



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:02 PM UTC

PDB ID : 5DUP / pdb_00005dup
Title : Influenza A virus H5 hemagglutinin globular head in complex with antibody AVFluIgG03
Authors : Zuo, T.; Sun, J.; Wang, G.; Zhou, P.; Wang, X.; Zhang, L.
Deposited on : 2015-09-20
Resolution : 3.05 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

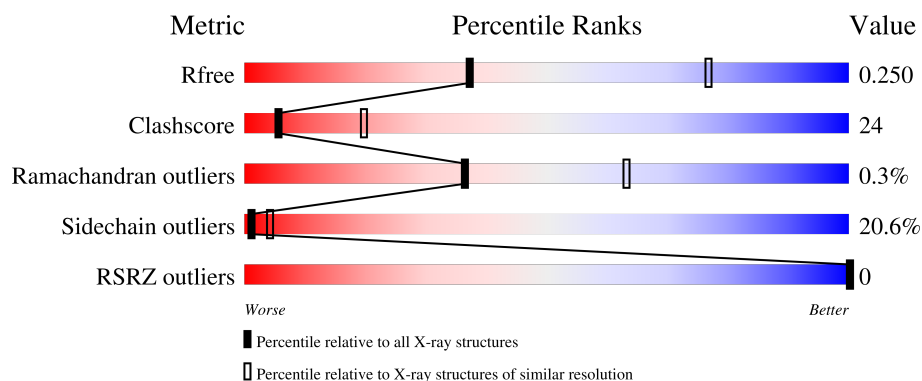
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

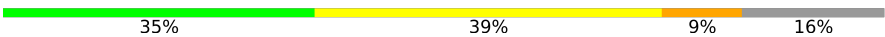
The reported resolution of this entry is 3.05 Å.

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}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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 $\leq 5\%$. 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	233	
2	H	234	
3	L	215	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4703 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1566	993	272	295	6			

There are 9 discrepancies between the modelled and reference sequences:

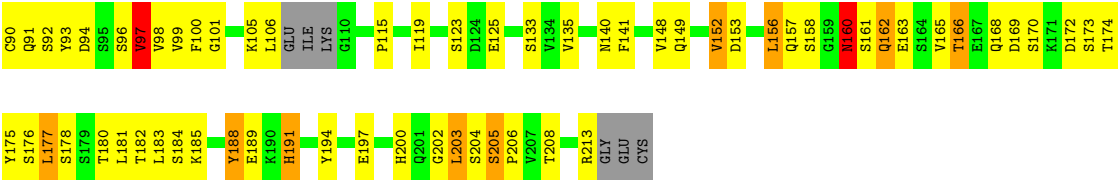
Chain	Residue	Modelled	Actual	Comment	Reference
A	42	ALA	-	expression tag	UNP Q1WDM0
A	43	ASP	-	expression tag	UNP Q1WDM0
A	44	PRO	-	expression tag	UNP Q1WDM0
A	269	HIS	-	expression tag	UNP Q1WDM0
A	270	HIS	-	expression tag	UNP Q1WDM0
A	271	HIS	-	expression tag	UNP Q1WDM0
A	272	HIS	-	expression tag	UNP Q1WDM0
A	273	HIS	-	expression tag	UNP Q1WDM0
A	274	HIS	-	expression tag	UNP Q1WDM0

- Molecule 2 is a protein called AVFluIgG03 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	208	Total	C	N	O	S	0	0	0
			1576	995	264	310	7			

- Molecule 3 is a protein called AVFluIgG03 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	209	Total	C	N	O	S	0	0	0
			1561	971	263	323	4			



4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	132.66Å 132.66Å 87.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.94 – 3.05 38.94 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (38.94-3.05) 99.7 (38.94-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.06Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.199 , 0.257 0.195 , 0.250	Depositor DCC
R_{free} test set	837 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4703	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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	0.53	0/1607	1.00	8/2182 (0.4%)
2	H	0.63	0/1615	1.02	6/2197 (0.3%)
3	L	0.58	0/1594	1.02	8/2168 (0.4%)
All	All	0.58	0/4816	1.01	22/6547 (0.3%)

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
2	H	0	3
3	L	0	1
All	All	0	4

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	215	LYS	CA-C-N	-8.51	109.21	119.84
2	H	215	LYS	C-N-CA	-8.51	109.21	119.84
1	A	84	ASN	CA-C-N	6.52	126.70	120.31
1	A	84	ASN	C-N-CA	6.52	126.70	120.31
2	H	108	HIS	N-CA-C	-6.06	105.65	113.16
1	A	185	ALA	N-CA-C	-5.92	104.77	112.23
3	L	205	SER	CA-C-N	5.66	126.92	119.84
3	L	205	SER	C-N-CA	5.66	126.92	119.84
2	H	139	ALA	CA-C-N	5.54	126.77	119.84
2	H	139	ALA	C-N-CA	5.54	126.77	119.84
3	L	188	TYR	CA-C-N	-5.54	115.05	122.42
3	L	188	TYR	C-N-CA	-5.54	115.05	122.42
2	H	130	THR	N-CA-C	5.36	116.83	110.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	41	LEU	CA-C-N	5.26	126.41	119.84
3	L	41	LEU	C-N-CA	5.26	126.41	119.84
3	L	160	ASN	N-CA-C	5.23	119.36	112.92
1	A	131	VAL	N-CA-C	-5.15	101.55	108.35
3	L	140	ASN	N-CA-C	5.09	116.87	110.91
1	A	234	LYS	CA-C-N	-5.06	114.78	120.14
1	A	234	LYS	C-N-CA	-5.06	114.78	120.14
1	A	132	SER	N-CA-C	5.02	117.04	109.41
1	A	169	GLN	N-CA-C	-5.00	106.96	113.16

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	109	TYR	Peptide
2	H	110	GLY	Peptide
2	H	216	PRO	Peptide
3	L	4	LEU	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	1566	0	1513	91	0
2	H	1576	0	1509	72	0
3	L	1561	0	1499	66	0
All	All	4703	0	4521	217	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 24.

All (217) 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:141:PRO:HD2	2:H:111:LEU:HG	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:5:THR:HB	3:L:23:THR:HG23	1.61	0.83
1:A:133:SER:HB3	2:H:109:TYR:HB3	1.61	0.83
2:H:113:ASN:O	3:L:93:TYR:OH	1.96	0.82
3:L:20:ILE:HB	3:L:75:LEU:HB3	1.63	0.81
1:A:179:HIS:O	1:A:246:ASN:ND2	2.17	0.78
1:A:152:LYS:HD3	1:A:192:GLN:HB2	1.66	0.77
1:A:170:GLU:OE1	1:A:255:LYS:NZ	2.20	0.75
1:A:167:THR:O	1:A:169:GLN:NE2	2.22	0.73
3:L:191:HIS:O	3:L:213:ARG:NH2	2.22	0.72
1:A:56:SER:OG	1:A:57:VAL:N	2.19	0.71
1:A:93:GLY:HA3	1:A:226:MET:H	1.56	0.70
3:L:161:SER:HB3	3:L:181:LEU:HD12	1.73	0.70
1:A:182:ASN:OD1	1:A:216:ARG:NH1	2.25	0.69
2:H:68:ARG:NH2	2:H:91:ASP:OD2	2.24	0.68
1:A:198:ILE:HB	1:A:209:LEU:HB2	1.76	0.67
1:A:65:PRO:HA	1:A:145:ARG:HH11	1.60	0.67
1:A:66:MET:HB2	1:A:87:ASN:HD22	1.59	0.66
3:L:63:ARG:NH1	3:L:79:GLY:O	2.29	0.66
1:A:183:ASP:OD1	1:A:183:ASP:N	2.29	0.65
3:L:20:ILE:HD12	3:L:75:LEU:HD23	1.78	0.65
3:L:23:THR:OG1	3:L:24:GLY:N	2.29	0.65
1:A:107:ARG:O	1:A:259:LYS:N	2.28	0.65
2:H:116:ASP:OD1	2:H:117:SER:N	2.30	0.65
3:L:160:ASN:OD1	3:L:160:ASN:N	2.29	0.65
2:H:75:ASN:OD1	2:H:75:ASN:N	2.27	0.64
2:H:111:LEU:HD13	2:H:112:HIS:CE1	2.33	0.64
2:H:131:LYS:O	2:H:217:SER:HB3	1.97	0.63
1:A:108:ILE:HD13	1:A:258:LYS:HA	1.81	0.63
2:H:161:PRO:O	2:H:214:HIS:NE2	2.20	0.63
1:A:172:LEU:HD23	1:A:174:ILE:HD11	1.79	0.63
1:A:182:ASN:HB3	1:A:215:THR:HA	1.79	0.63
2:H:109:TYR:OH	2:H:112:HIS:O	2.09	0.62
2:H:49:SER:OG	2:H:60:TYR:O	2.12	0.62
3:L:63:ARG:HH22	3:L:84:ASP:CG	2.06	0.62
1:A:116:ILE:HG13	1:A:117:ILE:H	1.65	0.62
2:H:11:LEU:HD21	2:H:127:SER:O	1.99	0.62
3:L:63:ARG:NH2	3:L:84:ASP:OD2	2.30	0.62
3:L:185:LYS:HA	3:L:188:TYR:HB3	1.82	0.61
2:H:178:HIS:HB2	2:H:195:VAL:HG23	1.83	0.61
1:A:179:HIS:HB2	1:A:248:ILE:HD11	1.81	0.61
3:L:135:VAL:HG22	3:L:180:THR:HG23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:VAL:O	2:H:126:VAL:HA	2.02	0.60
2:H:131:LYS:HG3	2:H:132:GLY:H	1.67	0.60
2:H:103:TYR:OH	3:L:52:GLY:HA3	2.02	0.60
1:A:87:ASN:OD1	1:A:87:ASN:N	2.35	0.59
3:L:169:ASP:HB3	3:L:172:ASP:OD1	2.03	0.59
2:H:113:ASN:N	2:H:113:ASN:OD1	2.36	0.59
1:A:101:LEU:O	1:A:105:LEU:HB2	2.03	0.58
3:L:157:GLN:CD	3:L:160:ASN:HD21	2.11	0.58
2:H:168:TRP:H	2:H:171:GLY:HA2	1.68	0.58
2:H:98:VAL:HG11	2:H:115:PHE:HB3	1.85	0.58
1:A:147:VAL:HG12	1:A:248:ILE:HG22	1.86	0.58
1:A:119:LYS:HA	1:A:122:TRP:HE1	1.67	0.58
2:H:98:VAL:CG1	2:H:115:PHE:HB3	2.34	0.58
1:A:98:TYR:O	1:A:102:LYS:HG3	2.04	0.58
1:A:59:GLY:O	1:A:63:GLY:N	2.35	0.57
1:A:65:PRO:HA	1:A:145:ARG:NH1	2.17	0.57
3:L:29:ILE:HG22	3:L:68:LYS:HZ2	1.69	0.57
3:L:63:ARG:HB3	3:L:78:THR:O	2.05	0.57
1:A:157:TYR:CZ	1:A:245:GLY:HA2	2.40	0.57
1:A:107:ARG:HB3	1:A:259:LYS:HD2	1.86	0.57
3:L:149:GLN:HG2	3:L:156:LEU:HD21	1.87	0.56
3:L:200:HIS:HB3	3:L:202:GLY:O	2.06	0.56
3:L:166:THR:OG1	3:L:176:SER:O	2.23	0.56
1:A:259:LYS:HZ2	1:A:259:LYS:HA	1.70	0.56
1:A:200:VAL:HA	1:A:240:ASN:O	2.06	0.55
3:L:197:GLU:HB2	3:L:208:THR:HG23	1.87	0.55
2:H:3:GLN:HB3	2:H:5:LEU:HD11	1.87	0.55
1:A:141:PRO:HG2	2:H:109:TYR:CD1	2.42	0.55
1:A:180:HIS:HB2	1:A:225:ARG:HB2	1.89	0.55
1:A:181:SER:O	1:A:216:ARG:NH2	2.36	0.55
3:L:185:LYS:O	3:L:188:TYR:HB3	2.08	0.54
2:H:92:THR:HG22	2:H:126:VAL:H	1.72	0.54
3:L:172:ASP:OD2	3:L:174:THR:OG1	2.19	0.54
1:A:198:ILE:O	1:A:209:LEU:N	2.33	0.54
2:H:89:ALA:O	2:H:92:THR:HG23	2.08	0.54
2:H:99:ARG:HB2	2:H:117:SER:HB2	1.90	0.53
1:A:154:ASN:O	1:A:154:ASN:ND2	2.35	0.53
1:A:159:THR:HG23	1:A:244:ASN:HB3	1.91	0.53
2:H:169:ASN:C	2:H:171:GLY:H	2.17	0.53
1:A:173:LEU:HB3	1:A:254:TYR:HB2	1.89	0.53
1:A:58:ALA:HB2	1:A:98:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:111:LEU:HD13	2:H:112:HIS:NE2	2.23	0.53
1:A:64:ASN:O	1:A:66:MET:N	2.42	0.53
1:A:182:ASN:O	1:A:213:ILE:HG23	2.10	0.52
2:H:167:SER:HB3	2:H:171:GLY:HA2	1.91	0.52
1:A:56:SER:HB2	1:A:85:PRO:HG3	1.92	0.52
2:H:29:PHE:HB2	2:H:78:ASN:ND2	2.25	0.52
3:L:115:PRO:HB3	3:L:141:PHE:CD2	2.45	0.52
1:A:58:ALA:HB2	1:A:98:TYR:HE2	1.74	0.51
1:A:152:LYS:HD2	1:A:155:ASN:HA	1.93	0.51
1:A:56:SER:HB2	1:A:85:PRO:CG	2.41	0.51
1:A:57:VAL:HB	1:A:98:TYR:OH	2.10	0.51
1:A:101:LEU:HD12	1:A:230:TRP:CE3	2.44	0.51
1:A:110:HIS:HB3	1:A:257:VAL:HB	1.92	0.51
1:A:111:PHE:HE1	1:A:254:TYR:HB3	1.76	0.51
1:A:119:LYS:O	1:A:122:TRP:HD1	1.93	0.51
2:H:131:LYS:HG3	2:H:132:GLY:N	2.26	0.51
2:H:209:ILE:HG23	2:H:223:LYS:C	2.36	0.50
3:L:28:ASN:HB3	3:L:94:ASP:HB2	1.93	0.50
2:H:168:TRP:CZ2	2:H:210:CYS:HB3	2.47	0.50
1:A:93:GLY:HA3	1:A:226:MET:N	2.27	0.50
2:H:29:PHE:HZ	2:H:80:MET:HB3	1.76	0.50
2:H:140:PRO:HD2	2:H:227:PRO:HD3	1.93	0.50
3:L:4:LEU:O	3:L:5:THR:OG1	2.23	0.50
3:L:169:ASP:OD1	3:L:170:SER:N	2.45	0.50
2:H:102:SER:HB2	2:H:113:ASN:HB3	1.93	0.50
3:L:203:LEU:O	3:L:204:SER:OG	2.23	0.50
1:A:97:ASP:HB2	1:A:230:TRP:HE1	1.77	0.49
2:H:95:TYR:O	2:H:121:GLY:HA2	2.12	0.49
3:L:163:GLU:HG3	3:L:177:LEU:HD11	1.95	0.49
3:L:152:VAL:HG13	3:L:194:TYR:HD1	1.77	0.49
3:L:29:ILE:HG22	3:L:68:LYS:NZ	2.27	0.49
2:H:4:LEU:HB2	2:H:119:GLY:HA2	1.94	0.49
3:L:56:ARG:HD3	3:L:64:PHE:HB2	1.95	0.49
3:L:97:VAL:HG12	3:L:98:VAL:H	1.78	0.49
1:A:157:TYR:CE2	1:A:245:GLY:HA2	2.48	0.48
2:H:111:LEU:O	2:H:112:HIS:ND1	2.46	0.48
3:L:169:ASP:O	3:L:173:SER:HA	2.12	0.48
2:H:209:ILE:HG12	2:H:224:LYS:HG3	1.95	0.48
3:L:168:GLN:NE2	3:L:173:SER:O	2.33	0.48
3:L:20:ILE:O	3:L:74:SER:HA	2.13	0.48
1:A:169:GLN:N	1:A:170:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:13:ALA:O	3:L:16:GLN:HB2	2.14	0.48
1:A:208:ARG:HE	1:A:208:ARG:HB2	1.46	0.47
3:L:4:LEU:N	3:L:100:PHE:O	2.47	0.47
3:L:105:LYS:C	3:L:106:LEU:HD12	2.39	0.47
2:H:92:THR:CG2	2:H:126:VAL:H	2.28	0.47
3:L:96:SER:HB3	3:L:97:VAL:H	1.51	0.47
1:A:125:HIS:NE2	1:A:158:PRO:HG2	2.28	0.47
2:H:72:SER:O	2:H:81:TYR:N	2.41	0.47
3:L:91:GLN:HG2	3:L:92:SER:N	2.29	0.47
2:H:131:LYS:NZ	2:H:158:ASP:O	2.44	0.47
2:H:27:PHE:CE2	2:H:34:MET:HE1	2.50	0.47
3:L:41:LEU:HA	3:L:42:PRO:HD3	1.76	0.47
3:L:63:ARG:O	3:L:77:ILE:HA	2.15	0.47
1:A:62:LEU:O	1:A:144:PHE:HB3	2.15	0.47
2:H:185:GLN:HG2	2:H:186:SER:H	1.79	0.46
1:A:124:ASP:HB3	1:A:158:PRO:HG3	1.96	0.46
2:H:65:VAL:HB	2:H:69:PHE:CG	2.50	0.46
1:A:141:PRO:HD2	2:H:111:LEU:CG	2.36	0.46
1:A:182:ASN:ND2	1:A:223:SER:OG	2.49	0.46
1:A:133:SER:HB3	2:H:109:TYR:CB	2.40	0.46
3:L:90:CYS:O	3:L:101:GLY:N	2.49	0.46
2:H:109:TYR:HE1	2:H:112:HIS:H	1.64	0.46
3:L:28:ASN:O	3:L:31:ALA:HB3	2.15	0.46
2:H:38:ARG:HD3	2:H:48:VAL:HG22	1.97	0.45
3:L:40:GLN:HB2	3:L:46:PRO:HA	1.98	0.45
2:H:183:VAL:HG11	3:L:162:GLN:HB2	1.98	0.45
2:H:167:SER:HB2	2:H:211:ASN:HB2	1.99	0.45
2:H:68:ARG:HH22	2:H:91:ASP:CG	2.22	0.45
2:H:18:LEU:HB3	2:H:84:MET:HE2	1.99	0.45
3:L:168:GLN:HB2	3:L:175:TYR:CE1	2.51	0.45
1:A:116:ILE:HG13	1:A:117:ILE:N	2.30	0.45
3:L:172:ASP:OD1	3:L:173:SER:N	2.50	0.45
1:A:197:TYR:O	1:A:243:SER:OG	2.31	0.44
2:H:51:ILE:HG12	2:H:73:ARG:HG2	1.99	0.44
3:L:50:ILE:HD13	3:L:56:ARG:HG2	1.99	0.44
3:L:191:HIS:C	3:L:213:ARG:HH21	2.21	0.44
1:A:53:ARG:O	1:A:82:LYS:HE2	2.17	0.44
1:A:56:SER:HB3	1:A:88:ASP:HA	2.00	0.44
2:H:168:TRP:CH2	2:H:210:CYS:HB3	2.52	0.44
1:A:203:SER:OG	1:A:237:ASP:OD2	2.32	0.44
3:L:58:SER:C	3:L:60:VAL:H	2.24	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:99:ARG:O	2:H:115:PHE:HA	2.18	0.44
2:H:169:ASN:HD21	2:H:208:TYR:HA	1.81	0.44
2:H:130:THR:HG22	2:H:131:LYS:H	1.83	0.44
2:H:157:LYS:NZ	3:L:133:SER:OG	2.50	0.43
1:A:178:ILE:HD12	1:A:209:LEU:HB3	1.99	0.43
1:A:220:ASN:OD1	1:A:220:ASN:N	2.50	0.43
3:L:168:GLN:HE21	3:L:173:SER:C	2.22	0.43
3:L:189:GLU:HG2	3:L:213:ARG:NE	2.33	0.43
1:A:99:GLU:H	1:A:99:GLU:HG3	1.55	0.43
1:A:122:TRP:CD1	1:A:122:TRP:H	2.35	0.43
2:H:136:PHE:CD1	3:L:125:GLU:HB2	2.54	0.43
2:H:159:TYR:CZ	2:H:190:TYR:HB2	2.52	0.43
2:H:68:ARG:O	2:H:69:PHE:HD1	2.02	0.43
2:H:109:TYR:O	2:H:109:TYR:CG	2.71	0.43
3:L:93:TYR:CE1	3:L:98:VAL:HG22	2.54	0.42
3:L:203:LEU:HD11	3:L:206:PRO:HG3	2.01	0.42
1:A:191:TYR:O	1:A:192:GLN:HB3	2.19	0.42
2:H:100:ASP:HB3	2:H:113:ASN:ND2	2.34	0.42
1:A:171:ASP:OD2	1:A:234:LYS:NZ	2.53	0.42
1:A:182:ASN:HB2	1:A:183:ASP:OD1	2.20	0.42
1:A:65:PRO:HB2	1:A:137:TYR:HB2	2.01	0.42
1:A:107:ARG:HA	1:A:259:LYS:NZ	2.35	0.42
3:L:185:LYS:CA	3:L:188:TYR:HB3	2.50	0.42
1:A:151:ILE:HG21	2:H:103:TYR:CE1	2.55	0.41
1:A:143:PHE:CG	1:A:144:PHE:N	2.88	0.41
2:H:176:GLY:O	2:H:197:THR:OG1	2.38	0.41
1:A:216:ARG:NH1	1:A:223:SER:O	2.52	0.41
2:H:68:ARG:C	2:H:69:PHE:HD1	2.28	0.41
1:A:95:PHE:CD1	1:A:98:TYR:HD2	2.38	0.41
3:L:184:SER:O	3:L:188:TYR:N	2.52	0.41
2:H:47:TRP:HB2	3:L:98:VAL:HB	2.01	0.41
2:H:18:LEU:O	2:H:84:MET:HG3	2.21	0.41
3:L:10:VAL:HG22	3:L:105:LYS:O	2.20	0.41
1:A:108:ILE:HG23	1:A:257:VAL:O	2.20	0.41
1:A:161:LYS:HE3	1:A:161:LYS:HB2	1.79	0.41
1:A:170:GLU:HB2	1:A:255:LYS:HE2	2.03	0.41
3:L:58:SER:O	3:L:60:VAL:HG23	2.21	0.41
1:A:175:LEU:O	1:A:250:PRO:HG3	2.21	0.40
2:H:4:LEU:HD12	2:H:118:TRP:C	2.46	0.40
3:L:205:SER:HA	3:L:206:PRO:HD3	1.82	0.40
1:A:64:ASN:H	1:A:144:PHE:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD22	1:A:105:LEU:HA	1.70	0.40
1:A:133:SER:O	1:A:136:PRO:HD3	2.22	0.40
3:L:13:ALA:HB3	3:L:16:GLN:CD	2.46	0.40
1:A:109:ASN:OD1	1:A:109:ASN:N	2.49	0.40
1:A:189:LYS:HG2	1:A:190:LEU:HD23	2.04	0.40
2:H:164:VAL:HG12	2:H:214:HIS:HB2	2.02	0.40
2:H:169:ASN:C	2:H:171:GLY:N	2.79	0.40
1:A:115:GLN:HA	1:A:252:TYR:HA	2.03	0.40
1:A:135:CYS:HB2	1:A:142:SER:O	2.22	0.40
1:A:53:ARG:HE	1:A:68:ASP:C	2.30	0.40
1:A:64:ASN:ND2	1:A:88:ASP:O	2.54	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	191/233 (82%)	169 (88%)	21 (11%)	1 (0%)	24	52
2	H	200/234 (86%)	181 (90%)	19 (10%)	0	100	100
3	L	205/215 (95%)	186 (91%)	18 (9%)	1 (0%)	24	52
All	All	596/682 (87%)	536 (90%)	58 (10%)	2 (0%)	36	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	97	VAL
1	A	83	ALA

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	174/208 (84%)	144 (83%)	30 (17%)	2	8
2	H	177/196 (90%)	130 (73%)	47 (27%)	0	1
3	L	177/182 (97%)	145 (82%)	32 (18%)	2	7
All	All	528/586 (90%)	419 (79%)	109 (21%)	1	4

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	67	CYS
1	A	84	ASN
1	A	87	ASN
1	A	99	GLU
1	A	104	LEU
1	A	105	LEU
1	A	106	SER
1	A	111	PHE
1	A	117	ILE
1	A	122	TRP
1	A	141	PRO
1	A	147	VAL
1	A	154	ASN
1	A	159	THR
1	A	175	LEU
1	A	178	ILE
1	A	182	ASN
1	A	183	ASP
1	A	195	THR
1	A	202	THR
1	A	203	SER
1	A	208	ARG
1	A	210	VAL
1	A	216	ARG
1	A	217	SER

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Mol	Chain	Res	Type
1	A	220	ASN
1	A	234	LYS
1	A	256	ILE
1	A	259	LYS
2	H	5	LEU
2	H	6	GLU
2	H	12	VAL
2	H	13	GLN
2	H	18	LEU
2	H	19	ARG
2	H	20	VAL
2	H	23	THR
2	H	28	THR
2	H	35	SER
2	H	45	LEU
2	H	64	SER
2	H	68	ARG
2	H	72	SER
2	H	73	ARG
2	H	75	ASN
2	H	85	ASN
2	H	90	GLU
2	H	98	VAL
2	H	100	ASP
2	H	101	ASP
2	H	102	SER
2	H	109	TYR
2	H	111	LEU
2	H	113	ASN
2	H	120	GLN
2	H	123	LEU
2	H	125	THR
2	H	128	SER
2	H	130	THR
2	H	152	LEU
2	H	155	LEU
2	H	165	THR
2	H	174	THR
2	H	177	VAL
2	H	192	LEU
2	H	195	VAL
2	H	196	VAL

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Mol	Chain	Res	Type
2	H	197	THR
2	H	198	VAL
2	H	211	ASN
2	H	215	LYS
2	H	218	ASN
2	H	220	LYS
2	H	222	ASP
2	H	223	LYS
2	H	226	GLU
3	L	19	THR
3	L	21	SER
3	L	23	THR
3	L	28	ASN
3	L	29	ILE
3	L	40	GLN
3	L	44	THR
3	L	58	SER
3	L	62	ASP
3	L	67	SER
3	L	69	SER
3	L	80	LEU
3	L	85	GLU
3	L	97	VAL
3	L	99	VAL
3	L	119	ILE
3	L	123	SER
3	L	148	VAL
3	L	152	VAL
3	L	153	ASP
3	L	156	LEU
3	L	158	SER
3	L	160	ASN
3	L	162	GLN
3	L	165	VAL
3	L	166	THR
3	L	177	LEU
3	L	178	SER
3	L	182	THR
3	L	183	LEU
3	L	191	HIS
3	L	203	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	138	GLN
1	A	182	ASN
2	H	13	GLN
2	H	24	ASN
2	H	85	ASN
3	L	28	ASN
3	L	154	ASN

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 oligosaccharides 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	195/233 (83%)	-1.46	0 100 100	57, 72, 96, 107	0
2	H	208/234 (88%)	-1.60	0 100 100	45, 55, 65, 70	0
3	L	209/215 (97%)	-1.56	0 100 100	49, 60, 72, 74	0
All	All	612/682 (89%)	-1.54	0 100 100	45, 62, 85, 107	0

There are no RSRZ outliers to report.

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 oligosaccharides 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.