



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:02 AM UTC

PDB ID : 9LV1 / pdb_00009lv1
Title : Crystal structure of H1 Haemagglutinin HN/18 from Influenza A virus
Authors : Deng, G.; Wei, X.; Sun, H.
Deposited on : 2025-02-11
Resolution : 2.40 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

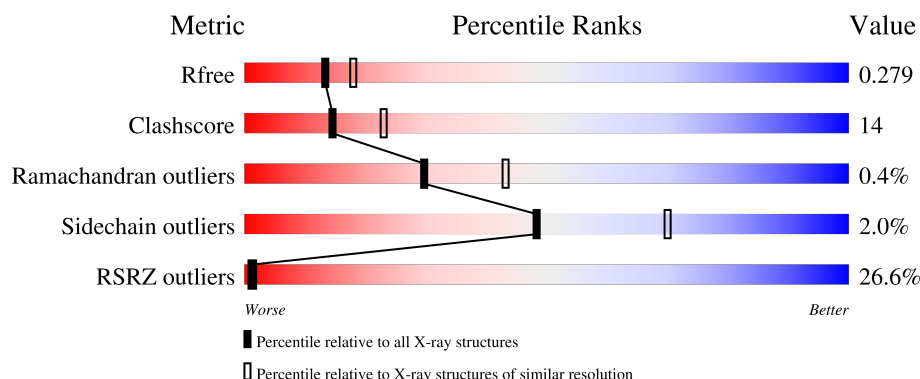
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	321	<div> <div>8%</div> <div>81%</div> <div>18%</div> <div>.</div> </div>
1	C	321	<div> <div>14%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
1	E	321	<div> <div>13%</div> <div>86%</div> <div>14%</div> </div>
2	B	154	<div> <div>64%</div> <div>75%</div> <div>22%</div> <div>..</div> </div>
2	D	154	<div> <div>72%</div> <div>56%</div> <div>38%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	154	<div><div></div><div>36%</div><div></div><div>71%</div><div></div><div>28%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11635 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	E	321	Total	C	N	O	S	0	0	0
			2515	1583	441	480	11			
1	A	321	Total	C	N	O	S	0	0	0
			2515	1583	441	480	11			
1	C	321	Total	C	N	O	S	0	0	0
			2515	1583	441	480	11			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	154	Total	C	N	O	S	0	0	0
			1229	771	211	240	7			
2	B	154	Total	C	N	O	S	0	0	0
			1229	771	211	240	7			
2	D	154	Total	C	N	O	S	0	0	0
			1229	771	211	240	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

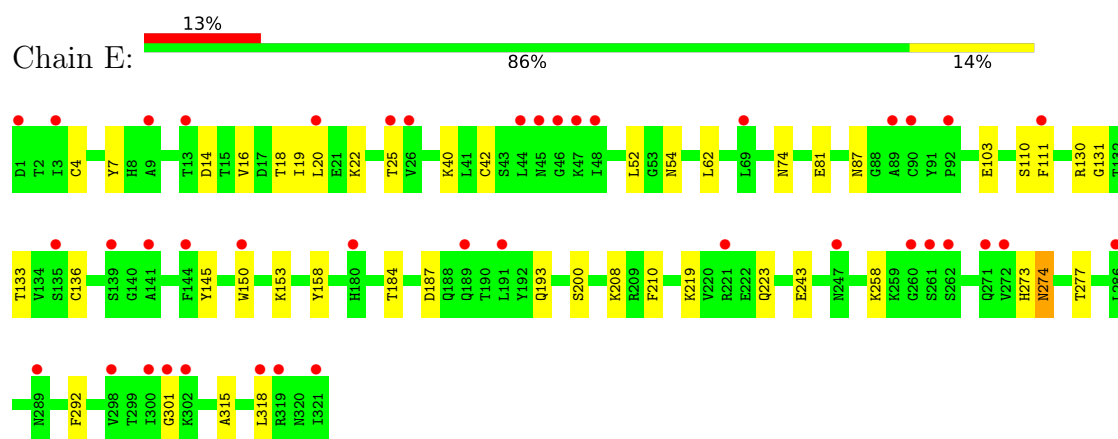
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	62	Total 62	O 62	0	0
4	A	65	Total 65	O 65	0	0
4	C	69	Total 69	O 69	0	0
4	F	16	Total 16	O 16	0	0
4	B	15	Total 15	O 15	0	0
4	D	8	Total 8	O 8	0	0

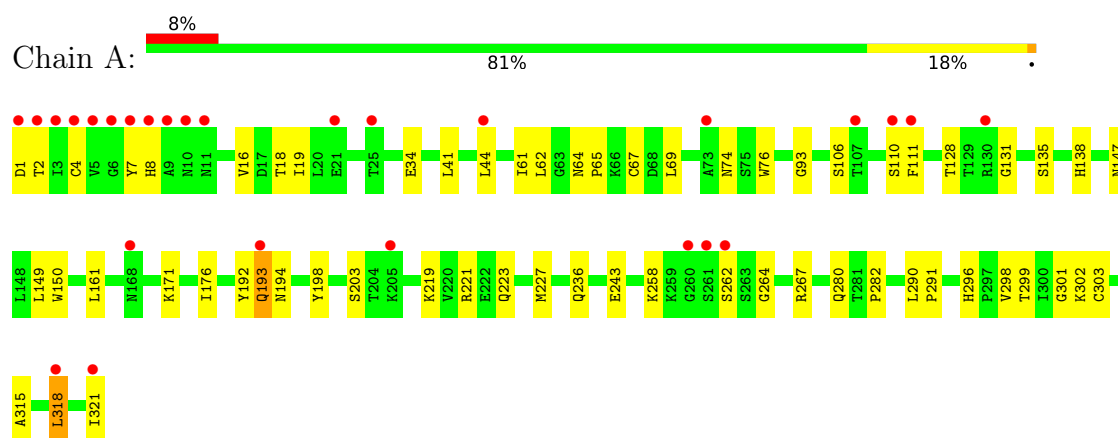
3 Residue-property plots [i](#)

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.

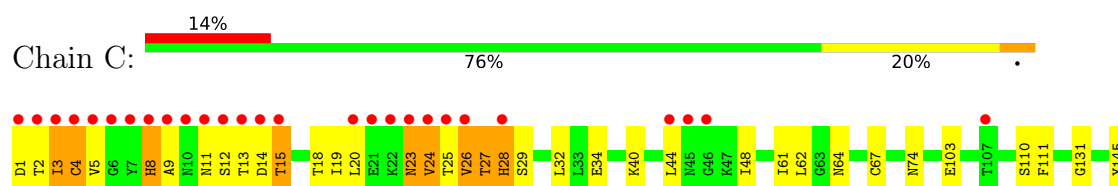
• Molecule 1: Hemagglutinin

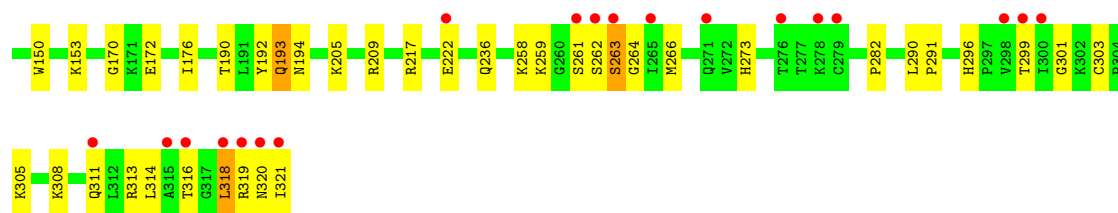


• Molecule 1: Hemagglutinin

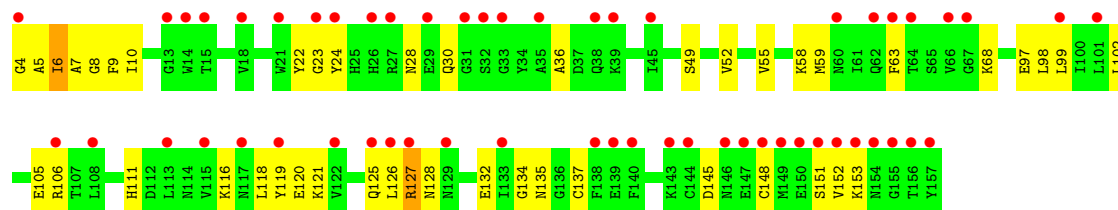


• Molecule 1: Hemagglutinin

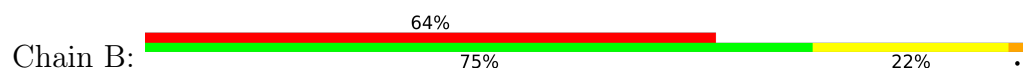




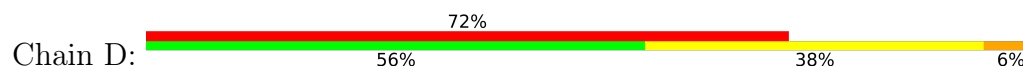
● Molecule 2: Hemagglutinin



● Molecule 2: Hemagglutinin



● Molecule 2: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.34Å 79.60Å 121.81Å 90.00° 95.34° 90.00°	Depositor
Resolution (Å)	50.01 – 2.40 50.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	75.8 (50.01-2.40) 75.8 (50.01-2.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.263 , 0.280 0.264 , 0.279	Depositor DCC
R_{free} test set	2984 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å ²)	36.6	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	11635	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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	A	0.33	0/2577	0.50	0/3506
1	C	0.41	0/2577	0.66	7/3506 (0.2%)
1	E	0.17	0/2577	0.41	0/3506
2	B	0.32	0/1252	0.73	5/1683 (0.3%)
2	D	0.32	0/1252	0.70	4/1683 (0.2%)
2	F	0.43	0/1252	0.59	0/1683
All	All	0.33	0/11487	0.58	16/15567 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	11	ASN	N-CA-C	10.23	124.21	108.96
2	B	143	LYS	N-CA-C	8.29	122.93	108.75
1	C	316	THR	N-CA-C	-7.06	104.54	113.43
1	C	15	THR	N-CA-C	7.03	120.10	109.41
2	B	127	ARG	CB-CA-C	-6.89	108.61	116.54
2	D	5	ALA	CA-C-N	-6.69	114.00	122.43
2	D	5	ALA	C-N-CA	-6.69	114.00	122.43
2	D	130	ALA	N-CA-C	-6.35	97.93	108.34
2	D	129	ASN	N-CA-C	-6.17	106.97	114.75
1	C	8	HIS	N-CA-C	6.14	118.29	108.41
1	C	28	HIS	N-CA-C	5.81	118.20	110.53
2	B	125	GLN	CA-C-N	5.53	130.07	120.68
2	B	125	GLN	C-N-CA	5.53	130.07	120.68
2	B	127	ARG	N-CA-C	5.50	116.67	108.31
1	C	222	GLU	CA-CB-CG	5.12	124.33	114.10
1	C	264	GLY	N-CA-C	5.06	125.18	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2515	0	2453	50	0
1	C	2515	0	2452	96	0
1	E	2515	0	2452	35	0
2	B	1229	0	1168	51	0
2	D	1229	0	1167	116	0
2	F	1229	0	1167	45	0
3	A	56	0	52	5	0
3	C	56	0	52	1	0
3	E	56	0	52	0	0
4	A	65	0	0	2	0
4	B	15	0	0	0	0
4	C	69	0	0	2	0
4	D	8	0	0	1	0
4	E	62	0	0	1	0
4	F	16	0	0	2	0
All	All	11635	0	11015	314	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 14.

All (314) 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)
2:D:113:LEU:HD13	2:D:114:ASN:N	1.30	1.46
1:A:4:CYS:SG	2:B:137:CYS:SG	1.34	1.34
1:C:13:THR:CG2	1:C:14:ASP:H	1.50	1.24
2:D:113:LEU:HD11	2:D:114:ASN:OD1	1.42	1.18
1:C:13:THR:HG22	1:C:14:ASP:N	1.48	1.17
2:D:113:LEU:CD1	2:D:114:ASN:OD1	1.97	1.13
2:D:131:LYS:HD3	2:D:141:TYR:CE1	1.88	1.08
2:D:110:PHE:O	2:D:113:LEU:HD12	1.52	1.08
1:C:15:THR:HG22	1:C:25:THR:HA	1.37	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:132:GLU:HB2	2:D:127:ARG:HH12	1.01	1.06
2:D:130:ALA:HB3	2:D:138:PHE:HB2	1.33	1.06
2:D:113:LEU:CD1	2:D:114:ASN:N	2.19	1.05
2:D:113:LEU:HD13	2:D:114:ASN:CA	1.89	1.00
2:D:130:ALA:HB2	2:D:140:PHE:CD1	1.97	1.00
3:A:401:NAG:H3	3:A:401:NAG:H83	1.43	0.99
1:C:2:THR:HG22	2:D:27:ARG:HB3	1.48	0.94
1:C:318:LEU:HD12	1:C:318:LEU:H	1.28	0.93
2:D:130:ALA:HB1	2:D:138:PHE:O	1.68	0.93
1:A:4:CYS:CB	2:B:137:CYS:SG	2.58	0.92
1:C:1:ASP:HA	2:D:27:ARG:O	1.67	0.92
2:D:113:LEU:HD13	2:D:114:ASN:H	1.31	0.92
2:D:130:ALA:CB	2:D:138:PHE:HB2	1.98	0.92
2:D:131:LYS:CD	2:D:141:TYR:CE1	2.53	0.92
1:C:5:VAL:HG22	2:D:24:TYR:CD1	2.05	0.91
2:F:132:GLU:CB	2:D:127:ARG:HH12	1.84	0.90
2:F:132:GLU:HB2	2:D:127:ARG:NH1	1.86	0.89
1:C:13:THR:HG22	1:C:14:ASP:OD1	1.73	0.88
2:B:122:VAL:O	2:B:126:LEU:HB2	1.73	0.88
1:A:1:ASP:HA	2:B:27:ARG:O	1.73	0.88
2:D:53:ASN:O	2:D:57:GLU:HB2	1.74	0.88
1:C:13:THR:CG2	1:C:14:ASP:OD1	2.22	0.88
2:D:130:ALA:HB2	2:D:140:PHE:CE1	2.08	0.87
2:F:106:ARG:HH11	2:D:106:ARG:HH12	1.19	0.87
1:C:26:VAL:HG22	1:C:318:LEU:O	1.74	0.87
2:D:130:ALA:HB1	2:D:138:PHE:C	2.00	0.87
1:C:2:THR:HA	2:D:140:PHE:CE2	2.09	0.87
1:C:15:THR:HG22	1:C:25:THR:CA	2.03	0.87
2:F:4:GLY:O	2:F:9:PHE:CD1	2.29	0.85
1:E:153:LYS:HD2	1:E:193:GLN:HG2	1.59	0.83
2:B:123:LYS:HA	2:B:126:LEU:HB3	1.61	0.83
1:A:110:SER:HB3	1:A:258:LYS:HB3	1.58	0.83
1:C:5:VAL:HG22	2:D:24:TYR:CE1	2.14	0.82
1:C:48:ILE:HD12	1:C:48:ILE:O	1.80	0.82
1:C:27:THR:HG23	1:C:319:ARG:O	1.80	0.82
1:C:172:GLU:OE2	1:C:259:LYS:HE2	1.80	0.81
1:C:26:VAL:O	1:C:27:THR:O	2.00	0.80
2:D:53:ASN:O	2:D:57:GLU:CB	2.30	0.79
1:C:170:GLY:C	1:C:236:GLN:HE21	1.91	0.79
2:D:130:ALA:HA	2:D:140:PHE:HA	1.65	0.79
3:C:404:NAG:H2	2:D:15:THR:HG21	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:TYR:CE2	2:D:37:ASP:OD1	2.36	0.78
1:C:153:LYS:HD3	1:C:193:GLN:H	1.47	0.78
1:C:8:HIS:CE1	2:D:17:MET:O	2.39	0.76
1:C:40:LYS:HB3	1:C:273:HIS:HD2	1.49	0.76
2:B:130:ALA:HA	2:B:139:GLU:O	1.85	0.75
1:C:318:LEU:HD12	1:C:318:LEU:N	2.02	0.75
2:F:4:GLY:O	2:F:9:PHE:HD1	1.70	0.74
1:C:26:VAL:CG2	1:C:318:LEU:O	2.36	0.74
1:C:153:LYS:HE3	1:C:190:THR:O	1.87	0.74
1:A:2:THR:HG22	2:B:27:ARG:HG2	1.68	0.74
2:F:116:LYS:NZ	2:F:120:GLU:OE2	2.20	0.74
2:B:131:LYS:NZ	2:B:139:GLU:OE1	2.21	0.73
2:D:127:ARG:HG2	2:D:128:ASN:OD1	1.87	0.73
1:C:13:THR:HG22	1:C:14:ASP:H	0.63	0.73
1:E:318:LEU:HD23	2:F:111:HIS:HB3	1.71	0.72
2:D:62:GLN:O	4:D:201:HOH:O	2.07	0.72
2:D:110:PHE:O	2:D:113:LEU:CD1	2.34	0.72
1:C:18:THR:HG22	2:D:104:ASN:HB3	1.69	0.72
1:A:171:LYS:HA	1:A:236:GLN:HE21	1.54	0.72
2:B:26:HIS:H	2:B:26:HIS:CD2	2.08	0.71
1:C:9:ALA:HB3	2:D:13:GLY:HA3	1.71	0.71
2:B:123:LYS:HA	2:B:126:LEU:HD23	1.73	0.71
2:B:122:VAL:O	2:B:126:LEU:CB	2.38	0.71
3:A:401:NAG:H3	3:A:401:NAG:C8	2.20	0.70
1:E:301:GLY:HA2	2:F:63:PHE:CE2	2.27	0.70
1:C:2:THR:HA	2:D:140:PHE:CD2	2.26	0.69
1:C:4:CYS:HB3	2:D:136:GLY:O	1.92	0.69
1:C:12:SER:O	1:C:13:THR:OG1	2.11	0.69
1:A:65:PRO:HB2	1:A:138:HIS:HB2	1.75	0.68
2:D:4:GLY:HA2	2:D:8:GLY:HA3	1.75	0.68
3:A:401:NAG:H82	3:A:401:NAG:C1	2.24	0.68
2:D:22:TYR:O	2:D:37:ASP:N	2.26	0.67
1:C:13:THR:CG2	1:C:14:ASP:N	2.25	0.66
1:C:3:ILE:HD13	2:D:152:VAL:CG1	2.27	0.65
2:F:118:LEU:HD12	2:F:121:LYS:HE3	1.78	0.65
1:A:2:THR:HG22	2:B:27:ARG:CG	2.27	0.65
1:C:48:ILE:HD12	1:C:48:ILE:C	2.21	0.65
2:D:21:TRP:HH2	2:D:48:ILE:HB	1.61	0.65
1:E:18:THR:HB	2:F:105:GLU:HB2	1.79	0.64
2:D:49:SER:O	2:D:52:VAL:HG12	1.97	0.64
1:C:29:SER:OG	1:C:313:ARG:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:LEU:HD13	2:D:113:LEU:C	2.16	0.64
1:C:308:LYS:HG2	2:D:93:THR:HG21	1.79	0.64
1:C:2:THR:HA	2:D:140:PHE:HE2	1.61	0.63
2:D:113:LEU:CD1	2:D:114:ASN:H	2.01	0.62
2:B:126:LEU:HD21	2:B:138:PHE:CD1	2.34	0.62
2:D:46:ASP:O	2:D:50:ASN:HB2	1.99	0.62
2:D:131:LYS:CD	2:D:141:TYR:HE1	2.12	0.62
1:C:20:LEU:HB2	2:D:105:GLU:OE2	2.00	0.62
2:F:4:GLY:HA3	2:D:117:ASN:HA	1.82	0.62
2:F:30:GLN:HE22	2:F:145:ASP:HB2	1.65	0.61
1:C:1:ASP:O	2:D:140:PHE:HD2	1.83	0.60
1:C:2:THR:HG21	2:D:137:CYS:SG	2.41	0.60
2:B:117:ASN:O	2:B:121:LYS:HG3	2.01	0.60
1:A:8:HIS:ND1	2:B:20:GLY:O	2.34	0.60
2:D:131:LYS:HD2	2:D:141:TYR:CE1	2.36	0.60
1:C:13:THR:HG21	1:C:27:THR:O	2.01	0.60
2:B:123:LYS:CA	2:B:126:LEU:HB3	2.30	0.59
2:D:24:TYR:CD2	2:D:37:ASP:OD1	2.55	0.59
2:F:106:ARG:NH1	2:D:106:ARG:HH12	1.95	0.59
2:B:97:GLU:O	2:B:100:ILE:HG13	2.03	0.58
1:C:3:ILE:CD1	2:D:152:VAL:HG13	2.34	0.58
2:D:131:LYS:HD3	2:D:141:TYR:HE1	1.61	0.58
2:B:4:GLY:HA2	2:B:112:ASP:OD2	2.04	0.58
2:D:126:LEU:HD21	2:D:140:PHE:CE1	2.39	0.57
1:A:7:TYR:CZ	2:B:12:GLY:O	2.58	0.57
2:D:22:TYR:OH	2:D:114:ASN:ND2	2.37	0.57
2:D:28:ASN:ND2	2:D:149:MET:SD	2.77	0.57
1:E:54:ASN:ND2	1:E:87:ASN:OD1	2.36	0.57
1:C:236:GLN:HB3	4:C:522:HOH:O	2.05	0.57
2:B:27:ARG:O	2:B:27:ARG:HG3	2.05	0.56
2:D:138:PHE:CD1	2:D:138:PHE:N	2.73	0.56
1:E:40:LYS:HD3	1:E:273:HIS:ND1	2.19	0.56
2:F:98:LEU:O	2:F:102:LEU:HG	2.06	0.56
1:E:7:TYR:HB2	1:E:318:LEU:HD13	1.87	0.56
1:C:110:SER:HB3	1:C:258:LYS:HB2	1.88	0.56
1:C:291:PRO:HD3	2:D:56:ILE:HG23	1.88	0.56
2:D:61:ILE:O	2:D:61:ILE:HG13	2.05	0.55
1:C:32:LEU:HD11	1:C:314:LEU:HD22	1.87	0.55
1:C:2:THR:CG2	2:D:137:CYS:SG	2.95	0.55
1:C:262:SER:O	1:C:262:SER:OG	2.19	0.55
2:B:58:LYS:NZ	2:D:97:GLU:OE1	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:THR:HB	2:D:105:GLU:HG2	1.90	0.54
1:A:62:LEU:HD23	1:A:176:ILE:HD12	1.90	0.54
1:C:74:ASN:HA	1:C:111:PHE:HB3	1.89	0.54
1:C:3:ILE:CD1	2:D:152:VAL:CG1	2.86	0.53
1:A:262:SER:HA	2:B:63:PHE:CZ	2.44	0.53
2:D:123:LYS:O	2:D:127:ARG:HB2	2.07	0.53
2:F:135:ASN:OD1	2:F:135:ASN:N	2.39	0.53
1:E:318:LEU:HD23	2:F:111:HIS:CB	2.39	0.53
1:A:193:GLN:NE2	1:A:193:GLN:HA	2.24	0.53
1:E:318:LEU:HD23	2:F:111:HIS:CG	2.44	0.53
1:E:274:ASN:OD1	1:E:274:ASN:N	2.42	0.53
1:C:15:THR:HB	1:C:24:VAL:O	2.09	0.52
2:D:131:LYS:N	2:D:139:GLU:O	2.35	0.52
1:A:8:HIS:CE1	2:B:20:GLY:O	2.62	0.52
2:B:26:HIS:CD2	2:B:26:HIS:N	2.77	0.52
1:A:106:SER:HB2	1:A:264:GLY:HA2	1.92	0.52
1:E:103:GLU:OE2	2:F:68:LYS:NZ	2.42	0.52
1:C:3:ILE:HD13	2:D:152:VAL:CG2	2.39	0.52
1:C:40:LYS:HB3	1:C:273:HIS:CD2	2.36	0.52
1:A:301:GLY:HA2	2:B:63:PHE:CD2	2.44	0.52
3:A:401:NAG:C8	3:A:401:NAG:C1	2.86	0.52
2:F:148:CYS:HA	2:F:151:SER:HB3	1.91	0.52
2:D:53:ASN:O	2:D:57:GLU:HB3	2.08	0.52
1:A:131:GLY:HA3	1:A:150:TRP:HB3	1.92	0.52
1:E:130:ARG:NH2	4:E:506:HOH:O	2.40	0.51
1:C:1:ASP:OD2	2:D:144:CYS:N	2.30	0.51
1:E:184:THR:OG1	1:E:187:ASP:OD1	2.29	0.51
1:A:16:VAL:HG21	1:A:315:ALA:HB2	1.92	0.51
2:B:59:MET:HE1	2:B:92:TRP:CZ3	2.45	0.51
1:A:135:SER:OG	1:A:221:ARG:O	2.29	0.51
1:C:110:SER:CB	1:C:258:LYS:HE3	2.41	0.51
1:A:93:GLY:HA3	1:A:227:MET:O	2.10	0.51
2:B:123:LYS:HA	2:B:126:LEU:CD2	2.40	0.50
1:C:5:VAL:CG2	2:D:24:TYR:CE1	2.89	0.50
1:C:28:HIS:N	1:C:28:HIS:CD2	2.79	0.50
1:E:4:CYS:HA	2:F:137:CYS:HA	1.92	0.50
2:D:27:ARG:HG3	2:D:27:ARG:HH11	1.76	0.50
1:E:7:TYR:OH	2:F:10:ILE:O	2.28	0.50
1:C:1:ASP:OD2	2:D:144:CYS:O	2.30	0.50
1:C:48:ILE:C	1:C:48:ILE:CD1	2.84	0.50
2:D:14:TRP:CH2	2:D:25:HIS:HB2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:LEU:HD13	2:D:114:ASN:OD1	2.05	0.50
1:E:292:PHE:CZ	2:F:59:MET:HE3	2.47	0.50
2:F:8:GLY:HA2	2:D:117:ASN:OD1	2.12	0.49
1:A:192:TYR:O	1:A:194:ASN:N	2.45	0.49
1:C:28:HIS:CD2	1:C:28:HIS:H	2.29	0.49
2:F:5:ALA:HA	2:F:9:PHE:CE1	2.48	0.49
1:E:52:LEU:HD12	1:E:81:GLU:HG3	1.94	0.49
1:C:318:LEU:H	1:C:318:LEU:CD1	2.11	0.49
2:F:49:SER:HA	2:F:52:VAL:HG12	1.93	0.49
2:B:9:PHE:HZ	2:B:116:LYS:HE2	1.77	0.49
1:E:22:LYS:HG3	2:D:50:ASN:HD21	1.76	0.49
1:C:27:THR:N	1:C:318:LEU:O	2.46	0.48
2:F:59:MET:HE2	2:B:94:TYR:CZ	2.48	0.48
1:E:42:CYS:HB2	1:E:277:THR:HG22	1.96	0.48
1:A:4:CYS:HA	2:B:136:GLY:O	2.13	0.48
2:F:125:GLN:NE2	2:F:152:VAL:O	2.47	0.48
2:D:106:ARG:HD2	2:D:106:ARG:HA	1.60	0.48
2:D:131:LYS:HG2	2:D:139:GLU:O	2.14	0.48
3:A:401:NAG:H83	3:A:401:NAG:C3	2.28	0.48
1:C:19:ILE:HG23	1:C:20:LEU:HG	1.95	0.48
2:D:125:GLN:NE2	2:D:157:TYR:C	2.72	0.48
2:D:113:LEU:CD1	2:D:113:LEU:C	2.82	0.48
1:C:15:THR:CG2	1:C:25:THR:HA	2.26	0.48
1:C:209:ARG:NH2	4:C:511:HOH:O	2.46	0.48
1:A:267:ARG:NH1	4:A:512:HOH:O	2.45	0.48
1:C:18:THR:HB	2:D:105:GLU:CG	2.44	0.48
1:E:208:LYS:HG2	1:E:210:PHE:CE2	2.49	0.47
1:E:301:GLY:HA2	2:F:63:PHE:CD2	2.49	0.47
2:D:130:ALA:HA	2:D:140:PHE:CA	2.42	0.47
1:C:26:VAL:C	1:C:27:THR:O	2.57	0.47
1:C:62:LEU:O	1:C:145:TYR:HB3	2.15	0.47
1:A:2:THR:CG2	2:B:27:ARG:HB3	2.44	0.47
1:A:262:SER:HA	2:B:63:PHE:CE1	2.50	0.47
2:F:28:ASN:HD21	2:F:145:ASP:C	2.21	0.47
1:C:311:GLN:OE1	1:C:313:ARG:N	2.41	0.47
2:D:130:ALA:CB	2:D:138:PHE:CB	2.84	0.47
1:C:3:ILE:HD13	2:D:152:VAL:HG13	1.96	0.47
2:B:58:LYS:O	2:D:94:TYR:HD1	1.98	0.47
1:A:203:SER:O	1:C:217:ARG:NH2	2.28	0.46
1:C:103:GLU:OE2	2:D:68:LYS:NZ	2.35	0.46
2:B:123:LYS:HA	2:B:126:LEU:CB	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:SER:HB3	1:E:258:LYS:HB2	1.97	0.46
2:B:144:CYS:SG	2:B:145:ASP:N	2.89	0.46
1:C:34:GLU:HG3	1:C:290:LEU:HD12	1.96	0.46
1:A:41:LEU:HA	1:A:280:GLN:NE2	2.31	0.46
1:E:219:LYS:HA	1:E:223:GLN:O	2.16	0.46
2:F:23:GLY:HA3	2:F:36:ALA:HA	1.97	0.46
1:A:34:GLU:HG3	1:A:290:LEU:HB2	1.97	0.46
2:F:6:ILE:O	2:F:7:ALA:HB3	2.16	0.45
2:B:145:ASP:N	2:B:145:ASP:OD1	2.46	0.45
1:E:318:LEU:HD21	2:F:22:TYR:HE1	1.81	0.45
2:F:119:TYR:OH	4:F:201:HOH:O	2.21	0.45
2:F:132:GLU:CB	2:D:127:ARG:NH1	2.63	0.45
1:E:16:VAL:HG21	1:E:315:ALA:HB2	1.98	0.45
2:D:21:TRP:CH2	2:D:48:ILE:HB	2.46	0.45
1:C:23:ASN:HD22	1:C:23:ASN:HA	1.52	0.45
2:B:127:ARG:HB3	2:B:128:ASN:H	1.52	0.45
2:F:134:GLY:HA3	2:D:124:SER:HA	1.97	0.45
1:C:61:ILE:HG22	1:C:176:ILE:HD13	1.98	0.45
2:F:24:TYR:HB2	2:F:153:LYS:HE2	1.99	0.45
2:B:117:ASN:OD1	2:D:4:GLY:N	2.49	0.45
1:E:14:ASP:O	1:E:25:THR:HA	2.17	0.45
1:A:298:VAL:HA	2:B:66:VAL:CG2	2.47	0.45
1:E:62:LEU:O	1:E:145:TYR:HB3	2.17	0.44
1:A:302:LYS:HA	2:B:62:GLN:O	2.17	0.44
1:A:76:TRP:NE1	4:A:501:HOH:O	2.28	0.44
1:C:305:LYS:HD3	1:C:305:LYS:HA	1.81	0.44
2:F:135:ASN:ND2	4:F:204:HOH:O	2.47	0.44
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.73	0.44
2:F:55:VAL:CG2	2:F:99:LEU:HD21	2.47	0.44
2:D:18:VAL:HG12	2:D:18:VAL:O	2.18	0.44
1:A:291:PRO:HB2	2:B:59:MET:HG3	2.00	0.44
1:C:3:ILE:HD13	2:D:152:VAL:HG11	1.99	0.44
2:B:118:LEU:HA	2:B:121:LYS:HE3	2.00	0.43
2:D:21:TRP:CZ2	2:D:45:ILE:HG12	2.52	0.43
2:D:130:ALA:HB1	2:D:138:PHE:HB2	1.94	0.43
2:B:123:LYS:C	2:B:126:LEU:HB3	2.43	0.43
1:E:19:ILE:HG23	1:E:20:LEU:HG	1.99	0.43
1:E:133:THR:HG23	1:E:136:CYS:H	1.83	0.43
1:E:200:SER:OG	1:E:243:GLU:HB3	2.18	0.43
1:A:74:ASN:HA	1:A:111:PHE:HB3	2.01	0.43
1:A:128:THR:HB	1:A:149:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:TYR:HB2	2:D:37:ASP:HB2	2.00	0.43
1:A:19:ILE:HB	2:B:102:LEU:HD23	2.00	0.43
1:A:282:PRO:HD3	1:A:298:VAL:O	2.19	0.43
1:C:14:ASP:O	1:C:25:THR:HG23	2.19	0.43
2:B:116:LYS:N	2:B:116:LYS:HD2	2.33	0.43
2:F:116:LYS:O	2:F:116:LYS:HG3	2.17	0.43
2:D:130:ALA:HA	2:D:139:GLU:O	2.18	0.43
1:E:318:LEU:CD2	2:F:111:HIS:HB3	2.45	0.43
1:A:299:THR:HB	1:A:303:CYS:SG	2.59	0.43
2:D:111:HIS:O	2:D:115:VAL:HG23	2.19	0.43
1:A:219:LYS:HA	1:A:223:GLN:O	2.18	0.43
1:C:40:LYS:HD3	1:C:273:HIS:CD2	2.54	0.43
1:E:74:ASN:HA	1:E:111:PHE:HB3	2.01	0.42
1:E:131:GLY:HA3	1:E:150:TRP:HB3	2.00	0.42
1:A:2:THR:HG22	2:B:27:ARG:CB	2.49	0.42
2:F:127:ARG:HB3	2:F:128:ASN:H	1.52	0.42
1:A:298:VAL:HA	2:B:66:VAL:HG22	2.01	0.42
1:C:4:CYS:HB3	2:D:137:CYS:CA	2.41	0.42
1:C:266:MET:HE3	1:C:266:MET:HB2	1.86	0.42
1:A:8:HIS:HB3	1:A:318:LEU:HD11	2.01	0.42
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.88	0.42
1:C:27:THR:HG22	1:C:320:ASN:OD1	2.20	0.42
1:C:301:GLY:HA2	2:D:63:PHE:CD2	2.55	0.42
1:C:263:SER:HB3	2:D:63:PHE:HZ	1.85	0.42
2:D:131:LYS:CD	2:D:141:TYR:CZ	3.01	0.42
1:C:44:LEU:HD12	1:C:44:LEU:HA	1.94	0.42
2:B:9:PHE:CZ	2:B:116:LYS:HE2	2.54	0.42
1:A:61:ILE:O	1:A:147:ASN:ND2	2.46	0.42
1:A:64:ASN:HB3	1:A:67:CYS:SG	2.60	0.42
1:C:131:GLY:HA3	1:C:150:TRP:HB3	2.01	0.42
1:C:205:LYS:HE3	1:C:205:LYS:HB3	1.75	0.42
2:D:5:ALA:HB3	2:D:112:ASP:OD1	2.20	0.42
2:D:113:LEU:HD13	2:D:114:ASN:HA	1.93	0.42
2:D:126:LEU:HD21	2:D:140:PHE:HE1	1.85	0.42
2:D:132:GLU:HG2	2:D:138:PHE:HD2	1.86	0.41
2:D:133:ILE:HD11	2:D:139:GLU:HB2	2.02	0.41
1:C:282:PRO:HG2	1:C:296:HIS:CD2	2.55	0.41
1:C:15:THR:HG22	1:C:25:THR:N	2.35	0.41
1:A:198:TYR:OH	1:A:243:GLU:OE2	2.32	0.41
1:C:19:ILE:HB	2:D:102:LEU:HD23	2.02	0.41
1:C:192:TYR:O	1:C:194:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:ASN:HB3	1:C:67:CYS:SG	2.60	0.41
1:A:161:LEU:O	1:A:243:GLU:HA	2.21	0.41
1:A:221:ARG:O	1:A:223:GLN:HG2	2.21	0.41
1:A:282:PRO:HD2	1:A:296:HIS:CG	2.55	0.41
1:C:14:ASP:N	1:C:14:ASP:OD1	2.53	0.41
1:C:4:CYS:CB	2:D:136:GLY:O	2.65	0.41
1:C:299:THR:HB	1:C:303:CYS:SG	2.61	0.41
2:B:126:LEU:HD21	2:B:138:PHE:CG	2.56	0.41
2:B:130:ALA:CB	2:B:138:PHE:HB3	2.50	0.41
2:D:130:ALA:HA	2:D:139:GLU:C	2.46	0.41
1:A:18:THR:HG22	2:B:104:ASN:HB3	2.02	0.41
1:E:19:ILE:HB	2:F:102:LEU:HD23	2.02	0.40
2:F:97:GLU:HB3	2:D:58:LYS:HD2	2.02	0.40
2:D:113:LEU:O	2:D:116:LYS:N	2.55	0.40
1:C:291:PRO:CB	2:D:59:MET:HG3	2.51	0.40
2:F:58:LYS:HD3	2:F:58:LYS:HA	1.88	0.40
1:E:158:TYR:CD1	1:E:158:TYR:C	3.00	0.40
2:D:118:LEU:HD12	2:D:118:LEU:HA	1.95	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	319/321 (99%)	301 (94%)	17 (5%)	1 (0%)	36	50
1	C	319/321 (99%)	295 (92%)	20 (6%)	4 (1%)	9	14
1	E	319/321 (99%)	304 (95%)	15 (5%)	0	100	100
2	B	152/154 (99%)	144 (95%)	8 (5%)	0	100	100
2	D	152/154 (99%)	137 (90%)	14 (9%)	1 (1%)	18	28
2	F	152/154 (99%)	146 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1413/1425 (99%)	1327 (94%)	80 (6%)	6 (0%)	30	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	27	THR
1	C	193	GLN
1	A	193	GLN
2	D	127	ARG
1	C	261	SER
1	C	3	ILE

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	282/282 (100%)	280 (99%)	2 (1%)	76	88
1	C	282/282 (100%)	275 (98%)	7 (2%)	42	64
1	E	282/282 (100%)	281 (100%)	1 (0%)	84	92
2	B	131/132 (99%)	126 (96%)	5 (4%)	29	49
2	D	131/132 (99%)	124 (95%)	7 (5%)	20	36
2	F	131/132 (99%)	128 (98%)	3 (2%)	44	66
All	All	1239/1242 (100%)	1214 (98%)	25 (2%)	48	70

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	274	ASN
1	A	318	LEU
1	A	321	ILE
1	C	4	CYS
1	C	23	ASN
1	C	24	VAL

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Mol	Chain	Res	Type
1	C	26	VAL
1	C	263	SER
1	C	318	LEU
1	C	321	ILE
2	F	6	ILE
2	F	126	LEU
2	F	127	ARG
2	B	26	HIS
2	B	127	ARG
2	B	128	ASN
2	B	141	TYR
2	B	143	LYS
2	D	37	ASP
2	D	62	GLN
2	D	100	ILE
2	D	113	LEU
2	D	129	ASN
2	D	131	LYS
2	D	138	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	51	GLN
1	E	196	ASN
1	E	289	ASN
1	A	181	HIS
1	A	189	GLN
1	A	193	GLN
1	A	236	GLN
1	A	271	GLN
1	C	10	ASN
1	C	28	HIS
1	C	31	ASN
1	C	196	ASN
1	C	236	GLN
1	C	271	GLN
1	C	273	HIS
2	F	28	ASN
2	F	30	GLN
2	F	114	ASN
2	B	26	HIS

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Mol	Chain	Res	Type
2	B	129	ASN
2	B	142	HIS
2	D	25	HIS
2	D	28	ASN
2	D	60	ASN
2	D	125	GLN
2	D	129	ASN
2	D	142	HIS

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](#)

12 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	$\# Z > 2$
3	NAG	C	403	1	14,14,15	0.27	0	17,19,21	0.55	0
3	NAG	A	404	1	14,14,15	0.30	0	17,19,21	1.02	1 (5%)
3	NAG	E	401	1	14,14,15	0.29	0	17,19,21	0.67	0
3	NAG	A	402	1	14,14,15	0.31	0	17,19,21	0.88	0
3	NAG	E	404	1	14,14,15	0.27	0	17,19,21	0.85	0
3	NAG	E	403	1	14,14,15	0.26	0	17,19,21	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	402	1	14,14,15	0.31	0	17,19,21	0.62	0
3	NAG	A	403	1	14,14,15	0.26	0	17,19,21	0.97	1 (5%)
3	NAG	C	404	1	14,14,15	0.26	0	17,19,21	0.95	2 (11%)
3	NAG	C	401	1	14,14,15	0.31	0	17,19,21	0.81	0
3	NAG	A	401	1	14,14,15	0.28	0	17,19,21	0.62	0
3	NAG	C	402	1	14,14,15	0.31	0	17,19,21	0.65	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
3	NAG	C	403	1	-	4/6/23/26	0/1/1/1
3	NAG	A	404	1	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	2/6/23/26	0/1/1/1
3	NAG	A	402	1	-	2/6/23/26	0/1/1/1
3	NAG	E	404	1	-	4/6/23/26	0/1/1/1
3	NAG	E	403	1	-	2/6/23/26	0/1/1/1
3	NAG	E	402	1	-	4/6/23/26	0/1/1/1
3	NAG	A	403	1	-	2/6/23/26	0/1/1/1
3	NAG	C	404	1	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	4/6/23/26	0/1/1/1
3	NAG	C	402	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	NAG	C2-N2-C7	-2.46	119.60	122.90
3	C	404	NAG	C2-N2-C7	-2.26	119.87	122.90
3	A	404	NAG	O5-C1-C2	-2.15	107.96	111.29
3	C	404	NAG	C4-C3-C2	-2.13	107.89	111.02

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	401	NAG	C8-C7-N2-C2
3	E	401	NAG	O7-C7-N2-C2
3	E	404	NAG	C8-C7-N2-C2
3	E	404	NAG	O7-C7-N2-C2
3	A	403	NAG	C8-C7-N2-C2
3	A	403	NAG	O7-C7-N2-C2
3	C	401	NAG	C8-C7-N2-C2
3	C	401	NAG	O7-C7-N2-C2
3	C	402	NAG	C8-C7-N2-C2
3	C	402	NAG	O7-C7-N2-C2
3	C	403	NAG	C8-C7-N2-C2
3	C	403	NAG	O7-C7-N2-C2
3	E	402	NAG	O7-C7-N2-C2
3	E	402	NAG	C8-C7-N2-C2
3	E	403	NAG	C8-C7-N2-C2
3	E	403	NAG	O7-C7-N2-C2
3	A	401	NAG	C8-C7-N2-C2
3	A	401	NAG	O7-C7-N2-C2
3	E	402	NAG	O5-C5-C6-O6
3	E	402	NAG	C4-C5-C6-O6
3	C	403	NAG	O5-C5-C6-O6
3	C	403	NAG	C4-C5-C6-O6
3	A	401	NAG	C1-C2-N2-C7
3	E	404	NAG	C4-C5-C6-O6
3	E	404	NAG	O5-C5-C6-O6
3	A	401	NAG	C3-C2-N2-C7
3	A	402	NAG	C8-C7-N2-C2
3	A	402	NAG	O7-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	404	NAG	1	0
3	A	401	NAG	5	0

5.7 Other polymers [i](#)

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	321/321 (100%)	0.73	27 (8%) 17 14	15, 31, 63, 149	0
1	C	321/321 (100%)	0.96	46 (14%) 6 5	15, 31, 76, 166	0
1	E	321/321 (100%)	0.91	41 (12%) 7 6	18, 40, 58, 71	0
2	B	154/154 (100%)	3.38	99 (64%) 0 0	17, 103, 135, 143	0
2	D	154/154 (100%)	4.20	111 (72%) 0 0	18, 124, 148, 156	0
2	F	154/154 (100%)	1.71	55 (35%) 1 1	17, 55, 79, 90	0
All	All	1425/1425 (100%)	1.59	379 (26%) 1 1	15, 41, 134, 166	0

All (379) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	CYS	20.7
1	C	7	TYR	17.0
1	C	6	GLY	16.6
1	A	3	ILE	16.3
2	D	25	HIS	14.9
1	C	5	VAL	13.9
2	D	10	ILE	13.5
2	D	135	ASN	12.5
2	B	21	TRP	12.5
2	B	138	PHE	10.7
2	D	115	VAL	10.5
2	D	5	ALA	10.5
1	A	4	CYS	10.3
2	B	22	TYR	10.2
2	D	9	PHE	10.2
2	D	6	ILE	9.7
2	B	24	TYR	9.4
1	A	2	THR	9.3
2	D	137	CYS	9.2

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Mol	Chain	Res	Type	RSRZ
2	D	43	ILE	8.9
2	D	141	TYR	8.8
2	D	14	TRP	8.8
2	B	35	ALA	8.8
2	B	9	PHE	8.6
2	F	152	VAL	8.5
2	B	23	GLY	8.4
2	D	52	VAL	8.4
2	B	26	HIS	8.4
2	D	110	PHE	8.3
2	D	15	THR	8.2
2	D	122	VAL	8.1
2	D	119	TYR	8.1
2	B	113	LEU	7.9
2	D	117	ASN	7.9
2	B	119	TYR	7.9
2	D	157	TYR	7.8
2	B	33	GLY	7.8
2	D	7	ALA	7.8
2	D	126	LEU	7.8
1	C	3	ILE	7.8
2	D	153	LYS	7.6
2	B	6	ILE	7.6
2	B	126	LEU	7.5
2	D	24	TYR	7.5
2	D	136	GLY	7.4
2	B	141	TYR	7.4
2	D	116	LYS	7.4
2	B	5	ALA	7.4
2	B	118	LEU	7.4
2	D	134	GLY	7.3
2	B	115	VAL	7.3
1	C	9	ALA	7.3
2	D	108	LEU	7.3
2	D	152	VAL	7.2
2	D	48	ILE	7.2
2	B	122	VAL	7.0
1	C	316	THR	7.0
2	B	7	ALA	7.0
2	D	21	TRP	6.9
2	D	111	HIS	6.9
2	D	4	GLY	6.9

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Mol	Chain	Res	Type	RSRZ
2	B	40	SER	6.8
2	D	13	GLY	6.8
2	D	133	ILE	6.8
2	B	131	LYS	6.8
2	F	157	TYR	6.8
1	C	1	ASP	6.6
1	A	5	VAL	6.6
2	F	126	LEU	6.5
2	B	25	HIS	6.4
2	D	26	HIS	6.4
2	B	43	ILE	6.4
2	D	112	ASP	6.4
2	B	114	ASN	6.4
2	D	118	LEU	6.3
2	D	22	TYR	6.3
2	D	156	THR	6.3
2	D	47	GLY	6.2
2	D	40	SER	6.2
2	D	32	SER	6.1
2	D	109	ASP	6.1
2	D	33	GLY	6.1
2	D	113	LEU	6.1
2	D	8	GLY	6.1
2	B	20	GLY	6.0
2	B	133	ILE	5.9
2	D	144	CYS	5.9
2	D	138	PHE	5.8
2	D	129	ASN	5.8
1	C	2	THR	5.7
2	D	41	THR	5.7
2	D	148	CYS	5.7
2	B	140	PHE	5.7
2	F	153	LYS	5.7
2	B	135	ASN	5.7
2	B	34	TYR	5.7
2	B	157	TYR	5.6
1	C	21	GLU	5.5
2	B	144	CYS	5.5
2	B	10	ILE	5.5
2	D	140	PHE	5.5
2	D	51	LYS	5.5
2	D	34	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	132	GLU	5.4
2	D	107	THR	5.4
1	A	6	GLY	5.4
2	D	125	GLN	5.3
2	B	14	TRP	5.3
2	B	116	LYS	5.3
2	B	8	GLY	5.2
2	D	44	ALA	5.2
2	B	136	GLY	5.2
2	B	117	ASN	5.1
2	B	152	VAL	5.1
2	B	125	GLN	5.1
2	B	17	MET	5.1
2	B	32	SER	5.1
2	D	18	VAL	5.1
2	B	46	ASP	5.0
2	D	12	GLY	5.0
2	B	112	ASP	5.0
2	F	150	GLU	5.0
2	B	149	MET	5.0
2	D	142	HIS	4.9
1	E	298	VAL	4.9
2	D	31	GLY	4.9
2	D	35	ALA	4.8
1	E	321	ILE	4.8
2	B	27	ARG	4.8
2	B	139	GLU	4.8
2	B	41	THR	4.8
1	C	318	LEU	4.8
2	D	114	ASN	4.8
1	A	9	ALA	4.7
1	A	321	ILE	4.7
2	B	129	ASN	4.7
1	A	7	TYR	4.7
2	F	156	THR	4.7
2	B	130	ALA	4.6
2	B	16	GLY	4.6
2	D	147	GLU	4.6
1	C	11	ASN	4.6
1	C	321	ILE	4.5
2	D	45	ILE	4.5
2	D	36	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	8	HIS	4.5
2	B	4	GLY	4.5
2	B	148	CYS	4.5
2	F	139	GLU	4.5
2	B	137	CYS	4.4
1	A	261	SER	4.4
1	E	221	ARG	4.4
1	A	262	SER	4.4
2	D	155	GLY	4.3
2	B	154	ASN	4.3
2	D	143	LYS	4.3
1	C	12	SER	4.3
2	B	31	GLY	4.2
2	B	28	ASN	4.2
2	B	156	THR	4.2
2	B	124	SER	4.2
2	D	123	LYS	4.2
1	C	10	ASN	4.2
2	D	149	MET	4.2
1	A	1	ASP	4.1
2	D	151	SER	4.1
2	D	42	GLN	4.1
2	D	56	ILE	4.1
2	B	15	THR	4.1
2	D	27	ARG	4.0
2	B	110	PHE	4.0
1	C	13	THR	4.0
2	F	21	TRP	4.0
2	D	19	ASP	4.0
2	D	17	MET	3.9
2	B	147	GLU	3.9
2	D	124	SER	3.9
2	B	12	GLY	3.9
1	C	8	HIS	3.9
2	F	38	GLN	3.9
2	B	42	GLN	3.9
1	C	26	VAL	3.9
2	B	146	ASN	3.8
2	B	153	LYS	3.8
1	E	261	SER	3.8
2	D	16	GLY	3.8
2	D	29	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	66	VAL	3.7
2	D	154	ASN	3.7
2	B	151	SER	3.7
2	D	49	SER	3.7
2	D	127	ARG	3.7
2	D	39	LYS	3.7
2	D	54	SER	3.7
1	A	111	PHE	3.7
2	D	50	ASN	3.7
2	B	120	GLU	3.7
2	D	132	GLU	3.7
1	C	261	SER	3.6
1	A	318	LEU	3.6
1	C	319	ARG	3.6
2	D	131	LYS	3.6
2	B	155	GLY	3.6
2	F	127	ARG	3.6
2	D	61	ILE	3.6
2	B	142	HIS	3.6
1	C	315	ALA	3.6
1	C	23	ASN	3.6
1	C	45	ASN	3.6
2	D	139	GLU	3.5
1	E	318	LEU	3.5
2	B	13	GLY	3.5
2	B	145	ASP	3.5
2	B	143	LYS	3.5
2	D	11	GLU	3.5
1	E	272	VAL	3.5
1	E	144	PHE	3.5
2	F	24	TYR	3.5
2	D	46	ASP	3.4
2	F	35	ALA	3.4
2	B	60	ASN	3.4
2	D	130	ALA	3.4
2	D	106	ARG	3.4
2	D	120	GLU	3.4
2	F	140	PHE	3.4
1	C	44	LEU	3.4
1	C	263	SER	3.4
2	F	62	GLN	3.3
2	F	31	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	29	GLU	3.3
1	E	135	SER	3.3
2	B	39	LYS	3.3
2	D	128	ASN	3.3
2	B	44	ALA	3.3
1	A	44	LEU	3.3
2	D	28	ASN	3.2
1	E	262	SER	3.2
1	C	262	SER	3.2
1	A	168	ASN	3.2
1	E	92	PRO	3.2
2	F	108	LEU	3.2
2	B	111	HIS	3.2
2	F	148	CYS	3.2
2	D	20	GLY	3.2
2	D	37	ASP	3.1
2	D	23	GLY	3.1
2	D	55	VAL	3.1
2	D	105	GLU	3.1
2	B	123	LYS	3.1
2	F	63	PHE	3.1
2	D	60	ASN	3.1
2	B	128	ASN	3.1
2	D	150	GLU	3.0
1	E	191	LEU	3.0
2	D	53	ASN	3.0
2	F	138	PHE	3.0
1	C	25	THR	3.0
2	F	64	THR	3.0
2	F	27	ARG	3.0
1	C	22	LYS	3.0
2	B	19	ASP	3.0
1	E	271	GLN	3.0
2	F	13	GLY	3.0
2	F	151	SER	2.9
1	A	10	ASN	2.9
2	F	4	GLY	2.9
2	B	121	LYS	2.9
2	D	121	LYS	2.9
1	E	247	ASN	2.8
1	E	300	ILE	2.8
2	D	146	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	122	VAL	2.8
2	B	62	GLN	2.8
1	E	44	LEU	2.8
1	C	14	ASP	2.8
1	E	46	GLY	2.8
2	F	146	ASN	2.8
2	B	47	GLY	2.8
1	E	3	ILE	2.8
1	E	139	SER	2.8
1	C	299	THR	2.8
2	F	144	CYS	2.8
1	C	24	VAL	2.7
2	D	30	GLN	2.7
1	E	13	THR	2.7
1	E	90	CYS	2.7
2	F	23	GLY	2.7
1	C	298	VAL	2.7
1	E	286	LEU	2.7
1	C	222	GLU	2.7
2	B	63	PHE	2.6
2	B	127	ARG	2.6
2	F	32	SER	2.6
2	D	38	GLN	2.6
2	F	133	ILE	2.6
1	C	278	LYS	2.6
1	A	130	ARG	2.5
1	E	301	GLY	2.5
2	F	67	GLY	2.5
2	B	99	LEU	2.5
1	A	193	GLN	2.5
2	F	125	GLN	2.5
1	A	205	LYS	2.5
1	E	1	ASP	2.5
2	B	45	ILE	2.5
1	E	111	PHE	2.5
2	F	143	LYS	2.5
1	E	319	ARG	2.5
2	F	113	LEU	2.4
1	E	189	GLN	2.4
1	A	11	ASN	2.4
2	B	11	GLU	2.4
1	E	47	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	260	GLY	2.4
1	C	279	CYS	2.4
2	D	145	ASP	2.4
2	B	30	GLN	2.4
1	A	21	GLU	2.4
2	F	39	LYS	2.4
2	B	134	GLY	2.4
1	A	110	SER	2.4
1	E	260	GLY	2.4
1	C	28	HIS	2.4
2	F	119	TYR	2.4
1	E	141	ALA	2.4
2	D	64	THR	2.3
1	E	20	LEU	2.3
2	B	48	ILE	2.3
1	C	320	ASN	2.3
2	F	147	GLU	2.3
2	B	38	GLN	2.3
2	B	29	GLU	2.3
2	F	117	ASN	2.3
1	C	15	THR	2.3
2	F	99	LEU	2.3
2	D	63	PHE	2.3
1	A	73	ALA	2.3
1	A	107	THR	2.3
1	C	271	GLN	2.3
2	F	33	GLY	2.3
1	E	150	TRP	2.2
2	F	154	ASN	2.2
1	C	265	ILE	2.2
2	F	26	HIS	2.2
1	E	25	THR	2.2
2	F	115	VAL	2.2
2	B	18	VAL	2.2
1	E	9	ALA	2.2
1	E	289	ASN	2.2
1	E	69	LEU	2.2
2	F	101	LEU	2.2
2	B	108	LEU	2.2
1	E	45	ASN	2.1
1	E	89	ALA	2.1
1	E	180	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	149	MET	2.1
1	A	25	THR	2.1
1	C	300	ILE	2.1
2	F	14	TRP	2.1
1	C	311	GLN	2.1
2	B	36	ALA	2.1
1	C	107	THR	2.1
2	F	155	GLY	2.1
1	E	26	VAL	2.1
2	F	18	VAL	2.1
2	B	55	VAL	2.1
2	F	129	ASN	2.1
1	C	276	THR	2.1
2	B	150	GLU	2.1
2	F	45	ILE	2.1
2	D	100	ILE	2.1
1	C	20	LEU	2.0
2	F	60	ASN	2.0
1	C	46	GLY	2.0
1	E	302	LYS	2.0
2	F	15	THR	2.0
2	F	106	ARG	2.0
1	E	48	ILE	2.0
2	B	64	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
3	NAG	E	404	14/15	-0.06	0.32	87,104,110,111	0
3	NAG	C	403	14/15	0.09	0.23	30,30,30,30	0
3	NAG	E	402	14/15	0.17	0.26	72,89,93,97	0
3	NAG	A	403	14/15	0.35	0.21	76,93,100,100	0
3	NAG	E	403	14/15	0.35	0.21	78,93,100,101	0
3	NAG	C	404	14/15	0.44	0.18	30,30,30,30	0
3	NAG	C	402	14/15	0.48	0.20	74,85,94,102	0
3	NAG	A	401	14/15	0.50	0.19	85,96,98,100	0
3	NAG	C	401	14/15	0.54	0.20	75,82,86,88	0
3	NAG	E	401	14/15	0.54	0.16	76,83,88,90	0
3	NAG	A	402	14/15	0.57	0.22	62,89,98,100	0
3	NAG	A	404	14/15	0.80	0.14	39,43,54,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.