



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 10:38 PM GMT

PDB ID : 5DUP
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
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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-20026982

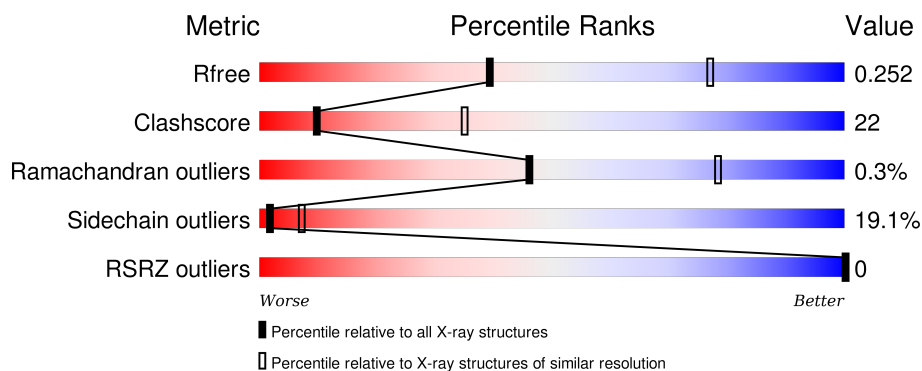
1 Overall quality at a glance

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}	91344	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (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 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	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			

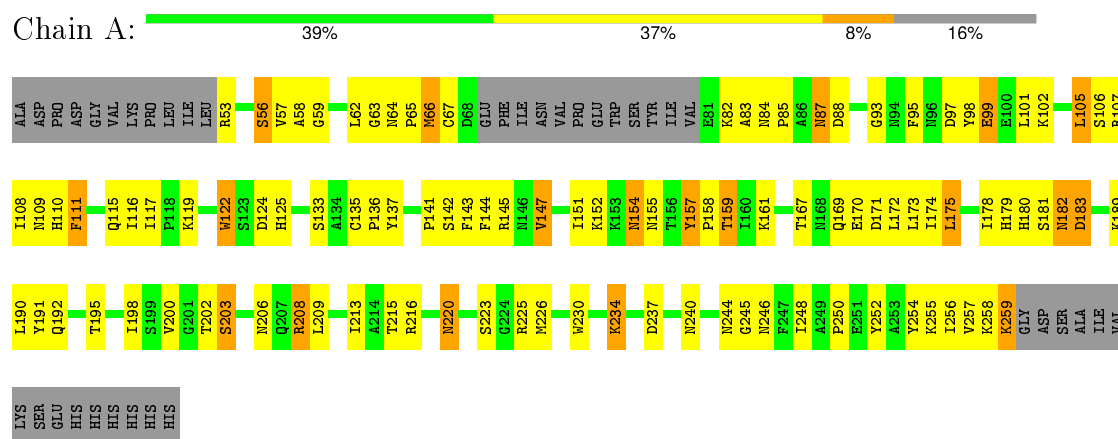
- Molecule 3 is a protein called AVFluIgG03 Light Chain.

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

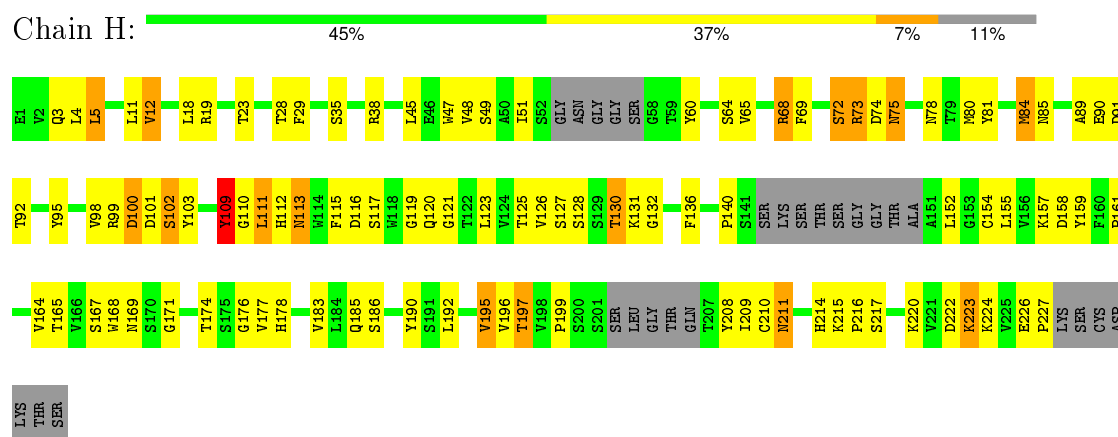
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

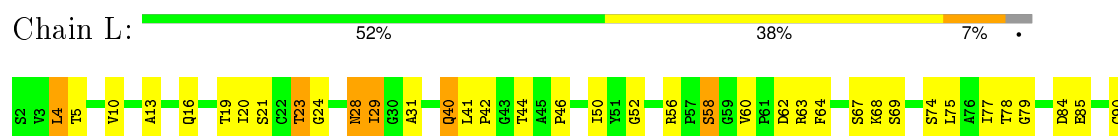
• Molecule 1: Hemagglutinin



• Molecule 2: AVFluIG03 Heavy Chain



• Molecule 3: AVFluIG03 Light Chain



S178	S179	T180	T181	T182	L183	S184	K185		Y188	E189	K190	H191	Y194	E197		H200	Q201	L203	S204	S205	P206	T207	T208		R213	GLY	GLU	CYS																												
Q91	S92	Y93	D94	S95	S96	V97	V98	V99	F100	G101		K105	L106	GLU	I107	L108	L109	S123	D124	E125		S133	V134	V135		F141	F142		V148	V149		V152	D153		L156	Q157	S158	G159	M160	S161	Q162	E163	S164	V165	T166	E167	Q168	D169	S170	K171	D172	S173	T174	Y175	S176	L177

4 Data and refinement statistics

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α , β , γ	132.66 Å 132.66 Å 87.96 Å 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 3.06 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.199 , 0.257 0.195 , 0.252	Depositor DCC
R_{free} test set	837 reflections (5.23%)	DCC
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 , 48.8	EDS
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 16855 reflections	Xtriage
F_o, F_c correlation	0.92	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.40	0/1607	0.61	0/2182
2	H	0.50	0/1615	0.67	0/2197
3	L	0.44	0/1594	0.63	0/2168
All	All	0.45	0/4816	0.64	0/6547

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.

There are no bond angle outliers.

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 [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	1566	0	1513	89	0
2	H	1576	0	1509	66	0
3	L	1561	0	1499	62	0
All	All	4703	0	4521	205	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 22.

All (205) 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
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: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:170:GLU:OE1	1:A:255:LYS:NZ	2.20	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:N	1:A:183:ASP:OD1	2.29	0.65
3:L:23:THR:OG1	3:L:24:GLY:N	2.29	0.65
3:L:20:ILE:HD12	3:L:75:LEU:HD23	1.78	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:PRO:O	2:H:214:HIS:NE2	2.20	0.63
1:A:182:ASN:HB3	1:A:215:THR:HA	1.79	0.63
1:A:172:LEU:HD23	1:A:174:ILE:HD11	1.79	0.63
2:H:109:TYR:OH	2:H:112:HIS:O	2.09	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
2:H:131:LYS:HG3	2:H:132:GLY:H	1.67	0.60
2:H:12:VAL:O	2:H:126:VAL:HA	2.02	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
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
2:H:98:VAL:CG1	2:H:115:PHE:HB3	2.34	0.58
1:A:119:LYS:HA	1:A:122:TRP:HE1	1.67	0.58
1:A:98:TYR:O	1:A:102:LYS:HG3	2.04	0.58
3:L:63:ARG:HH22	3:L:84:ASP:CG	2.06	0.57
1:A:65:PRO:HA	1:A:145:ARG:NH1	2.17	0.57
1:A:59:GLY:O	1:A:63:GLY:N	2.35	0.57
3:L:63:ARG:HB3	3:L:78:THR:O	2.05	0.57
3:L:29:ILE:HG22	3:L:68:LYS:HZ2	1.69	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:4:LEU:O	3:L:5:THR:OG1	2.23	0.56
3:L:166:THR:OG1	3:L:176:SER:O	2.23	0.56
3:L:197:GLU:HB2	3:L:208:THR:HG23	1.87	0.55
1:A:200:VAL:HA	1:A:240:ASN:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:L:157:GLN:CD	3:L:160:ASN:HD21	2.11	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
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
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
2:H:131:LYS:HG3	2:H:132:GLY:N	2.26	0.51
1:A:110:HIS:HB3	1:A:257:VAL:HB	1.92	0.51
1:A:119:LYS:O	1:A:122:TRP:HD1	1.93	0.51
1:A:111:PHE:HE1	1:A:254:TYR:HB3	1.76	0.51
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
3:L:169:ASP:OD1	3:L:170:SER:N	2.45	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
2:H:102:SER:HB2	2:H:113:ASN:HB3	1.93	0.50
1:A:97:ASP:HB2	1:A:230:TRP:HE1	1.77	0.49
3:L:163:GLU:HG3	3:L:177:LEU:HD11	1.95	0.49
2:H:95:TYR:O	2:H:121:GLY:HA2	2.12	0.49
3:L:152:VAL:HG13	3:L:194:TYR:HD1	1.77	0.49
1:A:53:ARG:N	1:A:82:LYS:HZ3	2.10	0.49
3:L:29:ILE:HG22	3:L:68:LYS:NZ	2.27	0.49
3:L:97:VAL:HG12	3:L:98:VAL:H	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:111:LEU:O	2:H:112:HIS:ND1	2.46	0.48
1:A:157:TYR:CE2	1:A:245:GLY:HA2	2.48	0.48
3:L:169:ASP:O	3:L:173:SER:HA	2.12	0.48
3:L:168:GLN:NE2	3:L:173:SER:O	2.33	0.48
2:H:209:ILE:HG12	2:H:224:LYS:HG3	1.95	0.48
2:H:169:ASN:C	2:H:171:GLY:H	2.17	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
3:L:13:ALA:O	3:L:16:GLN:HB2	2.14	0.48
1:A:208:ARG:HB2	1:A:208:ARG:HE	1.46	0.47
3:L:203:LEU:O	3:L:204:SER:OG	2.23	0.47
3:L:4:LEU:N	3:L:100:PHE:O	2.47	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
3:L:63:ARG:O	3:L:77:ILE:HA	2.15	0.47
3:L:41:LEU:HA	3:L:42:PRO:HD3	1.76	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
2:H:49:SER:OG	2:H:60:TYR:O	2.12	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:209:ILE:HG23	2:H:223:LYS:C	2.36	0.45
3:L:40:GLN:HB2	3:L:46:PRO:HA	1.98	0.45
2:H:38:ARG:HD3	2:H:48:VAL:HG22	1.97	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
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:220:ASN:N	1:A:220:ASN:OD1	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:50:ILE:HD13	3:L:56:ARG:HG2	1.99	0.44
2:H:51:ILE:HG12	2:H:73:ARG:HG2	1.99	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:53:ARG:O	1:A:82:LYS:HE2	2.17	0.44
1:A:203:SER:OG	1:A:237:ASP:OD2	2.32	0.44
2:H:131:LYS:NZ	2:H:158:ASP:O	2.44	0.44
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
3:L:189:GLU:HG2	3:L:213:ARG:NE	2.33	0.43
1:A:99:GLU:HG3	1:A:99:GLU:H	1.55	0.43
2:H:136:PHE:CD1	3:L:125:GLU:HB2	2.54	0.43
1:A:259:LYS:HA	1:A:259:LYS:HZ2	1.84	0.43
2:H:159:TYR:CZ	2:H:190:TYR:HB2	2.52	0.43
3:L:105:LYS:C	3:L:106:LEU:HD12	2.39	0.43
2:H:109:TYR:CG	2:H:109:TYR:O	2.71	0.43
2:H:68:ARG:O	2:H:69:PHE:HD1	2.02	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
2:H:100:ASP:HB3	2:H:113:ASN:ND2	2.34	0.42
1:A:191:TYR:O	1:A:192:GLN:HB3	2.19	0.42
1:A:182:ASN:HB2	1:A:183:ASP:OD1	2.20	0.42
1:A:171:ASP:OD2	1:A:234:LYS:NZ	2.53	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
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
3:L:10:VAL:HG22	3:L:105:LYS:O	2.20	0.41
2:H:18:LEU:O	2:H:84:MET:HG3	2.21	0.41
1:A:170:GLU:HB2	1:A:255:LYS:HE2	2.03	0.41
1:A:108:ILE:HG23	1:A:257:VAL:O	2.20	0.41
3:L:58:SER:O	3:L:60:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:LYS:HE3	1:A:161:LYS:HB2	1.79	0.41
3:L:205:SER:HA	3:L:206:PRO:HD3	1.82	0.40
1:A:175:LEU:O	1:A:250:PRO:HG3	2.21	0.40
1:A:133:SER:O	1:A:136:PRO:HD3	2.22	0.40
1:A:64:ASN:H	1:A:144:PHE:HA	1.87	0.40
1:A:105:LEU:HA	1:A:105:LEU:HD22	1.70	0.40
2:H:164:VAL:HG12	2:H:214:HIS:HB2	2.02	0.40
1:A:189:LYS:HG2	1:A:190:LEU:HD23	2.04	0.40
1:A:109:ASN:N	1:A:109:ASN:OD1	2.49	0.40
1:A:135:CYS:HB2	1:A:142:SER:O	2.22	0.40
1:A:115:GLN:HA	1:A:252:TYR:HA	2.03	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%)	34	70
2	H	200/234 (86%)	181 (90%)	19 (10%)	0	100	100
3	L	205/215 (95%)	186 (91%)	18 (9%)	1 (0%)	34	70
All	All	596/682 (87%)	536 (90%)	58 (10%)	2 (0%)	46	78

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%)	148 (85%)	26 (15%)	4	14
2	H	177/196 (90%)	133 (75%)	44 (25%)	1	2
3	L	177/182 (97%)	146 (82%)	31 (18%)	2	9
All	All	528/586 (90%)	427 (81%)	101 (19%)	2	7

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	A	66	MET
1	A	67	CYS
1	A	84	ASN
1	A	87	ASN
1	A	99	GLU
1	A	105	LEU
1	A	106	SER
1	A	111	PHE
1	A	122	TRP
1	A	147	VAL
1	A	154	ASN
1	A	157	TYR
1	A	159	THR
1	A	175	LEU
1	A	182	ASN
1	A	183	ASP
1	A	195	THR
1	A	202	THR
1	A	203	SER
1	A	206	ASN
1	A	208	ARG
1	A	220	ASN
1	A	234	LYS
1	A	256	ILE
1	A	259	LYS

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Mol	Chain	Res	Type
2	H	5	LEU
2	H	12	VAL
2	H	19	ARG
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	74	ASP
2	H	75	ASN
2	H	84	MET
2	H	85	ASN
2	H	90	GLU
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	154	CYS
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
2	H	197	THR
2	H	199	PRO
2	H	211	ASN
2	H	215	LYS
2	H	220	LYS
2	H	222	ASP

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Mol	Chain	Res	Type
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	85	GLU
3	L	123	SER
3	L	142	TYR
3	L	148	VAL
3	L	149	GLN
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	171	LYS
3	L	177	LEU
3	L	178	SER
3	L	182	THR
3	L	183	LEU
3	L	189	GLU
3	L	191	HIS
3	L	203	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	13	GLN
2	H	24	ASN
2	H	78	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 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	195/233 (83%)	-0.28	0 100 100	57, 72, 96, 107	0
2	H	208/234 (88%)	-0.35	0 100 100	45, 55, 65, 70	0
3	L	209/215 (97%)	-0.34	0 100 100	49, 60, 72, 74	0
All	All	612/682 (89%)	-0.32	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 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.