Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2017 – 11:27 AM EDT

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	:	unknown
Resolution	:	3.44 Å(reported)

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030345

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 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.
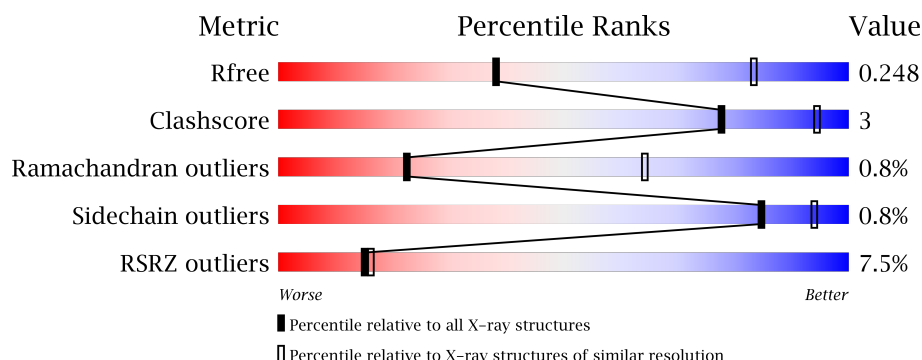
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1082 (3.52-3.36)
Clashscore	112137	1025 (3.50-3.38)
Ramachandran outliers	110173	1155 (3.52-3.36)
Sidechain outliers	110143	1156 (3.52-3.36)
RSRZ outliers	101464	1107 (3.52-3.36)

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 <=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	2% / 76% / 9% / 15%
1	B	490	2% / 78% / 7% / 14%
1	C	490	6% / 77% / 8% / 15%
1	D	490	3% / 77% / 7% / 16%
1	E	490	3% / 76% / 8% / 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	216	35% ... 76% ... 20% ··
3	L	213	15% ... 84% ... 11% · 5%

2 Entry composition (i)

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 3324	C 2120	N 553	O 632	S 19	0	0	0
1	B	420	Total 3345	C 2131	N 558	O 637	S 19	0	0	0
1	C	415	Total 3311	C 2113	N 550	O 629	S 19	0	0	0
1	D	414	Total 3305	C 2110	N 549	O 627	S 19	0	0	0
1	E	414	Total 3305	C 2110	N 549	O 627	S 19	0	0	0

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 1608	C 1018	N 264	O 319	S 7	0	0	0

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

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

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

• Molecule 1: Major capsid protein L1

Chain D:

• Molecule 1: Major capsid protein L1

Chain E:

• Molecule 2: heavy chain of Fab fragment of antibody A12A3
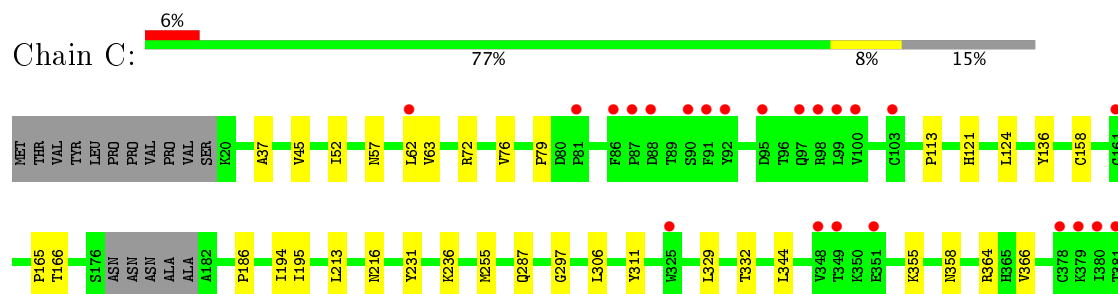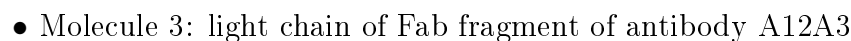
Chain H:

• Molecule 3: light chain of Fab fragment of antibody A12A3

Chain L:
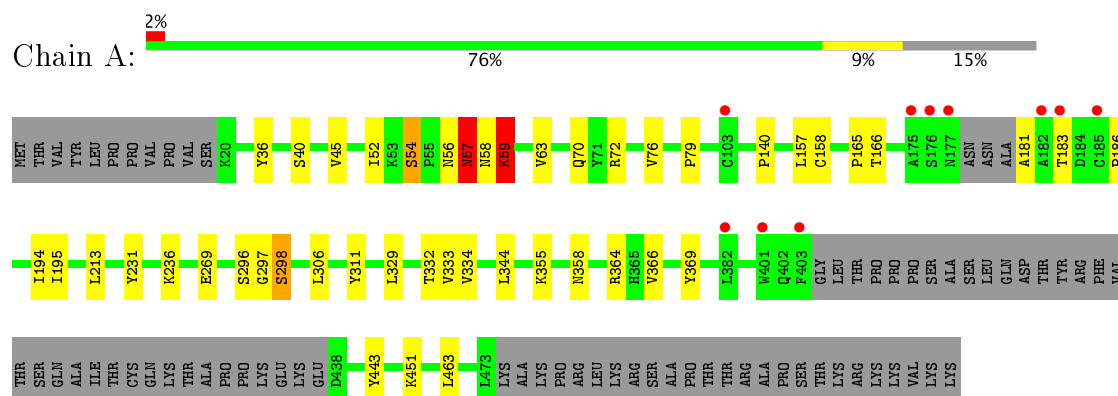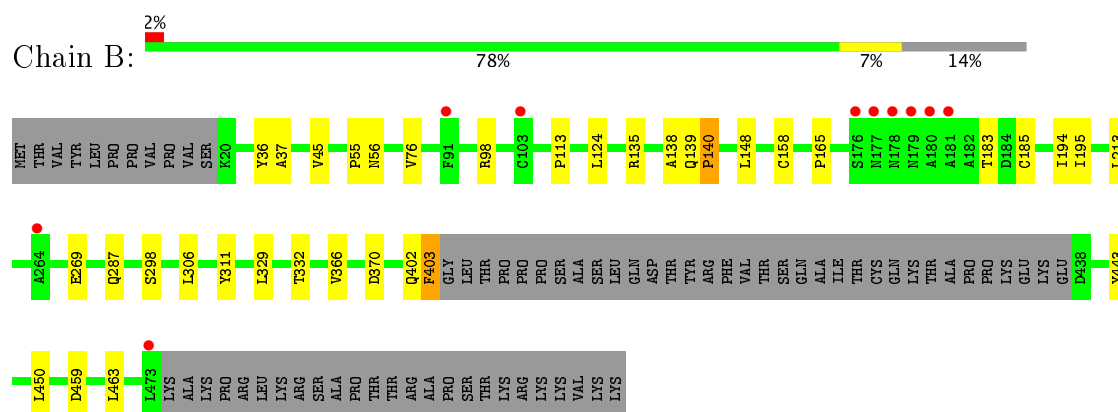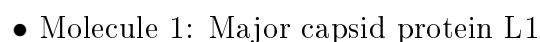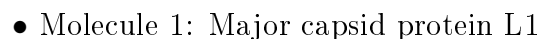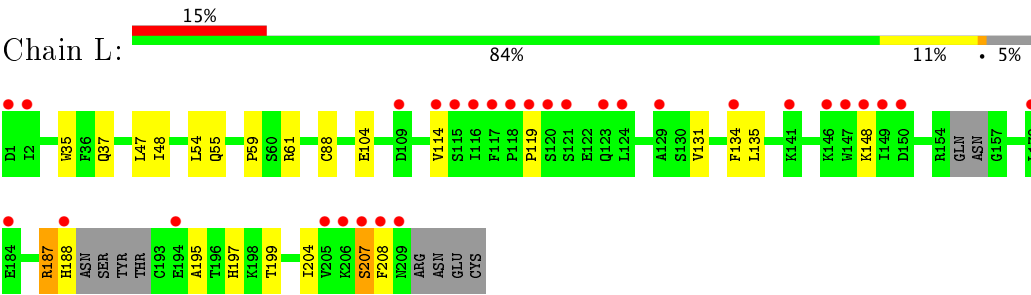
4   Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	3.05 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.202 , 0.249 0.201 , 0.248	Depositor DCC
R_{free} test set	2025 reflections (4.94%)	DCC
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]	$< |L| > = 0.48$, $< L^2 > = 0.31$	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.*

---

[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	0.25	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 ⓘ

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

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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:135:ARG:HH21	2:H:75:SER:HB3	1.82	0.44
1:B:55:PRO:HA	1:B:56:ASN:HA	1.51	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:C:76:VAL:HB	1:C:329:LEU:HB3	2.02	0.42
1:B:113:PRO:HB3	1:E:231:TYR:CD1	2.55	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

Continued on next page...

Continued from previous page...

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 (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	411/490 (84%)	387 (94%)	16 (4%)	8 (2%)	9	45
1	B	416/490 (85%)	394 (95%)	19 (5%)	3 (1%)	25	67
1	C	409/490 (84%)	390 (95%)	19 (5%)	0	100	100
1	D	408/490 (83%)	391 (96%)	15 (4%)	2 (0%)	32	72
1	E	408/490 (83%)	386 (95%)	19 (5%)	3 (1%)	25	67
2	H	206/216 (95%)	182 (88%)	21 (10%)	3 (2%)	12	51
3	L	197/213 (92%)	183 (93%)	14 (7%)	0	100	100
All	All	2455/2879 (85%)	2313 (94%)	123 (5%)	19 (1%)	22	64

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 (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	370/435 (85%)	366 (99%)	4 (1%)	78	91
1	B	372/435 (86%)	370 (100%)	2 (0%)	91	96
1	C	369/435 (85%)	368 (100%)	1 (0%)	94	98
1	D	368/435 (85%)	368 (100%)	0	100	100
1	E	368/435 (85%)	367 (100%)	1 (0%)	94	98
2	H	181/186 (97%)	174 (96%)	7 (4%)	37	72
3	L	179/189 (95%)	176 (98%)	3 (2%)	66	87
All	All	2207/2550 (86%)	2189 (99%)	18 (1%)	85	94

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 (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 carbohydrates 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	54	54, 87, 137, 172	0
1	B	420/490 (85%)	0.12	10 (2%)	59	54	48, 81, 134, 203	0
1	C	415/490 (84%)	0.37	27 (6%)	20	19	60, 93, 156, 212	0
1	D	414/490 (84%)	0.26	17 (4%)	38	34	53, 91, 153, 186	0
1	E	414/490 (84%)	0.32	16 (3%)	40	36	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	3	79, 110, 166, 189	0
All	All	2493/2879 (86%)	0.42	188 (7%)	15	16	48, 92, 155, 215	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	124	LEU	5.7
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	178	LEU	4.6
3	L	150	ASP	4.6
2	H	155	PRO	4.6
2	H	188	THR	4.6
3	L	109	ASP	4.6
2	H	168	SER	4.5
3	L	180	LEU	4.5
1	C	90	SER	4.5
1	C	403	PHE	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	183	MET	4.4
2	H	184	SER	4.3
1	C	378	CYS	4.3
2	H	185	SER	4.3
2	H	210	THR	4.3
1	A	403	PHE	4.2
2	H	140	SER	4.1
1	B	177	ASN	4.1
3	L	147	TRP	4.1
1	C	91	PHE	4.0
1	D	403	PHE	4.0
2	H	186	SER	3.9
1	C	380	ILE	3.8
3	L	1	ASP	3.8
1	C	381	THR	3.8
1	B	179	ASN	3.7
2	H	10	GLU	3.7
1	D	182	ALA	3.7
1	C	87	PRO	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	152	PHE	3.5
2	H	156	VAL	3.5
2	H	142	VAL	3.5
3	L	209	ASN	3.4
1	D	382	LEU	3.4
2	H	146	CYS	3.4
2	H	187	VAL	3.3
2	H	127	VAL	3.3
3	L	179	THR	3.3
2	H	198	THR	3.3
2	H	139	GLY	3.3
2	H	129	PRO	3.3
1	D	472	GLY	3.2
1	E	88	ASP	3.2
2	H	147	LEU	3.2
3	L	121	SER	3.2
2	H	145	GLY	3.2
3	L	120	SER	3.2
2	H	208	SER	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	88	ASP	3.1
2	H	195	PRO	3.1
2	H	189	VAL	3.1
1	B	181	ALA	3.1
1	E	473	LEU	3.1
2	H	12	VAL	3.1
1	C	379	LYS	3.1
1	E	91	PHE	3.1
2	H	201	CYS	3.1
2	H	211	THR	3.1
3	L	117	PHE	3.0
1	C	401	TRP	3.0
2	H	138	THR	3.0
1	C	99	LEU	3.0
3	L	116	ILE	3.0
3	L	207	SER	3.0
3	L	114	VAL	3.0
2	H	199	VAL	3.0
2	H	141	SER	2.9
1	C	86	PHE	2.9
1	C	92	TYR	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	2.8
1	C	351	GLU	2.8
2	H	215	LYS	2.8
1	C	100	VAL	2.8
1	E	403	PHE	2.8
1	D	87	PRO	2.8
2	H	148	VAL	2.8
2	H	179	GLY	2.8
3	L	129	ALA	2.8
2	H	143	THR	2.8
2	H	64	PHE	2.7
1	D	458	LEU	2.7
2	H	25	SER	2.7
2	H	67	LYS	2.7
1	E	87	PRO	2.7
2	H	11	LEU	2.7
3	L	149	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	L	194	GLU	2.7
3	L	118	PRO	2.7
1	B	178	ASN	2.6
2	H	194	TRP	2.6
3	L	115	SER	2.6
2	H	157	THR	2.6
2	H	116	LEU	2.6
1	A	176	SER	2.6
3	L	119	PRO	2.6
1	A	182	ALA	2.6
2	H	134	CYS	2.6
1	E	86	PHE	2.5
1	C	161	GLY	2.5
3	L	205	VAL	2.5
2	H	123	THR	2.5
1	A	185	CYS	2.5
1	B	103	CYS	2.5
1	C	471	SER	2.5
1	A	382	LEU	2.5
3	L	208	PHE	2.5
2	H	78	THR	2.5
2	H	84	SER	2.5
1	C	349	THR	2.5
2	H	213	ASP	2.5
1	B	264	ALA	2.4
2	H	173	PRO	2.4
3	L	148	LYS	2.4
3	L	146	LYS	2.4
2	H	135	GLY	2.4
2	H	216	LEU	2.4
2	H	161	ASN	2.4
2	H	172	PHE	2.4
2	H	81	LEU	2.3
2	H	150	GLY	2.3
2	H	203	VAL	2.3
2	H	197	GLN	2.3
1	B	176	SER	2.3
3	L	141	LYS	2.3
1	C	103	CYS	2.3
1	D	97	GLN	2.3
1	A	175	ALA	2.3
3	L	184	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	103	CYS	2.3
2	H	191	SER	2.3
3	L	206	LYS	2.3
1	E	458	LEU	2.3
2	H	177	GLN	2.3
1	C	348	VAL	2.3
1	D	401	TRP	2.3
1	B	473	LEU	2.3
1	E	62	LEU	2.3
2	H	1	GLU	2.3
1	A	103	CYS	2.2
2	H	20	LEU	2.2
1	B	91	PHE	2.2
1	C	97	GLN	2.2
1	A	183	THR	2.2
2	H	174	ALA	2.2
2	H	69	SER	2.2
1	A	177	ASN	2.2
1	C	95	ASP	2.2
2	H	159	THR	2.2
1	D	90	SER	2.2
1	E	56	ASN	2.2
1	C	325	TRP	2.2
2	H	115	THR	2.2
1	C	98	ARG	2.2
1	C	62	LEU	2.1
2	H	124	PRO	2.1
2	H	136	ASP	2.1
1	D	88	ASP	2.1
1	D	56	ASN	2.1
1	A	401	TRP	2.1
1	E	105	GLY	2.1
1	D	457	ASP	2.1
1	E	278	LYS	2.1
1	E	382	LEU	2.1
2	H	153	PRO	2.1
2	H	3	GLN	2.1
1	C	81	PRO	2.1
3	L	2	ILE	2.1
3	L	123	GLN	2.1
2	H	192	SER	2.1
1	D	379	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	55	PRO	2.0
2	H	193	THR	2.0
2	H	122	THR	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.