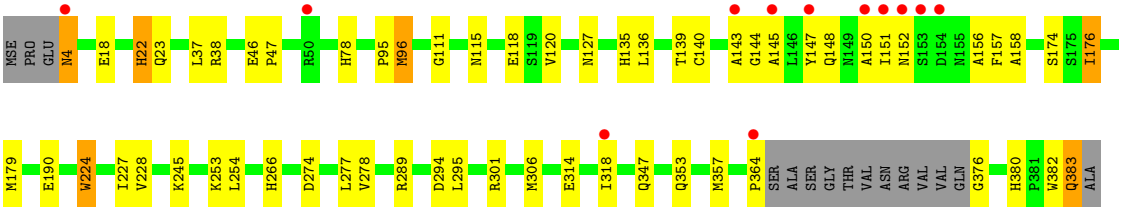
• Molecule 1: Putative tagatose-6-phosphate ketose/aldose isomerase

Chain D:

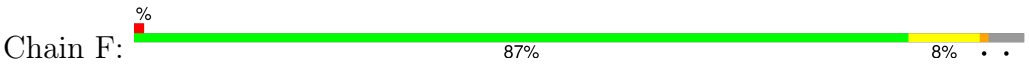


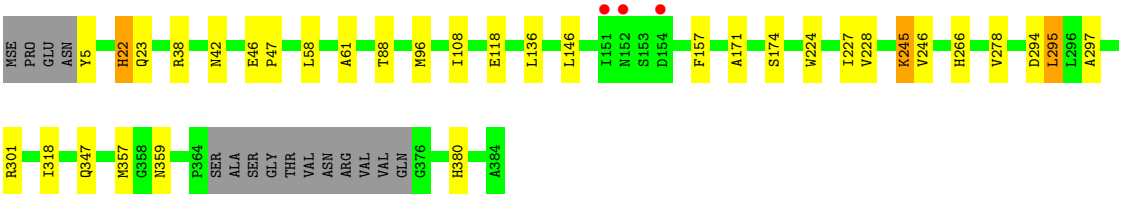
• Molecule 1: Putative tagatose-6-phosphate ketose/aldose isomerase





• Molecule 1: Putative tagatose-6-phosphate ketose/aldose isomerase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.94Å 81.21Å 138.32Å 90.00° 90.21° 90.00°	Depositor
Resolution (Å)	47.46 – 1.80 47.47 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.46-1.80) 99.5 (47.47-1.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.96 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.136 , 0.185 0.146 , 0.193	Depositor DCC
R_{free} test set	10357 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 66.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19285	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1382e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.65	0/2901	0.67	1/3945 (0.0%)
1	B	0.63	0/2893	0.70	2/3934 (0.1%)
1	C	0.64	0/2880	0.69	0/3915
1	D	0.64	1/2893 (0.0%)	0.69	1/3934 (0.0%)
1	E	0.63	0/2896	0.72	3/3938 (0.1%)
1	F	0.61	0/2893	0.68	4/3934 (0.1%)
All	All	0.63	1/17356 (0.0%)	0.69	11/23600 (0.0%)

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	E	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	228	VAL	CB-CG1	-5.34	1.41	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	E	38	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	F	295	LEU	CA-CB-CG	-7.02	99.15	115.30
1	B	38	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	E	38	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	E	383	GLN	N-CA-C	6.26	127.91	111.00
1	F	38	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	295	LEU	CA-CB-CG	-6.22	100.98	115.30
1	F	38	ARG	NE-CZ-NH2	-6.11	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	38	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	F	301	ARG	NE-CZ-NH1	5.37	122.99	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	E	383	GLN	CA

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	2840	0	2784	40	0
1	B	2832	0	2778	36	0
1	C	2820	0	2766	55	0
1	D	2832	0	2778	53	0
1	E	2835	0	2779	78	0
1	F	2832	0	2778	28	0
2	A	382	0	0	9	1
2	B	386	0	0	10	2
2	C	375	0	0	17	1
2	D	375	0	0	20	1
2	E	391	0	0	26	0
2	F	385	0	0	6	1
All	All	19285	0	16663	269	3

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 8.

All (269) 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:E:96:MSE:HE2	1:E:382:TRP:CH2	1.67	1.28
1:A:352:MSE:CE	1:A:355:LEU:HD12	1.78	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LEU:HG	1:A:352:MSE:HE3	1.12	1.09
1:A:352:MSE:HE1	1:A:355:LEU:HD12	1.09	1.07
1:B:351:LEU:HD23	1:B:352:MSE:HE2	1.33	1.04
1:E:140:CYS:SG	1:E:179:MSE:HE3	1.98	1.03
1:E:147:TYR:CE2	1:E:151:ILE:HD11	1.93	1.01
1:C:140:CYS:SG	1:C:179:MSE:HE3	2.00	1.00
1:D:96:MSE:HE3	1:D:382:TRP:HH2	1.25	1.00
1:B:352:MSE:SE	2:B:701:HOH:O	2.25	1.00
1:A:351:LEU:HG	1:A:352:MSE:CE	1.90	1.00
1:A:352:MSE:HE1	1:A:355:LEU:CD1	1.94	0.97
1:E:318:ILE:HG23	2:E:752:HOH:O	1.67	0.94
1:C:33:ASN:HB2	2:C:509:HOH:O	1.66	0.94
1:A:352:MSE:HA	1:A:352:MSE:HE2	1.47	0.94
1:D:318:ILE:HD12	2:D:445:HOH:O	1.72	0.90
1:E:96:MSE:CE	1:E:382:TRP:CH2	2.53	0.90
1:A:351:LEU:CG	1:A:352:MSE:HE3	2.02	0.90
1:F:246:VAL:HG13	2:F:763:HOH:O	1.70	0.90
1:E:96:MSE:CE	1:E:382:TRP:CZ3	2.56	0.89
1:E:115:ASN:HD21	1:E:144:GLY:HA2	1.32	0.88
1:C:253:LYS:HG3	1:C:357:MSE:HE1	1.55	0.88
1:E:96:MSE:HE2	1:E:382:TRP:HH2	1.37	0.87
1:D:227:ILE:HB	2:D:584:HOH:O	1.75	0.86
1:E:145:ALA:HB2	2:E:743:HOH:O	1.75	0.85
1:C:285:HIS:NE2	1:D:96:MSE:HE2	1.92	0.84
1:D:96:MSE:HE3	1:D:382:TRP:CH2	2.12	0.83
1:B:351:LEU:CD2	1:B:352:MSE:HE2	2.09	0.82
1:E:111:GLY:O	1:E:179:MSE:HE1	1.81	0.81
1:E:96:MSE:HE2	1:E:382:TRP:CZ3	2.14	0.80
1:B:46:GLU:HG2	1:B:47:PRO:HD3	1.63	0.80
1:E:96:MSE:HE1	1:E:382:TRP:CZ3	2.17	0.80
1:E:139:THR:HA	1:E:179:MSE:HE2	1.62	0.80
1:A:253:LYS:HG3	1:A:357:MSE:HE1	1.64	0.79
1:D:318:ILE:HG22	2:D:489:HOH:O	1.84	0.78
1:E:96:MSE:HE3	1:E:96:MSE:H	1.48	0.78
1:E:227:ILE:HB	2:E:454:HOH:O	1.81	0.78
1:E:145:ALA:CB	2:E:743:HOH:O	2.30	0.78
1:B:214:PHE:CD2	1:B:352:MSE:HE3	2.17	0.78
1:B:351:LEU:HD23	1:B:352:MSE:CE	2.13	0.77
1:C:272:VAL:HG12	1:C:304:GLN:HG3	1.67	0.77
1:E:139:THR:HA	1:E:179:MSE:CE	2.14	0.77
1:B:214:PHE:HD2	1:B:352:MSE:HE3	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:318:ILE:HG23	2:F:765:HOH:O	1.84	0.76
1:C:285:HIS:NE2	1:D:96:MSE:CE	2.48	0.76
1:E:78:HIS:HE1	1:E:190:GLU:OE2	1.68	0.76
1:E:120:VAL:HG23	2:E:692:HOH:O	1.87	0.74
1:C:285:HIS:CE1	1:D:96:MSE:HE1	2.23	0.74
1:C:78:HIS:HE1	1:C:190:GLU:OE2	1.72	0.73
1:E:143:ALA:C	2:E:508:HOH:O	2.27	0.73
1:D:221:TYR:CE2	2:D:754:HOH:O	2.40	0.73
1:C:363:THR:C	2:C:692:HOH:O	2.28	0.72
1:E:254:LEU:HD21	2:E:454:HOH:O	1.90	0.71
1:A:384:ALA:C	2:A:760:HOH:O	2.28	0.71
1:E:139:THR:CA	1:E:179:MSE:HE2	2.21	0.70
1:C:294:ASP:OD2	1:D:380:HIS:HE1	1.74	0.70
1:F:23:GLN:HE22	1:F:347:GLN:HE22	1.40	0.70
1:A:78:HIS:HE1	1:A:190:GLU:OE2	1.75	0.69
1:C:380:HIS:HE1	1:D:294:ASP:OD2	1.76	0.69
1:E:95:PRO:HG2	1:E:96:MSE:HE3	1.73	0.69
1:E:143:ALA:CB	2:E:508:HOH:O	2.39	0.69
1:C:139:THR:HA	1:C:179:MSE:HE2	1.75	0.69
1:C:23:GLN:HE22	1:C:347:GLN:HE22	1.41	0.69
1:C:228:VAL:CG2	1:C:271:LEU:HD11	2.23	0.69
1:C:111:GLY:O	1:C:179:MSE:HE1	1.94	0.68
1:E:176:ILE:HD13	1:E:176:ILE:C	2.13	0.68
1:E:118:GLU:OE2	1:F:266:HIS:HE1	1.75	0.68
1:C:176:ILE:HD13	2:C:716:HOH:O	1.94	0.68
1:A:380:HIS:HE1	1:B:294:ASP:OD2	1.76	0.67
1:E:23:GLN:HE22	1:E:347:GLN:HE22	1.42	0.67
1:A:294:ASP:OD2	1:B:380:HIS:HE1	1.78	0.67
1:D:151:ILE:HG23	2:D:521:HOH:O	1.95	0.66
2:A:564:HOH:O	1:D:22:HIS:HD2	1.79	0.66
1:C:143:ALA:HA	2:C:564:HOH:O	1.96	0.66
1:E:115:ASN:ND2	2:E:743:HOH:O	2.12	0.66
1:A:266:HIS:HE1	1:B:118:GLU:OE2	1.79	0.66
1:D:147:TYR:CD1	1:D:160:LEU:HD13	2.31	0.66
1:D:297:ALA:HB2	1:D:318:ILE:HD13	1.77	0.66
1:B:363:THR:HG23	1:B:363:THR:O	1.96	0.65
1:E:294:ASP:OD2	1:F:380:HIS:HE1	1.79	0.65
1:B:363:THR:HG22	2:B:598:HOH:O	1.97	0.64
1:D:23:GLN:HE22	1:D:347:GLN:HE22	1.45	0.64
1:E:148:GLN:HG3	2:E:534:HOH:O	1.97	0.64
1:A:352:MSE:CE	1:A:352:MSE:HA	2.24	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HB	2:A:518:HOH:O	1.97	0.64
1:D:221:TYR:C	2:D:685:HOH:O	2.35	0.64
1:C:148:GLN:CG	2:C:564:HOH:O	2.46	0.63
1:E:253:LYS:HG3	1:E:357:MSE:HE1	1.79	0.63
1:B:214:PHE:CB	1:B:352:MSE:HE3	2.27	0.63
1:E:95:PRO:HG2	1:E:96:MSE:CE	2.28	0.63
1:A:127:ASN:OD1	1:A:135:HIS:HE1	1.82	0.63
1:B:5:TYR:N	2:B:668:HOH:O	2.32	0.62
1:E:4:ASN:N	1:E:4:ASN:HD22	1.97	0.62
1:A:228:VAL:CG2	1:A:271:LEU:HD11	2.30	0.62
1:E:266:HIS:HE1	1:F:118:GLU:OE2	1.82	0.62
1:B:246:VAL:HG22	2:B:740:HOH:O	1.98	0.62
1:F:357:MSE:HE2	1:F:359:ASN:ND2	2.15	0.62
1:B:214:PHE:HD2	1:B:352:MSE:CE	2.13	0.61
1:B:285:HIS:HE1	1:D:142:GLU:OE1	1.82	0.61
1:E:143:ALA:HB1	2:E:508:HOH:O	2.00	0.61
1:E:115:ASN:ND2	1:E:144:GLY:HA2	2.11	0.61
1:F:295:LEU:O	1:F:295:LEU:HG	1.98	0.61
1:B:23:GLN:HE22	1:B:347:GLN:HE22	1.49	0.60
1:E:148:GLN:HG3	2:E:766:HOH:O	2.01	0.60
1:F:357:MSE:HE2	1:F:359:ASN:HD22	1.67	0.60
1:A:118:GLU:OE2	1:B:266:HIS:HE1	1.84	0.60
1:F:227:ILE:HB	2:F:464:HOH:O	2.02	0.60
1:C:139:THR:HA	1:C:179:MSE:CE	2.31	0.60
1:C:140:CYS:HG	1:C:179:MSE:HE3	1.67	0.59
1:F:171:ALA:HB1	1:F:245:LYS:HE2	1.85	0.59
1:C:228:VAL:HG21	1:C:271:LEU:HD11	1.83	0.59
1:C:148:GLN:HG3	2:C:564:HOH:O	2.02	0.59
1:E:380:HIS:HE1	1:F:294:ASP:OD2	1.86	0.58
1:C:285:HIS:CE1	1:D:96:MSE:CE	2.85	0.58
1:A:352:MSE:HE2	1:A:352:MSE:CA	2.28	0.58
1:A:228:VAL:HG21	1:A:271:LEU:HD11	1.85	0.57
1:E:150:ALA:HA	1:E:156:ALA:HB3	1.86	0.57
1:C:136:LEU:HD12	1:C:157:PHE:O	2.05	0.57
1:E:301:ARG:HG3	2:E:501:HOH:O	2.04	0.57
1:E:18:GLU:OE2	1:E:22:HIS:HD2	1.87	0.57
1:F:227:ILE:HG21	1:F:246:VAL:HG11	1.86	0.57
1:B:351:LEU:CD2	1:B:352:MSE:CE	2.79	0.57
1:D:221:TYR:CD2	2:D:754:HOH:O	2.57	0.57
1:A:23:GLN:HE22	1:A:347:GLN:HE22	1.51	0.57
1:E:120:VAL:HG13	2:E:613:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:LEU:O	1:A:295:LEU:HG	2.03	0.56
1:E:376:GLY:N	2:E:706:HOH:O	2.39	0.56
1:D:320:ALA:O	2:D:756:HOH:O	2.18	0.56
1:C:272:VAL:HG12	1:C:304:GLN:CG	2.35	0.56
1:C:115:ASN:ND2	1:C:145:ALA:H	2.04	0.56
1:E:115:ASN:ND2	1:E:145:ALA:H	2.04	0.56
1:C:266:HIS:HE1	1:D:118:GLU:OE2	1.88	0.55
1:C:357:MSE:HE2	2:C:497:HOH:O	2.06	0.55
1:D:5:TYR:N	2:D:668:HOH:O	2.40	0.55
1:D:228:VAL:CG1	1:D:278:VAL:HG22	2.37	0.55
1:F:228:VAL:CG1	1:F:278:VAL:HG22	2.36	0.55
1:C:285:HIS:HE2	1:D:96:MSE:HE2	1.69	0.55
1:E:364:PRO:C	2:E:688:HOH:O	2.45	0.55
1:C:254:LEU:HD21	2:C:597:HOH:O	2.06	0.55
1:E:95:PRO:HD2	1:E:96:MSE:HE1	1.88	0.55
1:E:148:GLN:CG	2:E:534:HOH:O	2.53	0.54
1:E:151:ILE:HB	2:E:703:HOH:O	2.07	0.54
1:E:4:ASN:N	2:E:745:HOH:O	2.40	0.54
1:E:115:ASN:HD21	1:E:144:GLY:CA	2.12	0.54
1:C:227:ILE:HB	2:C:597:HOH:O	2.07	0.54
1:C:139:THR:CA	1:C:179:MSE:HE2	2.38	0.54
1:E:147:TYR:CD2	1:E:151:ILE:HD11	2.42	0.54
1:A:18:GLU:OE2	1:A:22:HIS:HD2	1.92	0.53
1:A:352:MSE:HE2	1:A:355:LEU:HD12	1.85	0.53
1:A:22:HIS:HE1	1:A:174:SER:OG	1.90	0.53
1:A:254:LEU:HD13	2:A:580:HOH:O	2.07	0.53
1:F:357:MSE:SE	2:F:476:HOH:O	2.76	0.53
1:E:96:MSE:HE3	1:E:96:MSE:N	2.20	0.53
1:B:228:VAL:CG1	1:B:278:VAL:HG22	2.39	0.53
1:C:33:ASN:HB2	2:C:503:HOH:O	2.08	0.52
1:B:295:LEU:HG	1:B:295:LEU:O	2.09	0.52
1:E:96:MSE:CE	1:E:96:MSE:H	2.19	0.52
1:D:222:ALA:N	2:D:713:HOH:O	2.43	0.52
1:D:5:TYR:N	2:D:488:HOH:O	2.43	0.52
1:C:272:VAL:CG1	1:C:304:GLN:HG3	2.38	0.52
1:D:96:MSE:CE	1:D:382:TRP:CH2	2.91	0.52
1:E:152:ASN:HB2	2:E:695:HOH:O	2.10	0.51
1:A:171:ALA:HB1	1:A:245:LYS:HE3	1.92	0.51
1:E:4:ASN:N	1:E:4:ASN:ND2	2.58	0.51
1:E:139:THR:HA	1:E:179:MSE:HE1	1.91	0.51
1:E:357:MSE:HE2	2:E:774:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:HIS:HD2	2:B:592:HOH:O	1.94	0.51
1:C:33:ASN:CB	2:C:509:HOH:O	2.42	0.51
1:B:22:HIS:HE1	1:B:174:SER:OG	1.94	0.51
1:B:73:PRO:HG2	2:B:679:HOH:O	2.10	0.51
1:A:364:PRO:HB2	2:A:715:HOH:O	2.10	0.51
1:C:18:GLU:OE2	1:C:22:HIS:HD2	1.93	0.51
1:D:253:LYS:HG3	1:D:357:MSE:HE1	1.93	0.51
1:E:127:ASN:OD1	1:E:135:HIS:HE1	1.93	0.51
1:C:78:HIS:CE1	1:C:190:GLU:OE2	2.60	0.50
1:D:160:LEU:HD12	2:D:749:HOH:O	2.10	0.50
1:D:227:ILE:HD12	1:D:277:LEU:HD23	1.94	0.50
1:E:150:ALA:HA	1:E:156:ALA:CB	2.40	0.50
1:D:384:ALA:C	2:D:528:HOH:O	2.49	0.50
1:C:272:VAL:CG1	1:C:304:GLN:CG	2.90	0.50
1:E:295:LEU:O	1:E:295:LEU:HG	2.11	0.50
1:E:228:VAL:CG1	1:E:278:VAL:HG22	2.42	0.50
1:E:22:HIS:HE1	1:E:174:SER:OG	1.95	0.50
1:D:254:LEU:HD21	2:D:584:HOH:O	2.10	0.50
1:C:22:HIS:HE1	1:C:174:SER:OG	1.93	0.49
1:C:240:ARG:NH2	2:D:583:HOH:O	2.45	0.49
1:D:22:HIS:HE1	1:D:174:SER:OG	1.95	0.49
1:B:246:VAL:HG23	2:B:390:HOH:O	2.13	0.49
1:C:127:ASN:OD1	1:C:135:HIS:HE1	1.95	0.49
1:A:351:LEU:C	1:A:352:MSE:HE3	2.33	0.48
1:F:58:LEU:CD1	1:F:108:ILE:HD12	2.43	0.48
1:A:304:GLN:NE2	2:A:626:HOH:O	2.46	0.48
1:D:357:MSE:SE	2:D:486:HOH:O	2.81	0.47
1:A:227:ILE:HD12	1:A:277:LEU:HD23	1.95	0.47
1:A:352:MSE:CE	1:A:352:MSE:CA	2.91	0.47
1:D:285:HIS:HD2	1:D:287:TYR:H	1.61	0.47
1:E:78:HIS:CE1	1:E:190:GLU:OE2	2.58	0.47
1:E:380:HIS:HD2	2:E:587:HOH:O	1.97	0.47
1:F:136:LEU:HD12	1:F:157:PHE:O	2.15	0.47
1:E:96:MSE:HE1	1:E:382:TRP:HZ3	1.75	0.47
1:D:249:LEU:HD23	1:D:364:PRO:HG3	1.97	0.46
1:F:5:TYR:N	2:F:433:HOH:O	2.48	0.46
1:A:351:LEU:C	1:A:352:MSE:CE	2.84	0.46
1:C:150:ALA:HB3	1:C:158:ALA:HB2	1.98	0.46
1:D:227:ILE:HG21	1:D:246:VAL:HG11	1.98	0.46
1:E:150:ALA:HB3	1:E:158:ALA:HB2	1.97	0.46
1:A:216:GLU:HG2	2:A:437:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:VAL:HG13	2:B:740:HOH:O	2.15	0.46
1:B:285:HIS:HD2	1:B:288:THR:OG1	1.99	0.46
1:C:296:LEU:HD23	1:C:318:ILE:HG22	1.97	0.46
1:E:147:TYR:CZ	1:E:151:ILE:HD11	2.49	0.46
1:F:5:TYR:N	2:F:637:HOH:O	2.48	0.46
1:A:78:HIS:CE1	1:A:190:GLU:OE2	2.62	0.46
1:F:22:HIS:HE1	1:F:174:SER:OG	1.99	0.46
1:F:42:ASN:O	1:F:46:GLU:HG2	2.15	0.46
1:D:222:ALA:HB2	2:D:713:HOH:O	2.16	0.45
1:C:78:HIS:HD2	2:C:612:HOH:O	1.99	0.45
1:D:160:LEU:CD1	2:D:749:HOH:O	2.64	0.45
1:D:142:GLU:HA	1:D:160:LEU:HD11	1.99	0.45
1:A:4:ASN:ND2	2:A:531:HOH:O	2.49	0.45
1:C:304:GLN:HG2	2:C:425:HOH:O	2.17	0.45
1:B:363:THR:HB	2:B:751:HOH:O	2.17	0.45
1:C:111:GLY:C	1:C:179:MSE:HE1	2.36	0.45
1:C:363:THR:C	2:C:675:HOH:O	2.55	0.45
1:E:136:LEU:HD12	1:E:157:PHE:O	2.17	0.45
1:A:359:ASN:ND2	2:A:759:HOH:O	2.49	0.44
1:F:42:ASN:O	1:F:46:GLU:CG	2.66	0.44
1:D:149:ASN:O	1:D:152:ASN:ND2	2.51	0.44
1:F:46:GLU:N	1:F:47:PRO:CD	2.80	0.44
2:E:679:HOH:O	1:F:380:HIS:HD2	2.00	0.44
1:C:383:GLN:O	2:C:755:HOH:O	2.20	0.44
1:A:271:LEU:C	1:A:271:LEU:HD12	2.38	0.44
1:E:18:GLU:HG3	2:E:676:HOH:O	2.18	0.44
2:C:551:HOH:O	1:D:103:HIS:HE1	2.00	0.43
1:E:120:VAL:CG2	1:E:145:ALA:HB3	2.48	0.43
1:C:363:THR:HG22	2:C:692:HOH:O	2.18	0.43
1:F:61:ALA:HB2	1:F:88:THR:OG1	2.19	0.43
1:D:295:LEU:O	1:D:295:LEU:HG	2.18	0.43
1:E:46:GLU:N	1:E:47:PRO:HD2	2.33	0.43
1:E:227:ILE:HD12	1:E:277:LEU:HD23	2.00	0.43
1:B:316:SER:HB3	2:B:734:HOH:O	2.18	0.43
1:B:269:LYS:NZ	1:B:302:ASP:OD2	2.50	0.43
1:E:289:ARG:HH12	1:E:314:GLU:CB	2.32	0.43
1:F:297:ALA:HB2	1:F:318:ILE:HD12	2.00	0.42
1:D:293:LEU:HD22	1:D:318:ILE:HG23	2.00	0.42
1:A:115:ASN:ND2	1:A:145:ALA:H	2.18	0.42
1:D:138:ILE:HG23	1:D:161:MSE:HE3	2.02	0.42
1:B:297:ALA:HA	1:B:318:ILE:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:ARG:NH1	2:E:756:HOH:O	2.51	0.42
1:C:262:THR:HG21	2:D:686:HOH:O	2.19	0.42
1:D:171:ALA:HB1	1:D:245:LYS:HE2	2.02	0.42
1:D:236:GLN:NE2	2:D:583:HOH:O	2.42	0.41
1:C:294:ASP:OD2	1:D:380:HIS:CE1	2.64	0.41
1:F:357:MSE:HE2	1:F:359:ASN:HB2	2.02	0.41
1:B:46:GLU:CG	1:B:47:PRO:HD3	2.44	0.41
1:B:214:PHE:HB2	1:B:352:MSE:HE3	1.98	0.41
1:E:115:ASN:HB2	2:E:680:HOH:O	2.19	0.41
1:C:261:PRO:CA	1:C:295:LEU:HD22	2.50	0.41
1:C:285:HIS:CD2	1:D:96:MSE:HE2	2.55	0.41
1:C:82:ASN:HD21	1:D:55:ARG:HH21	1.67	0.41
1:E:224:TRP:HE1	1:E:353:GLN:NE2	2.18	0.41
1:E:274:ASP:O	1:E:306:MSE:HE3	2.20	0.41
1:F:58:LEU:HD12	1:F:108:ILE:HD12	2.03	0.40
1:A:176:ILE:C	1:A:176:ILE:HD13	2.41	0.40
1:B:214:PHE:CG	1:B:352:MSE:HE3	2.55	0.40
1:D:46:GLU:N	1:D:47:PRO:CD	2.85	0.40
1:C:82:ASN:HD21	1:D:55:ARG:NH2	2.19	0.40
1:E:150:ALA:HB1	1:E:156:ALA:HB1	2.02	0.40
1:B:253:LYS:HG3	1:B:357:MSE:HE1	2.03	0.40

All (3) 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:B:750:HOH:O	2:D:636:HOH:O[1_545]	2.11	0.09
2:A:545:HOH:O	2:C:746:HOH:O[2_646]	2.12	0.08
2:B:764:HOH:O	2:F:520:HOH:O[1_655]	2.19	0.01

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	366/384 (95%)	358 (98%)	8 (2%)	0	100	100
1	B	365/384 (95%)	358 (98%)	7 (2%)	0	100	100
1	C	363/384 (94%)	358 (99%)	5 (1%)	0	100	100
1	D	365/384 (95%)	360 (99%)	5 (1%)	0	100	100
1	E	365/384 (95%)	360 (99%)	5 (1%)	0	100	100
1	F	365/384 (95%)	357 (98%)	8 (2%)	0	100	100
All	All	2189/2304 (95%)	2151 (98%)	38 (2%)	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	302/304 (99%)	297 (98%)	5 (2%)	60	51
1	B	301/304 (99%)	296 (98%)	5 (2%)	60	51
1	C	300/304 (99%)	296 (99%)	4 (1%)	69	62
1	D	301/304 (99%)	292 (97%)	9 (3%)	41	27
1	E	302/304 (99%)	294 (97%)	8 (3%)	46	32
1	F	301/304 (99%)	296 (98%)	5 (2%)	60	51
All	All	1807/1824 (99%)	1771 (98%)	36 (2%)	55	44

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	96	MSE
1	A	176	ILE
1	A	224	TRP
1	A	352	MSE
1	B	22	HIS
1	B	96	MSE

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Mol	Chain	Res	Type
1	B	154	ASP
1	B	224	TRP
1	B	245	LYS
1	C	22	HIS
1	C	96	MSE
1	C	224	TRP
1	C	289	ARG
1	D	22	HIS
1	D	52	GLU
1	D	96	MSE
1	D	116	SER
1	D	151	ILE
1	D	154	ASP
1	D	160	LEU
1	D	224	TRP
1	D	245	LYS
1	E	4	ASN
1	E	22	HIS
1	E	37	LEU
1	E	96	MSE
1	E	176	ILE
1	E	224	TRP
1	E	245	LYS
1	E	383	GLN
1	F	22	HIS
1	F	96	MSE
1	F	146	LEU
1	F	224	TRP
1	F	245	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	22	HIS
1	A	23	GLN
1	A	78	HIS
1	A	82	ASN
1	A	94	ASN
1	A	115	ASN
1	A	135	HIS
1	A	266	HIS

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Mol	Chain	Res	Type
1	A	380	HIS
1	B	22	HIS
1	B	23	GLN
1	B	82	ASN
1	B	266	HIS
1	B	285	HIS
1	B	353	GLN
1	B	380	HIS
1	C	22	HIS
1	C	23	GLN
1	C	78	HIS
1	C	82	ASN
1	C	94	ASN
1	C	115	ASN
1	C	135	HIS
1	C	266	HIS
1	C	380	HIS
1	D	22	HIS
1	D	23	GLN
1	D	103	HIS
1	D	149	ASN
1	D	152	ASN
1	D	266	HIS
1	D	285	HIS
1	D	380	HIS
1	D	383	GLN
1	E	22	HIS
1	E	23	GLN
1	E	78	HIS
1	E	82	ASN
1	E	94	ASN
1	E	115	ASN
1	E	135	HIS
1	E	266	HIS
1	E	353	GLN
1	E	380	HIS
1	F	22	HIS
1	F	23	GLN
1	F	82	ASN
1	F	266	HIS
1	F	285	HIS
1	F	303	ASN

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Mol	Chain	Res	Type
1	F	353	GLN
1	F	380	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 monosaccharides 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	361/384 (94%)	-0.22	10 (2%)	53	47	12, 18, 28, 39	0
1	B	360/384 (93%)	-0.30	5 (1%)	75	72	11, 17, 28, 40	0
1	C	358/384 (93%)	-0.29	3 (0%)	86	84	11, 16, 27, 42	0
1	D	360/384 (93%)	-0.29	3 (0%)	86	84	11, 17, 29, 39	0
1	E	360/384 (93%)	-0.18	12 (3%)	46	40	11, 17, 29, 50	0
1	F	360/384 (93%)	-0.25	3 (0%)	86	84	12, 18, 29, 40	0
All	All	2159/2304 (93%)	-0.26	36 (1%)	70	66	11, 17, 28, 50	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	151	ILE	9.2
1	A	4	ASN	6.0
1	A	154	ASP	4.9
1	D	152	ASN	4.9
1	E	4	ASN	4.6
1	C	152	ASN	4.4
1	B	152	ASN	4.2
1	F	151	ILE	4.2
1	E	152	ASN	4.1
1	F	154	ASP	3.8
1	E	154	ASP	3.8
1	D	154	ASP	3.7
1	C	154	ASP	3.5
1	E	147	TYR	3.4
1	F	152	ASN	3.0
1	C	50	ARG	3.0
1	B	154	ASP	2.9
1	E	153	SER	2.8
1	A	153	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	50	ARG	2.8
1	E	318	ILE	2.7
1	A	52	GLU	2.6
1	E	143	ALA	2.5
1	A	152	ASN	2.5
1	B	301	ARG	2.4
1	B	153	SER	2.3
1	A	151	ILE	2.3
1	E	364	PRO	2.2
1	E	150	ALA	2.2
1	A	301	ARG	2.1
1	E	50	ARG	2.1
1	D	384	ALA	2.1
1	E	145	ALA	2.1
1	A	39	SER	2.0
1	A	364	PRO	2.0
1	B	52	GLU	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.