



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:56 PM UTC

PDB ID : 6A4K / pdb_00006a4k
Title : Human antibody 32D6 Fab in complex with H1N1 influenza A virus HA1
Authors : Lee, C.C.; Ko, T.P.; Lin, L.L.; Wang, A.H.J.
Deposited on : 2018-06-20
Resolution : 3.15 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

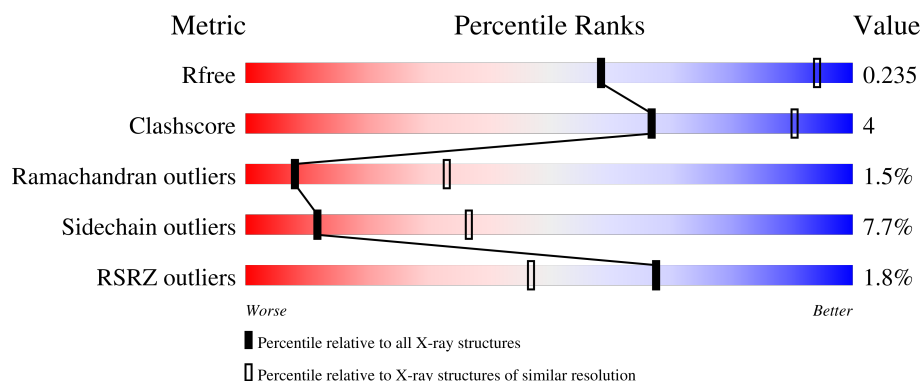
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	235	% 82% 11% • 5%
1	B	235	2% 80% 11% • 6%
1	C	235	% 83% 10% • 5%
1	D	235	% 82% 10% • 6%
2	H	238	% 85% 11% • •

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Mol	Chain	Length	Quality of chain
2	I	238	4% 77% 19%
2	J	238	2% 81% 13%
2	K	238	3% 76% 19%
3	L	216	83% 15%
3	M	216	4% 83% 16%
3	N	216	79% 19%
3	O	216	86% 13%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20618 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	223	Total	C	N	O	S	0	0	0
			1760	1123	296	335	6			
1	B	221	Total	C	N	O	S	0	0	0
			1745	1114	294	331	6			
1	C	223	Total	C	N	O	S	0	0	0
			1760	1123	296	335	6			
1	D	221	Total	C	N	O	S	0	0	0
			1745	1114	294	331	6			

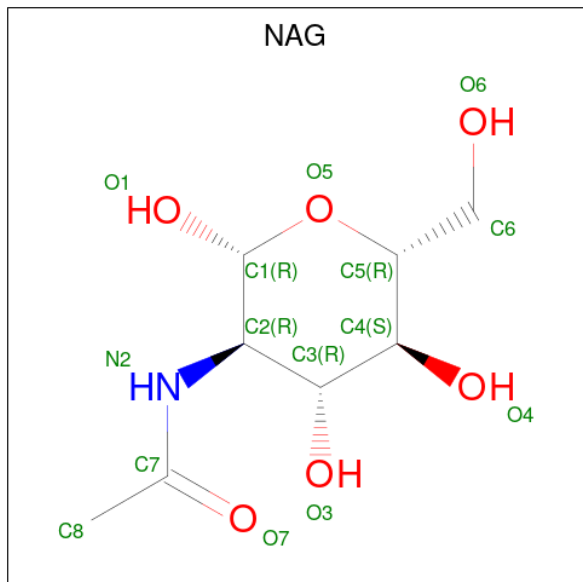
- Molecule 2 is a protein called immunoglobulin Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			
2	I	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			
2	J	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			
2	K	230	Total	C	N	O	S	0	0	0
			1722	1091	283	343	5			

- Molecule 3 is a protein called immunoglobulin Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			
3	M	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			
3	N	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			
3	O	216	Total	C	N	O	S	0	0	0
			1614	1000	277	330	7			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

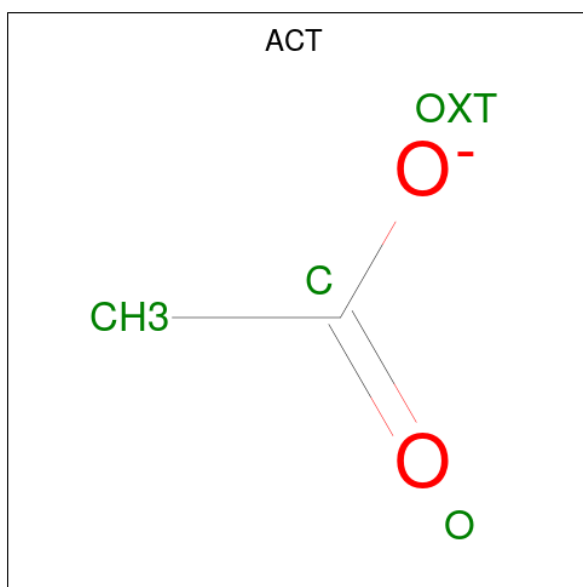


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	O	1	Total	Ca	0	0
			1	1		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			4	2	2		
6	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	28	Total	O	0	0
			28	28		
7	H	17	Total	O	0	0
			17	17		
7	L	29	Total	O	0	0
			29	29		
7	B	15	Total	O	0	0
			15	15		
7	I	6	Total	O	0	0
			6	6		
7	M	5	Total	O	0	0
			5	5		
7	C	24	Total	O	0	0
			24	24		
7	N	7	Total	O	0	0
			7	7		
7	D	31	Total	O	0	0
			31	31		
7	K	12	Total	O	0	0
			12	12		

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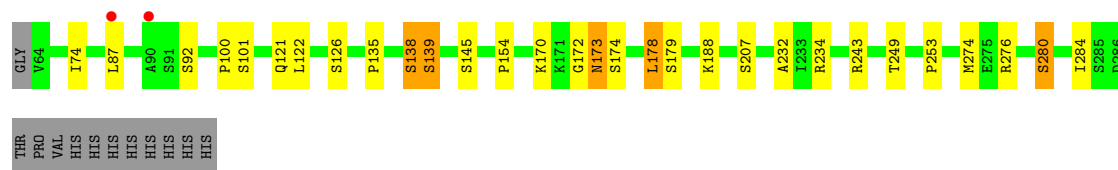
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	O	21	Total	O	0	0
			21	21		

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.

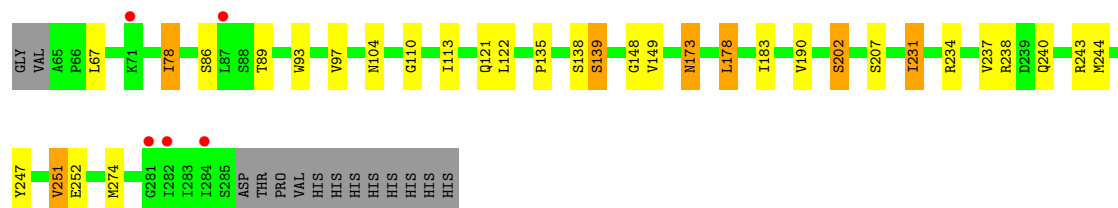
• Molecule 1: Hemagglutinin

Chain A: 



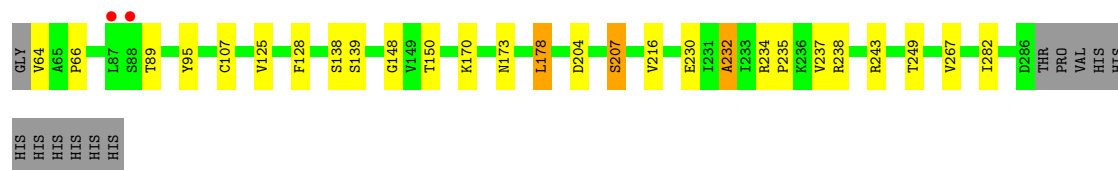
• Molecule 1: Hemagglutinin

Chain B: 



• Molecule 1: Hemagglutinin

Chain C: 



• Molecule 1: Hemagglutinin

Chain D: 



PRO
VAL
HIS
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HIS
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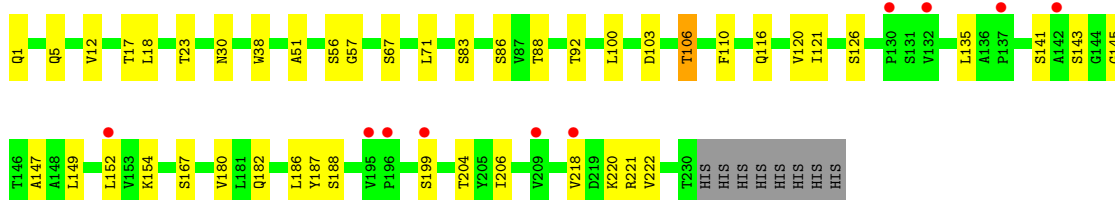
- Molecule 2: immunoglobulin Fab heavy chain

Chain H:  85% 11% . .



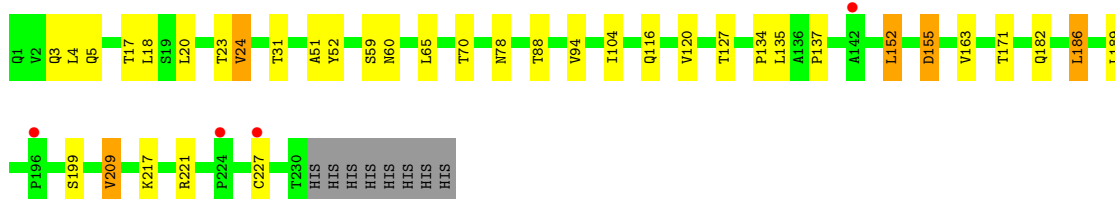
- Molecule 2: immunoglobulin Fab heavy chain

Chain I:  77% 19% .



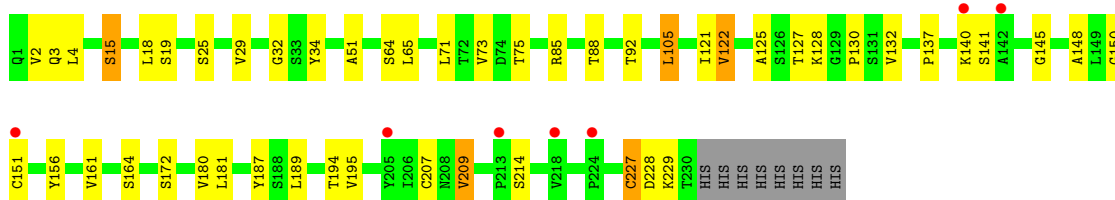
- Molecule 2: immunoglobulin Fab heavy chain

Chain J:  81% 13% . .



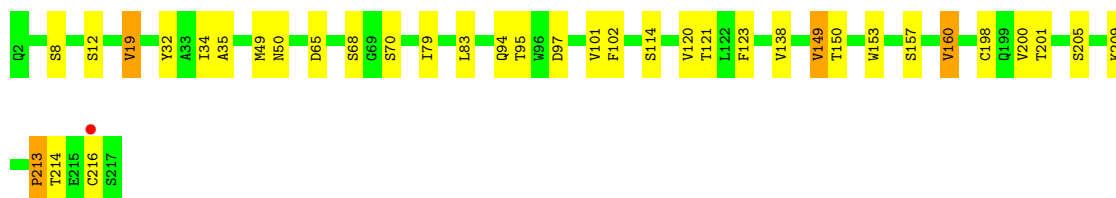
- Molecule 2: immunoglobulin Fab heavy chain

Chain K:  76% 19% . .

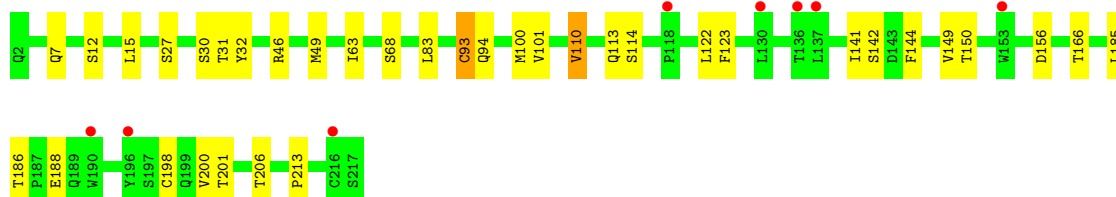
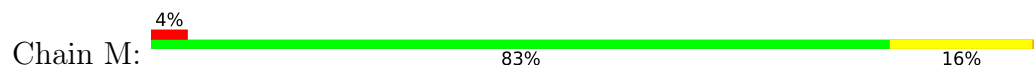


- Molecule 3: immunoglobulin Fab light chain

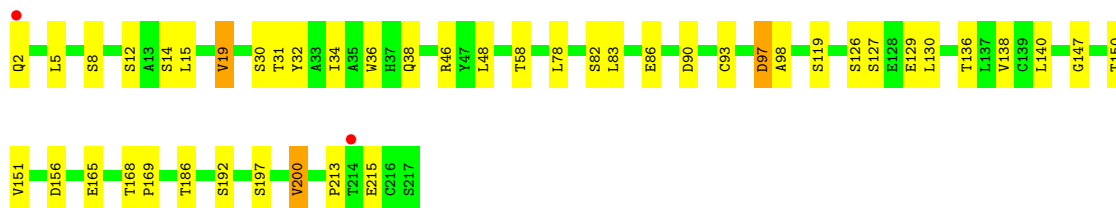
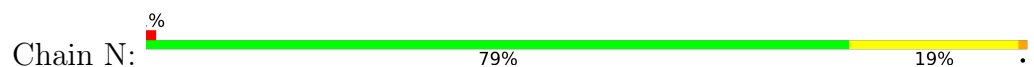
Chain L:  83% 15% .



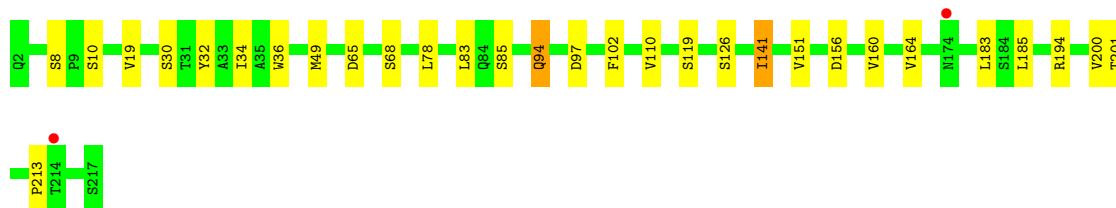
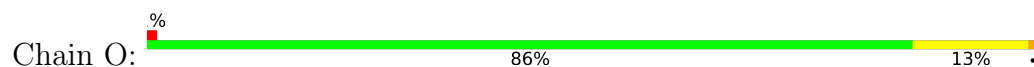
- Molecule 3: immunoglobulin Fab light chain



- Molecule 3: immunoglobulin Fab light chain



- Molecule 3: immunoglobulin Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	181.74Å 181.74Å 248.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.15 20.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	94.5 (20.00-3.15) 94.5 (20.00-3.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.15Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.175 , 0.233 0.178 , 0.235	Depositor DCC
R_{free} test set	3830 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20618	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.87% 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: CA, ACT, 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	A	0.70	0/1810	0.89	2/2457 (0.1%)
1	B	0.70	0/1795	0.90	1/2436 (0.0%)
1	C	0.69	0/1810	0.91	2/2457 (0.1%)
1	D	0.72	0/1795	0.92	1/2436 (0.0%)
2	H	0.72	0/1766	0.96	0/2414
2	I	0.80	0/1766	0.92	0/2414
2	J	0.71	0/1766	0.90	0/2414
2	K	0.78	0/1766	0.94	2/2414 (0.1%)
3	L	0.75	0/1651	0.97	0/2246
3	M	0.80	0/1651	0.95	1/2246 (0.0%)
3	N	0.73	0/1651	0.90	0/2246
3	O	0.79	0/1651	0.95	0/2246
All	All	0.74	0/20878	0.93	9/28426 (0.0%)

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	A	0	1
1	C	0	1
1	D	0	1
2	H	0	1
3	L	0	1
3	N	0	1
All	All	0	6

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	ASN	N-CA-CB	-7.55	101.01	110.98
2	K	150	GLY	N-CA-C	6.90	121.20	111.19
1	A	173	ASN	N-CA-CB	-6.75	102.03	111.00
1	C	232	ALA	N-CA-C	6.75	118.65	108.46
2	K	105	LEU	N-CA-C	6.34	117.86	111.07
3	M	93	CYS	N-CA-C	-5.95	100.00	109.59
1	C	150	THR	N-CA-C	5.52	117.79	109.23
1	B	173	ASN	N-CA-CB	-5.37	103.22	110.95
1	A	74	ILE	N-CA-CB	5.35	116.45	110.51

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	280	SER	Peptide
1	C	89	THR	Peptide
1	D	172	GLY	Peptide
2	H	198	SER	Peptide
3	L	213	PRO	Peptide
3	N	215	GLU	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	1760	0	1696	11	0
1	B	1745	0	1683	13	0
1	C	1760	0	1696	9	0
1	D	1745	0	1683	14	0
2	H	1722	0	1687	8	0
2	I	1722	0	1687	19	0
2	J	1722	0	1687	13	0
2	K	1722	0	1687	18	0
3	L	1614	0	1553	14	0
3	M	1614	0	1553	16	0
3	N	1614	0	1553	15	0
3	O	1614	0	1553	10	0
4	A	14	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	O	1	0	0	0	0
6	B	4	0	3	0	0
6	D	4	0	3	0	0
7	A	28	0	0	0	0
7	B	15	0	0	1	0
7	C	24	0	0	0	0
7	D	31	0	0	0	0
7	H	17	0	0	1	0
7	I	6	0	0	0	0
7	K	12	0	0	0	0
7	L	29	0	0	1	0
7	M	5	0	0	0	0
7	N	7	0	0	1	0
7	O	21	0	0	0	0
All	All	20618	0	19776	150	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 4.

All (150) 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:M:7:GLN:NE2	3:M:93:CYS:SG	2.48	0.87
3:M:7:GLN:HE22	3:M:93:CYS:H	1.31	0.78
2:I:218:VAL:HG12	2:I:220:LYS:HG2	1.73	0.71
3:O:151:VAL:HG12	3:O:200:VAL:HG12	1.72	0.70
2:H:110:PHE:HA	3:L:94:GLN:HE22	1.59	0.67
2:H:18:LEU:HD13	2:H:120:VAL:HG11	1.76	0.67
1:C:173:ASN:HB2	3:N:32:TYR:HA	1.76	0.66
1:D:122:LEU:HD23	1:D:274:MET:HE1	1.78	0.65
3:M:7:GLN:HE22	3:M:93:CYS:N	1.95	0.64
1:A:122:LEU:HD23	1:A:274:MET:HE1	1.80	0.64
1:C:230:GLU:O	1:C:234:ARG:NH2	2.29	0.64
2:H:30:ASN:HD21	2:H:75:THR:HG23	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ARG:HD3	1:B:243:ARG:HG3	1.80	0.64
2:I:110:PHE:HA	3:M:94:GLN:HE22	1.63	0.63
1:B:190:VAL:HG13	1:B:251:VAL:HG13	1.79	0.63
1:B:78:ILE:HD13	1:B:122:LEU:HD11	1.79	0.63
2:I:5:GLN:NE2	2:I:116:GLN:HE22	1.98	0.61
3:M:7:GLN:NE2	3:M:93:CYS:H	1.98	0.61
3:N:2:GLN:HE22	3:N:97:ASP:HB3	1.64	0.61
1:A:170:LYS:HE2	1:A:207:SER:O	2.01	0.60
3:N:138:VAL:HG12	3:N:140:LEU:HD11	1.83	0.60
1:A:122:LEU:CD2	1:A:274:MET:HE1	2.33	0.59
1:B:121:GLN:HE21	1:B:274:MET:HE2	1.68	0.58
2:K:132:VAL:HG21	2:K:209:VAL:HG11	1.86	0.58
1:C:235:PRO:O	1:C:243:ARG:NH2	2.37	0.57
2:K:92:THR:HG23	2:K:121:ILE:HA	1.85	0.57
3:O:141:ILE:HG12	3:O:200:VAL:HG11	1.87	0.57
2:I:149:LEU:HD13	2:I:222:VAL:HG11	1.88	0.55
1:A:173:ASN:HB2	3:L:32:TYR:HA	1.88	0.55
2:H:18:LEU:HD12	7:H:302:HOH:O	2.07	0.55
2:I:5:GLN:HE21	2:I:116:GLN:HE22	1.53	0.55
1:B:173:ASN:HB2	3:M:32:TYR:HA	1.88	0.54
1:B:178:LEU:HD12	1:B:178:LEU:C	2.32	0.54
2:I:141:SER:HB3	2:I:147:ALA:HA	1.89	0.54
2:K:64:SER:C	2:K:65:LEU:HD12	2.33	0.54
1:D:99:THR:HG22	1:D:100:PRO:HD2	1.91	0.53
2:I:18:LEU:HD12	2:I:120:VAL:HG11	1.91	0.53
2:K:148:ALA:HB2	2:K:194:THR:HG22	1.90	0.53
2:I:135:LEU:HD11	2:I:152:LEU:HB2	1.91	0.52
2:H:135:LEU:HD11	2:H:152:LEU:HB2	1.91	0.52
2:K:180:VAL:O	2:K:187:TYR:HA	2.09	0.52
2:I:92:THR:HG23	2:I:121:ILE:HA	1.91	0.51
2:K:3:GLN:O	2:K:4:LEU:HD23	2.10	0.51
1:C:232:ALA:O	1:C:234:ARG:NH1	2.43	0.51
2:I:206:ILE:HG22	2:I:221:ARG:HB2	1.92	0.51
1:C:178:LEU:C	1:C:178:LEU:HD12	2.36	0.51
3:N:151:VAL:HG12	3:N:200:VAL:HG12	1.92	0.51
3:N:2:GLN:NE2	3:N:2:GLN:HA	2.25	0.51
3:L:120:VAL:HG23	3:L:209:LYS:HG3	1.93	0.50
1:D:71:LYS:HE2	1:D:99:THR:HG21	1.93	0.50
1:A:121:GLN:HE22	1:A:276:ARG:HH11	1.59	0.50
1:A:135:PRO:O	1:A:139:SER:OG	2.30	0.50
2:J:155:ASP:HB3	2:J:186:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:LYS:O	1:A:253:PRO:HG3	2.13	0.49
3:M:200:VAL:O	3:M:200:VAL:HG23	2.12	0.49
3:M:122:LEU:HD22	3:M:198:CYS:HB2	1.95	0.49
2:J:3:GLN:C	2:J:4:LEU:HD12	2.38	0.49
1:B:135:PRO:O	1:B:139:SER:OG	2.31	0.49
2:I:51:ALA:HB3	2:I:71:LEU:HD11	1.94	0.48
2:K:181:LEU:HD13	2:K:187:TYR:CE2	2.49	0.48
2:H:30:ASN:ND2	2:H:75:THR:HG23	2.28	0.48
2:H:135:LEU:HB3	3:L:123:PHE:CD1	2.48	0.48
2:I:103:ASP:CG	2:I:106:THR:HG22	2.39	0.48
2:J:5:GLN:HG3	2:J:116:GLN:HE21	1.78	0.48
2:K:161:VAL:CG2	2:K:189:LEU:HD22	2.44	0.48
2:K:227:CYS:SG	2:K:228:ASP:N	2.87	0.47
3:O:49:MET:HE1	3:O:68:SER:N	2.29	0.47
1:D:67:LEU:HD13	1:D:90:ALA:CB	2.45	0.47
1:A:232:ALA:O	1:A:234:ARG:NH1	2.48	0.47
3:N:5:LEU:HD13	3:N:93:CYS:SG	2.54	0.47
1:D:234:ARG:HG3	1:D:243:ARG:HG3	1.96	0.47
1:B:238:ARG:O	1:B:240:GLN:HG2	2.15	0.47
1:D:104:ASN:HD22	1:D:104:ASN:N	2.11	0.47
3:N:138:VAL:HG12	3:N:140:LEU:CD1	2.44	0.46
2:K:127:THR:HG21	2:K:214:SER:HA	1.97	0.46
1:B:110:GLY:HA3	1:B:244:MET:O	2.16	0.46
2:I:135:LEU:HD23	3:M:123:PHE:CG	2.51	0.46
1:D:118:LEU:HD13	1:D:248:TRP:CD2	2.51	0.46
2:K:88:THR:O	2:K:122:VAL:HG11	2.15	0.46
3:O:194:ARG:O	3:O:213:PRO:HD2	2.15	0.46
3:N:19:VAL:CG2	3:N:83:LEU:HD22	2.46	0.45
3:N:38:GLN:HB2	3:N:48:LEU:HD11	1.98	0.45
1:A:234:ARG:HD3	1:A:243:ARG:HG3	1.98	0.45
3:L:94:GLN:HB3	3:L:102:PHE:CD1	2.51	0.45
2:I:18:LEU:CD1	2:I:120:VAL:HG11	2.46	0.45
2:J:52:TYR:CE2	2:J:60:ASN:HB3	2.52	0.45
3:N:147:GLY:O	3:N:169:PRO:HG2	2.16	0.45
2:K:51:ALA:HB3	2:K:71:LEU:HD11	1.97	0.45
3:L:149:VAL:HG22	3:L:200:VAL:HG13	2.00	0.44
3:M:83:LEU:HD21	3:M:110:VAL:CG1	2.47	0.44
1:C:170:LYS:HE2	1:C:207:SER:O	2.16	0.44
3:N:2:GLN:HE22	3:N:98:ALA:H	1.65	0.44
2:I:182:GLN:NE2	2:I:188:SER:OG	2.51	0.44
3:L:214:THR:HA	7:L:308:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:PRO:O	1:D:139:SER:OG	2.34	0.44
3:M:46:ARG:HE	3:M:63:ILE:HD11	1.82	0.44
2:J:135:LEU:HD11	2:J:152:LEU:HB3	2.00	0.44
3:O:94:GLN:HB3	3:O:102:PHE:CD1	2.53	0.44
2:I:180:VAL:O	2:I:187:TYR:HA	2.18	0.43
2:J:163:VAL:HG22	2:J:209:VAL:HG23	1.99	0.43
1:B:67:LEU:HD12	1:B:93:TRP:CD2	2.52	0.43
2:J:65:LEU:HD12	2:J:65:LEU:N	2.33	0.43
3:O:36:TRP:CE2	3:O:78:LEU:HB2	2.53	0.43
2:H:141:SER:HB3	2:H:147:ALA:HA	1.98	0.43
3:L:153:TRP:HB2	3:L:160:VAL:HG22	2.00	0.43
2:I:38:TRP:CD1	2:I:71:LEU:HD21	2.52	0.43
1:D:122:LEU:HD23	1:D:274:MET:CE	2.47	0.43
2:K:18:LEU:HD12	2:K:19:SER:N	2.34	0.43
2:J:24:VAL:O	2:J:78:ASN:ND2	2.52	0.43
2:J:155:ASP:OD1	2:J:182:GLN:NE2	2.50	0.43
3:N:129:GLU:OE1	3:N:136:THR:N	2.51	0.43
1:A:154:PRO:HD2	4:A:501:NAG:H83	2.00	0.43
2:I:5:GLN:HE21	2:I:116:GLN:NE2	2.17	0.43
3:M:201:THR:HG22	3:M:206:THR:OG1	2.19	0.42
2:K:65:LEU:HD12	2:K:65:LEU:N	2.34	0.42
3:N:36:TRP:CE2	3:N:78:LEU:HB2	2.55	0.42
1:D:134:PHE:CE1	1:D:180:LYS:HG2	2.55	0.42
3:L:19:VAL:CG2	3:L:83:LEU:HD13	2.50	0.42
2:K:130:PRO:HB3	2:K:156:TYR:HB3	2.01	0.42
3:O:164:VAL:HG22	3:O:183:LEU:HD13	2.02	0.42
3:L:35:ALA:HA	3:L:50:ASN:HA	2.02	0.41
3:L:49:MET:HE1	3:L:68:SER:N	2.35	0.41
1:B:113:ILE:HG13	1:B:247:TYR:CE2	2.55	0.41
3:M:49:MET:HE1	3:M:68:SER:N	2.35	0.41
1:C:125:VAL:HG11	1:C:128:PHE:HB2	2.02	0.41
3:L:79:ILE:HD12	3:L:79:ILE:N	2.34	0.41
1:B:202:SER:HA	1:B:231:ILE:HD12	2.03	0.41
1:B:252:GLU:HA	7:B:610:HOH:O	2.20	0.41
3:M:15:LEU:HD11	3:M:113:GLN:HG2	2.02	0.41
1:D:67:LEU:HD22	1:D:93:TRP:CD2	2.54	0.41
3:L:19:VAL:HG21	3:L:83:LEU:HD13	2.03	0.41
3:O:83:LEU:HD21	3:O:110:VAL:HG22	2.02	0.41
3:O:151:VAL:CG1	3:O:200:VAL:HG12	2.48	0.41
3:L:34:ILE:HG22	3:L:95:THR:HB	2.03	0.41
2:J:18:LEU:HD11	2:J:20:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:LEU:O	1:D:268:PRO:HB3	2.21	0.41
1:C:107:CYS:O	1:C:238:ARG:HD2	2.21	0.41
1:D:173:ASN:HB2	3:O:32:TYR:HA	2.03	0.41
2:J:18:LEU:HD11	2:J:20:LEU:HD11	2.02	0.41
2:J:134:PRO:O	3:N:126:SER:OG	2.32	0.41
2:K:29:VAL:HG11	2:K:73:VAL:CG1	2.50	0.41
3:M:141:ILE:HD11	3:M:200:VAL:HG11	2.03	0.41
1:C:66:PRO:HB3	1:C:95:TYR:CZ	2.56	0.40
2:K:32:GLY:HA3	2:K:34:TYR:CE2	2.56	0.40
1:D:70:GLY:O	1:D:99:THR:OG1	2.39	0.40
1:A:178:LEU:C	1:A:178:LEU:HD12	2.46	0.40
2:J:18:LEU:HD13	2:J:120:VAL:HG11	2.04	0.40
3:N:12:SER:N	7:N:301:HOH:O	2.48	0.40
2:K:127:THR:HG22	2:K:128:LYS:N	2.37	0.40
2:I:100:LEU:HD11	3:M:100:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/235 (94%)	202 (91%)	16 (7%)	3 (1%)	9	34
1	B	219/235 (93%)	197 (90%)	19 (9%)	3 (1%)	9	34
1	C	221/235 (94%)	203 (92%)	17 (8%)	1 (0%)	24	55
1	D	219/235 (93%)	201 (92%)	15 (7%)	3 (1%)	9	34
2	H	228/238 (96%)	200 (88%)	23 (10%)	5 (2%)	5	25
2	I	228/238 (96%)	198 (87%)	26 (11%)	4 (2%)	6	29
2	J	228/238 (96%)	203 (89%)	20 (9%)	5 (2%)	5	25
2	K	228/238 (96%)	197 (86%)	25 (11%)	6 (3%)	4	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	214/216 (99%)	200 (94%)	12 (6%)	2 (1%)	14	43
3	M	214/216 (99%)	193 (90%)	19 (9%)	2 (1%)	14	43
3	N	214/216 (99%)	201 (94%)	10 (5%)	3 (1%)	9	34
3	O	214/216 (99%)	204 (95%)	7 (3%)	3 (1%)	9	34
All	All	2648/2756 (96%)	2399 (91%)	209 (8%)	40 (2%)	8	33

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	15	SER
2	H	225	LYS
2	H	227	CYS
3	L	213	PRO
1	B	86	SER
2	I	57	GLY
2	J	227	CYS
3	O	65	ASP
1	B	89	THR
2	I	56	SER
2	I	145	GLY
1	D	148	GLY
2	K	15	SER
2	K	137	PRO
2	K	145	GLY
1	A	138	SER
1	B	148	GLY
2	I	143	SER
3	M	156	ASP
3	M	213	PRO
2	J	155	ASP
2	J	199	SER
2	K	125	ALA
3	O	97	ASP
3	O	156	ASP
2	H	197	SER
2	H	226	SER
3	L	97	ASP
3	N	156	ASP
1	D	100	PRO
2	J	51	ALA
2	J	137	PRO

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Mol	Chain	Res	Type
3	N	97	ASP
2	K	229	LYS
1	C	148	GLY
1	D	172	GLY
1	A	100	PRO
3	N	213	PRO
1	A	172	GLY
2	K	2	VAL

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	192/203 (95%)	179 (93%)	13 (7%)	14	41
1	B	190/203 (94%)	177 (93%)	13 (7%)	14	41
1	C	192/203 (95%)	181 (94%)	11 (6%)	18	47
1	D	190/203 (94%)	181 (95%)	9 (5%)	23	52
2	H	199/207 (96%)	184 (92%)	15 (8%)	12	38
2	I	199/207 (96%)	183 (92%)	16 (8%)	11	35
2	J	199/207 (96%)	182 (92%)	17 (8%)	10	33
2	K	199/207 (96%)	184 (92%)	15 (8%)	12	38
3	L	180/180 (100%)	163 (91%)	17 (9%)	8	29
3	M	180/180 (100%)	165 (92%)	15 (8%)	10	34
3	N	180/180 (100%)	158 (88%)	22 (12%)	5	19
3	O	180/180 (100%)	167 (93%)	13 (7%)	13	39
All	All	2280/2360 (97%)	2104 (92%)	176 (8%)	12	37

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	LEU
1	A	92	SER

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Mol	Chain	Res	Type
1	A	101	SER
1	A	126	SER
1	A	138	SER
1	A	139	SER
1	A	145	SER
1	A	174	SER
1	A	178	LEU
1	A	179	SER
1	A	249	THR
1	A	280	SER
1	A	284	ILE
2	H	23	THR
2	H	31	THR
2	H	58	THR
2	H	67	SER
2	H	141	SER
2	H	153	VAL
2	H	170	LEU
2	H	189	LEU
2	H	195	VAL
2	H	198	SER
2	H	199	SER
2	H	208	ASN
2	H	212	LYS
2	H	217	LYS
2	H	220	LYS
3	L	8	SER
3	L	12	SER
3	L	19	VAL
3	L	65	ASP
3	L	70	SER
3	L	101	VAL
3	L	114	SER
3	L	121	THR
3	L	138	VAL
3	L	149	VAL
3	L	150	THR
3	L	157	SER
3	L	160	VAL
3	L	198	CYS
3	L	201	THR
3	L	205	SER

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Mol	Chain	Res	Type
3	L	216	CYS
1	B	78	ILE
1	B	97	VAL
1	B	104	ASN
1	B	138	SER
1	B	139	SER
1	B	149	VAL
1	B	178	LEU
1	B	183	ILE
1	B	202	SER
1	B	207	SER
1	B	231	ILE
1	B	237	VAL
1	B	251	VAL
2	I	1	GLN
2	I	12	VAL
2	I	17	THR
2	I	23	THR
2	I	30	ASN
2	I	67	SER
2	I	83	SER
2	I	86	SER
2	I	88	THR
2	I	106	THR
2	I	126	SER
2	I	154	LYS
2	I	167	SER
2	I	186	LEU
2	I	199	SER
2	I	204	THR
3	M	12	SER
3	M	27	SER
3	M	30	SER
3	M	31	THR
3	M	101	VAL
3	M	110	VAL
3	M	114	SER
3	M	142	SER
3	M	144	PHE
3	M	149	VAL
3	M	150	THR
3	M	166	THR

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Mol	Chain	Res	Type
3	M	185	LEU
3	M	186	THR
3	M	188	GLU
1	C	64	VAL
1	C	138	SER
1	C	139	SER
1	C	178	LEU
1	C	204	ASP
1	C	207	SER
1	C	216	VAL
1	C	237	VAL
1	C	249	THR
1	C	267	VAL
1	C	282	ILE
2	J	17	THR
2	J	23	THR
2	J	24	VAL
2	J	31	THR
2	J	59	SER
2	J	70	THR
2	J	88	THR
2	J	94	VAL
2	J	104	ILE
2	J	127	THR
2	J	152	LEU
2	J	171	THR
2	J	186	LEU
2	J	189	LEU
2	J	209	VAL
2	J	217	LYS
2	J	221	ARG
3	N	8	SER
3	N	14	SER
3	N	15	LEU
3	N	19	VAL
3	N	30	SER
3	N	31	THR
3	N	34	ILE
3	N	46	ARG
3	N	58	THR
3	N	82	SER
3	N	86	GLU

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Mol	Chain	Res	Type
3	N	90	ASP
3	N	119	SER
3	N	127	SER
3	N	130	LEU
3	N	150	THR
3	N	165	GLU
3	N	168	THR
3	N	186	THR
3	N	192	SER
3	N	197	SER
3	N	200	VAL
1	D	99	THR
1	D	121	GLN
1	D	126	SER
1	D	139	SER
1	D	179	SER
1	D	180	LYS
1	D	216	VAL
1	D	251	VAL
1	D	275	GLU
2	K	15	SER
2	K	25	SER
2	K	75	THR
2	K	85	ARG
2	K	105	LEU
2	K	122	VAL
2	K	140	LYS
2	K	141	SER
2	K	151	CYS
2	K	164	SER
2	K	172	SER
2	K	195	VAL
2	K	207	CYS
2	K	209	VAL
2	K	227	CYS
3	O	8	SER
3	O	10	SER
3	O	19	VAL
3	O	30	SER
3	O	34	ILE
3	O	85	SER
3	O	94	GLN

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Mol	Chain	Res	Type
3	O	119	SER
3	O	126	SER
3	O	141	ILE
3	O	160	VAL
3	O	185	LEU
3	O	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	164	ASN
1	A	211	ASN
2	H	79	GLN
2	H	175	HIS
3	L	94	GLN
1	B	121	GLN
1	B	146	ASN
1	B	173	ASN
2	I	5	GLN
2	I	116	GLN
2	I	182	GLN
2	I	208	ASN
2	I	210	ASN
3	M	94	GLN
3	M	113	GLN
3	M	189	GLN
1	C	121	GLN
1	C	211	ASN
2	J	41	GLN
2	J	116	GLN
2	J	166	ASN
2	J	203	GLN
3	N	2	GLN
3	N	39	GLN
3	N	199	GLN
1	D	121	GLN
1	D	146	ASN
1	D	173	ASN
1	D	206	GLN
1	D	211	ASN
2	K	30	ASN

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Mol	Chain	Res	Type
2	K	166	ASN
2	K	175	HIS

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 ⓘ

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 for Mogul analysis.

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	501	1	14,14,15	0.58	0	17,19,21	1.99	2 (11%)
6	ACT	B	503	-	3,3,3	0.83	0	3,3,3	0.88	0
4	NAG	B	501	1	14,14,15	0.94	0	17,19,21	1.74	3 (17%)
4	NAG	C	501	1	14,14,15	0.58	0	17,19,21	1.06	1 (5%)
4	NAG	D	501	1	14,14,15	0.61	0	17,19,21	1.26	1 (5%)
6	ACT	D	503	-	3,3,3	0.80	0	3,3,3	0.79	0

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	C	501	1	-	2/6/23/26	0/1/1/1
4	NAG	D	501	1	-	0/6/23/26	0/1/1/1
4	NAG	B	501	1	-	2/6/23/26	0/1/1/1
4	NAG	A	501	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	NAG	C1-O5-C5	7.30	121.97	112.19
4	B	501	NAG	C2-N2-C7	3.77	127.96	122.90
4	C	501	NAG	C1-O5-C5	2.86	116.02	112.19
4	B	501	NAG	C1-O5-C5	2.71	115.82	112.19
4	B	501	NAG	C1-C2-N2	2.65	114.61	110.43
4	D	501	NAG	C2-N2-C7	2.48	126.23	122.90
4	A	501	NAG	O7-C7-C8	-2.21	118.12	122.05

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	501	NAG	C4-C5-C6-O6
4	B	501	NAG	O5-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6
4	C	501	NAG	O5-C5-C6-O6
4	A	501	NAG	C4-C5-C6-O6
4	C	501	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	223/235 (94%)	-0.59	2 (0%) 81 64	34, 55, 110, 171	0
1	B	221/235 (94%)	-0.32	5 (2%) 61 40	42, 72, 155, 183	0
1	C	223/235 (94%)	-0.49	2 (0%) 81 64	40, 62, 112, 169	0
1	D	221/235 (94%)	-0.57	3 (1%) 73 53	33, 60, 136, 196	0
2	H	230/238 (96%)	-0.46	2 (0%) 81 64	33, 67, 150, 226	0
2	I	230/238 (96%)	0.04	10 (4%) 40 23	43, 76, 223, 261	0
2	J	230/238 (96%)	-0.07	4 (1%) 69 48	46, 95, 186, 200	0
2	K	230/238 (96%)	-0.03	7 (3%) 52 32	33, 86, 182, 212	0
3	L	216/216 (100%)	-0.69	1 (0%) 87 75	32, 56, 88, 202	0
3	M	216/216 (100%)	0.04	8 (3%) 45 26	43, 81, 219, 268	0
3	N	216/216 (100%)	-0.19	2 (0%) 81 64	43, 95, 145, 197	0
3	O	216/216 (100%)	-0.32	2 (0%) 81 64	30, 65, 155, 191	0
All	All	2672/2756 (96%)	-0.30	48 (1%) 67 47	30, 69, 183, 268	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	227	CYS	4.7
2	I	218	VAL	4.1
2	J	142	ALA	4.1
1	D	282	ILE	3.7
1	C	87	LEU	3.6
1	A	87	LEU	3.5
1	C	88	SER	3.5
1	B	284	ILE	3.5
2	K	224	PRO	3.3
2	I	132	VAL	3.3
2	K	205	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
2	I	209	VAL	3.2
3	M	137	LEU	3.1
2	K	142	ALA	3.0
1	B	282	ILE	3.0
3	M	190	TRP	2.9
2	I	137	PRO	2.9
3	M	118	PRO	2.9
2	I	142	ALA	2.9
2	H	142	ALA	2.9
3	N	214	THR	2.8
2	K	140	LYS	2.7
3	L	216	CYS	2.7
2	I	152	LEU	2.6
2	K	218	VAL	2.5
3	M	136	THR	2.5
2	J	224	PRO	2.5
2	I	199	SER	2.4
2	K	151	CYS	2.4
3	M	196	TYR	2.4
3	O	214	THR	2.4
1	B	87	LEU	2.4
2	J	227	CYS	2.3
1	D	100	PRO	2.3
2	I	196	PRO	2.3
3	M	130	LEU	2.2
1	D	65	ALA	2.2
2	I	130	PRO	2.2
2	K	213	PRO	2.2
1	A	90	ALA	2.1
3	M	153	TRP	2.1
1	B	71	LYS	2.1
2	J	196	PRO	2.1
3	M	216	CYS	2.1
2	I	195	VAL	2.0
3	O	174	ASN	2.0
1	B	281	GLY	2.0
3	N	2	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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(Å ²)	Q<0.9
4	NAG	A	501	14/15	0.85	0.12	80,103,112,117	0
4	NAG	B	501	14/15	0.85	0.13	97,120,125,127	0
4	NAG	D	501	14/15	0.87	0.13	116,127,130,132	0
5	CA	O	301	1/1	0.89	0.36	122,122,122,122	1
4	NAG	C	501	14/15	0.90	0.12	111,122,127,129	0
6	ACT	B	503	4/4	0.93	0.15	58,60,63,66	0
5	CA	C	502	1/1	0.95	0.05	71,71,71,71	0
5	CA	B	502	1/1	0.97	0.06	72,72,72,72	0
6	ACT	D	503	4/4	0.97	0.08	51,51,57,58	0
5	CA	D	502	1/1	0.98	0.04	71,71,71,71	0
5	CA	A	502	1/1	0.99	0.08	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.