



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:59 AM UTC

PDB ID : 8B8I / pdb_00008b8i
Title : Nanobody (NbLumSyt1) bound to human Syt1
Authors : Liu, H.; Scaletti, E.; Stenmark, P.
Deposited on : 2022-10-04
Resolution : 2.75 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

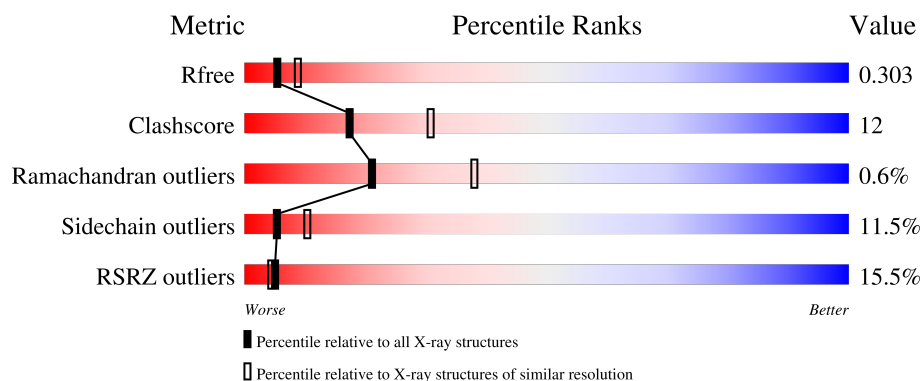
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	118	8% 70% 26% .
1	B	118	8% 68% 29% .
1	C	118	6% 72% 23% ..
1	D	118	18% 73% 22% ..
1	E	118	10% 71% 24% ..

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Mol	Chain	Length	Quality of chain
1	F	118	
1	G	118	
1	H	118	
2	I	60	
2	J	60	
2	K	60	
2	L	60	
2	M	60	
2	N	60	
2	O	60	
2	P	60	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7778 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 Nanobody (NbLumSyt1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total	C	N	O	S	0	0	0
			881	544	152	179	6			
1	B	118	Total	C	N	O	S	0	0	0
			881	544	152	179	6			
1	C	117	Total	C	N	O	S	0	0	0
			872	539	151	177	5			
1	D	117	Total	C	N	O	S	0	0	0
			874	539	151	179	5			
1	E	117	Total	C	N	O	S	0	0	0
			863	534	147	177	5			
1	F	117	Total	C	N	O	S	0	0	0
			863	534	148	176	5			
1	G	115	Total	C	N	O	S	0	0	0
			790	488	136	161	5			
1	H	113	Total	C	N	O	S	0	0	0
			751	464	130	152	5			

- Molecule 2 is a protein called Synaptotagmin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	17	Total	C	N	O	S	0	0	0
			146	94	24	27	1			
2	J	17	Total	C	N	O	S	0	0	0
			146	94	24	27	1			
2	K	16	Total	C	N	O	S	0	0	0
			132	84	21	26	1			
2	L	14	Total	C	N	O	S	0	0	0
			116	76	18	21	1			
2	M	15	Total	C	N	O	S	0	0	0
			116	74	18	23	1			
2	N	14	Total	C	N	O	S	0	0	0
			119	77	19	22	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	13	Total	C	N	O	S	0	0	0
			81	50	14	16	1			
2	P	14	Total	C	N	O		0	0	0
			74	43	14	17				

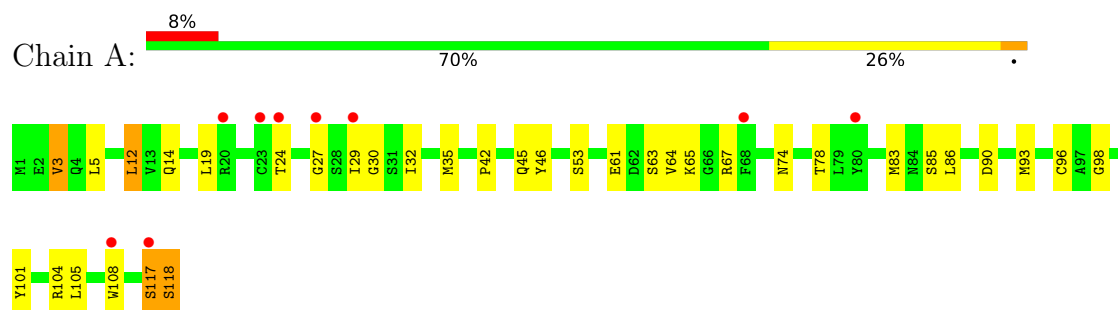
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	12	Total	O	0	0
			12	12		
3	B	5	Total	O	0	0
			5	5		
3	C	7	Total	O	0	0
			7	7		
3	D	7	Total	O	0	0
			7	7		
3	E	6	Total	O	0	0
			6	6		
3	F	13	Total	O	0	0
			13	13		
3	G	2	Total	O	0	0
			2	2		
3	H	1	Total	O	0	0
			1	1		
3	I	1	Total	O	0	0
			1	1		
3	J	1	Total	O	0	0
			1	1		
3	K	5	Total	O	0	0
			5	5		
3	L	5	Total	O	0	0
			5	5		
3	M	4	Total	O	0	0
			4	4		
3	N	4	Total	O	0	0
			4	4		

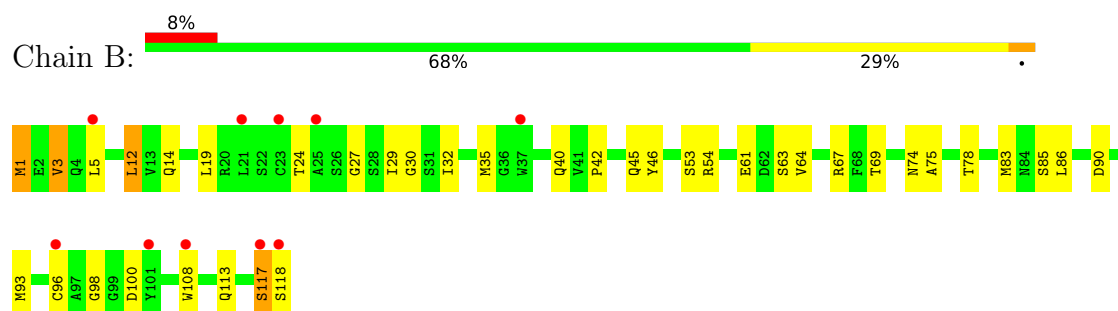
3 Residue-property plots [i](#)

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.

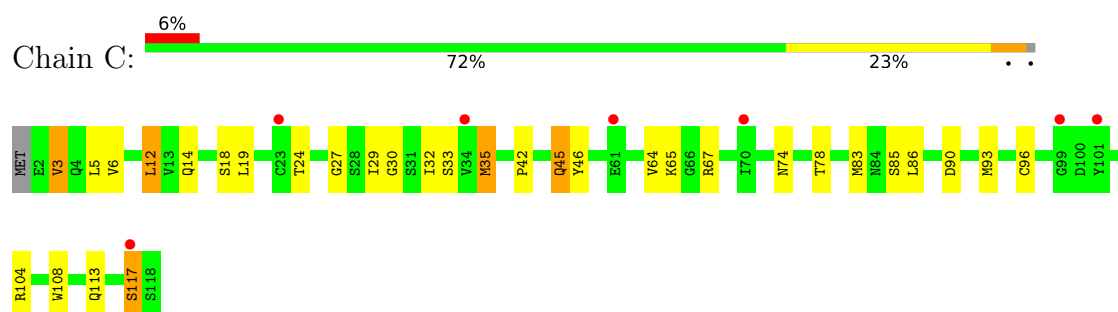
- Molecule 1: Nanobody (NbLumSyt1)



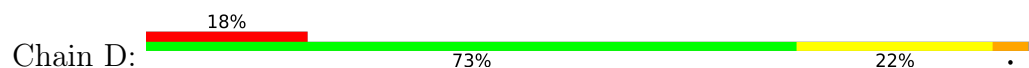
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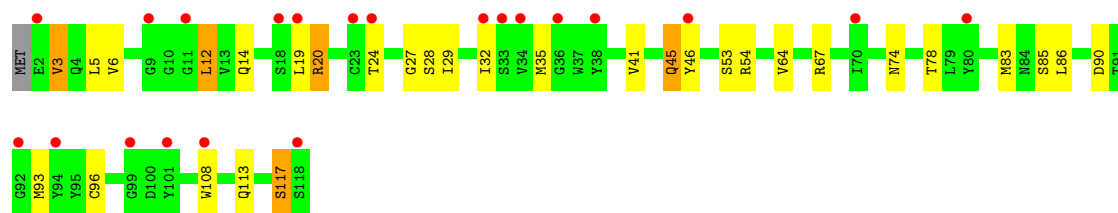


- Molecule 1: Nanobody (NbLumSyt1)

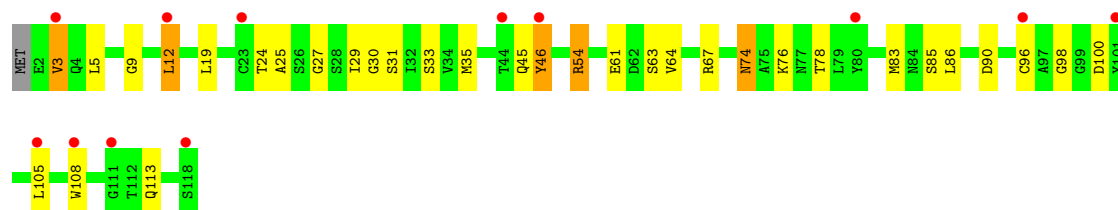


- Molecule 1: Nanobody (NbLumSyt1)

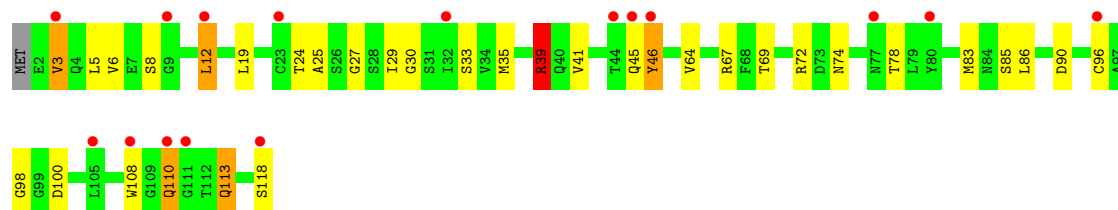




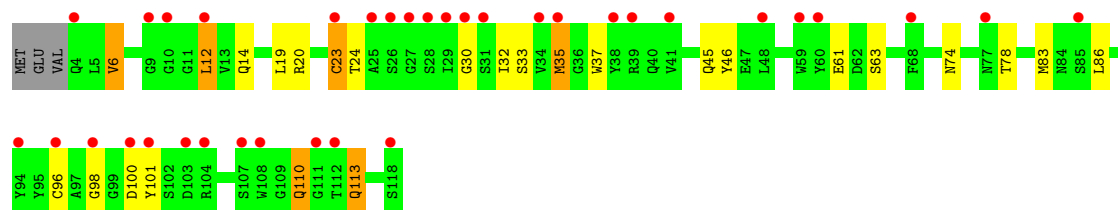
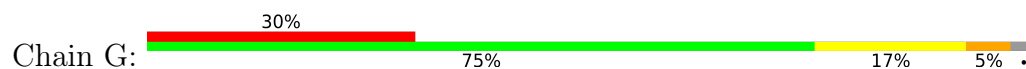
● Molecule 1: Nanobody (NbLumSyt1)



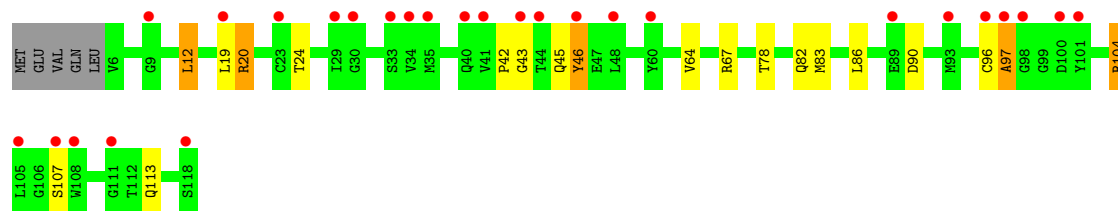
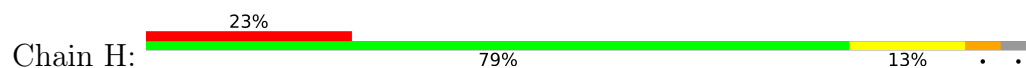
● Molecule 1: Nanobody (NbLumSyt1)



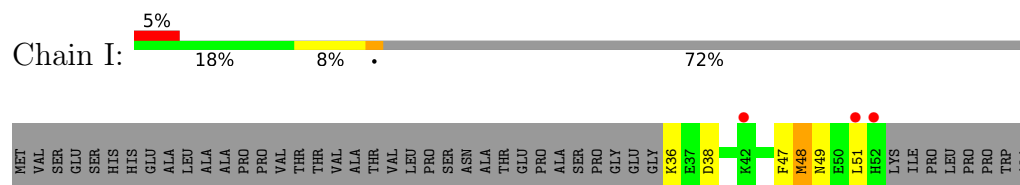
● Molecule 1: Nanobody (NbLumSyt1)



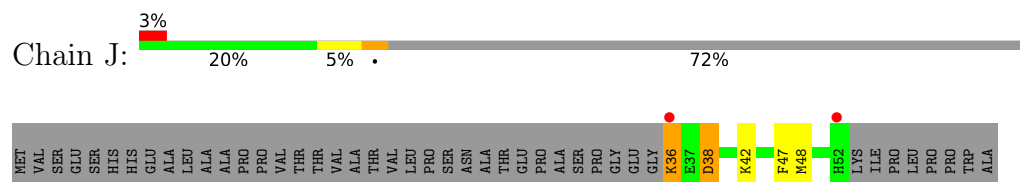
● Molecule 1: Nanobody (NbLumSyt1)



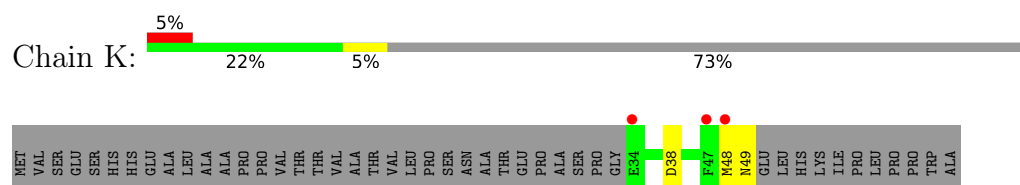
● Molecule 2: Synaptotagmin-1



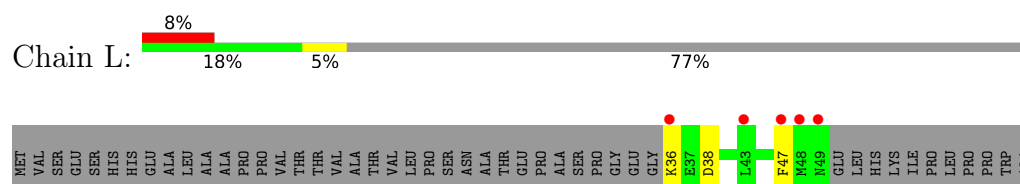
● Molecule 2: Synaptotagmin-1



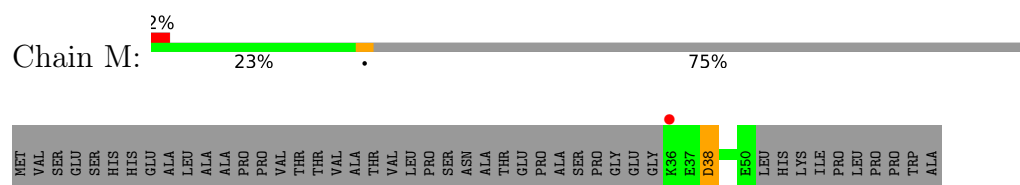
● Molecule 2: Synaptotagmin-1



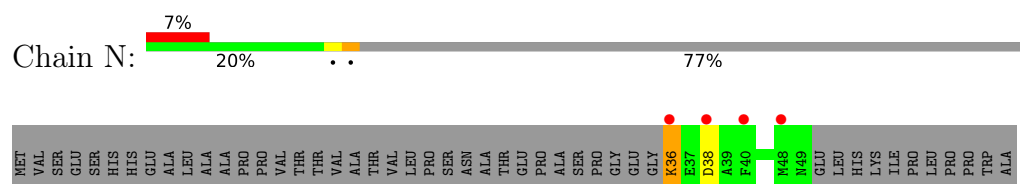
● Molecule 2: Synaptotagmin-1



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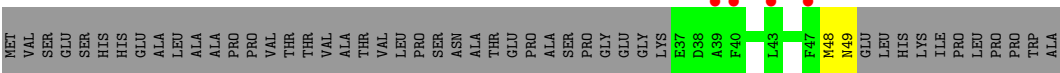


● Molecule 2: Synaptotagmin-1

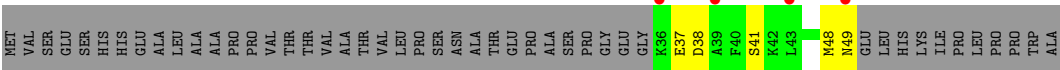


● Molecule 2: Synaptotagmin-1





● Molecule 2: Synaptotagmin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.95Å 100.23Å 103.94Å 90.00° 100.83° 90.00°	Depositor
Resolution (Å)	59.11 – 2.75 59.11 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.11-2.75) 99.8 (59.11-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.263 , 0.298 0.283 , 0.303	Depositor DCC
R_{free} test set	2370 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 84.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7778	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.49% 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	0.54	0/896	0.92	0/1210
1	B	0.53	0/896	0.88	0/1210
1	C	0.52	0/887	0.89	0/1199
1	D	0.51	0/889	0.89	0/1201
1	E	0.54	0/878	0.91	1/1188 (0.1%)
1	F	0.55	0/878	0.93	1/1188 (0.1%)
1	G	0.56	0/804	0.92	0/1095
1	H	0.58	0/765	0.92	1/1045 (0.1%)
2	I	0.54	0/148	1.03	0/193
2	J	0.51	0/148	1.05	0/193
2	K	0.49	0/133	1.03	0/172
2	L	0.43	0/117	1.03	0/151
2	M	0.50	0/117	1.06	0/154
2	N	0.52	0/120	1.06	0/155
2	O	0.71	0/81	1.28	0/109
2	P	0.51	0/73	1.11	0/100
All	All	0.54	0/7830	0.93	3/10563 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
1	G	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	113	GLN	CB-CG-CD	6.41	123.50	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	113	GLN	CB-CG-CD	6.26	123.24	112.60
1	E	113	GLN	CB-CG-CD	6.11	122.99	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	39	ARG	Sidechain
1	G	20	ARG	Sidechain

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	881	0	844	32	0
1	B	881	0	844	33	0
1	C	872	0	829	26	0
1	D	874	0	835	23	0
1	E	863	0	815	24	0
1	F	863	0	817	30	0
1	G	790	0	678	18	0
1	H	751	0	621	15	0
2	I	146	0	145	5	0
2	J	146	0	145	4	0
2	K	132	0	130	1	0
2	L	116	0	117	1	0
2	M	116	0	101	1	0
2	N	119	0	121	2	0
2	O	81	0	50	1	0
2	P	74	0	35	2	0
3	A	12	0	0	1	0
3	B	5	0	0	1	0
3	C	7	0	0	1	0
3	D	7	0	0	0	0
3	E	6	0	0	1	0
3	F	13	0	0	5	0
3	G	2	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	5	0	0	0	0
3	L	5	0	0	0	0
3	M	4	0	0	1	0
3	N	4	0	0	2	0
All	All	7778	0	7127	185	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 12.

All (185) 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:B:93:MET:HE3	1:H:12:LEU:HD13	1.54	0.89
1:D:93:MET:HE3	1:F:12:LEU:HD13	1.59	0.84
1:A:93:MET:HE3	1:G:12:LEU:HD13	1.58	0.83
1:C:93:MET:HE3	1:E:12:LEU:HD13	1.62	0.82
1:F:6:VAL:HG23	1:F:110:GLN:HE22	1.44	0.81
1:D:93:MET:HE3	1:F:12:LEU:CD1	2.13	0.79
1:E:30:GLY:CA	1:E:74:ASN:HD22	1.98	0.77
1:F:30:GLY:CA	1:F:74:ASN:HD22	1.98	0.76
1:B:30:GLY:CA	1:B:74:ASN:HD22	1.98	0.76
1:C:93:MET:HE3	1:E:12:LEU:CD1	2.16	0.76
1:A:30:GLY:CA	1:A:74:ASN:HD22	1.98	0.75
1:C:30:GLY:CA	1:C:74:ASN:HD22	1.99	0.75
1:A:45:GLN:HE22	2:I:36:LYS:HG2	1.52	0.75
1:G:30:GLY:CA	1:G:74:ASN:HD22	1.98	0.74
1:B:93:MET:HE3	1:H:12:LEU:CD1	2.19	0.72
1:E:25:ALA:CB	1:E:29:ILE:CG2	2.67	0.72
1:F:25:ALA:CB	1:F:29:ILE:CG2	2.68	0.71
1:A:93:MET:HE3	1:G:12:LEU:CD1	2.21	0.69
1:E:25:ALA:HB3	1:E:29:ILE:HG23	1.73	0.69
1:A:42:PRO:HB2	1:D:14:GLN:HB3	1.74	0.68
1:F:25:ALA:HB3	1:F:29:ILE:HG23	1.75	0.67
1:G:30:GLY:HA2	1:G:74:ASN:HD22	1.57	0.67
1:B:42:PRO:HB2	1:C:14:GLN:HB3	1.76	0.66
1:F:72:ARG:NH1	3:F:201:HOH:O	2.31	0.63
1:E:83:MET:HB3	1:E:86:LEU:HD21	1.80	0.63
1:E:30:GLY:HA3	1:E:74:ASN:HD22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:MET:HB3	1:F:86:LEU:HD21	1.80	0.62
1:F:110:GLN:H	1:F:110:GLN:HE21	1.47	0.62
1:F:118:SER:HB3	3:F:207:HOH:O	1.98	0.62
1:D:29:ILE:HG12	1:D:35:MET:HE1	1.82	0.62
1:C:29:ILE:HG12	1:C:35:MET:HE1	1.82	0.61
1:F:30:GLY:HA3	1:F:74:ASN:HD22	1.65	0.61
1:A:30:GLY:HA3	1:A:74:ASN:HD22	1.64	0.61
1:F:25:ALA:HB3	1:F:29:ILE:CG2	2.31	0.61
1:G:6:VAL:HG22	1:G:110:GLN:HE22	1.65	0.61
1:B:14:GLN:HB3	1:C:42:PRO:HB2	1.83	0.61
1:F:30:GLY:HA2	1:F:74:ASN:HD22	1.66	0.61
1:B:75:ALA:O	1:F:39:ARG:NH2	2.34	0.60
1:F:67:ARG:NH2	1:F:90:ASP:OD2	2.34	0.60
1:B:30:GLY:HA2	1:B:74:ASN:HD22	1.65	0.60
1:E:25:ALA:HB3	1:E:29:ILE:CG2	2.30	0.60
1:E:67:ARG:NH2	1:E:90:ASP:OD2	2.34	0.60
1:G:110:GLN:HE21	1:G:110:GLN:H	1.47	0.60
1:H:20:ARG:HH11	1:H:20:ARG:HB3	1.66	0.60
1:H:67:ARG:NH2	1:H:90:ASP:OD2	2.35	0.60
1:B:30:GLY:HA3	1:B:74:ASN:HD22	1.66	0.60
1:D:67:ARG:NH2	1:D:90:ASP:OD2	2.35	0.60
1:C:30:GLY:HA2	1:C:74:ASN:HD22	1.66	0.59
1:C:30:GLY:HA3	1:C:74:ASN:HD22	1.66	0.59
1:A:30:GLY:HA2	1:A:74:ASN:HD22	1.67	0.59
1:E:30:GLY:HA2	1:E:74:ASN:HD22	1.66	0.59
1:H:83:MET:HB3	1:H:86:LEU:HD21	1.84	0.59
1:A:29:ILE:HG12	1:A:35:MET:HE1	1.84	0.59
1:B:67:ARG:NH2	1:B:90:ASP:OD2	2.36	0.58
1:B:29:ILE:HG12	1:B:35:MET:HE1	1.85	0.58
1:A:83:MET:HB3	1:A:86:LEU:HD21	1.85	0.58
1:A:67:ARG:NH2	1:A:90:ASP:OD2	2.36	0.58
1:G:113:GLN:HG2	3:G:201:HOH:O	2.02	0.58
1:C:67:ARG:NH2	1:C:90:ASP:OD2	2.36	0.58
1:G:30:GLY:HA2	1:G:74:ASN:ND2	2.18	0.58
1:G:23:CYS:HB3	1:G:37:TRP:CH2	2.38	0.58
1:B:40:GLN:NE2	3:B:201:HOH:O	2.37	0.58
1:B:83:MET:HB3	1:B:86:LEU:HD21	1.85	0.58
1:C:104:ARG:HD3	3:C:205:HOH:O	2.04	0.58
1:D:83:MET:HB3	1:D:86:LEU:HD21	1.86	0.57
1:G:83:MET:HB3	1:G:86:LEU:HD21	1.84	0.57
1:H:104:ARG:HH21	2:P:37:GLU:CB	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:MET:HB3	1:C:86:LEU:HD21	1.85	0.57
1:E:9:GLY:O	3:E:201:HOH:O	2.17	0.56
1:C:18:SER:OG	1:H:20:ARG:NH1	2.39	0.56
1:B:113:GLN:HE22	1:C:12:LEU:HD12	1.71	0.56
1:C:5:LEU:HB2	1:C:108:TRP:O	2.06	0.56
1:D:5:LEU:HB2	1:D:108:TRP:O	2.06	0.56
1:A:5:LEU:HB2	1:A:108:TRP:O	2.06	0.56
1:D:20:ARG:HH11	1:D:20:ARG:HB3	1.71	0.55
1:B:5:LEU:HB2	1:B:108:TRP:O	2.06	0.55
1:B:1:MET:HE2	1:B:100:ASP:OD2	2.06	0.55
2:N:36:LYS:HD3	3:N:104:HOH:O	2.07	0.54
1:F:5:LEU:HB2	1:F:108:TRP:O	2.08	0.54
1:E:5:LEU:HB2	1:E:108:TRP:O	2.08	0.53
1:A:42:PRO:HD3	1:D:12:LEU:HD21	1.90	0.53
1:H:20:ARG:HH11	1:H:20:ARG:CB	2.21	0.53
2:J:38:ASP:O	2:J:42:LYS:HD3	2.08	0.53
1:D:20:ARG:HH11	1:D:20:ARG:CB	2.22	0.52
1:E:25:ALA:HB2	1:E:29:ILE:CG2	2.38	0.52
1:G:30:GLY:HA3	1:G:74:ASN:HD22	1.74	0.52
1:G:61:GLU:HG3	1:G:63:SER:OG	2.10	0.52
1:D:28:SER:HB2	1:H:43:GLY:HA3	1.91	0.52
1:E:105:LEU:N	1:E:105:LEU:HD12	2.26	0.51
1:B:30:GLY:HA2	1:B:74:ASN:ND2	2.25	0.51
1:F:30:GLY:HA2	1:F:74:ASN:ND2	2.25	0.51
1:A:12:LEU:HD12	1:D:113:GLN:HE22	1.75	0.51
1:C:14:GLN:HA	1:C:117:SER:O	2.10	0.51
1:F:25:ALA:HB2	1:F:29:ILE:CG2	2.39	0.51
1:E:30:GLY:HA2	1:E:74:ASN:ND2	2.26	0.50
1:A:45:GLN:NE2	2:I:36:LYS:HG2	2.23	0.50
1:B:14:GLN:HA	1:B:117:SER:O	2.11	0.50
1:D:14:GLN:HA	1:D:117:SER:O	2.12	0.50
1:H:20:ARG:HD3	1:H:82:GLN:OE1	2.11	0.50
1:B:12:LEU:HD12	1:C:113:GLN:HE22	1.76	0.49
1:A:30:GLY:HA2	1:A:74:ASN:ND2	2.27	0.49
1:G:113:GLN:CG	3:G:201:HOH:O	2.58	0.49
1:B:61:GLU:OE1	1:B:63:SER:CB	2.61	0.49
1:B:113:GLN:HE22	1:C:12:LEU:CD1	2.26	0.48
1:F:45:GLN:O	1:F:46:TYR:C	2.56	0.48
1:C:30:GLY:HA2	1:C:74:ASN:ND2	2.26	0.48
2:K:48:MET:O	2:K:49:ASN:ND2	2.46	0.48
2:O:48:MET:HG2	2:O:49:ASN:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:SER:C	3:A:202:HOH:O	2.56	0.48
1:A:14:GLN:OE1	1:F:8:SER:HB2	2.13	0.48
1:E:45:GLN:O	1:E:46:TYR:C	2.56	0.48
1:A:61:GLU:OE1	1:A:63:SER:CB	2.62	0.47
1:G:45:GLN:O	1:G:46:TYR:C	2.57	0.47
1:D:45:GLN:O	1:D:46:TYR:C	2.57	0.47
1:D:53:SER:HB3	2:L:47:PHE:CD1	2.50	0.47
1:H:45:GLN:O	1:H:46:TYR:C	2.57	0.47
1:B:45:GLN:OE1	2:J:36:LYS:HG2	2.14	0.47
1:C:24:THR:HG22	1:C:78:THR:OG1	2.15	0.47
1:F:24:THR:HG22	1:F:78:THR:OG1	2.15	0.47
1:G:24:THR:HG22	1:G:78:THR:OG1	2.15	0.47
1:H:24:THR:HG22	1:H:78:THR:OG1	2.15	0.47
1:B:24:THR:HG22	1:B:78:THR:OG1	2.15	0.47
1:E:31:SER:HA	1:E:54:ARG:NH1	2.30	0.47
1:D:24:THR:HG22	1:D:78:THR:OG1	2.14	0.47
1:C:45:GLN:O	1:C:46:TYR:C	2.57	0.46
1:E:24:THR:HG22	1:E:78:THR:OG1	2.15	0.46
1:A:3:VAL:HG23	1:A:27:GLY:H	1.80	0.46
1:A:24:THR:HG22	1:A:78:THR:OG1	2.15	0.46
1:B:45:GLN:O	1:B:46:TYR:C	2.58	0.46
1:F:118:SER:CB	3:F:207:HOH:O	2.59	0.46
1:B:3:VAL:HG23	1:B:27:GLY:H	1.81	0.46
1:E:25:ALA:HB2	1:E:29:ILE:HG21	1.97	0.46
1:H:97:ALA:HA	1:H:107:SER:O	2.16	0.46
1:C:3:VAL:HG23	1:C:27:GLY:H	1.80	0.46
1:E:35:MET:HG2	1:E:98:GLY:HA3	1.97	0.46
2:P:48:MET:O	2:P:49:ASN:C	2.58	0.46
1:C:29:ILE:HA	1:C:32:ILE:HD12	1.98	0.45
1:E:64:VAL:HA	1:E:67:ARG:NH1	2.31	0.45
1:F:64:VAL:HA	1:F:67:ARG:NH1	2.31	0.45
1:A:45:GLN:O	1:A:46:TYR:C	2.58	0.45
1:D:3:VAL:HG23	1:D:27:GLY:H	1.81	0.45
1:E:61:GLU:OE1	1:E:63:SER:CB	2.64	0.45
1:A:53:SER:HB3	2:I:47:PHE:CD1	2.52	0.45
1:C:29:ILE:CG1	1:C:35:MET:HE1	2.46	0.45
1:A:29:ILE:CG2	1:A:74:ASN:HA	2.47	0.45
1:C:64:VAL:HA	1:C:67:ARG:NH1	2.31	0.45
1:F:3:VAL:HG23	1:F:27:GLY:H	1.81	0.45
1:D:29:ILE:HA	1:D:32:ILE:HD12	1.99	0.45
1:C:29:ILE:CG2	1:C:74:ASN:HA	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:VAL:HA	1:D:67:ARG:NH1	2.32	0.44
1:A:45:GLN:HE22	2:I:36:LYS:CG	2.25	0.44
1:A:64:VAL:HA	1:A:67:ARG:NH1	2.32	0.44
1:B:29:ILE:HA	1:B:32:ILE:HD12	1.99	0.44
1:B:45:GLN:HE22	2:J:36:LYS:HE2	1.81	0.44
1:F:35:MET:HG2	1:F:98:GLY:HA3	1.99	0.44
1:F:113:GLN:HG2	3:F:208:HOH:O	2.16	0.44
1:F:25:ALA:HB2	1:F:29:ILE:HG21	1.98	0.44
1:B:12:LEU:CD1	1:C:113:GLN:HE22	2.31	0.44
1:D:29:ILE:CG2	1:D:74:ASN:HA	2.48	0.44
1:G:33:SER:OG	1:G:100:ASP:HA	2.18	0.44
1:A:104:ARG:HG3	1:A:105:LEU:HG	2.00	0.44
1:B:29:ILE:CG2	1:B:74:ASN:HA	2.48	0.44
1:H:64:VAL:HA	1:H:67:ARG:NH1	2.33	0.43
1:A:12:LEU:CD1	1:D:113:GLN:HE22	2.32	0.43
1:A:29:ILE:CG1	1:A:35:MET:HE1	2.47	0.43
1:E:3:VAL:HG23	1:E:27:GLY:H	1.82	0.43
1:F:41:VAL:HA	3:F:204:HOH:O	2.17	0.43
2:M:38:ASP:HA	3:M:102:HOH:O	2.18	0.43
1:D:29:ILE:CG1	1:D:35:MET:HE1	2.46	0.43
1:G:35:MET:HG3	1:G:98:GLY:HA3	2.00	0.43
1:B:64:VAL:HA	1:B:67:ARG:NH1	2.34	0.43
1:A:29:ILE:HA	1:A:32:ILE:HD12	2.00	0.43
1:B:29:ILE:CG1	1:B:35:MET:HE1	2.49	0.43
1:A:101:TYR:CE1	2:I:48:MET:HE2	2.54	0.42
1:B:35:MET:HG2	1:B:98:GLY:HA3	2.02	0.42
1:B:53:SER:HB3	2:J:47:PHE:CD1	2.55	0.41
1:B:1:MET:HE1	1:B:32:ILE:HA	2.02	0.41
1:A:35:MET:HG2	1:A:98:GLY:HA3	2.02	0.41
1:E:67:ARG:HH22	1:E:90:ASP:CG	2.29	0.41
1:F:6:VAL:HG23	1:F:110:GLN:NE2	2.25	0.41
1:F:67:ARG:HH22	1:F:90:ASP:CG	2.29	0.41
2:N:36:LYS:N	3:N:101:HOH:O	2.53	0.41
1:A:14:GLN:HA	1:A:117:SER:O	2.21	0.40
1:G:6:VAL:CG2	1:G:110:GLN:HE22	2.33	0.40
1:D:28:SER:HB2	1:H:42:PRO:O	2.21	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	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	B	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
1	C	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
1	D	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
1	E	115/118 (98%)	113 (98%)	1 (1%)	1 (1%)	14	28
1	F	115/118 (98%)	113 (98%)	1 (1%)	1 (1%)	14	28
1	G	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
1	H	111/118 (94%)	107 (96%)	1 (1%)	3 (3%)	4	7
2	I	15/60 (25%)	14 (93%)	0	1 (7%)	1	1
2	J	15/60 (25%)	13 (87%)	2 (13%)	0	100	100
2	K	14/60 (23%)	12 (86%)	2 (14%)	0	100	100
2	L	12/60 (20%)	12 (100%)	0	0	100	100
2	M	13/60 (22%)	13 (100%)	0	0	100	100
2	N	12/60 (20%)	12 (100%)	0	0	100	100
2	O	11/60 (18%)	11 (100%)	0	0	100	100
2	P	12/60 (20%)	12 (100%)	0	0	100	100
All	All	1020/1424 (72%)	996 (98%)	18 (2%)	6 (1%)	21	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	97	ALA
2	I	49	ASN
1	H	96	CYS
1	E	46	TYR
1	F	46	TYR
1	H	46	TYR

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	94/95 (99%)	86 (92%)	8 (8%)	10	18
1	B	94/95 (99%)	84 (89%)	10 (11%)	6	13
1	C	92/95 (97%)	81 (88%)	11 (12%)	5	8
1	D	94/95 (99%)	83 (88%)	11 (12%)	5	9
1	E	91/95 (96%)	81 (89%)	10 (11%)	6	11
1	F	91/95 (96%)	81 (89%)	10 (11%)	6	11
1	G	70/95 (74%)	59 (84%)	11 (16%)	2	4
1	H	62/95 (65%)	58 (94%)	4 (6%)	15	29
2	I	16/50 (32%)	13 (81%)	3 (19%)	1	3
2	J	16/50 (32%)	13 (81%)	3 (19%)	1	3
2	K	14/50 (28%)	13 (93%)	1 (7%)	13	25
2	L	12/50 (24%)	10 (83%)	2 (17%)	2	3
2	M	11/50 (22%)	10 (91%)	1 (9%)	9	17
2	N	13/50 (26%)	11 (85%)	2 (15%)	2	4
2	O	4/50 (8%)	4 (100%)	0	100	100
2	P	2/50 (4%)	0	2 (100%)	0	0
All	All	776/1160 (67%)	687 (88%)	89 (12%)	5	10

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	12	LEU
1	A	19	LEU
1	A	65	LYS
1	A	85	SER
1	A	96	CYS
1	A	117	SER
1	A	118	SER

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Mol	Chain	Res	Type
1	B	1	MET
1	B	3	VAL
1	B	12	LEU
1	B	19	LEU
1	B	54	ARG
1	B	69	THR
1	B	85	SER
1	B	96	CYS
1	B	117	SER
1	B	118	SER
1	C	3	VAL
1	C	6	VAL
1	C	12	LEU
1	C	19	LEU
1	C	33	SER
1	C	35	MET
1	C	45	GLN
1	C	65	LYS
1	C	85	SER
1	C	96	CYS
1	C	117	SER
1	D	3	VAL
1	D	6	VAL
1	D	12	LEU
1	D	19	LEU
1	D	20	ARG
1	D	41	VAL
1	D	45	GLN
1	D	54	ARG
1	D	85	SER
1	D	96	CYS
1	D	117	SER
1	E	3	VAL
1	E	12	LEU
1	E	19	LEU
1	E	33	SER
1	E	54	ARG
1	E	74	ASN
1	E	76	LYS
1	E	85	SER
1	E	96	CYS
1	E	100	ASP

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Mol	Chain	Res	Type
1	F	3	VAL
1	F	12	LEU
1	F	19	LEU
1	F	33	SER
1	F	39	ARG
1	F	69	THR
1	F	85	SER
1	F	96	CYS
1	F	100	ASP
1	F	110	GLN
1	G	6	VAL
1	G	12	LEU
1	G	14	GLN
1	G	19	LEU
1	G	23	CYS
1	G	32	ILE
1	G	35	MET
1	G	96	CYS
1	G	101	TYR
1	G	110	GLN
1	G	113	GLN
1	H	12	LEU
1	H	19	LEU
1	H	20	ARG
1	H	104	ARG
2	I	38	ASP
2	I	48	MET
2	I	51	LEU
2	J	36	LYS
2	J	38	ASP
2	J	48	MET
2	K	38	ASP
2	L	36	LYS
2	L	38	ASP
2	M	38	ASP
2	N	36	LYS
2	N	38	ASP
2	P	38	ASP
2	P	41	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	74	ASN
1	B	74	ASN
1	B	84	ASN
1	B	113	GLN
1	C	40	GLN
1	C	45	GLN
1	C	74	ASN
1	C	77	ASN
1	C	82	GLN
1	C	84	ASN
1	C	113	GLN
1	D	82	GLN
1	D	113	GLN
1	E	74	ASN
1	F	74	ASN
1	F	110	GLN
1	G	74	ASN
1	G	84	ASN
1	G	110	GLN
1	G	113	GLN
2	K	49	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	118/118 (100%)	0.98	9 (7%) 20 19	56, 81, 102, 120	0
1	B	118/118 (100%)	0.98	10 (8%) 16 17	58, 80, 103, 111	0
1	C	117/118 (99%)	1.10	7 (5%) 27 28	71, 99, 128, 144	0
1	D	117/118 (99%)	1.26	21 (17%) 3 3	75, 102, 133, 144	0
1	E	117/118 (99%)	1.02	12 (10%) 12 11	58, 86, 125, 134	0
1	F	117/118 (99%)	1.13	16 (13%) 6 5	62, 91, 127, 139	0
1	G	115/118 (97%)	1.65	35 (30%) 1 1	91, 143, 181, 201	0
1	H	113/118 (95%)	1.42	27 (23%) 2 1	79, 138, 175, 194	0
2	I	17/60 (28%)	1.17	3 (17%) 4 3	69, 93, 128, 128	0
2	J	17/60 (28%)	1.04	2 (11%) 9 7	74, 89, 125, 129	0
2	K	16/60 (26%)	1.25	3 (18%) 3 2	86, 100, 140, 145	0
2	L	14/60 (23%)	1.64	5 (35%) 1 0	92, 105, 130, 139	0
2	M	15/60 (25%)	1.21	1 (6%) 24 23	95, 105, 146, 157	0
2	N	14/60 (23%)	1.52	4 (28%) 1 1	101, 120, 144, 152	0
2	O	13/60 (21%)	1.45	4 (30%) 1 1	147, 167, 189, 207	0
2	P	14/60 (23%)	1.43	4 (28%) 1 1	141, 162, 181, 184	0
All	All	1052/1424 (73%)	1.21	163 (15%) 5 4	56, 99, 167, 207	0

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	29	ILE	5.9
1	H	98	GLY	5.3
1	G	100	ASP	4.8
1	F	23	CYS	4.7
1	G	9	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	H	105	LEU	4.5
1	F	44	THR	4.5
1	C	34	VAL	4.5
1	E	118	SER	4.4
1	H	100	ASP	4.4
1	H	118	SER	4.3
1	C	101	TYR	4.3
1	G	118	SER	4.2
1	B	23	CYS	4.2
1	E	96	CYS	4.1
1	B	117	SER	3.9
1	A	23	CYS	3.9
1	H	9	GLY	3.8
2	L	36	LYS	3.8
1	E	23	CYS	3.7
2	I	52	HIS	3.7
1	D	34	VAL	3.7
1	G	34	VAL	3.7
1	D	101	TYR	3.7
2	P	36	LYS	3.7
1	H	34	VAL	3.4
1	F	96	CYS	3.4
1	G	28	SER	3.4
1	G	112	THR	3.4
1	B	108	TRP	3.3
1	D	99	GLY	3.3
1	G	48	LEU	3.3
2	P	39	ALA	3.3
1	C	23	CYS	3.3
1	D	18	SER	3.3
1	G	107	SER	3.3
1	E	12	LEU	3.2
1	G	23	CYS	3.2
2	N	36	LYS	3.2
1	F	118	SER	3.1
2	J	52	HIS	3.1
1	H	41	VAL	3.1
1	A	80	TYR	3.1
1	E	111	GLY	3.1
2	O	39	ALA	3.1
2	K	47	PHE	3.1
1	C	117	SER	3.1

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Mol	Chain	Res	Type	RSRZ
2	L	48	MET	3.0
1	E	108	TRP	3.0
2	N	40	PHE	3.0
1	F	12	LEU	3.0
1	H	23	CYS	3.0
1	H	96	CYS	2.9
1	A	117	SER	2.9
1	G	98	GLY	2.9
1	A	108	TRP	2.9
1	H	107	SER	2.9
1	H	30	GLY	2.9
1	D	23	CYS	2.9
1	F	111	GLY	2.9
1	E	44	THR	2.8
1	F	108	TRP	2.8
2	M	36	LYS	2.8
1	H	35	MET	2.8
1	G	103	ASP	2.8
1	G	111	GLY	2.8
1	G	4	GLN	2.7
2	K	48	MET	2.7
2	K	34	GLU	2.7
1	G	27	GLY	2.7
1	H	108	TRP	2.7
1	G	101	TYR	2.7
1	C	99	GLY	2.7
1	E	80	TYR	2.6
1	H	33	SER	2.6
2	L	49	ASN	2.6
1	H	101	TYR	2.6
1	H	40	GLN	2.6
1	E	46	TYR	2.6
1	D	9	GLY	2.6
1	B	118	SER	2.6
1	F	45	GLN	2.6
1	G	104	ARG	2.6
1	G	25	ALA	2.6
1	G	41	VAL	2.6
2	O	40	PHE	2.6
2	O	47	PHE	2.6
1	H	44	THR	2.5
1	B	101	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	46	TYR	2.5
2	L	47	PHE	2.5
1	A	68	PHE	2.5
1	D	70	ILE	2.5
1	G	59	TRP	2.5
1	E	105	LEU	2.5
1	H	48	LEU	2.5
1	F	80	TYR	2.5
1	D	36	GLY	2.5
1	B	96	CYS	2.5
1	G	108	TRP	2.5
1	C	70	ILE	2.4
1	H	111	GLY	2.4
2	O	43	LEU	2.4
2	N	38	ASP	2.4
1	D	38	TYR	2.4
1	D	46	TYR	2.4
1	F	3	VAL	2.4
1	A	29	ILE	2.4
1	F	105	LEU	2.4
1	G	77	ASN	2.4
2	P	49	ASN	2.4
1	H	97	ALA	2.4
2	I	42	LYS	2.4
2	J	36	LYS	2.4
1	F	9	GLY	2.4
1	E	3	VAL	2.4
1	H	19	LEU	2.3
1	D	33	SER	2.3
1	D	11	GLY	2.3
1	B	25	ALA	2.3
1	G	12	LEU	2.3
1	H	60	TYR	2.3
1	F	77	ASN	2.3
1	G	26	SER	2.3
1	G	96	CYS	2.3
1	H	93	MET	2.3
1	F	46	TYR	2.3
1	G	31	SER	2.3
1	D	80	TYR	2.2
1	G	94	TYR	2.2
1	G	30	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	5	LEU	2.2
2	I	51	LEU	2.2
1	D	24	THR	2.2
1	G	39	ARG	2.2
1	A	27	GLY	2.2
1	D	118	SER	2.2
1	H	89	GLU	2.2
1	C	61	GLU	2.2
1	E	101	TYR	2.2
1	D	92	GLY	2.2
2	L	43	LEU	2.2
1	F	32	ILE	2.2
1	D	108	TRP	2.1
1	D	19	LEU	2.1
1	G	85	SER	2.1
1	G	10	GLY	2.1
1	D	2	GLU	2.1
1	G	35	MET	2.1
2	N	48	MET	2.1
1	G	38	TYR	2.1
1	H	43	GLY	2.1
1	D	32	ILE	2.1
1	G	68	PHE	2.1
1	B	37	TRP	2.1
2	P	43	LEU	2.1
1	D	94	TYR	2.1
1	H	29	ILE	2.1
1	A	20	ARG	2.0
1	A	24	THR	2.0
1	B	21	LEU	2.0
1	F	110	GLN	2.0
1	G	60	TYR	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.