



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:37 PM UTC

PDB ID : 1EAV / pdb_00001eav
Title : Crystal Structures of Human Gephyrin and Plant Cnx1 G domains - Comparative Analysis and Functional Implications
Authors : Schwarz, G.; Schrader, N.; Mendel, R.R.; Hecht, H.J.
Deposited on : 2001-07-17
Resolution : 2.60 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
Mogul : 2022.3.0, CSD as543be (2022)
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

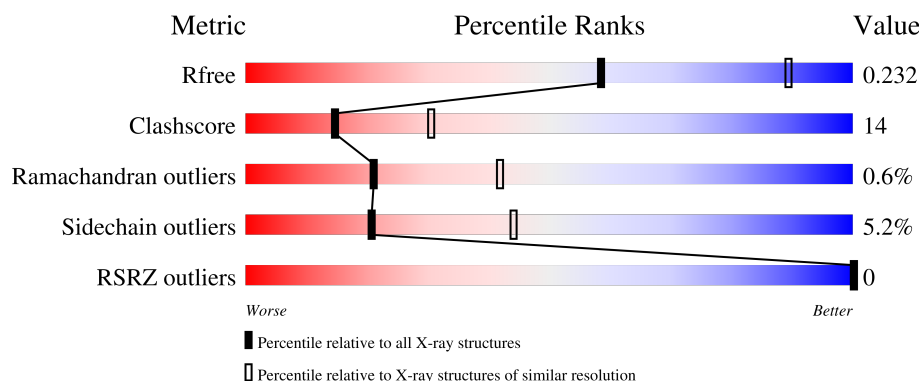
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

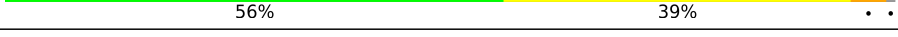
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	162	
1	B	162	
1	C	162	
1	D	162	
1	E	162	

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Mol	Chain	Length	Quality of chain
1	F	162	 59% 32% 7% •
1	G	162	 49% 41% 9% •
1	H	162	 53% 38% 7% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9501 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 MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	Se	0	0	0
			1181	745	200	229	1	6			
1	B	160	Total	C	N	O	S	Se	0	0	0
			1181	745	200	229	1	6			
1	C	160	Total	C	N	O	S	Se	0	0	0
			1181	745	200	229	1	6			
1	D	160	Total	C	N	O	S	Se	0	0	0
			1181	745	200	229	1	6			
1	E	160	Total	C	N	O	S	Se	0	0	0
			1181	745	200	229	1	6			
1	F	160	Total	C	N	O	S	Se	0	0	0
			1181	745	200	229	1	6			
1	G	160	Total	C	N	O	S	Se	0	0	0
			1183	745	200	231	1	6			
1	H	160	Total	C	N	O	S	Se	0	0	0
			1181	745	200	229	1	6			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	MSE	MET	modified residue	UNP Q39054
A	108	MSE	MET	modified residue	UNP Q39054
A	109	MSE	MET	modified residue	UNP Q39054
A	120	MSE	MET	modified residue	UNP Q39054
A	137	MSE	MET	modified residue	UNP Q39054
A	148	MSE	MET	modified residue	UNP Q39054
B	72	MSE	MET	modified residue	UNP Q39054
B	108	MSE	MET	modified residue	UNP Q39054
B	109	MSE	MET	modified residue	UNP Q39054
B	120	MSE	MET	modified residue	UNP Q39054
B	137	MSE	MET	modified residue	UNP Q39054
B	148	MSE	MET	modified residue	UNP Q39054
C	72	MSE	MET	modified residue	UNP Q39054

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Chain	Residue	Modelled	Actual	Comment	Reference
C	108	MSE	MET	modified residue	UNP Q39054
C	109	MSE	MET	modified residue	UNP Q39054
C	120	MSE	MET	modified residue	UNP Q39054
C	137	MSE	MET	modified residue	UNP Q39054
C	148	MSE	MET	modified residue	UNP Q39054
D	72	MSE	MET	modified residue	UNP Q39054
D	108	MSE	MET	modified residue	UNP Q39054
D	109	MSE	MET	modified residue	UNP Q39054
D	120	MSE	MET	modified residue	UNP Q39054
D	137	MSE	MET	modified residue	UNP Q39054
D	148	MSE	MET	modified residue	UNP Q39054
E	72	MSE	MET	modified residue	UNP Q39054
E	108	MSE	MET	modified residue	UNP Q39054
E	109	MSE	MET	modified residue	UNP Q39054
E	120	MSE	MET	modified residue	UNP Q39054
E	137	MSE	MET	modified residue	UNP Q39054
E	148	MSE	MET	modified residue	UNP Q39054
F	72	MSE	MET	modified residue	UNP Q39054
F	108	MSE	MET	modified residue	UNP Q39054
F	109	MSE	MET	modified residue	UNP Q39054
F	120	MSE	MET	modified residue	UNP Q39054
F	137	MSE	MET	modified residue	UNP Q39054
F	148	MSE	MET	modified residue	UNP Q39054
G	72	MSE	MET	modified residue	UNP Q39054
G	108	MSE	MET	modified residue	UNP Q39054
G	109	MSE	MET	modified residue	UNP Q39054
G	120	MSE	MET	modified residue	UNP Q39054
G	137	MSE	MET	modified residue	UNP Q39054
G	148	MSE	MET	modified residue	UNP Q39054
H	72	MSE	MET	modified residue	UNP Q39054
H	108	MSE	MET	modified residue	UNP Q39054
H	109	MSE	MET	modified residue	UNP Q39054
H	120	MSE	MET	modified residue	UNP Q39054
H	137	MSE	MET	modified residue	UNP Q39054
H	148	MSE	MET	modified residue	UNP Q39054

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	10	Total O 10 10	0	0
2	B	7	Total O 7 7	0	0

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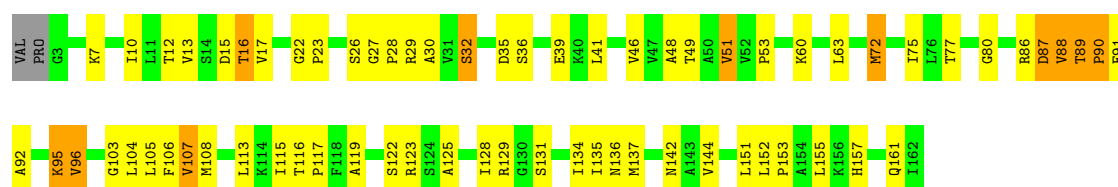
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	5	Total 5	O 5	0	0
2	D	3	Total 3	O 3	0	0
2	E	5	Total 5	O 5	0	0
2	F	8	Total 8	O 8	0	0
2	G	7	Total 7	O 7	0	0
2	H	6	Total 6	O 6	0	0

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.

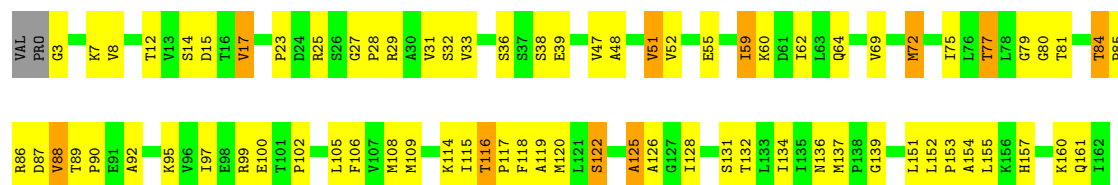
• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain A: 



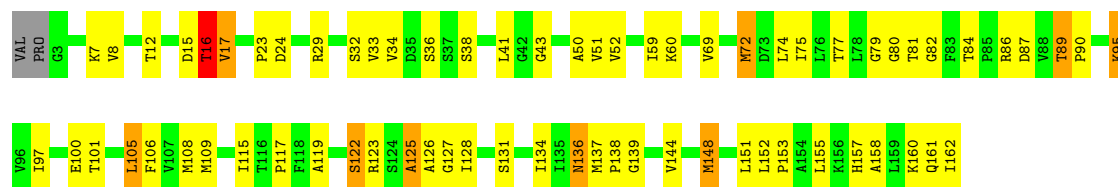
• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain B: 



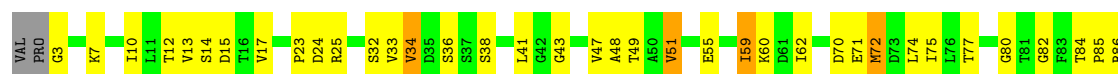
• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain C: 



• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain D: 





• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain E: 56% 35% 9%



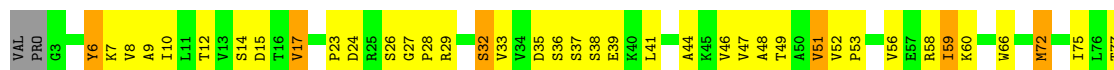
• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain F: 59% 32% 7%



• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain G: 49% 41% 9%



• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain H: 53% 38% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	175.30Å 175.30Å 175.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.00 – 2.60 27.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.8 (27.00-2.60) 90.8 (27.00-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.0.36	Depositor
R, R_{free}	0.223 , 0.251 (Not available) , 0.232	Depositor DCC
R_{free} test set	2582 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 20.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.457 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9501	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.11% 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	1.88	20/1192 (1.7%)	1.68	17/1608 (1.1%)
1	B	1.93	33/1192 (2.8%)	1.63	18/1608 (1.1%)
1	C	1.89	26/1192 (2.2%)	1.68	10/1608 (0.6%)
1	D	1.82	24/1192 (2.0%)	1.68	12/1608 (0.7%)
1	E	1.85	27/1192 (2.3%)	1.68	19/1608 (1.2%)
1	F	1.84	19/1192 (1.6%)	1.62	13/1608 (0.8%)
1	G	1.99	31/1194 (2.6%)	1.71	16/1609 (1.0%)
1	H	1.84	19/1192 (1.6%)	1.70	25/1608 (1.6%)
All	All	1.88	199/9538 (2.1%)	1.67	130/12865 (1.0%)

All (199) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	88	VAL	CA-CB	-13.77	1.40	1.54
1	G	75	ILE	CA-CB	-10.80	1.41	1.54
1	H	125	ALA	CA-CB	-10.34	1.37	1.53
1	H	75	ILE	CA-CB	-10.09	1.41	1.54
1	H	134	ILE	CA-CB	-9.70	1.42	1.54
1	E	134	ILE	CA-CB	-9.54	1.42	1.54
1	A	75	ILE	CA-CB	-9.51	1.42	1.54
1	G	97	ILE	CA-CB	-9.41	1.41	1.54
1	C	72	MSE	SE-CE	-9.35	1.67	1.95
1	B	134	ILE	CA-CB	-9.17	1.43	1.54
1	D	47	VAL	CA-CB	-9.17	1.42	1.54
1	D	75	ILE	CA-CB	-9.17	1.42	1.54
1	C	75	ILE	CA-CB	-9.14	1.42	1.54
1	B	69	VAL	CA-CB	-9.06	1.45	1.55
1	D	72	MSE	SE-CE	-8.87	1.68	1.95
1	C	24	ASP	CA-C	-8.77	1.41	1.52
1	C	134	ILE	CA-CB	-8.65	1.43	1.54
1	F	17	VAL	CA-CB	-8.54	1.44	1.54
1	B	109	MSE	SE-CE	-8.54	1.69	1.95
1	B	47	VAL	CA-CB	-8.46	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	59	ILE	CA-CB	-8.33	1.43	1.54
1	G	59	ILE	CA-CB	-8.28	1.43	1.54
1	E	75	ILE	CA-CB	-8.17	1.43	1.54
1	B	72	MSE	SE-CE	-8.14	1.71	1.95
1	C	82	GLY	C-O	-8.03	1.16	1.23
1	G	134	ILE	CA-CB	-7.98	1.44	1.54
1	F	52	VAL	C-O	-7.88	1.18	1.24
1	G	10	ILE	CA-CB	-7.83	1.44	1.54
1	C	148	MSE	SE-CE	7.76	2.18	1.95
1	A	92	ALA	CA-CB	-7.75	1.41	1.53
1	C	122	SER	C-O	-7.70	1.14	1.23
1	E	59	ILE	CA-CB	-7.66	1.44	1.54
1	G	51	VAL	N-CA	-7.60	1.37	1.46
1	B	8	VAL	CA-CB	-7.57	1.44	1.54
1	H	24	ASP	CA-C	-7.51	1.43	1.52
1	H	128	ILE	CA-CB	-7.47	1.45	1.54
1	E	17	VAL	CA-CB	-7.46	1.44	1.54
1	A	88	VAL	CA-CB	-7.45	1.44	1.54
1	E	25	ARG	CA-C	-7.37	1.43	1.52
1	D	47	VAL	CA-C	-7.28	1.43	1.52
1	G	108	MSE	SE-CE	-7.22	1.73	1.95
1	B	114	LYS	C-O	-7.19	1.14	1.24
1	H	48	ALA	CA-CB	-7.17	1.42	1.53
1	D	134	ILE	CA-CB	-7.15	1.45	1.54
1	C	69	VAL	CA-CB	-7.15	1.47	1.55
1	G	135	ILE	CA-CB	-7.12	1.45	1.54
1	E	128	ILE	CA-C	-7.12	1.44	1.52
1	G	126	ALA	CA-CB	-7.10	1.42	1.53
1	A	48	ALA	CA-CB	-7.09	1.42	1.53
1	G	48	ALA	CA-CB	-7.08	1.42	1.53
1	A	128	ILE	CA-CB	-7.03	1.45	1.54
1	C	126	ALA	CA-CB	-6.98	1.41	1.53
1	B	122	SER	C-O	-6.97	1.15	1.23
1	F	128	ILE	CA-CB	-6.94	1.45	1.54
1	F	125	ALA	CA-CB	-6.94	1.42	1.53
1	E	10	ILE	CA-CB	-6.91	1.45	1.54
1	F	8	VAL	CA-CB	-6.89	1.46	1.54
1	E	125	ALA	CA-CB	-6.84	1.42	1.54
1	C	136	ASN	C-O	-6.77	1.15	1.23
1	E	92	ALA	CA-CB	-6.75	1.42	1.53
1	F	72	MSE	SE-CE	-6.74	1.75	1.95
1	C	89	THR	N-CA	-6.68	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	59	ILE	CA-CB	-6.67	1.46	1.54
1	B	132	THR	CA-CB	-6.66	1.43	1.53
1	C	12	THR	CA-CB	-6.65	1.43	1.53
1	G	24	ASP	CA-C	-6.59	1.44	1.52
1	B	125	ALA	CA-CB	-6.55	1.43	1.53
1	D	59	ILE	CA-CB	-6.55	1.46	1.54
1	B	25	ARG	CA-C	-6.55	1.44	1.52
1	D	128	ILE	CA-CB	-6.50	1.46	1.54
1	H	92	ALA	CA-CB	-6.50	1.43	1.53
1	B	84	THR	CA-C	-6.48	1.46	1.53
1	A	89	THR	C-O	-6.47	1.18	1.24
1	H	33	VAL	CA-C	6.41	1.60	1.52
1	G	72	MSE	SE-CE	-6.41	1.76	1.95
1	C	109	MSE	SE-CE	-6.41	1.76	1.95
1	A	13	VAL	CA-CB	-6.37	1.46	1.54
1	H	52	VAL	CA-C	-6.33	1.45	1.52
1	G	12	THR	N-CA	-6.31	1.38	1.46
1	D	115	ILE	CA-C	-6.30	1.46	1.52
1	E	123	ARG	CA-C	-6.30	1.44	1.52
1	B	52	VAL	C-O	-6.29	1.19	1.24
1	F	136	ASN	C-O	-6.27	1.16	1.23
1	G	125	ALA	CA-CB	-6.25	1.44	1.53
1	B	12	THR	CA-CB	-6.24	1.44	1.53
1	C	115	ILE	N-CA	-6.24	1.38	1.46
1	B	97	ILE	CA-CB	-6.20	1.45	1.54
1	B	51	VAL	N-CA	-6.18	1.39	1.46
1	F	48	ALA	CA-CB	-6.18	1.43	1.53
1	D	136	ASN	C-O	-6.16	1.16	1.23
1	H	34	VAL	CA-CB	-6.16	1.47	1.54
1	C	95	LYS	C-O	-6.13	1.16	1.24
1	E	88	VAL	CA-CB	-6.10	1.46	1.54
1	H	108	MSE	SE-CE	-6.10	1.77	1.95
1	C	17	VAL	CA-CB	-6.09	1.47	1.54
1	G	109	MSE	SE-CE	-6.09	1.77	1.95
1	A	135	ILE	CA-CB	-6.07	1.46	1.54
1	B	154	ALA	CA-CB	-6.06	1.45	1.54
1	D	105	LEU	C-O	-6.03	1.17	1.24
1	H	115	ILE	CA-CB	-6.03	1.47	1.54
1	H	135	ILE	CA-CB	-6.00	1.47	1.54
1	C	79	GLY	C-O	6.00	1.31	1.23
1	E	135	ILE	CA-CB	-5.98	1.47	1.54
1	F	75	ILE	CA-CB	-5.98	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	48	ALA	CA-CB	-5.97	1.43	1.53
1	D	93	THR	CA-CB	-5.96	1.44	1.53
1	E	101	THR	CA-C	-5.96	1.45	1.52
1	D	51	VAL	N-CA	-5.95	1.39	1.46
1	E	13	VAL	CA-CB	-5.94	1.47	1.54
1	B	48	ALA	CA-CB	-5.94	1.44	1.53
1	G	9	ALA	CA-CB	-5.91	1.42	1.53
1	G	17	VAL	CA-CB	-5.90	1.47	1.54
1	H	59	ILE	C-O	-5.90	1.17	1.24
1	E	54	ASP	CA-CB	-5.89	1.45	1.52
1	G	8	VAL	CA-CB	-5.88	1.47	1.54
1	H	50	ALA	CA-CB	-5.88	1.43	1.53
1	E	97	ILE	CA-CB	-5.86	1.47	1.54
1	B	128	ILE	CA-CB	-5.86	1.47	1.54
1	B	59	ILE	CA-CB	-5.85	1.46	1.54
1	F	97	ILE	CA-CB	-5.84	1.46	1.54
1	A	108	MSE	CA-C	-5.83	1.45	1.52
1	B	75	ILE	CA-CB	-5.82	1.47	1.54
1	G	46	VAL	CA-CB	-5.81	1.47	1.54
1	A	72	MSE	SE-CE	-5.76	1.78	1.95
1	G	122	SER	C-O	-5.76	1.16	1.23
1	B	108	MSE	SE-CE	-5.75	1.78	1.95
1	G	101	THR	N-CA	-5.74	1.40	1.46
1	D	82	GLY	C-O	-5.73	1.17	1.24
1	A	88	VAL	CA-C	-5.71	1.45	1.52
1	F	87	ASP	C-O	-5.68	1.17	1.24
1	A	10	ILE	CA-CB	-5.68	1.47	1.54
1	E	128	ILE	CA-CB	-5.68	1.47	1.54
1	A	134	ILE	CA-CB	-5.64	1.47	1.54
1	F	24	ASP	CA-C	-5.64	1.45	1.52
1	D	148	MSE	SE-CE	5.63	2.12	1.95
1	C	128	ILE	CA-CB	-5.61	1.47	1.54
1	F	66	TRP	CA-C	-5.60	1.45	1.52
1	C	97	ILE	CA-CB	-5.60	1.46	1.54
1	D	60	LYS	C-O	-5.57	1.17	1.24
1	A	96	VAL	CA-C	-5.56	1.45	1.52
1	A	51	VAL	N-CA	-5.55	1.39	1.46
1	D	48	ALA	CA-C	-5.55	1.45	1.52
1	B	126	ALA	CA-CB	-5.54	1.44	1.53
1	E	34	VAL	CA-CB	-5.52	1.48	1.54
1	G	86	ARG	C-O	-5.52	1.16	1.24
1	D	128	ILE	N-CA	-5.51	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	66	TRP	CA-C	-5.51	1.45	1.52
1	G	100	GLU	CA-C	-5.51	1.45	1.52
1	G	93	THR	N-CA	-5.49	1.39	1.46
1	G	89	THR	C-O	-5.46	1.19	1.24
1	B	105	LEU	C-N	-5.46	1.26	1.33
1	D	34	VAL	CA-CB	-5.44	1.48	1.54
1	D	59	ILE	C-O	-5.43	1.17	1.24
1	E	72	MSE	SE-CE	-5.43	1.79	1.95
1	G	154	ALA	CA-CB	-5.41	1.46	1.54
1	F	88	VAL	CA-C	-5.41	1.45	1.52
1	D	13	VAL	C-O	-5.40	1.18	1.24
1	C	126	ALA	CA-C	-5.38	1.46	1.52
1	D	12	THR	CA-CB	-5.38	1.45	1.53
1	G	58	ARG	C-O	-5.35	1.17	1.24
1	C	52	VAL	C-O	-5.35	1.20	1.24
1	E	46	VAL	CA-CB	-5.35	1.47	1.54
1	H	88	VAL	CA-CB	-5.34	1.47	1.54
1	F	101	THR	C-O	-5.34	1.18	1.24
1	A	107	VAL	CA-CB	-5.33	1.47	1.54
1	D	24	ASP	CA-C	-5.31	1.46	1.52
1	H	34	VAL	N-CA	-5.29	1.40	1.46
1	D	10	ILE	CA-CB	-5.27	1.47	1.54
1	G	93	THR	CA-CB	-5.27	1.45	1.53
1	C	125	ALA	CA-CB	-5.26	1.45	1.53
1	E	122	SER	C-O	-5.26	1.17	1.23
1	B	115	ILE	CA-CB	-5.25	1.47	1.54
1	F	93	THR	CA-CB	-5.24	1.44	1.53
1	C	108	MSE	SE-CE	-5.24	1.79	1.95
1	G	48	ALA	CA-C	-5.23	1.45	1.52
1	B	92	ALA	CA-CB	-5.20	1.45	1.53
1	G	82	GLY	C-O	-5.20	1.18	1.23
1	H	89	THR	N-CA	-5.20	1.41	1.46
1	C	50	ALA	CA-C	-5.18	1.46	1.52
1	B	77	THR	N-CA	5.15	1.51	1.45
1	C	12	THR	CA-C	-5.15	1.46	1.52
1	E	82	GLY	C-O	-5.14	1.19	1.24
1	A	16	THR	N-CA	-5.13	1.40	1.46
1	E	105	LEU	C-O	-5.13	1.18	1.24
1	B	17	VAL	CA-CB	-5.13	1.47	1.54
1	B	99	ARG	N-CA	-5.13	1.40	1.46
1	H	95	LYS	C-O	-5.12	1.17	1.24
1	F	126	ALA	CA-CB	-5.09	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	137	MSE	CA-CB	-5.08	1.47	1.53
1	A	30	ALA	CA-C	-5.07	1.46	1.52
1	A	105	LEU	C-N	-5.05	1.27	1.33
1	F	95	LYS	C-O	-5.05	1.17	1.24
1	A	87	ASP	C-O	-5.02	1.17	1.24
1	D	108	MSE	SE-CE	-5.02	1.80	1.95
1	E	115	ILE	CA-CB	-5.02	1.49	1.54
1	E	84	THR	C-O	-5.01	1.17	1.24
1	B	12	THR	CA-C	-5.01	1.46	1.52
1	E	128	ILE	N-CA	-5.01	1.40	1.46
1	B	160	LYS	CD-CE	5.00	1.67	1.52

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	91	GLU	N-CA-C	-9.36	101.08	111.28
1	H	81	THR	N-CA-C	8.02	124.04	113.30
1	E	47	VAL	CB-CA-C	-7.65	101.72	111.20
1	H	81	THR	CB-CA-C	-7.56	97.40	110.17
1	B	31	VAL	N-CA-C	-7.32	103.39	110.42
1	E	75	ILE	CB-CA-C	-7.17	100.58	110.77
1	G	139	GLY	N-CA-C	7.12	122.74	113.27
1	H	95	LYS	CA-C-N	-6.97	114.41	122.14
1	H	95	LYS	C-N-CA	-6.97	114.41	122.14
1	E	152	LEU	CA-C-N	-6.92	112.50	119.56
1	E	152	LEU	C-N-CA	-6.92	112.50	119.56
1	C	105	LEU	N-CA-C	-6.81	103.94	111.36
1	E	105	LEU	N-CA-C	-6.79	103.96	111.36
1	H	47	VAL	CB-CA-C	-6.73	103.53	110.93
1	B	114	LYS	N-CA-C	-6.58	105.08	113.23
1	B	139	GLY	N-CA-C	6.48	121.89	113.27
1	E	95	LYS	CA-C-N	-6.44	113.99	121.71
1	E	95	LYS	C-N-CA	-6.44	113.99	121.71
1	F	91	GLU	N-CA-C	-6.43	104.27	111.28
1	D	139	GLY	N-CA-C	6.38	121.75	113.27
1	H	115	ILE	N-CA-C	-6.37	106.33	111.81
1	A	12	THR	CA-C-N	-6.36	114.86	123.12
1	A	12	THR	C-N-CA	-6.36	114.86	123.12
1	G	96	VAL	CA-C-N	-6.29	111.95	120.95
1	G	96	VAL	C-N-CA	-6.29	111.95	120.95
1	H	75	ILE	CB-CA-C	-6.29	101.85	110.77
1	E	157	HIS	N-CA-C	-6.24	104.48	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	ILE	CB-CA-C	-6.06	102.24	110.42
1	G	47	VAL	CB-CA-C	-6.04	103.71	111.20
1	G	59	ILE	CA-CB-CG1	-5.96	100.26	110.40
1	G	123	ARG	N-CA-C	-5.96	104.39	112.26
1	A	104	LEU	N-CA-C	-5.95	104.87	111.36
1	G	97	ILE	CB-CA-C	-5.94	105.06	111.59
1	H	34	VAL	N-CA-C	-5.93	104.73	110.42
1	F	81	THR	CB-CA-C	-5.91	100.73	110.72
1	G	95	LYS	CA-C-N	-5.89	114.64	121.71
1	G	95	LYS	C-N-CA	-5.89	114.64	121.71
1	B	47	VAL	CB-CA-C	-5.86	104.49	110.93
1	F	64	GLN	N-CA-C	-5.85	104.59	110.97
1	D	70	ASP	N-CA-C	5.85	120.03	113.01
1	A	22	GLY	N-CA-C	-5.85	100.41	112.34
1	C	95	LYS	CA-C-N	-5.82	115.67	122.14
1	C	95	LYS	C-N-CA	-5.82	115.67	122.14
1	D	47	VAL	CB-CA-C	-5.80	104.48	111.85
1	A	137	MSE	CA-C-N	-5.77	114.02	120.14
1	A	137	MSE	C-N-CA	-5.77	114.02	120.14
1	B	12	THR	CA-C-N	-5.75	115.61	123.14
1	B	12	THR	C-N-CA	-5.75	115.61	123.14
1	G	56	VAL	N-CA-C	5.73	116.46	110.62
1	E	69	VAL	CB-CA-C	-5.71	106.01	111.44
1	A	115	ILE	N-CA-C	-5.69	106.92	111.81
1	D	155	LEU	N-CA-C	-5.65	105.27	111.82
1	F	59	ILE	CA-CB-CG1	-5.65	100.80	110.40
1	D	75	ILE	CB-CA-C	-5.62	102.83	110.42
1	F	157	HIS	N-CA-C	-5.59	105.28	111.71
1	F	89	THR	CA-C-O	5.59	123.76	118.34
1	F	75	ILE	CB-CA-C	-5.58	102.81	110.96
1	E	129	ARG	CB-CA-C	-5.54	101.61	110.14
1	G	75	ILE	CB-CA-C	-5.53	102.45	110.63
1	H	69	VAL	CB-CA-C	-5.51	105.30	111.80
1	H	91	GLU	CA-C-N	-5.50	112.48	120.29
1	H	91	GLU	C-N-CA	-5.50	112.48	120.29
1	D	25	ARG	N-CA-C	-5.50	106.62	113.38
1	H	56	VAL	N-CA-CB	5.49	116.97	110.55
1	F	114	LYS	N-CA-C	-5.48	106.09	112.89
1	C	81	THR	CB-CA-C	-5.47	101.47	110.72
1	B	79	GLY	N-CA-C	5.45	120.88	112.81
1	D	98	GLU	CA-C-N	-5.45	114.35	122.74
1	D	98	GLU	C-N-CA	-5.45	114.35	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	88	VAL	N-CA-CB	-5.44	104.87	111.94
1	A	39	GLU	N-CA-C	-5.43	105.05	110.97
1	C	12	THR	CA-C-N	-5.42	116.07	123.12
1	C	12	THR	C-N-CA	-5.42	116.07	123.12
1	H	71	GLU	N-CA-C	5.42	118.87	111.39
1	C	139	GLY	N-CA-C	5.42	119.44	112.83
1	H	12	THR	CA-C-N	-5.41	115.90	123.10
1	H	12	THR	C-N-CA	-5.41	115.90	123.10
1	C	123	ARG	N-CA-C	-5.41	104.94	112.30
1	H	29	ARG	N-CA-C	-5.41	105.39	111.28
1	E	103	GLY	CA-C-N	-5.39	113.06	120.28
1	E	103	GLY	C-N-CA	-5.39	113.06	120.28
1	E	10	ILE	N-CA-C	5.36	115.57	107.80
1	G	6	TYR	CA-C-N	-5.33	115.10	122.30
1	G	6	TYR	C-N-CA	-5.33	115.10	122.30
1	B	81	THR	CB-CA-C	-5.33	101.72	110.72
1	D	62	ILE	N-CA-C	-5.32	105.31	110.42
1	A	53	PRO	CB-CA-C	-5.29	102.18	110.96
1	F	39	GLU	N-CA-C	-5.29	105.21	110.97
1	A	90	PRO	CA-C-N	-5.27	113.21	120.28
1	A	90	PRO	C-N-CA	-5.27	113.21	120.28
1	E	81	THR	N-CA-C	5.26	119.67	112.88
1	D	3	GLY	N-CA-C	-5.26	98.04	113.30
1	B	102	PRO	CB-CA-C	-5.25	104.01	111.68
1	F	95	LYS	CA-C-O	-5.25	112.22	119.05
1	H	116	THR	N-CA-C	5.24	114.87	108.11
1	H	111	GLU	CA-C-N	-5.23	111.98	120.72
1	H	111	GLU	C-N-CA	-5.23	111.98	120.72
1	D	71	GLU	N-CA-C	5.22	118.60	111.39
1	H	25	ARG	N-CA-C	-5.21	106.97	113.38
1	A	46	VAL	CB-CA-C	-5.18	104.69	110.96
1	A	142	ASN	N-CA-C	-5.17	106.82	113.23
1	H	134	ILE	N-CA-CB	-5.17	104.28	111.41
1	E	16	THR	OG1-CB-CG2	-5.17	98.96	109.30
1	H	39	GLU	N-CA-C	-5.17	105.34	110.97
1	D	49	THR	OG1-CB-CG2	-5.14	99.02	109.30
1	A	103	GLY	N-CA-C	-5.14	106.56	112.73
1	F	7	LYS	CA-C-O	5.14	126.18	120.43
1	B	25	ARG	CA-C-N	-5.13	112.90	122.09
1	B	25	ARG	C-N-CA	-5.13	112.90	122.09
1	E	81	THR	CB-CA-C	-5.12	102.07	110.72
1	H	19	ALA	N-CA-C	-5.12	106.99	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	ILE	N-CA-CB	-5.12	104.29	111.25
1	B	64	GLN	N-CA-C	-5.11	105.62	111.14
1	F	81	THR	N-CA-C	5.08	119.44	112.88
1	B	33	VAL	CB-CA-C	-5.08	105.28	112.14
1	E	69	VAL	N-CA-C	5.08	115.92	111.56
1	G	33	VAL	CB-CA-C	-5.07	105.29	112.14
1	A	95	LYS	N-CA-C	5.07	119.09	113.01
1	H	17	VAL	CB-CA-C	-5.07	105.22	112.22
1	C	16	THR	OG1-CB-CG2	-5.06	99.18	109.30
1	G	90	PRO	CA-C-N	-5.05	112.63	120.31
1	G	90	PRO	C-N-CA	-5.05	112.63	120.31
1	B	100	GLU	CA-C-O	-5.05	116.06	121.56
1	A	29	ARG	N-CA-C	-5.04	105.87	111.36
1	E	144	VAL	CB-CA-C	-5.03	104.36	112.16
1	E	91	GLU	N-CA-C	-5.01	105.26	111.33
1	B	118	PHE	N-CA-C	-5.01	107.00	113.01
1	A	75	ILE	CB-CA-C	-5.00	103.67	110.77
1	B	3	GLY	N-CA-C	-5.00	98.79	113.30
1	F	31	VAL	CB-CA-C	-5.00	105.48	111.88

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	1181	0	1228	37	0
1	B	1181	0	1228	29	0
1	C	1181	0	1228	39	0
1	D	1181	0	1228	30	0
1	E	1181	0	1228	29	0
1	F	1181	0	1228	37	0
1	G	1183	0	1228	43	0
1	H	1181	0	1228	39	0
2	A	10	0	0	1	0
2	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	3	0	0	0	0
2	E	5	0	0	0	0
2	F	8	0	0	1	0
2	G	7	0	0	0	0
2	H	6	0	0	1	0
All	All	9501	0	9824	267	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 14.

All (267) 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:C:148:MSE:SE	1:C:148:MSE:CE	2.18	1.41
1:A:32:SER:HB2	1:G:35:ASP:OD1	1.65	0.97
1:E:125:ALA:H	1:E:136:ASN:HD22	1.23	0.86
1:C:125:ALA:H	1:C:136:ASN:HD22	1.24	0.85
1:D:125:ALA:H	1:D:136:ASN:HD22	1.23	0.84
1:H:125:ALA:H	1:H:136:ASN:HD22	1.25	0.84
1:C:160:LYS:HE3	1:F:160:LYS:HZ1	1.49	0.77
1:A:32:SER:CB	1:G:35:ASP:OD1	2.32	0.76
1:F:35:ASP:OD1	1:H:32:SER:HB2	1.86	0.75
1:C:157:HIS:NE2	1:C:161:GLN:OE1	2.20	0.74
1:B:80:GLY:HA2	1:B:87:ASP:OD1	1.88	0.73
1:G:125:ALA:H	1:G:136:ASN:HD22	1.35	0.72
1:C:15:ASP:CG	1:C:86:ARG:HH21	1.97	0.71
1:F:35:ASP:OD2	2:F:2002:HOH:O	2.08	0.69
1:H:17:VAL:HG12	1:H:51:VAL:HG11	1.74	0.68
1:B:152:LEU:N	1:B:153:PRO:CD	2.56	0.68
1:F:7:LYS:HB3	1:F:72:MSE:HE1	1.76	0.67
1:C:125:ALA:H	1:C:136:ASN:ND2	1.93	0.67
1:E:125:ALA:H	1:E:136:ASN:ND2	1.92	0.67
1:G:89:THR:N	1:G:90:PRO:CD	2.57	0.67
1:C:84:THR:HB	1:C:87:ASP:OD2	1.96	0.66
1:A:51:VAL:O	2:A:2001:HOH:O	2.14	0.65
1:C:152:LEU:N	1:C:153:PRO:CD	2.59	0.65
1:B:15:ASP:CG	1:B:86:ARG:HH21	2.05	0.65
1:C:15:ASP:OD2	1:C:86:ARG:NH2	2.29	0.65
1:A:35:ASP:OD1	1:G:32:SER:HB2	1.96	0.64
1:F:7:LYS:HB3	1:F:72:MSE:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:HIS:NE2	1:F:161:GLN:OE1	2.31	0.63
1:G:17:VAL:HG12	1:G:51:VAL:HG11	1.80	0.63
1:C:160:LYS:HZ1	1:F:160:LYS:HE3	1.63	0.62
1:F:32:SER:HB2	1:H:35:ASP:OD1	1.98	0.62
1:F:152:LEU:N	1:F:153:PRO:CD	2.61	0.62
1:H:108:MSE:SE	2:H:2005:HOH:O	2.66	0.62
1:E:60:LYS:HZ3	1:E:95:LYS:HD3	1.64	0.62
1:B:84:THR:HG22	1:B:86:ARG:H	1.65	0.62
1:F:89:THR:N	1:F:90:PRO:CD	2.63	0.61
1:A:157:HIS:NE2	1:A:161:GLN:OE1	2.33	0.61
1:F:125:ALA:H	1:F:136:ASN:HD22	1.47	0.61
1:G:7:LYS:HB3	1:G:72:MSE:HE1	1.82	0.60
1:A:106:PHE:C	1:A:106:PHE:CD2	2.80	0.60
1:G:15:ASP:CG	1:G:86:ARG:HH21	2.10	0.60
1:A:152:LEU:N	1:A:153:PRO:CD	2.64	0.60
1:D:77:THR:OG1	1:D:136:ASN:HA	2.02	0.60
1:C:77:THR:OG1	1:C:136:ASN:HA	2.02	0.59
1:F:15:ASP:CG	1:F:86:ARG:HH21	2.09	0.59
1:B:84:THR:HG23	1:B:85:PRO:HD2	1.85	0.59
1:B:106:PHE:C	1:B:106:PHE:CD2	2.81	0.59
1:A:86:ARG:O	1:A:88:VAL:HG13	2.03	0.58
1:C:157:HIS:CE1	1:C:161:GLN:OE1	2.56	0.58
1:D:72:MSE:HE3	1:D:72:MSE:HA	1.84	0.58
1:B:125:ALA:H	1:B:136:ASN:HD22	1.52	0.58
1:G:157:HIS:NE2	1:G:161:GLN:OE1	2.37	0.57
1:D:38:SER:O	1:D:43:GLY:N	2.35	0.57
1:E:89:THR:N	1:E:90:PRO:CD	2.67	0.57
1:B:157:HIS:NE2	1:B:161:GLN:OE1	2.37	0.57
1:H:77:THR:OG1	1:H:136:ASN:HA	2.05	0.57
1:D:151:LEU:C	1:D:153:PRO:HD2	2.30	0.56
1:D:17:VAL:HG12	1:D:51:VAL:HG11	1.86	0.56
1:D:152:LEU:N	1:D:153:PRO:CD	2.69	0.56
1:H:89:THR:N	1:H:90:PRO:CD	2.69	0.56
1:B:151:LEU:C	1:B:153:PRO:HD2	2.31	0.56
1:F:151:LEU:C	1:F:153:PRO:HD2	2.31	0.56
1:A:89:THR:N	1:A:90:PRO:CD	2.69	0.55
1:C:89:THR:N	1:C:90:PRO:CD	2.70	0.55
1:C:7:LYS:HB3	1:C:72:MSE:CE	2.37	0.54
1:H:125:ALA:H	1:H:136:ASN:ND2	2.02	0.54
1:G:7:LYS:HB3	1:G:72:MSE:CE	2.37	0.54
1:B:60:LYS:HZ3	1:B:95:LYS:HD3	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:LYS:HB3	1:C:72:MSE:HE1	1.89	0.53
1:G:157:HIS:CD2	1:G:161:GLN:OE1	2.62	0.53
1:D:89:THR:HB	1:D:90:PRO:HD3	1.89	0.53
1:H:7:LYS:HB3	1:H:72:MSE:CE	2.38	0.53
1:H:113:LEU:HD23	1:H:119:ALA:HB3	1.91	0.53
1:C:38:SER:O	1:C:43:GLY:N	2.37	0.52
1:D:101:THR:HG23	1:D:127:GLY:HA2	1.90	0.52
1:F:15:ASP:OD2	1:F:86:ARG:NH2	2.38	0.52
1:E:158:ALA:O	1:E:162:ILE:HG13	2.09	0.52
1:B:17:VAL:HG12	1:B:51:VAL:HG11	1.90	0.52
1:E:113:LEU:HD23	1:E:119:ALA:HB3	1.90	0.52
1:G:152:LEU:N	1:G:153:PRO:CD	2.73	0.52
1:H:38:SER:O	1:H:43:GLY:N	2.35	0.52
1:A:7:LYS:HB3	1:A:72:MSE:CE	2.40	0.52
1:A:151:LEU:C	1:A:153:PRO:HD2	2.34	0.51
1:E:96:VAL:O	1:E:129:ARG:HD2	2.09	0.51
1:F:80:GLY:HA2	1:F:87:ASP:OD1	2.09	0.51
1:H:152:LEU:N	1:H:153:PRO:CD	2.74	0.51
1:D:157:HIS:NE2	1:D:161:GLN:OE1	2.43	0.51
1:E:17:VAL:HG12	1:E:51:VAL:HG11	1.91	0.51
1:E:157:HIS:NE2	1:E:161:GLN:OE1	2.43	0.51
1:F:35:ASP:OD1	1:H:32:SER:CB	2.58	0.51
1:H:90:PRO:O	1:H:91:GLU:C	2.51	0.51
1:H:96:VAL:O	1:H:129:ARG:HD2	2.11	0.51
1:E:106:PHE:C	1:E:106:PHE:CD2	2.88	0.51
1:A:77:THR:OG1	1:A:136:ASN:HA	2.11	0.50
1:E:80:GLY:HA2	1:E:87:ASP:OD1	2.11	0.50
1:E:86:ARG:O	1:E:88:VAL:HG13	2.11	0.50
1:F:32:SER:CB	1:H:35:ASP:OD1	2.59	0.50
1:A:35:ASP:OD1	1:G:32:SER:CB	2.60	0.50
1:D:80:GLY:HA2	1:D:87:ASP:OD1	2.11	0.50
1:D:113:LEU:HD23	1:D:119:ALA:HB3	1.94	0.50
1:E:7:LYS:HB3	1:E:72:MSE:CE	2.41	0.50
1:B:7:LYS:HB3	1:B:72:MSE:CE	2.41	0.50
1:C:151:LEU:C	1:C:153:PRO:HD2	2.36	0.50
1:G:84:THR:HG22	1:G:86:ARG:H	1.77	0.50
1:B:86:ARG:O	1:B:88:VAL:HG13	2.12	0.50
1:C:89:THR:HB	1:C:90:PRO:HD3	1.94	0.50
1:H:84:THR:HG23	1:H:85:PRO:HD2	1.92	0.49
1:A:60:LYS:HD3	1:A:95:LYS:HD3	1.93	0.49
1:G:89:THR:N	1:G:90:PRO:HD2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:ALA:O	1:C:162:ILE:HG13	2.13	0.49
1:D:106:PHE:C	1:D:106:PHE:CD2	2.88	0.49
1:B:89:THR:N	1:B:90:PRO:CD	2.76	0.49
1:H:89:THR:HB	1:H:90:PRO:HD3	1.95	0.49
1:H:117:PRO:C	1:H:119:ALA:N	2.69	0.48
1:B:116:THR:OG1	1:B:117:PRO:HD2	2.14	0.48
1:E:7:LYS:HB3	1:E:72:MSE:HE1	1.94	0.48
1:F:17:VAL:HG12	1:F:51:VAL:HG11	1.95	0.48
1:B:152:LEU:N	1:B:153:PRO:HD3	2.27	0.48
1:E:41:LEU:HD21	1:E:155:LEU:HD23	1.94	0.48
1:H:15:ASP:CG	1:H:86:ARG:HH21	2.21	0.48
1:B:29:ARG:HH11	1:B:29:ARG:HG3	1.79	0.48
1:B:77:THR:OG1	1:B:136:ASN:HA	2.14	0.48
1:F:89:THR:HB	1:F:90:PRO:HD3	1.96	0.48
1:A:7:LYS:HB3	1:A:72:MSE:HE1	1.95	0.48
1:D:151:LEU:C	1:D:153:PRO:CD	2.87	0.48
1:E:30:ALA:O	1:E:31:VAL:C	2.56	0.48
1:B:151:LEU:C	1:B:153:PRO:CD	2.87	0.47
1:C:160:LYS:CE	1:F:160:LYS:HZ1	2.25	0.47
1:A:90:PRO:O	1:A:91:GLU:C	2.57	0.47
1:A:15:ASP:CG	1:A:86:ARG:HH21	2.21	0.47
1:E:15:ASP:CG	1:E:86:ARG:HH21	2.23	0.47
1:A:96:VAL:O	1:A:129:ARG:HD2	2.14	0.47
1:F:49:THR:HG23	1:H:28:PRO:HG3	1.97	0.47
1:C:152:LEU:N	1:C:153:PRO:HD3	2.29	0.47
1:D:116:THR:OG1	1:D:117:PRO:HD2	2.15	0.47
1:F:135:ILE:HD13	1:F:135:ILE:HG21	1.58	0.47
1:G:77:THR:OG1	1:G:136:ASN:HA	2.15	0.47
1:A:17:VAL:HG12	1:A:51:VAL:HG11	1.96	0.47
1:C:60:LYS:NZ	1:C:95:LYS:HD3	2.30	0.47
1:A:113:LEU:HD23	1:A:119:ALA:HB3	1.97	0.46
1:G:59:ILE:H	1:G:59:ILE:HG13	1.47	0.46
1:G:105:LEU:HD23	1:G:108:MSE:CE	2.46	0.46
1:G:116:THR:OG1	1:G:117:PRO:HD2	2.15	0.46
1:G:151:LEU:C	1:G:153:PRO:HD2	2.41	0.46
1:B:88:VAL:O	1:B:89:THR:C	2.56	0.46
1:G:155:LEU:HD12	1:G:155:LEU:HA	1.56	0.46
1:A:60:LYS:HZ3	1:A:95:LYS:HD3	1.80	0.46
1:E:117:PRO:C	1:E:119:ALA:N	2.72	0.46
1:B:155:LEU:HD12	1:B:155:LEU:HA	1.69	0.46
1:D:89:THR:N	1:D:90:PRO:CD	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ALA:H	1:D:136:ASN:ND2	2.02	0.46
1:F:84:THR:HG22	1:F:86:ARG:H	1.80	0.46
1:H:151:LEU:C	1:H:153:PRO:HD2	2.41	0.46
1:A:125:ALA:H	1:A:136:ASN:HD22	1.63	0.45
1:A:151:LEU:C	1:A:153:PRO:CD	2.89	0.45
1:F:148:MSE:O	1:F:149:GLU:C	2.59	0.45
1:F:116:THR:OG1	1:F:117:PRO:HD2	2.16	0.45
1:F:125:ALA:H	1:F:136:ASN:ND2	2.14	0.45
1:H:29:ARG:HG3	1:H:29:ARG:HH11	1.81	0.45
1:A:80:GLY:HA2	1:A:87:ASP:OD1	2.17	0.45
1:D:80:GLY:O	1:D:90:PRO:HD3	2.16	0.45
1:G:38:SER:O	1:G:39:GLU:C	2.59	0.45
1:E:80:GLY:O	1:E:90:PRO:HD3	2.17	0.45
1:B:7:LYS:HB3	1:B:72:MSE:HE1	1.98	0.45
1:D:155:LEU:O	1:D:158:ALA:HB3	2.17	0.45
1:C:101:THR:HG23	1:C:127:GLY:HA2	1.98	0.45
1:H:97:ILE:HD12	1:H:127:GLY:HA3	1.99	0.44
1:C:15:ASP:O	1:C:16:THR:C	2.59	0.44
1:C:33:VAL:O	1:C:34:VAL:C	2.53	0.44
1:E:84:THR:HG22	1:E:86:ARG:H	1.82	0.44
1:G:140:ASN:O	1:G:143:ALA:HB3	2.18	0.44
1:E:59:ILE:O	1:E:60:LYS:C	2.59	0.44
1:H:140:ASN:O	1:H:143:ALA:HB3	2.18	0.44
1:C:16:THR:O	1:C:17:VAL:C	2.59	0.44
1:E:38:SER:O	1:E:43:GLY:N	2.38	0.44
1:F:104:LEU:HD22	1:F:151:LEU:HD22	1.98	0.44
1:A:125:ALA:H	1:A:136:ASN:ND2	2.16	0.44
1:C:8:VAL:HA	1:C:74:LEU:O	2.18	0.44
1:D:117:PRO:C	1:D:119:ALA:H	2.23	0.44
1:G:6:TYR:HB2	1:G:44:ALA:CB	2.48	0.44
1:G:52:VAL:HB	1:G:53:PRO:HD2	2.00	0.44
1:B:84:THR:CG2	1:B:85:PRO:HD2	2.48	0.43
1:A:41:LEU:HD21	1:A:155:LEU:HD23	2.00	0.43
1:A:123:ARG:HD2	1:C:100:GLU:O	2.18	0.43
1:F:55:GLU:O	1:F:59:ILE:HG13	2.19	0.43
1:H:106:PHE:C	1:H:106:PHE:CD2	2.96	0.43
1:G:125:ALA:H	1:G:136:ASN:ND2	2.08	0.43
1:H:84:THR:HB	1:H:87:ASP:OD2	2.18	0.43
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.81	0.43
1:F:151:LEU:C	1:F:153:PRO:CD	2.91	0.43
1:C:106:PHE:C	1:C:106:PHE:CD2	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:THR:HG22	1:D:86:ARG:H	1.82	0.43
1:H:7:LYS:HB3	1:H:72:MSE:HE1	1.99	0.43
1:A:107:VAL:HG21	1:B:120:MSE:HE2	2.01	0.43
1:D:117:PRO:C	1:D:119:ALA:N	2.71	0.43
1:E:105:LEU:HD23	1:E:105:LEU:HA	1.76	0.43
1:H:117:PRO:C	1:H:119:ALA:H	2.26	0.43
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.89	0.43
1:G:59:ILE:O	1:G:60:LYS:C	2.60	0.43
1:A:152:LEU:N	1:A:153:PRO:HD3	2.33	0.43
1:A:28:PRO:HG3	1:G:49:THR:HG23	2.01	0.42
1:A:49:THR:HG23	1:G:28:PRO:HG3	2.02	0.42
1:C:155:LEU:HD12	1:C:155:LEU:HA	1.73	0.42
1:H:155:LEU:HD12	1:H:155:LEU:HA	1.80	0.42
1:B:117:PRO:C	1:B:119:ALA:N	2.77	0.42
1:C:29:ARG:HD3	1:C:29:ARG:N	2.33	0.42
1:F:77:THR:OG1	1:F:136:ASN:HA	2.19	0.42
1:G:116:THR:OG1	1:G:118:PHE:HD1	2.02	0.42
1:C:117:PRO:C	1:C:119:ALA:N	2.77	0.42
1:F:148:MSE:C	1:F:150:ALA:N	2.76	0.42
1:E:26:SER:O	1:E:27:GLY:C	2.62	0.42
1:G:41:LEU:HD21	1:G:155:LEU:HD23	2.01	0.42
1:C:17:VAL:HG12	1:C:51:VAL:HG11	2.01	0.42
1:C:80:GLY:HA2	1:C:87:ASP:OD1	2.19	0.42
1:E:152:LEU:N	1:E:153:PRO:CD	2.83	0.42
1:D:84:THR:HG23	1:D:85:PRO:HD2	2.01	0.42
1:G:106:PHE:C	1:G:106:PHE:CD2	2.97	0.42
1:A:26:SER:O	1:A:27:GLY:C	2.63	0.42
1:H:6:TYR:HB2	1:H:44:ALA:HB2	2.01	0.42
1:H:86:ARG:O	1:H:88:VAL:HG13	2.20	0.42
1:E:90:PRO:O	1:E:91:GLU:C	2.62	0.42
1:G:26:SER:O	1:G:27:GLY:C	2.62	0.42
1:G:29:ARG:HH11	1:G:29:ARG:HG3	1.85	0.42
1:H:15:ASP:O	1:H:16:THR:C	2.63	0.42
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.82	0.42
1:C:117:PRO:C	1:C:119:ALA:H	2.28	0.42
1:C:137:MSE:HB3	1:C:138:PRO:CD	2.50	0.42
1:G:151:LEU:C	1:G:153:PRO:CD	2.93	0.42
1:D:15:ASP:CG	1:D:86:ARG:HH21	2.28	0.41
1:G:80:GLY:HA2	1:G:87:ASP:OD1	2.19	0.41
1:H:30:ALA:O	1:H:31:VAL:C	2.61	0.41
1:H:74:LEU:HD12	1:H:74:LEU:HA	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:24:ASP:OD2	1:H:26:SER:N	2.52	0.41
1:C:105:LEU:O	1:C:106:PHE:C	2.62	0.41
1:G:37:SER:O	1:G:38:SER:C	2.62	0.41
1:G:109:MSE:HB2	1:G:109:MSE:HE2	1.81	0.41
1:F:116:THR:HA	1:F:117:PRO:HD3	1.93	0.41
1:F:30:ALA:O	1:F:31:VAL:C	2.64	0.41
1:G:113:LEU:HD23	1:G:113:LEU:HA	1.91	0.41
1:F:106:PHE:CD2	1:F:106:PHE:C	2.99	0.41
1:G:15:ASP:OD2	1:G:86:ARG:NH2	2.48	0.41
1:B:38:SER:O	1:B:39:GLU:C	2.63	0.41
1:E:151:LEU:C	1:E:153:PRO:CD	2.93	0.41
1:H:59:ILE:O	1:H:60:LYS:C	2.60	0.41
1:B:55:GLU:O	1:B:59:ILE:HG13	2.21	0.41
1:B:62:ILE:HD13	1:B:62:ILE:HA	1.86	0.41
1:C:151:LEU:C	1:C:153:PRO:CD	2.92	0.41
1:D:33:VAL:O	1:D:34:VAL:C	2.60	0.41
1:D:55:GLU:O	1:D:59:ILE:HG13	2.20	0.41
1:D:74:LEU:HA	1:D:74:LEU:HD12	1.77	0.41
1:G:89:THR:HB	1:G:90:PRO:HD3	2.02	0.41
1:G:113:LEU:HD23	1:G:119:ALA:HB3	2.02	0.41
1:A:116:THR:HA	1:A:117:PRO:HD3	1.96	0.41
1:D:7:LYS:HB3	1:D:72:MSE:HE1	2.03	0.41
1:E:41:LEU:HD23	1:E:41:LEU:HA	1.98	0.40
1:F:152:LEU:N	1:F:153:PRO:HD3	2.36	0.40
1:F:113:LEU:HD23	1:F:119:ALA:HB3	2.02	0.40
1:G:6:TYR:HB2	1:G:44:ALA:HB2	2.01	0.40
1:E:117:PRO:C	1:E:119:ALA:H	2.29	0.40
1:F:26:SER:O	1:F:27:GLY:C	2.62	0.40
1:A:157:HIS:CD2	1:A:161:GLN:OE1	2.74	0.40
1:B:27:GLY:N	1:B:28:PRO:HD2	2.36	0.40
1:D:152:LEU:HD12	1:D:152:LEU:HA	1.93	0.40
1:H:29:ARG:HG3	1:H:29:ARG:NH1	2.37	0.40
1:A:116:THR:OG1	1:A:117:PRO:HD2	2.21	0.40
1:D:41:LEU:HD21	1:D:155:LEU:HD23	2.03	0.40
1:H:151:LEU:HA	1:H:151:LEU:HD23	1.83	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	158/162 (98%)	152 (96%)	6 (4%)	0	100	100
1	B	158/162 (98%)	152 (96%)	5 (3%)	1 (1%)	21	42
1	C	158/162 (98%)	149 (94%)	9 (6%)	0	100	100
1	D	158/162 (98%)	145 (92%)	11 (7%)	2 (1%)	9	21
1	E	158/162 (98%)	148 (94%)	9 (6%)	1 (1%)	21	42
1	F	158/162 (98%)	150 (95%)	7 (4%)	1 (1%)	21	42
1	G	158/162 (98%)	151 (96%)	6 (4%)	1 (1%)	21	42
1	H	158/162 (98%)	148 (94%)	9 (6%)	1 (1%)	21	42
All	All	1264/1296 (98%)	1195 (94%)	62 (5%)	7 (1%)	21	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	130	GLY
1	B	14	SER
1	D	14	SER
1	E	14	SER
1	F	14	SER
1	G	14	SER
1	H	43	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	131/127 (103%)	124 (95%)	7 (5%)	20	43
1	B	131/127 (103%)	125 (95%)	6 (5%)	24	49
1	C	131/127 (103%)	124 (95%)	7 (5%)	20	43
1	D	131/127 (103%)	125 (95%)	6 (5%)	24	49
1	E	131/127 (103%)	124 (95%)	7 (5%)	20	43
1	F	131/127 (103%)	123 (94%)	8 (6%)	17	37
1	G	131/127 (103%)	124 (95%)	7 (5%)	20	43
1	H	131/127 (103%)	125 (95%)	6 (5%)	24	49
All	All	1048/1016 (103%)	994 (95%)	54 (5%)	21	44

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	23	PRO
1	A	32	SER
1	A	36	SER
1	A	122	SER
1	A	131	SER
1	A	144	VAL
1	B	23	PRO
1	B	32	SER
1	B	36	SER
1	B	116	THR
1	B	122	SER
1	B	131	SER
1	C	16	THR
1	C	23	PRO
1	C	32	SER
1	C	36	SER
1	C	122	SER
1	C	131	SER
1	C	144	VAL
1	D	23	PRO
1	D	32	SER
1	D	36	SER
1	D	124	SER
1	D	131	SER
1	D	144	VAL
1	E	12	THR

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Mol	Chain	Res	Type
1	E	16	THR
1	E	23	PRO
1	E	32	SER
1	E	36	SER
1	E	131	SER
1	E	144	VAL
1	F	10	ILE
1	F	23	PRO
1	F	32	SER
1	F	36	SER
1	F	116	THR
1	F	122	SER
1	F	131	SER
1	F	144	VAL
1	G	23	PRO
1	G	32	SER
1	G	36	SER
1	G	116	THR
1	G	122	SER
1	G	131	SER
1	G	144	VAL
1	H	12	THR
1	H	23	PRO
1	H	32	SER
1	H	36	SER
1	H	131	SER
1	H	144	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	B	136	ASN
1	C	136	ASN
1	D	136	ASN
1	E	136	ASN
1	F	136	ASN
1	G	136	ASN
1	H	136	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 [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	154/162 (95%)	-1.41	0 100 100	33, 46, 77, 104	0
1	B	154/162 (95%)	-1.43	0 100 100	34, 46, 78, 105	0
1	C	154/162 (95%)	-1.44	0 100 100	35, 47, 76, 107	0
1	D	154/162 (95%)	-1.43	0 100 100	35, 47, 77, 104	0
1	E	154/162 (95%)	-1.43	0 100 100	35, 47, 77, 102	0
1	F	154/162 (95%)	-1.47	0 100 100	34, 46, 78, 106	0
1	G	154/162 (95%)	-1.41	0 100 100	34, 45, 77, 104	0
1	H	154/162 (95%)	-1.41	0 100 100	36, 48, 79, 104	0
All	All	1232/1296 (95%)	-1.43	0 100 100	33, 47, 78, 107	0

There are no RSRZ outliers to report.

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.