



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:35 PM UTC

PDB ID : 5DUR / pdb_00005dur
Title : Influenza A virus H5 hemagglutinin globular head in complex with antibody 100F4
Authors : Zuo, T.; Sun, J.; Wang, G.; Zhou, P.; Wang, X.; Zhang, L.
Deposited on : 2015-09-20
Resolution : 2.82 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
Mogul : 2022.3.0, CSD as543be (2022)
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

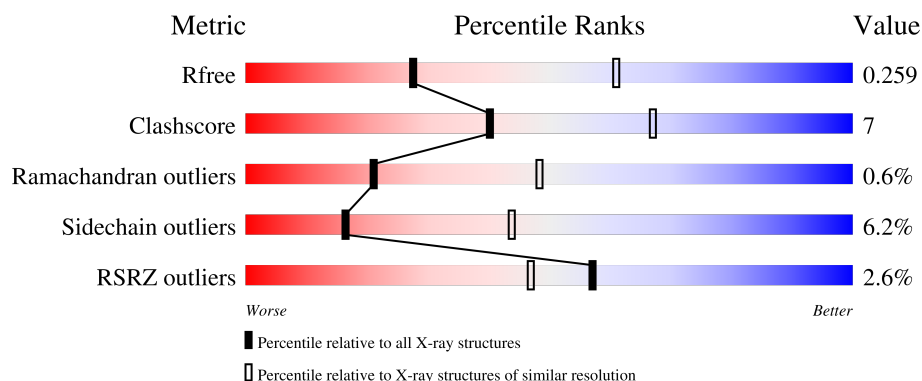
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	B	231	3% 76% 13% • 8%
1	H	231	4% 69% 19% • 7%
2	D	218	2% 79% 18% •
2	L	218	• 74% 23% •
3	A	233	• 80% 12% • 6%

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Mol	Chain	Length	Quality of chain
3	C	233	2% 73% 16% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10114 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 Heavy Chain of Antibody 100F4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	214	Total	C	N	O	S	0	0	0
			1604	1017	266	316	5			
1	B	213	Total	C	N	O	S	0	0	0
			1598	1013	265	315	5			

- Molecule 2 is a protein called Light Chain of Antibody 100F4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1562	975	266	317	4			
2	D	212	Total	C	N	O	S	0	0	0
			1562	975	266	317	4			

- Molecule 3 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	212	Total	C	N	O	S	0	1	0
			1708	1094	287	321	6			
3	A	218	Total	C	N	O	S	0	0	0
			1750	1118	298	328	6			

There are 18 discrepancies between the modelled and reference sequences:

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

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Chain	Residue	Modelled	Actual	Comment	Reference
C	274	HIS	-	expression tag	UNP Q1WDM0
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 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	47	Total	O	0	0
			47	47		
5	L	48	Total	O	0	0
			48	48		

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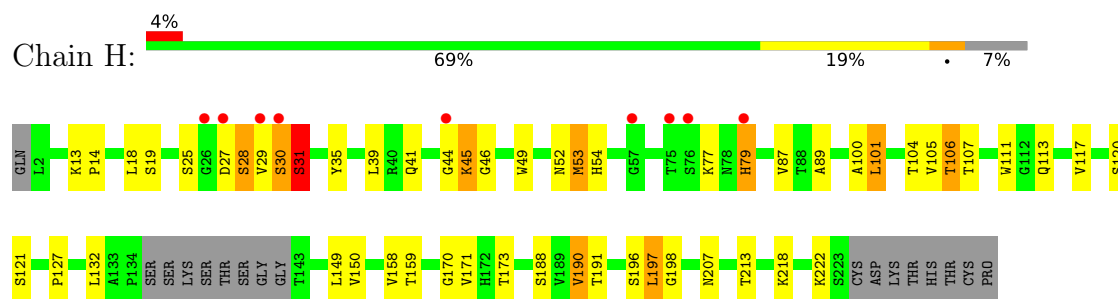
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	47	Total 47	O 47	0	0
5	B	43	Total 43	O 43	0	0
5	D	53	Total 53	O 53	0	0
5	A	64	Total 64	O 64	0	0

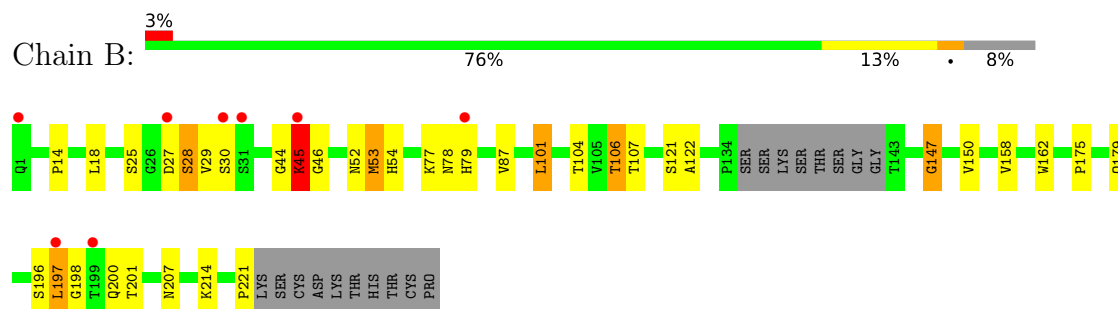
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

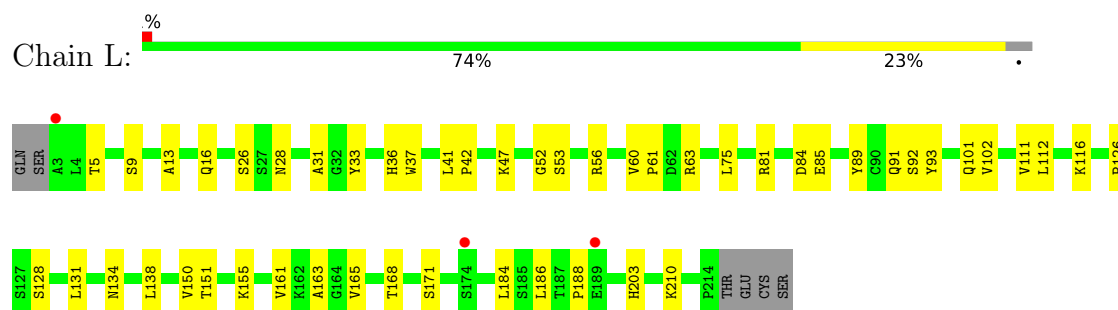
• Molecule 1: Heavy Chain of Antibody 100F4



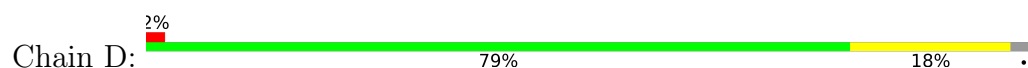
• Molecule 1: Heavy Chain of Antibody 100F4

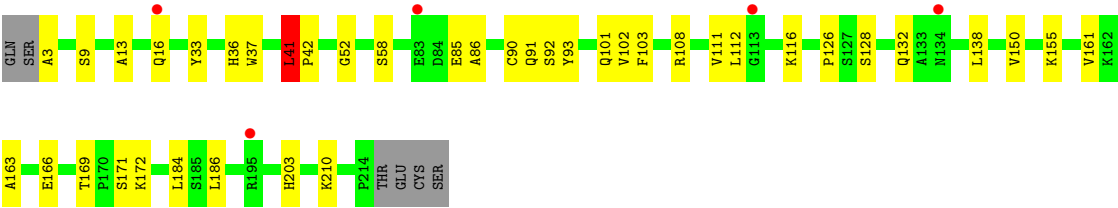


• Molecule 2: Light Chain of Antibody 100F4

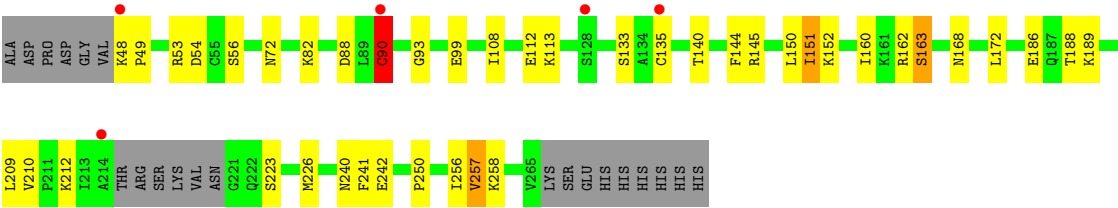


• Molecule 2: Light Chain of Antibody 100F4

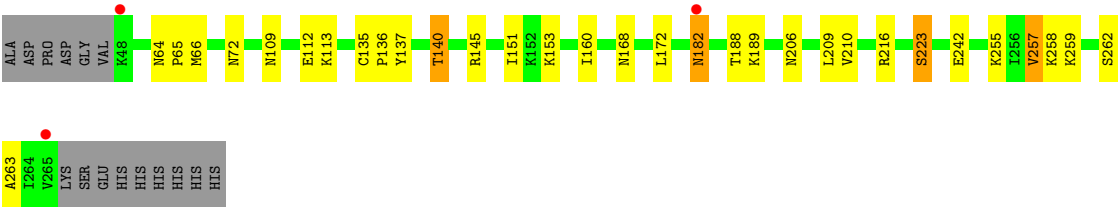
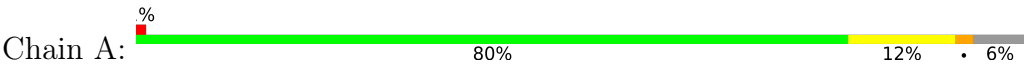




● Molecule 3: Hemagglutinin



● Molecule 3: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.09Å 101.22Å 206.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.50 – 2.82 40.50 – 2.82	Depositor EDS
% Data completeness (in resolution range)	99.2 (40.50-2.82) 99.3 (40.50-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.208 , 0.257 0.210 , 0.259	Depositor DCC
R_{free} test set	2259 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10114	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	B	0.65	0/1639	1.01	4/2244 (0.2%)
1	H	0.66	0/1645	0.99	5/2251 (0.2%)
2	D	0.60	0/1602	0.94	2/2190 (0.1%)
2	L	0.60	0/1602	0.94	2/2190 (0.1%)
3	A	0.63	0/1798	0.93	3/2447 (0.1%)
3	C	0.62	0/1758	0.91	3/2392 (0.1%)
All	All	0.62	0/10044	0.95	19/13714 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	197	LEU	N-CA-C	6.83	121.28	112.26
1	H	197	LEU	N-CA-C	6.68	121.08	112.26
3	A	135	CYS	CA-C-N	-6.48	113.27	120.14
3	A	135	CYS	C-N-CA	-6.48	113.27	120.14
1	H	41	GLN	CA-C-N	6.44	127.01	120.38
1	H	41	GLN	C-N-CA	6.44	127.01	120.38
3	A	182	ASN	N-CA-C	6.39	117.94	110.97
1	B	147	GLY	N-CA-C	6.22	120.21	111.19
3	C	135	CYS	CA-C-N	-6.04	113.74	120.14
3	C	135	CYS	C-N-CA	-6.04	113.74	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	41	LEU	CA-C-N	5.83	127.12	119.84
2	D	41	LEU	C-N-CA	5.83	127.12	119.84
1	H	46	GLY	N-CA-C	-5.42	100.32	113.18
3	C	54	ASP	N-CA-C	-5.42	105.29	112.94
1	B	29	VAL	N-CA-C	-5.39	106.24	112.98
2	L	41	LEU	CA-C-N	5.39	126.58	119.84
2	L	41	LEU	C-N-CA	5.39	126.58	119.84
1	B	45	LYS	N-CA-C	5.33	122.16	110.80
1	H	120	SER	N-CA-C	5.16	121.78	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	79	HIS	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	B	1598	0	1575	25	0
1	H	1604	0	1582	34	0
2	D	1562	0	1513	22	0
2	L	1562	0	1513	26	0
3	A	1750	0	1700	19	0
3	C	1708	0	1654	22	0
4	A	28	0	26	0	0
5	A	64	0	0	4	0
5	B	43	0	0	0	0
5	C	47	0	0	4	0
5	D	53	0	0	1	0
5	H	47	0	0	2	0
5	L	48	0	0	2	0
All	All	10114	0	9563	127	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 7.

All (127) 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)
3:A:206:ASN:ND2	5:A:401:HOH:O	2.08	0.86
3:A:216:ARG:NH2	5:A:402:HOH:O	2.11	0.84
2:L:63:ARG:NH2	2:L:84:ASP:OD2	2.12	0.82
1:B:104:THR:HG23	3:A:113:LYS:H	1.43	0.82
1:B:52:ASN:HD21	1:B:106:THR:HG21	1.48	0.79
2:L:9:SER:HB3	2:D:163:ALA:HB3	1.66	0.78
1:H:52:ASN:HD21	1:H:106:THR:HG21	1.50	0.74
3:C:168:ASN:O	5:C:301:HOH:O	2.06	0.73
2:L:85:GLU:HG3	2:L:111:VAL:HG23	1.71	0.73
1:H:104:THR:HG23	3:C:113:LYS:H	1.54	0.71
1:H:197:LEU:N	1:H:198:GLY:HA3	2.05	0.71
1:B:197:LEU:N	1:B:198:GLY:HA3	2.06	0.70
2:L:56:ARG:NH1	2:L:60:VAL:O	2.25	0.70
2:L:163:ALA:HB3	2:D:9:SER:HB3	1.75	0.69
1:H:104:THR:HG22	3:C:72:ASN:OD1	1.96	0.65
1:B:106:THR:HG23	2:D:101:GLN:CD	2.24	0.63
2:L:168:THR:O	5:L:301:HOH:O	2.16	0.63
1:B:104:THR:CG2	3:A:113:LYS:H	2.12	0.62
3:C:90:CYS:HB2	3:C:144:PHE:CZ	2.34	0.62
2:L:63:ARG:HD3	2:L:81:ARG:NH2	2.16	0.60
2:D:85:GLU:HG3	2:D:111:VAL:HG23	1.83	0.60
1:H:28:SER:O	1:H:30:SER:N	2.35	0.60
3:A:182:ASN:ND2	5:A:404:HOH:O	2.34	0.60
1:B:44:GLY:O	1:B:46:GLY:N	2.34	0.59
3:C:189:LYS:NZ	5:C:304:HOH:O	2.37	0.58
1:B:77:LYS:HB3	1:B:79:HIS:CD2	2.38	0.58
3:C:257:VAL:HG12	3:C:258:LYS:HG2	1.84	0.58
3:A:257:VAL:HG12	3:A:258:LYS:HG2	1.87	0.57
2:D:3:ALA:HA	5:D:331:HOH:O	2.04	0.56
3:A:137:TYR:O	3:A:140:THR:HG22	2.05	0.56
2:L:36:HIS:CD2	2:L:52:GLY:H	2.23	0.55
1:B:52:ASN:ND2	1:B:106:THR:HG21	2.21	0.55
1:H:101:LEU:HB2	1:H:107:THR:HB	1.87	0.55
2:L:150:VAL:HG12	2:L:203:HIS:HB2	1.88	0.54
2:D:13:ALA:O	2:D:16:GLN:HG2	2.06	0.54
1:H:196:SER:C	1:H:198:GLY:HA3	2.32	0.54
1:H:18:LEU:HB2	1:H:87:VAL:HG11	1.89	0.54
1:H:106:THR:HG23	2:L:101:GLN:CD	2.33	0.53
1:B:179:GLN:HG2	2:D:166:GLU:HG2	1.88	0.53
2:L:33:TYR:HA	3:C:112:GLU:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:113:GLN:NE2	5:H:302:HOH:O	2.42	0.53
3:C:152:LYS:HE2	3:C:189:LYS:O	2.09	0.52
2:D:126:PRO:HD3	2:D:138:LEU:HD23	1.90	0.52
1:B:104:THR:HG22	3:A:72:ASN:OD1	2.10	0.52
1:H:104:THR:CG2	3:C:113:LYS:H	2.22	0.52
2:D:138:LEU:HD12	2:D:184:LEU:HD23	1.92	0.52
1:B:196:SER:C	1:B:198:GLY:HA3	2.34	0.51
1:B:27:ASP:OD1	1:B:28:SER:N	2.44	0.51
1:H:218:LYS:NZ	5:H:303:HOH:O	2.43	0.51
2:L:13:ALA:O	2:L:16:GLN:HG2	2.10	0.51
3:A:168:ASN:HB3	3:A:255:LYS:HD3	1.92	0.51
1:H:28:SER:C	1:H:30:SER:H	2.18	0.51
3:C:99:GLU:H	3:C:99:GLU:CD	2.19	0.51
1:H:127:PRO:HD2	1:H:213:THR:HG21	1.93	0.50
3:A:216:ARG:NH1	5:A:408:HOH:O	2.44	0.50
2:L:134:ASN:HA	2:L:188:PRO:HG2	1.94	0.50
1:H:35:TYR:HB2	1:H:100:ALA:HB3	1.93	0.49
3:C:53:ARG:NH2	5:C:306:HOH:O	2.46	0.49
2:L:26:SER:O	2:L:31:ALA:HB2	2.13	0.49
3:A:160:ILE:O	3:A:242:GLU:HA	2.13	0.48
2:L:91:GLN:HG2	2:L:92:SER:N	2.29	0.47
1:H:53:MET:HG2	1:H:54:HIS:N	2.29	0.47
1:B:200:GLN:NE2	1:B:201:THR:O	2.42	0.47
1:H:39:LEU:HD22	1:H:111:TRP:CH2	2.49	0.47
1:H:105:VAL:HG22	2:L:93:TYR:HB2	1.97	0.47
2:D:128:SER:O	2:D:132:GLN:HG2	2.15	0.47
2:D:41:LEU:HD12	2:D:86:ALA:HB2	1.97	0.47
3:C:56:SER:OG	3:C:88:ASP:OD1	2.27	0.46
1:H:132:LEU:HD21	1:H:149:LEU:HB2	1.97	0.46
3:C:163:SER:HB2	3:C:240:ASN:OD1	2.16	0.46
2:L:126:PRO:HD3	2:L:138:LEU:HD23	1.98	0.46
1:B:18:LEU:HB2	1:B:87:VAL:HG11	1.98	0.45
1:B:150:VAL:HG11	1:B:158:VAL:HG11	1.97	0.45
3:A:262:SER:OG	3:A:263:ALA:N	2.49	0.45
1:B:45:LYS:NZ	2:D:108:ARG:HH22	2.13	0.45
1:B:104:THR:HG23	3:A:113:LYS:N	2.23	0.45
1:B:175:PRO:HG2	2:D:171:SER:OG	2.16	0.45
2:D:33:TYR:HA	3:A:112:GLU:OE1	2.17	0.45
3:C:48:LYS:HA	3:C:49:PRO:HD3	1.85	0.45
2:D:36:HIS:CD2	2:D:52:GLY:H	2.34	0.45
1:H:77:LYS:HD3	1:H:79:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:109:ASN:ND2	3:A:259:LYS:O	2.50	0.44
1:H:30:SER:OG	1:H:31:SER:N	2.49	0.44
1:H:150:VAL:HG11	1:H:158:VAL:HG11	1.99	0.44
1:H:171:VAL:HG22	1:H:190:VAL:HB	1.99	0.44
1:H:89:ALA:HB3	1:B:122:ALA:HB2	2.00	0.43
3:A:66:MET:HE2	3:A:66:MET:HA	1.98	0.43
2:D:150:VAL:HG12	2:D:203:HIS:HB2	2.00	0.43
2:L:60:VAL:HA	2:L:61:PRO:HD3	1.87	0.43
3:C:186:GLU:OE1	5:C:302:HOH:O	2.21	0.43
3:C:241:PHE:CZ	3:C:250:PRO:HG2	2.53	0.43
3:A:136:PRO:HA	3:A:140:THR:O	2.18	0.43
2:L:63:ARG:HH22	2:L:84:ASP:CG	2.17	0.42
1:B:14:PRO:HD2	1:B:121:SER:HB3	2.01	0.42
2:L:37:TRP:CE2	2:L:75:LEU:HB2	2.55	0.42
1:B:14:PRO:CD	1:B:121:SER:HB3	2.49	0.42
2:D:92:SER:OG	2:D:93:TYR:N	2.53	0.42
1:H:45:LYS:HD3	2:L:89:TYR:OH	2.20	0.42
1:H:170:GLY:O	1:H:190:VAL:HA	2.20	0.42
3:C:108:ILE:HD12	3:C:256:ILE:HG23	2.02	0.42
3:C:93:GLY:HA3	3:C:226:MET:O	2.20	0.42
1:H:13:LYS:HD3	1:H:121:SER:HA	2.02	0.42
2:L:165:VAL:HG22	2:L:184:LEU:HD13	2.01	0.42
2:D:91:GLN:HG2	2:D:92:SER:N	2.34	0.42
1:H:173:THR:HA	1:H:188:SER:HA	2.02	0.42
2:D:37:TRP:CH2	2:D:90:CYS:HB3	2.55	0.41
1:H:14:PRO:CG	1:H:121:SER:HB3	2.50	0.41
3:A:182:ASN:OD1	3:A:223:SER:HB2	2.19	0.41
1:B:101:LEU:HB2	1:B:107:THR:HB	2.02	0.41
1:H:45:LYS:HD3	2:L:89:TYR:HH	1.86	0.41
3:C:160:ILE:O	3:C:242:GLU:HA	2.20	0.41
2:L:210:LYS:HA	2:L:210:LYS:HD2	1.98	0.41
1:B:197:LEU:O	1:B:221:PRO:HG3	2.20	0.41
1:H:49:TRP:CG	2:L:101:GLN:HB2	2.54	0.41
2:D:91:GLN:HB2	2:D:103:PHE:CE2	2.56	0.41
2:L:47:LYS:NZ	5:L:302:HOH:O	2.53	0.41
2:D:85:GLU:OE1	2:D:172:LYS:NZ	2.54	0.41
1:H:18:LEU:HD23	1:H:19:SER:N	2.36	0.41
1:H:18:LEU:HD11	1:H:117:VAL:HG11	2.02	0.41
1:H:28:SER:C	1:H:30:SER:N	2.79	0.40
3:C:150:LEU:O	3:C:151:ILE:HD13	2.22	0.40
1:B:53:MET:HG2	1:B:54:HIS:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:GLY:HA2	1:B:162:TRP:CH2	2.57	0.40
3:C:53:ARG:O	3:C:82:LYS:HE3	2.21	0.40
3:C:162:ARG:HD3	3:C:162:ARG:HA	1.88	0.40
3:A:64:ASN:HA	3:A:65:PRO:HD2	1.95	0.40
2:D:210:LYS:HA	2:D:210:LYS:HD2	1.89	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	B	209/231 (90%)	195 (93%)	13 (6%)	1 (0%)	24	53
1	H	210/231 (91%)	195 (93%)	9 (4%)	6 (3%)	3	12
2	D	210/218 (96%)	206 (98%)	4 (2%)	0	100	100
2	L	210/218 (96%)	205 (98%)	5 (2%)	0	100	100
3	A	216/233 (93%)	205 (95%)	11 (5%)	0	100	100
3	C	209/233 (90%)	200 (96%)	8 (4%)	1 (0%)	24	53
All	All	1264/1364 (93%)	1206 (95%)	50 (4%)	8 (1%)	21	48

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	29	VAL
1	H	45	LYS
1	B	45	LYS
3	C	90	CYS
1	H	31	SER
1	H	27	ASP
1	H	44	GLY
1	H	30	SER

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	B	185/201 (92%)	176 (95%)	9 (5%)	22	53
1	H	186/201 (92%)	175 (94%)	11 (6%)	18	46
2	D	174/180 (97%)	164 (94%)	10 (6%)	18	47
2	L	174/180 (97%)	160 (92%)	14 (8%)	11	32
3	A	195/208 (94%)	184 (94%)	11 (6%)	19	48
3	C	190/208 (91%)	177 (93%)	13 (7%)	14	40
All	All	1104/1178 (94%)	1036 (94%)	68 (6%)	16	44

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	25	SER
1	H	28	SER
1	H	31	SER
1	H	53	MET
1	H	101	LEU
1	H	106	THR
1	H	159	THR
1	H	190	VAL
1	H	191	THR
1	H	207	ASN
1	H	222	LYS
2	L	5	THR
2	L	28	ASN
2	L	42	PRO
2	L	53	SER
2	L	102	VAL
2	L	112	LEU
2	L	116	LYS
2	L	128	SER
2	L	131	LEU
2	L	151	THR
2	L	155	LYS

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Mol	Chain	Res	Type
2	L	161	VAL
2	L	171	SER
2	L	186	LEU
3	C	90	CYS
3	C	133	SER
3	C	140	THR
3	C	145	ARG
3	C	151	ILE
3	C	163	SER
3	C	172	LEU
3	C	188	THR
3	C	209	LEU
3	C	210	VAL
3	C	212	LYS
3	C	223	SER
3	C	257	VAL
1	B	25	SER
1	B	28	SER
1	B	30	SER
1	B	53	MET
1	B	78	ASN
1	B	101	LEU
1	B	106	THR
1	B	207	ASN
1	B	214	LYS
2	D	41	LEU
2	D	42	PRO
2	D	58	SER
2	D	102	VAL
2	D	112	LEU
2	D	116	LYS
2	D	155	LYS
2	D	161	VAL
2	D	169	THR
2	D	186	LEU
3	A	140	THR
3	A	145	ARG
3	A	151	ILE
3	A	153	LYS
3	A	172	LEU
3	A	188	THR
3	A	189	LYS

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Mol	Chain	Res	Type
3	A	209	LEU
3	A	210	VAL
3	A	223	SER
3	A	257	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	41	GLN
1	H	79	HIS
1	H	113	GLN
1	H	179	GLN
2	L	40	GLN
2	L	114	GLN
2	L	118	ASN
2	L	190	GLN
2	L	200	GLN
3	C	94	ASN
3	C	115	GLN
3	C	146	ASN
1	B	52	ASN
1	B	79	HIS
1	B	113	GLN
1	B	207	ASN
2	D	176	ASN
3	A	206	ASN
3	A	220	ASN
3	A	240	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	302	3	14,14,15	0.59	1 (7%)	17,19,21	0.84	0
4	NAG	A	301	3	14,14,15	0.96	1 (7%)	17,19,21	1.01	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	302	3	-	2/6/23/26	0/1/1/1
4	NAG	A	301	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	NAG	O5-C1	3.23	1.49	1.43
4	A	302	NAG	O5-C1	2.01	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	NAG	C1-O5-C5	2.29	115.25	112.19
4	A	301	NAG	C3-C4-C5	-2.01	106.58	110.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	302	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	302	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	B	213/231 (92%)	0.07	8 (3%)	44 35	21, 29, 51, 65	0
1	H	214/231 (92%)	-0.05	9 (4%)	40 32	21, 29, 49, 57	0
2	D	212/218 (97%)	-0.07	5 (2%)	59 49	23, 32, 38, 48	0
2	L	212/218 (97%)	0.00	3 (1%)	73 64	24, 32, 44, 50	0
3	A	218/233 (93%)	-0.09	3 (1%)	73 64	23, 32, 47, 54	0
3	C	212/233 (90%)	-0.01	5 (2%)	59 49	20, 33, 47, 53	1 (0%)
All	All	1281/1364 (93%)	-0.02	33 (2%)	57 47	20, 31, 46, 65	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	27	ASP	4.6
2	D	113	GLY	4.0
1	B	45	LYS	3.7
1	B	197	LEU	3.3
1	B	30	SER	3.2
2	D	83	GLU	3.1
3	C	48	LYS	2.9
3	A	48	LYS	2.8
2	D	16	GLN	2.7
1	H	29	VAL	2.7
3	C	90	CYS	2.6
1	B	27	ASP	2.6
2	L	174	SER	2.6
1	H	57	GLY	2.5
1	H	44	GLY	2.5
3	A	265	VAL	2.5
1	B	79	HIS	2.5
1	H	76	SER	2.4
1	B	1	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	26	GLY	2.4
3	C	135	CYS	2.4
2	D	134	ASN	2.3
1	B	31	SER	2.3
1	H	79	HIS	2.3
1	B	199	THR	2.3
2	L	189	GLU	2.2
1	H	30	SER	2.2
3	A	182	ASN	2.2
3	C	128	SER	2.2
1	H	75	THR	2.1
2	L	3	ALA	2.1
3	C	214	ALA	2.0
2	D	195	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	301	14/15	0.85	0.15	27,27,27,27	0
4	NAG	A	302	14/15	0.88	0.11	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.