Full wwPDB X-ray Structure Validation Report (i)

Oct 24, 2023 – 04:53 AM EDT

PDB ID	:	2ZBL
Title	:	Functional annotation of Salmonella enterica yihS-encoded protein
Authors	:	Itoh, T.; Mikami, B.; Hashimoto, W.; Murata, K.
Deposited on	:	2007-10-24
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 (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:

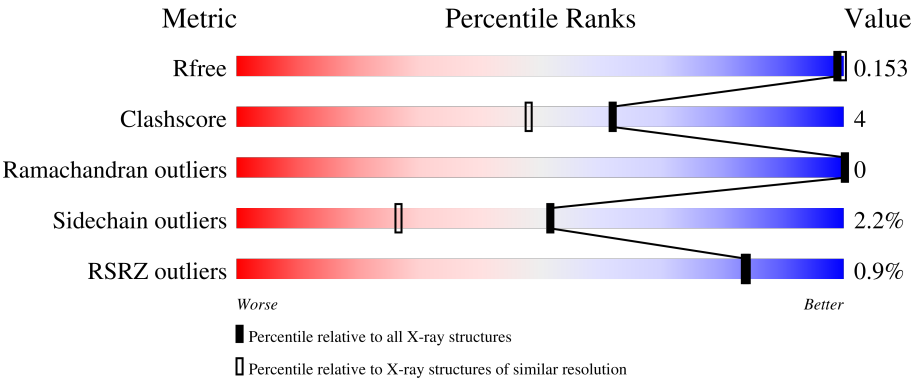
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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	421	92% 7%
1	B	421	91% 8%
1	C	421	89% 9%
1	D	421	89% 9%
1	E	421	2% 89% 10%

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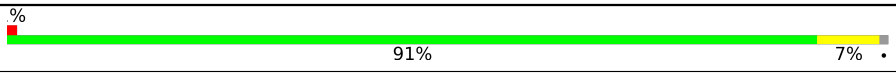
Mol	Chain	Length	Quality of chain
1	F	421	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23652 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 isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	4	0
			3415	2195	592	614	14			
1	B	418	Total	C	N	O	S	0	5	0
			3438	2210	596	618	14			
1	C	417	Total	C	N	O	S	8	10	0
			3454	2220	599	621	14			
1	D	416	Total	C	N	O	S	0	10	0
			3449	2216	597	622	14			
1	E	416	Total	C	N	O	S	0	10	0
			3447	2218	594	621	14			
1	F	416	Total	C	N	O	S	0	8	0
			3436	2206	590	626	14			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	ALA	HIS	engineered mutation	UNP Q8ZKT7
A	414	LEU	-	expression tag	UNP Q8ZKT7
A	415	GLU	-	expression tag	UNP Q8ZKT7
A	416	HIS	-	expression tag	UNP Q8ZKT7
A	417	HIS	-	expression tag	UNP Q8ZKT7
A	418	HIS	-	expression tag	UNP Q8ZKT7
A	419	HIS	-	expression tag	UNP Q8ZKT7
A	420	HIS	-	expression tag	UNP Q8ZKT7
A	421	HIS	-	expression tag	UNP Q8ZKT7
B	248	ALA	HIS	engineered mutation	UNP Q8ZKT7
B	414	LEU	-	expression tag	UNP Q8ZKT7
B	415	GLU	-	expression tag	UNP Q8ZKT7
B	416	HIS	-	expression tag	UNP Q8ZKT7
B	417	HIS	-	expression tag	UNP Q8ZKT7
B	418	HIS	-	expression tag	UNP Q8ZKT7
B	419	HIS	-	expression tag	UNP Q8ZKT7
B	420	HIS	-	expression tag	UNP Q8ZKT7

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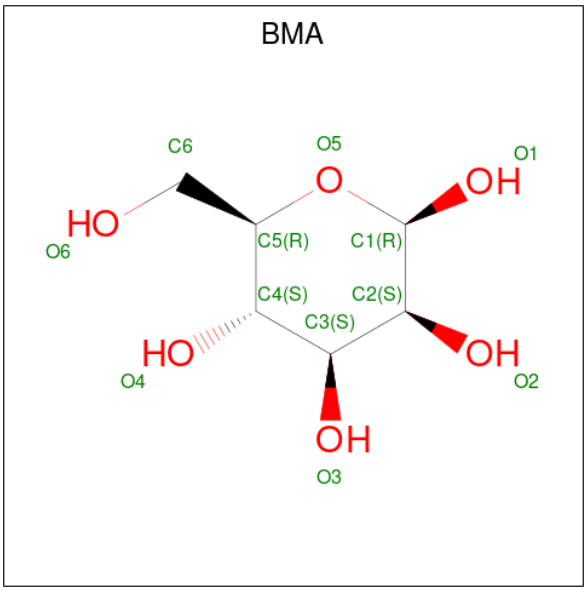
Chain	Residue	Modelled	Actual	Comment	Reference
B	421	HIS	-	expression tag	UNP Q8ZKT7
C	248	ALA	HIS	engineered mutation	UNP Q8ZKT7
C	414	LEU	-	expression tag	UNP Q8ZKT7
C	415	GLU	-	expression tag	UNP Q8ZKT7
C	416	HIS	-	expression tag	UNP Q8ZKT7
C	417	HIS	-	expression tag	UNP Q8ZKT7
C	418	HIS	-	expression tag	UNP Q8ZKT7
C	419	HIS	-	expression tag	UNP Q8ZKT7
C	420	HIS	-	expression tag	UNP Q8ZKT7
C	421	HIS	-	expression tag	UNP Q8ZKT7
D	248	ALA	HIS	engineered mutation	UNP Q8ZKT7
D	414	LEU	-	expression tag	UNP Q8ZKT7
D	415	GLU	-	expression tag	UNP Q8ZKT7
D	416	HIS	-	expression tag	UNP Q8ZKT7
D	417	HIS	-	expression tag	UNP Q8ZKT7
D	418	HIS	-	expression tag	UNP Q8ZKT7
D	419	HIS	-	expression tag	UNP Q8ZKT7
D	420	HIS	-	expression tag	UNP Q8ZKT7
D	421	HIS	-	expression tag	UNP Q8ZKT7
E	248	ALA	HIS	engineered mutation	UNP Q8ZKT7
E	414	LEU	-	expression tag	UNP Q8ZKT7
E	415	GLU	-	expression tag	UNP Q8ZKT7
E	416	HIS	-	expression tag	UNP Q8ZKT7
E	417	HIS	-	expression tag	UNP Q8ZKT7
E	418	HIS	-	expression tag	UNP Q8ZKT7
E	419	HIS	-	expression tag	UNP Q8ZKT7
E	420	HIS	-	expression tag	UNP Q8ZKT7
E	421	HIS	-	expression tag	UNP Q8ZKT7
F	248	ALA	HIS	engineered mutation	UNP Q8ZKT7
F	414	LEU	-	expression tag	UNP Q8ZKT7
F	415	GLU	-	expression tag	UNP Q8ZKT7
F	416	HIS	-	expression tag	UNP Q8ZKT7
F	417	HIS	-	expression tag	UNP Q8ZKT7
F	418	HIS	-	expression tag	UNP Q8ZKT7
F	419	HIS	-	expression tag	UNP Q8ZKT7
F	420	HIS	-	expression tag	UNP Q8ZKT7
F	421	HIS	-	expression tag	UNP Q8ZKT7

- Molecule 2 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0
2	E	1	Total C O 12 6 6	0	0
2	F	1	Total C O 12 6 6	0	0

- Molecule 3 is water.

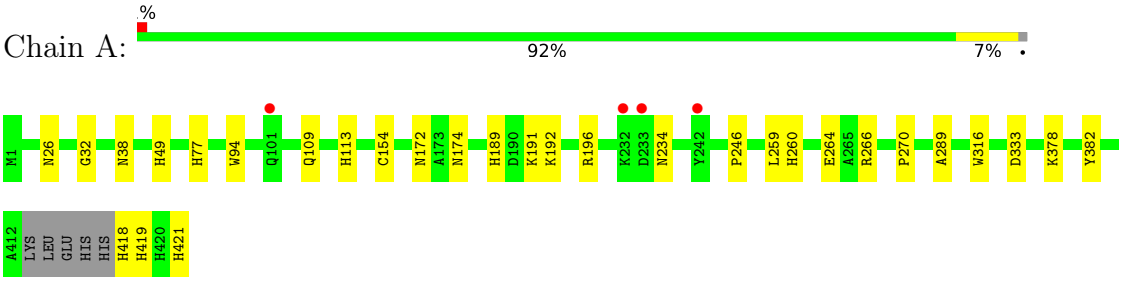
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	505	Total O 505 505	0	0
3	B	480	Total O 480 480	0	0
3	C	521	Total O 521 521	0	0
3	D	493	Total O 493 493	0	0
3	E	473	Total O 473 473	0	0
3	F	469	Total O 469 469	0	0

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.

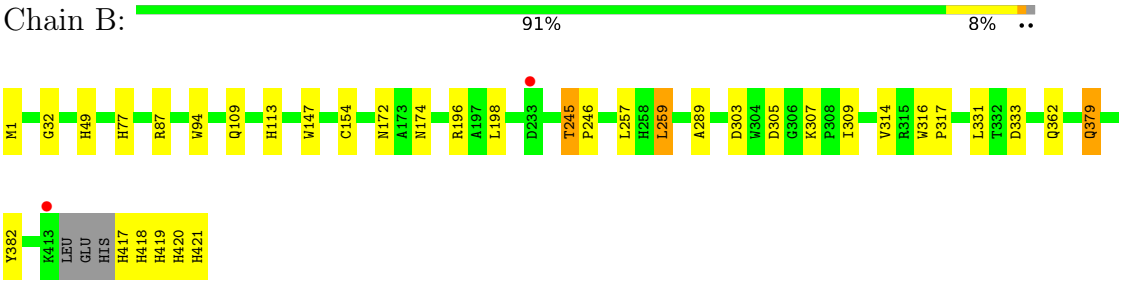
• Molecule 1: Putative isomerase

Chain A:



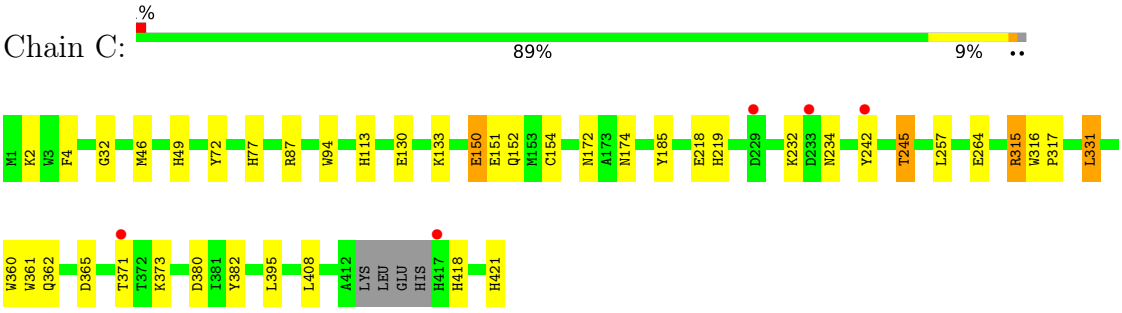
• Molecule 1: Putative isomerase

Chain B:



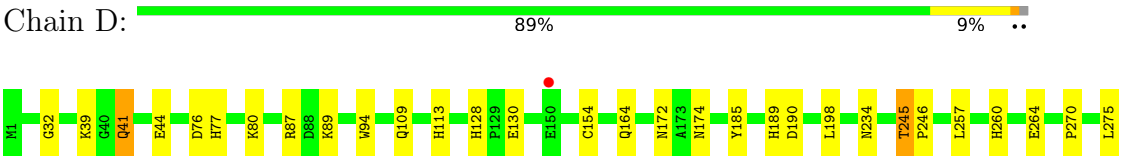
• Molecule 1: Putative isomerase

Chain C:

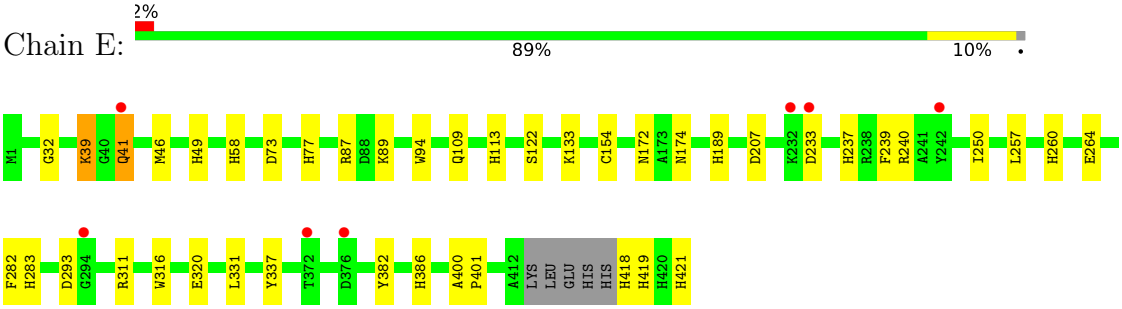


• Molecule 1: Putative isomerase

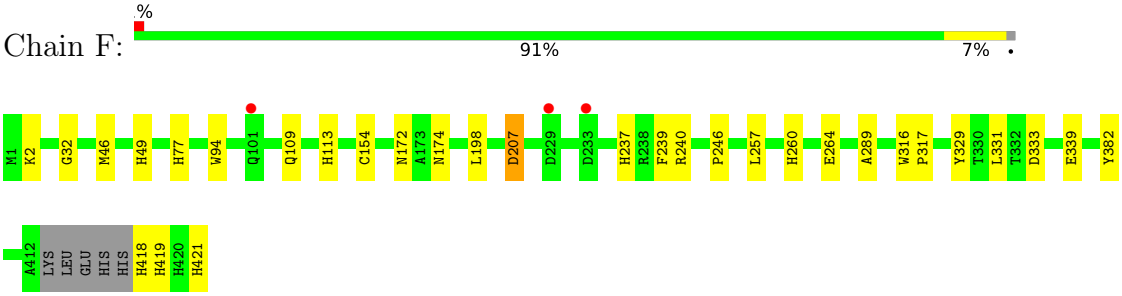
Chain D:



• Molecule 1: Putative isomerase



• Molecule 1: Putative isomerase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	88.23Å 89.81Å 94.73Å 106.86° 104.43° 110.31°	Depositor
Resolution (Å)	15.00 – 1.60 36.85 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.8 (15.00-1.60) 93.8 (36.85-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.152 , 0.182 0.153 , 0.153	Depositor DCC
R_{free} test set	15012 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	11.3	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	23652	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

Bond lengths and bond angles in the following residue types are not validated in this section: BMA

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	0.53	0/3538	0.59	0/4814
1	B	0.51	0/3565	0.59	0/4851
1	C	0.52	0/3595	0.67	4/4889 (0.1%)
1	D	0.52	0/3590	0.60	0/4884
1	E	0.52	0/3587	0.60	0/4878
1	F	0.51	0/3570	0.59	0/4857
All	All	0.52	0/21445	0.61	4/29173 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	315[A]	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	315[B]	ARG	NE-CZ-NH1	9.48	125.04	120.30
1	C	315[A]	ARG	NE-CZ-NH2	-9.07	115.76	120.30
1	C	315[B]	ARG	NE-CZ-NH2	-9.07	115.76	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3415	0	3235	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3438	0	3257	30	0
1	C	3454	0	3292	40	1
1	D	3449	0	3274	36	0
1	E	3447	0	3287	40	2
1	F	3436	0	3247	25	0
2	A	12	0	12	1	0
2	B	12	0	12	1	0
2	C	12	0	12	1	0
2	D	12	0	12	0	0
2	E	12	0	12	1	0
2	F	12	0	12	0	0
3	A	505	0	0	6	1
3	B	480	0	0	9	2
3	C	521	0	0	7	1
3	D	493	0	0	8	1
3	E	473	0	0	6	0
3	F	469	0	0	6	0
All	All	23652	0	19664	179	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 4.

All (179) 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:41[A]:GLN:NE2	1:E:41[A]:GLN:H	1.48	1.09
1:E:41[A]:GLN:H	1:E:41[A]:GLN:HE21	1.13	0.92
1:D:257:LEU:HD22	1:D:331[B]:LEU:HD22	1.54	0.89
1:B:421:HIS:HE1	3:B:740:HOH:O	1.57	0.87
1:C:315[A]:ARG:HD3	1:C:361:TRP:O	1.76	0.85
1:B:303[B]:ASP:OD2	1:B:305:ASP:OD2	1.96	0.83
1:D:39:LYS:HB2	1:D:41[A]:GLN:HE22	1.41	0.83
1:C:365:ASP:HB3	1:C:371[B]:THR:HG21	1.59	0.83
1:F:154:CYS:H	1:F:174:ASN:HD21	1.28	0.81
1:E:39[A]:LYS:CD	1:E:41[A]:GLN:OE1	2.30	0.80
1:D:303[A]:ASP:OD1	1:D:305:ASP:OD1	2.00	0.79
1:B:154:CYS:H	1:B:174:ASN:HD21	1.28	0.79
1:C:154:CYS:H	1:C:174:ASN:HD21	1.29	0.77
1:D:154:CYS:H	1:D:174:ASN:HD21	1.32	0.77
1:E:154:CYS:H	1:E:174:ASN:HD21	1.28	0.77
1:A:154:CYS:H	1:A:174:ASN:HD21	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:39[A]:LYS:HD2	1:E:39[A]:LYS:H	1.49	0.76
1:E:39[A]:LYS:HD3	1:E:41[A]:GLN:OE1	1.86	0.75
1:E:237:HIS:HD2	1:E:239:PHE:H	1.35	0.74
1:C:185:TYR:OH	1:E:189:HIS:HD2	1.69	0.74
1:F:237:HIS:HD2	1:F:239:PHE:H	1.36	0.74
1:C:371[A]:THR:HG21	3:C:719:HOH:O	1.87	0.73
1:E:320:GLU:OE2	1:E:386:HIS:HD2	1.71	0.71
1:B:257:LEU:HD22	1:B:331:LEU:HD12	1.74	0.70
1:F:333[B]:ASP:OD1	3:F:734:HOH:O	2.10	0.70
1:F:421:HIS:HE1	3:F:745:HOH:O	1.76	0.69
1:F:257:LEU:HD22	1:F:331:LEU:HD22	1.75	0.68
1:C:2[B]:LYS:HD2	1:C:418:HIS:CG	2.29	0.68
1:D:39:LYS:CB	1:D:41[A]:GLN:HE22	2.08	0.66
1:D:257:LEU:HD22	1:D:331[B]:LEU:CD2	2.22	0.66
1:E:237:HIS:CD2	1:E:240:ARG:H	2.13	0.66
1:D:245:THR:HG21	3:D:542:HOH:O	1.95	0.65
1:E:58:HIS:HD2	1:E:122:SER:OG	1.79	0.65
1:A:189:HIS:HD2	1:D:185:TYR:OH	1.81	0.64
1:B:245:THR:HG21	3:B:543:HOH:O	1.97	0.64
1:E:39[A]:LYS:HD2	1:E:41[A]:GLN:OE1	1.98	0.64
1:D:257:LEU:HD22	1:D:331[A]:LEU:HD13	1.81	0.62
1:E:421:HIS:HE1	3:E:930:HOH:O	1.81	0.62
1:F:237:HIS:CD2	1:F:240:ARG:H	2.17	0.62
1:F:237:HIS:CD2	1:F:239:PHE:H	2.18	0.61
1:F:2[A]:LYS:NZ	1:F:329:TYR:OH	2.32	0.61
1:E:283:HIS:HE1	1:E:337:TYR:OH	1.83	0.61
1:E:237:HIS:HD2	1:E:240:ARG:H	1.48	0.60
1:F:339:GLU:OE1	3:F:515:HOH:O	2.16	0.60
1:E:293:ASP:OD2	1:E:311:ARG:HD2	2.02	0.59
1:E:133[B]:LYS:HG3	3:E:547:HOH:O	2.02	0.59
1:F:237:HIS:HD2	1:F:240:ARG:H	1.49	0.59
1:C:315[A]:ARG:HD2	1:C:360:TRP:HB2	1.83	0.59
1:C:421:HIS:HD2	1:D:264:GLU:OE2	1.85	0.59
1:A:26:ASN:ND2	3:A:676:HOH:O	2.35	0.59
1:B:257:LEU:HD22	1:B:331:LEU:CD1	2.32	0.58
1:C:365:ASP:HB3	1:C:371[B]:THR:CG2	2.31	0.58
1:F:257:LEU:HD22	1:F:331:LEU:CD2	2.33	0.58
1:D:39:LYS:HB2	1:D:41[A]:GLN:NE2	2.16	0.57
1:E:237:HIS:CD2	1:E:239:PHE:H	2.19	0.57
1:D:419:HIS:H	1:D:419:HIS:CD2	2.22	0.57
1:B:421:HIS:CE1	3:B:740:HOH:O	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:LEU:HD22	1:E:331:LEU:HD12	1.87	0.56
1:B:303[B]:ASP:HB3	1:B:309:ILE:HD11	1.87	0.56
1:C:331:LEU:HD21	1:C:395:LEU:HD12	1.87	0.56
1:B:379:GLN:NE2	3:B:668:HOH:O	2.40	0.55
1:A:32:GLY:O	1:A:77:HIS:HE1	1.90	0.55
1:C:32:GLY:O	1:C:77:HIS:HE1	1.90	0.54
1:D:44:GLU:HG2	3:D:961:HOH:O	2.07	0.54
1:E:87:ARG:HB3	1:E:89:LYS:NZ	2.22	0.54
1:C:245:THR:HG21	3:C:619:HOH:O	2.08	0.53
1:A:266:ARG:HB3	1:D:189:HIS:CD2	2.43	0.53
1:E:419:HIS:H	1:E:419:HIS:CD2	2.27	0.53
1:B:77:HIS:HD2	3:B:968:HOH:O	1.92	0.53
1:D:189:HIS:HE1	3:D:717:HOH:O	1.91	0.53
1:E:87:ARG:HB3	1:E:89:LYS:HZ2	1.74	0.53
1:F:207[A]:ASP:OD1	3:F:937:HOH:O	2.18	0.53
1:C:315[A]:ARG:HD2	1:C:360:TRP:CB	2.39	0.53
1:E:32:GLY:O	1:E:77:HIS:HE1	1.91	0.52
1:D:41[A]:GLN:H	1:D:41[A]:GLN:CD	2.13	0.52
1:C:315[A]:ARG:CD	1:C:361:TRP:O	2.55	0.52
1:F:419:HIS:H	1:F:419:HIS:CD2	2.28	0.52
3:A:557:HOH:O	1:D:189:HIS:HD2	1.93	0.52
1:C:2[B]:LYS:HE2	1:C:4:PHE:O	2.09	0.52
1:D:32:GLY:O	1:D:77:HIS:HE1	1.92	0.51
1:C:362:GLN:HE21	1:C:362:GLN:HA	1.75	0.51
1:E:260:HIS:HD2	3:E:518:HOH:O	1.93	0.51
1:C:218[B]:GLU:HG3	1:C:219:HIS:CE1	2.46	0.51
1:C:130:GLU:HG3	3:C:784:HOH:O	2.10	0.51
1:C:150:GLU:HG3	1:C:151:GLU:N	2.26	0.50
1:F:260:HIS:HD2	3:F:539:HOH:O	1.95	0.50
1:E:58:HIS:HE1	3:E:511:HOH:O	1.94	0.50
1:D:303[A]:ASP:HB3	1:D:309:ILE:HD11	1.94	0.50
1:F:421:HIS:CE1	3:F:745:HOH:O	2.58	0.50
1:D:77:HIS:HD2	3:D:782:HOH:O	1.94	0.50
1:B:362:GLN:HE21	1:B:362:GLN:HA	1.77	0.50
1:D:418:HIS:N	3:D:812:HOH:O	2.45	0.49
1:B:1:MET:HE1	1:C:72:TYR:CD1	2.47	0.49
1:B:32:GLY:O	1:B:77:HIS:HE1	1.95	0.49
1:C:257:LEU:HD22	1:C:331:LEU:HD12	1.95	0.49
1:C:371[B]:THR:HG22	3:C:721:HOH:O	2.12	0.49
1:E:189:HIS:HE1	3:E:546:HOH:O	1.95	0.49
1:F:32:GLY:O	1:F:77:HIS:HE1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:HIS:H	1:B:419:HIS:CD2	2.32	0.48
1:C:371[A]:THR:HG23	3:C:790:HOH:O	2.13	0.48
1:A:419:HIS:H	1:A:419:HIS:CD2	2.31	0.48
1:C:232:LYS:HG2	1:C:242:TYR:CE1	2.48	0.48
1:D:76:ASP:O	1:D:80:LYS:HG2	2.14	0.48
1:A:109:GLN:O	1:A:113:HIS:HD2	1.96	0.47
1:C:245:THR:HG23	3:C:983:HOH:O	2.14	0.47
1:D:303[A]:ASP:CG	1:D:305:ASP:OD1	2.51	0.47
1:D:109:GLN:O	1:D:113:HIS:HD2	1.98	0.47
1:D:260:HIS:CE1	1:D:270:PRO:HG2	2.50	0.47
1:C:264:GLU:OE2	1:D:421:HIS:HD2	1.97	0.46
1:F:94:TRP:H	1:F:113:HIS:CE1	2.33	0.46
1:D:245:THR:CG2	3:D:956:HOH:O	2.63	0.46
1:D:190:ASP:OD1	1:D:190:ASP:C	2.54	0.46
1:F:2[A]:LYS:NZ	1:F:329:TYR:CZ	2.84	0.46
1:F:246:PRO:HG2	1:F:289:ALA:HB2	1.98	0.46
1:C:152:GLN:NE2	3:C:885:HOH:O	2.49	0.45
1:C:46:MET:O	1:C:49:HIS:CE1	2.69	0.45
1:A:264:GLU:OE2	1:F:421:HIS:HD2	1.98	0.45
1:C:316:TRP:CZ2	2:C:503:BMA:H3	2.52	0.45
1:D:419:HIS:H	1:D:419:HIS:HD2	1.64	0.45
1:E:257:LEU:HD22	1:E:331:LEU:CD1	2.47	0.45
1:C:94:TRP:H	1:C:113:HIS:CE1	2.35	0.45
1:B:419:HIS:HE1	3:E:615:HOH:O	1.99	0.44
1:D:128:HIS:HE1	1:D:130[B]:GLU:HG2	1.82	0.44
1:A:49:HIS:HD2	3:A:511:HOH:O	1.99	0.44
1:A:421:HIS:HD2	1:F:264:GLU:OE2	1.99	0.44
1:A:246:PRO:HG2	1:A:289:ALA:HB2	1.99	0.44
1:C:218[B]:GLU:CG	1:C:219:HIS:CE1	3.01	0.44
1:C:331:LEU:HD21	1:C:395:LEU:CD1	2.48	0.44
1:D:246:PRO:HG2	1:D:289:ALA:HB2	2.00	0.44
1:E:316:TRP:CZ2	2:E:505:BMA:H3	2.53	0.44
3:B:658:HOH:O	1:E:419:HIS:HE1	2.00	0.44
1:A:94:TRP:H	1:A:113:HIS:CE1	2.35	0.44
1:E:109:GLN:O	1:E:113:HIS:HD2	2.01	0.43
1:B:314:VAL:O	1:B:317:PRO:HD2	2.18	0.43
1:E:46:MET:O	1:E:49:HIS:CE1	2.71	0.43
1:F:46:MET:O	1:F:49:HIS:CE1	2.71	0.43
1:A:192:LYS:O	1:A:196:ARG:HG3	2.18	0.43
1:A:418:HIS:N	3:A:963:HOH:O	2.51	0.43
1:B:246:PRO:HG2	1:B:289:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:LEU:HD22	1:C:331:LEU:CD1	2.48	0.43
1:B:421:HIS:HD2	1:E:264:GLU:OE2	2.01	0.43
1:C:185:TYR:OH	1:E:189:HIS:CD2	2.60	0.43
1:A:333:ASP:CB	1:F:333[B]:ASP:OD2	2.67	0.42
1:A:421:HIS:HE1	3:A:970:HOH:O	2.02	0.42
1:B:109:GLN:O	1:B:113:HIS:HD2	2.02	0.42
1:C:46:MET:O	1:C:49:HIS:HE1	2.02	0.42
1:B:198[B]:LEU:HG	1:B:259:LEU:HD21	2.01	0.42
1:D:87[A]:ARG:NH2	3:D:733:HOH:O	2.53	0.42
1:B:49:HIS:HD2	3:B:738:HOH:O	2.02	0.42
1:B:333:ASP:OD1	3:B:974:HOH:O	2.22	0.42
1:D:164[A]:GLN:HG2	3:D:800:HOH:O	2.20	0.42
1:A:49:HIS:CD2	3:A:511:HOH:O	2.72	0.42
1:B:417:HIS:HD2	1:B:420:HIS:O	2.03	0.42
1:D:94:TRP:H	1:D:113:HIS:CE1	2.38	0.42
1:B:1:MET:HB2	1:B:1:MET:HE2	1.21	0.41
1:A:316:TRP:CZ2	2:A:501:BMA:H3	2.55	0.41
1:B:316:TRP:CZ2	2:B:502:BMA:H3	2.55	0.41
1:C:315[A]:ARG:NH2	1:C:380:ASP:O	2.48	0.41
1:E:250:ILE:HD11	1:E:282:PHE:CD1	2.56	0.41
1:B:147:TRP:CZ2	1:B:196:ARG:HG2	2.55	0.41
1:A:38:ASN:HD22	1:A:378:LYS:HG3	1.85	0.41
1:B:1:MET:CE	1:C:72:TYR:CD1	3.04	0.41
1:B:94:TRP:H	1:B:113:HIS:CE1	2.39	0.41
1:B:307:LYS:NZ	1:B:307:LYS:HB2	2.36	0.41
1:D:128:HIS:CE1	1:D:130[B]:GLU:HG2	2.55	0.41
1:D:275:LEU:HD13	1:D:331[B]:LEU:HD23	2.03	0.41
1:F:109:GLN:O	1:F:113:HIS:HD2	2.02	0.41
1:A:260:HIS:CE1	1:A:270:PRO:HG2	2.56	0.40
1:B:245:THR:CG2	3:B:931:HOH:O	2.68	0.40
1:C:232:LYS:HG2	1:C:242:TYR:CD1	2.56	0.40
1:E:94:TRP:H	1:E:113:HIS:CE1	2.38	0.40
1:C:316:TRP:CG	1:C:317:PRO:HD3	2.55	0.40
1:E:400:ALA:HB3	1:E:401:PRO:HD3	2.04	0.40
1:F:316:TRP:CG	1:F:317:PRO:HD3	2.56	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)
1:C:150:GLU:OE2	3:D:588:HOH:O[1_565]	1.40	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41[B]:GLN:OE1	3:B:608:HOH:O[1_655]	1.77	0.43
3:A:739:HOH:O	3:C:666:HOH:O[1_545]	2.11	0.09
1:E:39[A]:LYS:CE	3:B:604:HOH:O[1_655]	2.14	0.06

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	416/421 (99%)	402 (97%)	14 (3%)	0	100	100
1	B	419/421 (100%)	406 (97%)	13 (3%)	0	100	100
1	C	423/421 (100%)	412 (97%)	11 (3%)	0	100	100
1	D	422/421 (100%)	409 (97%)	13 (3%)	0	100	100
1	E	422/421 (100%)	410 (97%)	12 (3%)	0	100	100
1	F	420/421 (100%)	407 (97%)	13 (3%)	0	100	100
All	All	2522/2526 (100%)	2446 (97%)	76 (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	345/346 (100%)	340 (99%)	5 (1%)	67	47
1	B	348/346 (101%)	341 (98%)	7 (2%)	55	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	352/346 (102%)	342 (97%)	10 (3%)	43 18
1	D	351/346 (101%)	338 (96%)	13 (4%)	34 11
1	E	351/346 (101%)	340 (97%)	11 (3%)	40 15
1	F	349/346 (101%)	343 (98%)	6 (2%)	60 38
All	All	2096/2076 (101%)	2044 (98%)	52 (2%)	52 22

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	191	LYS
1	A	234	ASN
1	A	259	LEU
1	A	382	TYR
1	B	87	ARG
1	B	172	ASN
1	B	245	THR
1	B	259	LEU
1	B	379	GLN
1	B	382	TYR
1	B	418	HIS
1	C	87	ARG
1	C	133	LYS
1	C	150	GLU
1	C	172	ASN
1	C	234	ASN
1	C	245	THR
1	C	331	LEU
1	C	373	LYS
1	C	382	TYR
1	C	408	LEU
1	D	41[A]	GLN
1	D	41[B]	GLN
1	D	89	LYS
1	D	172	ASN
1	D	198	LEU
1	D	234	ASN
1	D	245	THR
1	D	331[A]	LEU
1	D	331[B]	LEU
1	D	379[A]	GLN

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Mol	Chain	Res	Type
1	D	379[B]	GLN
1	D	382	TYR
1	D	419	HIS
1	E	39[A]	LYS
1	E	39[B]	LYS
1	E	41[A]	GLN
1	E	41[B]	GLN
1	E	73	ASP
1	E	172	ASN
1	E	207[A]	ASP
1	E	207[B]	ASP
1	E	233	ASP
1	E	382	TYR
1	E	418	HIS
1	F	172	ASN
1	F	198	LEU
1	F	207[A]	ASP
1	F	207[B]	ASP
1	F	382	TYR
1	F	418	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	38	ASN
1	A	49	HIS
1	A	77	HIS
1	A	113	HIS
1	A	172	ASN
1	A	174	ASN
1	A	189	HIS
1	A	217	ASN
1	A	234	ASN
1	A	419	HIS
1	A	421	HIS
1	B	10	ASN
1	B	49	HIS
1	B	77	HIS
1	B	113	HIS
1	B	152	GLN
1	B	172	ASN

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Mol	Chain	Res	Type
1	B	174	ASN
1	B	217	ASN
1	B	362	GLN
1	B	379	GLN
1	B	419	HIS
1	B	421	HIS
1	C	38	ASN
1	C	49	HIS
1	C	77	HIS
1	C	113	HIS
1	C	152	GLN
1	C	164	GLN
1	C	172	ASN
1	C	174	ASN
1	C	217	ASN
1	C	234	ASN
1	C	362	GLN
1	C	419	HIS
1	C	421	HIS
1	D	49	HIS
1	D	77	HIS
1	D	83	ASN
1	D	101	GLN
1	D	113	HIS
1	D	152	GLN
1	D	172	ASN
1	D	174	ASN
1	D	189	HIS
1	D	217	ASN
1	D	234	ASN
1	D	419	HIS
1	D	421	HIS
1	E	38	ASN
1	E	49	HIS
1	E	58	HIS
1	E	77	HIS
1	E	113	HIS
1	E	172	ASN
1	E	174	ASN
1	E	189	HIS
1	E	217	ASN
1	E	231	ASN

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Mol	Chain	Res	Type
1	E	237	HIS
1	E	260	HIS
1	E	283	HIS
1	E	386	HIS
1	E	419	HIS
1	E	421	HIS
1	F	49	HIS
1	F	77	HIS
1	F	113	HIS
1	F	152	GLN
1	F	172	ASN
1	F	174	ASN
1	F	217	ASN
1	F	237	HIS
1	F	260	HIS
1	F	419	HIS
1	F	421	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

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BMA	A	501	-	12,12,12	0.50	0	17,17,17	0.69	0
2	BMA	D	504	-	12,12,12	0.48	0	17,17,17	0.60	0
2	BMA	B	502	-	12,12,12	0.52	0	17,17,17	0.75	0
2	BMA	C	503	-	12,12,12	0.49	0	17,17,17	0.79	0
2	BMA	F	506	-	12,12,12	0.47	0	17,17,17	0.59	0
2	BMA	E	505	-	12,12,12	0.51	0	17,17,17	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	A	501	-	-	0/2/22/22	0/1/1/1
2	BMA	D	504	-	-	0/2/22/22	0/1/1/1
2	BMA	B	502	-	-	0/2/22/22	0/1/1/1
2	BMA	C	503	-	-	0/2/22/22	0/1/1/1
2	BMA	F	506	-	-	0/2/22/22	0/1/1/1
2	BMA	E	505	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	BMA	1	0
2	B	502	BMA	1	0
2	C	503	BMA	1	0
2	E	505	BMA	1	0

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

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	416/421 (98%)	-0.26	4 (0%)	82	82	6, 10, 18, 25	0
1	B	418/421 (99%)	-0.23	2 (0%)	91	90	6, 11, 19, 27	0
1	C	417/421 (99%)	-0.24	5 (1%)	79	78	6, 9, 19, 30	0
1	D	416/421 (98%)	-0.26	1 (0%)	95	94	6, 10, 17, 23	0
1	E	416/421 (98%)	-0.19	7 (1%)	70	69	5, 10, 20, 33	0
1	F	416/421 (98%)	-0.22	3 (0%)	87	87	6, 10, 18, 25	0
All	All	2499/2526 (98%)	-0.23	22 (0%)	84	84	5, 10, 19, 33	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	233[A]	ASP	4.3
1	E	233	ASP	4.1
1	E	232	LYS	3.7
1	E	372	THR	3.7
1	B	413	LYS	3.3
1	B	233	ASP	3.0
1	C	229[A]	ASP	2.9
1	E	376	ASP	2.8
1	A	232	LYS	2.7
1	C	417	HIS	2.6
1	C	233	ASP	2.6
1	F	101	GLN	2.6
1	A	242	TYR	2.5
1	A	101	GLN	2.5
1	F	233[A]	ASP	2.4
1	C	242	TYR	2.4
1	E	41[A]	GLN	2.2
1	E	294	GLY	2.1
1	D	150	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	242	TYR	2.0
1	C	371[A]	THR	2.0
1	F	229	ASP	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BMA	E	505	12/12	0.97	0.08	9,11,11,12	0
2	BMA	B	502	12/12	0.98	0.10	8,9,10,10	0
2	BMA	C	503	12/12	0.98	0.07	9,11,12,13	0
2	BMA	D	504	12/12	0.98	0.12	7,8,9,9	0
2	BMA	A	501	12/12	0.98	0.09	7,9,10,10	0
2	BMA	F	506	12/12	0.98	0.10	8,9,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.