



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:31 AM UTC

PDB ID : 5XAJ / pdb_00005xaj
Title : Structural mimicry of the dengue virus envelope glycoprotein revealed by the crystallographic study of an idiotypic-anti-idiotypic Fab complex.
Authors : Wong, Y.H.; Goh, B.C.; Lescar, J.
Deposited on : 2017-03-13
Resolution : 2.50 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

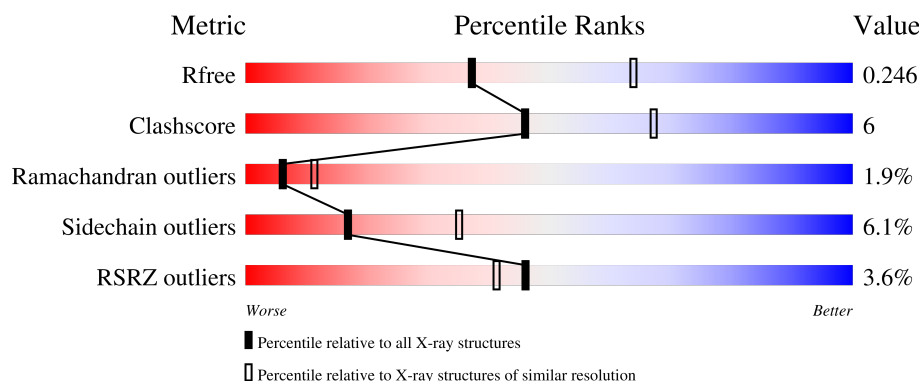
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	227	8% 81%15%..
1	H	227	5% 83%14%. .
2	B	214	81%13%5%.
2	L	214	% 79%18%. .
3	C	214	4% 88%11%

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Mol	Chain	Length	Quality of chain
3	D	214	% 86% 13%
4	E	215	6% 83% 15%
5	F	218	2% 82% 12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14313 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 FabHM14c10 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1678	1067	280	323	8			
1	H	227	Total	C	N	O	S	0	0	0
			1688	1073	282	325	8			

- Molecule 2 is a protein called FabHM14c10 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1646	1031	281	328	6			
2	L	214	Total	C	N	O	S	0	0	0
			1649	1032	281	330	6			

- Molecule 3 is a protein called Fab E1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	214	Total	C	N	O	S	0	0	0
			1613	1008	272	327	6			
3	D	213	Total	C	N	O	S	0	0	0
			1603	1002	270	326	5			

- Molecule 4 is a protein called Fab E1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	215	Total	C	N	O	S	0	0	0
			1578	998	258	316	6			

- Molecule 5 is a protein called Fab E1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	213	Total	C	N	O	S	0	0	0
			1565	991	256	311	7			

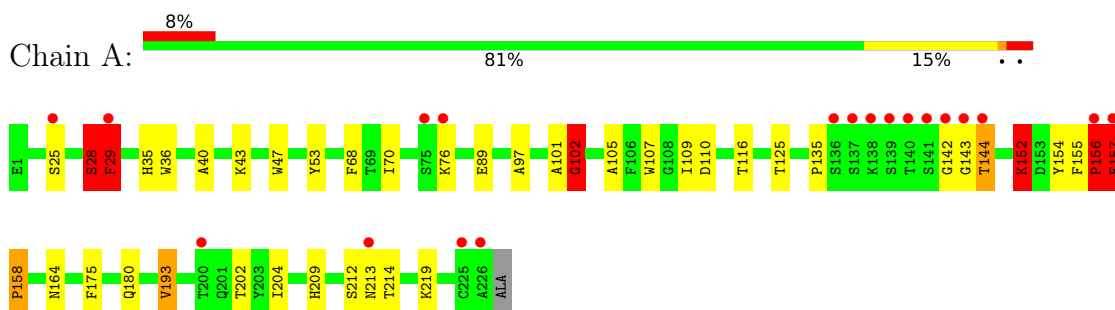
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	171	Total 171	O 171	0	0
6	B	190	Total 190	O 190	0	0
6	C	124	Total 124	O 124	0	0
6	D	151	Total 151	O 151	0	0
6	E	158	Total 158	O 158	0	0
6	F	157	Total 157	O 157	0	0
6	H	184	Total 184	O 184	0	0
6	L	158	Total 158	O 158	0	0

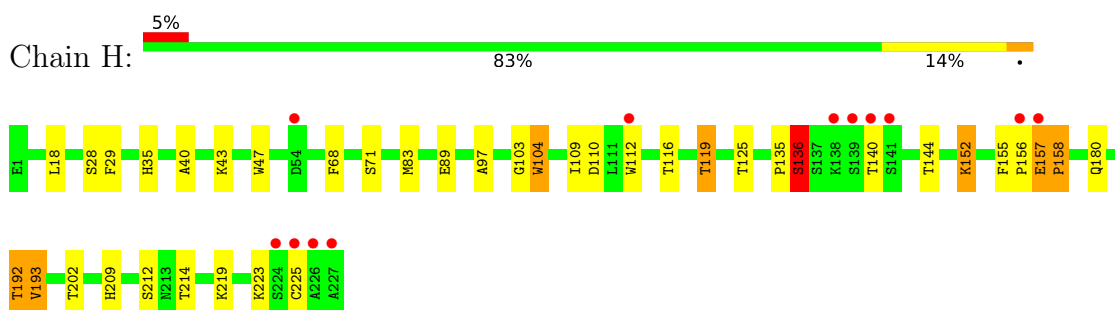
3 Residue-property plots

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.

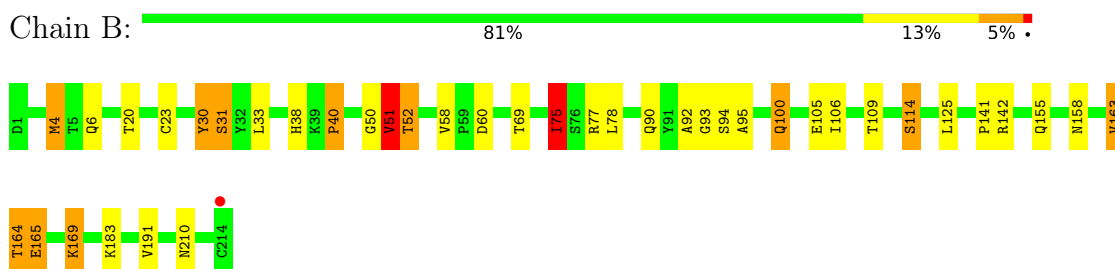
- Molecule 1: FabHM14c10 heavy chain



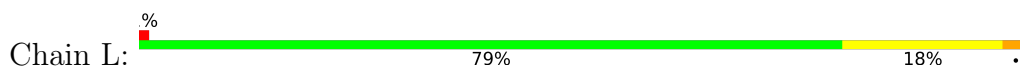
- Molecule 1: FabHM14c10 heavy chain

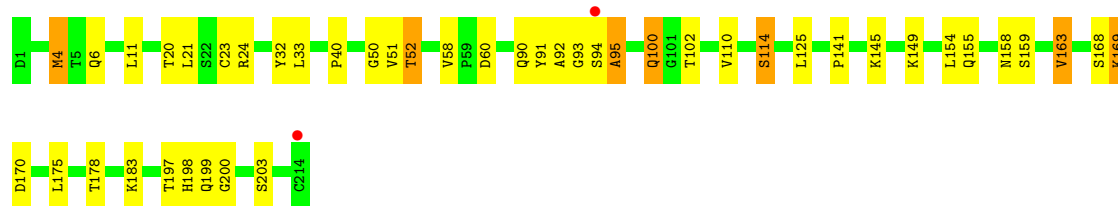


- Molecule 2: FabHM14c10 light chain

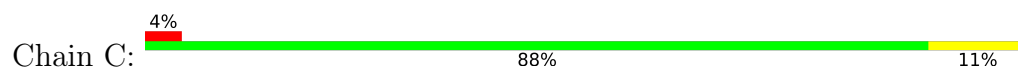


- Molecule 2: FabHM14c10 light chain

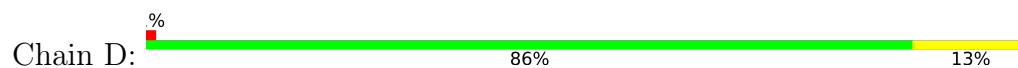




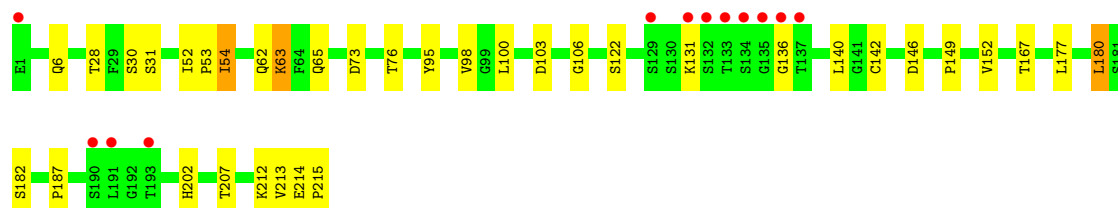
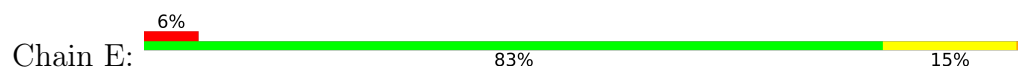
● Molecule 3: Fab E1 light chain



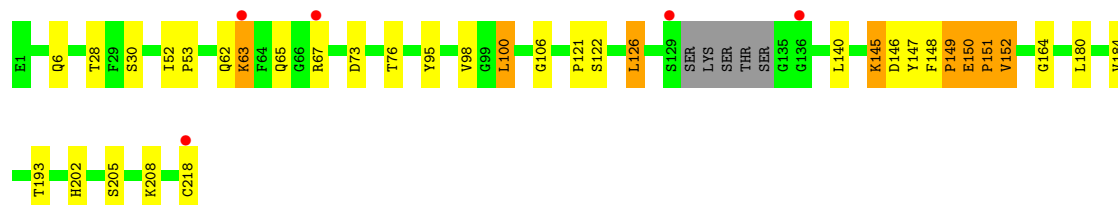
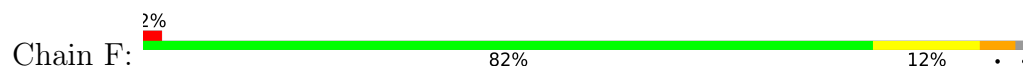
● Molecule 3: Fab E1 light chain



● Molecule 4: Fab E1 heavy chain



● Molecule 5: Fab E1 heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.30Å 47.59Å 220.76Å 90.00° 93.43° 90.00°	Depositor
Resolution (Å)	46.93 – 2.50 46.93 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.93-2.50) 99.7 (46.93-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.185 , 0.239 0.190 , 0.246	Depositor DCC
R_{free} test set	4183 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	33.0	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14313	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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](#)

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	0.85	1/1722 (0.1%)	1.33	18/2344 (0.8%)
1	H	0.83	1/1732 (0.1%)	1.29	15/2356 (0.6%)
2	B	0.90	1/1683 (0.1%)	1.29	12/2284 (0.5%)
2	L	0.80	1/1686 (0.1%)	1.22	11/2288 (0.5%)
3	C	0.80	0/1654	1.23	3/2261 (0.1%)
3	D	0.82	0/1644	1.19	3/2249 (0.1%)
4	E	0.81	0/1615	1.20	4/2204 (0.2%)
5	F	0.81	1/1601 (0.1%)	1.15	4/2183 (0.2%)
All	All	0.83	5/13337 (0.0%)	1.24	70/18169 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	MET	SD-CE	-5.64	1.65	1.79
1	A	157	GLU	CA-C	5.47	1.59	1.52
5	F	148	PHE	CA-C	-5.41	1.46	1.52
2	L	4	MET	SD-CE	-5.13	1.66	1.79
1	H	83	MET	SD-CE	-5.08	1.66	1.79

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	TYR	CA-C-N	11.72	136.94	120.29
1	A	53	TYR	C-N-CA	11.72	136.94	120.29
2	B	164	THR	N-CA-C	8.35	122.76	112.23
1	A	156	PRO	CA-C-N	7.84	140.93	121.80
1	A	156	PRO	C-N-CA	7.84	140.93	121.80
1	H	28	SER	CA-C-N	7.70	131.22	120.29
1	H	28	SER	C-N-CA	7.70	131.22	120.29
1	H	29	PHE	CA-CB-CG	7.57	121.36	113.80
2	L	94	SER	N-CA-C	-7.54	97.78	109.76
1	H	29	PHE	CB-CA-C	-7.41	98.25	110.85
2	B	94	SER	N-CA-C	-7.32	98.12	109.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	VAL	N-CA-CB	-7.06	104.08	111.64
3	C	93	ASN	CA-CB-CG	6.85	119.45	112.60
2	L	170	ASP	CA-C-N	-6.84	108.48	121.54
2	L	170	ASP	C-N-CA	-6.84	108.48	121.54
1	A	102	GLY	N-CA-C	6.66	128.97	113.18
2	B	75	ILE	CB-CA-C	6.66	120.19	111.53
1	H	193	VAL	N-CA-CB	-6.59	104.59	111.64
5	F	52	ILE	N-CA-C	-6.45	100.70	107.60
4	E	140	LEU	N-CA-CB	-6.36	100.13	110.81
4	E	52	ILE	N-CA-C	-6.31	100.85	107.60
1	H	136	SER	CA-C-N	6.30	128.72	120.28
1	H	136	SER	C-N-CA	6.30	128.72	120.28
1	H	192	THR	CB-CA-C	6.20	119.98	109.75
5	F	126	LEU	CA-C-N	6.18	129.47	120.51
5	F	126	LEU	C-N-CA	6.18	129.47	120.51
1	H	110	ASP	CA-CB-CG	6.16	118.76	112.60
1	H	223	LYS	CA-C-N	6.14	130.52	120.63
1	H	223	LYS	C-N-CA	6.14	130.52	120.63
1	A	143	GLY	CA-C-N	6.07	133.14	121.54
1	A	143	GLY	C-N-CA	6.07	133.14	121.54
1	A	110	ASP	CA-CB-CG	6.05	118.65	112.60
3	D	184	THR	N-CA-C	-6.01	101.99	110.29
2	L	114	SER	N-CA-C	-6.00	99.51	109.46
5	F	146	ASP	CA-CB-CG	5.92	118.53	112.60
2	B	141	PRO	CA-C-N	5.92	128.48	120.38
2	B	141	PRO	C-N-CA	5.92	128.48	120.38
2	L	60	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	135	PRO	CA-C-N	5.90	132.81	121.54
1	A	135	PRO	C-N-CA	5.90	132.81	121.54
3	C	29	GLY	CA-C-N	5.88	130.68	120.68
3	C	29	GLY	C-N-CA	5.88	130.68	120.68
2	B	52	THR	N-CA-CB	-5.84	100.63	110.49
2	B	50	GLY	CA-C-N	5.80	132.40	121.97
2	B	50	GLY	C-N-CA	5.80	132.40	121.97
3	D	29	GLY	CA-C-N	5.74	130.44	120.68
3	D	29	GLY	C-N-CA	5.74	130.44	120.68
1	H	193	VAL	CB-CA-C	5.66	114.88	109.33
2	B	114	SER	N-CA-C	-5.63	100.11	109.46
1	A	193	VAL	CB-CA-C	5.59	114.81	109.33
1	A	28	SER	CA-C-N	5.43	131.92	121.54
1	A	28	SER	C-N-CA	5.43	131.92	121.54
2	B	165	GLU	N-CA-CB	5.39	119.60	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	52	THR	N-CA-CB	-5.38	101.39	110.49
4	E	103	ASP	CA-CB-CG	5.37	117.97	112.60
4	E	122	SER	N-CA-C	-5.35	100.51	109.24
2	L	50	GLY	CA-C-N	5.34	131.59	121.97
2	L	50	GLY	C-N-CA	5.34	131.59	121.97
2	B	58	VAL	CB-CA-C	5.34	115.91	110.94
1	H	68	PHE	CA-CB-CG	5.31	119.11	113.80
1	A	68	PHE	CA-CB-CG	5.29	119.09	113.80
1	A	152	LYS	N-CA-C	5.20	118.22	109.95
2	B	60	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	156	PRO	N-CA-CB	-5.16	97.83	103.25
1	H	225	CYS	CA-C-N	5.16	129.24	121.40
1	H	225	CYS	C-N-CA	5.16	129.24	121.40
2	L	141	PRO	CA-C-N	5.12	127.14	120.28
2	L	141	PRO	C-N-CA	5.12	127.14	120.28
2	L	58	VAL	CB-CA-C	5.02	115.61	110.94
1	A	125	THR	CB-CA-C	5.01	117.37	110.16

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	1678	0	1633	34	0
1	H	1688	0	1653	19	0
2	B	1646	0	1593	20	0
2	L	1649	0	1596	24	0
3	C	1613	0	1551	15	0
3	D	1603	0	1535	11	0
4	E	1578	0	1558	21	0
5	F	1565	0	1545	19	0
6	A	171	0	0	0	0
6	B	190	0	0	2	0
6	C	124	0	0	0	0
6	D	151	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	158	0	0	0	0
6	F	157	0	0	0	0
6	H	184	0	0	2	0
6	L	158	0	0	0	0
All	All	14313	0	12664	149	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 6.

All (149) 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:156:PRO:HB3	1:A:209:HIS:CE1	1.67	1.29
1:A:157:GLU:HB2	1:A:158:PRO:HD3	1.16	1.16
5:F:150:GLU:HB3	5:F:151:PRO:HD3	1.18	1.10
1:H:157:GLU:HB3	1:H:158:PRO:HD3	1.13	1.09
1:A:156:PRO:CB	1:A:209:HIS:HE1	1.74	1.00
2:B:6:GLN:H	2:B:100:GLN:HE22	0.96	0.95
1:A:156:PRO:HB3	1:A:209:HIS:HE1	0.81	0.95
2:L:6:GLN:H	2:L:100:GLN:HE22	0.96	0.94
2:L:21:LEU:HD22	2:L:102:THR:HG21	1.49	0.94
5:F:150:GLU:HB3	5:F:151:PRO:CD	1.98	0.94
1:H:157:GLU:HB3	1:H:158:PRO:CD	1.98	0.93
1:H:119:THR:HG21	6:H:347:HOH:O	1.68	0.93
1:H:157:GLU:CB	1:H:158:PRO:HD3	2.00	0.91
5:F:150:GLU:CB	5:F:151:PRO:HD3	2.00	0.90
1:A:157:GLU:HB2	1:A:158:PRO:CD	2.03	0.86
1:H:35:HIS:HD2	1:H:47:TRP:HE1	1.21	0.85
4:E:136:GLY:HA2	4:E:187:PRO:HA	1.61	0.83
1:A:35:HIS:HD2	1:A:47:TRP:HE1	1.22	0.83
1:A:107:TRP:HH2	4:E:54:ILE:CD1	1.90	0.83
2:L:6:GLN:H	2:L:100:GLN:NE2	1.77	0.82
5:F:150:GLU:CB	5:F:151:PRO:CD	2.57	0.82
5:F:152:VAL:HG22	5:F:180:LEU:HD21	1.61	0.81
3:C:14:ALA:HB1	3:C:15:PRO:CA	2.11	0.80
2:B:6:GLN:H	2:B:100:GLN:NE2	1.78	0.80
1:A:157:GLU:CB	1:A:158:PRO:HD3	2.08	0.79
3:C:170:GLN:HE21	3:C:176:ALA:HB2	1.48	0.78
3:D:170:GLN:HE21	3:D:176:ALA:HB2	1.50	0.77
3:C:14:ALA:HB1	3:C:15:PRO:HA	1.67	0.76
5:F:149:PRO:HG2	5:F:150:GLU:HG3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:14:ALA:HB1	3:C:15:PRO:C	2.13	0.74
2:B:6:GLN:N	2:B:100:GLN:HE22	1.81	0.72
2:L:6:GLN:N	2:L:100:GLN:HE22	1.81	0.70
2:B:155:GLN:HE21	2:B:158:ASN:HD21	1.41	0.69
2:L:155:GLN:HE21	2:L:158:ASN:HD21	1.40	0.68
3:D:89:GLN:HE22	5:F:100:LEU:HD21	1.60	0.67
4:E:6:GLN:HE21	4:E:106:GLY:HA3	1.60	0.67
2:L:21:LEU:HD22	2:L:102:THR:CG2	2.25	0.66
5:F:6:GLN:HE21	5:F:106:GLY:HA3	1.59	0.65
3:D:211:PRO:HD3	6:D:374:HOH:O	1.97	0.64
1:A:107:TRP:HH2	4:E:54:ILE:HD11	1.62	0.64
1:A:152:LYS:HE2	1:A:180:GLN:HE22	1.63	0.64
2:B:31:SER:HA	2:B:51:VAL:HG12	1.80	0.64
4:E:214:GLU:HG3	4:E:215:PRO:HD2	1.78	0.63
3:C:89:GLN:HE22	4:E:100:LEU:HD21	1.63	0.62
1:H:152:LYS:HE2	1:H:180:GLN:HE22	1.63	0.62
1:H:209:HIS:HD2	1:H:212:SER:OG	1.83	0.62
1:H:119:THR:CG2	6:H:347:HOH:O	2.37	0.61
1:A:164:ASN:ND2	1:A:204:ILE:H	1.99	0.60
4:E:149:PRO:O	4:E:202:HIS:HE1	1.83	0.60
1:A:47:TRP:CZ3	2:B:95:ALA:HA	2.37	0.59
1:H:47:TRP:CZ3	2:L:95:ALA:HA	2.38	0.59
1:A:107:TRP:CH2	4:E:54:ILE:CD1	2.79	0.59
2:L:21:LEU:CD2	2:L:102:THR:HG21	2.29	0.58
1:A:212:SER:OG	1:A:214:THR:HG22	2.04	0.58
1:H:35:HIS:CD2	1:H:47:TRP:HE1	2.12	0.58
1:H:97:ALA:HB1	1:H:109:ILE:CG2	2.34	0.58
1:H:157:GLU:CB	1:H:158:PRO:CD	2.73	0.57
2:L:90:GLN:NE2	2:L:93:GLY:H	2.02	0.57
2:L:198:HIS:CD2	2:L:200:GLY:H	2.21	0.57
2:B:90:GLN:NE2	2:B:93:GLY:H	2.03	0.57
1:A:97:ALA:HB1	1:A:109:ILE:CG2	2.35	0.57
1:H:212:SER:OG	1:H:214:THR:HG22	2.04	0.56
2:B:38:HIS:HD2	6:B:326:HOH:O	1.88	0.56
1:A:209:HIS:HD2	1:A:212:SER:OG	1.86	0.56
1:A:107:TRP:CH2	4:E:54:ILE:HD13	2.40	0.56
2:L:4:MET:HE3	2:L:23:CYS:SG	2.47	0.55
1:A:101:ALA:O	1:A:105:ALA:O	2.25	0.54
1:A:154:TYR:CD2	1:A:156:PRO:HG3	2.41	0.54
2:L:90:GLN:HE21	2:L:92:ALA:H	1.56	0.54
2:B:90:GLN:HE21	2:B:92:ALA:N	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASN:HD21	1:A:204:ILE:H	1.54	0.54
1:A:154:TYR:HD2	1:A:156:PRO:HG3	1.73	0.53
2:B:4:MET:HE3	2:B:23:CYS:SG	2.48	0.53
5:F:6:GLN:HE22	5:F:95:TYR:HA	1.73	0.53
4:E:30:SER:O	4:E:54:ILE:HG13	2.08	0.53
2:L:149:LYS:HG2	2:L:154:LEU:HD22	1.91	0.53
3:D:141:ASP:H	3:D:170:GLN:HE22	1.57	0.52
4:E:6:GLN:HE22	4:E:95:TYR:HA	1.74	0.52
1:A:107:TRP:HH2	4:E:54:ILE:HD13	1.71	0.52
3:C:184:THR:HG23	3:C:187:GLN:H	1.74	0.52
5:F:121:PRO:HB3	5:F:147:TYR:HB3	1.92	0.52
3:C:14:ALA:CB	3:C:15:PRO:CA	2.86	0.51
4:E:167:THR:HA	4:E:182:SER:HA	1.92	0.51
3:D:189:LYS:HG2	6:D:444:HOH:O	2.11	0.51
2:L:90:GLN:HE21	2:L:92:ALA:N	2.09	0.51
3:C:147:VAL:HG12	3:C:200:HIS:HB2	1.92	0.51
5:F:202:HIS:HD2	5:F:205:SER:OG	1.94	0.51
2:B:90:GLN:HE21	2:B:92:ALA:H	1.59	0.50
3:C:141:ASP:H	3:C:170:GLN:HE22	1.58	0.50
1:A:156:PRO:CB	1:A:209:HIS:CE1	2.63	0.50
3:C:14:ALA:CB	3:C:15:PRO:HA	2.39	0.50
2:B:125:LEU:O	2:B:183:LYS:HD2	2.12	0.50
1:H:104:TRP:CD1	1:H:104:TRP:C	2.90	0.49
2:L:32:TYR:HB3	2:L:91:TYR:HB2	1.93	0.49
1:A:28:SER:O	1:A:29:PHE:HB2	2.11	0.49
2:L:125:LEU:O	2:L:183:LYS:HD2	2.12	0.49
2:L:11:LEU:HD22	2:L:21:LEU:HD23	1.95	0.49
4:E:180:LEU:C	4:E:180:LEU:HD23	2.38	0.48
3:C:14:ALA:HB2	3:C:17:GLN:HB2	1.95	0.48
4:E:30:SER:HA	4:E:53:PRO:HB2	1.96	0.48
5:F:164:GLY:O	5:F:184:VAL:HA	2.14	0.48
1:A:156:PRO:HG2	1:A:157:GLU:O	2.13	0.47
5:F:30:SER:HA	5:F:53:PRO:HB2	1.97	0.47
1:A:36:TRP:HD1	1:A:70:ILE:HD12	1.79	0.47
1:A:102:GLY:HA3	1:A:107:TRP:CD2	2.49	0.47
4:E:146:ASP:HB3	4:E:177:LEU:HD13	1.97	0.47
1:A:156:PRO:HB2	1:A:157:GLU:H	1.30	0.47
2:L:163:VAL:HG22	2:L:175:LEU:HD23	1.95	0.47
2:L:163:VAL:HG22	2:L:175:LEU:CD2	2.45	0.47
3:D:147:VAL:HG12	3:D:200:HIS:HB2	1.97	0.47
2:B:106:ILE:HD13	6:B:313:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:145:LYS:HB3	2:L:197:THR:HB	1.97	0.46
3:C:184:THR:CG2	3:C:187:GLN:H	2.29	0.46
5:F:152:VAL:CG2	5:F:180:LEU:HD21	2.41	0.46
1:A:35:HIS:CD2	1:A:47:TRP:HE1	2.13	0.45
3:C:89:GLN:HE22	4:E:100:LEU:CD2	2.29	0.45
1:A:155:PHE:HA	1:A:156:PRO:HD3	1.64	0.45
2:B:75:ILE:HG12	2:B:78:LEU:HD23	1.99	0.45
1:H:202:THR:HG23	1:H:219:LYS:HE3	1.99	0.45
3:D:122:PRO:HA	3:D:135:LEU:HD23	1.98	0.44
3:C:122:PRO:HA	3:C:135:LEU:HD23	1.98	0.44
4:E:62:GLN:O	4:E:63:LYS:HB2	2.17	0.44
2:B:100:GLN:NE2	2:B:100:GLN:H	2.15	0.44
4:E:73:ASP:HB3	4:E:76:THR:HG22	1.99	0.44
5:F:150:GLU:HB2	5:F:151:PRO:CD	2.46	0.44
2:B:169:LYS:H	2:B:169:LYS:HG3	1.69	0.44
1:H:135:PRO:O	1:H:136:SER:CB	2.65	0.44
2:L:169:LYS:H	2:L:169:LYS:HG3	1.63	0.44
2:L:100:GLN:NE2	2:L:100:GLN:H	2.15	0.43
5:F:73:ASP:HB3	5:F:76:THR:HG22	2.00	0.43
2:B:30:TYR:O	2:B:31:SER:CB	2.63	0.43
5:F:62:GLN:O	5:F:63:LYS:HB2	2.19	0.43
2:B:142:ARG:NH1	2:B:163:VAL:HG21	2.34	0.43
4:E:31:SER:HA	4:E:54:ILE:HD11	2.01	0.43
3:D:127:GLU:OE2	5:F:145:LYS:HE2	2.19	0.42
3:D:89:GLN:HE22	5:F:100:LEU:CD2	2.29	0.42
1:H:40:ALA:HB3	1:H:43:LYS:HD2	2.00	0.42
1:A:202:THR:HG23	1:A:219:LYS:HE3	2.01	0.42
1:A:40:ALA:HB3	1:A:43:LYS:HD2	2.03	0.41
2:L:110:VAL:HG21	2:L:199:GLN:NE2	2.35	0.41
1:A:102:GLY:HA2	4:E:31:SER:HB2	2.02	0.41
1:A:175:PHE:CE1	2:B:164:THR:HG23	2.55	0.41
1:H:209:HIS:CD2	1:H:212:SER:OG	2.68	0.41
1:H:125:THR:HA	1:H:156:PRO:HD3	2.02	0.41
2:B:191:VAL:HG22	2:B:210:ASN:HD22	1.86	0.40
3:D:46:LEU:HD21	3:D:49:TYR:HB3	2.02	0.40
3:C:184:THR:HG22	3:C:187:GLN:HG3	2.04	0.40
3:D:14:ALA:O	3:D:15:PRO:C	2.64	0.40
2:L:159:SER:HA	2:L:178:THR:O	2.22	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	224/227 (99%)	206 (92%)	10 (4%)	8 (4%)	2	3
1	H	225/227 (99%)	207 (92%)	12 (5%)	6 (3%)	4	6
2	B	212/214 (99%)	204 (96%)	4 (2%)	4 (2%)	6	11
2	L	212/214 (99%)	205 (97%)	4 (2%)	3 (1%)	9	17
3	C	212/214 (99%)	201 (95%)	9 (4%)	2 (1%)	14	27
3	D	211/214 (99%)	203 (96%)	4 (2%)	4 (2%)	6	11
4	E	213/215 (99%)	208 (98%)	4 (2%)	1 (0%)	24	43
5	F	209/218 (96%)	202 (97%)	3 (1%)	4 (2%)	6	11
All	All	1718/1743 (99%)	1636 (95%)	50 (3%)	32 (2%)	6	11

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	PHE
1	A	102	GLY
1	A	144	THR
1	A	156	PRO
1	A	157	GLU
1	A	158	PRO
2	B	165	GLU
5	F	149	PRO
5	F	150	GLU
1	H	136	SER
1	H	157	GLU
1	A	142	GLY
3	C	14	ALA
3	D	15	PRO
4	E	63	LYS
5	F	63	LYS

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Mol	Chain	Res	Type
1	H	103	GLY
3	C	118	VAL
3	D	118	VAL
1	H	155	PHE
1	H	158	PRO
3	D	16	GLY
5	F	151	PRO
1	H	140	THR
2	B	30	TYR
2	B	51	VAL
3	D	154	ASP
2	L	95	ALA
2	L	40	PRO
2	B	40	PRO
2	L	51	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	183/185 (99%)	174 (95%)	9 (5%)	22	45
1	H	185/185 (100%)	174 (94%)	11 (6%)	18	37
2	B	184/185 (100%)	169 (92%)	15 (8%)	10	23
2	L	185/185 (100%)	175 (95%)	10 (5%)	20	41
3	C	181/181 (100%)	172 (95%)	9 (5%)	22	44
3	D	179/181 (99%)	169 (94%)	10 (6%)	19	39
4	E	178/178 (100%)	167 (94%)	11 (6%)	16	34
5	F	176/181 (97%)	163 (93%)	13 (7%)	13	27
All	All	1451/1461 (99%)	1363 (94%)	88 (6%)	17	35

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	29	PHE
1	A	76	LYS
1	A	89	GLU
1	A	116	THR
1	A	144	THR
1	A	152	LYS
1	A	193	VAL
1	A	213	ASN
2	B	20	THR
2	B	31	SER
2	B	33	LEU
2	B	40	PRO
2	B	51	VAL
2	B	52	THR
2	B	69	THR
2	B	75	ILE
2	B	77	ARG
2	B	100	GLN
2	B	105	GLU
2	B	109	THR
2	B	114	SER
2	B	163	VAL
2	B	169	LYS
3	C	13	VAL
3	C	22	THR
3	C	30	THR
3	C	31	LYS
3	C	35	TRP
3	C	60	GLU
3	C	85	ASP
3	C	90	VAL
3	C	212	THR
3	D	13	VAL
3	D	15	PRO
3	D	30	THR
3	D	31	LYS
3	D	52	ARG
3	D	60	GLU
3	D	85	ASP
3	D	90	VAL
3	D	212	THR
3	D	213	GLU

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Mol	Chain	Res	Type
4	E	28	THR
4	E	54	ILE
4	E	65	GLN
4	E	98	VAL
4	E	131	LYS
4	E	142	CYS
4	E	152	VAL
4	E	180	LEU
4	E	207	THR
4	E	212	LYS
4	E	213	VAL
5	F	28	THR
5	F	65	GLN
5	F	67	ARG
5	F	98	VAL
5	F	100	LEU
5	F	122	SER
5	F	126	LEU
5	F	140	LEU
5	F	145	LYS
5	F	152	VAL
5	F	193	THR
5	F	208	LYS
5	F	218	CYS
1	H	18	LEU
1	H	71	SER
1	H	89	GLU
1	H	104	TRP
1	H	112	TRP
1	H	116	THR
1	H	119	THR
1	H	144	THR
1	H	152	LYS
1	H	192	THR
1	H	193	VAL
2	L	20	THR
2	L	24	ARG
2	L	33	LEU
2	L	52	THR
2	L	100	GLN
2	L	114	SER
2	L	163	VAL

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Mol	Chain	Res	Type
2	L	168	SER
2	L	169	LYS
2	L	203	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	HIS
1	A	164	ASN
1	A	180	GLN
1	A	209	HIS
2	B	38	HIS
2	B	90	GLN
2	B	100	GLN
2	B	152	ASN
2	B	155	GLN
2	B	199	GLN
2	B	210	ASN
3	C	89	GLN
3	C	170	GLN
3	D	42	GLN
3	D	89	GLN
3	D	170	GLN
3	D	173	ASN
4	E	6	GLN
4	E	173	GLN
4	E	202	HIS
5	F	6	GLN
5	F	173	GLN
5	F	202	HIS
1	H	35	HIS
1	H	80	ASN
1	H	180	GLN
1	H	208	ASN
1	H	209	HIS
1	H	213	ASN
2	L	37	GLN
2	L	38	HIS
2	L	90	GLN
2	L	100	GLN
2	L	152	ASN
2	L	155	GLN

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Mol	Chain	Res	Type
2	L	198	HIS
2	L	199	GLN
2	L	210	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](#)

There are no ligands in this entry.

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	226/227 (99%)	0.18	19 (8%) 17 15	15, 31, 76, 117	0
1	H	227/227 (100%)	-0.03	12 (5%) 32 28	16, 29, 62, 121	0
2	B	214/214 (100%)	-0.41	1 (0%) 87 85	13, 26, 49, 99	0
2	L	214/214 (100%)	-0.23	2 (0%) 81 78	17, 33, 54, 117	0
3	C	214/214 (100%)	0.11	8 (3%) 45 40	20, 39, 67, 130	0
3	D	213/214 (99%)	-0.02	3 (1%) 73 70	20, 36, 62, 127	0
4	E	215/215 (100%)	-0.02	12 (5%) 30 26	17, 32, 75, 104	0
5	F	213/218 (97%)	0.01	5 (2%) 61 57	19, 36, 67, 113	0
All	All	1736/1743 (99%)	-0.05	62 (3%) 46 41	13, 33, 66, 130	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	SER	6.1
1	A	141	SER	6.0
1	H	227	ALA	5.2
3	C	1	LEU	5.0
1	A	140	THR	5.0
1	H	226	ALA	4.8
1	A	143	GLY	4.5
3	D	1	LEU	4.5
1	A	226	ALA	4.3
4	E	135	GLY	4.3
1	A	142	GLY	4.2
4	E	134	SER	4.1
2	L	214	CYS	4.1
5	F	129	SER	4.0
1	H	157	GLU	3.9
1	A	156	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	157	GLU	3.8
3	C	212	THR	3.7
1	H	139	SER	3.6
5	F	218	CYS	3.5
1	H	140	THR	3.3
4	E	136	GLY	3.3
3	D	94	TYR	3.2
4	E	132	SER	3.1
1	A	144	THR	3.1
1	A	29	PHE	3.1
1	A	138	LYS	3.1
1	H	156	PRO	3.1
1	A	136	SER	3.1
3	D	212	THR	3.0
4	E	190	SER	3.0
1	H	54	ASP	3.0
4	E	137	THR	3.0
3	C	214	CYS	3.0
2	B	214	CYS	2.9
4	E	191	LEU	2.9
2	L	94	SER	2.7
4	E	133	THR	2.7
4	E	1	GLU	2.7
4	E	131	LYS	2.7
3	C	35	TRP	2.6
3	C	14	ALA	2.6
3	C	117	SER	2.6
1	H	112	TRP	2.5
1	H	225	CYS	2.5
5	F	67	ARG	2.5
1	A	25	SER	2.5
1	A	75	SER	2.5
1	H	224	SER	2.4
1	H	141	SER	2.4
1	A	225	CYS	2.3
1	A	213	ASN	2.3
1	A	139	SER	2.3
3	C	155	SER	2.3
4	E	193	THR	2.2
1	H	138	LYS	2.2
1	A	200	THR	2.1
5	F	136	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
4	E	129	SER	2.1
5	F	63	LYS	2.0
1	A	76	LYS	2.0
3	C	154	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.