Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 11:30 AM EST

PDB ID	:	2NZW
Title	:	Crystal Structure of alpha1,3-Fucosyltransferase
Authors	:	Sun, H.Y.; Ko, T.P.
Deposited on	:	2006-11-27
Resolution	:	1.90 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:

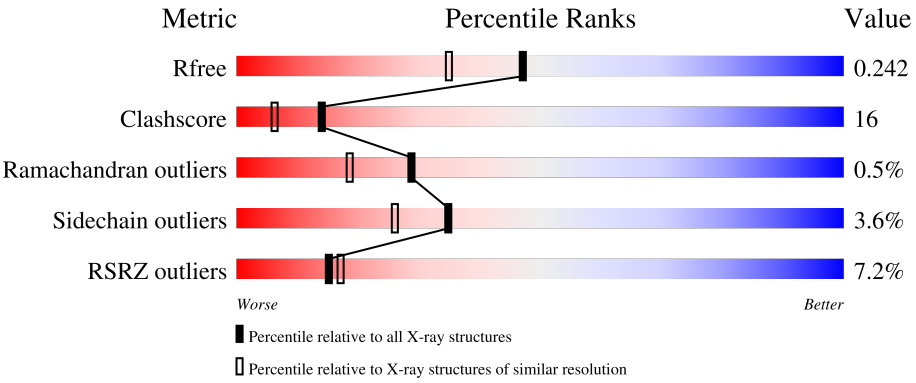
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	371	8% 69% 23% • 6%
1	B	371	7% 68% 21% •• 9%
1	C	371	5% 76% 16% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10265 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 Alpha1,3-fucosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2860	1852	467	534	7			
1	B	338	Total	C	N	O	S	0	0	0
			2776	1797	452	520	7			
1	C	351	Total	C	N	O	S	0	0	0
			2879	1867	469	536	7			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	364	LEU	-	expression tag	UNP O30511
A	365	GLU	-	expression tag	UNP O30511
A	366	HIS	-	expression tag	UNP O30511
A	367	HIS	-	expression tag	UNP O30511
A	368	HIS	-	expression tag	UNP O30511
A	369	HIS	-	expression tag	UNP O30511
A	370	HIS	-	expression tag	UNP O30511
A	371	HIS	-	expression tag	UNP O30511
B	364	LEU	-	expression tag	UNP O30511
B	365	GLU	-	expression tag	UNP O30511
B	366	HIS	-	expression tag	UNP O30511
B	367	HIS	-	expression tag	UNP O30511
B	368	HIS	-	expression tag	UNP O30511
B	369	HIS	-	expression tag	UNP O30511
B	370	HIS	-	expression tag	UNP O30511
B	371	HIS	-	expression tag	UNP O30511
C	364	LEU	-	expression tag	UNP O30511
C	365	GLU	-	expression tag	UNP O30511
C	366	HIS	-	expression tag	UNP O30511
C	367	HIS	-	expression tag	UNP O30511
C	368	HIS	-	expression tag	UNP O30511
C	369	HIS	-	expression tag	UNP O30511
C	370	HIS	-	expression tag	UNP O30511

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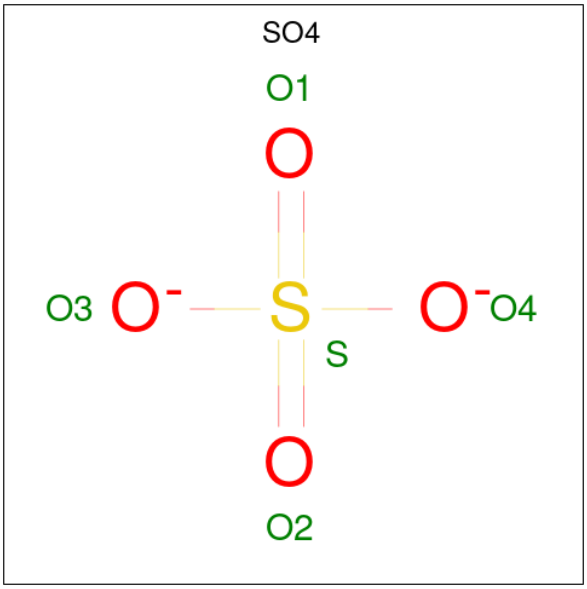
Chain	Residue	Modelled	Actual	Comment	Reference
C	371	HIS	-	expression tag	UNP O30511

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

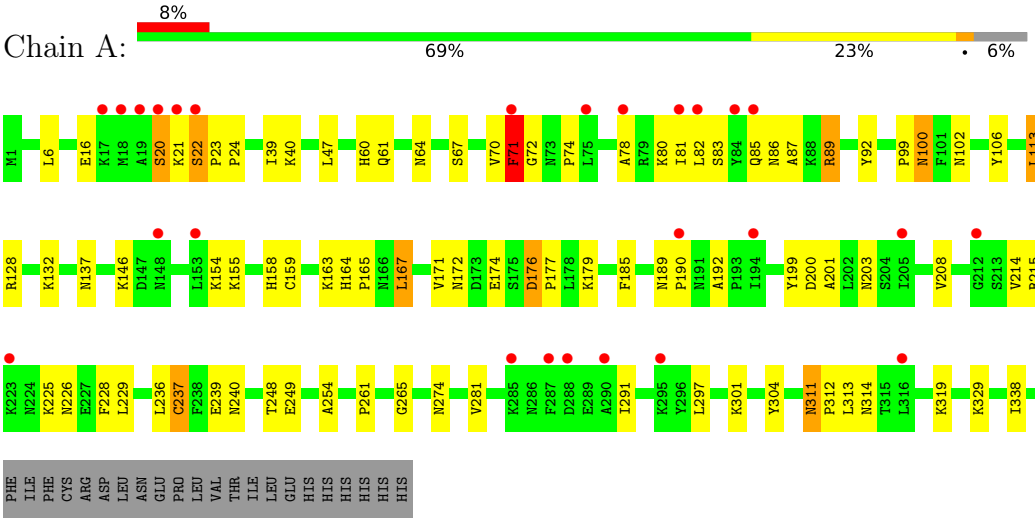
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	559	Total O 559 559	0	0
3	B	522	Total O 522 522	0	0
3	C	654	Total O 654 654	0	0

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.

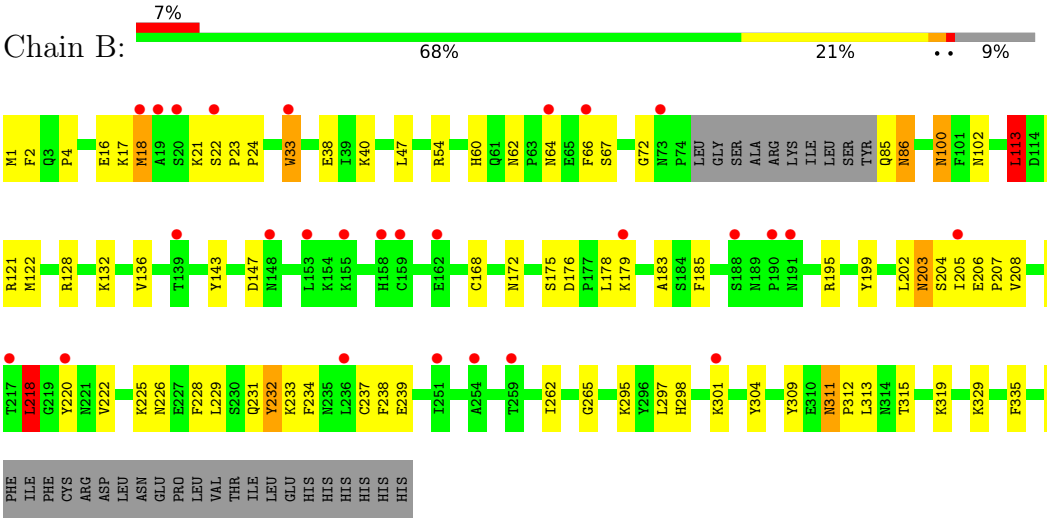
• Molecule 1: Alpha1,3-fucosyltransferase

Chain A:



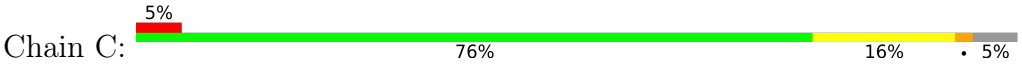
• Molecule 1: Alpha1,3-fucosyltransferase

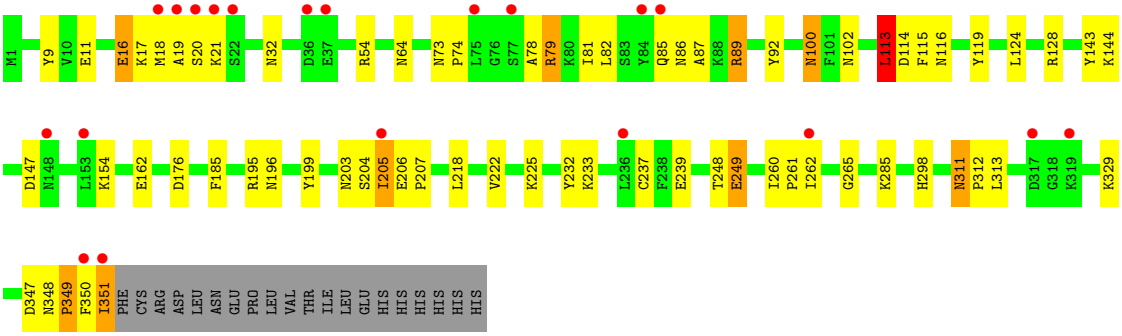
Chain B:



• Molecule 1: Alpha1,3-fucosyltransferase

Chain C:




M1 Y9 V10 E11 E16 K17 M18 A19 S20 K21 S22 N32 D36 E37 R54 N64 N73 P74 L75 G76 S77 A78 R79 K80 I81 L82 S83 Y84 Q85 N86 A87 K88 R89 Y92 N100 F101 N102 L113 D114 F115 N116 Y119 L124 R128 Y143 K144
D147 M148 L153 K154 E162 D176 F185 R195 N196 Y199 N203 S204 I205 E206 P207 L218 V222 K225 Y232 K233 L236 C237 F238 E239 T248 E249 I260 P261 I262 G265 K285 H298 N311 P312 L313 D317 G318 K319 K329
D347 N348 P349 F350 I351 PHE CYS ARG ASP LEU ASN GLU PRO LEU VAL THR ILE LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	104.55Å 136.20Å 96.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.54 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.9 (30.00-1.90) 92.1 (29.54-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 1.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.191 , 0.242 0.192 , 0.242	Depositor DCC
R_{free} test set	5075 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10265	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: SO4

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	0.93	2/2946 (0.1%)	0.87	4/3999 (0.1%)
1	B	0.88	1/2859 (0.0%)	0.85	3/3880 (0.1%)
1	C	1.01	2/2966 (0.1%)	0.93	7/4026 (0.2%)
All	All	0.94	5/8771 (0.1%)	0.89	14/11905 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	237	CYS	CB-SG	-8.98	1.67	1.82
1	C	249	GLU	CG-CD	6.81	1.62	1.51
1	A	71	PHE	CB-CG	-5.49	1.42	1.51
1	C	237	CYS	CB-SG	-5.35	1.73	1.81
1	B	237	CYS	CB-SG	-5.11	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	89	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	113	LEU	CA-CB-CG	7.57	132.71	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	113	LEU	CA-CB-CG	7.33	132.15	115.30
1	C	113	LEU	CA-CB-CG	7.15	131.75	115.30
1	B	121	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	20	SER	N-CA-C	6.27	127.94	111.00
1	C	79	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	C	176	ASP	CB-CG-OD1	5.95	123.66	118.30
1	C	262	ILE	N-CA-C	-5.88	95.12	111.00
1	B	262	ILE	N-CA-C	-5.63	95.78	111.00
1	C	79	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	C	89	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	176	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	137	ASN	N-CA-C	-5.08	97.27	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	TYR	Sidechain
1	B	232	TYR	Sidechain
1	C	232	TYR	Sidechain
1	C	9	TYR	Sidechain

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	2860	0	2747	95	0
1	B	2776	0	2653	92	0
1	C	2879	0	2767	79	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
3	A	559	0	0	27	0
3	B	522	0	0	13	1
3	C	654	0	0	23	0
All	All	10265	0	8167	262	1

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 16.

All (262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:MET:SD	1:B:122:MET:CE	2.02	1.48
1:C:87:ALA:HB1	3:C:2615:HOH:O	1.49	1.10
1:A:87:ALA:HB1	3:A:530:HOH:O	1.55	1.07
1:B:132:LYS:NZ	1:B:226:ASN:HD21	1.62	0.97
1:B:60:HIS:HD2	1:B:62:ASN:H	1.10	0.96
1:A:189:ASN:HD22	1:A:190:PRO:HD2	1.29	0.96
1:C:82:LEU:HD11	1:C:89:ARG:HD3	1.52	0.91
1:A:74:PRO:HD2	3:A:818:HOH:O	1.70	0.90
1:C:86:ASN:HA	1:C:89:ARG:HH21	1.37	0.90
1:C:86:ASN:CA	1:C:89:ARG:HH21	1.86	0.88
1:A:222:VAL:HG21	1:A:228:PHE:HB2	1.57	0.87
1:C:86:ASN:HA	1:C:89:ARG:NH2	1.89	0.87
1:B:176:ASP:OD2	1:B:179:LYS:HG3	1.75	0.85
1:A:74:PRO:CD	3:A:818:HOH:O	2.26	0.80
1:C:32:ASN:ND2	3:C:2594:HOH:O	2.15	0.80
1:C:347:ASP:O	1:C:349:PRO:HD3	1.82	0.79
1:C:16:GLU:H	1:C:16:GLU:CD	1.86	0.79
1:C:349:PRO:HA	3:C:2619:HOH:O	1.82	0.79
1:B:132:LYS:HZ1	1:B:226:ASN:HD21	1.30	0.77
1:B:203:ASN:HA	1:B:208:VAL:HG23	1.67	0.77
1:A:132:LYS:HZ2	1:A:226:ASN:HD21	1.31	0.77
1:B:315:THR:HG23	3:B:2073:HOH:O	1.85	0.76
1:B:132:LYS:HZ2	1:B:226:ASN:HD21	1.34	0.75
1:A:189:ASN:HD22	1:A:190:PRO:CD	2.01	0.73
1:B:168:CYS:O	1:B:172:ASN:HB2	1.88	0.73
1:A:132:LYS:NZ	1:A:226:ASN:HD21	1.87	0.73
1:B:100:ASN:C	1:B:100:ASN:HD22	1.92	0.72
1:A:72:GLY:N	3:A:895:HOH:O	2.22	0.71
1:C:351:ILE:HD13	1:C:351:ILE:O	1.91	0.71
1:B:72:GLY:HA3	3:B:2313:HOH:O	1.89	0.71
1:C:86:ASN:N	1:C:89:ARG:HH21	1.89	0.71
1:C:195:ARG:HH11	1:C:196:ASN:HD21	1.36	0.71
1:A:87:ALA:HA	3:A:804:HOH:O	1.90	0.70
1:B:16:GLU:OE2	1:B:329:LYS:HE2	1.90	0.70
1:C:21:LYS:HD2	3:C:2649:HOH:O	1.90	0.70
1:A:22:SER:N	1:A:23:PRO:HD3	2.08	0.69
1:C:351:ILE:C	3:C:2618:HOH:O	2.29	0.69
1:B:218:LEU:HD22	1:B:218:LEU:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASN:C	1:A:100:ASN:HD22	1.96	0.69
1:A:64:ASN:ND2	1:C:348:ASN:HD22	1.91	0.69
1:B:17:LYS:HG2	3:B:2513:HOH:O	1.91	0.69
1:A:87:ALA:CB	3:A:530:HOH:O	2.27	0.68
1:C:20:SER:HB3	3:C:2328:HOH:O	1.94	0.68
1:C:205:ILE:HG22	1:C:206:GLU:HB2	1.74	0.67
1:B:18:MET:HE3	1:B:21:LYS:HG3	1.75	0.67
1:B:222:VAL:HG21	1:B:228:PHE:HB2	1.75	0.67
1:C:128:ARG:HB2	1:C:249:GLU:HB3	1.77	0.67
1:B:16:GLU:CD	1:B:16:GLU:H	1.96	0.66
1:C:162:GLU:HG3	3:C:2213:HOH:O	1.95	0.66
1:C:116:ASN:ND2	3:C:2599:HOH:O	2.07	0.66
1:C:154:LYS:HE2	3:C:2341:HOH:O	1.95	0.66
1:B:60:HIS:CD2	1:B:62:ASN:H	2.03	0.65
1:B:132:LYS:HZ2	1:B:226:ASN:ND2	1.93	0.65
1:C:206:GLU:OE1	1:C:298:HIS:HE1	1.80	0.65
1:C:18:MET:HA	3:C:2656:HOH:O	1.96	0.65
1:B:348:ASN:C	3:B:2504:HOH:O	2.35	0.64
1:A:21:LYS:C	1:A:23:PRO:HD3	2.18	0.64
1:B:33:TRP:HH2	3:B:2314:HOH:O	1.79	0.64
1:B:203:ASN:ND2	1:B:207:PRO:HA	2.13	0.64
1:B:311:ASN:ND2	1:B:313:LEU:H	1.96	0.63
1:B:100:ASN:HD21	1:B:102:ASN:HB2	1.62	0.63
1:C:82:LEU:CD1	1:C:89:ARG:HD3	2.27	0.63
1:A:64:ASN:HD22	1:C:348:ASN:HD22	1.45	0.63
1:B:206:GLU:HG2	1:B:207:PRO:HD2	1.81	0.62
1:A:87:ALA:CA	3:A:530:HOH:O	2.46	0.62
1:B:18:MET:CE	1:B:21:LYS:HG3	2.31	0.61
1:B:178:LEU:HD11	1:B:301:LYS:HB2	1.83	0.61
1:B:311:ASN:HD22	1:B:313:LEU:H	1.48	0.61
1:B:18:MET:HE1	1:B:21:LYS:HE3	1.83	0.61
1:C:204:SER:HB2	3:C:2144:HOH:O	2.01	0.61
1:A:189:ASN:ND2	1:A:190:PRO:HD2	2.09	0.61
1:B:100:ASN:HD22	1:B:102:ASN:H	1.50	0.60
1:C:86:ASN:H	1:C:89:ARG:HH21	1.49	0.60
1:C:85:GLN:O	1:C:86:ASN:C	2.39	0.60
1:C:195:ARG:HH11	1:C:196:ASN:ND2	1.99	0.60
1:A:39:ILE:HD11	1:A:61:GLN:OE1	2.03	0.59
1:C:100:ASN:C	1:C:100:ASN:HD22	2.05	0.59
1:B:225:LYS:O	1:B:229:LEU:HG	2.02	0.59
1:B:100:ASN:ND2	1:B:102:ASN:H	2.00	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:O	1:B:4:PRO:HD2	2.03	0.58
1:B:311:ASN:HD22	1:B:312:PRO:N	2.01	0.58
1:C:16:GLU:OE2	1:C:54:ARG:NH2	2.37	0.57
1:C:78:ALA:HB1	3:C:2594:HOH:O	2.04	0.57
1:B:132:LYS:NZ	1:B:226:ASN:ND2	2.42	0.57
1:C:100:ASN:HD21	1:C:102:ASN:HB2	1.68	0.57
1:A:81:ILE:HG22	1:C:350:PHE:CZ	2.40	0.57
1:B:185:PHE:CE1	1:B:195:ARG:HD3	2.40	0.57
1:A:100:ASN:ND2	1:A:102:ASN:H	2.03	0.57
1:B:215:ARG:H	1:B:215:ARG:HD3	1.70	0.56
1:A:200:ASP:OD1	1:A:215:ARG:NH1	2.38	0.56
1:B:38:GLU:N	1:B:38:GLU:OE1	2.39	0.56
1:B:233:LYS:HB3	1:B:304:TYR:CE2	2.40	0.56
1:A:82:LEU:HD11	1:A:89:ARG:HD3	1.85	0.56
1:A:248:THR:HB	1:A:249:GLU:OE2	2.06	0.56
1:A:70:VAL:HG23	1:A:87:ALA:HB3	1.88	0.56
1:A:85:GLN:O	1:A:86:ASN:C	2.45	0.56
1:A:239:GLU:HG3	1:A:265:GLY:HA3	1.88	0.56
1:B:195:ARG:HG3	1:B:238:PHE:HB2	1.88	0.56
1:A:176:ASP:OD2	1:A:179:LYS:HG3	2.06	0.55
1:A:100:ASN:HD22	1:A:102:ASN:H	1.54	0.55
1:C:205:ILE:HG22	1:C:206:GLU:N	2.20	0.55
1:C:100:ASN:HD22	1:C:102:ASN:H	1.53	0.55
1:C:249:GLU:HG2	3:C:2101:HOH:O	2.05	0.55
1:A:222:VAL:HG21	1:A:228:PHE:CB	2.34	0.55
1:A:47:LEU:HD21	1:A:71:PHE:HZ	1.71	0.55
1:B:218:LEU:H	1:B:218:LEU:CD2	2.19	0.54
1:C:32:ASN:HB2	3:C:2309:HOH:O	2.07	0.54
1:C:81:ILE:O	1:C:85:GLN:HG3	2.07	0.54
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.71	0.54
1:B:232:TYR:N	1:B:232:TYR:CD1	2.75	0.54
1:B:215:ARG:HD3	1:B:215:ARG:N	2.21	0.54
1:C:92:TYR:C	1:C:92:TYR:CD2	2.80	0.54
1:B:33:TRP:CD1	1:B:33:TRP:N	2.75	0.54
1:B:22:SER:OG	3:B:2516:HOH:O	2.19	0.54
1:C:87:ALA:HA	3:C:2534:HOH:O	2.07	0.54
1:B:231:GLN:HB2	1:B:232:TYR:CE1	2.42	0.54
1:A:311:ASN:HD22	1:A:312:PRO:N	2.06	0.53
1:C:311:ASN:HD22	1:C:312:PRO:N	2.06	0.53
1:A:132:LYS:NZ	3:A:702:HOH:O	2.41	0.53
1:B:203:ASN:ND2	1:B:208:VAL:H	2.04	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:PHE:HD2	3:B:2413:HOH:O	1.91	0.53
1:A:281:VAL:HG12	1:A:281:VAL:O	2.09	0.53
1:B:205:ILE:HD11	1:B:295:LYS:HG3	1.90	0.53
1:A:80:LYS:O	1:A:83:SER:HB2	2.09	0.53
1:C:82:LEU:HA	1:C:85:GLN:HE21	1.75	0.52
1:A:20:SER:HB3	3:A:930:HOH:O	2.09	0.52
1:C:100:ASN:ND2	1:C:102:ASN:H	2.07	0.52
1:B:62:ASN:OD1	1:B:64:ASN:HB2	2.09	0.52
1:B:233:LYS:HD3	1:B:298:HIS:CE1	2.44	0.52
1:A:132:LYS:HZ2	1:A:226:ASN:ND2	2.03	0.52
1:C:195:ARG:NH1	1:C:196:ASN:HD21	2.07	0.52
1:A:100:ASN:HD21	1:A:102:ASN:HB2	1.75	0.52
1:A:86:ASN:ND2	1:A:346:HIS:NE2	2.58	0.51
1:A:60:HIS:HD2	1:A:67:SER:OG	1.94	0.51
1:B:218:LEU:CD2	1:B:218:LEU:N	2.73	0.51
1:C:73:ASN:OD1	1:C:79:ARG:NH1	2.44	0.51
1:A:297:LEU:O	1:A:304:TYR:HB2	2.11	0.51
1:A:85:GLN:C	1:A:87:ALA:N	2.58	0.51
1:C:78:ALA:CB	3:C:2594:HOH:O	2.59	0.51
1:A:199:TYR:CD1	1:A:199:TYR:C	2.84	0.51
1:A:146:LYS:HE3	3:A:884:HOH:O	2.10	0.50
1:A:311:ASN:ND2	1:A:313:LEU:H	2.10	0.50
1:C:85:GLN:C	1:C:87:ALA:N	2.62	0.50
1:B:16:GLU:OE1	1:B:54:ARG:NH2	2.37	0.50
1:C:218:LEU:CD2	1:C:222:VAL:HG13	2.42	0.50
1:B:40:LYS:HA	3:B:2439:HOH:O	2.10	0.50
1:A:254:ALA:HB3	1:A:261:PRO:HG3	1.93	0.50
1:B:311:ASN:HD22	1:B:311:ASN:C	2.14	0.50
1:B:205:ILE:HG12	1:B:295:LYS:HG2	1.94	0.50
1:B:202:LEU:C	1:B:204:SER:H	2.15	0.49
1:B:38:GLU:HG2	3:B:2171:HOH:O	2.10	0.49
1:B:113:LEU:HD22	1:B:119:TYR:CD2	2.48	0.49
1:A:116:ASN:ND2	3:A:497:HOH:O	2.26	0.49
1:A:249:GLU:CD	1:A:249:GLU:H	2.16	0.49
1:B:1:MET:HE2	3:B:2060:HOH:O	2.11	0.49
1:B:297:LEU:O	1:B:304:TYR:HB2	2.13	0.49
1:A:70:VAL:CG2	1:A:87:ALA:HB3	2.42	0.49
1:A:154:LYS:HE3	3:A:548:HOH:O	2.13	0.49
1:C:124:LEU:HB2	1:C:248:THR:HA	1.93	0.49
1:C:113:LEU:C	1:C:113:LEU:HD23	2.32	0.49
1:A:78:ALA:HA	1:A:81:ILE:CD1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ALA:HA	1:A:81:ILE:HD11	1.94	0.49
1:B:17:LYS:O	1:B:18:MET:C	2.50	0.49
1:A:106:TYR:CD2	1:A:338:ILE:HG12	2.48	0.48
1:A:167:LEU:HD12	1:A:167:LEU:O	2.13	0.48
1:A:146:LYS:CE	3:A:884:HOH:O	2.60	0.48
1:A:72:GLY:CA	3:A:895:HOH:O	2.60	0.48
1:A:201:ALA:O	1:A:291:ILE:HD12	2.13	0.48
1:B:199:TYR:CD1	1:B:199:TYR:C	2.86	0.48
1:A:348:ASN:HD22	1:C:64:ASN:HD22	1.61	0.48
1:C:86:ASN:CA	1:C:89:ARG:NH2	2.60	0.48
1:C:74:PRO:O	1:C:79:ARG:HB2	2.14	0.48
1:A:71:PHE:C	3:A:895:HOH:O	2.52	0.48
1:A:214:VAL:HG12	1:A:215:ARG:HG2	1.96	0.48
1:A:22:SER:N	1:A:23:PRO:CD	2.75	0.47
1:C:87:ALA:O	1:C:89:ARG:HG3	2.14	0.47
1:B:205:ILE:CD1	1:B:295:LYS:HG3	2.44	0.47
1:B:218:LEU:HG	1:B:220:TYR:CE2	2.50	0.47
1:A:192:ALA:HB2	3:A:624:HOH:O	2.15	0.47
1:B:185:PHE:HE1	1:B:195:ARG:HD3	1.79	0.47
1:C:143:TYR:C	1:C:144:LYS:HD3	2.35	0.47
1:C:185:PHE:CZ	1:C:195:ARG:HD3	2.50	0.47
1:C:185:PHE:HZ	1:C:195:ARG:HD3	1.79	0.47
1:C:285:LYS:CG	3:C:2380:HOH:O	2.63	0.47
1:B:215:ARG:HG3	1:B:215:ARG:NH1	2.29	0.47
1:C:285:LYS:HD3	3:C:2380:HOH:O	2.13	0.47
1:A:329:LYS:HG2	3:A:387:HOH:O	2.15	0.46
1:B:346:HIS:HD2	1:B:347:ASP:O	1.98	0.46
1:B:100:ASN:C	1:B:100:ASN:ND2	2.65	0.46
1:C:16:GLU:OE1	1:C:329:LYS:HE2	2.15	0.46
1:A:128:ARG:HB2	1:A:249:GLU:HB3	1.98	0.46
1:B:85:GLN:N	3:B:2414:HOH:O	2.48	0.46
1:A:281:VAL:O	1:A:281:VAL:CG1	2.64	0.46
1:B:60:HIS:HD2	1:B:62:ASN:N	1.94	0.46
1:A:311:ASN:HD22	1:A:313:LEU:H	1.63	0.45
1:B:86:ASN:HD22	1:B:86:ASN:HA	1.36	0.45
1:B:218:LEU:O	1:B:220:TYR:CD2	2.68	0.45
1:C:311:ASN:ND2	1:C:313:LEU:H	2.14	0.45
1:A:225:LYS:HE2	1:A:229:LEU:HD11	1.98	0.45
1:C:311:ASN:HD22	1:C:313:LEU:H	1.65	0.45
1:A:82:LEU:HD22	3:A:818:HOH:O	2.16	0.45
1:A:349:PRO:HD2	3:C:2559:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:PRO:HA	1:B:24:PRO:HD2	1.91	0.45
1:B:2:PHE:HB3	1:B:143:TYR:CE2	2.52	0.45
1:C:79:ARG:O	1:C:82:LEU:HB3	2.17	0.45
1:A:20:SER:CB	3:A:930:HOH:O	2.65	0.45
1:A:226:ASN:HB2	3:A:559:HOH:O	2.17	0.44
1:C:113:LEU:HD23	1:C:114:ASP:N	2.33	0.44
1:A:254:ALA:CB	1:A:261:PRO:HG3	2.46	0.44
1:A:329:LYS:HE2	3:A:387:HOH:O	2.17	0.44
1:B:22:SER:OG	1:B:23:PRO:HD2	2.17	0.44
1:B:122:MET:CE	1:B:122:MET:CG	2.92	0.44
1:C:203:ASN:OD1	1:C:207:PRO:HA	2.16	0.44
1:B:183:ALA:HA	1:B:234:PHE:O	2.18	0.44
1:A:172:ASN:O	1:A:174:GLU:HG3	2.18	0.44
1:C:113:LEU:HD22	1:C:119:TYR:CD2	2.53	0.44
1:B:47:LEU:HD11	1:B:335:PHE:CE2	2.52	0.44
1:B:60:HIS:HE1	1:B:67:SER:OG	2.01	0.44
1:B:168:CYS:O	1:B:172:ASN:CB	2.62	0.44
1:B:202:LEU:C	1:B:204:SER:N	2.71	0.44
1:A:87:ALA:HA	3:A:530:HOH:O	2.14	0.43
1:C:199:TYR:CD1	1:C:199:TYR:C	2.91	0.43
1:A:23:PRO:HA	1:A:24:PRO:HD2	1.88	0.43
1:B:319:LYS:NZ	3:B:2291:HOH:O	2.52	0.43
1:C:124:LEU:HD12	1:C:248:THR:HG22	2.01	0.43
1:C:78:ALA:HA	1:C:81:ILE:HD12	1.99	0.43
1:C:239:GLU:CG	1:C:265:GLY:HA3	2.49	0.43
1:A:155:LYS:HA	1:A:155:LYS:HD3	1.59	0.43
1:A:203:ASN:HA	1:A:208:VAL:HG23	2.01	0.43
1:B:205:ILE:HG12	1:B:295:LYS:CG	2.49	0.43
1:C:233:LYS:NZ	1:C:298:HIS:HD2	2.17	0.43
1:C:285:LYS:HG3	3:C:2380:HOH:O	2.17	0.43
1:A:21:LYS:HB3	1:A:21:LYS:HE2	1.87	0.43
1:B:22:SER:O	1:B:24:PRO:HD3	2.19	0.42
1:C:11:GLU:HB3	3:C:2423:HOH:O	2.19	0.42
1:C:21:LYS:HG2	3:C:2591:HOH:O	2.20	0.42
1:A:176:ASP:HA	1:A:177:PRO:HD2	1.89	0.42
1:A:165:PRO:HG3	3:A:608:HOH:O	2.19	0.42
1:A:86:ASN:HA	1:A:89:ARG:HH21	1.85	0.42
1:A:6:LEU:HG	3:A:573:HOH:O	2.19	0.42
1:C:128:ARG:HG2	1:C:249:GLU:HB2	2.02	0.41
1:A:185:PHE:CD1	1:A:236:LEU:HD23	2.55	0.41
1:A:189:ASN:ND2	1:A:190:PRO:CD	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLU:CG	1:B:265:GLY:HA3	2.51	0.41
1:A:159:CYS:HB2	1:A:163:LYS:HE3	2.01	0.41
1:A:100:ASN:C	1:A:100:ASN:ND2	2.70	0.41
1:B:128:ARG:NH2	1:B:132:LYS:NZ	2.67	0.41
1:A:167:LEU:HD12	1:A:171:VAL:HG23	2.03	0.41
1:C:347:ASP:C	1:C:349:PRO:HD3	2.40	0.41
1:C:225:LYS:NZ	3:C:2041:HOH:O	2.52	0.41
1:A:236:LEU:HD12	1:A:236:LEU:HA	1.88	0.41
1:A:240:ASN:ND2	3:A:925:HOH:O	2.45	0.41
1:B:1:MET:CE	1:B:1:MET:HA	2.50	0.41
1:B:231:GLN:NE2	3:B:2368:HOH:O	2.50	0.41
1:C:260:ILE:HA	1:C:261:PRO:HD3	1.94	0.41
1:B:18:MET:HE1	1:B:21:LYS:CE	2.51	0.40
1:A:40:LYS:CD	3:A:698:HOH:O	2.69	0.40
1:A:164:HIS:N	1:A:165:PRO:HD3	2.36	0.40
1:A:274:ASN:HA	1:A:314:ASN:ND2	2.37	0.40
1:A:158:HIS:HE1	3:A:920:HOH:O	2.03	0.40
1:B:1:MET:HG2	1:B:309:TYR:HA	2.03	0.40
1:A:239:GLU:OE1	1:A:248:THR:OG1	2.35	0.40

All (1) 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)
3:B:2249:HOH:O	3:B:2249:HOH:O[2_665]	2.12	0.08

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	347/371 (94%)	326 (94%)	20 (6%)	1 (0%)	41 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	334/371 (90%)	317 (95%)	14 (4%)	3 (1%)	17 7
1	C	349/371 (94%)	333 (95%)	15 (4%)	1 (0%)	41 31
All	All	1030/1113 (92%)	976 (95%)	49 (5%)	5 (0%)	29 18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	19	ALA
1	A	301	LYS
1	B	18	MET
1	B	213	SER
1	B	218	LEU

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	312/334 (93%)	300 (96%)	12 (4%)	33 24
1	B	303/334 (91%)	292 (96%)	11 (4%)	35 26
1	C	314/334 (94%)	304 (97%)	10 (3%)	39 30
All	All	929/1002 (93%)	896 (96%)	33 (4%)	35 26

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	22	SER
1	A	71	PHE
1	A	99	PRO
1	A	100	ASN
1	A	113	LEU
1	A	115	PHE
1	A	167	LEU
1	A	176	ASP

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Mol	Chain	Res	Type
1	A	237	CYS
1	A	311	ASN
1	A	319	LYS
1	B	33	TRP
1	B	86	ASN
1	B	100	ASN
1	B	113	LEU
1	B	115	PHE
1	B	136	VAL
1	B	147	ASP
1	B	175	SER
1	B	203	ASN
1	B	218	LEU
1	B	311	ASN
1	C	16	GLU
1	C	17	LYS
1	C	100	ASN
1	C	113	LEU
1	C	115	PHE
1	C	147	ASP
1	C	205	ILE
1	C	311	ASN
1	C	349	PRO
1	C	351	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	64	ASN
1	A	85	GLN
1	A	86	ASN
1	A	100	ASN
1	A	148	ASN
1	A	172	ASN
1	A	189	ASN
1	A	196	ASN
1	A	221	ASN
1	A	226	ASN
1	A	235	ASN
1	A	240	ASN
1	A	300	HIS

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Mol	Chain	Res	Type
1	A	311	ASN
1	A	314	ASN
1	B	60	HIS
1	B	61	GLN
1	B	64	ASN
1	B	86	ASN
1	B	100	ASN
1	B	172	ASN
1	B	196	ASN
1	B	203	ASN
1	B	226	ASN
1	B	258	HIS
1	B	300	HIS
1	B	311	ASN
1	B	314	ASN
1	C	44	ASN
1	C	60	HIS
1	C	64	ASN
1	C	85	GLN
1	C	86	ASN
1	C	100	ASN
1	C	131	HIS
1	C	172	ASN
1	C	196	ASN
1	C	235	ASN
1	C	298	HIS
1	C	300	HIS
1	C	311	ASN
1	C	314	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

3 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	SO4	B	2001	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	C	2003	-	4,4,4	0.22	0	6,6,6	0.21	0
2	SO4	C	2002	-	4,4,4	0.34	0	6,6,6	0.77	0

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.

No monomer is involved in short contacts.

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	349/371 (94%)	0.38	28 (8%)	12	13	18, 37, 67, 81	0
1	B	338/371 (91%)	0.39	27 (7%)	12	13	18, 37, 69, 80	0
1	C	351/371 (94%)	0.15	20 (5%)	23	26	16, 28, 54, 78	0
All	All	1038/1113 (93%)	0.30	75 (7%)	15	17	16, 33, 66, 81	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	SER	8.1
1	C	20	SER	7.6
1	C	84	TYR	6.3
1	C	351	ILE	5.5
1	A	19	ALA	5.5
1	C	19	ALA	5.5
1	C	75	LEU	4.8
1	A	205	ILE	4.8
1	C	22	SER	4.7
1	A	18	MET	4.6
1	B	139	THR	4.6
1	B	205	ILE	4.5
1	A	75	LEU	4.4
1	B	153	LEU	4.4
1	B	191	ASN	4.3
1	A	84	TYR	3.8
1	A	17	LYS	3.7
1	A	316	LEU	3.5
1	A	82	LEU	3.4
1	A	22	SER	3.3
1	B	73	ASN	3.2
1	A	285	LYS	3.2
1	B	217	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	236	LEU	3.1
1	B	19	ALA	3.1
1	A	81	ILE	3.1
1	B	190	PRO	3.0
1	B	64	ASN	3.0
1	B	251	ILE	2.9
1	B	33	TRP	2.9
1	B	22	SER	2.8
1	B	220	TYR	2.8
1	C	37	GLU	2.8
1	C	350	PHE	2.8
1	A	21	LYS	2.8
1	C	21	LYS	2.7
1	B	148	ASN	2.7
1	C	77	SER	2.7
1	C	317	ASP	2.6
1	B	254	ALA	2.6
1	B	188	SER	2.6
1	A	194	ILE	2.6
1	A	288	ASP	2.5
1	A	212	GLY	2.5
1	A	222	VAL	2.5
1	A	85	GLN	2.5
1	C	319	LYS	2.5
1	C	18	MET	2.4
1	A	78	ALA	2.4
1	C	148	ASN	2.4
1	C	205	ILE	2.4
1	B	20	SER	2.4
1	A	148	ASN	2.4
1	B	301	LYS	2.4
1	C	85	GLN	2.4
1	B	179	LYS	2.4
1	A	71	PHE	2.4
1	A	287	PHE	2.3
1	B	66	PHE	2.3
1	A	223	LYS	2.3
1	C	153	LEU	2.3
1	B	158	HIS	2.3
1	A	153	LEU	2.3
1	A	290	ALA	2.3
1	C	236	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	190	PRO	2.2
1	A	295	LYS	2.2
1	B	155	LYS	2.2
1	B	259	THR	2.2
1	A	219	GLY	2.2
1	C	262	ILE	2.2
1	C	36	ASP	2.1
1	B	159	CYS	2.1
1	B	18	MET	2.1
1	B	162	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)

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	SO4	B	2001	5/5	0.95	0.12	76,76,77,77	0
2	SO4	C	2002	5/5	0.97	0.10	45,48,49,50	0
2	SO4	C	2003	5/5	0.98	0.10	61,62,63,63	0

6.5 Other polymers (i)

There are no such residues in this entry.