Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:27 pm BST

PDB ID	:	6EWJ
Title	:	Putative sugar aminotransferase Spr1654 from Streptococcus pneumoniae, apo-form
Authors	:	Achour, A.; Sun, R.; Sandalova, T.; Han, X.
Deposited on	:	2017-11-04
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 ⓘ symbol.

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

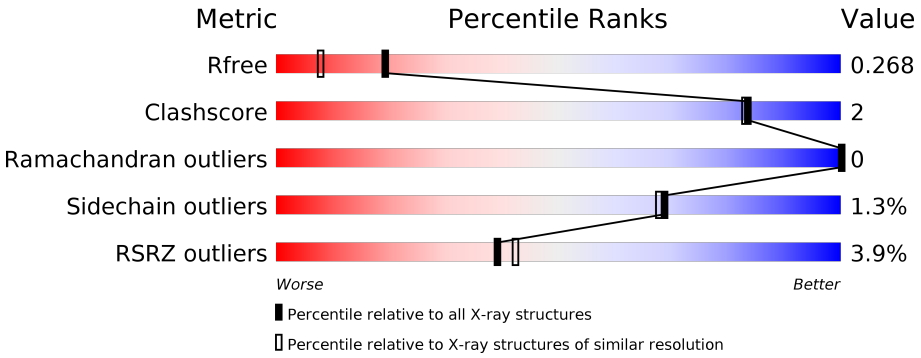
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.90 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 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	427	2% 88% 5% 7%
1	B	427	4% 86% 7% • 7%
1	C	427	4% 88% 5% 7%
1	D	427	4% 89% 5% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13277 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 capsular polysaccharide biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	399	Total	C	N	O	S	0	0	0
			3135	2002	513	608	12			
1	D	401	Total	C	N	O	S	0	0	0
			3155	2015	516	612	12			
1	C	398	Total	C	N	O	S	0	0	0
			3135	2002	513	609	11			
1	B	398	Total	C	N	O	S	0	0	0
			3139	2004	514	610	11			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	initiating methionine	UNP A0A0H2URM1
A	-4	ALA	-	expression tag	UNP A0A0H2URM1
A	-3	SER	-	expression tag	UNP A0A0H2URM1
A	-2	MET	-	expression tag	UNP A0A0H2URM1
A	-1	THR	-	expression tag	UNP A0A0H2URM1
A	0	GLY	-	expression tag	UNP A0A0H2URM1
A	178	THR	ILE	conflict	UNP A0A0H2URM1
A	409	LYS	-	expression tag	UNP A0A0H2URM1
A	410	LEU	-	expression tag	UNP A0A0H2URM1
A	411	ALA	-	expression tag	UNP A0A0H2URM1
A	412	ALA	-	expression tag	UNP A0A0H2URM1
A	413	ALA	-	expression tag	UNP A0A0H2URM1
A	414	LEU	-	expression tag	UNP A0A0H2URM1
A	415	GLU	-	expression tag	UNP A0A0H2URM1
A	416	HIS	-	expression tag	UNP A0A0H2URM1
A	417	HIS	-	expression tag	UNP A0A0H2URM1
A	418	HIS	-	expression tag	UNP A0A0H2URM1
A	419	HIS	-	expression tag	UNP A0A0H2URM1
A	420	HIS	-	expression tag	UNP A0A0H2URM1
A	421	HIS	-	expression tag	UNP A0A0H2URM1
D	-5	MET	-	initiating methionine	UNP A0A0H2URM1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	ALA	-	expression tag	UNP A0A0H2URM1
D	-3	SER	-	expression tag	UNP A0A0H2URM1
D	-2	MET	-	expression tag	UNP A0A0H2URM1
D	-1	THR	-	expression tag	UNP A0A0H2URM1
D	0	GLY	-	expression tag	UNP A0A0H2URM1
D	178	THR	ILE	conflict	UNP A0A0H2URM1
D	409	LYS	-	expression tag	UNP A0A0H2URM1
D	410	LEU	-	expression tag	UNP A0A0H2URM1
D	411	ALA	-	expression tag	UNP A0A0H2URM1
D	412	ALA	-	expression tag	UNP A0A0H2URM1
D	413	ALA	-	expression tag	UNP A0A0H2URM1
D	414	LEU	-	expression tag	UNP A0A0H2URM1
D	415	GLU	-	expression tag	UNP A0A0H2URM1
D	416	HIS	-	expression tag	UNP A0A0H2URM1
D	417	HIS	-	expression tag	UNP A0A0H2URM1
D	418	HIS	-	expression tag	UNP A0A0H2URM1
D	419	HIS	-	expression tag	UNP A0A0H2URM1
D	420	HIS	-	expression tag	UNP A0A0H2URM1
D	421	HIS	-	expression tag	UNP A0A0H2URM1
C	-5	MET	-	initiating methionine	UNP A0A0H2URM1
C	-4	ALA	-	expression tag	UNP A0A0H2URM1
C	-3	SER	-	expression tag	UNP A0A0H2URM1
C	-2	MET	-	expression tag	UNP A0A0H2URM1
C	-1	THR	-	expression tag	UNP A0A0H2URM1
C	0	GLY	-	expression tag	UNP A0A0H2URM1
C	178	THR	ILE	conflict	UNP A0A0H2URM1
C	409	LYS	-	expression tag	UNP A0A0H2URM1
C	410	LEU	-	expression tag	UNP A0A0H2URM1
C	411	ALA	-	expression tag	UNP A0A0H2URM1
C	412	ALA	-	expression tag	UNP A0A0H2URM1
C	413	ALA	-	expression tag	UNP A0A0H2URM1
C	414	LEU	-	expression tag	UNP A0A0H2URM1
C	415	GLU	-	expression tag	UNP A0A0H2URM1
C	416	HIS	-	expression tag	UNP A0A0H2URM1
C	417	HIS	-	expression tag	UNP A0A0H2URM1
C	418	HIS	-	expression tag	UNP A0A0H2URM1
C	419	HIS	-	expression tag	UNP A0A0H2URM1
C	420	HIS	-	expression tag	UNP A0A0H2URM1
C	421	HIS	-	expression tag	UNP A0A0H2URM1
B	-5	MET	-	initiating methionine	UNP A0A0H2URM1
B	-4	ALA	-	expression tag	UNP A0A0H2URM1
B	-3	SER	-	expression tag	UNP A0A0H2URM1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	MET	-	expression tag	UNP A0A0H2URM1
B	-1	THR	-	expression tag	UNP A0A0H2URM1
B	0	GLY	-	expression tag	UNP A0A0H2URM1
B	178	THR	ILE	conflict	UNP A0A0H2URM1
B	409	LYS	-	expression tag	UNP A0A0H2URM1
B	410	LEU	-	expression tag	UNP A0A0H2URM1
B	411	ALA	-	expression tag	UNP A0A0H2URM1
B	412	ALA	-	expression tag	UNP A0A0H2URM1
B	413	ALA	-	expression tag	UNP A0A0H2URM1
B	414	LEU	-	expression tag	UNP A0A0H2URM1
B	415	GLU	-	expression tag	UNP A0A0H2URM1
B	416	HIS	-	expression tag	UNP A0A0H2URM1
B	417	HIS	-	expression tag	UNP A0A0H2URM1
B	418	HIS	-	expression tag	UNP A0A0H2URM1
B	419	HIS	-	expression tag	UNP A0A0H2URM1
B	420	HIS	-	expression tag	UNP A0A0H2URM1
B	421	HIS	-	expression tag	UNP A0A0H2URM1

- Molecule 2 is water.

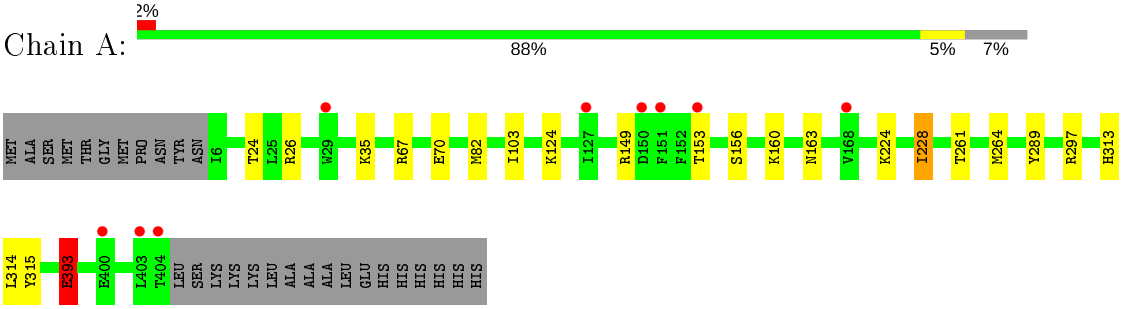
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	174	Total	O	0	0
			174	174		
2	D	167	Total	O	0	0
			167	167		
2	C	194	Total	O	0	0
			194	194		
2	B	178	Total	O	0	0
			178	178		

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.

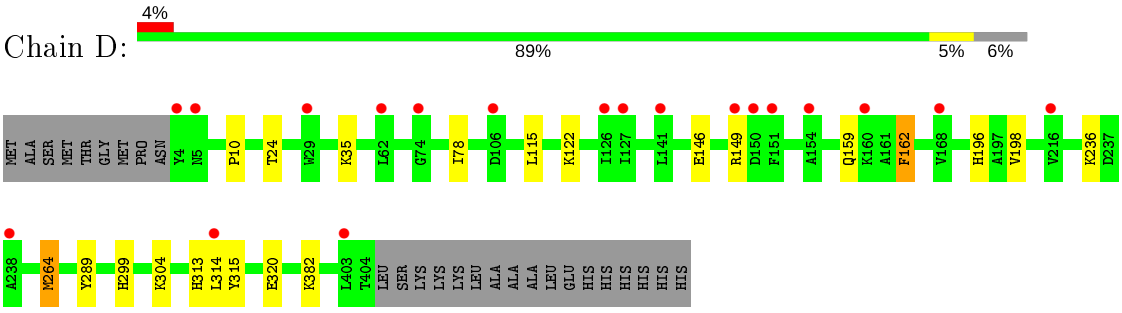
- Molecule 1: Putative capsular polysaccharide biosynthesis protein

Chain A:



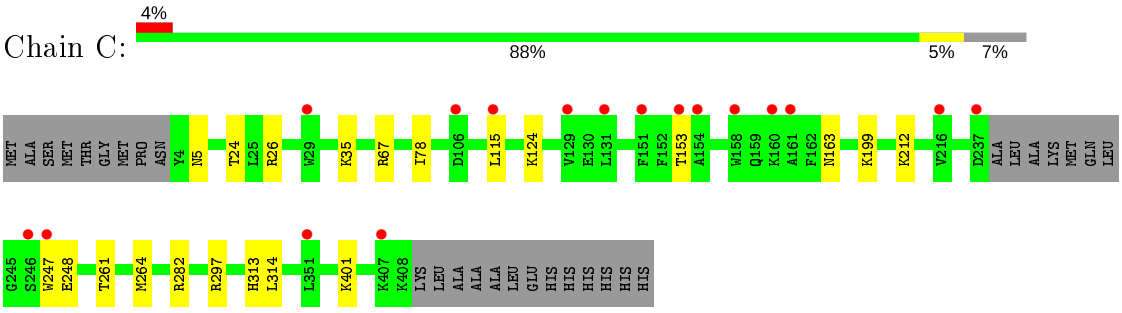
- Molecule 1: Putative capsular polysaccharide biosynthesis protein

Chain D:



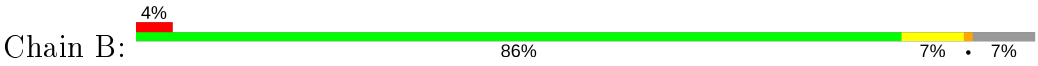
- Molecule 1: Putative capsular polysaccharide biosynthesis protein

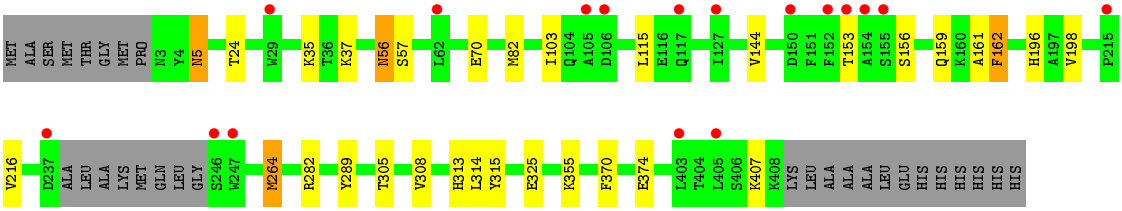
Chain C:



- Molecule 1: Putative capsular polysaccharide biosynthesis protein

Chain B:




MET ALA SER MET THR GLY MET PRO N3 Y4 N5 T24 W29 K35 T36 K37 N56 S57 L62 E70 M82 I103 Q104 A105 D106 L115 E116 Q117 I127 V144 D150 F151 F152 T153 A154 S155 S156 Q159 K160 A161 F162 H196 A197 V198 P215
V216 D237 ALA LEU ALA LYS MET GLN LEU GLY S246 W247 M264 R282 Y289 T305 V308 H313 L314 Y315 E325 K355 F370 E374 L403 T404 L405 S406 K407 K408 LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.33Å 99.98Å 110.42Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 29.95 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.00-1.90) 97.5 (29.95-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.236 , 0.265 0.240 , 0.268	Depositor DCC
R_{free} test set	6467 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13277	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.47% 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	0.70	0/3201	0.81	3/4350 (0.1%)
1	B	0.70	0/3205	0.81	2/4354 (0.0%)
1	C	0.71	0/3201	0.83	3/4348 (0.1%)
1	D	0.68	0/3222	0.81	2/4379 (0.0%)
All	All	0.70	0/12829	0.81	10/17431 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	162	PHE	N-CA-C	-6.42	93.66	111.00
1	C	297	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	162	PHE	N-CA-C	-6.33	93.90	111.00
1	A	297	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	282	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	67	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	393	GLU	CB-CA-C	5.35	121.11	110.40
1	D	236	LYS	CD-CE-NZ	5.31	123.92	111.70
1	B	282	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	67	ARG	NE-CZ-NH1	5.21	122.90	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	3135	0	3122	16	0
1	B	3139	0	3119	19	0
1	C	3135	0	3116	15	0
1	D	3155	0	3137	13	0
2	A	174	0	0	0	0
2	B	178	0	0	1	0
2	C	194	0	0	3	0
2	D	167	0	0	0	0
All	All	13277	0	12494	59	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:THR:OG1	1:A:264:MET:HE2	1.47	1.14
1:C:261:THR:OG1	1:C:264:MET:HE2	1.50	1.09
1:C:261:THR:OG1	1:C:264:MET:CE	2.00	1.09
1:A:261:THR:OG1	1:A:264:MET:CE	2.00	1.09
1:C:261:THR:HG1	1:C:264:MET:HE2	1.25	1.00
1:B:305:THR:OG1	1:B:308:VAL:HG22	1.75	0.87
1:A:261:THR:HG1	1:A:264:MET:HE2	1.43	0.83
1:B:159:GLN:O	1:B:162:PHE:O	2.00	0.80
1:D:159:GLN:O	1:D:162:PHE:O	2.01	0.79
1:C:261:THR:OG1	1:C:264:MET:HE1	1.84	0.77
1:B:115:LEU:CD2	1:B:144:VAL:HG11	2.18	0.72
1:A:261:THR:OG1	1:A:264:MET:HE1	1.87	0.72
1:A:224:LYS:O	1:A:228:ILE:HD13	1.94	0.67
1:D:196:HIS:HE1	2:C:654:HOH:O	1.81	0.64
1:D:10:PRO:HG2	1:D:382:LYS:HD3	1.83	0.59
1:B:161:ALA:HB1	1:B:216:VAL:CG1	2.33	0.58
1:B:56:ASN:HD22	1:B:56:ASN:C	2.07	0.57
1:A:26:ARG:NE	1:C:26:ARG:NH1	2.54	0.56
1:B:115:LEU:HD23	1:B:144:VAL:HG11	1.86	0.56
1:B:5:ASN:ND2	2:B:503:HOH:O	2.42	0.52
1:A:70:GLU:OE1	1:A:156:SER:HB2	2.12	0.49
1:B:161:ALA:HB1	1:B:216:VAL:HG11	1.95	0.49
1:A:124:LYS:NZ	1:A:153:THR:O	2.46	0.48
1:B:70:GLU:OE1	1:B:156:SER:HB2	2.13	0.48
1:A:393:GLU:OE1	1:A:393:GLU:C	2.53	0.47
1:D:264:MET:HE1	1:C:264:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASN:HD22	1:B:57:SER:N	2.13	0.46
1:B:24:THR:OG1	1:B:35:LYS:HE2	2.15	0.46
1:B:196:HIS:HD2	1:B:198:VAL:HG22	1.80	0.46
1:C:124:LYS:NZ	1:C:153:THR:O	2.49	0.45
1:C:24:THR:OG1	1:C:35:LYS:HE2	2.17	0.45
1:B:313:HIS:CD2	1:B:314:LEU:HG	2.52	0.44
1:A:24:THR:OG1	1:A:35:LYS:HE2	2.17	0.44
1:C:247:TRP:CH2	1:C:248:GLU:HG2	2.53	0.44
1:D:313:HIS:CD2	1:D:314:LEU:HG	2.52	0.44
1:D:10:PRO:CG	1:D:382:LYS:HD3	2.47	0.43
1:C:78:ILE:HG21	1:C:115:LEU:CD1	2.49	0.43
1:B:305:THR:HG1	1:B:308:VAL:HG22	1.78	0.43
1:A:26:ARG:CZ	1:C:26:ARG:NH1	2.81	0.43
1:D:24:THR:OG1	1:D:35:LYS:HE2	2.19	0.43
1:D:382:LYS:HE2	1:D:382:LYS:HB3	1.85	0.43
1:A:228:ILE:N	1:A:228:ILE:CD1	2.81	0.42
1:D:299:HIS:HE1	1:D:320:GLU:OE1	2.03	0.42
1:B:161:ALA:HB1	1:B:216:VAL:HG12	2.01	0.42
1:D:289:TYR:HB3	1:D:315:TYR:CZ	2.55	0.42
1:C:313:HIS:CD2	1:C:314:LEU:HG	2.54	0.42
1:C:212:LYS:NZ	2:C:501:HOH:O	2.44	0.42
1:B:289:TYR:HB3	1:B:315:TYR:CZ	2.55	0.41
1:D:196:HIS:HD2	1:D:198:VAL:HG22	1.85	0.41
1:C:401:LYS:HE2	2:C:685:HOH:O	2.20	0.41
1:A:264:MET:HE1	1:B:264:MET:HE1	2.02	0.41
1:D:146:GLU:OE1	1:D:149:ARG:NH1	2.53	0.41
1:C:199:LYS:HA	1:C:313:HIS:CE1	2.56	0.41
1:B:82:MET:HB3	1:B:103:ILE:HG21	2.03	0.41
1:D:78:ILE:HG21	1:D:115:LEU:CD1	2.51	0.41
1:A:289:TYR:HB3	1:A:315:TYR:CZ	2.56	0.40
1:A:82:MET:HB3	1:A:103:ILE:HG21	2.03	0.40
1:A:313:HIS:CD2	1:A:314:LEU:HG	2.56	0.40
1:B:370:PHE:O	1:B:374:GLU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	397/427 (93%)	383 (96%)	14 (4%)	0	100	100
1	B	394/427 (92%)	379 (96%)	15 (4%)	0	100	100
1	C	394/427 (92%)	380 (96%)	14 (4%)	0	100	100
1	D	399/427 (93%)	386 (97%)	13 (3%)	0	100	100
All	All	1584/1708 (93%)	1528 (96%)	56 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	346/371 (93%)	341 (99%)	5 (1%)	67	65
1	B	348/371 (94%)	340 (98%)	8 (2%)	50	45
1	C	347/371 (94%)	345 (99%)	2 (1%)	86	87
1	D	348/371 (94%)	345 (99%)	3 (1%)	78	79
All	All	1389/1484 (94%)	1371 (99%)	18 (1%)	69	68

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ARG
1	A	160	LYS

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Mol	Chain	Res	Type
1	A	163	ASN
1	A	228	ILE
1	A	393	GLU
1	D	122	LYS
1	D	264	MET
1	D	304	LYS
1	C	5	ASN
1	C	163	ASN
1	B	5	ASN
1	B	37	LYS
1	B	56	ASN
1	B	153	THR
1	B	264	MET
1	B	325	GLU
1	B	355	LYS
1	B	407	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	143	GLN
1	D	196	HIS
1	D	299	HIS
1	C	5	ASN
1	B	5	ASN
1	B	56	ASN
1	B	196	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 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	399/427 (93%)	0.38	9 (2%) 60 63	15, 25, 43, 64	0
1	B	398/427 (93%)	0.53	17 (4%) 35 38	17, 28, 47, 64	0
1	C	398/427 (93%)	0.45	17 (4%) 35 38	15, 27, 49, 69	0
1	D	401/427 (93%)	0.52	19 (4%) 31 34	17, 29, 50, 73	0
All	All	1596/1708 (93%)	0.47	62 (3%) 39 42	15, 28, 48, 73	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	TRP	6.5
1	C	153	THR	5.5
1	C	160	LYS	5.3
1	B	153	THR	4.7
1	B	154	ALA	4.2
1	C	246	SER	4.1
1	C	216	VAL	4.1
1	C	154	ALA	4.0
1	D	403	LEU	3.9
1	D	127	ILE	3.9
1	A	403	LEU	3.7
1	D	151	PHE	3.5
1	D	150	ASP	3.4
1	D	4	TYR	3.4
1	C	407	LYS	3.3
1	A	404	THR	3.3
1	C	106	ASP	3.3
1	D	29	TRP	3.2
1	B	237	ASP	3.2
1	C	237	ASP	3.1
1	D	106	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	151	PHE	3.0
1	D	168	VAL	3.0
1	B	247	TRP	2.9
1	C	29	TRP	2.9
1	A	150	ASP	2.8
1	B	155	SER	2.8
1	C	161	ALA	2.7
1	C	247	TRP	2.7
1	B	215	PRO	2.6
1	C	158	TRP	2.6
1	D	126	ILE	2.6
1	B	246	SER	2.6
1	C	129	VAL	2.6
1	A	127	ILE	2.5
1	D	74	GLY	2.5
1	A	400	GLU	2.5
1	B	152	PHE	2.5
1	A	29	TRP	2.4
1	C	131	LEU	2.4
1	A	153	THR	2.4
1	A	168	VAL	2.4
1	A	151	PHE	2.4
1	B	106	ASP	2.3
1	B	117	GLN	2.3
1	B	105	ALA	2.3
1	D	154	ALA	2.3
1	B	403	LEU	2.3
1	D	216	VAL	2.2
1	D	62	LEU	2.2
1	B	405	LEU	2.2
1	D	5	ASN	2.1
1	B	127	ILE	2.1
1	B	150	ASP	2.1
1	D	149	ARG	2.1
1	D	314	LEU	2.1
1	B	62	LEU	2.1
1	D	238	ALA	2.1
1	C	115	LEU	2.0
1	D	141	LEU	2.0
1	C	351	LEU	2.0
1	D	160	LYS	2.0

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.