



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:19 AM BST

PDB ID : 5IBL
Title : Human antibody 6639 in complex with influenza hemagglutinin H1 X-181
Authors : Raymond, D.D.; Harrison, S.C.
Deposited on : 2016-02-22
Resolution : 3.39 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

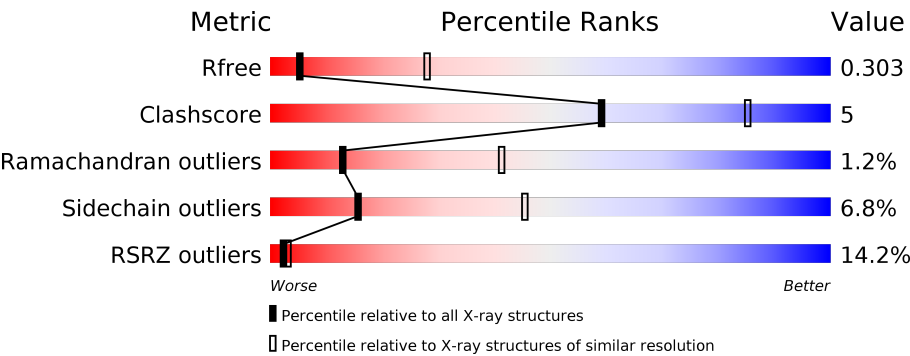
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 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}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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	176	
1	E	176	
2	B	328	
2	F	328	
3	C	230	
3	H	230	

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Mol	Chain	Length	Quality of chain
4	D	215	 20% 81% 18% •
4	L	215	 20% 84% 15% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13181 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	106	Total	C	N	O	S	0	0	0
			858	534	141	179	4			
1	E	115	Total	C	N	O	S	0	0	0
			931	584	152	191	4			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total	C	N	O	S	0	0	0
			2336	1480	401	445	10			
2	F	306	Total	C	N	O	S	0	0	0
			2398	1517	416	455	10			

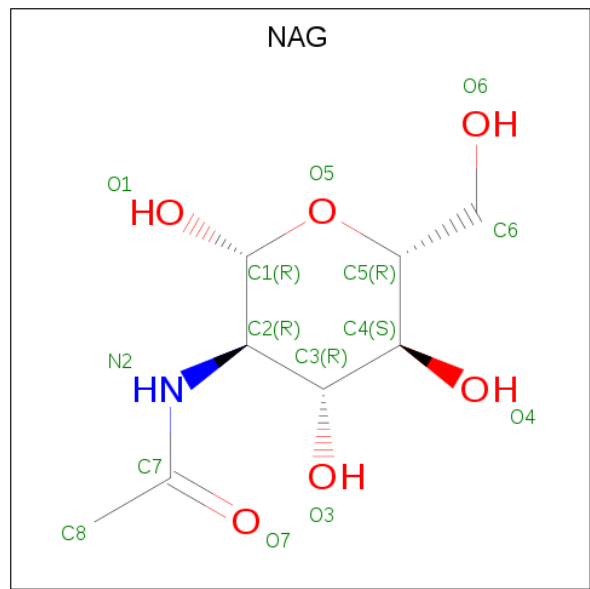
- Molecule 3 is a protein called 6639 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	1	0
			1643	1043	273	319	8			
3	H	216	Total	C	N	O	S	0	0	0
			1639	1041	271	319	8			

- Molecule 4 is a protein called 6639 Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	215	Total	C	N	O	S	0	0	0
			1639	1022	278	333	6			
4	L	215	Total	C	N	O	S	0	0	0
			1639	1022	278	333	6			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

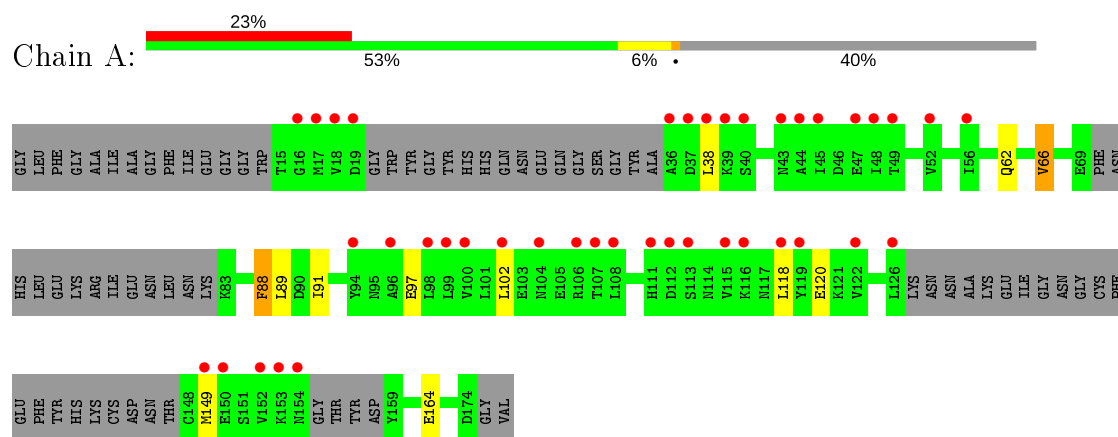


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

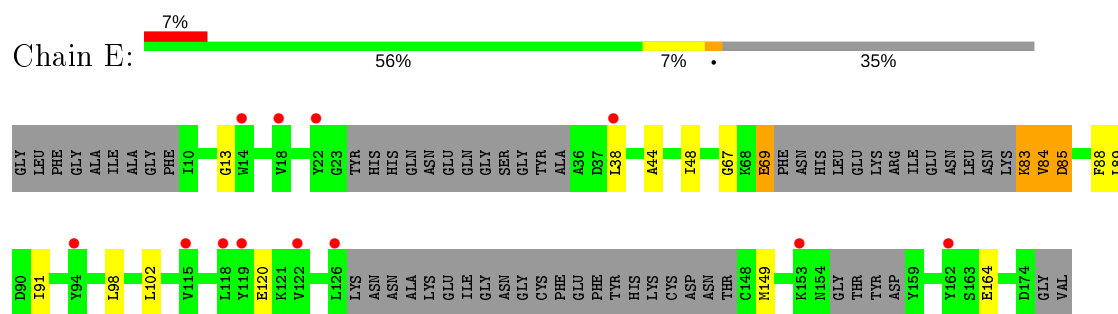
3 Residue-property plots [i](#)

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.

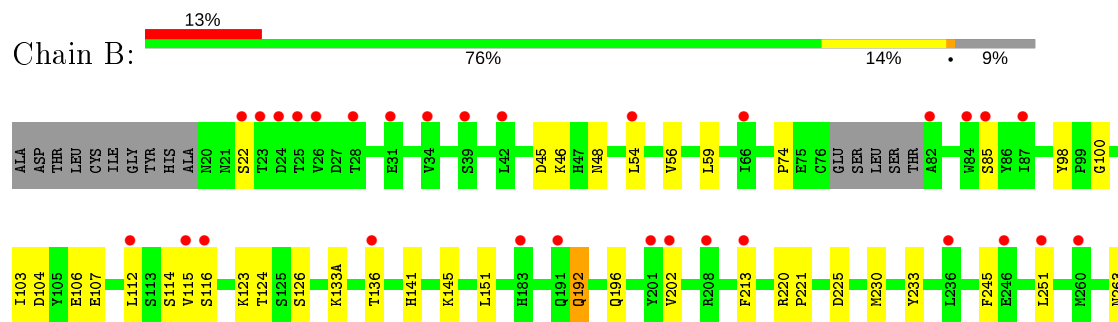
• Molecule 1: Hemagglutinin

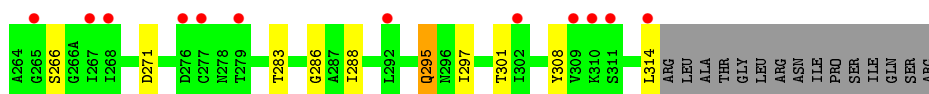


• Molecule 1: Hemagglutinin

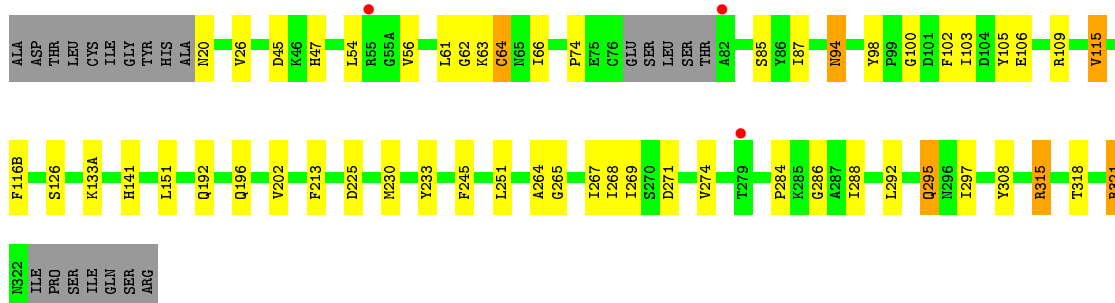
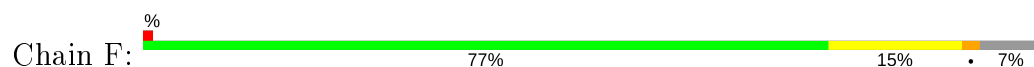


• Molecule 2: Hemagglutinin

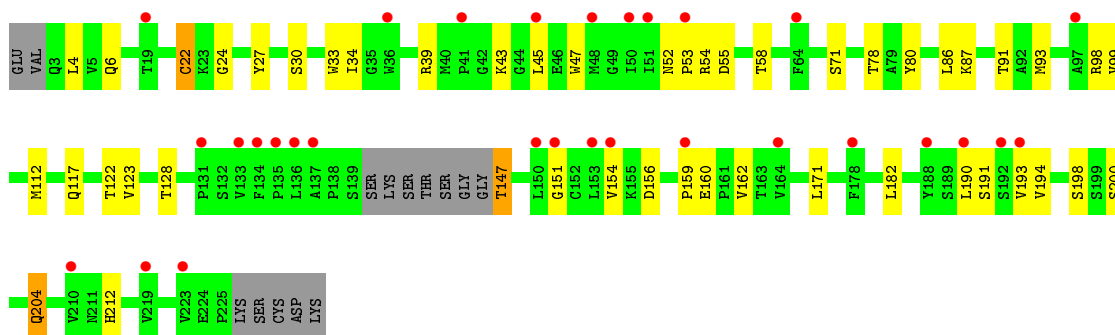
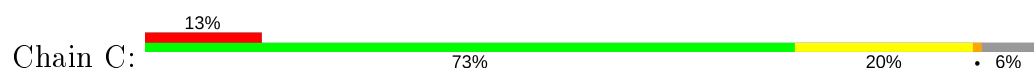




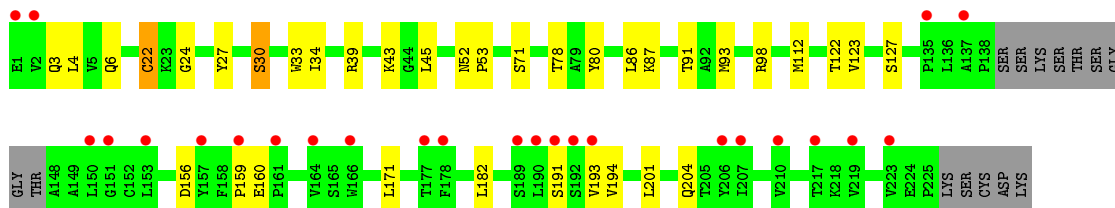
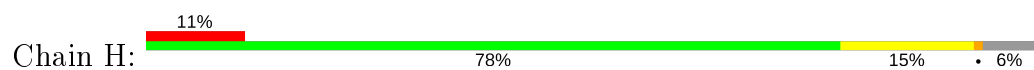
• Molecule 2: Hemagglutinin



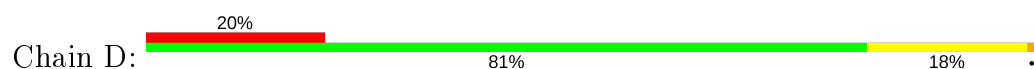
• Molecule 3: 6639 Heavy Chain

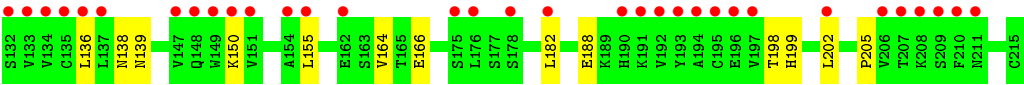


• Molecule 3: 6639 Heavy Chain

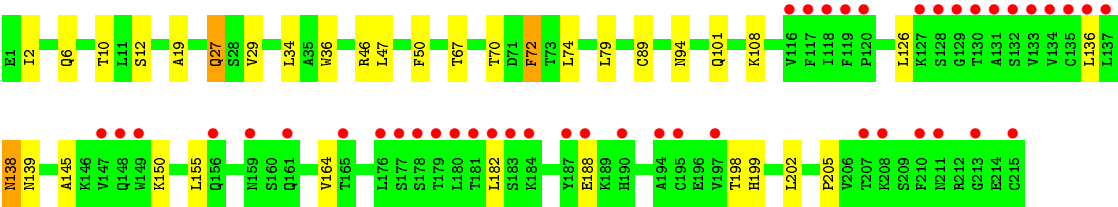
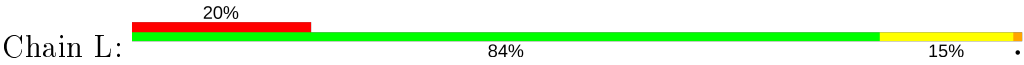


• Molecule 4: 6639 Light Chain





● Molecule 4: 6639 Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.13Å 104.72Å 116.66Å 101.95° 95.33° 98.36°	Depositor
Resolution (Å)	44.81 – 3.39 46.40 – 3.39	Depositor EDS
% Data completeness (in resolution range)	95.4 (44.81-3.39) 95.6 (46.40-3.39)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.214 , 0.257 0.252 , 0.303	Depositor DCC
R_{free} test set	1637 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	113.2	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 107.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13181	wwPDB-VP
Average B, all atoms (Å ²)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.16% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.41	0/864	0.57	0/1159
1	E	0.41	0/942	0.58	0/1266
2	B	0.39	0/2396	0.63	0/3255
2	F	0.41	0/2458	0.67	0/3338
3	C	0.38	0/1690	0.61	0/2302
3	H	0.40	0/1682	0.64	0/2291
4	D	0.38	0/1674	0.60	0/2273
4	L	0.39	0/1674	0.60	0/2273
All	All	0.39	0/13380	0.62	0/18157

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	858	0	834	4	0
1	E	931	0	892	13	0
2	B	2336	0	2281	21	0
2	F	2398	0	2347	23	0
3	C	1643	0	1598	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1639	0	1597	12	0
4	D	1639	0	1591	15	0
4	L	1639	0	1591	16	0
5	B	28	0	26	0	0
5	F	70	0	65	2	0
All	All	13181	0	12822	121	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 5.

All (121) 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:E:69:GLU:OE1	1:E:69:GLU:N	2.06	0.87
1:E:83:LYS:HD3	1:E:83:LYS:C	2.00	0.80
4:L:2:ILE:HD11	4:L:94:ASN:HB3	1.64	0.79
2:B:74:PRO:HB2	2:B:141:HIS:HB2	1.72	0.72
1:E:83:LYS:O	1:E:83:LYS:HD3	1.91	0.70
2:B:114:SER:HA	2:B:266:SER:HB2	1.74	0.67
2:F:63:LYS:O	2:F:94:ASN:HB2	1.95	0.66
1:E:83:LYS:O	1:E:85:ASP:N	2.30	0.65
4:D:21:LEU:HD13	4:D:74:LEU:HD23	1.82	0.61
2:F:74:PRO:HB2	2:F:141:HIS:HB2	1.81	0.61
2:F:47:HIS:HD2	2:F:286:GLY:HA3	1.65	0.60
3:C:147:THR:N	3:C:198:SER:HG	2.00	0.59
1:E:88:PHE:HD1	1:E:89:LEU:N	2.01	0.59
3:C:128:THR:HG23	3:C:159:PRO:HD3	1.84	0.58
2:B:295:GLN:HG2	2:B:297:ILE:H	1.69	0.57
2:F:268:ILE:HG12	2:F:284:PRO:HG3	1.85	0.57
2:F:295:GLN:HG2	2:F:297:ILE:H	1.68	0.57
3:C:30:SER:HB3	3:C:54:ARG:HG2	1.88	0.56
1:A:88:PHE:HA	1:A:91:ILE:HD12	1.88	0.56
3:C:6:GLN:HB2	3:C:117:GLN:HG2	1.87	0.56
2:F:115:VAL:HG11	2:F:116(B):PHE:HB2	1.87	0.56
1:E:88:PHE:CD1	1:E:89:LEU:N	2.75	0.55
2:B:54:LEU:HB3	2:B:85:SER:HB2	1.87	0.55
3:H:30:SER:HA	3:H:53:PRO:HB2	1.87	0.55
4:L:2:ILE:CD1	4:L:94:ASN:HB3	2.37	0.55
3:C:71:SER:HB2	3:C:80:TYR:HB2	1.89	0.55
3:H:71:SER:HB2	3:H:80:TYR:HB2	1.89	0.54
2:B:136:THR:HA	2:B:145:LYS:HE3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:LEU:HD23	2:B:115:VAL:HG21	1.91	0.53
3:C:30:SER:HA	3:C:53:PRO:HB2	1.91	0.53
4:L:136:LEU:HD11	4:L:138:ASN:HD22	1.74	0.52
2:F:103:ILE:HG13	2:F:233:TYR:CE2	2.45	0.52
3:C:154:VAL:HG11	3:C:162:VAL:HG21	1.93	0.51
1:A:91:ILE:HG23	1:E:98:LEU:HD11	1.92	0.51
1:E:88:PHE:C	1:E:88:PHE:CD1	2.84	0.51
4:L:198:THR:HG22	4:L:205:PRO:HB3	1.92	0.51
3:H:33:TRP:CE2	3:H:52:ASN:HB2	2.46	0.51
2:B:103:ILE:HG13	2:B:233:TYR:CE2	2.46	0.50
3:C:91:THR:HG23	3:C:122:THR:HA	1.94	0.50
3:H:91:THR:HG23	3:H:122:THR:HA	1.93	0.50
3:C:171:LEU:HD21	3:C:194:VAL:HG21	1.93	0.50
4:D:49:ILE:HG21	4:D:65:GLY:HA3	1.94	0.50
4:L:34:LEU:HB3	4:L:72:PHE:CZ	2.48	0.49
3:H:171:LEU:HD21	3:H:194:VAL:HG21	1.94	0.49
4:L:12:SER:HB3	4:L:108:LYS:HG2	1.94	0.49
4:D:198:THR:HG22	4:D:205:PRO:HB3	1.93	0.48
2:F:321:ARG:HD2	2:F:321:ARG:H	1.79	0.48
1:E:48:ILE:HG21	2:F:318:THR:HG23	1.96	0.48
2:B:98:TYR:CD1	2:B:230:MET:HB2	2.50	0.47
4:D:47:LEU:HD21	4:D:50:PHE:HB3	1.97	0.47
2:F:98:TYR:CD1	2:F:230:MET:HB2	2.50	0.47
3:C:200:SER:OG	3:C:204:GLN:HB2	2.15	0.47
4:D:31:SER:HA	4:D:34:LEU:HD12	1.97	0.46
4:L:150:LYS:HG2	4:L:155:LEU:HG	1.97	0.46
2:F:54:LEU:HB3	2:F:85:SER:HB2	1.98	0.46
2:B:220:ARG:HB3	2:B:221:PRO:HD2	1.98	0.46
1:E:67:GLY:O	1:E:69:GLU:OE1	2.33	0.45
4:L:47:LEU:HD21	4:L:50:PHE:HB3	1.98	0.45
3:H:34:ILE:HD13	3:H:98:ARG:HA	1.98	0.45
4:D:150:LYS:HG2	4:D:155:LEU:HG	1.97	0.45
1:E:13:GLY:HA2	5:F:404:NAG:H62	1.99	0.45
2:B:104:ASP:HB3	2:B:107:GLU:HB2	1.99	0.45
2:F:109:ARG:HH22	2:F:269:ILE:HD11	1.82	0.45
3:C:39:ARG:HB2	3:C:45:LEU:HD23	1.99	0.44
3:H:6:GLN:HA	3:H:22:CYS:HA	1.99	0.44
2:F:245:PHE:HD2	2:F:251:LEU:HD21	1.83	0.44
4:L:6:GLN:H	4:L:101:GLN:HG3	1.82	0.44
1:A:97:GLU:HG2	2:B:314:LEU:HD21	2.00	0.44
4:D:6:GLN:H	4:D:101:GLN:HG3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:193:VAL:HG11	4:D:136:LEU:HD22	2.00	0.44
4:D:34:LEU:HB3	4:D:72:PHE:CE1	2.53	0.44
3:C:86:LEU:HB3	3:C:123:VAL:HG11	2.00	0.44
3:C:34:ILE:HD13	3:C:98:ARG:HA	1.98	0.44
2:F:66:ILE:HD11	2:F:267:ILE:HG21	2.00	0.44
3:H:39:ARG:HB2	3:H:45:LEU:HD23	2.00	0.44
2:F:20:ASN:OD1	5:F:404:NAG:H2	2.18	0.43
2:B:192:GLN:HA	2:B:196:GLN:HA	2.00	0.43
3:C:162:VAL:HG12	3:C:212:HIS:HA	1.99	0.43
3:C:47:TRP:HB3	4:D:97:TRP:O	2.18	0.43
3:H:86:LEU:HB3	3:H:123:VAL:HG11	2.00	0.43
3:C:33:TRP:HB2	3:C:99:VAL:HB	2.00	0.43
3:H:4:LEU:HD23	3:H:24:GLY:HA2	2.01	0.43
4:L:19:ALA:HB2	4:L:79:LEU:HD11	2.01	0.43
3:C:6:GLN:HA	3:C:22:CYS:HA	2.00	0.43
4:D:2:ILE:HG23	4:D:27:GLN:HG2	2.01	0.43
3:C:27:TYR:OH	3:C:34:ILE:HD11	2.18	0.42
3:H:27:TYR:OH	3:H:34:ILE:HD11	2.19	0.42
4:L:36:TRP:CE2	4:L:74:LEU:HB2	2.54	0.42
2:B:202:VAL:HB	2:B:213:PHE:HB2	2.01	0.42
2:B:48:ASN:O	2:B:286:GLY:HA3	2.20	0.42
3:C:52:ASN:ND2	3:C:55:ASP:H	2.17	0.42
2:F:61:LEU:HB3	2:F:64:CYS:HB3	2.01	0.42
3:C:4:LEU:HD23	3:C:24:GLY:HA2	2.02	0.42
3:H:193:VAL:HG11	4:L:136:LEU:HD22	2.01	0.42
2:B:295:GLN:OE1	2:B:308:TYR:HD1	2.03	0.42
3:C:162:VAL:HG23	3:C:190:LEU:HD21	2.01	0.42
1:A:62:GLN:O	1:A:66:VAL:HG23	2.19	0.42
2:F:202:VAL:HG11	2:F:251:LEU:HD13	2.02	0.41
2:F:26:VAL:HG12	2:F:315:ARG:HG2	2.00	0.41
2:B:100:GLY:HA3	2:B:230:MET:O	2.20	0.41
2:B:114:SER:HB2	2:B:263:ASN:O	2.20	0.41
2:B:116:SER:HB2	2:B:263:ASN:HB2	2.01	0.41
2:F:94:ASN:HD22	2:F:94:ASN:HA	1.48	0.41
2:B:245:PHE:HD2	2:B:251:LEU:HD21	1.85	0.41
4:D:19:ALA:HB2	4:D:79:LEU:HD11	2.00	0.41
4:L:36:TRP:CZ3	4:L:89:CYS:HB3	2.56	0.41
3:C:47:TRP:CG	4:D:97:TRP:HB2	2.56	0.41
4:D:36:TRP:CZ3	4:D:89:CYS:HB3	2.56	0.41
4:L:199:HIS:HB3	4:L:202:LEU:HD12	2.03	0.41
2:B:202:VAL:HG11	2:B:251:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:2:ILE:HG23	4:L:27:GLN:HG2	2.03	0.41
2:F:202:VAL:HB	2:F:213:PHE:HB2	2.02	0.41
4:L:145:ALA:HB2	4:L:199:HIS:HD2	1.86	0.41
4:D:199:HIS:HB3	4:D:202:LEU:HD12	2.03	0.41
1:E:83:LYS:C	1:E:85:ASP:N	2.74	0.40
2:F:295:GLN:OE1	2:F:308:TYR:HD1	2.03	0.40
1:E:44:ALA:O	1:E:48:ILE:HG12	2.22	0.40
2:B:283:THR:HG22	2:B:301:THR:HG22	2.03	0.40
2:F:100:GLY:HA3	2:F:230:MET:O	2.20	0.40
2:F:102:PHE:HB3	2:F:105:TYR:HB2	2.03	0.40
3:C:151:GLY:HA2	3:C:193:VAL:HG12	2.04	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	96/176 (54%)	93 (97%)	2 (2%)	1 (1%)	15	46
1	E	105/176 (60%)	92 (88%)	10 (10%)	3 (3%)	4	24
2	B	294/328 (90%)	261 (89%)	31 (10%)	2 (1%)	22	55
2	F	302/328 (92%)	265 (88%)	32 (11%)	5 (2%)	9	34
3	C	213/230 (93%)	194 (91%)	18 (8%)	1 (0%)	29	61
3	H	212/230 (92%)	191 (90%)	18 (8%)	3 (1%)	11	37
4	D	213/215 (99%)	194 (91%)	16 (8%)	3 (1%)	11	37
4	L	213/215 (99%)	195 (92%)	16 (8%)	2 (1%)	17	49
All	All	1648/1898 (87%)	1485 (90%)	143 (9%)	20 (1%)	13	41

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	126	SER
4	D	71	ASP
4	D	139	ASN
1	E	85	ASP
2	F	126	SER
3	H	159	PRO
4	L	139	ASN
1	E	84	VAL
2	F	62	GLY
2	F	264	ALA
2	F	265	GLY
4	L	72	PHE
3	C	156	ASP
4	D	94	ASN
2	F	196	GLN
3	H	156	ASP
2	B	124	THR
3	H	160	GLU
1	E	91	ILE
1	A	66	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	98/151 (65%)	90 (92%)	8 (8%)	11	37
1	E	103/151 (68%)	95 (92%)	8 (8%)	12	39
2	B	262/287 (91%)	248 (95%)	14 (5%)	22	52
2	F	268/287 (93%)	250 (93%)	18 (7%)	16	46
3	C	184/195 (94%)	172 (94%)	12 (6%)	17	46
3	H	183/195 (94%)	170 (93%)	13 (7%)	14	44
4	D	186/186 (100%)	170 (91%)	16 (9%)	10	35
4	L	186/186 (100%)	175 (94%)	11 (6%)	19	49
All	All	1470/1638 (90%)	1370 (93%)	100 (7%)	16	45

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	A	88	PHE
1	A	89	LEU
1	A	102	LEU
1	A	118	LEU
1	A	120	GLU
1	A	149	MET
1	A	164	GLU
2	B	22	SER
2	B	45	ASP
2	B	46	LYS
2	B	56	VAL
2	B	59	LEU
2	B	106	GLU
2	B	123	LYS
2	B	133(A)	LYS
2	B	151	LEU
2	B	192	GLN
2	B	225	ASP
2	B	271	ASP
2	B	288	ILE
2	B	295	GLN
3	C	22	CYS
3	C	43	LYS
3	C	58	THR
3	C	78	THR
3	C	87	LYS
3	C	93	MET
3	C	112	MET
3	C	147	THR
3	C	160	GLU
3	C	182	LEU
3	C	191	SER
3	C	204	GLN
4	D	5	THR
4	D	10	THR
4	D	27	GLN
4	D	29	VAL
4	D	46	ARG
4	D	62	ARG
4	D	71	ASP
4	D	72	PHE

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Mol	Chain	Res	Type
4	D	73	THR
4	D	103	THR
4	D	126	LEU
4	D	138	ASN
4	D	164	VAL
4	D	166	GLU
4	D	182	LEU
4	D	188	GLU
1	E	38	LEU
1	E	69	GLU
1	E	83	LYS
1	E	84	VAL
1	E	102	LEU
1	E	120	GLU
1	E	149	MET
1	E	164	GLU
2	F	45	ASP
2	F	56	VAL
2	F	64	CYS
2	F	87	ILE
2	F	94	ASN
2	F	106	GLU
2	F	115	VAL
2	F	133(A)	LYS
2	F	151	LEU
2	F	192	GLN
2	F	225	ASP
2	F	271	ASP
2	F	274	VAL
2	F	288	ILE
2	F	292	LEU
2	F	295	GLN
2	F	315	ARG
2	F	321	ARG
3	H	3	GLN
3	H	22	CYS
3	H	30	SER
3	H	43	LYS
3	H	78	THR
3	H	87	LYS
3	H	93	MET
3	H	112	MET

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Mol	Chain	Res	Type
3	H	127	SER
3	H	182	LEU
3	H	191	SER
3	H	201	LEU
3	H	204	GLN
4	L	10	THR
4	L	27	GLN
4	L	29	VAL
4	L	46	ARG
4	L	67	THR
4	L	70	THR
4	L	126	LEU
4	L	138	ASN
4	L	164	VAL
4	L	182	LEU
4	L	188	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
3	C	52	ASN
4	D	38	GLN
1	E	114	ASN
2	F	47	HIS
4	L	38	GLN
4	L	138	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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$
5	NAG	F	404	2	14,14,15	0.39	0	17,19,21	1.03	2 (11%)
5	NAG	F	405	2	14,14,15	0.42	0	17,19,21	1.93	2 (11%)
5	NAG	F	403	2	14,14,15	0.38	0	17,19,21	0.63	0
5	NAG	F	402	2	14,14,15	0.33	0	17,19,21	0.68	1 (5%)
5	NAG	B	401	2	14,14,15	0.35	0	17,19,21	0.58	0
5	NAG	F	401	2	14,14,15	0.32	0	17,19,21	0.51	0
5	NAG	B	402	2	14,14,15	0.36	0	17,19,21	1.22	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	F	404	2	-	1/6/23/26	0/1/1/1
5	NAG	F	405	2	-	0/6/23/26	0/1/1/1
5	NAG	F	403	2	-	0/6/23/26	0/1/1/1
5	NAG	F	402	2	-	0/6/23/26	0/1/1/1
5	NAG	B	401	2	-	0/6/23/26	0/1/1/1
5	NAG	F	401	2	-	1/6/23/26	0/1/1/1
5	NAG	B	402	2	-	0/6/23/26	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(°)
5	F	405	NAG	C1-O5-C5	5.70	119.92	112.19
5	F	405	NAG	O5-C1-C2	5.19	119.49	111.29
5	B	402	NAG	O5-C1-C2	-3.54	105.69	111.29
5	F	404	NAG	C1-C2-N2	-2.91	105.51	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	402	NAG	C1-C2-N2	2.86	115.38	110.49
5	F	404	NAG	O5-C1-C2	2.06	114.54	111.29
5	F	402	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	404	NAG	O5-C5-C6-O6
5	F	401	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	404	NAG	2	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	106/176 (60%)	1.59	41 (38%) 0 0	131, 184, 216, 242	0
1	E	115/176 (65%)	0.72	12 (10%) 6 8	107, 153, 210, 221	0
2	B	298/328 (90%)	0.92	42 (14%) 2 3	85, 126, 174, 200	0
2	F	306/328 (93%)	0.51	3 (0%) 82 81	81, 113, 140, 160	0
3	C	216/230 (93%)	0.95	30 (13%) 2 3	103, 154, 195, 210	0
3	H	216/230 (93%)	0.79	25 (11%) 4 5	79, 130, 197, 218	0
4	D	215/215 (100%)	1.19	42 (19%) 1 1	105, 143, 197, 211	0
4	L	215/215 (100%)	1.12	44 (20%) 1 1	96, 137, 202, 229	0
All	All	1687/1898 (88%)	0.92	239 (14%) 2 3	79, 136, 198, 242	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	195	CYS	7.1
4	L	182	LEU	7.0
4	L	118	ILE	6.9
4	D	192	VAL	6.5
1	A	19	ASP	6.1
4	D	197	VAL	6.0
1	A	18	VAL	5.7
4	D	134	VAL	5.6
2	B	39	SER	5.5
4	L	135	CYS	5.3
4	D	119	PHE	5.3
4	D	209	SER	5.2
4	L	134	VAL	5.2
4	D	149	TRP	5.2
4	D	202	LEU	5.1
4	D	117	PHE	5.1

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Mol	Chain	Res	Type	RSRZ
3	C	153	LEU	5.1
4	L	149	TRP	5.1
4	L	131	ALA	5.0
3	C	131	PRO	5.0
4	D	118	ILE	5.0
3	C	154	VAL	4.9
3	H	151	GLY	4.9
2	B	31	GLU	4.8
1	A	108	LEU	4.6
3	H	219	VAL	4.6
3	H	217	THR	4.5
4	D	207	THR	4.4
4	L	211	ASN	4.4
3	H	150	LEU	4.4
4	L	195	CYS	4.3
1	A	118	LEU	4.3
4	L	136	LEU	4.3
1	A	126	LEU	4.2
1	A	36	ALA	4.1
4	L	119	PHE	4.1
4	L	133	VAL	4.1
1	A	107	THR	4.1
2	B	279	THR	4.0
4	L	178	SER	4.0
4	L	130	THR	3.9
4	L	210	PHE	3.9
1	A	122	VAL	3.8
4	L	215	CYS	3.8
1	A	38	LEU	3.8
1	A	40	SER	3.8
1	E	122	VAL	3.8
4	D	94	ASN	3.8
1	A	52	VAL	3.8
4	L	132	SER	3.8
3	C	223	VAL	3.7
4	L	129	GLY	3.7
4	D	176	LEU	3.6
2	B	26	VAL	3.6
3	C	219	VAL	3.6
1	E	162	TYR	3.6
3	C	164	VAL	3.6
3	C	135	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	154	ASN	3.5
1	A	115	VAL	3.5
2	B	310	LYS	3.5
3	C	133	VAL	3.5
4	D	191	LYS	3.5
1	E	126	LEU	3.5
3	H	206	TYR	3.5
4	D	193	TYR	3.5
3	H	192	SER	3.4
2	B	260	MET	3.4
1	A	100	VAL	3.4
2	B	24	ASP	3.3
1	E	18	VAL	3.3
2	B	54	LEU	3.3
3	H	161	PRO	3.3
3	C	190	LEU	3.3
4	L	194	ALA	3.3
2	B	115	VAL	3.3
3	H	153	LEU	3.3
3	H	2	VAL	3.3
3	C	137	ALA	3.3
3	H	178	PHE	3.2
4	D	133	VAL	3.2
1	A	104	ASN	3.2
3	C	192	SER	3.2
3	H	166	TRP	3.2
4	L	181	THR	3.2
4	L	184	LYS	3.2
1	A	45	ILE	3.2
3	H	210	VAL	3.1
4	L	187	TYR	3.1
2	B	265	GLY	3.1
1	A	152	VAL	3.1
1	A	116	LYS	3.1
3	H	189	SER	3.1
2	B	25	THR	3.1
4	D	120	PRO	3.1
4	D	178	SER	3.1
1	A	102	LEU	3.1
4	D	190	HIS	3.1
4	D	132	SER	3.0
2	B	309	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
4	L	116	VAL	3.0
4	L	117	PHE	3.0
4	L	156	GLN	3.0
2	B	116	SER	3.0
4	D	210	PHE	3.0
4	L	190	HIS	3.0
3	C	136	LEU	2.9
4	D	147	VAL	2.9
4	L	159	ASN	2.9
4	L	208	LYS	2.9
3	H	223	VAL	2.9
1	A	112	ASP	2.9
1	A	113	SER	2.9
4	D	182	LEU	2.9
4	D	208	LYS	2.8
1	A	150	GLU	2.8
4	D	175	SER	2.8
2	B	201	TYR	2.8
4	D	116	VAL	2.8
3	C	178	PHE	2.8
4	D	151	VAL	2.8
2	B	34	VAL	2.8
3	C	210	VAL	2.8
4	L	161	GLN	2.7
1	E	14	TRP	2.7
2	B	191	GLN	2.7
3	C	159	PRO	2.7
3	H	177	THR	2.7
4	D	19	ALA	2.7
2	B	112	LEU	2.7
3	C	51	ILE	2.7
1	A	98	LEU	2.7
1	A	96	ALA	2.7
3	H	190	LEU	2.7
4	D	155	LEU	2.7
2	B	202	VAL	2.7
4	L	197	VAL	2.7
3	H	207	ILE	2.7
4	D	211	ASN	2.6
1	A	99	LEU	2.6
2	F	82	ALA	2.6
3	H	193	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	188	TYR	2.6
4	L	128	SER	2.6
3	C	45	LEU	2.6
1	A	119	TYR	2.6
2	B	213	PHE	2.6
4	L	147	VAL	2.6
1	A	149	MET	2.6
3	C	36	TRP	2.6
2	B	251	LEU	2.5
1	A	153	LYS	2.5
1	A	56	ILE	2.5
2	B	276	ASP	2.5
1	E	115	VAL	2.5
2	B	292	LEU	2.5
1	A	111	HIS	2.5
2	F	279	THR	2.5
4	D	136	LEU	2.5
1	E	22	TYR	2.5
4	D	196	GLU	2.5
1	A	43	ASN	2.5
2	B	28	THR	2.5
2	B	183	HIS	2.5
4	D	135	CYS	2.4
2	F	55	ARG	2.4
1	E	153	LYS	2.4
2	B	136	THR	2.4
3	C	193	VAL	2.4
2	B	42	LEU	2.4
2	B	85	SER	2.4
3	C	41	PRO	2.4
3	H	159	PRO	2.4
1	E	94	TYR	2.4
1	A	37	ASP	2.4
2	B	22	SER	2.4
1	A	48	ILE	2.4
4	D	150	LYS	2.4
4	L	176	LEU	2.4
4	D	206	VAL	2.4
3	H	164	VAL	2.3
2	B	277	CYS	2.3
4	L	207	THR	2.3
4	L	177	SER	2.3

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Mol	Chain	Res	Type	RSRZ
4	L	183	SER	2.3
4	L	188	GLU	2.3
2	B	314	LEU	2.3
3	H	135	PRO	2.3
1	A	16	GLY	2.3
2	B	267	ILE	2.3
1	E	38	LEU	2.3
4	D	194	ALA	2.3
4	L	127	LYS	2.3
4	L	213	GLY	2.3
1	A	49	THR	2.3
4	L	165	THR	2.3
4	L	137	LEU	2.3
2	B	268	ILE	2.3
3	C	19	THR	2.2
2	B	66	ILE	2.2
4	D	123	ASP	2.2
3	H	137	ALA	2.2
3	C	150	LEU	2.2
2	B	87	ILE	2.2
4	D	137	LEU	2.2
1	A	39	LYS	2.2
1	A	44	ALA	2.2
4	D	125	GLN	2.2
2	B	236	LEU	2.2
3	H	157	TYR	2.2
3	C	48	MET	2.2
3	C	50	ILE	2.2
2	B	311	SER	2.2
1	A	106	ARG	2.2
3	C	134	PHE	2.2
4	D	148	GLN	2.2
3	C	53	PRO	2.2
1	A	94	TYR	2.1
2	B	208	ARG	2.1
1	E	119	TYR	2.1
3	C	97	ALA	2.1
3	H	1	GLU	2.1
4	L	120	PRO	2.1
2	B	84	TRP	2.1
4	L	179	THR	2.1
4	D	154	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	118	LEU	2.1
2	B	23	THR	2.1
3	H	191	SER	2.1
2	B	302	ILE	2.1
4	L	180	LEU	2.1
2	B	82	ALA	2.0
3	C	64	PHE	2.0
4	D	162	GLU	2.0
4	L	148	GLN	2.0
3	C	151	GLY	2.0
1	A	47	GLU	2.0
1	A	17	MET	2.0
2	B	246	GLU	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 monosaccharides 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
5	NAG	F	405	14/15	0.58	0.27	159,160,161,161	0
5	NAG	F	402	14/15	0.70	0.28	147,148,154,155	0
5	NAG	F	404	14/15	0.79	0.31	144,145,148,149	0
5	NAG	F	401	14/15	0.79	0.39	173,180,184,186	0
5	NAG	B	401	14/15	0.81	0.26	160,166,175,175	0
5	NAG	B	402	14/15	0.81	0.30	173,176,179,179	0
5	NAG	F	403	14/15	0.84	0.24	126,136,140,140	0

6.5 Other polymers

There are no such residues in this entry.