



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:33 PM GMT

PDB ID : 3ZTN
Title : STRUCTURE OF INFLUENZA A NEUTRALIZING ANTIBODY SELECTED FROM CULTURES OF SINGLE HUMAN PLASMA CELLS IN COMPLEX WITH HUMAN H1 INFLUENZA HAEMAGGLUTININ.
Authors : Hubbard, P.A.; Ritchie, A.J.; Corti, D.; Voss, J.E.; Gamblin, S.J.; Codoni, G.; Macagno, A.; Jarrossay, D.; Pinna, D.; Minola, A.; Vanzetta, F.; Silacci, C.; Fernandez-Rodriguez, B.M.; Agatic, G.; Giacchetto-Sasselli, I.; Vachieri, S.G.; Sallusto, F.; Collins, P.J.; Haire, L.F.; Temperton, N.; Langedijk, J.P.M.; Skehel, J.J.; Lanzavecchia, A.
Deposited on : 2011-07-12
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

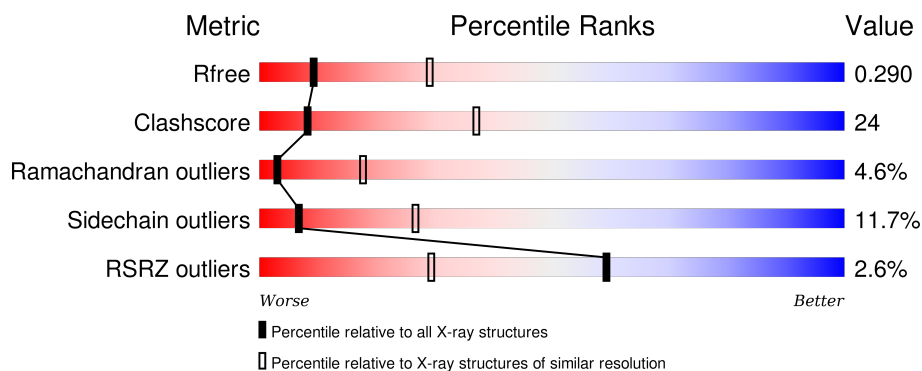
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	<div> <div>53%</div> <div>41%</div> <div>6%</div> </div>
2	B	176	<div> <div>66%</div> <div>28%</div> <div>• •</div> </div>
3	H	226	<div> <div>5%</div> <div>39%</div> <div>31%</div> <div>7%</div> <div>23%</div> </div>
4	L	218	<div> <div>4%</div> <div>33%</div> <div>31%</div> <div>5%</div> <div>31%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	640	X	-	-	-
7	BMA	A	622	X	-	-	-
8	SO4	A	1331	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 6361 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 HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2469	1567	416	475	11			

- Molecule 2 is a protein called HAEMAGGLUTININ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total	C	N	O	S	0	0	0
			1320	833	218	263	6			

- Molecule 3 is a protein called FI6V3 ANTIBODY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	173	Total	C	N	O	S	0	0	0
			1334	853	220	256	5			

- Molecule 4 is a protein called FI6V3 ANTIBODY LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	150	Total	C	N	O	S	0	0	0
			1084	685	177	219	3			

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).

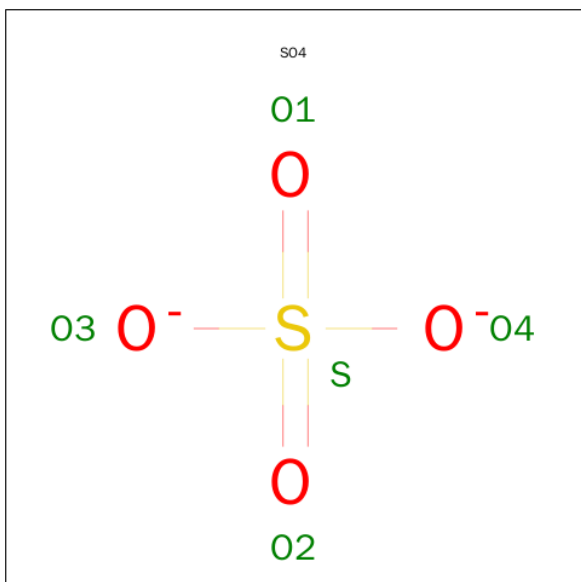


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

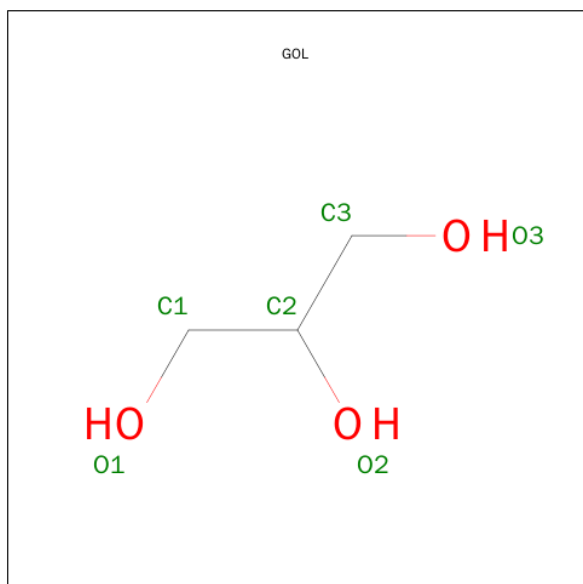
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

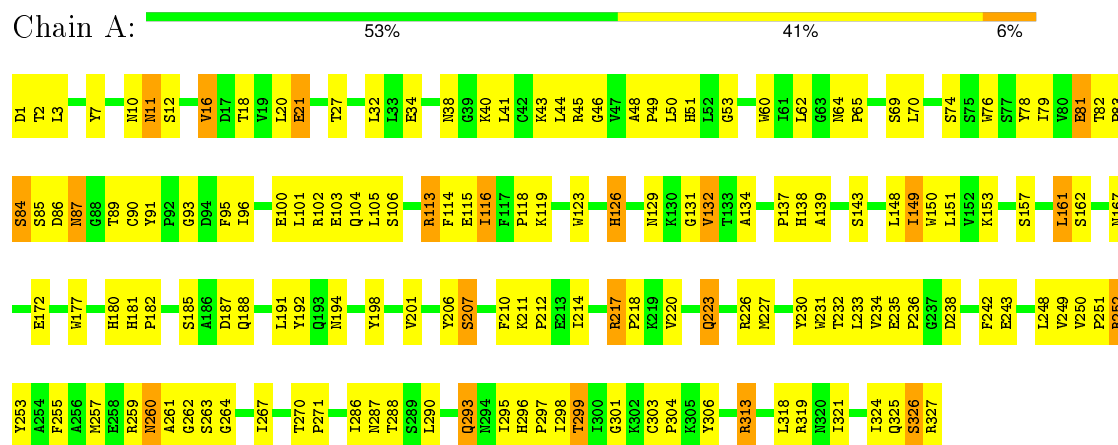


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		

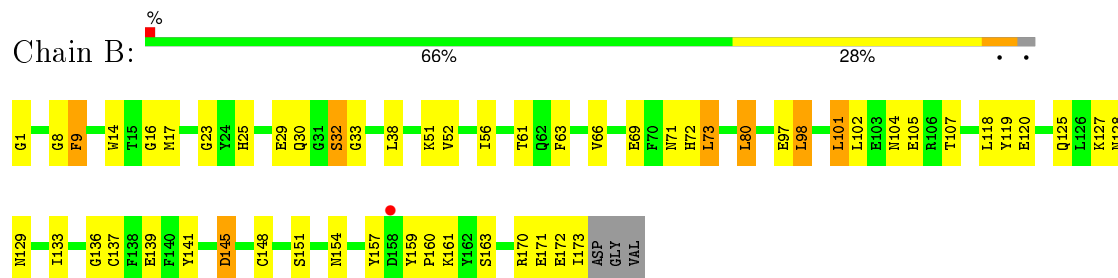
3 Residue-property plots

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

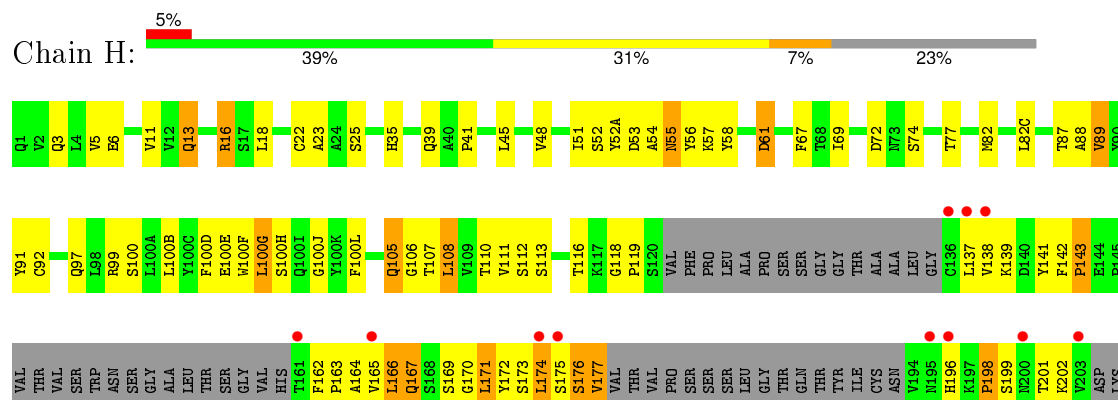
• Molecule 1: HAEMAGGLUTININ

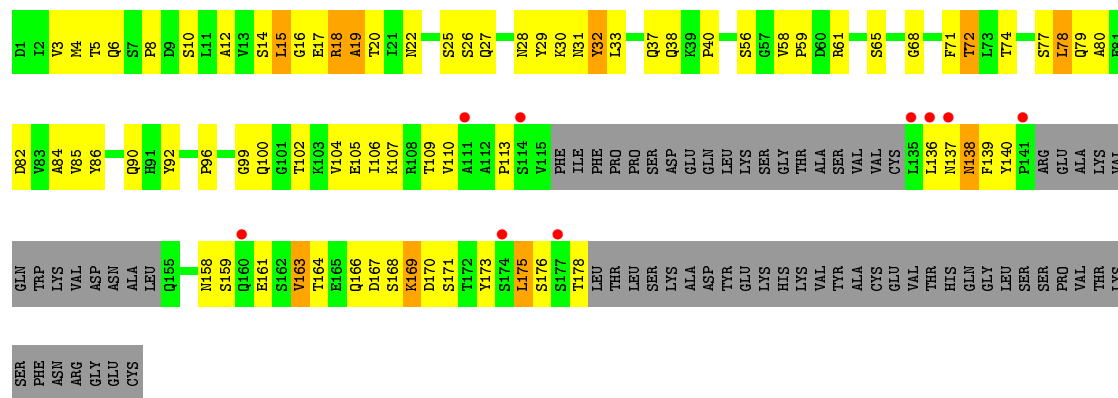


• Molecule 2: HAEMAGGLUTININ



• Molecule 3: FI6V3 ANTIBODY LIGHT CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	206.10 Å 206.10 Å 206.10 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.16 – 3.00 57.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (57.16-3.00) 99.7 (57.16-3.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.01 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7_650)	Depositor
R, R_{free}	0.214 , 0.289 0.210 , 0.290	Depositor DCC
R_{free} test set	1529 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 80.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 30436 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6361	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, SO4

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	0.45	0/2533	0.65	0/3465
2	B	0.45	0/1348	0.59	0/1830
3	H	0.43	0/1367	0.60	0/1860
4	L	0.39	0/1109	0.59	0/1518
All	All	0.44	0/6357	0.62	0/8673

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
7	A	3	0

There are no bond length outliers.

There are no bond angle outliers.

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	622	BMA	C2,C5,C3

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2469	0	2297	143	0
2	B	1320	0	1159	46	0
3	H	1334	0	1255	67	0
4	L	1084	0	950	55	0
5	A	56	0	50	5	0
6	A	28	0	26	1	0
7	A	39	0	34	6	0
8	A	20	0	0	0	0
8	L	5	0	0	0	0
9	A	6	0	8	0	0
All	All	6361	0	5779	296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ARG:HH11	1:A:313:ARG:HG2	1.08	1.18
4:L:12:ALA:HB1	4:L:107:LYS:HB2	1.31	1.07
1:A:116:ILE:O	1:A:118:PRO:HD3	1.63	0.98
4:L:163:VAL:HG12	4:L:164:THR:H	1.31	0.96
1:A:182:PRO:HD2	1:A:214:ILE:HD13	1.51	0.93
3:H:87:THR:HG23	3:H:110:THR:HA	1.53	0.90
1:A:16:VAL:HG23	1:A:313:ARG:HB3	1.57	0.87
1:A:287:ASN:ND2	7:A:620:NAG:C1	2.40	0.85
3:H:196:HIS:CD2	3:H:198:PRO:HD2	2.11	0.85
1:A:43:LYS:HD3	1:A:46:GLY:O	1.82	0.80
1:A:313:ARG:NH1	1:A:313:ARG:HG2	1.81	0.79
1:A:287:ASN:HD21	7:A:620:NAG:C1	1.97	0.78
1:A:87:ASN:OD1	5:A:600:NAG:C1	2.31	0.78
3:H:18:LEU:HB3	3:H:82:MET:HE3	1.67	0.75
1:A:87:ASN:CG	5:A:600:NAG:C1	2.55	0.75
1:A:119:LYS:HG3	1:A:149:ILE:HD11	1.68	0.74
2:B:133:ILE:HG12	2:B:137:CYS:O	1.87	0.74
3:H:170:GLY:C	3:H:171:LEU:HD23	2.07	0.73
1:A:87:ASN:ND2	5:A:600:NAG:C1	2.52	0.72
4:L:159:SER:HA	4:L:178:THR:O	1.89	0.72
1:A:235:GLU:HB2	1:A:236:PRO:HD2	1.70	0.72
4:L:175:LEU:HG	4:L:176:SER:H	1.54	0.71
1:A:126:HIS:HB2	1:A:151:LEU:HD22	1.71	0.71
3:H:82:MET:HB3	3:H:82(C):LEU:HD21	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ILE:HG22	1:A:324:ILE:O	1.90	0.71
1:A:260:ASN:O	1:A:262:GLY:N	2.26	0.69
2:B:128:ASN:HB2	2:B:159:TYR:OH	1.93	0.69
2:B:133:ILE:HD13	2:B:139:GLU:HG3	1.73	0.69
1:A:287:ASN:CG	7:A:620:NAG:C1	2.61	0.68
4:L:163:VAL:HG12	4:L:164:THR:N	2.07	0.68
3:H:72:ASP:OD1	3:H:74:SER:HB3	1.92	0.68
1:A:327:ARG:C	2:B:1:GLY:N	2.48	0.68
1:A:287:ASN:OD1	7:A:620:NAG:C1	2.42	0.68
4:L:37:GLN:HG3	4:L:86:TYR:CE1	2.29	0.67
1:A:327:ARG:O	2:B:1:GLY:HA3	1.94	0.67
3:H:89:VAL:HA	3:H:108:LEU:HA	1.76	0.67
1:A:299:THR:HG23	1:A:303:CYS:SG	2.35	0.67
1:A:82:THR:HG22	1:A:84:SER:H	1.59	0.67
2:B:9:PHE:H	2:B:9:PHE:HD1	1.40	0.67
1:A:50:LEU:HD12	1:A:76:TRP:CE3	2.29	0.67
3:H:201:THR:HG22	3:H:202:LYS:H	1.59	0.67
1:A:50:LEU:HD12	1:A:76:TRP:CD2	2.30	0.67
4:L:18:ARG:HG2	4:L:19:ALA:H	1.59	0.66
4:L:113:PRO:HD3	4:L:139:PHE:HB3	1.77	0.66
4:L:175:LEU:HG	4:L:176:SER:N	2.12	0.65
1:A:115:GLU:HB2	1:A:253:TYR:CE1	2.33	0.64
3:H:171:LEU:N	3:H:171:LEU:HD23	2.12	0.63
1:A:10:ASN:OD1	1:A:12:SER:HB3	1.98	0.63
1:A:49:PRO:HB3	1:A:78:TYR:CZ	2.33	0.63
1:A:131:GLY:HA3	1:A:150:TRP:HB3	1.79	0.63
2:B:30:GLN:OE1	2:B:145:ASP:HB2	1.99	0.63
3:H:137:LEU:HD12	3:H:138:VAL:H	1.63	0.63
1:A:327:ARG:O	2:B:1:GLY:CA	2.48	0.62
1:A:234:VAL:HG12	1:A:238:ASP:HB3	1.80	0.62
1:A:182:PRO:HD2	1:A:214:ILE:CD1	2.28	0.62
3:H:5:VAL:O	3:H:22:CYS:HA	2.00	0.62
4:L:163:VAL:HA	4:L:175:LEU:HA	1.80	0.62
4:L:163:VAL:HG22	4:L:175:LEU:HD12	1.82	0.61
1:A:64:ASN:HD21	1:A:90:CYS:HB3	1.64	0.61
1:A:177:TRP:CE2	1:A:201:VAL:HG21	2.35	0.61
1:A:287:ASN:HD21	7:A:620:NAG:C2	2.13	0.61
1:A:206:TYR:O	1:A:207:SER:HB2	2.00	0.61
3:H:23:ALA:HA	3:H:77:THR:HG22	1.81	0.61
1:A:248:LEU:HD12	1:A:249:VAL:N	2.16	0.61
3:H:35:HIS:CD2	3:H:100(L):PHE:HE1	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:107:LYS:HA	4:L:140:TYR:OH	2.00	0.61
1:A:149:ILE:HG23	1:A:149:ILE:O	2.01	0.61
1:A:248:LEU:HD12	1:A:249:VAL:H	1.65	0.61
4:L:79:GLN:HG2	4:L:80:ALA:H	1.65	0.61
1:A:234:VAL:CG1	1:A:238:ASP:HB3	2.29	0.61
1:A:250:VAL:CG1	1:A:251:PRO:HD2	2.31	0.61
1:A:161:LEU:HD12	1:A:161:LEU:C	2.21	0.61
1:A:211:LYS:HG3	1:A:212:PRO:HD2	1.82	0.60
3:H:112:SER:HB3	3:H:142:PHE:HZ	1.66	0.60
2:B:80:LEU:HD12	2:B:80:LEU:O	2.02	0.59
3:H:105:GLN:O	3:H:105:GLN:HG3	2.01	0.59
2:B:71:ASN:O	2:B:73:LEU:N	2.35	0.59
1:A:18:THR:HG23	2:B:105:GLU:HA	1.86	0.58
1:A:250:VAL:HG13	1:A:251:PRO:HD2	1.85	0.57
2:B:9:PHE:CD1	2:B:9:PHE:N	2.71	0.57
1:A:20:LEU:C	1:A:21:GLU:HG3	2.25	0.57
4:L:6:GLN:H	4:L:100:GLN:HE22	1.51	0.57
1:A:3:LEU:HD12	2:B:25:HIS:O	2.05	0.56
1:A:132:VAL:HG22	1:A:143:SER:HA	1.86	0.56
2:B:17:MET:SD	2:B:23:GLY:HA3	2.46	0.56
3:H:13:GLN:HB2	3:H:16:ARG:NH1	2.20	0.56
1:A:41:LEU:HG	1:A:270:THR:HG22	1.88	0.56
1:A:123:TRP:CZ2	1:A:250:VAL:HG11	2.41	0.55
1:A:288:THR:HG22	1:A:304:PRO:HD3	1.87	0.55
1:A:286:ILE:CD1	1:A:293:GLN:HG3	2.35	0.55
4:L:85:VAL:HA	4:L:102:THR:O	2.06	0.55
4:L:79:GLN:HG2	4:L:80:ALA:N	2.21	0.55
1:A:177:TRP:CZ2	1:A:201:VAL:HG21	2.42	0.55
3:H:35:HIS:CD2	3:H:100(L):PHE:CE1	2.95	0.55
3:H:97:GLN:HG2	3:H:100(J):GLY:HA3	1.89	0.54
1:A:11:ASN:HD22	1:A:11:ASN:N	2.06	0.54
4:L:71:PHE:O	4:L:72:THR:HG23	2.08	0.54
1:A:60:TRP:CD1	1:A:70:LEU:HD23	2.43	0.54
3:H:100(H):SER:HB3	4:L:92:TYR:O	2.07	0.54
2:B:9:PHE:N	2:B:9:PHE:HD1	2.05	0.54
1:A:313:ARG:CG	1:A:313:ARG:NH1	2.60	0.54
2:B:71:ASN:C	2:B:73:LEU:H	2.11	0.54
3:H:139:LYS:HG3	3:H:173:SER:HB3	1.90	0.54
3:H:167:GLN:HG2	3:H:171:LEU:O	2.07	0.53
4:L:175:LEU:CG	4:L:176:SER:N	2.72	0.53
1:A:96:ILE:HG13	1:A:230:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:137:LEU:HD12	3:H:138:VAL:N	2.23	0.53
1:A:167:ASN:ND2	1:A:236:PRO:HA	2.24	0.53
1:A:260:ASN:ND2	1:A:260:ASN:H	2.06	0.53
3:H:53:ASP:O	3:H:54:ALA:HB3	2.09	0.53
3:H:112:SER:HB3	3:H:142:PHE:CZ	2.44	0.53
4:L:80:ALA:C	4:L:82:ASP:H	2.11	0.53
1:A:296:HIS:CE1	1:A:298:ILE:HB	2.44	0.53
1:A:48:ALA:HB1	1:A:49:PRO:HD2	1.91	0.53
1:A:161:LEU:O	1:A:243:GLU:HA	2.08	0.52
1:A:286:ILE:HG21	1:A:295:ILE:HG13	1.91	0.52
1:A:242:PHE:HD2	1:A:248:LEU:HD21	1.75	0.52
3:H:118:GLY:HA2	3:H:199:SER:OG	2.09	0.52
3:H:3:GLN:HB3	3:H:25:SER:HB3	1.92	0.52
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.92	0.51
2:B:159:TYR:N	2:B:160:PRO:HD2	2.25	0.51
4:L:3:VAL:H	4:L:26:SER:CB	2.24	0.51
1:A:327:ARG:HB3	2:B:1:GLY:H3	1.76	0.51
1:A:11:ASN:OD1	6:A:610:NAG:O5	2.28	0.51
1:A:82:THR:HG22	1:A:83:PRO:HD2	1.92	0.51
3:H:57:LYS:HD3	3:H:69:ILE:O	2.11	0.51
4:L:4:MET:O	4:L:99:GLY:HA2	2.11	0.51
4:L:32:TYR:HB2	4:L:92:TYR:HB2	1.93	0.51
1:A:84:SER:O	1:A:86:ASP:N	2.44	0.51
1:A:299:THR:HG21	1:A:303:CYS:HB2	1.92	0.51
1:A:60:TRP:HD1	1:A:70:LEU:HD23	1.74	0.50
3:H:100(D):PHE:HB2	3:H:100(G):LEU:HG	1.93	0.50
1:A:93:GLY:HA3	1:A:227:MET:O	2.10	0.50
1:A:87:ASN:HD21	5:A:600:NAG:C1	2.23	0.50
2:B:159:TYR:O	2:B:163:SER:HB3	2.11	0.50
4:L:104:VAL:HG12	4:L:104:VAL:O	2.09	0.50
1:A:172:GLU:OE2	1:A:233:LEU:HD13	2.11	0.50
3:H:119:PRO:HA	3:H:141:TYR:HB3	1.93	0.50
1:A:250:VAL:HG12	1:A:251:PRO:N	2.26	0.50
1:A:270:THR:HG23	1:A:271:PRO:HD2	1.92	0.50
3:H:58:TYR:HE2	3:H:100(B):LEU:HB3	1.77	0.50
1:A:16:VAL:HG22	2:B:104:ASN:HD21	1.76	0.50
1:A:123:TRP:HZ2	1:A:250:VAL:HG11	1.76	0.50
4:L:38:GLN:O	4:L:84:ALA:HB1	2.11	0.50
1:A:11:ASN:HD22	1:A:11:ASN:H	1.58	0.50
1:A:177:TRP:HZ3	1:A:232:THR:HG22	1.77	0.49
1:A:286:ILE:HD12	1:A:293:GLN:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:31:ASN:O	4:L:33:LEU:N	2.46	0.49
1:A:113:ARG:HB2	1:A:255:PHE:CD2	2.48	0.49
1:A:100:GLU:O	1:A:104:GLN:HB2	2.13	0.49
4:L:12:ALA:CB	4:L:107:LYS:HB2	2.22	0.49
2:B:125:GLN:OE1	2:B:157:TYR:HB3	2.13	0.49
2:B:172:GLU:O	2:B:173:ILE:O	2.31	0.49
1:A:16:VAL:HG22	2:B:104:ASN:ND2	2.27	0.49
4:L:3:VAL:H	4:L:26:SER:HB3	1.78	0.48
1:A:62:LEU:HD12	1:A:89:THR:HG22	1.95	0.48
4:L:14:SER:O	4:L:16:GLY:N	2.46	0.48
1:A:299:THR:CG2	1:A:303:CYS:SG	3.01	0.48
4:L:32:TYR:H	4:L:32:TYR:HD1	1.61	0.48
1:A:217:ARG:HD2	1:A:226:ARG:CG	2.43	0.48
1:A:325:GLN:HG3	1:A:326:SER:N	2.28	0.48
1:A:49:PRO:HB3	1:A:78:TYR:CE2	2.48	0.48
1:A:327:ARG:C	2:B:1:GLY:H1	2.15	0.48
1:A:38:ASN:O	1:A:40:LYS:HG2	2.13	0.47
4:L:12:ALA:HA	4:L:105:GLU:O	2.15	0.47
3:H:52(A):TYR:CD2	3:H:99:ARG:HA	2.49	0.47
1:A:138:HIS:O	1:A:139:ALA:HB3	2.14	0.47
2:B:98:LEU:O	2:B:102:LEU:HG	2.15	0.47
2:B:63:PHE:CD1	2:B:63:PHE:C	2.87	0.47
1:A:50:LEU:HD23	1:A:50:LEU:C	2.35	0.47
1:A:91:TYR:CE2	1:A:223:GLN:HG2	2.49	0.47
1:A:119:LYS:O	1:A:119:LYS:HG2	2.15	0.47
1:A:248:LEU:HG	1:A:250:VAL:HG22	1.95	0.47
4:L:14:SER:O	4:L:17:GLU:HG3	2.15	0.47
3:H:116:THR:O	3:H:116:THR:HG22	2.13	0.47
3:H:162:PHE:HB3	3:H:163:PRO:HD2	1.96	0.47
1:A:134:ALA:O	1:A:137:PRO:HD3	2.15	0.47
1:A:148:LEU:HB3	1:A:249:VAL:HG12	1.97	0.46
1:A:210:PHE:HE2	1:A:230:TYR:CZ	2.32	0.46
1:A:252:ARG:HD2	1:A:253:TYR:CE2	2.50	0.46
4:L:8:PRO:HG2	4:L:10:SER:O	2.15	0.46
1:A:79:ILE:HD12	1:A:106:SER:HA	1.96	0.46
3:H:201:THR:HG22	3:H:202:LYS:N	2.28	0.46
1:A:82:THR:CG2	1:A:83:PRO:HD2	2.45	0.46
1:A:11:ASN:H	1:A:11:ASN:ND2	2.14	0.46
4:L:90:GLN:NE2	4:L:96:PRO:HA	2.31	0.46
1:A:113:ARG:O	1:A:113:ARG:HG3	2.16	0.46
1:A:198:TYR:C	1:A:198:TYR:CD1	2.89	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:HD13	1:A:231:TRP:CD2	2.51	0.46
1:A:182:PRO:HG2	1:A:188:GLN:OE1	2.16	0.46
4:L:22:ASN:HA	4:L:72:THR:CG2	2.46	0.46
3:H:53:ASP:OD1	3:H:55:ASN:OD1	2.34	0.46
4:L:15:LEU:HD23	4:L:78:LEU:O	2.16	0.46
5:A:600:NAG:O4	5:A:601:NAG:H62	2.16	0.46
1:A:297:PRO:HG3	1:A:306:TYR:CE2	2.50	0.46
2:B:14:TRP:C	2:B:16:GLY:H	2.18	0.45
2:B:14:TRP:C	2:B:16:GLY:N	2.69	0.45
3:H:97:GLN:HG2	3:H:100(J):GLY:CA	2.46	0.45
1:A:65:PRO:HB3	1:A:138:HIS:HB2	1.99	0.45
1:A:102:ARG:C	1:A:104:GLN:H	2.20	0.45
1:A:114:PHE:CE2	1:A:116:ILE:HG23	2.52	0.45
4:L:4:MET:SD	4:L:25:SER:HB2	2.56	0.45
4:L:28:ASN:C	4:L:30:LYS:H	2.20	0.45
3:H:167:GLN:HG3	3:H:169:SER:OG	2.17	0.45
4:L:22:ASN:HA	4:L:72:THR:HG22	1.99	0.45
4:L:166:GLN:CG	4:L:173:TYR:CE1	3.00	0.45
1:A:7:TYR:HB2	1:A:318:LEU:CD2	2.46	0.45
4:L:32:TYR:N	4:L:32:TYR:CD1	2.85	0.45
3:H:51:ILE:HG13	3:H:57:LYS:HG2	1.97	0.45
1:A:217:ARG:HD2	1:A:226:ARG:HG3	1.98	0.45
3:H:162:PHE:CE2	4:L:176:SER:HB2	2.52	0.44
3:H:176:SER:O	3:H:177:VAL:HG13	2.17	0.44
1:A:181:HIS:HA	1:A:182:PRO:HD3	1.79	0.44
1:A:82:THR:HG22	1:A:83:PRO:N	2.32	0.44
1:A:250:VAL:HG12	1:A:251:PRO:CD	2.47	0.44
4:L:167:ASP:C	4:L:169:LYS:H	2.20	0.44
3:H:162:PHE:CD1	3:H:162:PHE:N	2.84	0.44
3:H:88:ALA:O	3:H:108:LEU:HD12	2.16	0.44
1:A:82:THR:HG22	1:A:83:PRO:CD	2.47	0.44
3:H:105:GLN:HE21	3:H:105:GLN:HB2	1.63	0.44
3:H:141:TYR:O	3:H:142:PHE:HB2	2.18	0.44
4:L:166:GLN:HG3	4:L:173:TYR:CE1	2.53	0.44
3:H:82:MET:CB	3:H:82(C):LEU:HD21	2.43	0.44
2:B:52:VAL:O	2:B:56:ILE:HG13	2.18	0.44
2:B:133:ILE:CD1	2:B:139:GLU:HG3	2.44	0.44
2:B:118:LEU:HA	2:B:118:LEU:HD23	1.75	0.44
2:B:32:SER:OG	2:B:33:GLY:N	2.51	0.44
4:L:136:LEU:HD13	4:L:175:LEU:CD2	2.47	0.44
3:H:91:TYR:CE1	3:H:106:GLY:HA3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:HIS:HD2	1:A:53:GLY:H	1.65	0.44
2:B:119:TYR:CE1	2:B:136:GLY:HA2	2.53	0.43
2:B:38:LEU:HD22	3:H:100(F):TRP:CZ2	2.52	0.43
3:H:165:VAL:HG23	3:H:165:VAL:O	2.18	0.43
4:L:163:VAL:O	4:L:164:THR:HG23	2.19	0.43
1:A:287:ASN:HD21	7:A:620:NAG:C7	2.32	0.43
1:A:32:LEU:HA	1:A:290:LEU:HD22	2.01	0.43
3:H:100(F):TRP:O	3:H:100(G):LEU:O	2.35	0.43
1:A:263:SER:OG	1:A:264:GLY:N	2.47	0.43
4:L:80:ALA:C	4:L:82:ASP:N	2.72	0.43
1:A:149:ILE:CG2	1:A:149:ILE:O	2.67	0.43
4:L:170:ASP:O	4:L:171:SER:HB2	2.18	0.43
3:H:11:VAL:HA	3:H:110:THR:O	2.19	0.43
1:A:131:GLY:CA	1:A:150:TRP:HB3	2.46	0.43
3:H:53:ASP:CG	3:H:55:ASN:OD1	2.57	0.43
2:B:38:LEU:HB3	3:H:100(F):TRP:CH2	2.54	0.43
1:A:115:GLU:OE2	1:A:118:PRO:HA	2.19	0.43
1:A:206:TYR:O	1:A:207:SER:CB	2.65	0.43
4:L:33:LEU:HD13	4:L:71:PHE:CD1	2.54	0.42
1:A:319:ARG:O	1:A:321:ILE:HG13	2.19	0.42
3:H:82(C):LEU:HB3	3:H:111:VAL:HG21	2.01	0.42
1:A:296:HIS:HA	1:A:297:PRO:HD3	1.64	0.42
3:H:142:PHE:HA	3:H:143:PRO:HA	1.75	0.42
4:L:170:ASP:OD1	4:L:171:SER:N	2.52	0.42
1:A:206:TYR:CD2	1:A:207:SER:N	2.88	0.42
2:B:98:LEU:HA	2:B:98:LEU:HD12	1.84	0.42
4:L:28:ASN:O	4:L:30:LYS:N	2.51	0.42
1:A:191:LEU:HB3	1:A:192:TYR:CE1	2.54	0.42
2:B:129:ASN:HD21	2:B:163:SER:HA	1.84	0.42
3:H:52(A):TYR:CD1	3:H:53:ASP:N	2.88	0.42
3:H:175:SER:O	3:H:176:SER:HB2	2.19	0.42
1:A:49:PRO:HB3	1:A:78:TYR:CE1	2.55	0.42
1:A:220:VAL:O	1:A:223:GLN:HB2	2.19	0.42
3:H:119:PRO:HD3	3:H:201:THR:OG1	2.19	0.42
1:A:327:ARG:C	2:B:1:GLY:H3	2.23	0.42
1:A:299:THR:HG21	1:A:303:CYS:CB	2.50	0.42
3:H:18:LEU:HA	3:H:18:LEU:HD12	1.91	0.41
4:L:77:SER:O	4:L:79:GLN:N	2.53	0.41
2:B:141:TYR:CE2	2:B:170:ARG:HG2	2.55	0.41
1:A:10:ASN:ND2	1:A:27:THR:HB	2.35	0.41
2:B:105:GLU:OE1	2:B:105:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:164:ALA:HA	3:H:174:LEU:HB3	2.02	0.41
3:H:67:PHE:CZ	3:H:82:MET:HG2	2.54	0.41
1:A:60:TRP:HZ3	1:A:105:LEU:HD13	1.84	0.41
1:A:319:ARG:HD2	1:A:321:ILE:HD11	2.03	0.41
3:H:52:SER:HB3	3:H:56:TYR:HB2	2.02	0.41
1:A:38:ASN:OD1	1:A:38:ASN:C	2.58	0.41
3:H:11:VAL:HG21	3:H:142:PHE:HE2	1.86	0.41
1:A:298:ILE:HA	1:A:298:ILE:HD13	1.71	0.41
2:B:101:LEU:HA	2:B:101:LEU:HD12	1.57	0.41
1:A:153:LYS:HB2	1:A:157:SER:O	2.20	0.41
1:A:114:PHE:CD1	1:A:114:PHE:N	2.89	0.41
3:H:67:PHE:CE1	3:H:82:MET:HG2	2.56	0.41
1:A:301:GLY:O	2:B:63:PHE:HA	2.21	0.41
4:L:161:GLU:H	4:L:161:GLU:CD	2.24	0.41
4:L:58:VAL:HA	4:L:59:PRO:HD3	1.86	0.41
1:A:250:VAL:CG1	1:A:251:PRO:CD	2.97	0.41
3:H:6:GLU:OE2	3:H:91:TYR:HA	2.21	0.41
2:B:61:THR:O	2:B:61:THR:HG23	2.21	0.41
1:A:150:TRP:HZ2	1:A:180:HIS:CE1	2.40	0.40
2:B:14:TRP:HE3	2:B:17:MET:HE2	1.85	0.40
4:L:137:ASN:O	4:L:138:ASN:HB2	2.21	0.40
3:H:141:TYR:CE1	3:H:172:TYR:O	2.75	0.40
1:A:7:TYR:HA	2:B:17:MET:HE1	2.03	0.40
2:B:71:ASN:C	2:B:73:LEU:N	2.73	0.40
3:H:165:VAL:O	3:H:166:LEU:C	2.60	0.40
1:A:81:GLU:O	1:A:267:ILE:HA	2.21	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	325/327 (99%)	271 (83%)	45 (14%)	9 (3%)	6	30
2	B	171/176 (97%)	143 (84%)	20 (12%)	8 (5%)	3	17
3	H	165/226 (73%)	138 (84%)	20 (12%)	7 (4%)	3	20
4	L	144/218 (66%)	103 (72%)	28 (19%)	13 (9%)	1	4
All	All	805/947 (85%)	655 (81%)	113 (14%)	37 (5%)	3	18

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	LEU
1	A	85	SER
1	A	207	SER
1	A	261	ALA
2	B	72	HIS
2	B	127	LYS
3	H	100(G)	LEU
4	L	15	LEU
4	L	19	ALA
4	L	32	TYR
4	L	78	LEU
4	L	163	VAL
1	A	45	ARG
2	B	8	GLY
2	B	145	ASP
2	B	161	LYS
4	L	56	SER
4	L	138	ASN
1	A	69	SER
2	B	148	CYS
3	H	166	LEU
3	H	198	PRO
4	L	40	PRO
4	L	168	SER
2	B	29	GLU
3	H	61	ASP
4	L	18	ARG
4	L	68	GLY
3	H	176	SER
4	L	169	LYS
1	A	218	PRO
1	A	326	SER
4	L	29	TYR

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Mol	Chain	Res	Type
2	B	66	VAL
1	A	149	ILE
3	H	41	PRO
3	H	143	PRO

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	258/288 (90%)	227 (88%)	31 (12%)	6	26
2	B	126/151 (83%)	112 (89%)	14 (11%)	8	29
3	H	141/191 (74%)	124 (88%)	17 (12%)	6	25
4	L	105/193 (54%)	93 (89%)	12 (11%)	7	28
All	All	630/823 (76%)	556 (88%)	74 (12%)	7	27

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	2	THR
1	A	11	ASN
1	A	16	VAL
1	A	21	GLU
1	A	34	GLU
1	A	74	SER
1	A	81	GLU
1	A	84	SER
1	A	87	ASN
1	A	95	PHE
1	A	103	GLU
1	A	113	ARG
1	A	116	ILE
1	A	126	HIS
1	A	129	ASN
1	A	132	VAL

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Mol	Chain	Res	Type
1	A	161	LEU
1	A	162	SER
1	A	185	SER
1	A	187	ASP
1	A	194	ASN
1	A	217	ARG
1	A	223	GLN
1	A	252	ARG
1	A	257	MET
1	A	259	ARG
1	A	260	ASN
1	A	293	GLN
1	A	299	THR
1	A	313	ARG
2	B	9	PHE
2	B	32	SER
2	B	51	LYS
2	B	69	GLU
2	B	73	LEU
2	B	80	LEU
2	B	97	GLU
2	B	98	LEU
2	B	101	LEU
2	B	107	THR
2	B	120	GLU
2	B	151	SER
2	B	154	ASN
2	B	171	GLU
3	H	13	GLN
3	H	16	ARG
3	H	48	VAL
3	H	55	ASN
3	H	61	ASP
3	H	89	VAL
3	H	92	CYS
3	H	100	SER
3	H	100(E)	GLU
3	H	105	GLN
3	H	107	THR
3	H	108	LEU
3	H	113	SER
3	H	167	GLN

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Mol	Chain	Res	Type
3	H	171	LEU
3	H	174	LEU
3	H	177	VAL
4	L	5	THR
4	L	20	THR
4	L	27	GLN
4	L	61	ARG
4	L	65	SER
4	L	72	THR
4	L	74	THR
4	L	106	ILE
4	L	109	THR
4	L	110	VAL
4	L	158	ASN
4	L	175	LEU

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

Mol	Chain	Res	Type
1	A	11	ASN
1	A	64	ASN
1	A	87	ASN
1	A	138	HIS
1	A	147	ASN
1	A	156	ASN
1	A	167	ASN
1	A	223	GLN
1	A	260	ASN
1	A	287	ASN
1	A	325	GLN
2	B	60	ASN
2	B	114	ASN
2	B	129	ASN
3	H	76	ASN
3	H	81	GLN
3	H	105	GLN
4	L	100	GLN
4	L	158	ASN
4	L	160	GLN

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 ⓘ

7 carbohydrates 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	$\# Z > 2$
5	NAG	A	600	5	14,14,15	0.54	0	15,19,21	1.02	1 (6%)
5	NAG	A	601	5	14,14,15	0.51	0	15,19,21	0.80	0
7	NAG	A	620	7	14,14,15	0.49	0	15,19,21	1.94	3 (20%)
7	NAG	A	621	7	14,14,15	0.61	0	15,19,21	0.95	0
7	BMA	A	622	7	11,11,12	0.45	0	14,15,17	1.30	1 (7%)
5	NAG	A	630	1,5	14,14,15	0.42	0	15,19,21	1.53	2 (13%)
5	NAG	A	631	5	14,14,15	0.43	0	15,19,21	1.29	2 (13%)

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
5	NAG	A	600	5	-	0/6/23/26	0/1/1/1
5	NAG	A	601	5	-	0/6/23/26	0/1/1/1
7	NAG	A	620	7	-	0/6/23/26	0/1/1/1
7	NAG	A	621	7	-	0/6/23/26	0/1/1/1
7	BMA	A	622	7	3/3/4/5	0/2/19/22	0/1/1/1
5	NAG	A	630	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	631	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	620	NAG	C2-N2-C7	-2.88	119.33	123.04
5	A	600	NAG	C2-N2-C7	-2.33	120.05	123.04
5	A	631	NAG	C4-C3-C2	-2.19	107.83	111.23
5	A	630	NAG	C3-C4-C5	2.12	113.90	110.20
7	A	620	NAG	C3-C4-C5	2.12	113.90	110.20
5	A	631	NAG	C1-O5-C5	2.97	116.02	112.25
7	A	622	BMA	C1-O5-C5	3.98	117.31	112.25
5	A	630	NAG	C1-O5-C5	4.64	118.13	112.25
7	A	620	NAG	C1-O5-C5	5.86	119.69	112.25

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	622	BMA	C2
7	A	622	BMA	C5
7	A	622	BMA	C3

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	NAG	5	0
5	A	601	NAG	1	0
7	A	620	NAG	6	0

5.6 Ligand geometry

8 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
8	SO4	A	1328	-	4,4,4	0.20	0	6,6,6	0.13	0
8	SO4	A	1329	-	4,4,4	0.17	0	6,6,6	0.14	0
8	SO4	A	1330	-	4,4,4	0.20	0	6,6,6	0.12	0
8	SO4	A	1331	-	4,4,4	0.20	0	6,6,6	0.11	0
9	GOL	A	1332	-	5,5,5	0.36	0	5,5,5	0.86	0
6	NAG	A	610	-	14,14,15	0.70	1 (7%)	15,19,21	1.60	1 (6%)
6	NAG	A	640	1	14,14,15	0.49	0	15,19,21	0.79	1 (6%)
8	SO4	L	1179	-	4,4,4	0.21	0	6,6,6	0.09	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
8	SO4	A	1328	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1329	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1330	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1331	-	-	0/0/0/0	0/0/0/0
9	GOL	A	1332	-	-	0/4/4/4	0/0/0/0
6	NAG	A	610	-	-	0/6/23/26	0/1/1/1
6	NAG	A	640	1	1/1/5/7	0/6/23/26	0/1/1/1
8	SO4	L	1179	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	610	NAG	C1-C2	2.21	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	640	NAG	C1-O5-C5	2.13	114.95	112.25
6	A	610	NAG	C1-O5-C5	4.81	118.35	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	640	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	610	NAG	1	0

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	A	327/327 (100%)	-0.39	0 100 100	43, 69, 107, 130	0
2	B	173/176 (98%)	-0.37	1 (0%) 90 73	40, 74, 125, 146	0
3	H	173/226 (76%)	-0.07	11 (6%) 23 8	43, 71, 152, 191	0
4	L	150/218 (68%)	0.05	9 (6%) 25 9	58, 99, 150, 168	0
All	All	823/947 (86%)	-0.24	21 (2%) 59 29	40, 74, 137, 191	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	138	VAL	7.3
4	L	174	SER	4.8
4	L	137	ASN	4.5
4	L	111	ALA	4.2
4	L	135	LEU	3.8
3	H	175	SER	3.7
3	H	161	THR	3.4
3	H	137	LEU	3.2
4	L	177	SER	3.0
3	H	174	LEU	2.7
3	H	196	HIS	2.6
3	H	200	ASN	2.6
3	H	203	VAL	2.6
4	L	136	LEU	2.5
4	L	141	PRO	2.5
2	B	158	ASP	2.4
4	L	114	SER	2.3
4	L	160	GLN	2.3
3	H	165	VAL	2.2
3	H	195	ASN	2.2
3	H	136	CYS	2.1

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	A	620	14/15	0.94	0.21	0.88	46,63,81,85	0
7	NAG	A	621	14/15	0.95	0.22	0.87	64,73,81,83	0
5	NAG	A	600	14/15	0.90	0.21	0.35	72,94,106,109	0
5	NAG	A	601	14/15	0.93	0.27	-	118,126,131,134	0
5	NAG	A	630	14/15	0.89	0.16	-	82,101,119,135	0
7	BMA	A	622	11/12	0.88	0.18	-	91,99,108,119	0
5	NAG	A	631	14/15	0.72	0.26	-	138,145,155,160	0

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
8	SO4	A	1331	5/5	0.93	0.24	3.03	153,153,154,154	0
8	SO4	A	1329	5/5	0.92	0.23	1.02	151,152,155,156	0
9	GOL	A	1332	6/6	0.95	0.18	1.00	61,68,69,70	0
8	SO4	L	1179	5/5	0.90	0.22	-	139,146,149,151	0
8	SO4	A	1330	5/5	0.87	0.19	-	138,140,144,149	0
6	NAG	A	610	14/15	0.75	0.22	-	110,128,136,138	0
8	SO4	A	1328	5/5	0.93	0.29	-	154,155,156,160	0
6	NAG	A	640	14/15	0.88	0.19	-	90,107,117,121	0

6.5 Other polymers [i](#)

There are no such residues in this entry.