Full wwPDB X-ray Structure Validation Report (i)

May 27, 2020 – 02:36 am BST

PDB ID	:	1EAV
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

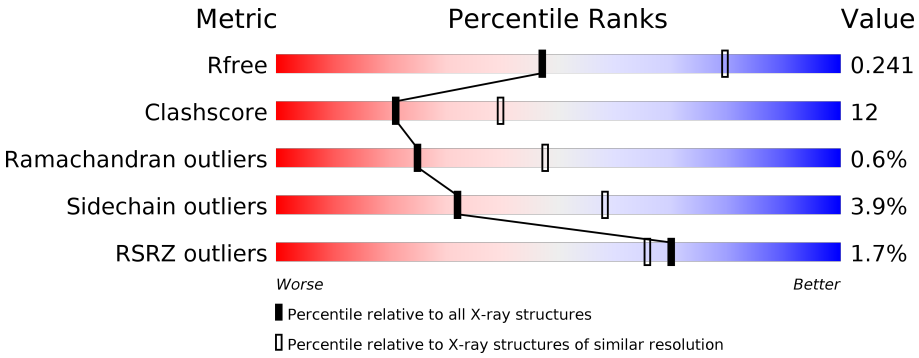
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 on 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 <=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	2% 68% 27%
1	B	162	2% 70% 26%
1	C	162	2% 67% 30%
1	D	162	% 66% 31%
1	E	162	% 69% 29%
1	F	162	% 71% 25%

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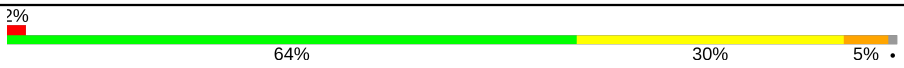
Mol	Chain	Length	Quality of chain
1	G	162	
1	H	162	

2 Entry composition (i)

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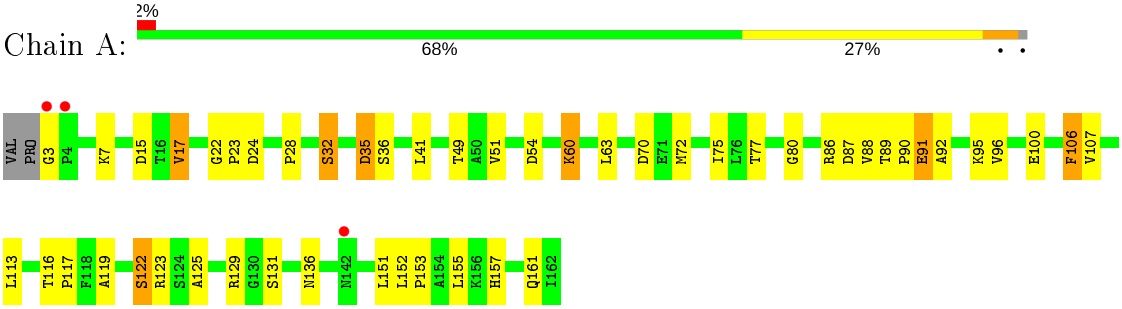
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	5	Total O 5 5	0	0
2	D	3	Total O 3 3	0	0
2	E	5	Total O 5 5	0	0
2	F	8	Total O 8 8	0	0
2	G	7	Total O 7 7	0	0
2	H	6	Total O 6 6	0	0

3 Residue-property plots (i)

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

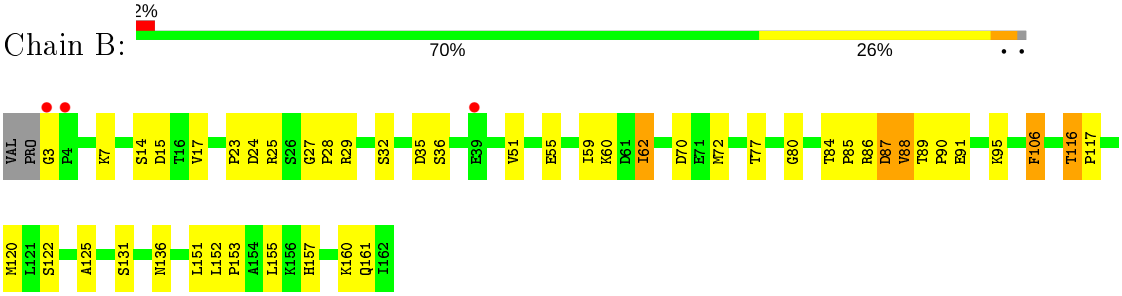
- Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain A:



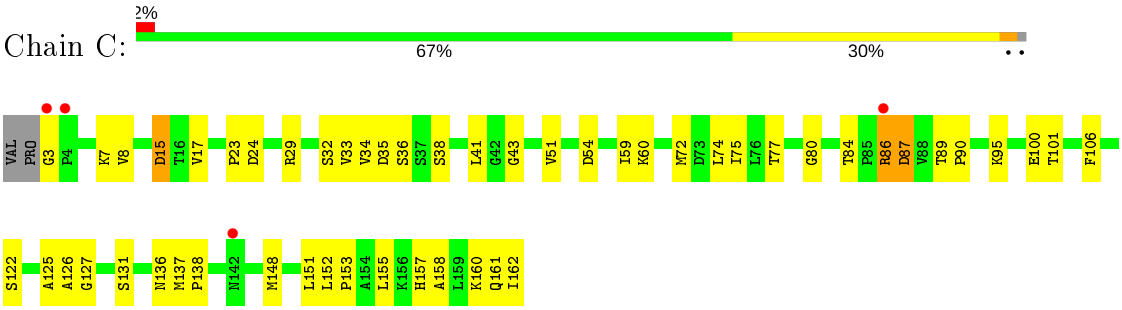
- Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain B:



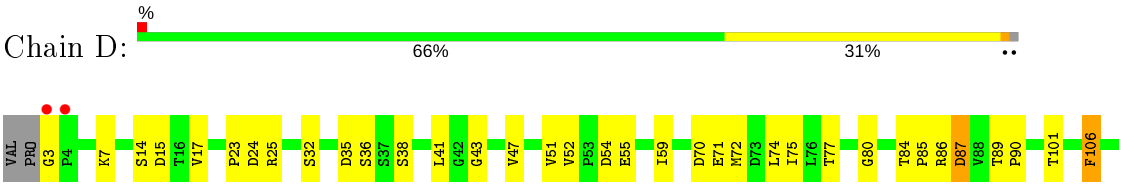
- Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

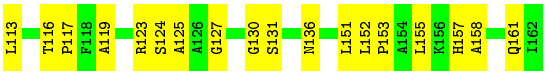
Chain C:



- Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

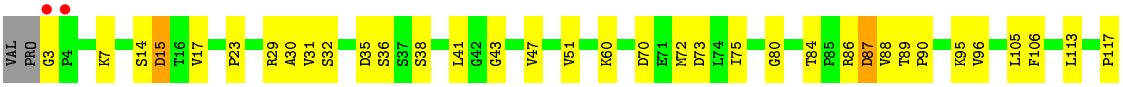
Chain D:





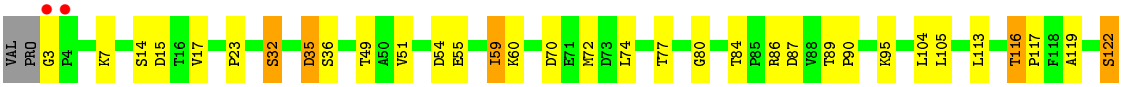
• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain E:



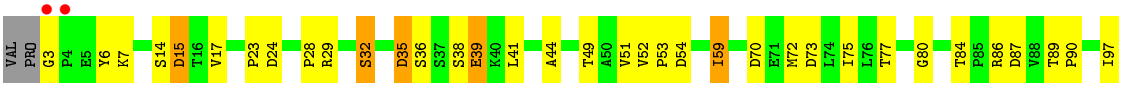
• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain F:



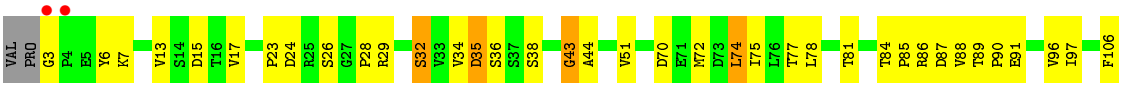
• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

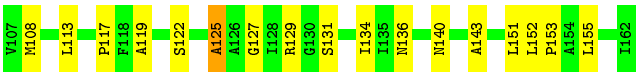
Chain G:



• Molecule 1: MOLYBDOPTERIN BIOSYNTHESIS CNX1 PROTEIN

Chain H:





4 Data and refinement statistics (i)

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 26.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.8 (27.00-2.60) 90.8 (26.43-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.0.36	Depositor
R, R_{free}	0.223 , 0.251 0.219 , 0.241	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)	0.30 , 13.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.457 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.44	8/1192 (0.7%)	1.32	6/1608 (0.4%)
1	B	1.37	4/1192 (0.3%)	1.30	9/1608 (0.6%)
1	C	1.36	4/1192 (0.3%)	1.36	7/1608 (0.4%)
1	D	1.32	5/1192 (0.4%)	1.36	10/1608 (0.6%)
1	E	1.36	1/1192 (0.1%)	1.30	11/1608 (0.7%)
1	F	1.34	1/1192 (0.1%)	1.29	7/1608 (0.4%)
1	G	1.46	4/1194 (0.3%)	1.40	12/1609 (0.7%)
1	H	1.36	7/1192 (0.6%)	1.31	6/1608 (0.4%)
All	All	1.38	34/9538 (0.4%)	1.33	68/12865 (0.5%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	125	ALA	CA-CB	-7.19	1.37	1.52
1	D	71	GLU	CD-OE1	7.03	1.33	1.25
1	B	88	VAL	CA-CB	-6.99	1.40	1.54
1	A	122	SER	CB-OG	6.85	1.51	1.42
1	G	122	SER	CB-OG	6.85	1.51	1.42
1	B	160	LYS	CD-CE	6.49	1.67	1.51
1	A	17	VAL	CB-CG1	-6.39	1.39	1.52
1	A	106	PHE	CB-CG	-6.38	1.40	1.51
1	H	106	PHE	CG-CD2	-6.37	1.29	1.38
1	H	34	VAL	CB-CG1	-6.09	1.40	1.52
1	D	47	VAL	CA-CB	-5.95	1.42	1.54
1	G	75	ILE	CA-CB	-5.93	1.41	1.54
1	C	106	PHE	CB-CG	-5.92	1.41	1.51
1	G	97	ILE	CA-CB	-5.85	1.41	1.54
1	H	75	ILE	CA-CB	-5.82	1.41	1.54
1	D	106	PHE	CB-CG	-5.80	1.41	1.51
1	B	106	PHE	CB-CG	-5.74	1.41	1.51
1	A	60	LYS	CE-NZ	5.73	1.63	1.49
1	A	91	GLU	CG-CD	5.67	1.60	1.51
1	A	75	ILE	CA-CB	-5.50	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	92	ALA	CA-CB	-5.48	1.41	1.52
1	G	39	GLU	CD-OE1	5.46	1.31	1.25
1	D	75	ILE	CA-CB	-5.42	1.42	1.54
1	C	75	ILE	CA-CB	-5.40	1.42	1.54
1	H	134	ILE	CA-CB	-5.35	1.42	1.54
1	H	122	SER	CB-OG	5.28	1.49	1.42
1	E	134	ILE	CA-CB	-5.26	1.42	1.54
1	C	59	ILE	CA-CB	-5.16	1.43	1.54
1	F	122	SER	CB-OG	5.15	1.49	1.42
1	H	13	VAL	CB-CG1	-5.13	1.42	1.52
1	C	126	ALA	CA-CB	-5.11	1.41	1.52
1	B	91	GLU	CG-CD	5.07	1.59	1.51
1	D	52	VAL	CB-CG2	-5.07	1.42	1.52
1	A	100	GLU	CD-OE2	5.03	1.31	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	35	ASP	CB-CG-OD2	12.88	129.90	118.30
1	A	35	ASP	CB-CG-OD2	11.81	128.93	118.30
1	B	35	ASP	CB-CG-OD2	11.21	128.39	118.30
1	C	35	ASP	CB-CG-OD2	10.18	127.46	118.30
1	G	24	ASP	CB-CG-OD2	9.50	126.85	118.30
1	G	73	ASP	CB-CG-OD2	9.26	126.64	118.30
1	A	70	ASP	CB-CG-OD2	8.92	126.33	118.30
1	C	54	ASP	CB-CG-OD2	8.73	126.16	118.30
1	D	35	ASP	CB-CG-OD2	8.39	125.85	118.30
1	C	24	ASP	CB-CG-OD2	8.25	125.72	118.30
1	H	70	ASP	CB-CG-OD2	8.21	125.69	118.30
1	G	129	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	C	87	ASP	CB-CG-OD1	8.07	125.56	118.30
1	D	24	ASP	CB-CG-OD2	7.94	125.45	118.30
1	B	35	ASP	CB-CG-OD1	-7.50	111.55	118.30
1	F	74	LEU	CB-CG-CD2	7.40	123.58	111.00
1	D	70	ASP	CB-CG-OD2	6.96	124.56	118.30
1	F	105	LEU	CB-CG-CD2	-6.76	99.51	111.00
1	E	70	ASP	CB-CG-OD2	6.69	124.32	118.30
1	C	15	ASP	CB-CG-OD2	6.59	124.23	118.30
1	F	35	ASP	CB-CG-OD2	6.50	124.15	118.30
1	A	24	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	24	ASP	CB-CG-OD2	6.41	124.06	118.30
1	E	35	ASP	CB-CG-OD2	6.27	123.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	15	ASP	CB-CG-OD1	6.25	123.93	118.30
1	D	123	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	54	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	3	GLY	N-CA-C	-6.02	98.04	113.10
1	H	35	ASP	CB-CG-OD2	5.99	123.69	118.30
1	E	29	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	F	70	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	15	ASP	CB-CG-OD2	5.87	123.58	118.30
1	G	35	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	B	62	ILE	CG1-CB-CG2	-5.86	98.52	111.40
1	D	123	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	B	3	GLY	N-CA-C	-5.72	98.79	113.10
1	C	3	GLY	N-CA-C	-5.72	98.80	113.10
1	E	87	ASP	CB-CG-OD2	5.72	123.45	118.30
1	E	133	LEU	CB-CG-CD2	-5.67	101.37	111.00
1	D	54	ASP	CB-CG-OD2	5.65	123.39	118.30
1	G	59	ILE	CA-CB-CG1	-5.65	100.26	111.00
1	B	70	ASP	CB-CG-OD2	5.60	123.34	118.30
1	F	54	ASP	CB-CG-OD2	5.58	123.32	118.30
1	E	75	ILE	CB-CA-C	-5.51	100.58	111.60
1	E	3	GLY	N-CA-C	-5.51	99.33	113.10
1	F	3	GLY	N-CA-C	-5.49	99.37	113.10
1	H	78	LEU	CB-CG-CD2	5.43	120.23	111.00
1	A	3	GLY	N-CA-C	-5.43	99.53	113.10
1	G	54	ASP	CB-CG-OD2	5.41	123.17	118.30
1	H	3	GLY	N-CA-C	-5.40	99.60	113.10
1	F	59	ILE	CA-CB-CG1	-5.37	100.80	111.00
1	G	3	GLY	N-CA-C	-5.35	99.73	113.10
1	G	70	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	87	ASP	CB-CG-OD1	5.27	123.04	118.30
1	H	81	THR	CB-CA-C	-5.26	97.40	111.60
1	E	15	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	107	VAL	CG1-CB-CG2	-5.20	102.58	110.90
1	D	87	ASP	CB-CG-OD2	5.18	122.97	118.30
1	B	25	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	88	VAL	CG1-CB-CG2	-5.14	102.67	110.90
1	H	74	LEU	CB-CG-CD1	-5.12	102.29	111.00
1	E	47	VAL	CB-CA-C	-5.10	101.72	111.40
1	E	73	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	86	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	A	22	GLY	N-CA-C	-5.07	100.41	113.10
1	E	35	ASP	CB-CG-OD1	-5.05	113.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	25	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	G	155	LEU	CB-CG-CD1	-5.00	102.50	111.00

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	35	0
1	B	1181	0	1228	27	0
1	C	1181	0	1228	31	0
1	D	1181	0	1228	28	0
1	E	1181	0	1228	24	0
1	F	1181	0	1228	32	0
1	G	1183	0	1228	38	0
1	H	1181	0	1228	34	0
2	A	10	0	0	1	0
2	B	7	0	0	0	0
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	234	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 (234) 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:CE	1:C:148:MSE:SE	2.18	1.41
1:A:32:SER:HB2	1:G:35:ASP:OD1	1.65	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:160:LYS:HE3	1:F:160:LYS:HZ1	1.51	0.73
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: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:15:ASP:CG	1:C:86:ARG:HH21	1.97	0.66
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: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
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:F:152:LEU:N	1:F:153:PRO:CD	2.61	0.62
1:F:32:SER:HB2	1:H:35:ASP:OD1	1.98	0.62
1:H:108:MSE:SE	2:H:2005:HOH:O	2.66	0.62
1:B:84:THR:HG22	1:B:86:ARG:H	1.65	0.62
1:E:60:LYS:HZ3	1:E:95:LYS:HD3	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:B:15:ASP:CG	1:B:86:ARG:HH21	2.05	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:B:84:THR:HG23	1:B:85:PRO:HD2	1.85	0.59
1:A:86:ARG:O	1:A:88:VAL:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:106:PHE:CD2	1:A:106:PHE:C	2.80	0.56
1:C:160:LYS:HZ1	1:F:160:LYS:HE3	1.70	0.56
1:G:15:ASP:CG	1:G:86:ARG:HH21	2.10	0.55
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:F:15:ASP:CG	1:F:86:ARG:HH21	2.09	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:B:106:PHE:C	1:B:106:PHE:CD2	2.81	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
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:D:151:LEU:C	1:D:153:PRO:HD2	2.30	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:151:LEU:C	1:B:153:PRO:HD2	2.31	0.51
1:F:151:LEU:C	1:F:153:PRO:HD2	2.31	0.51
1:H:96:VAL:O	1:H:129:ARG:HD2	2.11	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: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
1:C:158:ALA:O	1:C:162:ILE:HG13	2.13	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: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: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: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:F:135:ILE:HD13	1:F:135:ILE:HG21	1.58	0.47
1:D:116:THR:OG1	1:D:117:PRO:HD2	2.15	0.47
1:G:77:THR:OG1	1:G:136:ASN:HA	2.15	0.47
1:A:151:LEU:C	1:A:153:PRO:HD2	2.34	0.47
1:A:17:VAL:HG12	1:A:51:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LYS:NZ	1:C:95:LYS:HD3	2.30	0.47
1:H:90:PRO:O	1:H:91:GLU:C	2.51	0.46
1:A:113:LEU:HD23	1:A:119:ALA:HB3	1.97	0.46
1:G:105:LEU:HD23	1:G:108:MSE:CE	2.46	0.46
1:G:59:ILE:H	1:G:59:ILE:HG13	1.47	0.46
1:E:106:PHE:C	1:E:106:PHE:CD2	2.88	0.46
1:G:116:THR:OG1	1:G:117:PRO:HD2	2.15	0.46
1:G:155:LEU:HA	1:G:155:LEU:HD12	1.56	0.46
1:B:155:LEU:HA	1:B:155:LEU:HD12	1.69	0.46
1:D:125:ALA:H	1:D:136:ASN:ND2	2.02	0.46
1:D:89:THR:N	1:D:90:PRO:CD	2.78	0.46
1:F:84:THR:HG22	1:F:86:ARG:H	1.80	0.46
1:A:125:ALA:H	1:A:136:ASN:HD22	1.63	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:HH11	1:H:29:ARG:HG3	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:C:151:LEU:C	1:C:153:PRO:HD2	2.36	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: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:D:106:PHE:C	1:D:106:PHE:CD2	2.88	0.44
1:H:140:ASN:O	1:H:143:ALA:HB3	2.18	0.44
1:E:38:SER:O	1:E:43:GLY:N	2.38	0.44
1:D:117:PRO:C	1:D:119:ALA:N	2.71	0.44
1:F:104:LEU:HD22	1:F:151:LEU:HD22	1.98	0.44
1:H:117:PRO:C	1:H:119:ALA:N	2.69	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:G:52:VAL:HB	1:G:53:PRO:HD2	2.00	0.44
1:G:6:TYR:HB2	1:G:44:ALA:CB	2.48	0.44
1:B:84:THR:CG2	1:B:85:PRO:HD2	2.48	0.43
1:H:15:ASP:CG	1:H:86:ARG:HH21	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:63:LEU:HD23	1.81	0.43
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:151:LEU:C	1:D:153:PRO:CD	2.87	0.43
1:E:105:LEU:HA	1:E:105:LEU:HD23	1.76	0.43
1:B:151:LEU:C	1:B:153:PRO:CD	2.87	0.43
1:C:41:LEU:HA	1:C:41:LEU:HD23	1.89	0.43
1:E:30:ALA:O	1:E:31:VAL:C	2.56	0.43
1:A:152:LEU:N	1:A:153:PRO:HD3	2.33	0.43
1:A:49:THR:HG23	1:G:28:PRO:HG3	2.02	0.42
1:A:90:PRO:O	1:A:91:GLU:C	2.57	0.42
1:C:155:LEU:HA	1:C:155:LEU:HD12	1.73	0.42
1:A:28:PRO:HG3	1:G:49:THR:HG23	2.01	0.42
1:H:155:LEU:HD12	1:H:155:LEU:HA	1.80	0.42
1:A:15:ASP:CG	1:A:86:ARG:HH21	2.21	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: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:C:33:VAL:O	1:C:34:VAL:C	2.53	0.42
1:E:117:PRO:C	1:E:119:ALA:N	2.72	0.42
1:H:6:TYR:HB2	1:H:44:ALA:HB2	2.01	0.42
1:E:15:ASP:CG	1:E:86:ARG:HH21	2.23	0.42
1:H:86:ARG:O	1:H:88:VAL:HG13	2.20	0.42
1:G:29:ARG:HH11	1:G:29:ARG:HG3	1.85	0.42
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.82	0.42
1:C:137:MSE:HB3	1:C:138:PRO:CD	2.50	0.42
1:G:80:GLY:HA2	1:G:87:ASP:OD1	2.19	0.41
1:H:74:LEU:HD12	1:H:74:LEU:HA	1.73	0.41
1:G:151:LEU:C	1:G:153:PRO:HD2	2.41	0.41
1:H:24:ASP:OD2	1:H:26:SER:N	2.52	0.41
1:G:109:MSE:HE2	1:G:109:MSE:HB2	1.81	0.41
1:B:88:VAL:O	1:B:89:THR:C	2.56	0.41
1:F:116:THR:HA	1:F:117:PRO:HD3	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:LEU:HA	1:G:113:LEU:HD23	1.91	0.41
1:G:15:ASP:OD2	1:G:86:ARG:NH2	2.48	0.41
1:H:151:LEU:C	1:H:153:PRO:HD2	2.41	0.41
1:A:151:LEU:C	1:A:153:PRO:CD	2.89	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: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:F:148:MSE:O	1:F:149:GLU:C	2.59	0.41
1:G:113:LEU:HD23	1:G:119:ALA:HB3	2.02	0.41
1:G:89:THR:HB	1:G:90:PRO:HD3	2.02	0.41
1:A:116:THR:HA	1:A:117:PRO:HD3	1.96	0.41
1:D:117:PRO:C	1:D:119:ALA:H	2.23	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:G:38:SER:O	1:G:39:GLU:C	2.59	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: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:F:60:LYS:HZ3	1:F:95:LYS:HD3	1.86	0.40
1:H:29:ARG:NH1	1:H:29:ARG:HG3	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:HD23	1:H:151:LEU:HA	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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%)	25	47
1	C	158/162 (98%)	149 (94%)	9 (6%)	0	100	100
1	D	158/162 (98%)	145 (92%)	11 (7%)	2 (1%)	12	24
1	E	158/162 (98%)	148 (94%)	9 (6%)	1 (1%)	25	47
1	F	158/162 (98%)	150 (95%)	7 (4%)	1 (1%)	25	47
1	G	158/162 (98%)	151 (96%)	6 (4%)	1 (1%)	25	47
1	H	158/162 (98%)	148 (94%)	9 (6%)	1 (1%)	25	47
All	All	1264/1296 (98%)	1195 (94%)	62 (5%)	7 (1%)	25	47

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 (i)

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%)	126 (96%)	5 (4%)	33	59
1	B	131/127 (103%)	125 (95%)	6 (5%)	27	51
1	C	131/127 (103%)	126 (96%)	5 (4%)	33	59
1	D	131/127 (103%)	126 (96%)	5 (4%)	33	59
1	E	131/127 (103%)	127 (97%)	4 (3%)	40	66
1	F	131/127 (103%)	125 (95%)	6 (5%)	27	51
1	G	131/127 (103%)	125 (95%)	6 (5%)	27	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	131/127 (103%)	127 (97%)	4 (3%)	40 66
All	All	1048/1016 (103%)	1007 (96%)	41 (4%)	32 58

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	PRO
1	A	32	SER
1	A	36	SER
1	A	122	SER
1	A	131	SER
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	23	PRO
1	C	32	SER
1	C	36	SER
1	C	122	SER
1	C	131	SER
1	D	23	PRO
1	D	32	SER
1	D	36	SER
1	D	124	SER
1	D	131	SER
1	E	23	PRO
1	E	32	SER
1	E	36	SER
1	E	131	SER
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	G	23	PRO
1	G	32	SER
1	G	36	SER
1	G	116	THR
1	G	122	SER

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Mol	Chain	Res	Type
1	G	131	SER
1	H	23	PRO
1	H	32	SER
1	H	36	SER
1	H	131	SER

Some 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

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.10	3 (1%)	66	62	33, 46, 77, 104	0
1	B	154/162 (95%)	-0.07	3 (1%)	66	62	34, 46, 78, 105	0
1	C	154/162 (95%)	-0.07	4 (2%)	56	50	35, 47, 76, 107	0
1	D	154/162 (95%)	-0.10	2 (1%)	77	73	35, 47, 77, 104	0
1	E	154/162 (95%)	-0.02	2 (1%)	77	73	35, 47, 77, 102	0
1	F	154/162 (95%)	-0.12	2 (1%)	77	73	34, 46, 78, 106	0
1	G	154/162 (95%)	-0.08	3 (1%)	66	62	34, 45, 77, 104	0
1	H	154/162 (95%)	-0.10	2 (1%)	77	73	36, 48, 79, 104	0
All	All	1232/1296 (95%)	-0.08	21 (1%)	70	66	33, 47, 78, 107	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	3	GLY	11.9
1	F	4	PRO	8.4
1	D	3	GLY	8.4
1	G	3	GLY	8.1
1	B	3	GLY	7.5
1	B	4	PRO	6.5
1	H	3	GLY	6.5
1	C	4	PRO	6.2
1	G	4	PRO	5.5
1	D	4	PRO	5.1
1	E	3	GLY	5.1
1	C	3	GLY	4.9
1	E	4	PRO	4.7
1	A	3	GLY	4.6
1	A	4	PRO	4.2
1	A	142	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	142	ASN	2.8
1	H	4	PRO	2.7
1	C	86	ARG	2.4
1	B	39	GLU	2.2
1	G	142	ASN	2.2

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.