



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:29 AM UTC

PDB ID : 1NMP / pdb_00001nmp
Title : Structural genomics, ybgI protein, unknown function
Authors : Ladner, J.E.; Obmolova, G.; Teplyakov, A.; Khil, P.P.; Camerini-Otero, R.D.;
Gilliland, G.L.; Structure 2 Function Project (S2F)
Deposited on : 2003-01-10
Resolution : 2.20 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

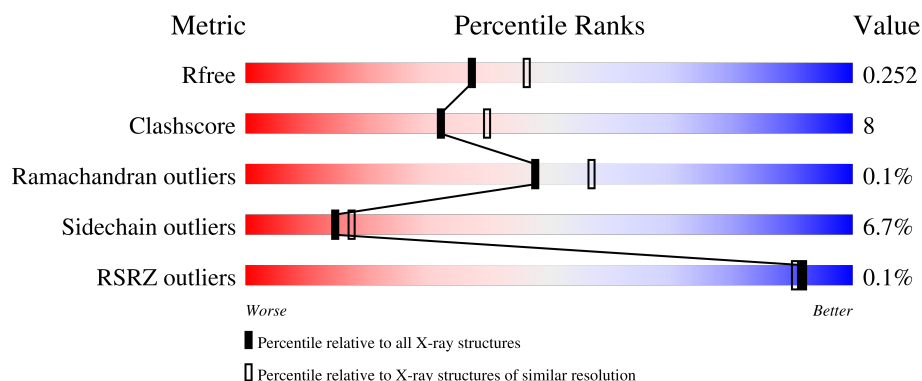
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	247	 72% 23% .
1	B	247	 67% 26% 6% .
1	C	247	 70% 24% 6%
1	D	247	 77% 21% .
1	E	247	 81% 17% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	247	77% 19% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11969 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 Hypothetical protein ybgI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	B	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	C	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	D	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	E	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			
1	F	247	Total	C	N	O	S	0	0	0
			1897	1200	332	359	6			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	1	Total	Mg	0	0
			1	1		
2	C	2	Total	Mg	0	0
			2	2		
2	D	2	Total	Mg	0	0
			2	2		
2	E	2	Total	Mg	0	0
			2	2		
2	F	2	Total	Mg	0	0
			2	2		

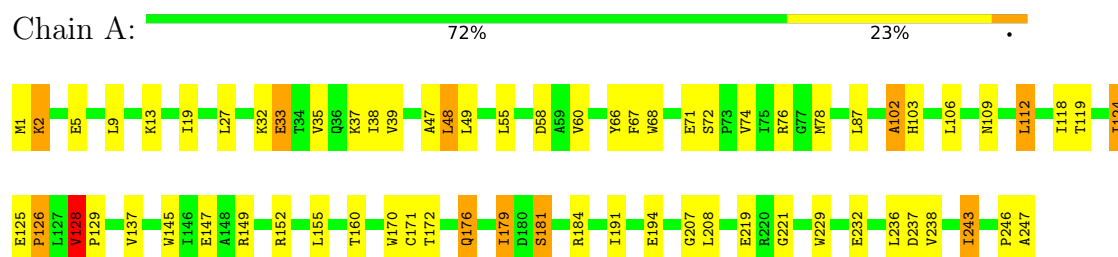
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	78	Total 78	O 78	0	0
3	B	79	Total 79	O 79	0	0
3	C	95	Total 95	O 95	0	0
3	D	87	Total 87	O 87	0	0
3	E	124	Total 124	O 124	0	0
3	F	113	Total 113	O 113	0	0

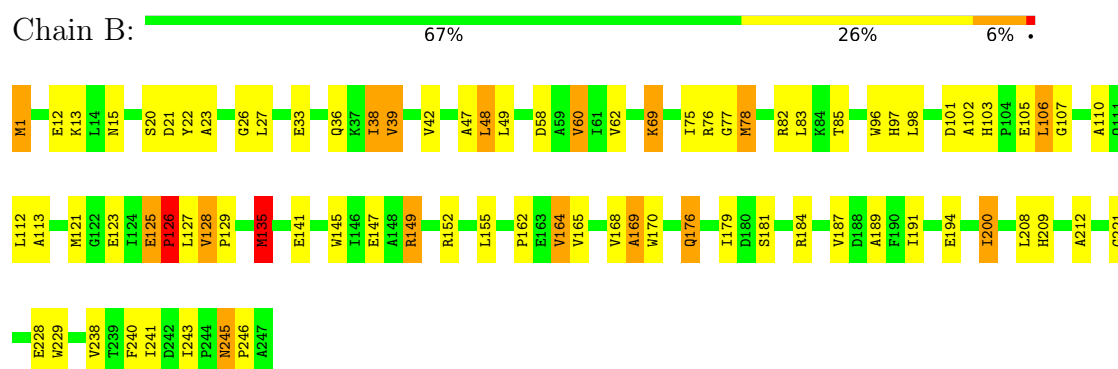
3 Residue-property plots

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

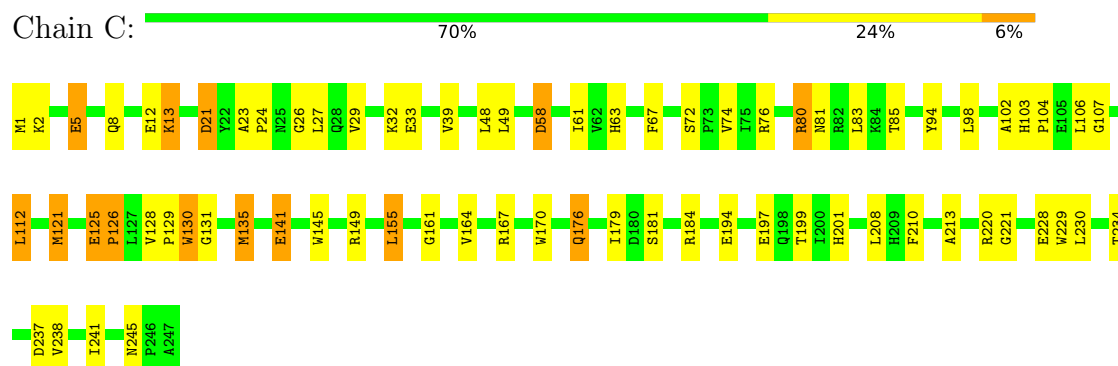
• Molecule 1: Hypothetical protein ybgI



• Molecule 1: Hypothetical protein ybgI

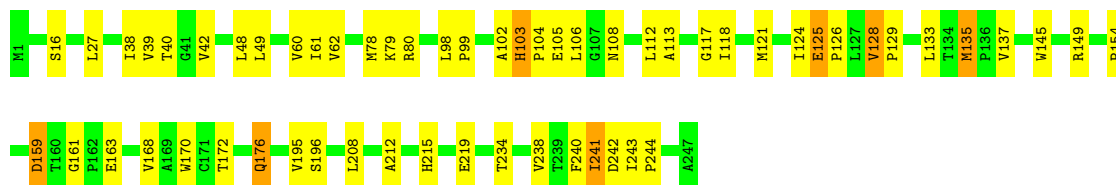


• Molecule 1: Hypothetical protein ybgI



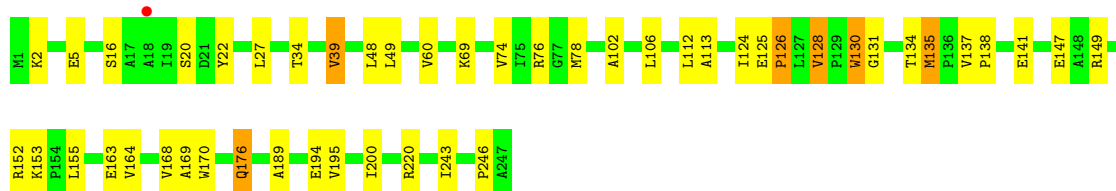
• Molecule 1: Hypothetical protein ybgI

Chain D:  77% 21% .



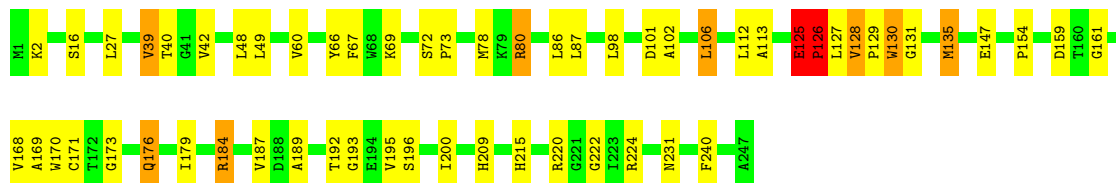
• Molecule 1: Hypothetical protein ybgI

Chain E:  81% 17% .



• Molecule 1: Hypothetical protein ybgI

Chain F:  77% 19% . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	156.73Å 156.73Å 57.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.76 – 2.20 19.76 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.9 (19.76-2.20) 96.7 (19.76-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.253 0.212 , 0.252	Depositor DCC
R_{free} test set	7004 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l 0.029 for h,-h-k,-l 0.009 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11969	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	1.49	7/1940 (0.4%)	1.41	18/2641 (0.7%)
1	B	1.57	17/1940 (0.9%)	1.46	25/2641 (0.9%)
1	C	1.41	8/1940 (0.4%)	1.50	31/2641 (1.2%)
1	D	1.36	5/1940 (0.3%)	1.41	20/2641 (0.8%)
1	E	1.38	5/1940 (0.3%)	1.44	16/2641 (0.6%)
1	F	1.38	5/1940 (0.3%)	1.45	17/2641 (0.6%)
All	All	1.43	47/11640 (0.4%)	1.44	127/15846 (0.8%)

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	B	0	1
1	E	0	1
All	All	0	2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	135	MET	SD-CE	13.52	2.13	1.79
1	B	135	MET	SD-CE	12.60	2.11	1.79
1	F	135	MET	SD-CE	12.47	2.10	1.79
1	A	128	VAL	CA-CB	10.19	1.67	1.54
1	C	121	MET	SD-CE	10.06	2.04	1.79
1	D	135	MET	SD-CE	9.51	2.03	1.79
1	B	1	MET	SD-CE	8.91	2.01	1.79
1	E	135	MET	SD-CE	8.80	2.01	1.79
1	A	243	ILE	N-CA	8.13	1.52	1.46
1	B	126	PRO	C-O	8.00	1.34	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	62	VAL	CA-CB	7.67	1.66	1.54
1	A	191	ILE	CA-CB	7.36	1.64	1.54
1	D	78	MET	SD-CE	7.19	1.97	1.79
1	C	126	PRO	C-O	6.82	1.32	1.24
1	D	126	PRO	C-O	6.60	1.32	1.24
1	B	243	ILE	CA-C	6.59	1.58	1.53
1	B	200	ILE	CA-CB	6.50	1.62	1.54
1	C	1	MET	SD-CE	6.48	1.95	1.79
1	B	38	ILE	CA-CB	6.47	1.62	1.54
1	E	137	VAL	CA-CB	6.36	1.62	1.54
1	B	121	MET	SD-CE	6.31	1.95	1.79
1	C	61	ILE	CA-CB	-6.16	1.46	1.54
1	C	29	VAL	CA-CB	-6.07	1.46	1.54
1	F	80	ARG	CZ-NH2	5.98	1.41	1.33
1	C	213	ALA	CA-CB	5.98	1.64	1.53
1	F	231	ASN	CA-C	5.90	1.60	1.52
1	F	126	PRO	C-O	5.86	1.31	1.24
1	D	121	MET	SD-CE	5.75	1.94	1.79
1	E	78	MET	SD-CE	5.65	1.93	1.79
1	E	200	ILE	CA-CB	5.58	1.61	1.54
1	B	110	ALA	CA-CB	5.56	1.61	1.53
1	C	13	LYS	CA-C	5.53	1.59	1.52
1	A	47	ALA	CA-CB	5.52	1.61	1.53
1	A	119	THR	CA-CB	5.50	1.60	1.53
1	B	48	LEU	N-CA	5.47	1.53	1.46
1	B	191	ILE	CA-CB	5.42	1.61	1.54
1	E	126	PRO	C-O	5.42	1.31	1.24
1	B	47	ALA	CA-CB	5.39	1.61	1.53
1	B	36	GLN	CA-C	5.33	1.59	1.52
1	B	60	VAL	CA-CB	5.28	1.61	1.54
1	A	126	PRO	CA-C	5.23	1.59	1.52
1	B	165	VAL	CA-CB	5.17	1.60	1.54
1	B	103	HIS	CA-C	5.13	1.59	1.53
1	B	39	VAL	CA-C	5.13	1.58	1.52
1	F	86	LEU	C-O	5.08	1.29	1.24
1	D	137	VAL	CA-CB	5.07	1.60	1.54
1	A	181	SER	CA-C	5.05	1.59	1.52

All (127) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	245	ASN	CA-C-N	11.82	131.54	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	245	ASN	C-N-CA	11.82	131.54	119.24
1	F	16	SER	N-CA-C	9.98	122.23	111.36
1	B	245	ASN	CA-C-N	9.43	129.65	119.28
1	B	245	ASN	C-N-CA	9.43	129.65	119.28
1	B	102	ALA	N-CA-C	9.18	124.61	113.23
1	C	72	SER	CA-C-N	9.13	128.87	119.19
1	C	72	SER	C-N-CA	9.13	128.87	119.19
1	E	102	ALA	N-CA-C	9.12	124.54	113.23
1	C	102	ALA	N-CA-C	8.85	124.20	113.23
1	C	220	ARG	N-CA-C	-8.58	102.59	113.23
1	B	101	ASP	N-CA-C	-8.32	101.25	111.40
1	F	102	ALA	N-CA-C	8.28	123.49	113.23
1	B	23	ALA	CA-C-N	7.96	128.26	119.90
1	B	23	ALA	C-N-CA	7.96	128.26	119.90
1	C	161	GLY	CA-C-N	7.94	128.42	119.92
1	C	161	GLY	C-N-CA	7.94	128.42	119.92
1	B	212	ALA	N-CA-C	-7.80	94.18	107.99
1	B	125	GLU	N-CA-C	-7.65	101.34	108.22
1	B	42	VAL	N-CA-C	7.61	117.73	110.42
1	C	103	HIS	CA-C-N	7.60	128.28	119.47
1	C	103	HIS	C-N-CA	7.60	128.28	119.47
1	E	220	ARG	N-CA-C	-7.50	102.78	112.23
1	F	98	LEU	CA-C-N	-7.42	112.07	119.56
1	F	98	LEU	C-N-CA	-7.42	112.07	119.56
1	F	125	GLU	N-CA-C	-7.27	99.78	108.14
1	C	128	VAL	CA-C-N	7.18	127.14	120.03
1	C	128	VAL	C-N-CA	7.18	127.14	120.03
1	F	125	GLU	CA-C-N	6.97	128.56	119.84
1	F	125	GLU	C-N-CA	6.97	128.56	119.84
1	D	42	VAL	N-CA-C	6.96	117.75	110.72
1	C	228	GLU	N-CA-C	-6.96	103.77	111.36
1	F	161	GLY	CA-C-N	6.94	128.51	119.84
1	F	161	GLY	C-N-CA	6.94	128.51	119.84
1	A	179	ILE	N-CA-C	6.91	117.67	110.62
1	D	176	GLN	CB-CA-C	-6.86	97.94	110.63
1	B	33	GLU	N-CA-C	6.85	118.75	111.28
1	B	221	GLY	N-CA-C	6.77	121.09	112.83
1	E	126	PRO	CA-C-N	-6.77	111.86	122.49
1	E	126	PRO	C-N-CA	-6.77	111.86	122.49
1	C	107	GLY	N-CA-C	6.69	119.69	112.33
1	E	243	ILE	N-CA-C	-6.67	100.46	107.60
1	A	102	ALA	N-CA-C	6.66	121.69	113.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	125	GLU	CB-CA-C	-6.65	101.26	110.37
1	C	125	GLU	N-CA-C	-6.64	102.24	108.22
1	A	137	VAL	CA-C-N	6.63	126.61	119.78
1	A	137	VAL	C-N-CA	6.63	126.61	119.78
1	F	222	GLY	N-CA-C	6.59	120.15	112.50
1	D	102	ALA	N-CA-C	6.54	121.55	113.50
1	C	179	ILE	N-CA-C	6.51	117.26	110.62
1	E	243	ILE	CA-C-N	6.44	127.89	119.84
1	E	243	ILE	C-N-CA	6.44	127.89	119.84
1	A	112	LEU	N-CA-C	-6.41	104.21	111.07
1	C	112	LEU	N-CA-C	-6.38	104.24	111.07
1	D	168	VAL	N-CA-C	6.37	117.87	108.45
1	D	212	ALA	N-CA-C	-6.30	96.03	107.75
1	A	155	LEU	N-CA-C	-6.30	99.62	109.25
1	A	219	GLU	N-CA-C	6.23	120.19	112.59
1	C	125	GLU	CB-CA-C	-6.23	102.00	110.22
1	D	234	THR	N-CA-C	-6.19	100.19	108.74
1	A	72	SER	CA-C-N	6.18	125.88	119.64
1	A	72	SER	C-N-CA	6.18	125.88	119.64
1	C	155	LEU	N-CA-C	-6.12	100.02	109.76
1	C	58	ASP	N-CA-C	-6.10	105.87	113.38
1	F	220	ARG	N-CA-C	-6.10	104.91	112.90
1	E	164	VAL	CA-C-N	-6.08	115.27	122.93
1	E	164	VAL	C-N-CA	-6.08	115.27	122.93
1	B	155	LEU	N-CA-C	-6.05	99.99	109.25
1	B	176	GLN	CB-CA-C	-6.04	99.45	110.63
1	D	78	MET	N-CA-C	6.04	117.53	111.07
1	D	219	GLU	N-CA-C	6.00	120.18	112.26
1	C	230	LEU	CA-C-N	-5.89	111.92	120.29
1	C	230	LEU	C-N-CA	-5.89	111.92	120.29
1	E	163	GLU	CA-C-N	-5.89	114.93	123.06
1	E	163	GLU	C-N-CA	-5.89	114.93	123.06
1	D	16	SER	N-CA-C	5.88	117.36	111.07
1	F	87	LEU	N-CA-C	5.88	117.77	111.36
1	D	243	ILE	CA-C-N	5.82	127.11	119.84
1	D	243	ILE	C-N-CA	5.82	127.11	119.84
1	D	103	HIS	CA-C-N	5.81	126.21	119.47
1	D	103	HIS	C-N-CA	5.81	126.21	119.47
1	B	243	ILE	CA-C-N	5.72	126.99	119.84
1	B	243	ILE	C-N-CA	5.72	126.99	119.84
1	D	161	GLY	CA-C-N	5.69	126.00	119.92
1	D	161	GLY	C-N-CA	5.69	126.00	119.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	VAL	N-CA-C	5.67	116.11	108.17
1	A	221	GLY	N-CA-C	5.66	119.49	112.64
1	E	134	THR	N-CA-C	-5.66	106.22	113.01
1	D	126	PRO	N-CA-C	5.62	124.05	112.47
1	B	103	HIS	CA-C-N	5.62	125.99	119.47
1	B	103	HIS	C-N-CA	5.62	125.99	119.47
1	A	48	LEU	N-CA-C	-5.57	105.30	111.36
1	B	125	GLU	CB-CA-C	-5.51	102.94	110.22
1	F	106	LEU	N-CA-C	5.49	119.98	113.28
1	C	201	HIS	N-CA-C	-5.45	105.42	111.36
1	E	155	LEU	N-CA-C	-5.42	101.14	109.76
1	E	16	SER	N-CA-C	5.42	116.86	111.07
1	A	78	MET	N-CA-C	5.36	117.12	111.28
1	C	21	ASP	N-CA-C	5.33	116.38	108.86
1	C	234	THR	N-CA-C	-5.31	101.41	108.74
1	E	153	LYS	CA-C-N	-5.29	115.14	120.85
1	E	153	LYS	C-N-CA	-5.29	115.14	120.85
1	F	101	ASP	N-CA-C	-5.25	105.15	112.45
1	B	58	ASP	N-CA-C	-5.25	107.01	113.41
1	F	78	MET	N-CA-C	5.24	117.67	111.33
1	A	191	ILE	CB-CA-C	-5.23	102.83	110.62
1	A	171	CYS	N-CA-C	-5.22	99.69	110.80
1	B	107	GLY	CA-C-O	-5.22	115.32	122.31
1	B	78	MET	N-CA-C	5.21	117.63	111.33
1	C	67	PHE	N-CA-C	5.20	118.89	111.92
1	C	63	HIS	N-CA-C	-5.20	106.09	112.90
1	F	179	ILE	N-CA-C	5.18	116.52	110.62
1	C	213	ALA	N-CA-C	5.18	119.69	113.17
1	C	181	SER	N-CA-C	-5.17	105.72	111.36
1	D	117	GLY	CA-C-N	-5.15	116.81	123.19
1	D	117	GLY	C-N-CA	-5.15	116.81	123.19
1	B	169	ALA	N-CA-C	-5.14	101.55	109.52
1	A	137	VAL	CB-CA-C	-5.13	104.35	109.89
1	A	33	GLU	N-CA-C	5.13	116.68	111.14
1	B	228	GLU	N-CA-C	-5.12	105.61	111.14
1	A	19	ILE	N-CA-C	5.11	115.34	107.77
1	B	179	ILE	N-CA-C	5.10	115.82	110.62
1	A	124	ILE	N-CA-C	-5.09	105.88	110.82
1	B	85	THR	N-CA-C	-5.08	105.74	111.28
1	F	42	VAL	N-CA-C	5.06	115.29	110.53
1	D	62	VAL	N-CA-C	5.04	115.96	108.65
1	C	85	THR	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	22	TYR	Sidechain
1	E	22	TYR	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	1897	0	1866	42	0
1	B	1897	0	1866	41	0
1	C	1897	0	1866	35	0
1	D	1897	0	1866	24	0
1	E	1897	0	1866	21	0
1	F	1897	0	1866	28	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	78	0	0	2	0
3	B	79	0	0	1	0
3	C	95	0	0	2	0
3	D	87	0	0	0	0
3	E	124	0	0	0	0
3	F	113	0	0	3	0
All	All	11969	0	11196	181	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 8.

All (181) 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:1:MET:CE	1:B:1:MET:SD	2.01	1.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:MET:CE	1:E:135:MET:SD	2.01	1.47
1:D:135:MET:CE	1:D:135:MET:SD	2.03	1.47
1:C:121:MET:CE	1:C:121:MET:SD	2.04	1.44
1:B:135:MET:CE	1:B:135:MET:SD	2.11	1.39
1:F:135:MET:CE	1:F:135:MET:SD	2.10	1.39
1:C:135:MET:SD	1:C:135:MET:CE	2.13	1.36
1:E:246:PRO:HD2	1:F:200:ILE:HG12	1.59	0.83
1:D:128:VAL:O	1:D:128:VAL:HG23	1.78	0.80
1:A:37:LYS:HG3	1:A:237:ASP:OD2	1.83	0.77
1:A:2:LYS:HB2	1:A:2:LYS:NZ	2.02	0.75
1:C:74:VAL:HG12	1:C:76:ARG:HG3	1.69	0.73
1:C:39:VAL:HG13	1:C:241:ILE:HD12	1.70	0.73
1:F:125:GLU:HG3	1:F:128:VAL:HG11	1.72	0.71
1:F:130:TRP:CD1	1:F:131:GLY:N	2.59	0.71
1:F:125:GLU:HG3	1:F:128:VAL:CG1	2.21	0.70
1:C:145:TRP:O	1:C:149:ARG:HG2	1.92	0.69
1:A:38:ILE:HD11	1:A:236:LEU:HD22	1.77	0.66
1:C:8:GLN:O	1:C:12:GLU:HG3	1.95	0.66
1:C:130:TRP:CD1	1:C:131:GLY:N	2.64	0.66
1:A:184:ARG:HH22	1:B:76:ARG:NE	1.95	0.65
1:A:39:VAL:O	1:A:60:VAL:HA	1.98	0.64
1:A:125:GLU:HB2	1:A:128:VAL:HG13	1.80	0.62
1:D:240:PHE:C	1:D:241:ILE:HD12	2.24	0.62
1:C:176:GLN:HG3	1:C:194:GLU:O	2.00	0.62
1:B:13:LYS:HE2	1:B:229:TRP:CE2	2.35	0.61
1:B:75:ILE:HD12	1:B:83:LEU:CD1	2.30	0.61
1:A:2:LYS:HB2	1:A:2:LYS:HZ2	1.63	0.61
1:B:75:ILE:HD12	1:B:83:LEU:HD12	1.80	0.61
1:F:129:PRO:HD2	1:F:170:TRP:O	2.02	0.59
1:A:208:LEU:C	1:A:208:LEU:HD12	2.28	0.59
1:A:74:VAL:HG12	1:A:76:ARG:HG3	1.84	0.59
1:C:74:VAL:CG1	1:C:76:ARG:HG3	2.33	0.59
1:D:124:ILE:HB	1:D:128:VAL:HG23	1.84	0.58
1:B:189:ALA:HA	1:B:209:HIS:O	2.05	0.57
1:B:75:ILE:CD1	1:B:83:LEU:HD12	2.34	0.57
1:A:38:ILE:CD1	1:A:236:LEU:HD22	2.34	0.56
1:E:168:VAL:HG22	1:E:189:ALA:HB3	1.86	0.56
1:B:176:GLN:HG3	1:B:194:GLU:O	2.05	0.56
1:F:113:ALA:HB2	1:F:170:TRP:CZ2	2.41	0.56
1:E:76:ARG:HB2	1:F:184:ARG:HH12	1.71	0.56
1:C:237:ASP:OD1	1:C:237:ASP:C	2.49	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:GLU:HB2	1:D:128:VAL:HG22	1.88	0.56
1:A:87:LEU:HA	3:A:322:HOH:O	2.06	0.56
1:F:126:PRO:HB2	3:F:327:HOH:O	2.05	0.56
1:E:138:PRO:HB2	1:E:141:GLU:OE1	2.06	0.56
1:A:160:THR:OG1	1:A:207:GLY:HA2	2.07	0.55
1:A:124:ILE:HB	1:A:128:VAL:HG22	1.89	0.55
1:B:13:LYS:HE2	1:B:229:TRP:CZ2	2.42	0.55
1:B:145:TRP:O	1:B:149:ARG:HG2	2.06	0.55
1:C:121:MET:CE	1:C:121:MET:CG	2.84	0.55
1:E:125:GLU:HB2	1:E:128:VAL:HG13	1.89	0.55
1:F:169:ALA:HB2	1:F:187:VAL:HG11	1.89	0.54
1:F:224:ARG:HD3	3:F:354:HOH:O	2.08	0.54
1:C:32:LYS:HD2	1:C:58:ASP:HB3	1.90	0.54
1:D:145:TRP:O	1:D:149:ARG:HG2	2.08	0.53
1:E:130:TRP:CD1	1:E:131:GLY:N	2.75	0.53
1:D:242:ASP:O	1:D:244:PRO:HD3	2.09	0.53
1:E:74:VAL:HG12	1:E:76:ARG:HG3	1.91	0.53
1:B:39:VAL:O	1:B:60:VAL:HA	2.09	0.52
1:F:176:GLN:H	1:F:176:GLN:CD	2.17	0.52
1:D:98:LEU:HB2	1:D:99:PRO:HD3	1.92	0.52
1:E:176:GLN:HG3	1:E:194:GLU:O	2.10	0.52
1:A:184:ARG:NH2	1:B:76:ARG:NE	2.57	0.52
1:C:13:LYS:HD3	1:C:229:TRP:CZ2	2.45	0.51
1:D:118:ILE:HG12	1:D:133:LEU:HD23	1.92	0.51
1:A:176:GLN:HG3	1:A:194:GLU:O	2.10	0.51
1:D:38:ILE:HB	1:D:238:VAL:HG13	1.92	0.51
1:D:129:PRO:HD2	1:D:170:TRP:O	2.10	0.51
1:F:147:GLU:HB2	1:F:154:PRO:HD2	1.93	0.51
1:D:195:VAL:HG22	1:D:196:SER:N	2.25	0.51
1:D:128:VAL:O	1:D:128:VAL:CG2	2.51	0.51
1:C:130:TRP:CD1	1:C:130:TRP:C	2.89	0.51
1:A:2:LYS:HG3	1:A:33:GLU:HG2	1.93	0.50
1:A:37:LYS:HD3	1:A:55:LEU:O	2.11	0.50
1:A:1:MET:HE1	1:A:9:LEU:HD22	1.93	0.50
1:A:87:LEU:HD23	3:A:322:HOH:O	2.11	0.50
1:E:176:GLN:HG2	1:E:195:VAL:HA	1.93	0.50
1:A:184:ARG:NH2	1:B:76:ARG:HE	2.10	0.49
1:A:68:TRP:O	1:A:71:GLU:HB3	2.12	0.49
1:B:21:ASP:OD2	1:B:97:HIS:HB3	2.13	0.49
1:F:106:LEU:HD22	1:F:106:LEU:N	2.27	0.49
1:F:130:TRP:CD1	1:F:130:TRP:C	2.90	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:HG22	1:A:128:VAL:O	2.13	0.49
1:D:113:ALA:HB2	1:D:170:TRP:CZ2	2.48	0.49
1:D:103:HIS:CE1	1:D:105:GLU:HB3	2.48	0.49
1:A:129:PRO:HD2	1:A:170:TRP:O	2.12	0.49
1:C:39:VAL:CG1	1:C:241:ILE:HD12	2.39	0.49
1:E:124:ILE:HB	1:E:128:VAL:HG22	1.93	0.49
1:A:145:TRP:O	1:A:149:ARG:HG2	2.14	0.48
1:A:118:ILE:HG21	1:A:170:TRP:CZ3	2.48	0.48
1:B:240:PHE:C	1:B:241:ILE:HD13	2.38	0.48
1:C:199:THR:HG21	1:C:210:PHE:CZ	2.48	0.48
1:C:221:GLY:HA3	3:C:320:HOH:O	2.12	0.48
1:B:125:GLU:HB3	1:B:126:PRO:HD2	1.95	0.48
1:B:69:LYS:HD3	1:B:69:LYS:HA	1.61	0.48
1:A:35:VAL:HG12	1:A:38:ILE:HD11	1.96	0.48
1:C:129:PRO:HD2	1:C:170:TRP:O	2.14	0.48
1:B:78:MET:O	1:B:82:ARG:HG3	2.13	0.48
1:A:109:ASN:OD1	1:A:172:THR:HG23	2.13	0.48
1:B:26:GLY:HA2	1:B:96:TRP:CZ2	2.49	0.47
1:C:2:LYS:HG2	1:C:33:GLU:HG2	1.97	0.47
1:C:208:LEU:HD23	1:C:208:LEU:H	1.79	0.47
1:F:176:GLN:HG2	1:F:195:VAL:HA	1.96	0.47
1:A:147:GLU:HA	1:A:152:ARG:O	2.15	0.46
1:A:179:ILE:HD11	1:A:208:LEU:HD11	1.97	0.46
1:F:66:TYR:O	1:F:67:PHE:HB2	2.16	0.46
1:A:66:TYR:O	1:A:67:PHE:HB2	2.16	0.46
1:A:129:PRO:HB2	1:A:170:TRP:CZ2	2.51	0.46
1:F:195:VAL:HG22	1:F:196:SER:N	2.29	0.46
1:B:38:ILE:HB	1:B:238:VAL:HG22	1.98	0.46
1:D:124:ILE:HB	1:D:128:VAL:CG2	2.46	0.46
1:E:2:LYS:O	1:E:5:GLU:HB2	2.15	0.46
1:B:129:PRO:HD2	1:B:170:TRP:O	2.17	0.45
1:A:106:LEU:N	1:A:106:LEU:HD22	2.31	0.45
1:C:26:GLY:O	1:C:94:TYR:HA	2.16	0.45
1:D:39:VAL:O	1:D:60:VAL:HA	2.16	0.45
1:A:102:ALA:O	1:A:103:HIS:C	2.59	0.45
1:A:128:VAL:O	1:A:128:VAL:CG2	2.65	0.45
1:B:168:VAL:HG12	1:B:169:ALA:N	2.32	0.45
1:C:2:LYS:O	1:C:5:GLU:N	2.50	0.45
1:A:247:ALA:HB2	1:B:200:ILE:HD13	1.98	0.45
1:E:69:LYS:HD3	1:E:69:LYS:HA	1.76	0.45
1:C:80:ARG:HG3	1:C:81:ASN:N	2.31	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:LYS:HB3	1:D:79:LYS:HE3	1.86	0.44
1:F:39:VAL:O	1:F:60:VAL:HA	2.18	0.44
1:A:38:ILE:HB	1:A:238:VAL:HG22	2.00	0.44
1:A:128:VAL:HA	1:A:129:PRO:HD3	1.77	0.44
1:B:75:ILE:HD11	1:B:83:LEU:HB2	1.99	0.44
1:B:125:GLU:OE2	1:B:181:SER:OG	2.22	0.44
1:B:147:GLU:HA	1:B:152:ARG:O	2.18	0.43
1:D:40:THR:HG22	1:D:61:ILE:HB	2.00	0.43
1:B:162:PRO:HD2	1:B:209:HIS:CD2	2.53	0.43
1:D:159:ASP:OD1	1:D:159:ASP:N	2.51	0.43
1:C:167:ARG:HE	1:C:167:ARG:HB2	1.66	0.43
1:C:197:GLU:HB2	1:D:215:HIS:CG	2.53	0.43
1:D:103:HIS:HA	1:D:104:PRO:HD3	1.83	0.43
1:B:1:MET:CE	1:B:1:MET:CG	2.94	0.43
1:B:245:ASN:HA	1:B:246:PRO:HD3	1.82	0.43
1:D:80:ARG:O	1:D:80:ARG:HG2	2.18	0.43
1:E:130:TRP:CD1	1:E:130:TRP:C	2.94	0.43
1:C:32:LYS:NZ	3:C:391:HOH:O	2.52	0.43
1:E:39:VAL:O	1:E:60:VAL:HA	2.17	0.43
1:B:169:ALA:HB2	1:B:187:VAL:HG11	2.00	0.43
1:A:246:PRO:HD2	1:B:200:ILE:HG12	2.00	0.43
1:C:208:LEU:HD23	1:C:208:LEU:N	2.33	0.43
1:F:127:LEU:N	3:F:327:HOH:O	2.05	0.43
1:A:13:LYS:HD3	1:A:229:TRP:CZ2	2.54	0.42
1:F:168:VAL:HG12	1:F:169:ALA:N	2.33	0.42
1:B:76:ARG:O	1:B:77:GLY:C	2.62	0.42
1:B:123:GLU:O	1:B:123:GLU:HG3	2.20	0.42
1:C:21:ASP:OD1	1:C:98:LEU:HG	2.19	0.42
1:B:241:ILE:HD13	1:B:241:ILE:N	2.33	0.42
1:B:145:TRP:O	1:B:149:ARG:CG	2.68	0.42
1:C:23:ALA:HB1	1:C:24:PRO:CD	2.50	0.42
1:A:2:LYS:HB2	1:A:2:LYS:HZ3	1.79	0.42
1:F:171:CYS:O	1:F:192:THR:HA	2.19	0.42
1:A:2:LYS:NZ	1:A:2:LYS:CB	2.75	0.42
1:F:40:THR:OG1	1:F:240:PHE:HA	2.19	0.42
1:F:72:SER:HA	1:F:73:PRO:HD3	1.87	0.42
1:C:141:GLU:HG3	1:E:135:MET:SD	2.60	0.41
1:E:76:ARG:HB2	1:F:184:ARG:NH1	2.33	0.41
1:B:164:VAL:HG13	3:B:323:HOH:O	2.19	0.41
1:B:113:ALA:HB2	1:B:170:TRP:CZ2	2.55	0.41
1:C:106:LEU:HD22	1:C:106:LEU:N	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ALA:HB2	1:E:170:TRP:CZ2	2.56	0.41
1:F:189:ALA:HA	1:F:209:HIS:O	2.21	0.41
1:B:105:GLU:HG2	1:B:106:LEU:HD13	2.02	0.41
1:C:164:VAL:HG13	1:C:164:VAL:O	2.20	0.41
1:D:108:ASN:HB3	1:D:172:THR:HG21	2.02	0.41
1:A:32:LYS:NZ	1:A:58:ASP:OD1	2.44	0.41
1:B:98:LEU:HD22	1:B:127:LEU:HD11	2.03	0.41
1:C:125:GLU:HB3	1:C:126:PRO:HD2	2.02	0.41
1:E:168:VAL:HG12	1:E:169:ALA:N	2.35	0.41
1:E:147:GLU:HA	1:E:152:ARG:O	2.21	0.41
1:E:149:ARG:HD2	1:E:149:ARG:HA	1.67	0.40
1:F:173:GLY:HA2	1:F:215:HIS:CD2	2.55	0.40
1:B:128:VAL:O	1:B:128:VAL:HG22	2.22	0.40
1:F:192:THR:HG23	1:F:193:GLY:N	2.36	0.40
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.85	0.40
1:C:129:PRO:HB2	1:C:170:TRP:CZ2	2.56	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	245/247 (99%)	231 (94%)	14 (6%)	0	100	100
1	B	245/247 (99%)	236 (96%)	8 (3%)	1 (0%)	30	34
1	C	245/247 (99%)	237 (97%)	8 (3%)	0	100	100
1	D	245/247 (99%)	238 (97%)	7 (3%)	0	100	100
1	E	245/247 (99%)	236 (96%)	9 (4%)	0	100	100
1	F	245/247 (99%)	233 (95%)	11 (4%)	1 (0%)	30	34
All	All	1470/1482 (99%)	1411 (96%)	57 (4%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	159	ASP
1	B	126	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	197/197 (100%)	185 (94%)	12 (6%)	17	20
1	B	197/197 (100%)	180 (91%)	17 (9%)	10	10
1	C	197/197 (100%)	185 (94%)	12 (6%)	17	20
1	D	197/197 (100%)	185 (94%)	12 (6%)	17	20
1	E	197/197 (100%)	185 (94%)	12 (6%)	17	20
1	F	197/197 (100%)	183 (93%)	14 (7%)	13	16
All	All	1182/1182 (100%)	1103 (93%)	79 (7%)	15	17

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	5	GLU
1	A	27	LEU
1	A	48	LEU
1	A	49	LEU
1	A	112	LEU
1	A	126	PRO
1	A	128	VAL
1	A	176	GLN
1	A	181	SER
1	A	232	GLU
1	A	243	ILE
1	B	12	GLU
1	B	15	ASN
1	B	20	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	27	LEU
1	B	48	LEU
1	B	49	LEU
1	B	69	LYS
1	B	106	LEU
1	B	112	LEU
1	B	126	PRO
1	B	128	VAL
1	B	135	MET
1	B	141	GLU
1	B	149	ARG
1	B	164	VAL
1	B	184	ARG
1	B	208	LEU
1	C	5	GLU
1	C	27	LEU
1	C	48	LEU
1	C	49	LEU
1	C	80	ARG
1	C	104	PRO
1	C	112	LEU
1	C	130	TRP
1	C	141	GLU
1	C	155	LEU
1	C	176	GLN
1	C	184	ARG
1	D	27	LEU
1	D	48	LEU
1	D	49	LEU
1	D	106	LEU
1	D	112	LEU
1	D	128	VAL
1	D	154	PRO
1	D	159	ASP
1	D	163	GLU
1	D	176	GLN
1	D	208	LEU
1	D	241	ILE
1	E	20	SER
1	E	27	LEU
1	E	34	THR
1	E	39	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	48	LEU
1	E	49	LEU
1	E	106	LEU
1	E	112	LEU
1	E	126	PRO
1	E	128	VAL
1	E	130	TRP
1	E	176	GLN
1	F	2	LYS
1	F	27	LEU
1	F	39	VAL
1	F	48	LEU
1	F	49	LEU
1	F	69	LYS
1	F	80	ARG
1	F	112	LEU
1	F	125	GLU
1	F	126	PRO
1	F	128	VAL
1	F	130	TRP
1	F	176	GLN
1	F	184	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	166	GLN
1	B	36	GLN
1	B	64	HIS
1	B	166	GLN
1	B	201	HIS
1	C	36	GLN
1	C	166	GLN
1	C	206	GLN
1	D	36	GLN
1	D	206	GLN
1	E	36	GLN
1	E	46	GLN
1	E	166	GLN
1	E	206	GLN
1	F	46	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	166	GLN

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](#)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	247/247 (100%)	-0.33	0 100 100	7, 14, 23, 29	0
1	B	247/247 (100%)	-0.30	0 100 100	7, 14, 24, 28	0
1	C	247/247 (100%)	-0.49	0 100 100	5, 12, 22, 28	0
1	D	247/247 (100%)	-0.46	0 100 100	5, 12, 23, 27	0
1	E	247/247 (100%)	-0.52	1 (0%) 88 87	4, 11, 21, 28	0
1	F	247/247 (100%)	-0.54	0 100 100	5, 11, 20, 26	0
All	All	1482/1482 (100%)	-0.44	1 (0%) 92 90	4, 12, 22, 29	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	18	ALA	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	301	1/1	0.65	0.28	55,55,55,55	0
2	MG	E	301	1/1	0.69	0.35	49,49,49,49	0
2	MG	B	302	1/1	0.70	0.24	41,41,41,41	0
2	MG	D	301	1/1	0.71	0.31	48,48,48,48	0
2	MG	C	301	1/1	0.74	0.34	58,58,58,58	0
2	MG	F	301	1/1	0.75	0.28	55,55,55,55	0
2	MG	C	302	1/1	0.87	0.12	27,27,27,27	0
2	MG	F	302	1/1	0.88	0.09	23,23,23,23	0
2	MG	A	302	1/1	0.89	0.11	24,24,24,24	0
2	MG	D	302	1/1	0.91	0.04	15,15,15,15	0
2	MG	E	302	1/1	0.94	0.17	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.