



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 01:28 pm GMT

PDB ID : 5Y9C
Title : Crystal structure of HPV58 pentamer in complex with the Fab fragment of antibody A12A3
Authors : Li, S.W.; Li, Z.H.
Deposited on : 2017-08-24
Resolution : 3.44 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

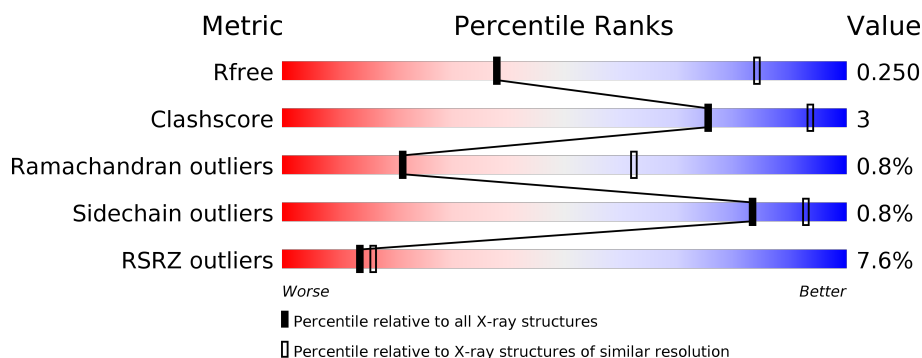
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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}	111664	1073 (3.50-3.38)
Clashscore	122126	1149 (3.50-3.38)
Ramachandran outliers	120053	1120 (3.50-3.38)
Sidechain outliers	120020	1121 (3.50-3.38)
RSRZ outliers	108989	1170 (3.52-3.36)

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. 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 $\leq 5\%$. 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	490	<div> <div>2%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>
1	B	490	<div> <div>2%</div> <div>78%</div> <div>7%</div> <div>14%</div> </div>
1	C	490	<div> <div>6%</div> <div>77%</div> <div>8%</div> <div>15%</div> </div>
1	D	490	<div> <div>3%</div> <div>77%</div> <div>7%</div> <div>16%</div> </div>
1	E	490	<div> <div>3%</div> <div>76%</div> <div>8%</div> <div>16%</div> </div>
2	H	216	<div> <div>35%</div> <div>76%</div> <div>20%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
3	L	213	<div><div></div><div>15%</div><div>84%</div><div>11%</div><div>• 5%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19783 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 Major capsid protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	417	Total	C	N	O	S	0	0	0
			3324	2120	553	632	19			
1	B	420	Total	C	N	O	S	0	0	0
			3345	2131	558	637	19			
1	C	415	Total	C	N	O	S	0	0	0
			3311	2113	550	629	19			
1	D	414	Total	C	N	O	S	0	0	0
			3305	2110	549	627	19			
1	E	414	Total	C	N	O	S	0	0	0
			3305	2110	549	627	19			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	MET	-	initiating methionine	UNP P26535
A	176	SER	CYS	engineered mutation	UNP P26535
B	9	MET	-	initiating methionine	UNP P26535
B	176	SER	CYS	engineered mutation	UNP P26535
C	9	MET	-	initiating methionine	UNP P26535
C	176	SER	CYS	engineered mutation	UNP P26535
D	9	MET	-	initiating methionine	UNP P26535
D	176	SER	CYS	engineered mutation	UNP P26535
E	9	MET	-	initiating methionine	UNP P26535
E	176	SER	CYS	engineered mutation	UNP P26535

- Molecule 2 is a protein called heavy chain of Fab fragment of antibody A12A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	210	Total	C	N	O	S	0	0	0
			1608	1018	264	319	7			

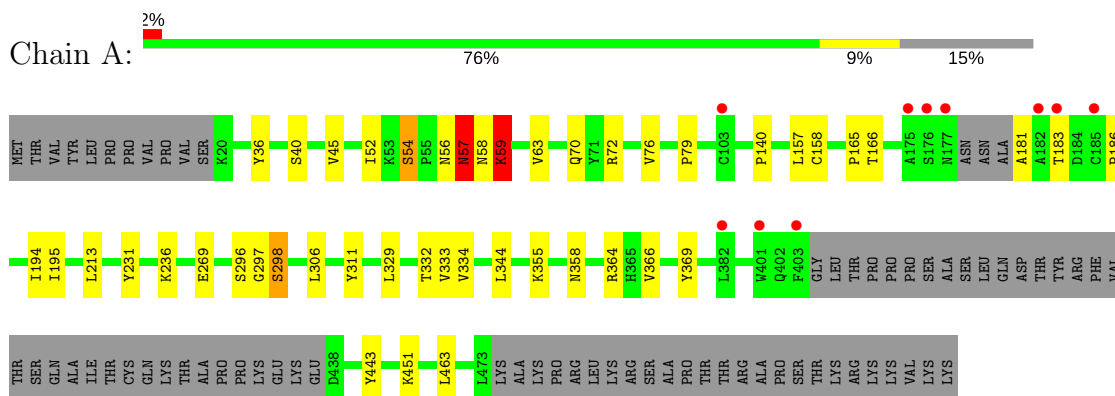
- Molecule 3 is a protein called light chain of Fab fragment of antibody A12A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	203	Total	C	N	O	S	0	0	0
			1585	1003	264	312	6			

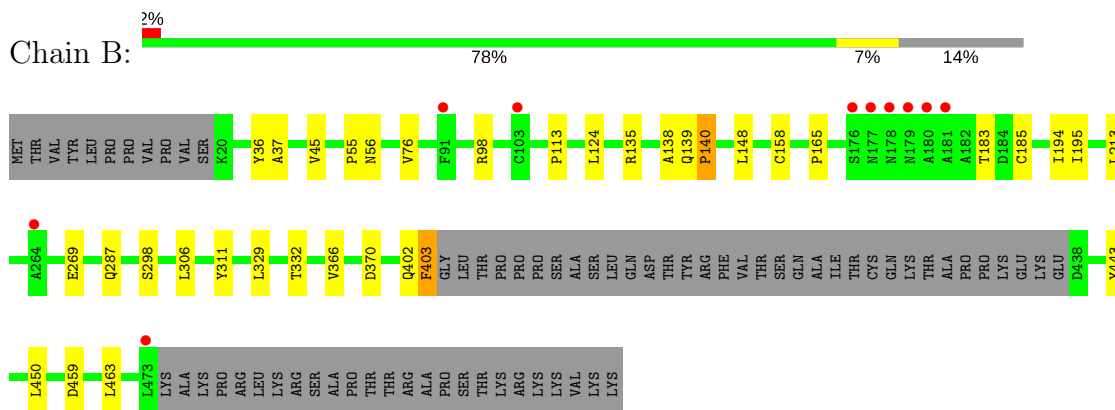
3 Residue-property plots

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.

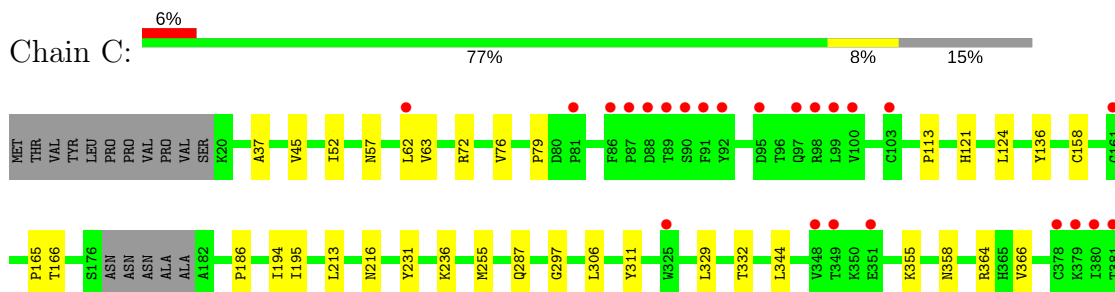
• Molecule 1: Major capsid protein L1

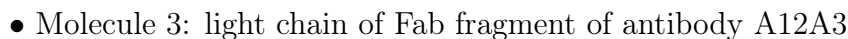
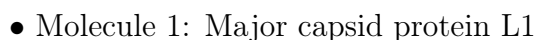
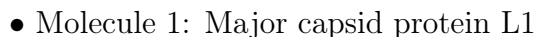


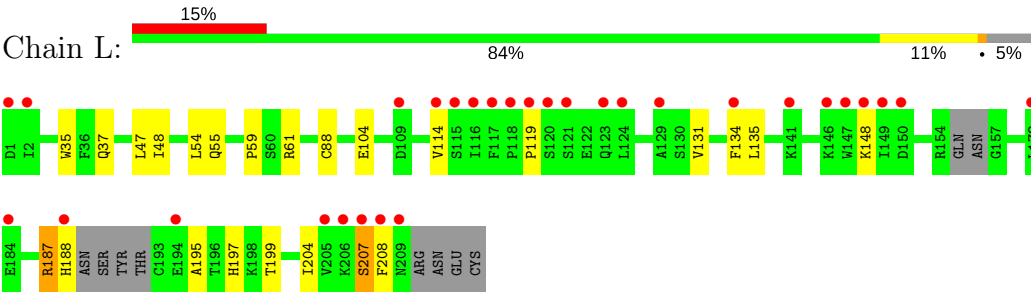
• Molecule 1: Major capsid protein L1



• Molecule 1: Major capsid protein L1







4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.57Å 102.60Å 138.03Å 90.00° 114.52° 90.00°	Depositor
Resolution (Å)	47.86 – 3.44 47.86 – 3.44	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.86-3.44) 99.6 (47.86-3.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.202 , 0.249 0.202 , 0.250	Depositor DCC
R_{free} test set	2025 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	77.3	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	19783	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/3410	0.44	0/4625
1	B	0.25	0/3432	0.44	0/4657
1	C	0.25	0/3397	0.44	0/4607
1	D	0.25	0/3391	0.43	0/4599
1	E	0.25	0/3391	0.44	0/4599
2	H	0.24	0/1652	0.44	0/2260
3	L	0.25	0/1624	0.44	0/2199
All	All	0.25	0/20297	0.44	0/27546

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3324	0	3204	24	0
1	B	3345	0	3222	20	0
1	C	3311	0	3193	24	0
1	D	3305	0	3188	23	0
1	E	3305	0	3188	23	0
2	H	1608	0	1551	23	0
3	L	1585	0	1531	14	0
All	All	19783	0	19077	131	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 3.

All (131) 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:296:SER:O	1:A:298:SER:N	2.20	0.74
1:B:306:LEU:O	1:B:311:TYR:OH	2.08	0.69
3:L:183:ASP:OD2	3:L:187:ARG:NE	2.24	0.68
1:A:306:LEU:O	1:A:311:TYR:OH	2.11	0.67
1:D:306:LEU:O	1:D:311:TYR:OH	2.12	0.62
1:C:165:PRO:HG2	1:C:195:ILE:HB	1.83	0.61
1:A:52:ILE:HB	1:A:63:VAL:HB	1.82	0.61
1:C:255:MET:HA	1:C:297:GLY:HA2	1.83	0.60
1:A:70:GLN:OE1	1:A:72:ARG:NH2	2.35	0.60
1:C:306:LEU:O	1:C:311:TYR:OH	2.13	0.60
1:E:306:LEU:O	1:E:311:TYR:OH	2.13	0.58
2:H:35:HIS:CD2	2:H:50:TRP:HB2	2.38	0.58
2:H:29:ILE:HG12	2:H:53:PRO:HG2	1.85	0.58
1:B:37:ALA:HB1	1:B:450:LEU:HD13	1.85	0.58
1:D:54:SER:HB2	1:D:62:LEU:HG	1.87	0.56
3:L:195:ALA:HB3	3:L:204:ILE:HG23	1.88	0.55
3:L:48:ILE:HG12	3:L:54:LEU:HD23	1.88	0.55
1:A:364:ARG:NH2	1:B:269:GLU:OE1	2.40	0.54
2:H:38:LYS:HB2	2:H:48:ILE:HD11	1.88	0.54
1:B:138:ALA:HB2	1:B:287:GLN:HG2	1.89	0.54
1:D:231:TYR:CG	1:E:113:PRO:HG3	2.43	0.53
2:H:20:LEU:HD21	2:H:116:LEU:HD21	1.90	0.53
1:C:52:ILE:HB	1:C:63:VAL:HB	1.91	0.52
2:H:193:THR:O	2:H:197:GLN:N	2.37	0.52
1:E:45:VAL:HG22	1:E:366:VAL:HG12	1.91	0.52
1:A:213:LEU:HB3	1:C:344:LEU:HD22	1.92	0.52
1:D:158:CYS:HA	1:D:332:THR:O	2.10	0.51
1:D:45:VAL:HG22	1:D:366:VAL:HG12	1.92	0.51
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.92	0.51
1:C:194:ILE:HD12	1:C:443:TYR:CZ	2.46	0.50
2:H:52:ASP:HB3	2:H:57:LYS:HB2	1.93	0.50
1:A:165:PRO:HG2	1:A:195:ILE:HB	1.93	0.50
2:H:125:PRO:HB3	2:H:151:TYR:HB3	1.93	0.49
1:D:135:ARG:NH1	2:H:31:ASP:OD1	2.44	0.49
2:H:20:LEU:HD11	2:H:116:LEU:HD11	1.94	0.49
1:A:344:LEU:HD22	1:B:213:LEU:HB3	1.95	0.49
1:C:213:LEU:HB3	1:D:344:LEU:HD22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ASN:HB2	1:D:354:TYR:HE2	1.77	0.49
2:H:91:ALA:HB2	2:H:118:VAL:HG23	1.95	0.49
1:D:76:VAL:HB	1:D:329:LEU:HB3	1.95	0.48
1:E:127:PHE:CZ	1:E:139:GLN:HB2	2.48	0.48
3:L:37:GLN:HB2	3:L:47:LEU:HD11	1.96	0.48
1:B:158:CYS:HA	1:B:332:THR:O	2.13	0.48
3:L:119:PRO:HD3	3:L:131:VAL:HG22	1.95	0.48
2:H:159:THR:OG1	2:H:202:SER:OG	2.22	0.48
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.48	0.48
3:L:114:VAL:HG22	3:L:135:LEU:HG	1.94	0.48
1:E:70:GLN:OE1	1:E:72:ARG:NH2	2.47	0.48
3:L:148:LYS:O	3:L:188:HIS:NE2	2.47	0.48
1:E:55:PRO:HA	1:E:56:ASN:HA	1.49	0.47
1:A:59:LYS:HA	1:A:59:LYS:HD3	1.54	0.47
1:C:186:PRO:HG2	1:D:344:LEU:HD13	1.97	0.47
1:B:124:LEU:HD23	1:B:148:LEU:HD12	1.95	0.47
1:C:355:LYS:HB2	1:C:358:ASN:ND2	2.30	0.47
2:H:144:SER:HB3	2:H:216:LEU:HD13	1.95	0.47
1:A:36:TYR:HE1	1:A:463:LEU:HB3	1.80	0.47
1:E:165:PRO:HG2	1:E:195:ILE:HB	1.97	0.47
1:C:231:TYR:CD1	1:D:113:PRO:HB3	2.50	0.46
1:A:186:PRO:HG2	1:C:344:LEU:HD13	1.98	0.46
3:L:59:PRO:HB2	3:L:61:ARG:HG2	1.98	0.46
1:E:29:SER:HB2	1:E:379:LYS:HG3	1.96	0.46
3:L:114:VAL:HA	3:L:134:PHE:O	2.16	0.46
1:B:194:ILE:HD12	1:B:443:TYR:CZ	2.50	0.46
1:A:166:THR:HG21	1:A:236:LYS:HD3	1.98	0.46
1:E:76:VAL:HB	1:E:329:LEU:HB3	1.98	0.46
1:D:183:THR:HG22	1:D:185:CYS:H	1.81	0.46
1:D:110:ARG:NH1	1:D:368:GLU:O	2.48	0.45
1:D:72:ARG:HD3	1:D:72:ARG:HA	1.79	0.45
1:C:158:CYS:HA	1:C:332:THR:O	2.17	0.45
1:D:141:GLY:N	1:D:144:ASN:OD1	2.47	0.45
1:D:317:GLN:O	1:E:465:ARG:NH1	2.49	0.45
2:H:11:LEU:HD13	2:H:153:PRO:HG3	1.98	0.45
1:E:157:LEU:HG	1:E:334:VAL:HB	1.97	0.45
1:A:45:VAL:HG22	1:A:366:VAL:HG12	1.98	0.45
1:C:136:TYR:CE2	1:C:287:GLN:HG3	2.52	0.45
1:B:138:ALA:O	1:B:140:PRO:HD3	2.17	0.45
1:B:45:VAL:HG22	1:B:366:VAL:HG12	1.97	0.45
1:A:76:VAL:HB	1:A:329:LEU:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ARG:HA	1:C:72:ARG:HD3	1.80	0.44
1:B:55:PRO:HA	1:B:56:ASN:HA	1.51	0.44
1:B:135:ARG:HH21	2:H:75:SER:HB3	1.82	0.44
1:C:79:PRO:HD3	1:C:451:LYS:HA	1.99	0.44
2:H:14:PRO:HA	2:H:15:GLY:HA2	1.46	0.44
1:E:36:TYR:HE1	1:E:463:LEU:HB3	1.82	0.44
1:A:157:LEU:HG	1:A:334:VAL:HB	2.00	0.44
1:A:194:ILE:HD12	1:A:443:TYR:CZ	2.52	0.44
1:B:165:PRO:HG2	1:B:195:ILE:HB	2.00	0.44
3:L:119:PRO:HD2	3:L:187:ARG:NH2	2.32	0.44
1:B:183:THR:HG22	1:B:185:CYS:H	1.83	0.43
1:B:76:VAL:HB	1:B:329:LEU:HB3	2.00	0.43
1:E:153:LYS:HG3	1:E:255:MET:HB3	2.01	0.43
1:E:72:ARG:HA	1:E:72:ARG:HD3	1.78	0.43
1:D:79:PRO:HD3	1:D:451:LYS:HA	2.00	0.43
2:H:23:LYS:HB3	2:H:78:THR:HG23	1.99	0.43
1:A:181:ALA:N	1:C:62:LEU:HD13	2.33	0.43
1:A:158:CYS:HA	1:A:332:THR:O	2.18	0.43
2:H:50:TRP:CD1	2:H:50:TRP:C	2.92	0.43
1:C:45:VAL:HG22	1:C:366:VAL:HG12	2.01	0.42
1:A:231:TYR:CD1	1:C:113:PRO:HB3	2.54	0.42
1:D:315:ARG:NH1	1:E:469:LEU:HD11	2.34	0.42
1:D:110:ARG:NH2	1:D:367:GLU:OE1	2.52	0.42
1:E:333:VAL:HG11	1:E:369:TYR:HE2	1.84	0.42
1:B:113:PRO:HB3	1:E:231:TYR:CD1	2.55	0.42
1:C:76:VAL:HB	1:C:329:LEU:HB3	2.02	0.42
1:B:459:ASP:O	1:E:319:HIS:NE2	2.51	0.42
1:A:269:GLU:OE1	1:C:364:ARG:NH2	2.47	0.42
1:A:355:LYS:HB2	1:A:358:ASN:ND2	2.34	0.42
1:B:98:ARG:HH21	1:B:403:PHE:HB3	1.85	0.42
1:D:124:LEU:HD23	1:D:148:LEU:HD12	2.01	0.42
1:A:333:VAL:HG11	1:A:369:TYR:HE2	1.85	0.42
1:A:54:SER:O	1:A:57:ASN:HB3	2.20	0.42
1:B:36:TYR:HE1	1:B:463:LEU:HB3	1.85	0.41
3:L:197:HIS:HB3	3:L:199:THR:HG22	2.02	0.41
2:H:194:TRP:HA	2:H:195:PRO:HA	1.87	0.41
1:E:194:ILE:HD12	1:E:443:TYR:CZ	2.55	0.41
1:A:79:PRO:HD3	1:A:451:LYS:HA	2.02	0.41
1:C:166:THR:HG21	1:C:236:LYS:HD3	2.02	0.41
1:C:37:ALA:HB1	1:C:450:LEU:HD13	2.03	0.41
2:H:36:TRP:CE2	2:H:81:LEU:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ASP:HB2	1:E:235:LEU:HD13	2.03	0.41
1:E:355:LYS:HB2	1:E:358:ASN:ND2	2.36	0.41
3:L:207:SER:OG	3:L:208:PHE:N	2.53	0.41
2:H:105:ARG:CZ	3:L:55:GLN:HE22	2.33	0.41
1:E:59:LYS:HA	1:E:59:LYS:HD3	1.87	0.41
1:C:121:HIS:HB3	1:C:124:LEU:HB2	2.03	0.40
1:D:54:SER:O	1:D:57:ASN:HB2	2.21	0.40
1:D:194:ILE:HD12	1:D:443:TYR:CZ	2.56	0.40
1:D:355:LYS:HB2	1:D:358:ASN:ND2	2.37	0.40
1:E:79:PRO:HD3	1:E:451:LYS:HA	2.04	0.40
2:H:152:PHE:HA	2:H:153:PRO:HA	1.82	0.40
2:H:47:TRP:HH2	2:H:59:ILE:HG22	1.86	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	411/490 (84%)	387 (94%)	16 (4%)	8 (2%)	9	43
1	B	416/490 (85%)	394 (95%)	19 (5%)	3 (1%)	24	65
1	C	409/490 (84%)	390 (95%)	19 (5%)	0	100	100
1	D	408/490 (83%)	391 (96%)	15 (4%)	2 (0%)	31	71
1	E	408/490 (83%)	386 (95%)	19 (5%)	3 (1%)	24	65
2	H	206/216 (95%)	182 (88%)	21 (10%)	3 (2%)	11	48
3	L	197/213 (92%)	183 (93%)	14 (7%)	0	100	100
All	All	2455/2879 (85%)	2313 (94%)	123 (5%)	19 (1%)	21	62

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	58	ASN
1	A	297	GLY
1	D	298	SER
1	E	40	SER
1	A	140	PRO
1	A	298	SER
1	B	140	PRO
1	E	58	ASN
1	A	54	SER
1	B	402	GLN
1	E	298	SER
1	A	40	SER
2	H	137	THR
1	A	59	LYS
1	B	298	SER
1	D	40	SER
2	H	140	SER
2	H	139	GLY

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	370/435 (85%)	366 (99%)	4 (1%)	76	89
1	B	372/435 (86%)	370 (100%)	2 (0%)	90	95
1	C	369/435 (85%)	368 (100%)	1 (0%)	93	97
1	D	368/435 (85%)	368 (100%)	0	100	100
1	E	368/435 (85%)	367 (100%)	1 (0%)	93	97
2	H	181/186 (97%)	174 (96%)	7 (4%)	35	68
3	L	179/189 (95%)	176 (98%)	3 (2%)	63	84
All	All	2207/2550 (86%)	2189 (99%)	18 (1%)	83	93

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

Mol	Chain	Res	Type
1	A	56	ASN
1	A	57	ASN
1	A	59	LYS
1	A	183	THR
1	B	139	GLN
1	B	403	PHE
1	C	57	ASN
1	E	59	LYS
2	H	11	LEU
2	H	13	ARG
2	H	28	ASN
2	H	50	TRP
2	H	54	GLU
2	H	136	ASP
2	H	138	THR
3	L	104	GLU
3	L	187	ARG
3	L	207	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	112	GLN
2	H	6	GLN
2	H	35	HIS
2	H	197	GLN

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, 95th 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	417/490 (85%)	0.24	10 (2%) 59 56	54, 87, 137, 172	0
1	B	420/490 (85%)	0.12	10 (2%) 59 56	48, 81, 134, 203	0
1	C	415/490 (84%)	0.37	28 (6%) 18 19	60, 93, 156, 212	0
1	D	414/490 (84%)	0.26	17 (4%) 37 36	53, 91, 153, 186	0
1	E	414/490 (84%)	0.32	16 (3%) 39 38	55, 90, 147, 197	0
2	H	210/216 (97%)	1.61	76 (36%) 0 0	74, 125, 184, 215	0
3	L	203/213 (95%)	0.89	32 (15%) 2 2	79, 110, 166, 189	0
All	All	2493/2879 (86%)	0.43	189 (7%) 14 16	48, 92, 155, 215	0

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	124	LEU	5.8
2	H	130	LEU	5.7
1	D	473	LEU	5.5
1	E	182	ALA	5.4
2	H	160	TRP	5.0
1	C	473	LEU	4.8
2	H	151	TYR	4.8
1	D	91	PHE	4.8
3	L	150	ASP	4.7
3	L	178	LEU	4.6
2	H	168	SER	4.6
2	H	155	PRO	4.6
3	L	109	ASP	4.6
2	H	188	THR	4.6
3	L	180	LEU	4.5
1	C	90	SER	4.4
1	C	403	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
2	H	183	MET	4.4
2	H	184	SER	4.3
2	H	210	THR	4.3
1	C	378	CYS	4.3
1	A	403	PHE	4.3
2	H	185	SER	4.3
1	B	177	ASN	4.1
3	L	147	TRP	4.1
2	H	140	SER	4.1
1	C	91	PHE	4.1
1	D	403	PHE	4.0
2	H	186	SER	3.9
1	C	380	ILE	3.9
3	L	1	ASP	3.8
1	C	381	THR	3.8
1	B	179	ASN	3.7
1	C	87	PRO	3.7
2	H	10	GLU	3.7
1	D	182	ALA	3.6
1	B	180	ALA	3.6
2	H	158	VAL	3.6
3	L	188	HIS	3.5
3	L	134	PHE	3.5
2	H	156	VAL	3.5
2	H	142	VAL	3.5
2	H	152	PHE	3.5
3	L	209	ASN	3.5
1	D	382	LEU	3.4
2	H	187	VAL	3.4
2	H	146	CYS	3.4
2	H	127	VAL	3.3
3	L	179	THR	3.3
2	H	129	PRO	3.3
2	H	198	THR	3.3
1	E	88	ASP	3.2
1	D	472	GLY	3.2
2	H	139	GLY	3.2
2	H	145	GLY	3.2
2	H	147	LEU	3.2
3	L	121	SER	3.2
3	L	120	SER	3.2
1	C	88	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	208	SER	3.1
2	H	195	PRO	3.1
2	H	189	VAL	3.1
2	H	12	VAL	3.1
1	B	181	ALA	3.1
2	H	201	CYS	3.1
1	E	91	PHE	3.1
2	H	138	THR	3.1
2	H	211	THR	3.1
3	L	117	PHE	3.1
1	C	379	LYS	3.1
1	C	401	TRP	3.1
1	E	473	LEU	3.1
3	L	116	ILE	3.0
1	C	99	LEU	3.0
3	L	114	VAL	3.0
3	L	207	SER	3.0
2	H	199	VAL	2.9
2	H	141	SER	2.9
1	C	92	TYR	2.9
1	C	86	PHE	2.9
2	H	214	LYS	2.9
1	E	183	THR	2.9
1	D	103	CYS	2.9
2	H	68	ALA	2.9
1	D	377	LEU	2.9
1	C	351	GLU	2.8
2	H	215	LYS	2.8
1	C	100	VAL	2.8
2	H	148	VAL	2.8
1	D	87	PRO	2.8
1	E	403	PHE	2.8
3	L	129	ALA	2.7
2	H	64	PHE	2.7
2	H	67	LYS	2.7
2	H	179	GLY	2.7
1	D	458	LEU	2.7
2	H	11	LEU	2.7
2	H	143	THR	2.7
2	H	25	SER	2.7
1	E	87	PRO	2.7
3	L	149	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	194	GLU	2.7
1	B	178	ASN	2.6
3	L	118	PRO	2.6
1	A	176	SER	2.6
3	L	115	SER	2.6
2	H	157	THR	2.6
2	H	194	TRP	2.6
2	H	116	LEU	2.6
3	L	119	PRO	2.6
1	A	182	ALA	2.6
2	H	134	CYS	2.6
1	E	86	PHE	2.6
1	C	161	GLY	2.6
2	H	123	THR	2.6
3	L	205	VAL	2.5
3	L	208	PHE	2.5
1	A	185	CYS	2.5
1	B	103	CYS	2.5
2	H	78	THR	2.5
1	A	382	LEU	2.5
1	C	471	SER	2.5
2	H	84	SER	2.5
1	B	264	ALA	2.4
3	L	148	LYS	2.4
1	C	349	THR	2.4
2	H	213	ASP	2.4
2	H	173	PRO	2.4
2	H	172	PHE	2.4
3	L	146	LYS	2.4
2	H	135	GLY	2.4
2	H	216	LEU	2.4
2	H	150	GLY	2.4
2	H	161	ASN	2.4
2	H	203	VAL	2.3
2	H	81	LEU	2.3
2	H	197	GLN	2.3
1	B	176	SER	2.3
3	L	141	LYS	2.3
1	D	97	GLN	2.3
1	C	103	CYS	2.3
3	L	206	LYS	2.3
2	H	1	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	191	SER	2.3
1	C	348	VAL	2.3
1	E	458	LEU	2.3
1	A	175	ALA	2.3
1	D	401	TRP	2.3
3	L	184	GLU	2.3
1	C	97	GLN	2.3
2	H	177	GLN	2.3
1	E	103	CYS	2.3
1	E	62	LEU	2.3
1	A	103	CYS	2.2
1	B	473	LEU	2.2
2	H	20	LEU	2.2
1	A	177	ASN	2.2
1	B	91	PHE	2.2
1	C	95	ASP	2.2
2	H	159	THR	2.2
2	H	69	SER	2.2
1	A	183	THR	2.2
2	H	174	ALA	2.2
1	D	90	SER	2.2
1	C	325	TRP	2.2
1	C	98	ARG	2.2
1	E	56	ASN	2.2
1	C	62	LEU	2.1
2	H	115	THR	2.1
1	D	88	ASP	2.1
2	H	136	ASP	2.1
1	E	105	GLY	2.1
2	H	124	PRO	2.1
1	D	56	ASN	2.1
1	E	278	LYS	2.1
1	D	457	ASP	2.1
2	H	3	GLN	2.1
1	C	81	PRO	2.1
2	H	153	PRO	2.1
1	A	401	TRP	2.1
1	E	382	LEU	2.1
3	L	123	GLN	2.1
3	L	2	ILE	2.1
1	D	379	LYS	2.0
1	E	55	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	122	THR	2.0
1	C	89	THR	2.0
2	H	193	THR	2.0
2	H	192	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.