



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 12:14 PM EDT

PDB ID : 2QR0
Title : Structure of VEGF complexed to a Fab containing TYR and SER in the CDRs
Authors : Wiesmann, C.
Deposited on : unknown
Resolution : 3.50 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

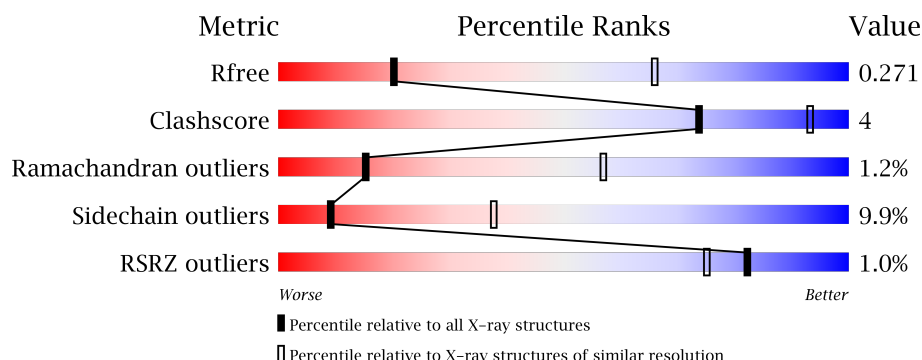
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	213	<div> <div>81%</div> <div>15%</div> <div>•</div> </div>
1	E	213	<div> <div>5%</div> <div>84%</div> <div>12%</div> <div>•</div> </div>
1	G	213	<div> <div>82%</div> <div>14%</div> <div>•</div> </div>
1	K	213	<div> <div>84%</div> <div>13%</div> <div>•</div> </div>
1	M	213	<div> <div>85%</div> <div>12%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	Q	213	 85%12%.
1	S	213	 85%12%.
1	W	213	 87%9%.
2	B	221	 82%14%..
2	F	221	 6%84%14%.
2	H	221	 81%16%.
2	L	221	 0%82%14%..
2	N	221	 83%14%.
2	R	221	 82%15%.
2	T	221	 0%83%14%..
2	X	221	 82%16%.
3	C	97	 0%85%11%..
3	D	97	 0%88%12%.
3	I	97	 0%79%19%.
3	J	97	 2%85%14%.
3	O	97	 85%11%..
3	P	97	 3%86%12%.
3	U	97	 84%14%.
3	V	97	 3%85%13%.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32356 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 Fab-Fragment Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1654	1042	273	334	5			
1	E	213	Total	C	N	O	S	0	0	0
			1654	1042	273	334	5			
1	G	213	Total	C	N	O	S	0	0	0
			1654	1042	273	334	5			
1	K	213	Total	C	N	O	S	0	0	0
			1654	1042	273	334	5			
1	M	213	Total	C	N	O	S	0	0	0
			1654	1042	273	334	5			
1	Q	213	Total	C	N	O	S	0	0	0
			1654	1042	273	334	5			
1	S	213	Total	C	N	O	S	0	0	0
			1654	1042	273	334	5			
1	W	213	Total	C	N	O	S	0	0	0
			1654	1042	273	334	5			

- Molecule 2 is a protein called Fab-Fragment Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1612	1020	265	320	7			
2	F	216	Total	C	N	O	S	0	0	0
			1612	1020	265	320	7			
2	H	216	Total	C	N	O	S	0	0	0
			1612	1020	265	320	7			
2	L	216	Total	C	N	O	S	0	0	0
			1612	1020	265	320	7			
2	N	216	Total	C	N	O	S	0	0	0
			1612	1020	265	320	7			
2	R	216	Total	C	N	O	S	0	0	0
			1612	1020	265	320	7			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	216	Total	C	N	O	S	0	0	0
			1612	1020	265	320	7			
2	X	216	Total	C	N	O	S	0	0	0
			1612	1020	265	320	7			

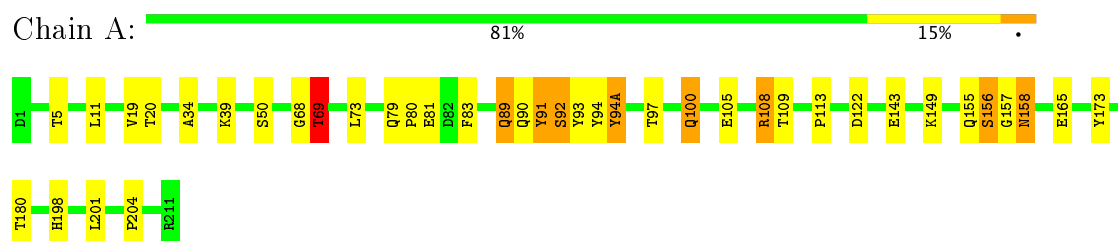
- Molecule 3 is a protein called Vascular endothelial growth factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	95	Total	C	N	O	S	0	0	0
			770	483	129	145	13			
3	D	97	Total	C	N	O	S	0	0	0
			787	493	132	149	13			
3	I	95	Total	C	N	O	S	0	0	0
			770	483	129	145	13			
3	J	97	Total	C	N	O	S	0	0	0
			787	493	132	149	13			
3	O	95	Total	C	N	O	S	0	0	0
			770	483	129	145	13			
3	P	97	Total	C	N	O	S	0	0	0
			787	493	132	149	13			
3	U	95	Total	C	N	O	S	0	0	0
			770	483	129	145	13			
3	V	97	Total	C	N	O	S	0	0	0
			787	493	132	149	13			

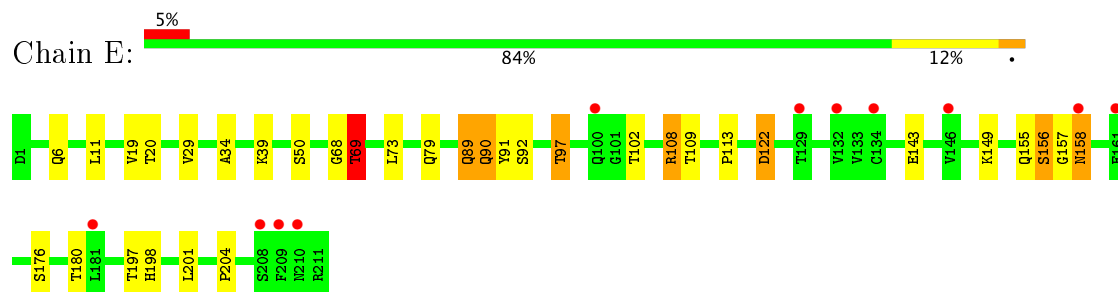
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

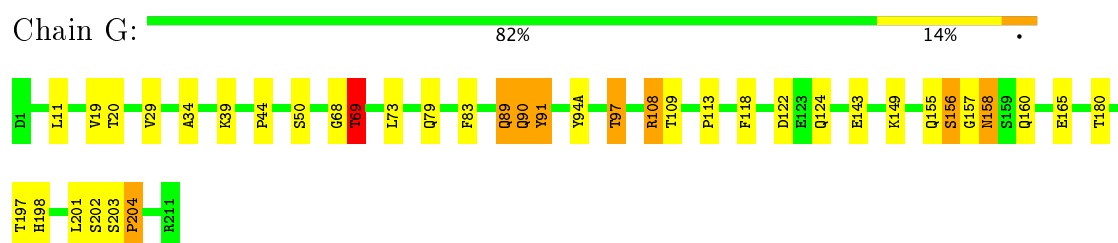
- Molecule 1: Fab-Fragment Light Chain



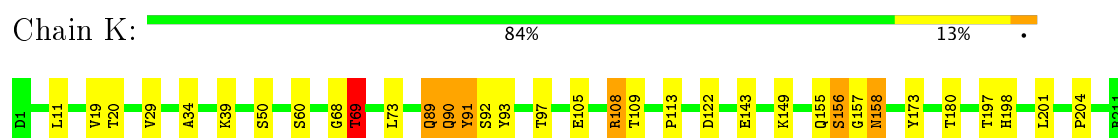
- Molecule 1: Fab-Fragment Light Chain



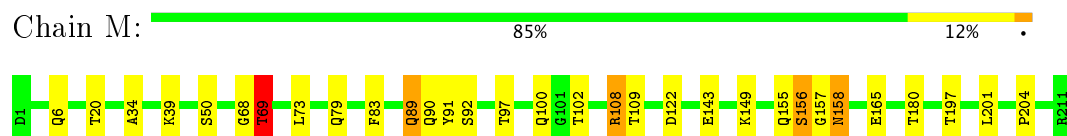
- Molecule 1: Fab-Fragment Light Chain



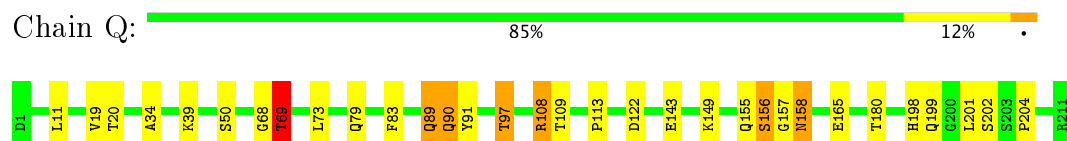
- Molecule 1: Fab-Fragment Light Chain



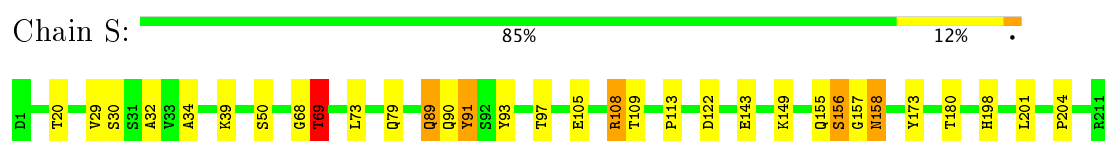
- Molecule 1: Fab-Fragment Light Chain



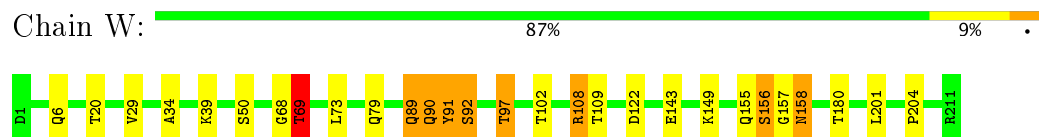
- Molecule 1: Fab-Fragment Light Chain



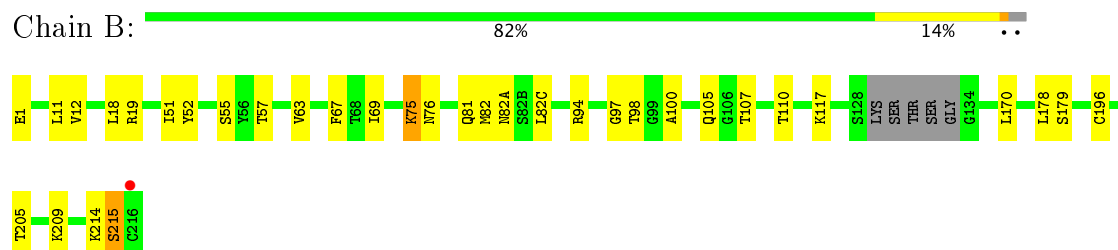
- Molecule 1: Fab-Fragment Light Chain



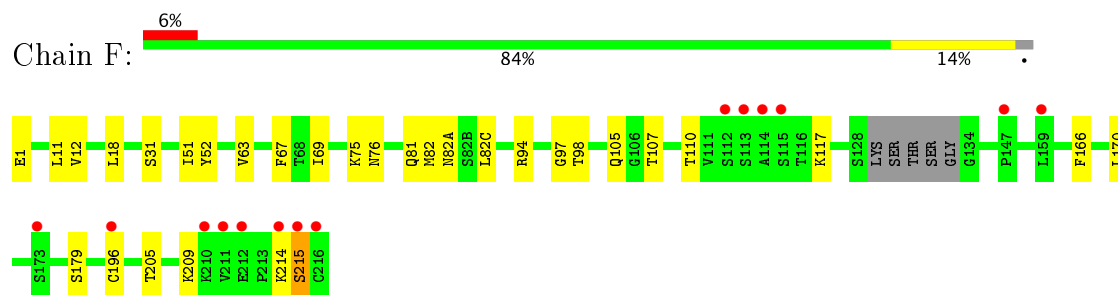
- Molecule 1: Fab-Fragment Light Chain



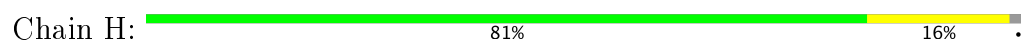
- Molecule 2: Fab-Fragment Heavy Chain

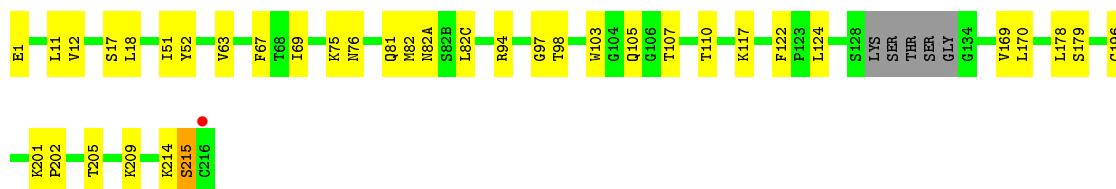


- Molecule 2: Fab-Fragment Heavy Chain

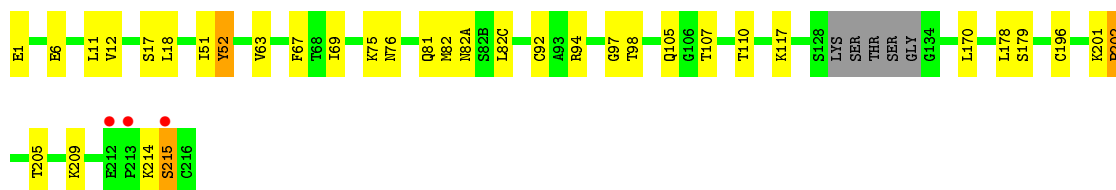
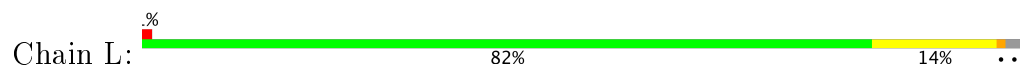


- Molecule 2: Fab-Fragment Heavy Chain

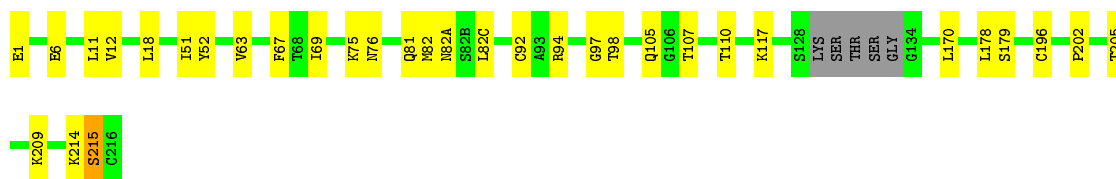
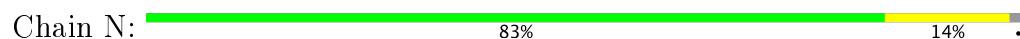




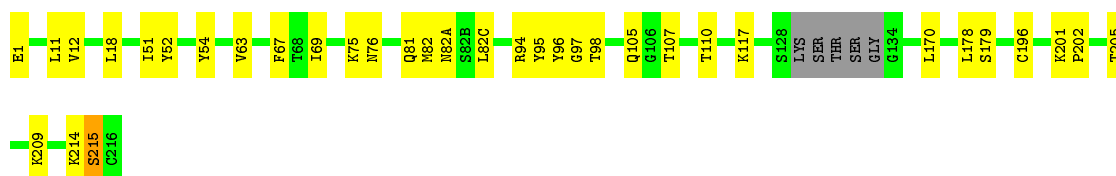
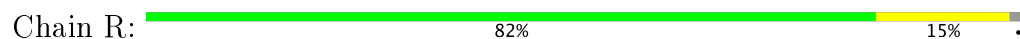
• Molecule 2: Fab-Fragment Heavy Chain



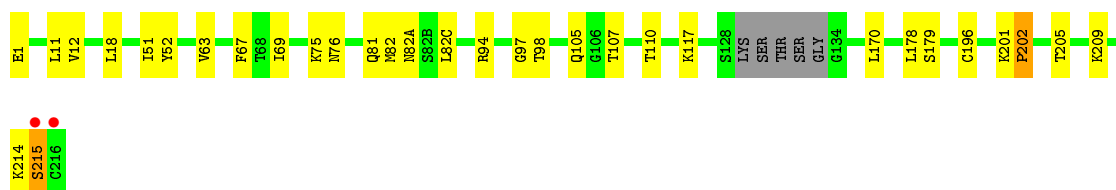
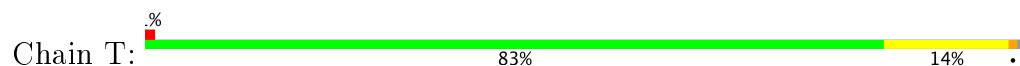
• Molecule 2: Fab-Fragment Heavy Chain



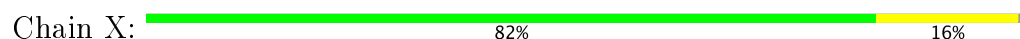
• Molecule 2: Fab-Fragment Heavy Chain

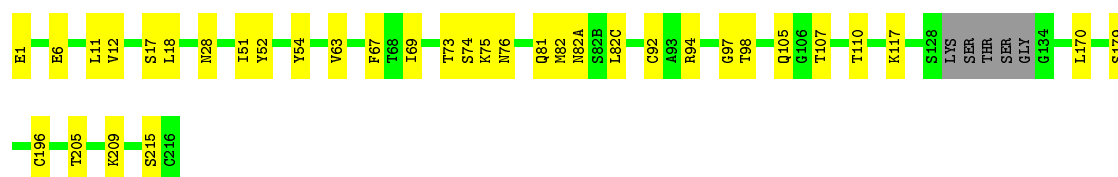


• Molecule 2: Fab-Fragment Heavy Chain

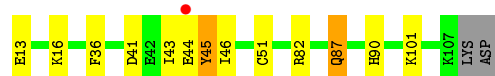
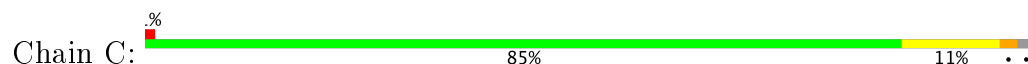


• Molecule 2: Fab-Fragment Heavy Chain

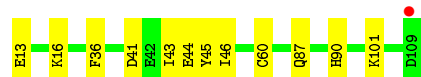
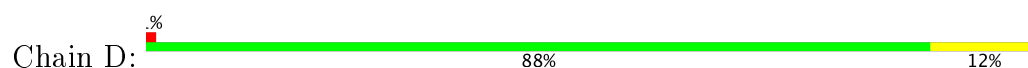




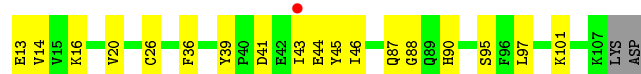
- Molecule 3: Vascular endothelial growth factor A



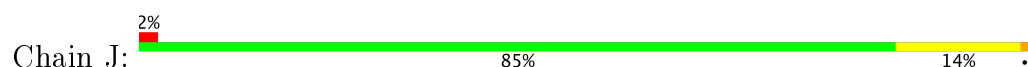
- Molecule 3: Vascular endothelial growth factor A



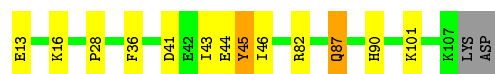
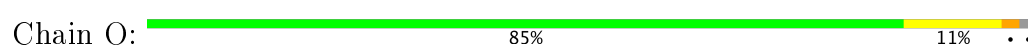
- Molecule 3: Vascular endothelial growth factor A



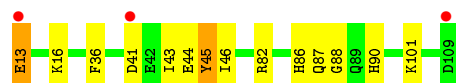
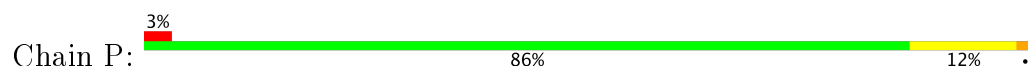
- Molecule 3: Vascular endothelial growth factor A



- Molecule 3: Vascular endothelial growth factor A

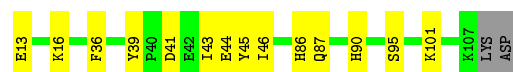


- Molecule 3: Vascular endothelial growth factor A




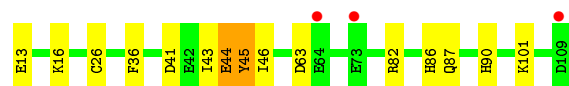
- Molecule 3: Vascular endothelial growth factor A

Chain U: 84% 14%



- Molecule 3: Vascular endothelial growth factor A

Chain V: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	154.45Å 90.22Å 205.56Å 90.00° 90.85° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 48.97 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.1 (20.00-3.50) 96.1 (48.97-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.65 (at 3.48Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.291 , 0.312 0.255 , 0.271	Depositor DCC
R_{free} test set	3496 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	80.2	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	32356	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.90% 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

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	0.40	0/1693	0.55	0/2300
1	E	0.36	0/1693	0.53	0/2300
1	G	0.40	0/1693	0.55	0/2300
1	K	0.39	0/1693	0.56	0/2300
1	M	0.39	0/1693	0.55	0/2300
1	Q	0.41	0/1693	0.55	0/2300
1	S	0.41	0/1693	0.55	0/2300
1	W	0.42	0/1693	0.54	0/2300
2	B	0.37	0/1653	0.54	0/2253
2	F	0.36	0/1653	0.53	0/2253
2	H	0.38	0/1653	0.54	0/2253
2	L	0.37	0/1653	0.53	0/2253
2	N	0.36	0/1653	0.53	0/2253
2	R	0.40	0/1653	0.54	0/2253
2	T	0.38	0/1653	0.54	0/2253
2	X	0.36	0/1653	0.53	0/2253
3	C	0.37	0/788	0.53	0/1062
3	D	0.36	0/805	0.53	0/1084
3	I	0.38	0/788	0.54	0/1062
3	J	0.37	0/805	0.53	0/1084
3	O	0.39	0/788	0.54	0/1062
3	P	0.36	0/805	0.54	0/1084
3	U	0.38	0/788	0.53	0/1062
3	V	0.38	0/805	0.53	0/1084
All	All	0.38	0/33140	0.54	0/45008

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	1654	0	1602	18	0
1	E	1654	0	1602	20	0
1	G	1654	0	1602	21	0
1	K	1654	0	1602	18	0
1	M	1654	0	1602	9	0
1	Q	1654	0	1602	22	0
1	S	1654	0	1602	12	0
1	W	1654	0	1602	11	0
2	B	1612	0	1561	18	0
2	F	1612	0	1561	16	0
2	H	1612	0	1561	14	0
2	L	1612	0	1561	13	0
2	N	1612	0	1561	9	0
2	R	1612	0	1561	17	0
2	T	1612	0	1561	11	0
2	X	1612	0	1561	13	0
3	C	770	0	732	4	0
3	D	787	0	749	2	0
3	I	770	0	732	18	0
3	J	787	0	749	5	0
3	O	770	0	732	3	0
3	P	787	0	749	14	0
3	U	770	0	732	4	0
3	V	787	0	749	8	0
All	All	32356	0	31228	240	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 4.

All (240) 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)
3:I:39:TYR:CE2	1:Q:202:SER:HB2	1.78	1.19
2:B:75:LYS:NZ	3:V:44:GLU:HB3	1.83	0.94
3:P:86:HIS:H	2:R:97:GLY:HA2	1.36	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:39:TYR:CZ	1:Q:202:SER:CB	2.54	0.90
3:I:39:TYR:CE2	1:Q:202:SER:CB	2.58	0.87
1:K:90:GLN:NE2	1:K:97:THR:OG1	2.07	0.87
1:G:202:SER:O	3:P:13:GLU:HA	1.77	0.84
3:C:87:GLN:HG3	2:F:31:SER:O	1.78	0.84
3:I:39:TYR:CZ	1:Q:202:SER:HB2	2.16	0.81
2:T:97:GLY:HA2	3:U:86:HIS:H	1.45	0.80
1:Q:90:GLN:NE2	1:Q:97:THR:OG1	2.15	0.77
1:G:204:PRO:HD2	3:P:13:GLU:HB3	1.66	0.77
3:P:45:TYR:HH	2:R:54:TYR:HH	1.26	0.76
1:E:122:ASP:CG	2:F:214:LYS:HE3	2.07	0.75
3:I:39:TYR:OH	1:Q:202:SER:HA	1.87	0.73
2:B:75:LYS:HZ3	3:V:44:GLU:HB3	1.52	0.72
3:P:86:HIS:N	2:R:97:GLY:HA2	2.05	0.69
1:E:122:ASP:HB2	2:F:214:LYS:HE2	1.75	0.68
2:T:97:GLY:HA2	3:U:86:HIS:N	2.09	0.68
3:I:39:TYR:CZ	1:Q:202:SER:HB3	2.30	0.66
1:S:158:ASN:HD22	1:S:158:ASN:H	1.43	0.65
1:A:158:ASN:H	1:A:158:ASN:HD22	1.43	0.65
1:W:6:GLN:NE2	1:W:102:THR:OG1	2.29	0.65
3:I:88:GLY:HA3	2:L:52:TYR:CE2	2.33	0.64
1:Q:158:ASN:HD22	1:Q:158:ASN:H	1.46	0.64
1:A:5:THR:HA	1:A:100:GLN:HE22	1.63	0.63
1:M:158:ASN:H	1:M:158:ASN:HD22	1.46	0.63
1:E:122:ASP:HB2	2:F:214:LYS:CE	2.29	0.62
2:B:55:SER:HB3	2:X:28:ASN:OD1	2.00	0.61
1:G:158:ASN:HD22	1:G:158:ASN:H	1.48	0.61
1:K:158:ASN:HD22	1:K:158:ASN:H	1.46	0.61
1:E:158:ASN:H	1:E:158:ASN:HD22	1.50	0.60
3:P:82:ARG:NH2	2:R:54:TYR:CE2	2.69	0.60
1:W:158:ASN:HD22	1:W:158:ASN:H	1.47	0.60
1:S:105:GLU:OE1	1:S:173:TYR:OH	2.20	0.59
3:P:45:TYR:OH	2:R:54:TYR:OH	2.08	0.57
2:B:75:LYS:NZ	3:V:44:GLU:CB	2.62	0.57
1:G:204:PRO:CD	3:P:13:GLU:HB3	2.33	0.57
1:W:90:GLN:NE2	1:W:97:THR:OG1	2.33	0.57
2:B:75:LYS:HZ2	3:V:44:GLU:HB3	1.65	0.56
3:I:39:TYR:OH	3:I:95:SER:O	2.15	0.56
1:A:80:PRO:HG2	1:K:60:SER:OG	2.05	0.56
1:E:90:GLN:HE22	1:E:97:THR:CB	2.18	0.56
1:E:6:GLN:NE2	1:E:102:THR:OG1	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:97:GLY:O	2:L:98:THR:HG22	2.07	0.55
3:I:20:VAL:HG12	3:J:49:PRO:HG3	1.89	0.54
3:I:39:TYR:CE1	1:Q:202:SER:HB3	2.42	0.54
2:B:97:GLY:O	2:B:98:THR:HG22	2.08	0.53
1:E:122:ASP:CB	2:F:214:LYS:HE3	2.37	0.53
1:A:91:TYR:CE2	2:B:100:ALA:HB2	2.44	0.52
1:S:32:ALA:HB1	1:S:91:TYR:CD1	2.44	0.52
2:T:97:GLY:O	2:T:98:THR:HG22	2.08	0.52
3:I:39:TYR:CZ	1:Q:202:SER:CA	2.93	0.52
2:H:97:GLY:O	2:H:98:THR:HG22	2.09	0.52
1:A:105:GLU:OE1	1:A:173:TYR:OH	2.29	0.51
3:V:86:HIS:H	2:X:97:GLY:HA2	1.75	0.51
1:G:108:ARG:HD3	1:G:109:THR:O	2.10	0.51
1:A:94:TYR:O	1:A:94(A):TYR:CB	2.57	0.51
2:B:57:THR:HG22	2:X:74:SER:HA	1.93	0.51
3:I:88:GLY:HA3	2:L:52:TYR:CD2	2.46	0.51
1:S:108:ARG:HD3	1:S:109:THR:O	2.11	0.51
1:M:68:GLY:O	1:M:69:THR:HG23	2.12	0.50
1:Q:68:GLY:O	1:Q:69:THR:HG23	2.11	0.50
1:G:90:GLN:NE2	1:G:97:THR:OG1	2.43	0.50
1:K:68:GLY:O	1:K:69:THR:HG23	2.11	0.50
2:X:97:GLY:O	2:X:98:THR:HG22	2.11	0.50
1:A:108:ARG:HD3	1:A:109:THR:O	2.11	0.50
3:I:88:GLY:CA	2:L:52:TYR:CE2	2.94	0.50
1:S:156:SER:O	1:S:158:ASN:N	2.45	0.50
1:A:156:SER:O	1:A:158:ASN:N	2.45	0.49
1:K:105:GLU:OE2	1:K:173:TYR:OH	2.27	0.49
1:E:68:GLY:O	1:E:69:THR:HG23	2.13	0.49
1:E:108:ARG:HD3	1:E:109:THR:O	2.12	0.49
2:R:97:GLY:O	2:R:98:THR:HG22	2.12	0.49
1:A:68:GLY:O	1:A:69:THR:HG23	2.13	0.49
1:G:68:GLY:O	1:G:69:THR:HG23	2.12	0.49
1:Q:108:ARG:HD3	1:Q:109:THR:O	2.12	0.49
1:A:81:GLU:OE1	1:K:60:SER:N	2.39	0.49
1:W:108:ARG:HD3	1:W:109:THR:O	2.14	0.48
1:A:91:TYR:O	1:A:92:SER:CB	2.62	0.48
3:I:39:TYR:CZ	1:Q:202:SER:HA	2.49	0.48
1:K:91:TYR:O	1:K:92:SER:OG	2.20	0.48
2:R:81:GLN:HG3	2:R:82(A):ASN:HD21	1.79	0.47
1:K:90:GLN:HG2	1:K:91:TYR:O	2.14	0.47
1:W:68:GLY:O	1:W:69:THR:HG23	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:ASP:CB	2:F:214:LYS:CE	2.92	0.47
1:M:108:ARG:HD3	1:M:109:THR:O	2.15	0.47
2:N:97:GLY:O	2:N:98:THR:HG22	2.14	0.47
2:B:57:THR:HG21	2:X:73:THR:HG22	1.95	0.47
2:H:51:ILE:HB	2:H:69:ILE:HG21	1.96	0.47
3:O:90:HIS:N	3:O:90:HIS:HD1	2.13	0.47
2:X:63:VAL:HG13	2:X:67:PHE:CG	2.49	0.47
2:H:81:GLN:HG3	2:H:82(A):ASN:HD21	1.80	0.47
2:F:97:GLY:O	2:F:98:THR:HG22	2.14	0.47
2:B:63:VAL:HG13	2:B:67:PHE:CG	2.50	0.47
3:I:39:TYR:OH	1:Q:202:SER:CA	2.59	0.47
2:L:51:ILE:HB	2:L:69:ILE:HG21	1.97	0.47
2:X:51:ILE:HB	2:X:69:ILE:HG21	1.97	0.47
1:Q:156:SER:O	1:Q:158:ASN:N	2.48	0.46
1:W:156:SER:O	1:W:158:ASN:N	2.48	0.46
2:F:63:VAL:HG13	2:F:67:PHE:CG	2.50	0.46
1:K:108:ARG:HD3	1:K:109:THR:O	2.15	0.46
2:B:63:VAL:CG1	2:B:67:PHE:HB2	2.46	0.46
3:P:86:HIS:HE1	2:R:96:TYR:CE2	2.34	0.46
2:X:63:VAL:CG1	2:X:67:PHE:HB2	2.46	0.46
2:F:63:VAL:CG1	2:F:67:PHE:HB2	2.45	0.46
2:N:51:ILE:HB	2:N:69:ILE:HG21	1.97	0.46
3:C:51:CYS:N	3:D:60:CYS:SG	2.89	0.46
1:K:34:ALA:HB3	1:K:89:GLN:HE21	1.80	0.46
2:R:63:VAL:HG13	2:R:67:PHE:CG	2.51	0.46
1:E:176:SER:HB3	2:F:166:PHE:CZ	2.50	0.46
3:J:90:HIS:N	3:J:90:HIS:HD1	2.14	0.46
2:N:81:GLN:HG3	2:N:82(A):ASN:HD21	1.81	0.46
2:B:55:SER:HB3	2:X:28:ASN:HA	1.98	0.46
2:T:51:ILE:HB	2:T:69:ILE:HG21	1.97	0.46
3:V:90:HIS:N	3:V:90:HIS:HD1	2.14	0.46
1:M:156:SER:O	1:M:158:ASN:N	2.48	0.45
2:R:51:ILE:HB	2:R:69:ILE:HG21	1.97	0.45
1:S:68:GLY:O	1:S:69:THR:HG23	2.15	0.45
1:A:81:GLU:OE1	1:K:60:SER:CB	2.64	0.45
3:D:90:HIS:N	3:D:90:HIS:HD1	2.14	0.45
2:N:63:VAL:HG13	2:N:67:PHE:CG	2.52	0.45
1:Q:34:ALA:HB3	1:Q:89:GLN:HE21	1.81	0.45
2:F:51:ILE:HB	2:F:69:ILE:HG21	1.98	0.45
1:G:118:PHE:CD1	2:H:124:LEU:HB3	2.52	0.45
1:M:6:GLN:NE2	1:M:102:THR:OG1	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:81:GLN:HG3	2:X:82(A):ASN:HD21	1.82	0.45
2:L:81:GLN:HG3	2:L:82(A):ASN:HD21	1.81	0.45
1:S:34:ALA:HB3	1:S:89:GLN:HE21	1.80	0.45
2:T:81:GLN:HG3	2:T:82(A):ASN:HD21	1.82	0.45
2:L:63:VAL:CG1	2:L:67:PHE:HB2	2.47	0.45
2:R:63:VAL:CG1	2:R:67:PHE:HB2	2.47	0.45
3:C:90:HIS:HD1	3:C:90:HIS:N	2.15	0.45
2:L:63:VAL:HG13	2:L:67:PHE:CG	2.52	0.45
2:B:51:ILE:HB	2:B:69:ILE:HG21	1.97	0.45
3:P:90:HIS:HD1	3:P:90:HIS:N	2.15	0.45
2:T:63:VAL:CG1	2:T:67:PHE:HB2	2.47	0.45
2:T:63:VAL:HG13	2:T:67:PHE:CG	2.52	0.45
2:N:63:VAL:CG1	2:N:67:PHE:HB2	2.46	0.45
3:I:97:LEU:HD13	1:Q:199:GLN:HG3	1.99	0.45
2:B:81:GLN:HG3	2:B:82(A):ASN:HD21	1.82	0.44
1:E:89:GLN:HB3	1:E:89:GLN:HE21	1.67	0.44
2:H:63:VAL:HG13	2:H:67:PHE:CG	2.52	0.44
3:I:14:VAL:CG1	3:J:79:GLN:HG3	2.47	0.44
2:F:81:GLN:HG3	2:F:82(A):ASN:HD21	1.83	0.44
2:B:178:LEU:C	2:B:178:LEU:HD12	2.38	0.44
1:E:176:SER:HB3	2:F:166:PHE:CE1	2.52	0.44
2:H:63:VAL:CG1	2:H:67:PHE:HB2	2.48	0.44
1:K:156:SER:O	1:K:158:ASN:N	2.51	0.44
3:U:90:HIS:N	3:U:90:HIS:HD1	2.16	0.44
1:G:156:SER:O	1:G:158:ASN:N	2.51	0.44
2:H:178:LEU:C	2:H:178:LEU:HD12	2.38	0.44
2:F:82:MET:HB3	2:F:82(C):LEU:HD21	2.00	0.44
2:X:82:MET:HB3	2:X:82(C):LEU:HD21	1.99	0.44
1:E:122:ASP:OD1	2:F:214:LYS:HE3	2.17	0.44
1:E:156:SER:O	1:E:158:ASN:N	2.51	0.44
2:T:82:MET:HB3	2:T:82(C):LEU:HD21	1.99	0.44
1:G:203:SER:HA	3:P:13:GLU:CB	2.48	0.43
2:H:82:MET:HB3	2:H:82(C):LEU:HD21	1.99	0.43
1:S:158:ASN:HD22	1:S:158:ASN:N	2.09	0.43
1:G:124:GLN:HG3	2:H:122:PHE:CE2	2.53	0.43
1:G:113:PRO:HD3	1:G:198:HIS:CD2	2.53	0.43
1:G:29:VAL:HG12	1:G:29:VAL:O	2.18	0.43
2:B:82:MET:HB3	2:B:82(C):LEU:HD21	1.99	0.43
1:K:155:GLN:HB3	1:K:158:ASN:HD21	1.84	0.43
2:L:82:MET:HB3	2:L:82(C):LEU:HD21	2.00	0.43
2:N:82:MET:HB3	2:N:82(C):LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLN:HB3	1:A:158:ASN:HD21	1.84	0.43
3:I:90:HIS:N	3:I:90:HIS:HD1	2.16	0.43
1:K:29:VAL:HG12	1:K:29:VAL:O	2.20	0.42
1:M:89:GLN:HB3	1:M:89:GLN:HE21	1.65	0.42
1:W:91:TYR:O	1:W:92:SER:OG	2.28	0.42
1:E:113:PRO:HD3	1:E:198:HIS:CD2	2.55	0.42
3:P:88:GLY:HA2	2:R:95:TYR:CE2	2.55	0.42
1:S:30:SER:HB2	3:V:63:ASP:OD2	2.19	0.42
1:G:34:ALA:HB3	1:G:89:GLN:HE21	1.84	0.42
1:M:155:GLN:HB3	1:M:158:ASN:HD21	1.84	0.42
2:R:82:MET:HB3	2:R:82(C):LEU:HD21	2.00	0.42
1:W:34:ALA:HB3	1:W:89:GLN:HE21	1.84	0.42
1:G:44:PRO:HD2	2:H:103:TRP:CE3	2.54	0.42
1:K:158:ASN:HD22	1:K:158:ASN:N	2.11	0.42
3:U:39:TYR:OH	3:U:95:SER:O	2.24	0.42
1:K:11:LEU:HD21	1:K:19:VAL:HG13	2.01	0.42
2:N:6:GLU:OE2	2:N:92:CYS:N	2.43	0.42
1:G:160:GLN:HB3	2:H:169:VAL:HG11	2.02	0.42
2:T:178:LEU:HD12	2:T:178:LEU:C	2.40	0.42
2:B:214:LYS:O	2:B:215:SER:C	2.59	0.42
1:E:34:ALA:HB3	1:E:89:GLN:HE21	1.82	0.42
1:Q:155:GLN:HB3	1:Q:158:ASN:HD21	1.85	0.42
2:H:214:LYS:O	2:H:215:SER:C	2.58	0.41
2:L:178:LEU:C	2:L:178:LEU:HD12	2.41	0.41
1:G:155:GLN:HB3	1:G:158:ASN:HD21	1.86	0.41
1:K:89:GLN:HE21	1:K:89:GLN:HB3	1.66	0.41
2:N:214:LYS:O	2:N:215:SER:C	2.58	0.41
1:S:155:GLN:HB3	1:S:158:ASN:HD21	1.85	0.41
1:S:113:PRO:HD3	1:S:198:HIS:CD2	2.55	0.41
2:B:19:ARG:CZ	2:X:54:TYR:CE2	3.03	0.41
1:G:124:GLN:HA	2:H:122:PHE:CE1	2.55	0.41
2:L:214:LYS:O	2:L:215:SER:C	2.59	0.41
1:Q:113:PRO:HD3	1:Q:198:HIS:CD2	2.56	0.41
1:W:155:GLN:HB3	1:W:158:ASN:HD21	1.84	0.41
1:A:34:ALA:HB3	1:A:89:GLN:HE21	1.84	0.41
2:R:214:LYS:O	2:R:215:SER:C	2.59	0.41
1:E:11:LEU:HD21	1:E:19:VAL:HG13	2.01	0.41
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.56	0.41
1:K:113:PRO:HD3	1:K:198:HIS:CD2	2.55	0.41
1:M:34:ALA:HB3	1:M:89:GLN:HE21	1.84	0.41
3:C:45:TYR:HD1	3:C:82:ARG:HB3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:83:PHE:CZ	1:M:165:GLU:HG3	2.56	0.41
2:N:178:LEU:HD12	2:N:178:LEU:C	2.40	0.41
3:O:87:GLN:HB2	3:O:87:GLN:HE21	1.66	0.41
1:Q:11:LEU:HD21	1:Q:19:VAL:HG13	2.02	0.41
3:J:87:GLN:HE21	3:J:87:GLN:HB2	1.67	0.41
2:R:201:LYS:N	2:R:202:PRO:CD	2.83	0.41
3:V:45:TYR:HD1	3:V:82:ARG:HB3	1.86	0.41
1:W:29:VAL:O	1:W:29:VAL:HG12	2.20	0.41
2:X:6:GLU:OE2	2:X:92:CYS:N	2.42	0.41
1:A:11:LEU:HD21	1:A:19:VAL:HG13	2.02	0.41
1:E:155:GLN:HB3	1:E:158:ASN:HD21	1.84	0.41
3:P:45:TYR:HD1	3:P:82:ARG:HB3	1.86	0.41
1:S:29:VAL:O	1:S:29:VAL:HG12	2.20	0.41
1:A:83:PHE:CZ	1:A:165:GLU:HG3	2.56	0.41
2:F:214:LYS:O	2:F:215:SER:C	2.59	0.41
2:T:214:LYS:O	2:T:215:SER:C	2.59	0.41
2:H:201:LYS:N	2:H:202:PRO:CD	2.84	0.41
3:O:45:TYR:HD1	3:O:82:ARG:HB3	1.86	0.41
1:G:90:GLN:HG2	1:G:91:TYR:O	2.21	0.40
1:E:29:VAL:O	1:E:29:VAL:HG12	2.21	0.40
3:J:39:TYR:OH	3:J:95:SER:O	2.26	0.40
1:Q:83:PHE:CZ	1:Q:165:GLU:HG3	2.56	0.40
1:G:83:PHE:CZ	1:G:165:GLU:HG3	2.57	0.40
3:P:90:HIS:CD2	2:R:54:TYR:CG	3.09	0.40
1:W:89:GLN:HB3	1:W:89:GLN:HE21	1.65	0.40
2:L:6:GLU:OE2	2:L:92:CYS:N	2.42	0.40
1:Q:158:ASN:HD22	1:Q:158:ASN:N	2.11	0.40
2:T:201:LYS:N	2:T:202:PRO:CD	2.85	0.40
1:A:91:TYR:O	1:A:92:SER:OG	2.31	0.40
1:G:11:LEU:HD21	1:G:19:VAL:HG13	2.02	0.40
2:L:201:LYS:N	2:L:202:PRO:CD	2.84	0.40
2:R:178:LEU:C	2:R:178:LEU:HD12	2.41	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	211/213 (99%)	188 (89%)	16 (8%)	7 (3%)	4	35
1	E	211/213 (99%)	190 (90%)	16 (8%)	5 (2%)	7	42
1	G	211/213 (99%)	188 (89%)	19 (9%)	4 (2%)	9	47
1	K	211/213 (99%)	188 (89%)	18 (8%)	5 (2%)	7	42
1	M	211/213 (99%)	189 (90%)	17 (8%)	5 (2%)	7	42
1	Q	211/213 (99%)	189 (90%)	18 (8%)	4 (2%)	9	47
1	S	211/213 (99%)	188 (89%)	18 (8%)	5 (2%)	7	42
1	W	211/213 (99%)	189 (90%)	17 (8%)	5 (2%)	7	42
2	B	212/221 (96%)	203 (96%)	8 (4%)	1 (0%)	32	73
2	F	212/221 (96%)	203 (96%)	8 (4%)	1 (0%)	32	73
2	H	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	32	73
2	L	212/221 (96%)	201 (95%)	10 (5%)	1 (0%)	32	73
2	N	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	32	73
2	R	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	32	73
2	T	212/221 (96%)	203 (96%)	8 (4%)	1 (0%)	32	73
2	X	212/221 (96%)	202 (95%)	9 (4%)	1 (0%)	32	73
3	C	93/97 (96%)	88 (95%)	5 (5%)	0	100	100
3	D	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
3	I	93/97 (96%)	86 (92%)	6 (6%)	1 (1%)	17	59
3	J	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
3	O	93/97 (96%)	87 (94%)	6 (6%)	0	100	100
3	P	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
3	U	93/97 (96%)	87 (94%)	6 (6%)	0	100	100
3	V	95/97 (98%)	90 (95%)	4 (4%)	1 (1%)	17	59
All	All	4136/4248 (97%)	3832 (93%)	254 (6%)	50 (1%)	15	57

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	94(A)	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	69	THR
1	A	92	SER
1	A	93	TYR
1	A	143	GLU
1	A	157	GLY
2	B	215	SER
1	E	69	THR
1	E	143	GLU
1	E	157	GLY
2	F	215	SER
1	G	69	THR
1	G	143	GLU
1	G	157	GLY
2	H	215	SER
1	K	69	THR
1	K	93	TYR
1	K	143	GLU
1	K	157	GLY
2	L	215	SER
1	M	69	THR
1	M	143	GLU
1	M	157	GLY
2	N	215	SER
1	Q	69	THR
1	Q	143	GLU
1	Q	157	GLY
2	R	215	SER
1	S	69	THR
1	S	143	GLU
1	S	157	GLY
2	T	215	SER
1	W	69	THR
1	W	143	GLU
1	W	157	GLY
2	X	215	SER
1	E	92	SER
1	M	92	SER
1	S	93	TYR
1	W	92	SER
1	A	204	PRO
1	E	204	PRO
1	G	204	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	26	CYS
1	K	204	PRO
1	M	204	PRO
1	Q	204	PRO
1	S	204	PRO
3	V	26	CYS
1	W	204	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	189/189 (100%)	171 (90%)	18 (10%)	10	40
1	E	189/189 (100%)	171 (90%)	18 (10%)	10	40
1	G	189/189 (100%)	170 (90%)	19 (10%)	9	37
1	K	189/189 (100%)	173 (92%)	16 (8%)	12	45
1	M	189/189 (100%)	170 (90%)	19 (10%)	9	37
1	Q	189/189 (100%)	172 (91%)	17 (9%)	11	42
1	S	189/189 (100%)	172 (91%)	17 (9%)	11	42
1	W	189/189 (100%)	172 (91%)	17 (9%)	11	42
2	B	179/183 (98%)	162 (90%)	17 (10%)	10	40
2	F	179/183 (98%)	162 (90%)	17 (10%)	10	40
2	H	179/183 (98%)	161 (90%)	18 (10%)	9	37
2	L	179/183 (98%)	160 (89%)	19 (11%)	8	35
2	N	179/183 (98%)	161 (90%)	18 (10%)	9	37
2	R	179/183 (98%)	162 (90%)	17 (10%)	10	40
2	T	179/183 (98%)	161 (90%)	18 (10%)	9	37
2	X	179/183 (98%)	161 (90%)	18 (10%)	9	37
3	C	90/92 (98%)	80 (89%)	10 (11%)	7	32
3	D	92/92 (100%)	82 (89%)	10 (11%)	7	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	90/92 (98%)	80 (89%)	10 (11%)	7	32
3	J	92/92 (100%)	82 (89%)	10 (11%)	7	33
3	O	90/92 (98%)	79 (88%)	11 (12%)	6	27
3	P	92/92 (100%)	82 (89%)	10 (11%)	7	33
3	U	90/92 (98%)	80 (89%)	10 (11%)	7	32
3	V	92/92 (100%)	82 (89%)	10 (11%)	7	33
All	All	3672/3712 (99%)	3308 (90%)	364 (10%)	9	38

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	39	LYS
1	A	50	SER
1	A	69	THR
1	A	73	LEU
1	A	79	GLN
1	A	89	GLN
1	A	90	GLN
1	A	91	TYR
1	A	97	THR
1	A	100	GLN
1	A	108	ARG
1	A	122	ASP
1	A	149	LYS
1	A	156	SER
1	A	158	ASN
1	A	180	THR
1	A	201	LEU
2	B	1	GLU
2	B	11	LEU
2	B	12	VAL
2	B	18	LEU
2	B	52	TYR
2	B	75	LYS
2	B	76	ASN
2	B	94	ARG
2	B	105	GLN
2	B	107	THR
2	B	110	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	117	LYS
2	B	170	LEU
2	B	179	SER
2	B	196	CYS
2	B	205	THR
2	B	209	LYS
3	C	13	GLU
3	C	16	LYS
3	C	36	PHE
3	C	41	ASP
3	C	43	ILE
3	C	44	GLU
3	C	45	TYR
3	C	46	ILE
3	C	87	GLN
3	C	101	LYS
3	D	13	GLU
3	D	16	LYS
3	D	36	PHE
3	D	41	ASP
3	D	43	ILE
3	D	44	GLU
3	D	45	TYR
3	D	46	ILE
3	D	87	GLN
3	D	101	LYS
1	E	20	THR
1	E	39	LYS
1	E	50	SER
1	E	69	THR
1	E	73	LEU
1	E	79	GLN
1	E	89	GLN
1	E	90	GLN
1	E	91	TYR
1	E	97	THR
1	E	108	ARG
1	E	122	ASP
1	E	149	LYS
1	E	156	SER
1	E	158	ASN
1	E	180	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	197	THR
1	E	201	LEU
2	F	1	GLU
2	F	11	LEU
2	F	12	VAL
2	F	18	LEU
2	F	52	TYR
2	F	75	LYS
2	F	76	ASN
2	F	94	ARG
2	F	105	GLN
2	F	107	THR
2	F	110	THR
2	F	117	LYS
2	F	170	LEU
2	F	179	SER
2	F	196	CYS
2	F	205	THR
2	F	209	LYS
1	G	20	THR
1	G	39	LYS
1	G	50	SER
1	G	69	THR
1	G	73	LEU
1	G	79	GLN
1	G	89	GLN
1	G	90	GLN
1	G	91	TYR
1	G	94(A)	TYR
1	G	97	THR
1	G	108	ARG
1	G	122	ASP
1	G	149	LYS
1	G	156	SER
1	G	158	ASN
1	G	180	THR
1	G	197	THR
1	G	201	LEU
2	H	1	GLU
2	H	11	LEU
2	H	12	VAL
2	H	17	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	18	LEU
2	H	52	TYR
2	H	75	LYS
2	H	76	ASN
2	H	94	ARG
2	H	105	GLN
2	H	107	THR
2	H	110	THR
2	H	117	LYS
2	H	170	LEU
2	H	179	SER
2	H	196	CYS
2	H	205	THR
2	H	209	LYS
3	I	13	GLU
3	I	16	LYS
3	I	36	PHE
3	I	41	ASP
3	I	43	ILE
3	I	44	GLU
3	I	45	TYR
3	I	46	ILE
3	I	87	GLN
3	I	101	LYS
3	J	13	GLU
3	J	16	LYS
3	J	36	PHE
3	J	41	ASP
3	J	43	ILE
3	J	44	GLU
3	J	45	TYR
3	J	46	ILE
3	J	87	GLN
3	J	101	LYS
1	K	20	THR
1	K	39	LYS
1	K	50	SER
1	K	69	THR
1	K	73	LEU
1	K	89	GLN
1	K	90	GLN
1	K	91	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	108	ARG
1	K	122	ASP
1	K	149	LYS
1	K	156	SER
1	K	158	ASN
1	K	180	THR
1	K	197	THR
1	K	201	LEU
2	L	1	GLU
2	L	11	LEU
2	L	12	VAL
2	L	17	SER
2	L	18	LEU
2	L	52	TYR
2	L	75	LYS
2	L	76	ASN
2	L	94	ARG
2	L	105	GLN
2	L	107	THR
2	L	110	THR
2	L	117	LYS
2	L	170	LEU
2	L	179	SER
2	L	196	CYS
2	L	202	PRO
2	L	205	THR
2	L	209	LYS
1	M	20	THR
1	M	39	LYS
1	M	50	SER
1	M	69	THR
1	M	73	LEU
1	M	79	GLN
1	M	89	GLN
1	M	90	GLN
1	M	91	TYR
1	M	97	THR
1	M	100	GLN
1	M	108	ARG
1	M	122	ASP
1	M	149	LYS
1	M	156	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	158	ASN
1	M	180	THR
1	M	197	THR
1	M	201	LEU
2	N	1	GLU
2	N	11	LEU
2	N	12	VAL
2	N	18	LEU
2	N	52	TYR
2	N	75	LYS
2	N	76	ASN
2	N	94	ARG
2	N	105	GLN
2	N	107	THR
2	N	110	THR
2	N	117	LYS
2	N	170	LEU
2	N	179	SER
2	N	196	CYS
2	N	202	PRO
2	N	205	THR
2	N	209	LYS
3	O	13	GLU
3	O	16	LYS
3	O	28	PRO
3	O	36	PHE
3	O	41	ASP
3	O	43	ILE
3	O	44	GLU
3	O	45	TYR
3	O	46	ILE
3	O	87	GLN
3	O	101	LYS
3	P	13	GLU
3	P	16	LYS
3	P	36	PHE
3	P	41	ASP
3	P	43	ILE
3	P	44	GLU
3	P	45	TYR
3	P	46	ILE
3	P	87	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	P	101	LYS
1	Q	20	THR
1	Q	39	LYS
1	Q	50	SER
1	Q	69	THR
1	Q	73	LEU
1	Q	79	GLN
1	Q	89	GLN
1	Q	90	GLN
1	Q	91	TYR
1	Q	97	THR
1	Q	108	ARG
1	Q	122	ASP
1	Q	149	LYS
1	Q	156	SER
1	Q	158	ASN
1	Q	180	THR
1	Q	201	LEU
2	R	1	GLU
2	R	11	LEU
2	R	12	VAL
2	R	18	LEU
2	R	52	TYR
2	R	75	LYS
2	R	76	ASN
2	R	94	ARG
2	R	105	GLN
2	R	107	THR
2	R	110	THR
2	R	117	LYS
2	R	170	LEU
2	R	179	SER
2	R	196	CYS
2	R	205	THR
2	R	209	LYS
1	S	20	THR
1	S	39	LYS
1	S	50	SER
1	S	69	THR
1	S	73	LEU
1	S	79	GLN
1	S	89	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	90	GLN
1	S	91	TYR
1	S	97	THR
1	S	108	ARG
1	S	122	ASP
1	S	149	LYS
1	S	156	SER
1	S	158	ASN
1	S	180	THR
1	S	201	LEU
2	T	1	GLU
2	T	11	LEU
2	T	12	VAL
2	T	18	LEU
2	T	52	TYR
2	T	75	LYS
2	T	76	ASN
2	T	94	ARG
2	T	105	GLN
2	T	107	THR
2	T	110	THR
2	T	117	LYS
2	T	170	LEU
2	T	179	SER
2	T	196	CYS
2	T	202	PRO
2	T	205	THR
2	T	209	LYS
3	U	13	GLU
3	U	16	LYS
3	U	36	PHE
3	U	41	ASP
3	U	43	ILE
3	U	44	GLU
3	U	45	TYR
3	U	46	ILE
3	U	87	GLN
3	U	101	LYS
3	V	13	GLU
3	V	16	LYS
3	V	36	PHE
3	V	41	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	V	43	ILE
3	V	44	GLU
3	V	45	TYR
3	V	46	ILE
3	V	87	GLN
3	V	101	LYS
1	W	20	THR
1	W	39	LYS
1	W	50	SER
1	W	69	THR
1	W	73	LEU
1	W	79	GLN
1	W	89	GLN
1	W	90	GLN
1	W	91	TYR
1	W	97	THR
1	W	108	ARG
1	W	122	ASP
1	W	149	LYS
1	W	156	SER
1	W	158	ASN
1	W	180	THR
1	W	201	LEU
2	X	1	GLU
2	X	11	LEU
2	X	12	VAL
2	X	17	SER
2	X	18	LEU
2	X	52	TYR
2	X	75	LYS
2	X	76	ASN
2	X	94	ARG
2	X	105	GLN
2	X	107	THR
2	X	110	THR
2	X	117	LYS
2	X	170	LEU
2	X	179	SER
2	X	196	CYS
2	X	205	THR
2	X	209	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	90	GLN
1	A	100	GLN
1	A	158	ASN
1	A	198	HIS
2	B	3	GLN
2	B	76	ASN
2	B	192	GLN
2	B	200	HIS
3	C	87	GLN
3	D	87	GLN
1	E	79	GLN
1	E	89	GLN
1	E	90	GLN
1	E	158	ASN
1	E	198	HIS
2	F	3	GLN
2	F	76	ASN
2	F	192	GLN
2	F	200	HIS
1	G	79	GLN
1	G	89	GLN
1	G	90	GLN
1	G	158	ASN
1	G	160	GLN
1	G	198	HIS
2	H	3	GLN
2	H	192	GLN
2	H	200	HIS
3	I	62	ASN
3	I	87	GLN
3	J	87	GLN
1	K	79	GLN
1	K	89	GLN
1	K	90	GLN
1	K	158	ASN
1	K	198	HIS
2	L	3	GLN
2	L	76	ASN
2	L	192	GLN
2	L	200	HIS
1	M	79	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	89	GLN
1	M	90	GLN
1	M	100	GLN
1	M	158	ASN
1	M	198	HIS
2	N	3	GLN
2	N	76	ASN
2	N	192	GLN
2	N	200	HIS
3	O	87	GLN
3	P	87	GLN
1	Q	89	GLN
1	Q	90	GLN
1	Q	158	ASN
1	Q	160	GLN
1	Q	198	HIS
2	R	3	GLN
2	R	76	ASN
2	R	192	GLN
2	R	200	HIS
1	S	89	GLN
1	S	90	GLN
1	S	158	ASN
1	S	198	HIS
2	T	3	GLN
2	T	76	ASN
2	T	192	GLN
2	T	200	HIS
3	U	62	ASN
3	U	87	GLN
3	V	87	GLN
1	W	79	GLN
1	W	89	GLN
1	W	90	GLN
1	W	158	ASN
1	W	198	HIS
2	X	3	GLN
2	X	76	ASN
2	X	192	GLN
2	X	200	HIS

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 carbohydrates 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	213/213 (100%)	-0.16	0 100 100	16, 60, 93, 109	0
1	E	213/213 (100%)	0.39	11 (5%) 28 23	16, 62, 93, 109	0
1	G	213/213 (100%)	-0.14	0 100 100	16, 62, 93, 109	0
1	K	213/213 (100%)	0.02	0 100 100	16, 60, 93, 109	0
1	M	213/213 (100%)	-0.05	0 100 100	16, 61, 93, 109	0
1	Q	213/213 (100%)	-0.04	0 100 100	16, 62, 93, 109	0
1	S	213/213 (100%)	-0.16	0 100 100	16, 62, 93, 109	0
1	W	213/213 (100%)	-0.02	0 100 100	16, 61, 93, 109	0
2	B	216/221 (97%)	-0.13	1 (0%) 90 86	25, 63, 111, 150	0
2	F	216/221 (97%)	0.58	14 (6%) 20 16	25, 63, 111, 150	0
2	H	216/221 (97%)	0.07	1 (0%) 90 86	25, 63, 111, 150	0
2	L	216/221 (97%)	0.01	3 (1%) 75 67	25, 63, 111, 150	0
2	N	216/221 (97%)	-0.09	0 100 100	25, 63, 111, 150	0
2	R	216/221 (97%)	0.09	0 100 100	25, 63, 111, 150	0
2	T	216/221 (97%)	-0.11	2 (0%) 84 77	25, 63, 111, 150	0
2	X	216/221 (97%)	-0.02	0 100 100	25, 63, 111, 150	0
3	C	95/97 (97%)	0.16	1 (1%) 80 72	52, 84, 125, 135	0
3	D	97/97 (100%)	0.08	1 (1%) 82 75	52, 84, 130, 142	0
3	I	95/97 (97%)	0.14	1 (1%) 80 72	52, 84, 125, 135	0
3	J	97/97 (100%)	0.22	2 (2%) 64 55	52, 84, 130, 135	0
3	O	95/97 (97%)	0.10	0 100 100	52, 84, 125, 135	0
3	P	97/97 (100%)	0.20	3 (3%) 49 41	52, 84, 130, 140	0
3	U	95/97 (97%)	0.04	0 100 100	52, 84, 125, 135	0
3	V	97/97 (100%)	0.09	3 (3%) 49 41	52, 84, 130, 135	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	4200/4248 (98%)	0.04	43 (1%) 82 75	16, 66, 110, 150	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	P	109	ASP	7.6
3	D	109	ASP	7.5
3	V	109	ASP	4.3
1	E	181	LEU	4.2
2	H	216	CYS	3.6
2	F	210	LYS	3.5
1	E	161	GLU	3.4
2	F	214	LYS	3.4
2	F	112	SER	3.3
3	J	109	ASP	3.2
3	J	64	GLU	3.1
2	F	196	CYS	3.0
3	P	13	GLU	2.9
2	F	215	SER	2.9
2	B	216	CYS	2.9
1	E	210	ASN	2.8
2	F	147	PRO	2.8
3	P	41	ASP	2.8
2	F	216	CYS	2.7
2	F	115	SER	2.7
2	T	216	CYS	2.6
1	E	132	VAL	2.6
2	L	215	SER	2.6
2	F	212	GLU	2.5
3	C	44	GLU	2.5
1	E	129	THR	2.3
1	E	100	GLN	2.2
3	V	64	GLU	2.2
2	F	211	VAL	2.2
1	E	134	CYS	2.2
2	L	213	PRO	2.1
3	I	43	ILE	2.1
3	V	73	GLU	2.1
1	E	146	VAL	2.1
2	F	113	SER	2.1
2	T	215	SER	2.1
1	E	208	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	159	LEU	2.0
1	E	158	ASN	2.0
2	F	173	SER	2.0
2	F	114	ALA	2.0
1	E	209	PHE	2.0
2	L	212	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.