



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:43 PM UTC

PDB ID : 8V50 / pdb_00008v50
Title : Crystal structure of a HLA-B*35:01-NP6 with D1 TCR
Authors : Littler, D.R.; Rossjohn, J.; Gras, S.
Deposited on : 2023-11-30
Resolution : 2.65 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

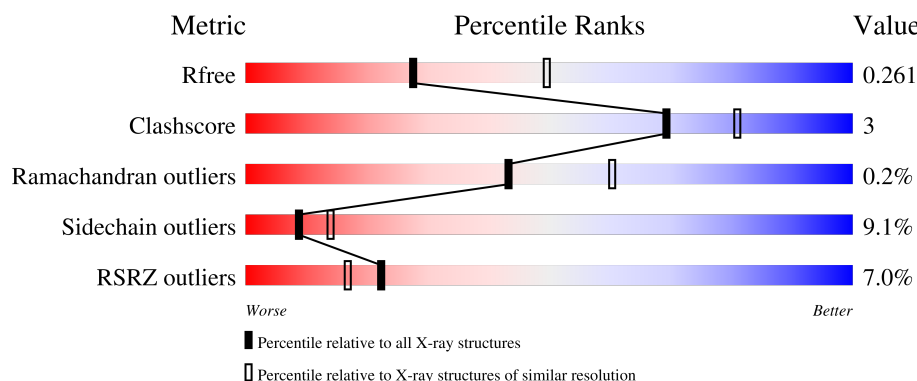
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	274	% 80% 15% .
1	F	274	6% 81% 16% .
1	K	274	5% 79% 19% .
1	P	274	3% 84% 13% ..
2	B	100	% 72% 20% 7% .

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Mol	Chain	Length	Quality of chain
2	G	100	
2	L	100	
2	Q	100	
3	C	9	
3	H	9	
3	M	9	
3	R	9	
4	D	197	
4	I	197	
4	N	197	
4	S	197	
5	E	242	
5	J	242	
5	O	242	
5	T	242	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27419 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 HLA-B35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	1	0
			2241	1397	409	428	7			
1	F	273	Total	C	N	O	S	0	1	0
			2241	1397	409	428	7			
1	K	273	Total	C	N	O	S	0	0	0
			2233	1393	408	425	7			
1	P	271	Total	C	N	O	S	0	0	0
			2221	1386	406	422	7			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	G	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	L	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	Q	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
G	0	MET	-	initiating methionine	UNP P61769
L	0	MET	-	initiating methionine	UNP P61769
Q	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called NP6 epitope H1N1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			
3	H	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			
3	M	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			
3	R	9	Total	C	N	O	S	0	0	0
			72	47	10	14	1			

- Molecule 4 is a protein called D1 TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	197	Total	C	N	O	S	0	2	0
			1546	970	249	317	10			
4	I	197	Total	C	N	O	S	0	2	0
			1546	970	249	317	10			
4	N	197	Total	C	N	O	S	0	2	0
			1546	970	249	317	10			
4	S	197	Total	C	N	O	S	0	2	0
			1546	970	249	317	10			

- Molecule 5 is a protein called D1 TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	242	Total	C	N	O	S	0	2	0
			1933	1216	338	372	7			
5	J	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			
5	O	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			
5	T	242	Total	C	N	O	S	0	3	0
			1942	1221	339	375	7			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	61	Total	O	0	0
			61	61		
6	B	29	Total	O	0	0
			29	29		
6	C	1	Total	O	0	0
			1	1		

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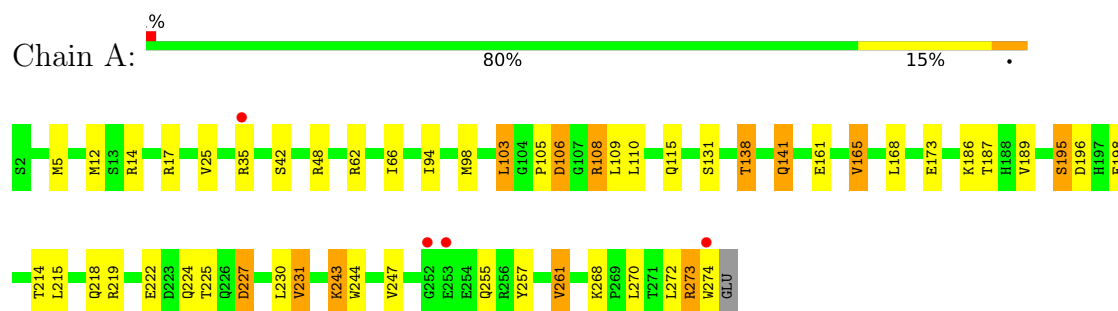
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	44	Total 44	O 44	0	0
6	E	50	Total 50	O 50	0	0
6	F	83	Total 83	O 83	0	0
6	G	22	Total 22	O 22	0	0
6	H	6	Total 6	O 6	0	0
6	I	65	Total 65	O 65	0	0
6	J	73	Total 73	O 73	0	0
6	K	86	Total 86	O 86	0	0
6	L	14	Total 14	O 14	0	0
6	M	5	Total 5	O 5	0	0
6	N	58	Total 58	O 58	0	0
6	O	73	Total 73	O 73	0	0
6	P	89	Total 89	O 89	0	0
6	Q	31	Total 31	O 31	0	0
6	R	6	Total 6	O 6	0	0
6	S	54	Total 54	O 54	0	0
6	T	86	Total 86	O 86	0	0

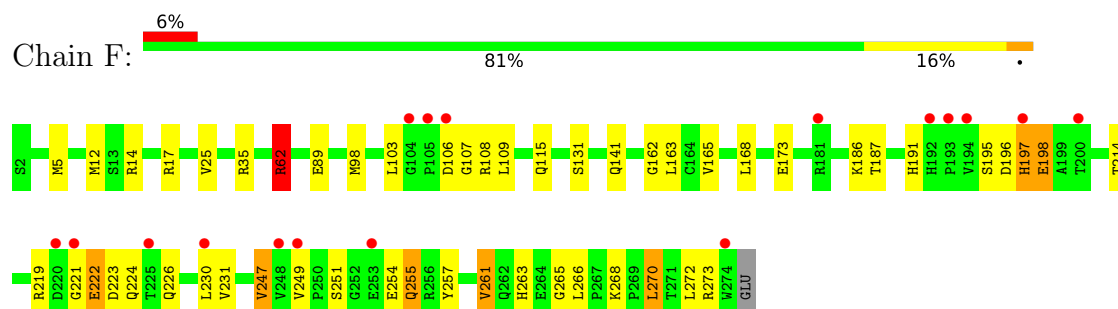
3 Residue-property plots [i](#)

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

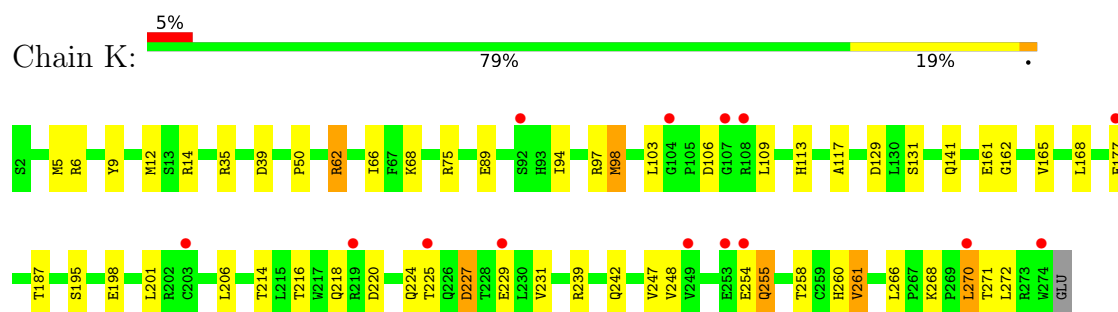
- Molecule 1: HLA-B35



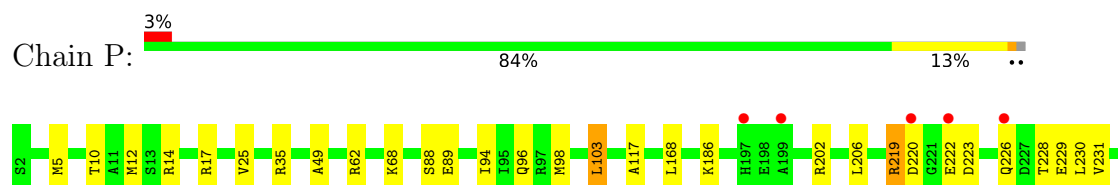
- Molecule 1: HLA-B35

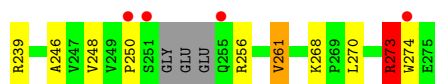


- Molecule 1: HLA-B35

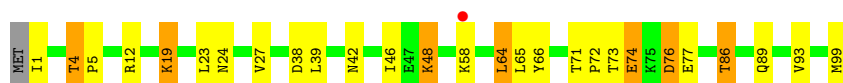


- Molecule 1: HLA-B35

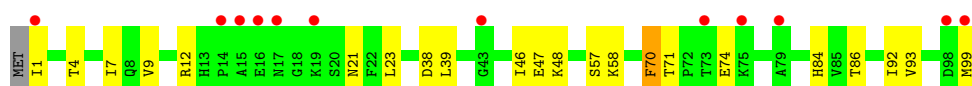
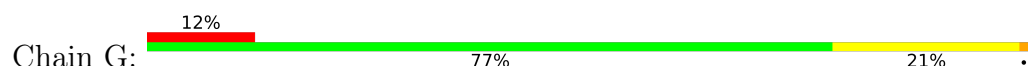




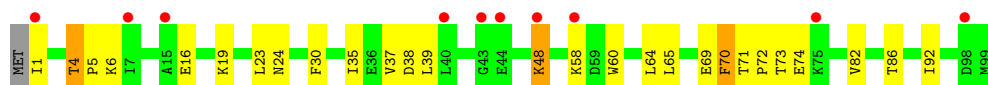
- Molecule 2: Beta-2-microglobulin



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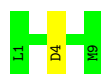
- Molecule 2: Beta-2-microglobulin



- Molecule 3: NP6 epitope H1N1



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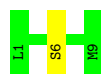
- Molecule 3: NP6 epitope H1N1

Chain M:  78% 22%



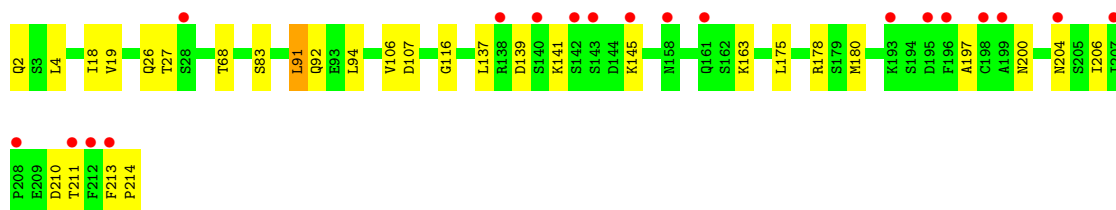
- Molecule 3: NP6 epitope H1N1

Chain R:  89% 11%



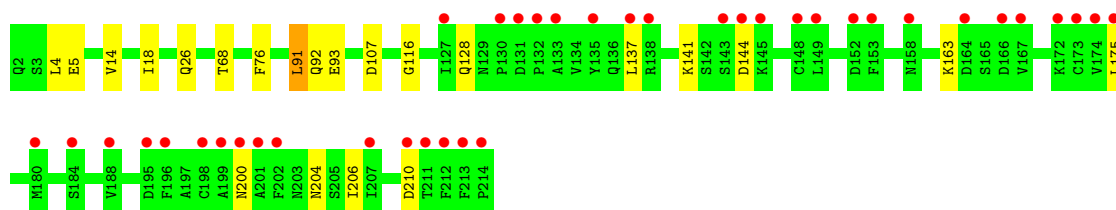
- Molecule 4: D1 TCR alpha chain

Chain D:  10% 85% 15%



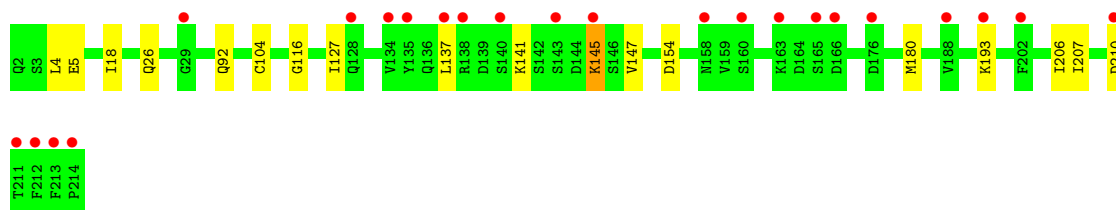
- Molecule 4: D1 TCR alpha chain

Chain I:  20% 89% 11%



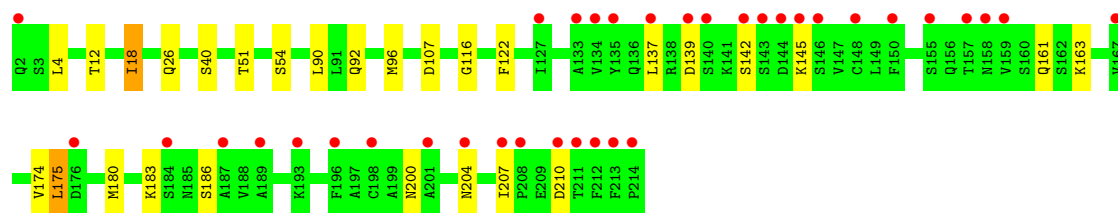
- Molecule 4: D1 TCR alpha chain

Chain N:  12% 91% 9%

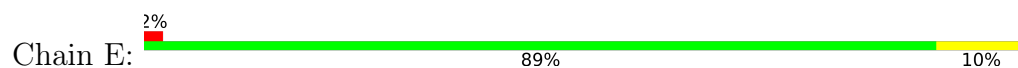


- Molecule 4: D1 TCR alpha chain

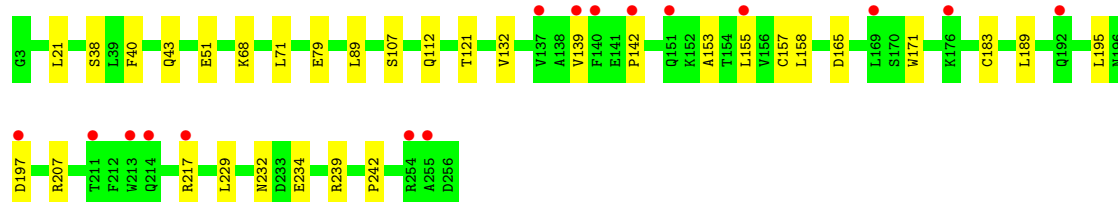
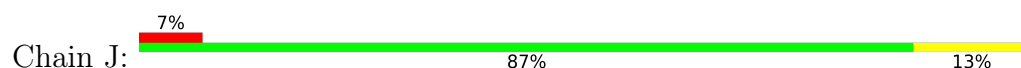
Chain S:  18% 86% 13%



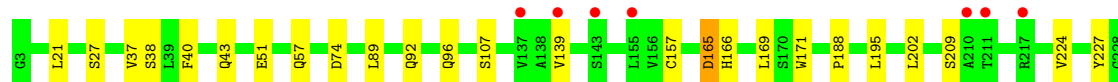
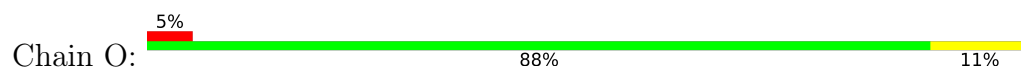
● Molecule 5: D1 TCR beta chain



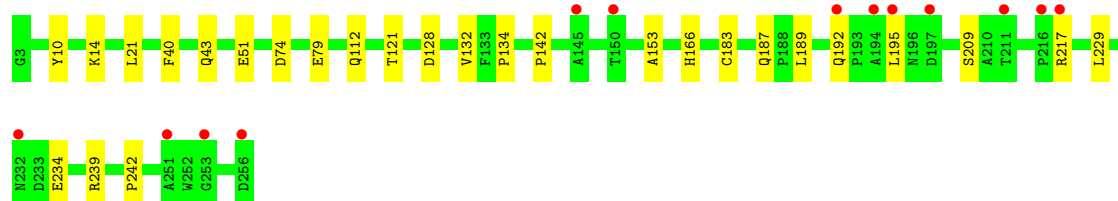
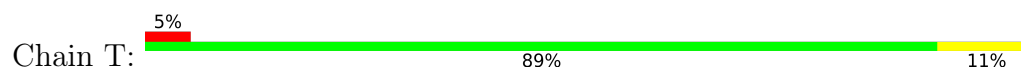
● Molecule 5: D1 TCR beta chain



● Molecule 5: D1 TCR beta chain



● Molecule 5: D1 TCR beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	78.58Å 192.16Å 252.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.59 – 2.65 38.59 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.59-2.65) 99.9 (38.59-2.65)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.65Å)	Xtrriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, R_{free}	0.218 , 0.265 0.215 , 0.261	Depositor DCC
R_{free} test set	5599 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtrriage
Anisotropy	0.644	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27419	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.9819e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

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	0.69	0/2303	1.19	7/3132 (0.2%)
1	F	0.72	0/2303	1.22	5/3132 (0.2%)
1	K	0.70	0/2295	1.20	3/3121 (0.1%)
1	P	0.69	0/2282	1.19	5/3101 (0.2%)
2	B	0.67	0/852	1.17	0/1152
2	G	0.72	0/852	1.17	3/1152 (0.3%)
2	L	0.68	0/852	1.18	3/1152 (0.3%)
2	Q	0.67	0/852	1.20	6/1152 (0.5%)
3	C	0.81	0/73	0.86	0/96
3	H	0.68	0/73	1.04	0/96
3	M	0.87	0/73	1.04	0/96
3	R	0.68	0/73	0.98	0/96
4	D	0.71	0/1580	1.09	1/2139 (0.0%)
4	I	0.70	0/1580	1.09	3/2139 (0.1%)
4	N	0.70	0/1580	1.12	1/2139 (0.0%)
4	S	0.70	0/1580	1.10	3/2139 (0.1%)
5	E	0.65	0/1985	1.07	2/2700 (0.1%)
5	J	0.64	0/1994	1.10	4/2712 (0.1%)
5	O	0.66	0/1994	1.09	2/2712 (0.1%)
5	T	0.63	0/1994	1.08	3/2712 (0.1%)
All	All	0.68	0/27170	1.14	51/36870 (0.1%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	220	ASP	CA-CB-CG	8.54	121.14	112.60
1	K	162	GLY	N-CA-C	8.03	117.51	110.21
2	Q	76	ASP	CA-CB-CG	7.47	120.07	112.60
5	J	79	GLU	CA-C-N	7.29	128.70	122.28
5	J	79	GLU	C-N-CA	7.29	128.70	122.28
4	N	145	LYS	N-CA-C	7.12	119.01	110.19
5	T	79	GLU	CA-C-N	6.73	128.63	122.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	T	79	GLU	C-N-CA	6.73	128.63	122.37
2	G	70	PHE	CA-CB-CG	6.45	120.25	113.80
1	F	224	GLN	CA-C-N	6.39	129.13	120.38
1	F	224	GLN	C-N-CA	6.39	129.13	120.38
2	L	70	PHE	CA-CB-CG	6.09	119.89	113.80
5	O	165	ASP	CA-CB-CG	6.09	118.69	112.60
2	Q	96	ASP	CA-C-N	5.64	127.84	120.28
2	Q	96	ASP	C-N-CA	5.64	127.84	120.28
5	E	165	ASP	CA-CB-CG	5.56	118.16	112.60
1	A	105	PRO	CA-C-N	5.55	129.48	120.60
1	A	105	PRO	C-N-CA	5.55	129.48	120.60
1	P	273	ARG	CA-C-N	5.48	132.00	121.54
1	P	273	ARG	C-N-CA	5.48	132.00	121.54
5	J	40	PHE	CA-CB-CG	5.46	119.26	113.80
5	T	40	PHE	CA-CB-CG	5.38	119.18	113.80
1	A	165	VAL	CA-C-N	5.37	127.42	120.44
1	A	165	VAL	C-N-CA	5.37	127.42	120.44
5	J	165	ASP	CA-CB-CG	5.34	117.94	112.60
1	F	62	ARG	CB-CG-CD	5.33	123.57	111.30
2	L	73	THR	CA-C-N	5.33	128.82	120.82
2	L	73	THR	C-N-CA	5.33	128.82	120.82
4	S	200	ASN	CA-C-N	5.33	127.68	120.38
4	S	200	ASN	C-N-CA	5.33	127.68	120.38
4	I	144	ASP	CA-CB-CG	5.32	117.92	112.60
5	O	40	PHE	CA-CB-CG	5.27	119.07	113.80
2	G	57	SER	CA-C-N	5.22	127.54	120.38
2	G	57	SER	C-N-CA	5.22	127.54	120.38
1	K	129	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	195	SER	CA-C-N	5.20	127.51	120.44
1	A	195	SER	C-N-CA	5.20	127.51	120.44
1	F	162	GLY	CA-C-N	5.19	127.54	120.54
1	F	162	GLY	C-N-CA	5.19	127.54	120.54
1	K	227	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	227	ASP	CA-CB-CG	5.13	117.73	112.60
4	S	139	ASP	CA-CB-CG	5.09	117.69	112.60
1	P	219	ARG	CA-C-N	5.08	131.25	121.54
1	P	219	ARG	C-N-CA	5.08	131.25	121.54
2	Q	57	SER	CA-C-N	5.05	127.55	120.28
2	Q	57	SER	C-N-CA	5.05	127.55	120.28
2	Q	70	PHE	CA-CB-CG	5.04	118.84	113.80
4	D	139	ASP	CA-CB-CG	5.03	117.63	112.60
5	E	40	PHE	CA-CB-CG	5.03	118.83	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	200	ASN	CA-C-N	5.03	128.36	120.82
4	I	200	ASN	C-N-CA	5.03	128.36	120.82

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	2241	0	2101	21	0
1	F	2241	0	2103	18	0
1	K	2233	0	2100	25	0
1	P	2221	0	2090	11	0
2	B	829	0	794	11	0
2	G	829	0	794	4	0
2	L	829	0	794	8	0
2	Q	829	0	794	17	0
3	C	72	0	76	2	0
3	H	72	0	76	1	0
3	M	72	0	76	1	0
3	R	72	0	76	0	0
4	D	1546	0	1437	11	0
4	I	1546	0	1437	8	0
4	N	1546	0	1437	8	0
4	S	1546	0	1437	9	0
5	E	1933	0	1832	10	0
5	J	1942	0	1837	15	0
5	O	1942	0	1837	10	0
5	T	1942	0	1837	14	0
6	A	61	0	0	0	0
6	B	29	0	0	0	0
6	C	1	0	0	0	0
6	D	44	0	0	0	0
6	E	50	0	0	0	0
6	F	83	0	0	0	0
6	G	22	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	6	0	0	0	0
6	I	65	0	0	0	0
6	J	73	0	0	0	0
6	K	86	0	0	1	0
6	L	14	0	0	0	0
6	M	5	0	0	0	0
6	N	58	0	0	0	0
6	O	73	0	0	0	0
6	P	89	0	0	0	0
6	Q	31	0	0	0	0
6	R	6	0	0	0	0
6	S	54	0	0	0	0
6	T	86	0	0	0	0
All	All	27419	0	24965	178	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 3.

All (178) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:42:ASN:HD21	2:Q:76:ASP:HB2	1.20	1.05
2:Q:42:ASN:HD21	2:Q:76:ASP:CB	1.71	1.03
2:Q:42:ASN:ND2	2:Q:76:ASP:HB2	1.82	0.92
1:A:255:GLN:HG3	1:K:255:GLN:HG2	1.53	0.86
2:G:4:THR:HA	2:G:86:THR:HG21	1.60	0.84
2:L:4:THR:HA	2:L:86:THR:HG21	1.60	0.82
1:F:251:SER:HA	1:F:254:GLU:OE2	1.80	0.80
1:F:62:ARG:NH1	3:H:4:ASP:OD2	2.16	0.79
2:Q:4:THR:HA	2:Q:86:THR:HG21	1.65	0.78
2:B:4:THR:HA	2:B:86:THR:HG21	1.67	0.77
1:K:201:LEU:HD11	1:K:254:GLU:HG3	1.67	0.76
1:A:62:ARG:NH2	3:C:4:ASP:OD2	2.21	0.73
1:K:62:ARG:HG2	1:K:62:ARG:HH11	1.52	0.73
1:K:255:GLN:H	1:K:255:GLN:CD	1.96	0.72
1:A:273:ARG:HH11	1:A:273:ARG:HG3	1.55	0.71
1:A:255:GLN:HG3	1:K:255:GLN:CG	2.21	0.70
5:T:21:LEU:HD22	5:T:121:THR:HG21	1.75	0.69
1:F:195:SER:HB3	1:F:198:GLU:HB3	1.75	0.69
2:Q:42:ASN:HD21	2:Q:76:ASP:HB3	1.58	0.68
1:K:113:HIS:HD2	6:K:301:HOH:O	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:132:VAL:HG23	5:J:242:PRO:HG2	1.81	0.63
1:K:62:ARG:HH11	1:K:62:ARG:CG	2.12	0.62
1:P:49:ALA:HA	1:P:239:ARG:HH12	1.64	0.62
5:J:21:LEU:HD22	5:J:121:THR:HG21	1.82	0.61
1:P:261:VAL:HG13	1:P:270:LEU:HB3	1.82	0.61
4:S:175:LEU:HB3	5:T:183[A]:CYS:HB2	1.83	0.60
1:F:221:GLY:HA3	1:K:258:THR:HG21	1.84	0.60
2:Q:27:VAL:HG21	2:Q:37:VAL:HG21	1.83	0.60
4:S:175:LEU:HB3	5:T:183[B]:CYS:HB2	1.83	0.60
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.84	0.59
4:S:180:MET:HE1	5:T:209:SER:HB3	1.83	0.59
1:A:195:SER:HB3	1:A:198:GLU:HB2	1.85	0.59
1:P:202:ARG:HD3	1:P:246:ALA:HB2	1.85	0.58
1:A:255:GLN:HG3	1:K:255:GLN:CD	2.28	0.58
1:F:255:GLN:H	1:F:255:GLN:CD	2.11	0.58
1:K:187:THR:HG21	1:K:261:VAL:HG11	1.85	0.58
1:K:50:PRO:HD3	1:K:239:ARG:HH12	1.68	0.57
1:A:12:MET:HG3	1:A:94:ILE:HG12	1.86	0.57
4:D:175:LEU:HB3	5:E:183[A]:CYS:HB2	1.85	0.57
4:D:175:LEU:HB3	5:E:183[B]:CYS:HB2	1.85	0.57
1:K:62:ARG:HG2	1:K:62:ARG:NH1	2.19	0.56
5:T:132:VAL:HG23	5:T:242:PRO:HG2	1.86	0.56
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.87	0.56
1:F:222:GLU:HB3	1:K:271:THR:HG21	1.88	0.56
1:A:187:THR:HG21	1:A:261:VAL:HG11	1.88	0.55
2:L:24:ASN:HB3	2:L:65:LEU:HD11	1.89	0.55
1:F:5:MET:HB2	1:F:168:LEU:HD13	1.88	0.55
1:P:5:MET:HB2	1:P:168:LEU:HD13	1.89	0.55
4:I:4:LEU:HD11	4:I:116:GLY:HA3	1.90	0.54
5:O:157:CYS:HB2	5:O:171:TRP:CZ2	2.42	0.54
4:D:180:MET:HE1	5:E:209:SER:HB3	1.89	0.54
5:J:157:CYS:HB2	5:J:171:TRP:CZ2	2.43	0.54
2:Q:64:LEU:HD13	2:Q:66:TYR:HE1	1.72	0.54
4:S:18:ILE:HG13	4:S:92:GLN:HA	1.90	0.53
1:A:109:LEU:HD22	1:A:161:GLU:HA	1.90	0.53
2:Q:24:ASN:HB3	2:Q:65:LEU:HD11	1.90	0.53
2:L:5:PRO:HB3	2:L:30:PHE:HB3	1.89	0.53
1:A:66:ILE:HG12	3:C:4:ASP:OD1	2.08	0.53
4:I:137:LEU:HD22	5:J:142:PRO:HA	1.90	0.52
5:T:14:LYS:HG3	5:T:128:ASP:HA	1.90	0.52
2:Q:39:LEU:HD23	2:Q:68:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:N:4:LEU:HD11	4:N:116:GLY:CA	2.40	0.52
1:F:197:HIS:HA	1:F:251:SER:HB3	1.92	0.51
4:N:4:LEU:HD11	4:N:116:GLY:HA3	1.91	0.51
4:I:4:LEU:HD11	4:I:116:GLY:CA	2.41	0.51
1:F:187:THR:HG21	1:F:261:VAL:HG11	1.93	0.51
4:N:180:MET:HE1	5:O:209:SER:HB3	1.92	0.51
1:A:261:VAL:HG13	1:A:270:LEU:HB3	1.93	0.50
5:J:239:ARG:HH12	5:J:242:PRO:HG3	1.77	0.50
2:B:73:THR:HB	2:B:76:ASP:OD1	2.11	0.50
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.94	0.50
4:N:4:LEU:HD13	4:N:104[A]:CYS:SG	2.51	0.50
2:Q:12:ARG:HB2	2:Q:22:PHE:HB2	1.93	0.50
4:S:12:THR:HG23	4:S:122:PHE:HB2	1.92	0.50
4:D:107:ASP:HB3	5:E:112:GLN:OE1	2.12	0.49
4:N:18:ILE:HG22	4:N:92:GLN:HA	1.94	0.49
1:F:109:LEU:HB2	1:F:165:VAL:HG21	1.95	0.49
1:F:249:VAL:HG11	1:F:257:TYR:CE2	2.47	0.49
1:P:12:MET:HG3	1:P:94:ILE:HG12	1.94	0.49
1:K:218:GLN:HB2	1:K:260:HIS:HE1	1.78	0.49
1:K:12:MET:HG3	1:K:94:ILE:HG12	1.95	0.49
4:D:91:LEU:HD12	4:D:94:LEU:HD21	1.95	0.48
5:O:188:PRO:HB3	5:O:202:LEU:HB2	1.96	0.48
5:O:43:GLN:O	5:O:51[A]:GLU:HG2	2.14	0.48
1:A:14:ARG:HB2	1:A:17:ARG:HB2	1.96	0.48
4:I:175:LEU:HB3	5:J:183[A]:CYS:HB2	1.96	0.48
4:I:175:LEU:HB3	5:J:183[B]:CYS:HB2	1.96	0.48
2:Q:84:HIS:HB3	2:Q:86:THR:HG22	1.96	0.48
4:D:4:LEU:HD11	4:D:116:GLY:CA	2.44	0.48
1:P:14:ARG:HB2	1:P:17:ARG:HB2	1.97	0.47
5:J:68:LYS:HB2	5:J:71:LEU:HD12	1.96	0.47
4:S:137:LEU:HD22	5:T:142:PRO:HA	1.96	0.47
5:T:10:TYR:HB3	5:T:166:HIS:CD2	2.50	0.47
2:B:64:LEU:HD13	2:B:66:TYR:HE1	1.78	0.47
2:G:9:VAL:HG12	2:G:93:VAL:HG12	1.96	0.47
2:Q:48:LYS:HD3	2:Q:48:LYS:HA	1.45	0.47
1:F:247:VAL:HB	1:F:249:VAL:HG13	1.95	0.47
1:K:117:ALA:HB2	2:L:60:TRP:CE2	2.50	0.47
2:L:19:LYS:O	2:L:72:PRO:HD2	2.15	0.47
2:B:5:PRO:HD3	2:B:86:THR:HG21	1.97	0.47
1:K:195:SER:HB3	1:K:198:GLU:HB2	1.97	0.46
1:K:255:GLN:CD	1:K:255:GLN:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:37:VAL:HG22	2:L:82:VAL:HG22	1.96	0.46
2:L:48:LYS:HA	2:L:48:LYS:HD3	1.49	0.46
4:N:137:LEU:HD12	4:N:147:VAL:HG12	1.98	0.46
5:J:38:SER:HB2	5:J:107:SER:HB2	1.98	0.46
1:F:191:HIS:CD2	1:F:254:GLU:HG2	2.51	0.46
5:T:239:ARG:HH12	5:T:242:PRO:HG3	1.80	0.46
1:A:103:LEU:HD11	1:A:165:VAL:HG13	1.97	0.46
5:E:21:LEU:HD12	5:E:89:LEU:HD23	1.99	0.45
1:K:266:LEU:HD22	1:K:270:LEU:HD13	1.98	0.45
2:G:23:LEU:HD23	2:G:39:LEU:HD23	1.99	0.45
5:T:229:LEU:HD22	5:T:242:PRO:HD2	1.97	0.45
5:E:157:CYS:HB2	5:E:171:TRP:CZ2	2.52	0.45
5:J:142:PRO:HD3	5:J:155:LEU:HG	1.98	0.45
1:P:273:ARG:O	1:P:273:ARG:HG2	2.15	0.45
1:P:103:LEU:HD13	1:P:168:LEU:HD23	1.99	0.45
5:E:192:GLN:HE21	5:E:195:LEU:HD22	1.81	0.45
1:F:14:ARG:HB2	1:F:17:ARG:HB2	1.99	0.45
4:S:107:ASP:HB3	5:T:112:GLN:OE1	2.17	0.45
5:T:142:PRO:HG2	5:T:153:ALA:HB1	1.99	0.45
5:E:68:LYS:HB2	5:E:71:LEU:HD12	1.99	0.45
2:B:48:LYS:HD3	2:B:48:LYS:HA	1.44	0.44
1:K:66:ILE:HG12	3:M:4:ASP:OD1	2.18	0.44
1:P:10:THR:HG21	2:Q:62:PHE:HE1	1.83	0.44
4:I:18:ILE:HG22	4:I:92:GLN:HA	2.00	0.44
4:I:107:ASP:HB3	5:J:112:GLN:OE1	2.18	0.44
4:D:4:LEU:HD23	4:D:106:VAL:HG12	1.99	0.43
5:E:14:LYS:HG3	5:E:128:ASP:HA	2.00	0.43
4:I:76:PHE:CD2	4:I:91:LEU:HD22	2.53	0.43
1:P:10:THR:HG22	1:P:96:GLN:HG2	2.00	0.43
1:F:266:LEU:HD22	1:F:270:LEU:HD13	1.98	0.43
4:D:4:LEU:HD11	4:D:116:GLY:HA3	2.00	0.43
1:K:6:ARG:HB3	1:K:98:MET:HE3	2.00	0.43
5:O:38:SER:HB2	5:O:107:SER:HB2	2.01	0.43
2:Q:36:GLU:HB2	2:Q:83:ASN:HB3	2.01	0.43
5:T:134:PRO:HD3	5:T:242:PRO:HB3	2.00	0.43
1:A:218:GLN:HA	1:A:222:GLU:O	2.19	0.43
1:K:9:TYR:HB2	1:K:97:ARG:HB3	2.01	0.43
2:Q:42:ASN:ND2	2:Q:76:ASP:CB	2.52	0.43
2:B:39:LEU:HB3	2:B:46:ILE:HD12	2.01	0.42
4:N:145:LYS:HD3	4:N:145:LYS:H	1.84	0.42
1:A:219:ARG:HG3	1:A:257:TYR:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASP:HB2	1:A:108:ARG:HG2	2.02	0.42
5:O:229:LEU:HD13	5:O:242:PRO:HG2	2.00	0.42
5:O:21:LEU:HD12	5:O:89:LEU:HD23	2.02	0.42
5:T:43:GLN:O	5:T:51[A]:GLU:HG2	2.20	0.42
2:B:19:LYS:O	2:B:72:PRO:HD2	2.20	0.42
4:D:2:GLN:HA	4:D:27:THR:HG22	2.02	0.42
5:E:192:GLN:HB3	5:E:195:LEU:HD13	2.01	0.42
1:F:251:SER:HA	1:F:254:GLU:CD	2.44	0.42
4:N:127:ILE:HD13	4:N:154:ASP:HA	2.02	0.42
1:A:215:LEU:HD12	1:A:243:LYS:HD2	2.02	0.42
2:B:74:GLU:H	2:B:74:GLU:HG3	1.69	0.41
4:D:197:ALA:HB3	4:D:200:ASN:HD21	1.85	0.41
5:J:153:ALA:O	5:J:207:ARG:HA	2.19	0.41
1:K:109:LEU:HB2	1:K:165:VAL:HG21	2.00	0.41
5:J:43:GLN:HB3	5:J:51[A]:GLU:HG3	2.02	0.41
1:A:138:THR:HA	1:A:141:GLN:HG3	2.02	0.41
2:B:23:LEU:HD23	2:B:39:LEU:HD23	2.01	0.41
5:O:169:LEU:HG	5:O:224:VAL:HG22	2.02	0.41
2:B:42:ASN:HA	2:B:77:GLU:HG3	2.01	0.41
2:G:84:HIS:ND1	2:G:86:THR:HG22	2.36	0.41
1:A:103:LEU:HD13	1:A:168:LEU:HD23	2.02	0.41
4:D:213:PHE:HA	4:D:214:PRO:HD3	1.92	0.41
1:F:263:HIS:HD1	1:F:265:GLY:H	1.69	0.41
1:P:117:ALA:HB2	2:Q:60:TRP:CE2	2.56	0.41
1:A:231:VAL:HG12	1:A:244:TRP:H	1.86	0.41
1:K:109:LEU:HD22	1:K:161:GLU:HA	2.01	0.41
2:L:23:LEU:HD23	2:L:39:LEU:HD23	2.03	0.41
5:O:37:VAL:HG12	5:O:57:GLN:HG2	2.02	0.41
4:S:4:LEU:HD11	4:S:116:GLY:CA	2.50	0.41
2:Q:7:ILE:CG2	2:Q:93:VAL:HG11	2.50	0.41
5:J:21:LEU:HD12	5:J:89:LEU:HD23	2.03	0.40
5:O:166:HIS:HB3	5:O:227:TYR:HB2	2.03	0.40
4:S:96:MET:HE3	4:S:183:LYS:HD3	2.02	0.40
1:F:197:HIS:CA	1:F:251:SER:HB3	2.51	0.40
5:J:132:VAL:HG21	5:J:229:LEU:CD1	2.51	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	272/274 (99%)	266 (98%)	6 (2%)	0	100	100
1	F	272/274 (99%)	262 (96%)	8 (3%)	2 (1%)	18	30
1	K	271/274 (99%)	259 (96%)	12 (4%)	0	100	100
1	P	267/274 (97%)	255 (96%)	10 (4%)	2 (1%)	18	30
2	B	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	G	97/100 (97%)	91 (94%)	6 (6%)	0	100	100
2	L	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
2	Q	97/100 (97%)	92 (95%)	4 (4%)	1 (1%)	12	20
3	C	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	H	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	M	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	R	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
4	D	197/197 (100%)	187 (95%)	10 (5%)	0	100	100
4	I	197/197 (100%)	185 (94%)	12 (6%)	0	100	100
4	N	197/197 (100%)	182 (92%)	15 (8%)	0	100	100
4	S	197/197 (100%)	183 (93%)	13 (7%)	1 (0%)	24	39
5	E	242/242 (100%)	228 (94%)	14 (6%)	0	100	100
5	J	243/242 (100%)	234 (96%)	9 (4%)	0	100	100
5	O	243/242 (100%)	234 (96%)	8 (3%)	1 (0%)	30	45
5	T	243/242 (100%)	233 (96%)	10 (4%)	0	100	100
All	All	3257/3288 (99%)	3101 (95%)	149 (5%)	7 (0%)	43	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	274	TRP

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Mol	Chain	Res	Type
1	P	250	PRO
2	Q	18	GLY
4	S	142	SER
5	O	165	ASP
1	F	196	ASP
1	F	107	GLY

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	233/233 (100%)	203 (87%)	30 (13%)	4	6
1	F	233/233 (100%)	202 (87%)	31 (13%)	4	6
1	K	232/233 (100%)	202 (87%)	30 (13%)	4	6
1	P	231/233 (99%)	208 (90%)	23 (10%)	7	11
2	B	94/95 (99%)	78 (83%)	16 (17%)	2	2
2	G	94/95 (99%)	80 (85%)	14 (15%)	3	4
2	L	94/95 (99%)	80 (85%)	14 (15%)	3	4
2	Q	94/95 (99%)	79 (84%)	15 (16%)	2	3
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	1
3	H	9/9 (100%)	9 (100%)	0	100	100
3	M	9/9 (100%)	8 (89%)	1 (11%)	6	9
3	R	9/9 (100%)	8 (89%)	1 (11%)	6	9
4	D	173/171 (101%)	157 (91%)	16 (9%)	8	14
4	I	173/171 (101%)	161 (93%)	12 (7%)	14	24
4	N	173/171 (101%)	166 (96%)	7 (4%)	28	47
4	S	173/171 (101%)	158 (91%)	15 (9%)	9	16
5	E	210/208 (101%)	198 (94%)	12 (6%)	18	32
5	J	211/208 (101%)	203 (96%)	8 (4%)	29	49
5	O	211/208 (101%)	204 (97%)	7 (3%)	33	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	T	211/208 (101%)	204 (97%)	7 (3%)	33	55
All	All	2876/2864 (100%)	2615 (91%)	261 (9%)	9	14

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	VAL
1	A	35	ARG
1	A	42	SER
1	A	48	ARG
1	A	98	MET
1	A	103	LEU
1	A	106	ASP
1	A	108	ARG
1	A	110	LEU
1	A	115	GLN
1	A	131	SER
1	A	138	THR
1	A	141	GLN
1	A	173	GLU
1	A	186	LYS
1	A	189	VAL
1	A	196	ASP
1	A	214	THR
1	A	224	GLN
1	A	225	THR
1	A	227	ASP
1	A	230	LEU
1	A	231	VAL
1	A	243	LYS
1	A	247	VAL
1	A	261	VAL
1	A	268	LYS
1	A	272	LEU
1	A	273	ARG
1	A	274	TRP
2	B	1	ILE
2	B	4	THR
2	B	12	ARG
2	B	19	LYS
2	B	27	VAL
2	B	38	ASP

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Mol	Chain	Res	Type
2	B	48	LYS
2	B	58	LYS
2	B	64	LEU
2	B	71	THR
2	B	74	GLU
2	B	76	ASP
2	B	86	THR
2	B	89	GLN
2	B	93	VAL
2	B	99	MET
3	C	6	SER
3	C	7	THR
4	D	18	ILE
4	D	19	VAL
4	D	26	GLN
4	D	68	THR
4	D	83	SER
4	D	91	LEU
4	D	92	GLN
4	D	137	LEU
4	D	141	LYS
4	D	145	LYS
4	D	163	LYS
4	D	178	ARG
4	D	204	ASN
4	D	206	ILE
4	D	210	ASP
4	D	211	THR
5	E	57	GLN
5	E	74	ASP
5	E	83	GLU
5	E	92	GLN
5	E	96	GLN
5	E	131	ASN
5	E	158	LEU
5	E	160	THR
5	E	192	GLN
5	E	203	SER
5	E	223	GLN
5	E	254	ARG
1	F	12	MET
1	F	25	VAL

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Mol	Chain	Res	Type
1	F	35	ARG
1	F	62	ARG
1	F	89	GLU
1	F	98	MET
1	F	103	LEU
1	F	106	ASP
1	F	108	ARG
1	F	115	GLN
1	F	131	SER
1	F	141	GLN
1	F	163	LEU
1	F	173	GLU
1	F	186	LYS
1	F	197	HIS
1	F	198	GLU
1	F	214	THR
1	F	219	ARG
1	F	222	GLU
1	F	223	ASP
1	F	226	GLN
1	F	230	LEU
1	F	231	VAL
1	F	247	VAL
1	F	255	GLN
1	F	261	VAL
1	F	268	LYS
1	F	270	LEU
1	F	272	LEU
1	F	273	ARG
2	G	1	ILE
2	G	7	ILE
2	G	12	ARG
2	G	21	ASN
2	G	38	ASP
2	G	46	ILE
2	G	47	GLU
2	G	48	LYS
2	G	58	LYS
2	G	70	PHE
2	G	71	THR
2	G	74	GLU
2	G	92	ILE

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Mol	Chain	Res	Type
2	G	99	MET
4	I	5	GLU
4	I	14	VAL
4	I	26	GLN
4	I	68	THR
4	I	91	LEU
4	I	93	GLU
4	I	128	GLN
4	I	141	LYS
4	I	163	LYS
4	I	204	ASN
4	I	206	ILE
4	I	210	ASP
5	J	139	VAL
5	J	158	LEU
5	J	189	LEU
5	J	195	LEU
5	J	197	ASP
5	J	217	ARG
5	J	232	ASN
5	J	234	GLU
1	K	14	ARG
1	K	35	ARG
1	K	39	ASP
1	K	62	ARG
1	K	68	LYS
1	K	75	ARG
1	K	89	GLU
1	K	98	MET
1	K	103	LEU
1	K	106	ASP
1	K	131	SER
1	K	141	GLN
1	K	177	GLU
1	K	206	LEU
1	K	214	THR
1	K	216	THR
1	K	220	ASP
1	K	224	GLN
1	K	225	THR
1	K	227	ASP
1	K	229	GLU

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Mol	Chain	Res	Type
1	K	231	VAL
1	K	242	GLN
1	K	247	VAL
1	K	248	VAL
1	K	255	GLN
1	K	261	VAL
1	K	268	LYS
1	K	270	LEU
1	K	272	LEU
2	L	1	ILE
2	L	4	THR
2	L	6	LYS
2	L	16	GLU
2	L	35	ILE
2	L	38	ASP
2	L	48	LYS
2	L	58	LYS
2	L	64	LEU
2	L	69	GLU
2	L	70	PHE
2	L	71	THR
2	L	74	GLU
2	L	92	ILE
3	M	6	SER
4	N	5	GLU
4	N	26	GLN
4	N	141	LYS
4	N	193	LYS
4	N	206	ILE
4	N	207	ILE
4	N	210	ASP
5	O	27	SER
5	O	74	ASP
5	O	92	GLN
5	O	96	GLN
5	O	139	VAL
5	O	195	LEU
5	O	230	SER
1	P	25	VAL
1	P	35	ARG
1	P	62	ARG
1	P	68	LYS

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Mol	Chain	Res	Type
1	P	88	SER
1	P	89	GLU
1	P	98	MET
1	P	103	LEU
1	P	186	LYS
1	P	206	LEU
1	P	219	ARG
1	P	222	GLU
1	P	223	ASP
1	P	226	GLN
1	P	228	THR
1	P	229	GLU
1	P	230	LEU
1	P	231	VAL
1	P	248	VAL
1	P	256	ARG
1	P	261	VAL
1	P	268	LYS
1	P	273	ARG
2	Q	4	THR
2	Q	6	LYS
2	Q	7	ILE
2	Q	12	ARG
2	Q	19	LYS
2	Q	27	VAL
2	Q	38	ASP
2	Q	40	LEU
2	Q	41	LYS
2	Q	48	LYS
2	Q	58	LYS
2	Q	64	LEU
2	Q	69	GLU
2	Q	74	GLU
2	Q	75	LYS
3	R	6	SER
4	S	18	ILE
4	S	26	GLN
4	S	40	SER
4	S	51	THR
4	S	54	SER
4	S	90	LEU
4	S	145	LYS

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Mol	Chain	Res	Type
4	S	161	GLN
4	S	163	LYS
4	S	174	VAL
4	S	175	LEU
4	S	186	SER
4	S	204	ASN
4	S	207	ILE
4	S	210	ASP
5	T	74	ASP
5	T	187	GLN
5	T	189	LEU
5	T	192	GLN
5	T	195	LEU
5	T	217	ARG
5	T	234	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	65	GLN
1	A	72	GLN
1	A	141	GLN
1	A	180	GLN
1	A	188	HIS
1	A	260	HIS
2	B	13	HIS
4	D	20	GLN
4	D	26	GLN
4	D	43	GLN
4	D	200	ASN
5	E	57	GLN
5	E	58	ASN
5	E	179	HIS
5	E	192	GLN
1	F	72	GLN
1	F	86	ASN
1	F	141	GLN
1	F	144	GLN
1	F	180	GLN
1	F	197	HIS
4	I	2	GLN

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Mol	Chain	Res	Type
4	I	20	GLN
4	I	92	GLN
4	I	95	GLN
5	J	57	GLN
5	J	58	ASN
5	J	179	HIS
5	J	225	GLN
1	K	87	GLN
1	K	113	HIS
1	K	180	GLN
1	K	260	HIS
4	N	2	GLN
4	N	26	GLN
4	N	44	GLN
4	N	56	ASN
5	O	44	GLN
5	O	115	GLN
5	O	151	GLN
5	O	166	HIS
5	O	232	ASN
1	P	32	GLN
1	P	180	GLN
1	P	191	HIS
1	P	192	HIS
2	Q	8	GLN
2	Q	13	HIS
2	Q	42	ASN
4	S	2	GLN
4	S	20	GLN
4	S	43	GLN
4	S	126	ASN
4	S	128	GLN
4	S	204	ASN
5	T	58	ASN
5	T	115	GLN
5	T	225	GLN

5.3.3 RNA ⓘ

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	273/274 (99%)	0.26	4 (1%) 72 67	19, 39, 74, 110	2 (0%)
1	F	273/274 (99%)	0.35	17 (6%) 26 20	18, 36, 89, 123	3 (1%)
1	K	273/274 (99%)	0.44	14 (5%) 33 26	20, 38, 90, 114	2 (0%)
1	P	271/274 (98%)	0.18	9 (3%) 49 40	20, 33, 77, 108	1 (0%)
2	B	99/100 (99%)	0.20	1 (1%) 79 76	25, 41, 70, 80	0
2	G	99/100 (99%)	0.79	12 (12%) 8 7	21, 48, 84, 97	0
2	L	99/100 (99%)	0.74	10 (10%) 12 10	23, 54, 95, 104	0
2	Q	99/100 (99%)	0.26	2 (2%) 65 59	21, 38, 76, 84	0
3	C	9/9 (100%)	-0.02	0 100 100	24, 26, 31, 33	0
3	H	9/9 (100%)	-0.12	0 100 100	20, 21, 23, 27	0
3	M	9/9 (100%)	-0.02	0 100 100	22, 23, 26, 29	0
3	R	9/9 (100%)	-0.18	0 100 100	21, 21, 26, 29	0
4	D	197/197 (100%)	0.54	19 (9%) 13 11	11, 39, 117, 136	2 (1%)
4	I	197/197 (100%)	0.83	39 (19%) 3 2	11, 39, 128, 149	2 (1%)
4	N	197/197 (100%)	0.65	23 (11%) 9 7	11, 39, 120, 146	2 (1%)
4	S	197/197 (100%)	0.81	36 (18%) 3 2	11, 40, 129, 157	2 (1%)
5	E	242/242 (100%)	0.24	5 (2%) 63 57	13, 41, 78, 118	2 (0%)
5	J	242/242 (100%)	0.55	16 (6%) 24 18	12, 51, 102, 149	3 (1%)
5	O	242/242 (100%)	0.35	11 (4%) 38 31	12, 45, 88, 134	3 (1%)
5	T	242/242 (100%)	0.35	13 (5%) 31 25	11, 41, 96, 137	3 (1%)
All	All	3278/3288 (99%)	0.44	231 (7%) 22 17	11, 40, 105, 157	27 (0%)

All (231) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	S	211	THR	4.3
5	E	143	SER	4.1
1	K	254	GLU	4.0
1	F	274	TRP	3.9
4	I	211	THR	3.9
1	P	255	GLN	3.7
1	K	225	THR	3.7
4	I	210	ASP	3.7
5	J	255	ALA	3.7
4	D	213	PHE	3.6
4	I	143	SER	3.6
5	J	137	VAL	3.6
1	K	104	GLY	3.5
2	G	16	GLU	3.5
1	K	253	GLU	3.4
4	N	137	LEU	3.4
4	S	204	ASN	3.4
1	A	274	TRP	3.3
4	S	143	SER	3.3
4	S	210	ASP	3.3
5	J	197	ASP	3.3
4	S	137	LEU	3.2
1	K	274	TRP	3.2
4	N	145	LYS	3.2
1	A	253	GLU	3.2
4	D	143	SER	3.2
4	D	199	ALA	3.2
4	N	143	SER	3.2
4	N	213	PHE	3.2
1	P	251	SER	3.1
4	S	134	VAL	3.1
4	I	145	LYS	3.1
5	J	192	GLN	3.1
4	S	176	ASP	3.0
4	N	158	ASN	3.0
4	N	140	SER	3.0
4	D	195	ASP	3.0
1	F	221	GLY	3.0
4	S	133	ALA	3.0
4	N	210	ASP	2.9
2	L	7	ILE	2.9
5	O	253	GLY	2.9
4	I	133	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
4	I	201	ALA	2.9
4	D	193	LYS	2.9
4	I	148	CYS	2.9
1	F	253	GLU	2.9
1	F	181	ARG	2.9
4	S	207	ILE	2.9
5	O	255	ALA	2.9
4	I	167	VAL	2.9
4	I	212	PHE	2.9
4	S	213	PHE	2.9
5	J	155	LEU	2.8
4	I	202	PHE	2.8
2	Q	44	GLU	2.8
1	P	274	TRP	2.8
2	G	17	ASN	2.8
4	N	211	THR	2.8
4	D	198	CYS	2.8
4	S	142	SER	2.8
4	S	155	SER	2.8
4	I	158	ASN	2.8
4	S	144	ASP	2.8
4	N	188	VAL	2.8
5	O	210	ALA	2.8
2	Q	43	GLY	2.7
4	I	164	ASP	2.7
1	K	108	ARG	2.7
4	I	213	PHE	2.7
4	S	196	PHE	2.7
5	J	211	THR	2.7
2	L	44	GLU	2.7
4	N	138	ARG	2.6
1	P	199	ALA	2.6
4	I	199	ALA	2.6
4	D	211	THR	2.6
2	G	99	MET	2.6
1	F	230	LEU	2.6
1	K	270	LEU	2.6
1	F	197	HIS	2.6
4	D	145	LYS	2.6
4	I	195	ASP	2.6
4	I	137	LEU	2.6
5	O	217	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
5	J	176	LYS	2.6
2	G	73	THR	2.5
4	S	2	GLN	2.6
1	F	106	ASP	2.5
5	O	155	LEU	2.5
2	B	58	LYS	2.5
1	F	194	VAL	2.5
4	S	198	CYS	2.5
5	E	192	GLN	2.5
5	J	151	GLN	2.5
4	S	140	SER	2.5
4	I	144	ASP	2.5
2	L	58	LYS	2.5
4	N	135	TYR	2.5
2	L	43	GLY	2.5
1	P	250	PRO	2.5
4	I	196	PHE	2.5
4	N	212	PHE	2.5
5	T	192	GLN	2.5
4	I	200	ASN	2.5
4	N	163	LYS	2.5
2	G	14	PRO	2.5
4	S	201	ALA	2.5
5	T	251	ALA	2.5
4	D	204	ASN	2.5
2	L	1	ILE	2.5
4	D	28	SER	2.5
4	I	149	LEU	2.5
1	F	249	VAL	2.5
4	N	128	GLN	2.5
5	J	139	VAL	2.5
5	J	217	ARG	2.4
1	F	192	HIS	2.4
2	G	98	ASP	2.4
4	S	139	ASP	2.4
5	T	197	ASP	2.4
1	F	248	VAL	2.4
1	P	226	GLN	2.4
4	I	188	VAL	2.4
2	L	15	ALA	2.4
4	D	196	PHE	2.4
4	S	158	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	105	PRO	2.4
4	I	130	PRO	2.4
2	G	79	ALA	2.4
4	D	140	SER	2.4
2	G	75	LYS	2.4
4	I	132	PRO	2.4
2	G	15	ALA	2.4
4	I	153	PHE	2.4
1	P	222	GLU	2.4
1	F	220	ASP	2.4
1	K	203	CYS	2.4
2	G	19	LYS	2.4
5	E	92	GLN	2.4
4	S	150	PHE	2.4
2	G	1	ILE	2.3
4	I	127	ILE	2.3
4	I	135	TYR	2.3
4	I	166	ASP	2.3
4	N	165	SER	2.3
4	N	29	GLY	2.3
5	O	137	VAL	2.3
5	O	139	VAL	2.3
4	I	175	LEU	2.3
4	S	189	ALA	2.3
5	E	251	ALA	2.3
5	J	169	LEU	2.3
5	T	195	LEU	2.3
5	T	211	THR	2.3
4	I	180	MET	2.3
4	S	145	LYS	2.3
1	F	193	PRO	2.3
4	N	166	ASP	2.3
1	K	219	ARG	2.3
5	J	214	GLN	2.3
4	D	212	PHE	2.3
4	N	202	PHE	2.3
4	I	207	ILE	2.3
4	S	187	ALA	2.3
4	S	157	THR	2.3
1	K	229	GLU	2.3
4	I	138	ARG	2.3
4	D	161	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
4	I	174	VAL	2.3
4	S	167	VAL	2.3
5	J	140	PHE	2.3
4	I	173	CYS	2.2
5	T	194	ALA	2.2
4	N	176	ASP	2.2
4	S	184	SER	2.2
1	A	252	GLY	2.2
2	G	43	GLY	2.2
2	L	40	LEU	2.2
4	S	212	PHE	2.2
1	P	197	HIS	2.2
1	A	35	ARG	2.2
4	D	208	PRO	2.2
5	T	145	ALA	2.2
1	K	177	GLU	2.2
5	J	254	ARG	2.2
5	T	216	PRO	2.2
1	F	104	GLY	2.2
1	P	220	ASP	2.2
4	D	142	SER	2.2
4	I	184	SER	2.2
5	O	143	SER	2.2
5	T	256	ASP	2.2
4	N	134	VAL	2.2
4	D	158	ASN	2.2
4	S	135	TYR	2.2
5	E	151	GLN	2.2
4	N	193	LYS	2.2
5	T	253	GLY	2.2
4	S	159	VAL	2.2
5	T	217	ARG	2.1
2	L	75	LYS	2.1
4	I	131	ASP	2.1
5	T	232	ASN	2.1
4	I	152	ASP	2.1
1	K	92	SER	2.1
2	L	48	LYS	2.1
4	S	193	LYS	2.1
4	I	214	PRO	2.1
5	O	232	ASN	2.1
1	F	225	THR	2.1

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Mol	Chain	Res	Type	RSRZ
5	T	150	THR	2.1
2	L	98	ASP	2.0
4	D	138	ARG	2.0
5	J	213	TRP	2.0
4	N	214	PRO	2.0
4	S	208	PRO	2.0
1	K	107	GLY	2.0
4	S	127	ILE	2.0
1	K	249	VAL	2.0
4	I	198	CYS	2.0
4	S	148	CYS	2.0
5	O	234	GLU	2.0
4	I	172	LYS	2.0
4	N	160	SER	2.0
4	S	146	SER	2.0
1	F	200	THR	2.0
4	S	214	PRO	2.0
5	J	142	PRO	2.0
5	O	211	THR	2.0
4	D	207	ILE	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.