Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 06:48 PM JST

PDB ID	:	5XU0
Title	:	Structure of the membrane fusion protein Spr0693 from Streptococcus pneumoniae R6
Authors	:	Yang, H.B.; Jiang, Y.L.; Hou, W.T.; Chen, M.T.; Chen, Y.; Zhou, C.Z.
Deposited on	:	2017-06-22
Resolution	:	2.95 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:

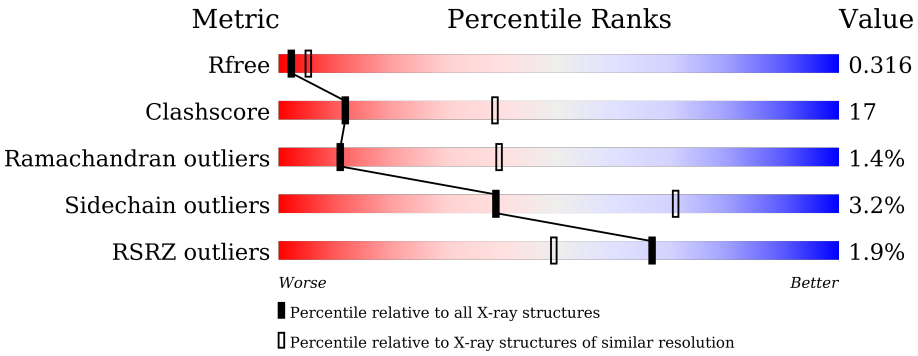
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	273	2% 57% 25% • 17%
1	B	273	% 63% 20% • 15%
1	C	273	% 59% 21% • 18%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5102 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 Membrane-fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	Se	0	0	0
			1698	1047	289	359	3			
1	B	231	Total	C	N	O	Se	0	0	0
			1732	1064	297	368	3			
1	C	223	Total	C	N	O	Se	0	0	0
			1672	1029	285	355	3			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	MSE	-	expression tag	UNP A0A0Y3EE53
A	197	MSE	THR	engineered mutation	UNP A0A0Y3EE53
A	317	MSE	ILE	engineered mutation	UNP A0A0Y3EE53
A	325	HIS	-	expression tag	UNP A0A0Y3EE53
A	326	HIS	-	expression tag	UNP A0A0Y3EE53
A	327	HIS	-	expression tag	UNP A0A0Y3EE53
A	328	HIS	-	expression tag	UNP A0A0Y3EE53
A	329	HIS	-	expression tag	UNP A0A0Y3EE53
A	330	HIS	-	expression tag	UNP A0A0Y3EE53
B	58	MSE	-	expression tag	UNP A0A0Y3EE53
B	197	MSE	THR	engineered mutation	UNP A0A0Y3EE53
B	317	MSE	ILE	engineered mutation	UNP A0A0Y3EE53
B	325	HIS	-	expression tag	UNP A0A0Y3EE53
B	326	HIS	-	expression tag	UNP A0A0Y3EE53
B	327	HIS	-	expression tag	UNP A0A0Y3EE53
B	328	HIS	-	expression tag	UNP A0A0Y3EE53
B	329	HIS	-	expression tag	UNP A0A0Y3EE53
B	330	HIS	-	expression tag	UNP A0A0Y3EE53
C	58	MSE	-	expression tag	UNP A0A0Y3EE53
C	197	MSE	THR	engineered mutation	UNP A0A0Y3EE53
C	317	MSE	ILE	engineered mutation	UNP A0A0Y3EE53
C	325	HIS	-	expression tag	UNP A0A0Y3EE53
C	326	HIS	-	expression tag	UNP A0A0Y3EE53

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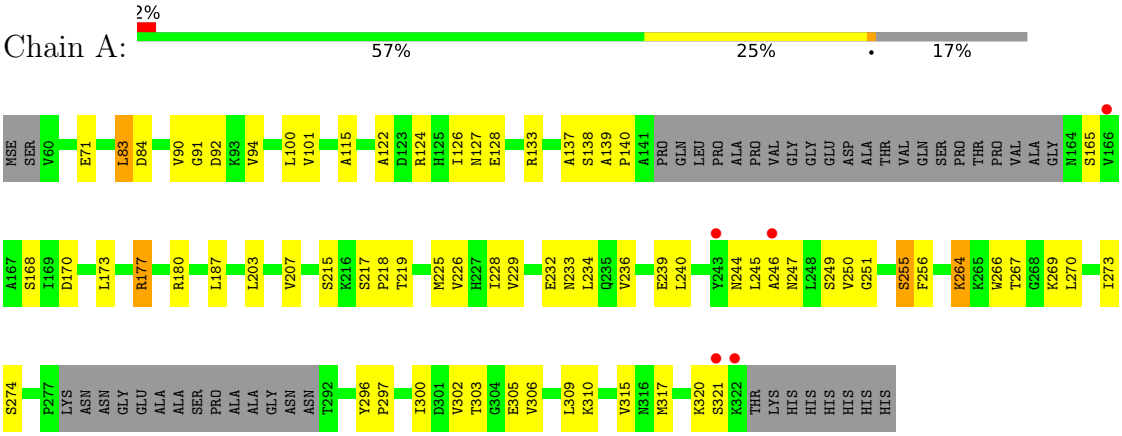
Chain	Residue	Modelled	Actual	Comment	Reference
C	327	HIS	-	expression tag	UNP A0A0Y3EE53
C	328	HIS	-	expression tag	UNP A0A0Y3EE53
C	329	HIS	-	expression tag	UNP A0A0Y3EE53
C	330	HIS	-	expression tag	UNP A0A0Y3EE53

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.

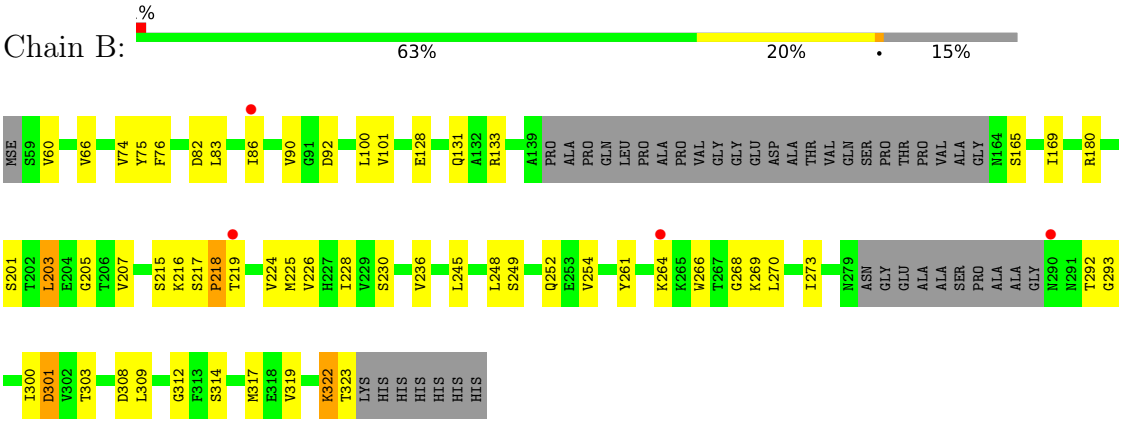
• Molecule 1: Membrane-fusion protein

Chain A:



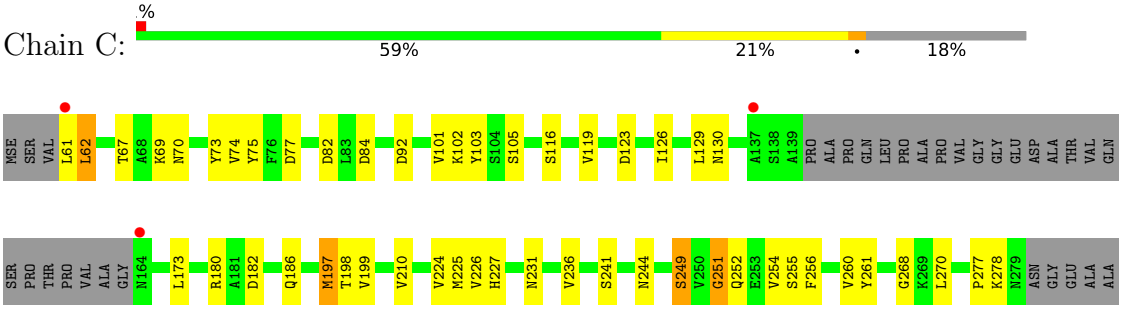
• Molecule 1: Membrane-fusion protein

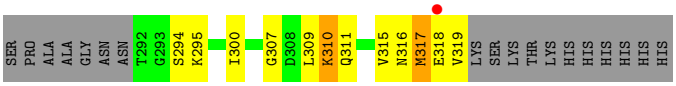
Chain B:



• Molecule 1: Membrane-fusion protein

Chain C:




SER
PRO
ALA
ALA
GLY
ASN
ASN
T292
G293
S294
K295
I300
G307
D308
L309
K310
Q311
V315
N316
M317
E318
V319
LYS
SER
LYS
THR
LYS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.21Å 159.21Å 99.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.98 – 2.95 48.98 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.98-2.95) 99.9 (48.98-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.248 , 0.305 0.264 , 0.316	Depositor DCC
R_{free} test set	1306 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	89.8	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 61.9	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	0.93	EDS
Total number of atoms	5102	wwPDB-VP
Average B, all atoms (Å^2)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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	0.31	0/1714	0.54	1/2315 (0.0%)
1	B	0.29	0/1747	0.53	0/2358
1	C	0.30	0/1687	0.55	1/2278 (0.0%)
All	All	0.30	0/5148	0.54	2/6951 (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	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	129	LEU	CA-CB-CG	-5.94	101.64	115.30
1	A	177	ARG	NE-CZ-NH1	-5.50	117.55	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	310	LYS	Peptide

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	1698	0	1662	61	0
1	B	1732	0	1692	51	0
1	C	1672	0	1629	66	0
All	All	5102	0	4983	174	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 17.

All (174) 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:215:SER:OG	1:B:219:THR:CG2	1.83	1.26
1:C:61:LEU:N	1:C:318:GLU:HG3	1.51	1.23
1:B:215:SER:OG	1:B:219:THR:HG21	1.35	1.21
1:A:247:ASN:OD1	1:A:321:SER:HB2	1.37	1.20
1:C:256:PHE:HB3	1:C:317:MSE:HG2	1.29	1.12
1:C:254:VAL:HG21	1:C:317:MSE:CE	1.80	1.10
1:C:61:LEU:HD23	1:C:318:GLU:HB2	1.30	1.10
1:A:247:ASN:OD1	1:A:321:SER:CB	2.07	1.01
1:B:217:SER:O	1:B:219:THR:HG23	1.60	1.00
1:B:217:SER:O	1:B:219:THR:CG2	2.10	0.99
1:A:203:LEU:HD11	1:A:228:ILE:CG2	1.95	0.97
1:C:61:LEU:CD2	1:C:318:GLU:HB2	1.95	0.96
1:B:215:SER:OG	1:B:219:THR:HG23	1.65	0.93
1:A:203:LEU:HD11	1:A:228:ILE:HG22	1.50	0.91
1:C:254:VAL:HG21	1:C:317:MSE:HE2	1.54	0.89
1:C:256:PHE:HB3	1:C:317:MSE:CG	2.03	0.89
1:C:101:VAL:HG22	1:C:199:VAL:HG12	1.54	0.88
1:A:266:TRP:CE2	1:A:309:LEU:HD11	2.11	0.85
1:B:269:LYS:HE3	1:B:303:THR:HG21	1.59	0.84
1:C:254:VAL:CG2	1:C:317:MSE:HE2	2.09	0.82
1:B:215:SER:CB	1:B:219:THR:HG21	2.10	0.82
1:C:231:ASN:HD21	1:C:310:LYS:HD2	1.44	0.80
1:C:254:VAL:CG2	1:C:317:MSE:CE	2.58	0.79
1:C:61:LEU:HB2	1:C:318:GLU:CD	2.03	0.79
1:C:61:LEU:N	1:C:318:GLU:CG	2.43	0.78
1:C:254:VAL:HG21	1:C:317:MSE:HE1	1.65	0.77
1:A:137:ALA:C	1:A:139:ALA:H	1.88	0.76
1:A:203:LEU:HD11	1:A:228:ILE:HG21	1.69	0.75
1:A:133:ARG:NH1	1:A:170:ASP:OD2	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ALA:O	1:A:139:ALA:N	2.16	0.74
1:A:234:LEU:HD23	1:A:306:VAL:HG21	1.69	0.73
1:A:245:LEU:HD12	1:A:296:TYR:HD2	1.55	0.72
1:A:124:ARG:O	1:A:128:GLU:OE2	2.08	0.71
1:A:267:THR:HG23	1:A:303:THR:HB	1.72	0.71
1:A:100:LEU:HD23	1:A:226:VAL:HG11	1.72	0.71
1:C:61:LEU:C	1:C:61:LEU:HD13	2.13	0.69
1:B:236:VAL:HG23	1:B:300:ILE:HG12	1.74	0.68
1:B:60:VAL:HG11	1:B:248:LEU:HD21	1.75	0.67
1:B:322:LYS:HA	1:B:322:LYS:HE2	1.76	0.66
1:A:245:LEU:HD12	1:A:296:TYR:CD2	2.30	0.66
1:C:61:LEU:HA	1:C:318:GLU:HB2	1.78	0.66
1:B:215:SER:HG	1:B:219:THR:CG2	2.07	0.64
1:C:61:LEU:CA	1:C:318:GLU:HG3	2.26	0.64
1:A:266:TRP:CD2	1:A:309:LEU:HD11	2.33	0.64
1:C:101:VAL:HG22	1:C:199:VAL:CG1	2.27	0.64
1:B:270:LEU:HD23	1:B:300:ILE:HG22	1.79	0.64
1:C:61:LEU:HA	1:C:318:GLU:CB	2.30	0.62
1:C:102:LYS:HG3	1:C:198:THR:HG22	1.81	0.62
1:B:203:LEU:HD21	1:B:228:ILE:HD11	1.81	0.61
1:C:61:LEU:HD23	1:C:318:GLU:CB	2.19	0.61
1:C:67:THR:HA	1:C:311:GLN:HG3	1.82	0.61
1:C:256:PHE:HA	1:C:317:MSE:HB3	1.83	0.60
1:B:74:VAL:HG22	1:B:226:VAL:HB	1.84	0.60
1:A:217:SER:O	1:A:219:THR:N	2.36	0.59
1:C:311:GLN:O	1:C:311:GLN:HG2	2.03	0.59
1:A:94:VAL:HG21	1:A:228:ILE:HD13	1.85	0.59
1:A:137:ALA:C	1:A:139:ALA:N	2.50	0.59
1:A:203:LEU:CD1	1:A:228:ILE:CG2	2.78	0.58
1:C:241:SER:N	1:C:244:ASN:OD1	2.36	0.58
1:C:251:GLY:HA2	1:C:270:LEU:HB3	1.86	0.58
1:B:66:VAL:HA	1:B:236:VAL:HG12	1.85	0.57
1:A:270:LEU:HD22	1:A:300:ILE:HG12	1.87	0.57
1:B:312:GLY:HA3	1:C:277:PRO:HG3	1.87	0.56
1:C:61:LEU:HB2	1:C:318:GLU:OE1	2.05	0.56
1:C:75:TYR:CE2	1:C:224:VAL:HG12	2.41	0.56
1:B:216:LYS:HD2	1:C:77:ASP:OD2	2.07	0.55
1:A:310:LYS:HG3	1:B:245:LEU:HD13	1.89	0.54
1:B:82:ASP:OD1	1:B:216:LYS:HE2	2.07	0.54
1:B:254:VAL:HG22	1:B:319:VAL:HG22	1.88	0.54
1:A:234:LEU:HD23	1:A:306:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:PHE:HB3	1:A:317:MSE:HG2	1.90	0.54
1:A:83:LEU:HD12	1:A:84:ASP:N	2.23	0.53
1:B:261:TYR:HE2	1:B:308:ASP:HB2	1.72	0.53
1:C:84:ASP:HB3	1:C:102:LYS:O	2.09	0.53
1:B:270:LEU:HD13	1:B:273:ILE:HD11	1.91	0.53
1:B:100:LEU:HD11	1:B:201:SER:HB2	1.92	0.52
1:A:236:VAL:HG21	1:A:315:VAL:HG21	1.91	0.52
1:A:101:VAL:HG11	1:A:225:MSE:HE1	1.90	0.52
1:A:203:LEU:CD1	1:A:228:ILE:HG21	2.39	0.52
1:B:228:ILE:C	1:B:228:ILE:HD12	2.29	0.52
1:A:124:ARG:O	1:A:127:ASN:N	2.40	0.52
1:C:315:VAL:C	1:C:316:ASN:OD1	2.48	0.52
1:C:61:LEU:CA	1:C:318:GLU:CG	2.87	0.51
1:B:128:GLU:HA	1:B:131:GLN:HG3	1.91	0.51
1:C:75:TYR:HE2	1:C:224:VAL:HG12	1.76	0.51
1:B:86:ILE:HG23	1:B:101:VAL:HG12	1.93	0.51
1:A:128:GLU:OE2	1:A:128:GLU:N	2.41	0.51
1:C:103:TYR:N	1:C:197:MSE:O	2.40	0.51
1:B:83:LEU:HD22	1:B:225:MSE:SE	2.61	0.50
1:A:255:SER:HA	1:A:267:THR:HA	1.94	0.50
1:C:123:ASP:O	1:C:126:ILE:HG13	2.12	0.50
1:C:101:VAL:HG11	1:C:225:MSE:HE3	1.94	0.49
1:A:115:ALA:HB3	1:A:187:LEU:HD12	1.93	0.49
1:B:248:LEU:HD12	1:B:270:LEU:HD11	1.93	0.49
1:A:91:GLY:H	1:A:207:VAL:HG13	1.76	0.48
1:B:76:PHE:HA	1:B:225:MSE:HE2	1.95	0.48
1:B:264:LYS:HB3	1:B:264:LYS:HE3	1.63	0.48
1:B:292:THR:OG1	1:B:293:GLY:N	2.46	0.48
1:A:264:LYS:HZ3	1:A:266:TRP:HE1	1.61	0.48
1:A:274:SER:HB3	1:A:297:PRO:HD2	1.94	0.48
1:B:322:LYS:HD3	1:B:323:THR:HG22	1.94	0.48
1:A:203:LEU:CD1	1:A:228:ILE:HG22	2.34	0.48
1:B:90:VAL:HA	1:B:207:VAL:HG23	1.95	0.48
1:C:182:ASP:O	1:C:186:GLN:HG2	2.13	0.48
1:C:231:ASN:ND2	1:C:310:LYS:HD2	2.23	0.48
1:A:240:LEU:HB2	1:A:244:ASN:HB3	1.96	0.48
1:B:217:SER:O	1:B:219:THR:HG22	2.07	0.48
1:A:165:SER:HB3	1:A:168:SER:HB3	1.95	0.47
1:A:251:GLY:O	1:A:269:LYS:NZ	2.47	0.47
1:A:305:GLU:OE1	1:A:305:GLU:N	2.28	0.47
1:B:74:VAL:CG2	1:B:226:VAL:HB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ARG:HB2	1:B:169:ILE:HG21	1.96	0.47
1:C:294:SER:C	1:C:295:LYS:HE2	2.34	0.47
1:C:74:VAL:HG22	1:C:226:VAL:HB	1.95	0.47
1:C:318:GLU:HG2	1:C:319:VAL:N	2.29	0.47
1:C:268:GLY:C	1:C:300:ILE:HD11	2.35	0.47
1:A:244:ASN:HA	1:A:247:ASN:ND2	2.30	0.47
1:C:73:TYR:HE2	1:C:227:HIS:CE1	2.34	0.46
1:C:73:TYR:HE2	1:C:227:HIS:CG	2.33	0.46
1:B:128:GLU:O	1:B:131:GLN:NE2	2.49	0.46
1:C:249:SER:HG	1:C:252:GLN:H	1.60	0.46
1:C:309:LEU:O	1:C:310:LYS:HD3	2.15	0.45
1:A:83:LEU:HD22	1:A:225:MSE:SE	2.66	0.45
1:A:94:VAL:HG21	1:A:228:ILE:CD1	2.45	0.45
1:C:249:SER:HB2	1:C:252:GLN:OE1	2.15	0.45
1:A:232:GLU:CD	1:A:233:ASN:H	2.20	0.45
1:C:130:ASN:HB3	1:C:173:LEU:HD11	1.98	0.45
1:A:245:LEU:C	1:A:247:ASN:H	2.20	0.45
1:C:105:SER:O	1:C:105:SER:OG	2.28	0.45
1:A:122:ALA:O	1:A:126:ILE:HG23	2.17	0.44
1:B:207:VAL:HG12	1:B:228:ILE:HG22	1.98	0.44
1:A:234:LEU:O	1:A:302:VAL:HG22	2.17	0.44
1:A:247:ASN:HB3	1:A:321:SER:HA	1.98	0.44
1:B:75:TYR:CE1	1:B:224:VAL:HG22	2.53	0.44
1:A:239:GLU:HA	1:A:296:TYR:O	2.16	0.44
1:A:245:LEU:O	1:A:247:ASN:N	2.47	0.44
1:A:270:LEU:HA	1:A:300:ILE:HG23	1.99	0.44
1:C:116:SER:O	1:C:119:VAL:HG22	2.17	0.44
1:C:74:VAL:CG2	1:C:226:VAL:HB	2.48	0.43
1:B:217:SER:HA	1:B:218:PRO:HD2	1.67	0.43
1:B:248:LEU:CD1	1:B:319:VAL:HG11	2.48	0.43
1:B:268:GLY:HA2	1:B:303:THR:HG23	2.01	0.43
1:B:92:ASP:H	1:B:207:VAL:HG22	1.82	0.43
1:B:322:LYS:HD3	1:B:323:THR:N	2.33	0.43
1:A:247:ASN:OD1	1:A:321:SER:HB3	2.12	0.43
1:C:101:VAL:HG21	1:C:225:MSE:HE1	2.00	0.43
1:B:207:VAL:HG12	1:B:228:ILE:CG2	2.49	0.43
1:C:260:VAL:HG22	1:C:261:TYR:CD2	2.54	0.43
1:C:260:VAL:HG13	1:C:261:TYR:H	1.83	0.43
1:C:69:LYS:HG2	1:C:70:ASN:OD1	2.19	0.43
1:A:249:SER:HB3	1:A:250:VAL:H	1.59	0.43
1:C:61:LEU:HA	1:C:61:LEU:HD22	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:LEU:O	1:A:245:LEU:HD23	2.20	0.42
1:A:247:ASN:CB	1:A:321:SER:HA	2.49	0.42
1:C:236:VAL:HB	1:C:300:ILE:HG23	2.01	0.42
1:A:264:LYS:NZ	1:A:266:TRP:HE1	2.18	0.42
1:C:61:LEU:C	1:C:61:LEU:CD1	2.85	0.42
1:C:82:ASP:OD2	1:C:82:ASP:N	2.53	0.42
1:C:310:LYS:HD3	1:C:310:LYS:HA	1.74	0.42
1:C:210:VAL:HA	1:C:225:MSE:O	2.20	0.42
1:A:270:LEU:HD11	1:A:273:ILE:HG13	2.01	0.41
1:B:205:GLY:HA2	1:B:230:SER:HA	2.03	0.41
1:A:92:ASP:O	1:A:207:VAL:HG12	2.20	0.41
1:C:61:LEU:CA	1:C:318:GLU:HB2	2.49	0.41
1:C:61:LEU:HD13	1:C:62:LEU:N	2.35	0.41
1:B:269:LYS:O	1:B:300:ILE:HB	2.21	0.41
1:A:173:LEU:O	1:A:177:ARG:HG3	2.20	0.41
1:B:301:ASP:N	1:B:301:ASP:OD2	2.54	0.41
1:C:123:ASP:OD2	1:C:180:ARG:NH1	2.54	0.41
1:A:71:GLU:HG2	1:A:229:VAL:HG12	2.01	0.41
1:C:61:LEU:CA	1:C:318:GLU:CB	2.99	0.41
1:A:215:SER:HB3	1:B:75:TYR:CD2	2.56	0.40
1:B:266:TRP:CZ2	1:B:309:LEU:HB2	2.56	0.40
1:B:249:SER:O	1:B:252:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

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	221/273 (81%)	203 (92%)	13 (6%)	5 (2%)	6 27
1	B	225/273 (82%)	215 (96%)	9 (4%)	1 (0%)	34 69
1	C	217/273 (80%)	193 (89%)	21 (10%)	3 (1%)	11 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	663/819 (81%)	611 (92%)	43 (6%)	9 (1%)	11 39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	218	PRO
1	C	249	SER
1	C	307	GLY
1	A	138	SER
1	A	140	PRO
1	A	218	PRO
1	A	246	ALA
1	C	251	GLY
1	A	90	VAL

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	186/216 (86%)	181 (97%)	5 (3%)	44 74
1	B	191/216 (88%)	184 (96%)	7 (4%)	34 66
1	C	183/216 (85%)	177 (97%)	6 (3%)	38 70
All	All	560/648 (86%)	542 (97%)	18 (3%)	39 71

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

Mol	Chain	Res	Type
1	A	83	LEU
1	A	180	ARG
1	A	255	SER
1	A	264	LYS
1	A	320	LYS
1	B	165	SER
1	B	180	ARG

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Mol	Chain	Res	Type
1	B	203	LEU
1	B	301	ASP
1	B	314	SER
1	B	317	MSE
1	B	322	LYS
1	C	62	LEU
1	C	92	ASP
1	C	197	MSE
1	C	255	SER
1	C	278	LYS
1	C	317	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	GLN
1	C	172	GLN
1	C	223	GLN
1	C	231	ASN
1	C	311	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	224/273 (82%)	0.17	5 (2%)	62	45	74, 97, 130, 150	0
1	B	228/273 (83%)	0.36	4 (1%)	68	51	73, 91, 125, 180	0
1	C	220/273 (80%)	0.20	4 (1%)	68	51	30, 105, 143, 162	0
All	All	672/819 (82%)	0.25	13 (1%)	66	49	30, 97, 136, 180	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	THR	7.7
1	A	322	LYS	5.2
1	C	61	LEU	3.9
1	A	321	SER	3.7
1	C	164	ASN	3.6
1	B	264	LYS	3.4
1	C	137	ALA	3.4
1	C	318	GLU	2.8
1	A	246	ALA	2.6
1	B	290	ASN	2.3
1	A	243	TYR	2.2
1	B	86	ILE	2.1
1	A	166	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides 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.