



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:45 PM UTC

PDB ID : 5IBL / pdb_00005ibl
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 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

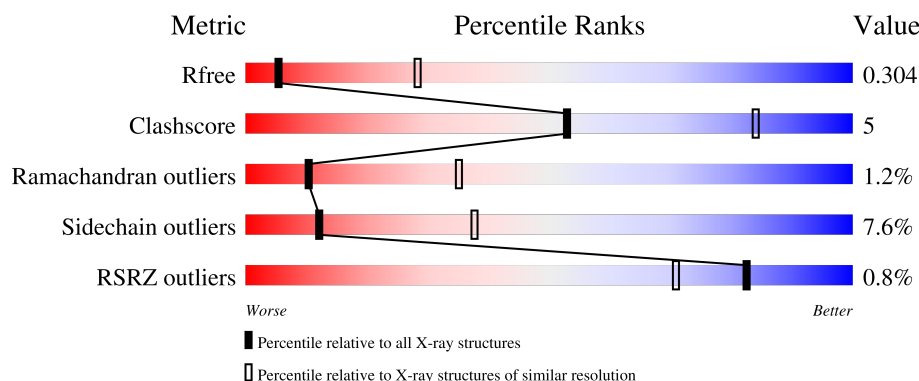
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	176	52% 7% 40%
1	E	176	53% 9% 35%
2	B	328	74% 16% 9%
2	F	328	75% 16% 7%
3	C	230	71% 22% 6%

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Mol	Chain	Length	Quality of chain
3	H	230	% 76%17%6%
4	D	215	80%19%•
4	L	215	82%16%•

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			

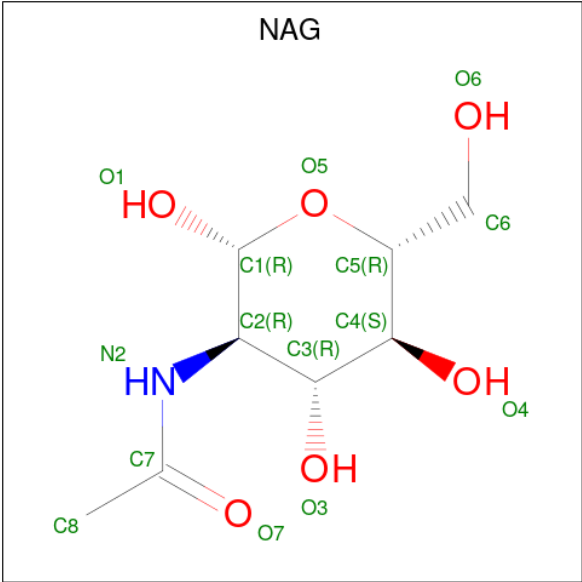
- Molecule 3 is a protein called 6639 Heavy Chain.

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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).

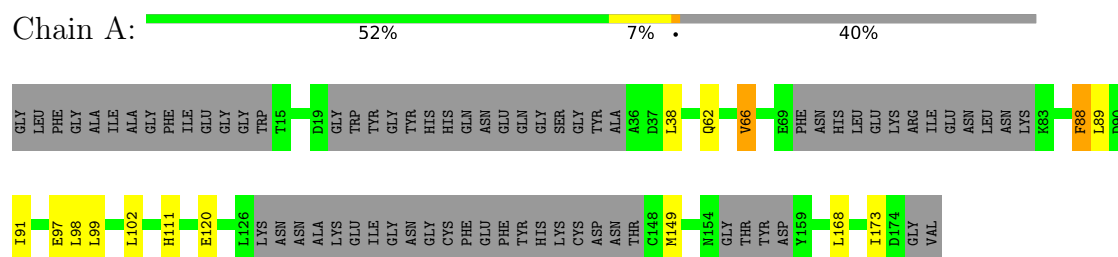


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

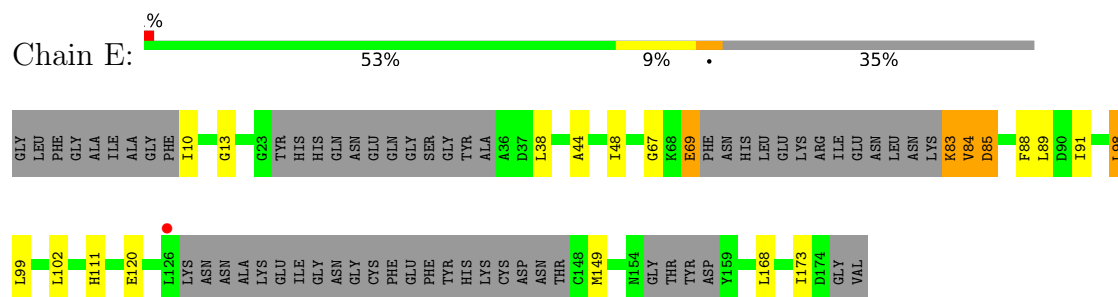
3 Residue-property plots [i](#)

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.

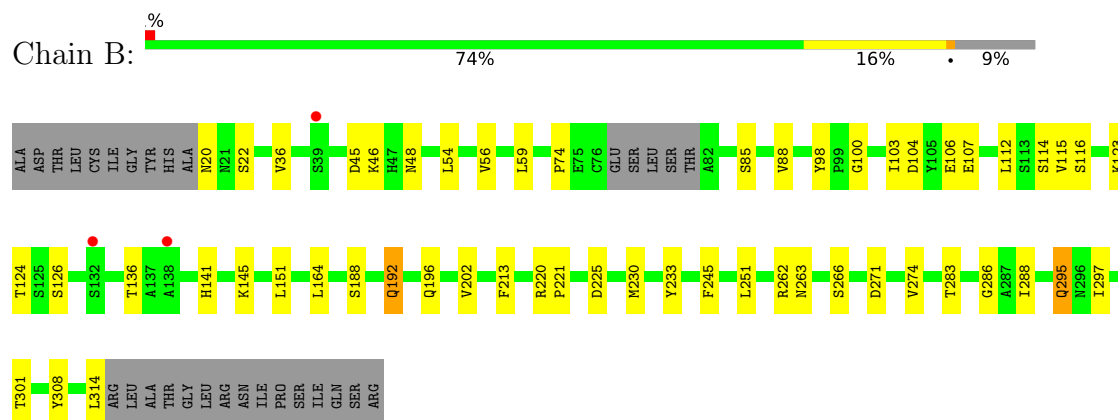
• Molecule 1: Hemagglutinin



• Molecule 1: Hemagglutinin

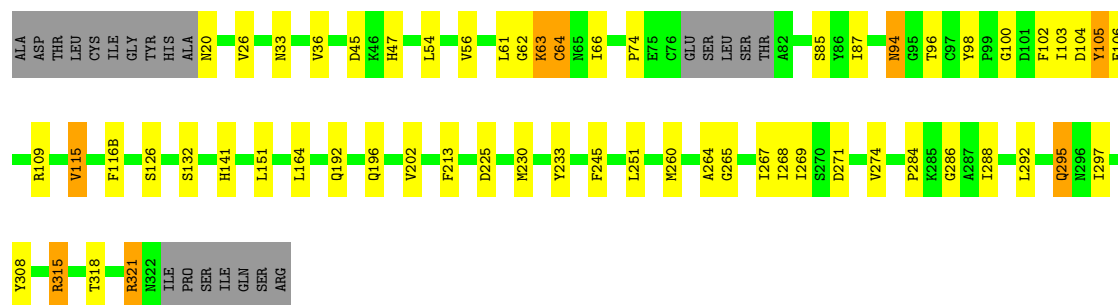


• Molecule 2: Hemagglutinin

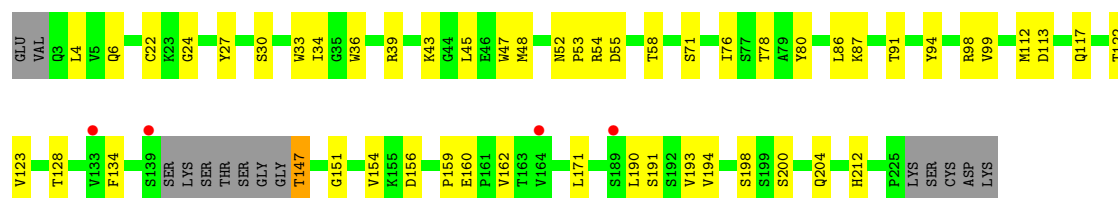


• Molecule 2: Hemagglutinin

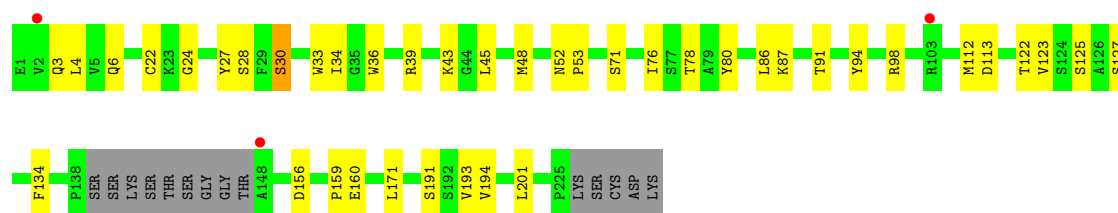
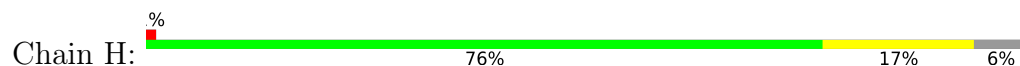




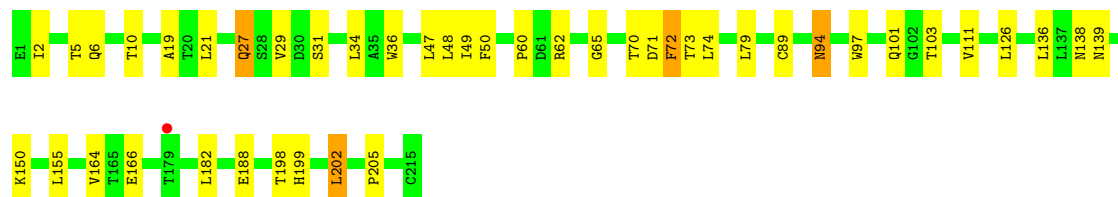
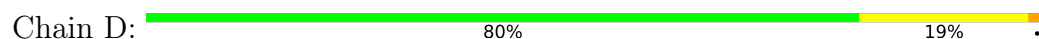
• Molecule 3: 6639 Heavy Chain



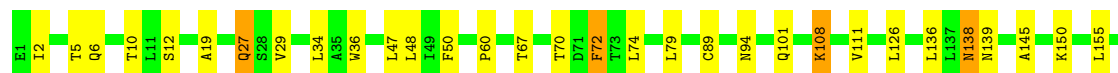
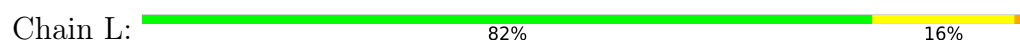
• Molecule 3: 6639 Heavy Chain

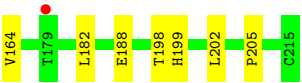


• Molecule 4: 6639 Light Chain



• 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 44.81 – 3.39	Depositor EDS
% Data completeness (in resolution range)	95.4 (44.81-3.39) 95.5 (44.81-3.39)	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 , 0.304	Depositor DCC
R_{free} test set	1637 reflections (4.79%)	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 , 112.0	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

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	0.75	0/864	1.44	2/1159 (0.2%)
1	E	0.73	0/942	1.37	2/1266 (0.2%)
2	B	0.72	0/2396	1.21	4/3255 (0.1%)
2	F	0.75	0/2458	1.25	6/3338 (0.2%)
3	C	0.72	0/1690	1.16	2/2302 (0.1%)
3	H	0.75	0/1682	1.18	6/2291 (0.3%)
4	D	0.72	0/1674	1.15	6/2273 (0.3%)
4	L	0.73	0/1674	1.14	2/2273 (0.1%)
All	All	0.73	0/13380	1.22	30/18157 (0.2%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	125	SER	CA-C-N	6.61	130.74	120.82
3	H	125	SER	C-N-CA	6.61	130.74	120.82
3	H	113	ASP	CA-CB-CG	6.36	118.96	112.60
2	B	20	ASN	CA-C-N	6.34	129.64	120.38
2	B	20	ASN	C-N-CA	6.34	129.64	120.38
3	C	113	ASP	CA-CB-CG	6.16	118.76	112.60
2	F	104	ASP	CA-CB-CG	5.83	118.43	112.60
2	F	105	TYR	CA-C-N	5.68	127.89	120.28
2	F	105	TYR	C-N-CA	5.68	127.89	120.28
3	C	134	PHE	CA-CB-CG	5.33	119.13	113.80
2	F	33	ASN	OD1-CG-ND2	-5.25	117.34	122.60
2	F	96	THR	CA-C-N	5.24	127.56	120.38
2	F	96	THR	C-N-CA	5.24	127.56	120.38
3	H	28	SER	CA-C-N	5.14	127.42	120.38
3	H	28	SER	C-N-CA	5.14	127.42	120.38
3	H	134	PHE	CA-CB-CG	5.12	118.92	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	60	PRO	CA-C-N	5.11	127.84	120.38
4	D	60	PRO	C-N-CA	5.11	127.84	120.38
2	B	188	SER	CA-C-N	5.11	127.12	120.28
2	B	188	SER	C-N-CA	5.11	127.12	120.28
4	L	60	PRO	CA-C-N	5.10	127.83	120.38
4	L	60	PRO	C-N-CA	5.10	127.83	120.38
4	D	70	THR	CA-C-N	5.08	131.24	121.54
4	D	70	THR	C-N-CA	5.08	131.24	121.54
4	D	138	ASN	CA-C-N	5.06	131.21	121.54
4	D	138	ASN	C-N-CA	5.06	131.21	121.54
1	A	111	HIS	CA-C-N	5.03	127.02	120.28
1	A	111	HIS	C-N-CA	5.03	127.02	120.28
1	E	111	HIS	CA-C-N	5.03	127.02	120.28
1	E	111	HIS	C-N-CA	5.03	127.02	120.28

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	858	0	834	4	0
1	E	931	0	892	15	0
2	B	2336	0	2281	21	0
2	F	2398	0	2347	25	0
3	C	1643	0	1598	26	0
3	H	1639	0	1597	14	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	129	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 (129) 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:C	1:E:83:LYS:HD3	2.00	0.85
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:HD3	1:E:83:LYS:O	1.91	0.70
3:C:36:TRP:HB3	3:C:48:MET:HE3	1.73	0.69
3:H:36:TRP:HB3	3:H:48:MET:HE3	1.73	0.68
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
2:F:116(B):PHE:HE1	2:F:260:MET:HE2	1.64	0.62
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
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
1:E:88:PHE:CD1	1:E:88:PHE:C	2.84	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
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
3:C:147:THR:N	3:C:198:SER:HG	2.08	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	2:F:321:ARG:HD2	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
1:E:69:GLU:N	1:E:69:GLU:CD	2.73	0.45
4:L:47:LEU:HD21	4:L:50:PHE:HB3	1.98	0.45
1:E:83:LYS:C	1:E:85:ASP:N	2.74	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
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:34:ILE:HD13	3:C:98:ARG:HA	1.98	0.44
3:C:86:LEU:HB3	3:C:123:VAL:HG11	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:116(B):PHE:CE1	2:F:260:MET:HE2	2.48	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:48:ASN:O	2:B:286:GLY:HA3	2.20	0.42
2:B:202:VAL:HB	2:B:213:PHE:HB2	2.01	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
3:C:48:MET:HE1	3:C:94:TYR:HD2	1.85	0.42
2:F:26:VAL:HG12	2:F:315:ARG:HG2	2.00	0.41
2:F:202:VAL:HG11	2:F:251:LEU:HD13	2.02	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
3:H:48:MET:HE1	3:H:94:TYR:HD2	1.85	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
2:F:202:VAL:HB	2:F:213:PHE:HB2	2.02	0.41
4:L:2:ILE:HG23	4:L:27:GLN:HG2	2.03	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
2:F:295:GLN:OE1	2:F:308:TYR:HD1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:83:LYS:C	1:E:85:ASP:H	2.29	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%)	12	40
1	E	105/176 (60%)	92 (88%)	10 (10%)	3 (3%)	3	19
2	B	294/328 (90%)	261 (89%)	31 (10%)	2 (1%)	18	47
2	F	302/328 (92%)	265 (88%)	32 (11%)	5 (2%)	7	28
3	C	213/230 (93%)	194 (91%)	18 (8%)	1 (0%)	24	54
3	H	212/230 (92%)	191 (90%)	18 (8%)	3 (1%)	9	31
4	D	213/215 (99%)	194 (91%)	16 (8%)	3 (1%)	9	31
4	L	213/215 (99%)	195 (92%)	16 (8%)	2 (1%)	14	42
All	All	1648/1898 (87%)	1485 (90%)	143 (9%)	20 (1%)	10	35

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

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Mol	Chain	Res	Type
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%)	88 (90%)	10 (10%)	7	25
1	E	103/151 (68%)	91 (88%)	12 (12%)	5	20
2	B	262/287 (91%)	244 (93%)	18 (7%)	14	40
2	F	268/287 (93%)	247 (92%)	21 (8%)	11	37
3	C	184/195 (94%)	175 (95%)	9 (5%)	22	49
3	H	183/195 (94%)	173 (94%)	10 (6%)	19	46
4	D	186/186 (100%)	169 (91%)	17 (9%)	9	30
4	L	186/186 (100%)	172 (92%)	14 (8%)	12	38
All	All	1470/1638 (90%)	1359 (92%)	111 (8%)	12	38

All (111) 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	98	LEU
1	A	99	LEU
1	A	102	LEU
1	A	120	GLU
1	A	149	MET
1	A	168	LEU
1	A	173	ILE
2	B	22	SER
2	B	36	VAL
2	B	45	ASP
2	B	46	LYS
2	B	56	VAL
2	B	59	LEU
2	B	88	VAL
2	B	106	GLU
2	B	123	LYS
2	B	151	LEU
2	B	164	LEU
2	B	192	GLN
2	B	225	ASP
2	B	262	ARG
2	B	271	ASP
2	B	274	VAL
2	B	288	ILE
2	B	295	GLN
3	C	43	LYS
3	C	58	THR
3	C	76	ILE
3	C	78	THR
3	C	87	LYS
3	C	112	MET
3	C	147	THR
3	C	160	GLU
3	C	191	SER
4	D	5	THR
4	D	10	THR
4	D	27	GLN
4	D	29	VAL
4	D	48	LEU
4	D	62	ARG

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Mol	Chain	Res	Type
4	D	72	PHE
4	D	73	THR
4	D	94	ASN
4	D	103	THR
4	D	111	VAL
4	D	126	LEU
4	D	164	VAL
4	D	166	GLU
4	D	182	LEU
4	D	188	GLU
4	D	202	LEU
1	E	10	ILE
1	E	38	LEU
1	E	69	GLU
1	E	83	LYS
1	E	84	VAL
1	E	98	LEU
1	E	99	LEU
1	E	102	LEU
1	E	120	GLU
1	E	149	MET
1	E	168	LEU
1	E	173	ILE
2	F	36	VAL
2	F	45	ASP
2	F	56	VAL
2	F	63	LYS
2	F	64	CYS
2	F	87	ILE
2	F	94	ASN
2	F	106	GLU
2	F	115	VAL
2	F	132	SER
2	F	151	LEU
2	F	164	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

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Mol	Chain	Res	Type
2	F	315	ARG
2	F	321	ARG
3	H	3	GLN
3	H	30	SER
3	H	43	LYS
3	H	76	ILE
3	H	78	THR
3	H	87	LYS
3	H	112	MET
3	H	127	SER
3	H	191	SER
3	H	201	LEU
4	L	5	THR
4	L	10	THR
4	L	27	GLN
4	L	29	VAL
4	L	48	LEU
4	L	67	THR
4	L	70	THR
4	L	108	LYS
4	L	111	VAL
4	L	126	LEU
4	L	138	ASN
4	L	164	VAL
4	L	182	LEU
4	L	188	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	114	ASN
1	A	125	GLN
2	B	192	GLN
2	B	197	ASN
2	B	295	GLN
3	C	3	GLN
3	C	52	ASN
3	C	82	GLN
3	C	117	GLN
4	D	38	GLN
4	D	43	GLN

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Mol	Chain	Res	Type
4	D	101	GLN
4	D	161	GLN
1	E	60	ASN
1	E	114	ASN
1	E	125	GLN
1	E	154	ASN
2	F	47	HIS
2	F	111	GLN
2	F	192	GLN
2	F	295	GLN
3	H	82	GLN
4	L	38	GLN
4	L	138	ASN

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](#)

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	B	402	2	14,14,15	0.38	0	17,19,21	1.28	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	F	405	2	14,14,15	0.43	0	17,19,21	1.96	2 (11%)
5	NAG	B	401	2	14,14,15	0.37	0	17,19,21	0.61	0
5	NAG	F	401	2	14,14,15	0.34	0	17,19,21	0.52	0
5	NAG	F	404	2	14,14,15	0.41	0	17,19,21	1.08	2 (11%)
5	NAG	F	402	2	14,14,15	0.35	0	17,19,21	0.72	1 (5%)
5	NAG	F	403	2	14,14,15	0.38	0	17,19,21	0.64	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
5	NAG	B	402	2	-	0/6/23/26	0/1/1/1
5	NAG	F	405	2	-	0/6/23/26	0/1/1/1
5	NAG	B	401	2	-	1/6/23/26	0/1/1/1
5	NAG	F	401	2	-	1/6/23/26	0/1/1/1
5	NAG	F	404	2	-	1/6/23/26	0/1/1/1
5	NAG	F	402	2	-	0/6/23/26	0/1/1/1
5	NAG	F	403	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	5.77	119.92	112.19
5	F	405	NAG	O5-C1-C2	5.30	119.49	111.29
5	B	402	NAG	O5-C1-C2	-3.62	105.69	111.29
5	B	402	NAG	C1-C2-N2	3.14	115.38	110.43
5	F	404	NAG	C1-C2-N2	-3.12	105.51	110.43
5	F	404	NAG	O5-C1-C2	2.10	114.54	111.29
5	F	402	NAG	C1-O5-C5	2.06	114.94	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	404	NAG	O5-C5-C6-O6
5	B	401	NAG	C1-C2-N2-C7
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%)	-0.10	0 100 100	131, 184, 216, 242	0
1	E	115/176 (65%)	-0.12	1 (0%) 81 68	107, 153, 210, 221	0
2	B	298/328 (90%)	-0.14	3 (1%) 79 66	85, 126, 174, 200	0
2	F	306/328 (93%)	-0.22	0 100 100	81, 113, 140, 160	0
3	C	216/230 (93%)	-0.04	4 (1%) 66 51	83, 154, 195, 210	1 (0%)
3	H	216/230 (93%)	-0.12	3 (1%) 73 59	79, 130, 197, 218	0
4	D	215/215 (100%)	-0.07	1 (0%) 87 78	105, 143, 197, 211	0
4	L	215/215 (100%)	-0.10	1 (0%) 87 78	96, 137, 202, 229	0
All	All	1687/1898 (88%)	-0.12	13 (0%) 82 71	79, 136, 198, 242	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	179	THR	4.0
3	H	148	ALA	3.4
3	H	2	VAL	3.2
3	C	133	VAL	2.9
4	L	179	THR	2.9
3	H	103	ARG	2.9
3	C	189	SER	2.2
1	E	126	LEU	2.2
3	C	139	SER	2.1
2	B	39	SER	2.1
2	B	138	ALA	2.1
3	C	164	VAL	2.1
2	B	132	SER	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	NAG	B	401	14/15	0.44	0.09	160,166,175,175	0
5	NAG	F	405	14/15	0.50	0.12	159,160,161,161	0
5	NAG	F	402	14/15	0.61	0.10	147,148,154,155	0
5	NAG	F	401	14/15	0.61	0.09	173,180,184,186	0
5	NAG	B	402	14/15	0.64	0.09	173,176,179,179	0
5	NAG	F	404	14/15	0.75	0.13	144,145,148,149	0
5	NAG	F	403	14/15	0.88	0.09	126,136,140,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.