



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:42 PM UTC

PDB ID : 1YF1 / pdb_00001yfl
Title : Structural and biochemical analysis of the link between enzymatic activity and oligomerization in AhpC, a bacterial peroxiredoxin.
Authors : Parsonage, D.; Youngblood, D.S.; Sarma, G.N.; Wood, Z.A.; Karplus, P.A.; Poole, L.B.
Deposited on : 2004-12-29
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
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

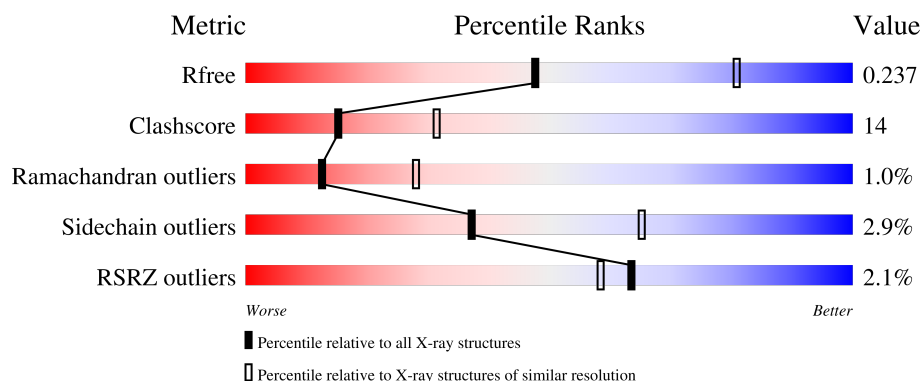
1 Overall quality at a glance

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.



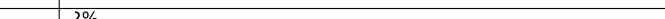
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	186	3% 65% 23% • 11%
1	B	186	0% 63% 23% • 11%
1	C	186	2% 62% 24% • 12%
1	D	186	0% 53% 33% •• 11%
1	E	186	2% 60% 24% •• 11%

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Mol	Chain	Length	Quality of chain
1	F	186	
1	G	186	
1	H	186	
1	I	186	
1	J	186	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13819 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 Alkyl hydroperoxide reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1306	832	217	253	4			
1	B	165	Total	C	N	O	S	0	0	0
			1299	827	216	252	4			
1	C	163	Total	C	N	O	S	0	0	0
			1286	819	214	250	3			
1	D	166	Total	C	N	O	S	0	0	0
			1306	832	217	253	4			
1	E	165	Total	C	N	O	S	0	0	0
			1299	827	216	252	4			
1	F	166	Total	C	N	O	S	0	0	0
			1306	832	217	253	4			
1	G	165	Total	C	N	O	S	0	0	0
			1299	827	216	252	4			
1	H	163	Total	C	N	O	S	0	0	0
			1286	819	214	250	3			
1	I	166	Total	C	N	O	S	0	0	0
			1306	832	217	253	4			
1	J	165	Total	C	N	O	S	0	0	0
			1299	827	216	252	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	VAL	THR	engineered mutation	UNP P0A251
B	77	VAL	THR	engineered mutation	UNP P0A251
C	77	VAL	THR	engineered mutation	UNP P0A251
D	77	VAL	THR	engineered mutation	UNP P0A251
E	77	VAL	THR	engineered mutation	UNP P0A251
F	77	VAL	THR	engineered mutation	UNP P0A251
G	77	VAL	THR	engineered mutation	UNP P0A251
H	77	VAL	THR	engineered mutation	UNP P0A251
I	77	VAL	THR	engineered mutation	UNP P0A251

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Chain	Residue	Modelled	Actual	Comment	Reference
J	77	VAL	THR	engineered mutation	UNP P0A251

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0

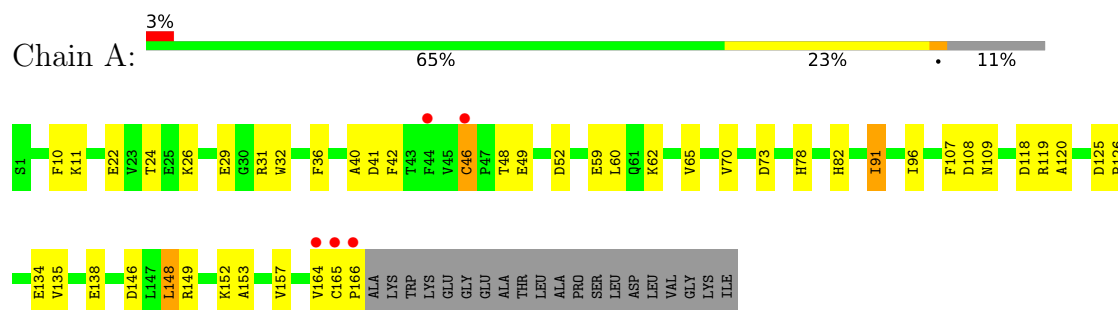
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	112	Total O 112 112	0	0
3	B	95	Total O 95 95	0	0
3	C	94	Total O 94 94	0	0
3	D	67	Total O 67 67	0	0
3	E	32	Total O 32 32	0	0
3	F	100	Total O 100 100	0	0
3	G	101	Total O 101 101	0	0
3	H	96	Total O 96 96	0	0
3	I	89	Total O 89 89	0	0
3	J	40	Total O 40 40	0	0

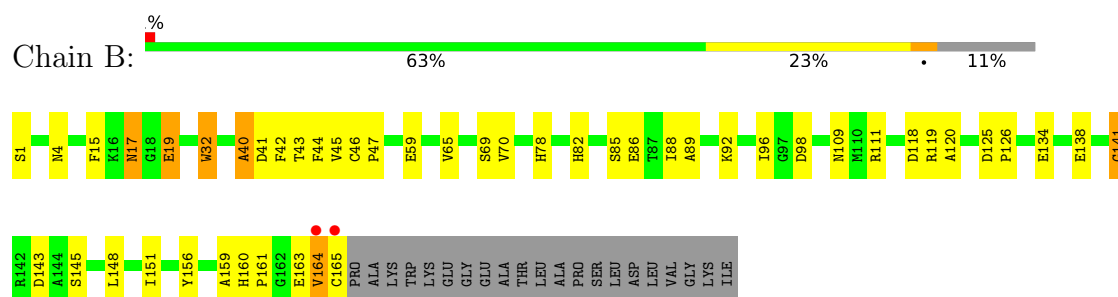
3 Residue-property plots

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.

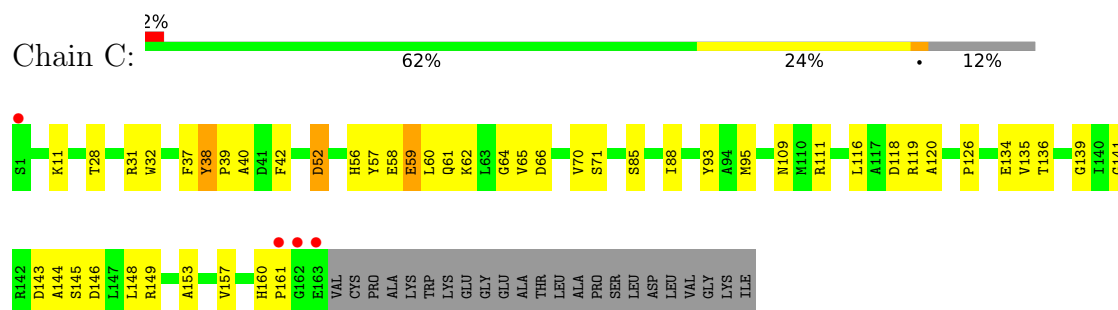
- Molecule 1: Alkyl hydroperoxide reductase subunit C



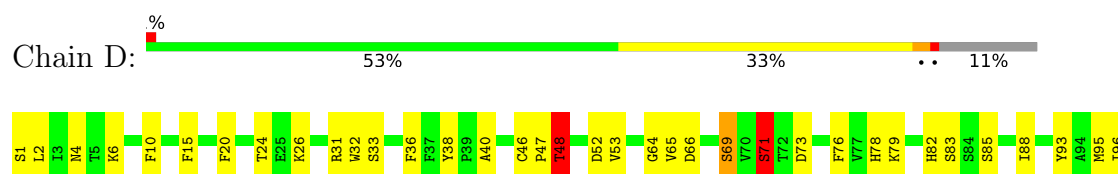
- Molecule 1: Alkyl hydroperoxide reductase subunit C

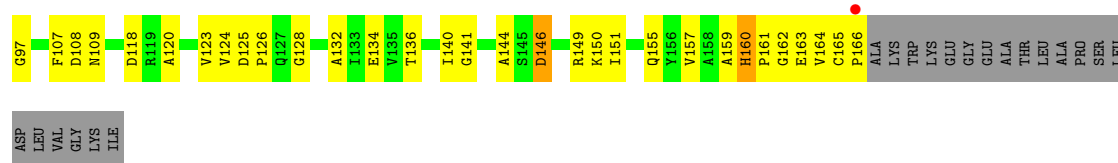


- Molecule 1: Alkyl hydroperoxide reductase subunit C

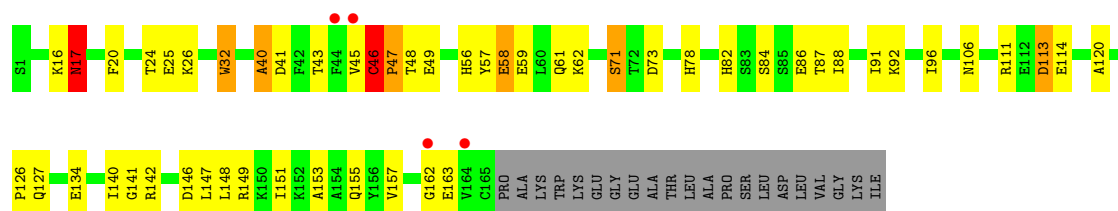


- Molecule 1: Alkyl hydroperoxide reductase subunit C

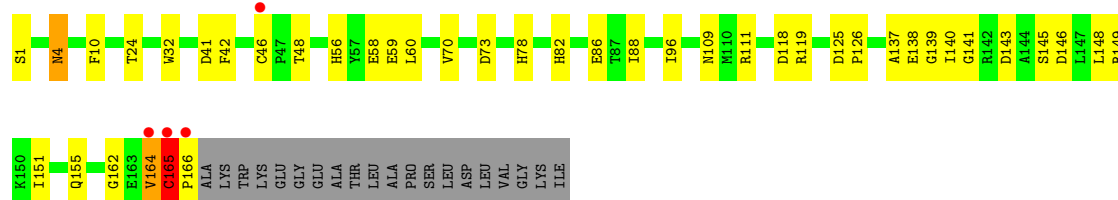




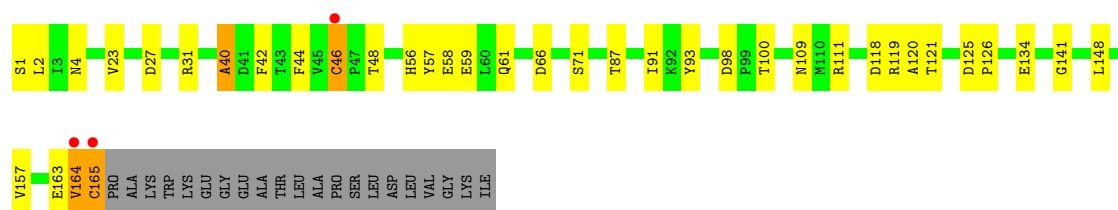
• Molecule 1: Alkyl hydroperoxide reductase subunit C



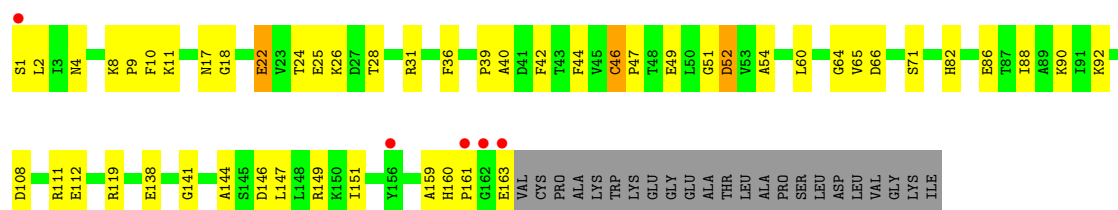
• Molecule 1: Alkyl hydroperoxide reductase subunit C



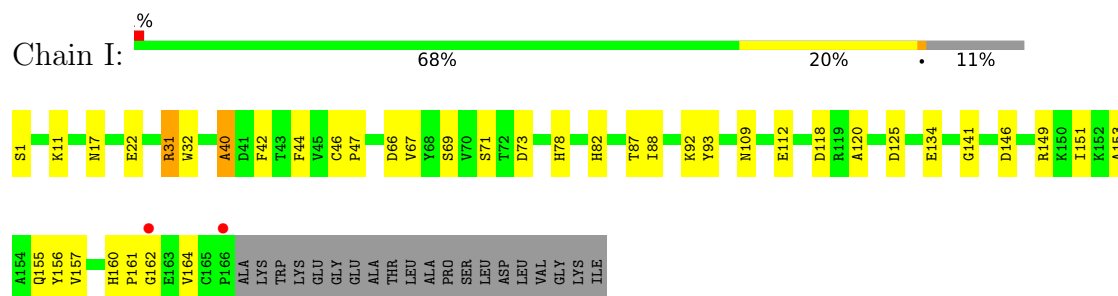
• Molecule 1: Alkyl hydroperoxide reductase subunit C



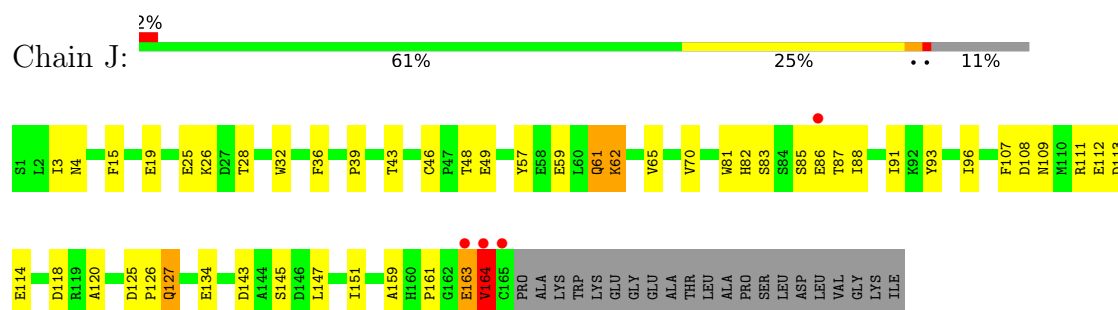
• Molecule 1: Alkyl hydroperoxide reductase subunit C



- Molecule 1: Alkyl hydroperoxide reductase subunit C



- Molecule 1: Alkyl hydroperoxide reductase subunit C



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	136.35Å 169.96Å 117.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.60 100.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-2.60) 93.5 (100.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.237 0.181 , 0.237	Depositor DCC
R_{free} test set	7964 reflections (9.50%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13819	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2860e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.62	0/1337	1.07	4/1813 (0.2%)
1	B	0.62	0/1329	1.03	6/1801 (0.3%)
1	C	0.63	1/1316 (0.1%)	1.07	5/1783 (0.3%)
1	D	0.53	0/1337	1.02	7/1813 (0.4%)
1	E	0.48	0/1329	1.03	8/1801 (0.4%)
1	F	0.62	0/1337	1.00	4/1813 (0.2%)
1	G	0.62	0/1329	1.00	6/1801 (0.3%)
1	H	0.57	0/1316	1.05	9/1783 (0.5%)
1	I	0.59	0/1337	1.05	9/1813 (0.5%)
1	J	0.52	0/1329	0.99	2/1801 (0.1%)
All	All	0.58	1/13296 (0.0%)	1.03	60/18022 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	MET	SD-CE	7.09	1.97	1.79

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	46	CYS	CA-C-N	7.78	129.57	119.84
1	I	46	CYS	C-N-CA	7.78	129.57	119.84
1	A	42	PHE	N-CA-C	7.63	121.94	112.47
1	C	38	TYR	CA-C-N	7.39	126.65	118.97
1	C	38	TYR	C-N-CA	7.39	126.65	118.97
1	G	91	ILE	N-CA-C	7.06	118.16	108.84
1	B	40	ALA	N-CA-C	6.85	119.58	108.76
1	A	91	ILE	N-CA-C	6.75	117.74	109.30
1	H	2	LEU	N-CA-C	-6.67	105.71	114.31
1	F	42	PHE	N-CA-C	6.66	120.69	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ASP	N-CA-C	-6.41	101.89	110.55
1	B	19	GLU	N-CA-C	6.32	118.79	109.69
1	E	96	ILE	N-CA-C	6.26	117.65	109.58
1	F	141	GLY	N-CA-C	6.23	121.09	112.37
1	H	39	PRO	N-CA-C	6.22	122.37	113.47
1	C	40	ALA	N-CA-C	6.16	117.88	108.52
1	C	111	ARG	N-CA-C	-6.12	97.70	108.23
1	I	73	ASP	N-CA-C	-6.11	102.89	110.41
1	C	42	PHE	N-CA-C	6.08	120.02	112.47
1	B	69	SER	N-CA-C	-6.02	101.57	110.48
1	E	91	ILE	N-CA-C	5.99	117.01	108.93
1	D	48	THR	N-CA-C	5.95	118.25	111.11
1	I	42	PHE	N-CA-C	5.93	120.09	112.86
1	E	20	PHE	N-CA-C	-5.87	100.14	109.76
1	E	32	TRP	N-CA-C	-5.83	99.74	109.24
1	I	141	GLY	N-CA-C	5.71	119.51	112.14
1	H	46	CYS	CA-C-N	5.70	126.96	119.84
1	H	46	CYS	C-N-CA	5.70	126.96	119.84
1	B	111	ARG	N-CA-C	-5.65	98.72	108.56
1	H	86	GLU	N-CA-C	-5.61	105.24	111.36
1	H	111	ARG	N-CA-C	-5.61	97.32	107.75
1	H	112	GLU	N-CA-C	5.60	117.38	111.28
1	J	19	GLU	N-CA-C	5.59	117.75	109.69
1	D	69	SER	N-CA-C	-5.38	101.76	110.32
1	D	40	ALA	N-CA-C	5.38	117.26	108.76
1	I	40	ALA	N-CA-C	5.37	117.25	108.76
1	G	40	ALA	N-CA-C	5.32	117.17	108.76
1	I	32	TRP	N-CA-C	-5.32	101.04	109.76
1	G	100	THR	N-CA-C	-5.31	106.75	113.18
1	E	40	ALA	N-CA-C	5.29	116.58	108.42
1	I	112	GLU	N-CA-C	5.28	117.72	111.33
1	F	4	ASN	N-CA-C	5.26	120.88	113.56
1	E	140	ILE	N-CA-C	-5.26	100.75	108.54
1	B	32	TRP	N-CA-C	-5.20	101.23	109.76
1	D	160	HIS	CA-C-N	5.19	125.48	119.93
1	D	160	HIS	C-N-CA	5.19	125.48	119.93
1	D	146	ASP	N-CA-C	-5.16	105.73	112.23
1	G	111	ARG	N-CA-C	-5.14	99.61	108.56
1	H	42	PHE	N-CA-C	5.12	118.80	112.24
1	A	40	ALA	N-CA-C	5.12	116.85	108.76
1	J	62	LYS	N-CA-C	-5.11	105.40	110.97
1	F	73	ASP	N-CA-C	-5.11	103.65	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	18	GLY	N-CA-C	5.10	121.15	115.08
1	D	71	SER	N-CA-C	-5.09	101.55	109.24
1	E	46	CYS	N-CA-C	5.08	117.57	108.47
1	G	87	THR	N-CA-C	5.07	116.50	111.07
1	B	141	GLY	N-CA-C	5.05	119.01	112.54
1	E	106	ASN	N-CA-C	-5.04	105.97	111.82
1	G	42	PHE	N-CA-C	5.03	118.70	112.47
1	I	69	SER	N-CA-C	-5.01	102.35	110.32

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	1306	0	1261	35	0
1	B	1299	0	1254	50	0
1	C	1286	0	1240	31	0
1	D	1306	0	1261	54	0
1	E	1299	0	1255	39	0
1	F	1306	0	1260	31	0
1	G	1299	0	1253	30	0
1	H	1286	0	1240	32	0
1	I	1306	0	1261	24	0
1	J	1299	0	1255	44	0
2	A	1	0	0	0	0
3	A	112	0	0	1	0
3	B	95	0	0	4	0
3	C	94	0	0	4	0
3	D	67	0	0	3	0
3	E	32	0	0	0	0
3	F	100	0	0	4	0
3	G	101	0	0	6	0
3	H	96	0	0	6	0
3	I	89	0	0	3	0
3	J	40	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13819	0	12540	347	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 (347) 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:119:ARG:HD3	3:B:2004:HOH:O	1.79	0.81
1:C:52:ASP:HB3	1:C:144:ALA:HB2	1.63	0.80
1:F:164:VAL:HG12	1:F:165:CYS:H	1.47	0.79
1:J:111:ARG:HH11	1:J:118:ASP:HA	1.50	0.77
1:C:119:ARG:HD3	3:C:3004:HOH:O	1.88	0.74
1:I:109:ASN:HD21	1:I:118:ASP:HB2	1.53	0.74
1:D:15:PHE:CE1	1:D:79:LYS:HG3	2.23	0.74
1:B:109:ASN:ND2	1:B:118:ASP:HB2	2.03	0.73
1:H:44:PHE:HB3	1:I:164:VAL:HG13	1.71	0.73
1:E:82:HIS:HA	1:E:88:ILE:HG22	1.70	0.73
1:F:164:VAL:HG12	1:F:165:CYS:N	2.02	0.72
1:I:109:ASN:ND2	1:I:118:ASP:HB2	2.05	0.72
1:G:56:HIS:HD2	1:G:148:LEU:HD12	1.54	0.71
1:H:160:HIS:N	1:H:161:PRO:HD3	2.04	0.71
1:G:119:ARG:HD3	3:G:2504:HOH:O	1.90	0.70
1:D:46:CYS:HB3	1:D:48:THR:HG22	1.72	0.70
1:J:82:HIS:HA	1:J:88:ILE:HG22	1.75	0.68
1:B:59:GLU:CD	1:B:148:LEU:HD21	2.19	0.68
1:G:164:VAL:HG12	1:G:165:CYS:H	1.59	0.68
1:A:164:VAL:HG11	1:B:45:VAL:HG13	1.76	0.67
1:J:15:PHE:HE2	1:J:82:HIS:CD2	2.13	0.67
1:J:147:LEU:O	1:J:151:ILE:HG13	1.93	0.67
1:F:149:ARG:NH2	1:G:141:GLY:O	2.27	0.67
1:H:28:THR:HA	3:H:3545:HOH:O	1.95	0.67
1:H:141:GLY:O	1:I:149:ARG:NH2	2.27	0.66
1:C:11:LYS:HD3	3:C:3295:HOH:O	1.96	0.66
1:G:31:ARG:HD3	1:G:66:ASP:OD2	1.95	0.66
1:B:44:PHE:CD1	1:F:166:PRO:HD3	2.32	0.65
1:G:164:VAL:HG12	1:G:165:CYS:N	2.11	0.65
1:H:1:SER:HA	3:H:3649:HOH:O	1.97	0.65
1:D:164:VAL:O	1:D:166:PRO:HD3	1.96	0.64
1:J:85:SER:HB3	1:J:88:ILE:HB	1.77	0.64
1:D:164:VAL:HG12	1:D:165:CYS:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ARG:NH2	1:H:64:GLY:HA2	2.13	0.64
1:H:31:ARG:HD3	1:H:66:ASP:OD2	1.99	0.63
1:A:149:ARG:NH2	1:B:141:GLY:O	2.30	0.63
1:A:59:GLU:OE2	1:A:148:LEU:HD22	1.99	0.63
1:D:46:CYS:CB	1:D:48:THR:HG22	2.29	0.63
1:E:45:VAL:HG12	1:E:46:CYS:H	1.61	0.63
1:E:46:CYS:C	1:E:48:THR:H	2.05	0.63
1:C:143:ASP:OD2	1:C:145:SER:HB2	1.99	0.63
1:C:160:HIS:N	1:C:161:PRO:HD3	2.13	0.63
1:E:163:GLU:OE1	1:E:163:GLU:HA	1.97	0.63
1:H:25:GLU:HG2	1:H:26:LYS:N	2.13	0.63
1:I:40:ALA:HB1	3:I:4597:HOH:O	1.99	0.63
1:B:17:ASN:ND2	1:B:92:LYS:HA	2.14	0.63
1:A:164:VAL:CG1	1:B:45:VAL:HG13	2.29	0.62
1:D:24:THR:OG1	1:D:26:LYS:HD2	1.99	0.62
1:J:61:GLN:OE1	1:J:61:GLN:HA	2.00	0.62
1:F:1:SER:HB2	3:F:1649:HOH:O	1.99	0.61
1:I:82:HIS:HA	1:I:88:ILE:HG22	1.81	0.61
1:A:109:ASN:ND2	1:A:118:ASP:HB2	2.15	0.61
1:G:109:ASN:ND2	1:G:118:ASP:HB2	2.15	0.61
1:E:16:LYS:C	1:E:17:ASN:HD22	2.08	0.61
1:G:163:GLU:OE1	1:G:163:GLU:HA	2.00	0.61
1:E:32:TRP:CE2	1:E:126:PRO:HD3	2.35	0.60
1:B:109:ASN:HD21	1:B:118:ASP:HB2	1.64	0.60
1:C:153:ALA:O	1:C:157:VAL:HG23	2.02	0.60
1:D:159:ALA:HB2	3:D:4077:HOH:O	2.01	0.60
1:E:151:ILE:O	1:E:155:GLN:HG3	2.02	0.59
1:D:159:ALA:C	1:D:161:PRO:HD3	2.28	0.59
1:C:139:GLY:HA3	1:D:157:VAL:HG21	1.84	0.59
1:E:82:HIS:HA	1:E:88:ILE:CG2	2.32	0.59
1:F:146:ASP:OD1	1:F:149:ARG:NH1	2.35	0.59
1:E:134:GLU:CD	1:E:142:ARG:HG2	2.27	0.59
1:B:164:VAL:O	1:B:165:CYS:HB2	2.02	0.59
1:J:46:CYS:C	1:J:48:THR:H	2.10	0.59
1:J:39:PRO:HG3	1:J:111:ARG:HH12	1.69	0.58
1:E:56:HIS:CD2	1:E:148:LEU:HD12	2.38	0.58
1:D:82:HIS:HA	1:D:88:ILE:HG22	1.86	0.58
1:I:31:ARG:HD3	1:I:66:ASP:OD2	2.03	0.58
1:E:120:ALA:HA	1:E:134:GLU:O	2.03	0.58
3:D:5097:HOH:O	1:E:40:ALA:HB1	2.04	0.57
1:J:59:GLU:O	1:J:62:LYS:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:PHE:O	1:F:24:THR:HA	2.03	0.57
1:D:46:CYS:C	1:D:48:THR:H	2.13	0.56
1:D:76:PHE:CD1	1:E:43:THR:HG22	2.40	0.56
1:A:26:LYS:HA	1:A:29:GLU:HG3	1.87	0.56
1:E:16:LYS:C	1:E:17:ASN:ND2	2.63	0.56
1:B:40:ALA:HB1	3:B:2097:HOH:O	2.05	0.55
1:C:146:ASP:OD1	1:C:149:ARG:NH1	2.39	0.55
1:E:45:VAL:HG12	1:E:46:CYS:N	2.22	0.55
1:J:127:GLN:NE2	1:J:127:GLN:N	2.54	0.55
1:D:85:SER:HB3	1:D:88:ILE:HG12	1.86	0.55
1:F:164:VAL:CG1	1:F:165:CYS:H	2.09	0.55
1:C:141:GLY:O	1:D:149:ARG:NH2	2.40	0.55
1:F:70:VAL:HG22	1:F:96:ILE:HB	1.89	0.55
1:B:125:ASP:HB2	1:B:126:PRO:HD2	1.89	0.55
1:B:156:TYR:CE1	1:B:160:HIS:HD2	2.25	0.55
1:B:156:TYR:CZ	1:B:160:HIS:HD2	2.25	0.55
1:E:86:GLU:OE1	1:E:86:GLU:HA	2.07	0.55
1:E:147:LEU:O	1:E:151:ILE:HG13	2.07	0.55
1:H:36:PHE:HZ	1:H:49:GLU:HB3	1.72	0.54
1:C:59:GLU:OE2	1:C:148:LEU:HD13	2.07	0.54
1:F:111:ARG:HH12	1:F:138:GLU:CG	2.20	0.54
1:G:1:SER:HB2	3:G:2649:HOH:O	2.06	0.54
1:B:163:GLU:HB3	3:B:2279:HOH:O	2.07	0.54
1:D:109:ASN:ND2	1:D:118:ASP:HB2	2.23	0.54
1:J:111:ARG:HD2	1:J:114:GLU:CD	2.33	0.54
1:A:119:ARG:NE	1:A:138:GLU:OE1	2.41	0.54
1:D:125:ASP:HB2	1:D:126:PRO:CD	2.38	0.54
1:A:31:ARG:O	1:A:126:PRO:HA	2.07	0.54
1:D:78:HIS:HB3	1:D:95:MET:HE2	1.90	0.54
1:J:15:PHE:CE2	1:J:82:HIS:CD2	2.96	0.54
1:D:71:SER:OG	1:D:73:ASP:HB2	2.08	0.54
1:F:1:SER:N	3:F:1701:HOH:O	2.41	0.54
1:A:153:ALA:O	1:A:157:VAL:HG23	2.07	0.53
1:C:149:ARG:NH2	1:D:141:GLY:O	2.41	0.53
1:J:36:PHE:HZ	1:J:49:GLU:HB3	1.73	0.53
1:B:85:SER:HB3	1:B:88:ILE:HG12	1.89	0.53
1:D:78:HIS:CD2	1:D:95:MET:HB3	2.44	0.53
1:B:44:PHE:CD1	1:F:165:CYS:HA	2.44	0.53
1:D:82:HIS:HA	1:D:88:ILE:CG2	2.38	0.53
1:E:61:GLN:OE1	1:E:61:GLN:HA	2.08	0.53
1:A:164:VAL:HG11	1:B:45:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:GLU:OE2	1:E:26:LYS:HE3	2.09	0.53
1:A:36:PHE:HZ	1:A:49:GLU:HB3	1.74	0.53
1:F:164:VAL:O	1:F:165:CYS:HB3	2.08	0.53
1:G:61:GLN:HA	1:G:61:GLN:NE2	2.25	0.52
1:C:109:ASN:ND2	1:C:118:ASP:HB2	2.25	0.52
1:C:58:GLU:O	1:C:62:LYS:HG3	2.10	0.52
1:G:57:TYR:CE1	1:G:93:TYR:HB3	2.45	0.52
1:B:17:ASN:HD21	1:B:92:LYS:HA	1.73	0.52
1:J:159:ALA:C	1:J:161:PRO:HD3	2.35	0.52
1:A:165:CYS:HB3	1:B:46:CYS:SG	2.50	0.52
1:F:60:LEU:HG	1:F:148:LEU:HD21	1.92	0.52
1:C:56:HIS:HD2	1:C:148:LEU:HD12	1.74	0.51
1:E:134:GLU:OE1	1:E:142:ARG:HG2	2.09	0.51
1:G:109:ASN:HD21	1:G:118:ASP:HB2	1.74	0.51
1:C:31:ARG:HD3	1:C:66:ASP:OD2	2.11	0.51
1:G:59:GLU:OE2	1:G:148:LEU:HD13	2.11	0.51
1:H:10:PHE:O	1:H:24:THR:HA	2.11	0.51
1:A:46:CYS:C	1:A:48:THR:H	2.19	0.51
1:B:44:PHE:CE1	1:F:166:PRO:HD3	2.45	0.51
1:E:24:THR:OG1	1:E:26:LYS:HD2	2.11	0.51
1:E:58:GLU:O	1:E:62:LYS:HG3	2.11	0.51
1:J:109:ASN:ND2	1:J:118:ASP:HB2	2.26	0.51
1:H:60:LEU:HD22	1:H:65:VAL:HG11	1.93	0.51
1:H:82:HIS:HD2	3:H:3808:HOH:O	1.92	0.51
1:H:90:LYS:HE2	3:H:3784:HOH:O	2.09	0.50
1:A:82:HIS:HE1	1:A:91:ILE:O	1.95	0.50
1:B:41:ASP:OD2	1:B:78:HIS:ND1	2.36	0.50
1:E:59:GLU:O	1:E:62:LYS:HB2	2.11	0.50
1:H:163:GLU:HG3	1:I:44:PHE:O	2.11	0.50
1:J:70:VAL:HG22	1:J:96:ILE:HB	1.94	0.50
1:B:163:GLU:OE1	1:B:163:GLU:HA	2.11	0.50
1:F:58:GLU:HG2	3:F:1703:HOH:O	2.12	0.50
1:B:65:VAL:HG21	1:B:151:ILE:HG21	1.93	0.50
1:C:56:HIS:CD2	1:C:148:LEU:HD12	2.46	0.50
1:D:38:TYR:CZ	1:D:71:SER:HB3	2.47	0.50
1:F:41:ASP:OD2	1:F:78:HIS:ND1	2.43	0.50
1:F:109:ASN:ND2	1:F:118:ASP:HB2	2.26	0.50
1:G:56:HIS:CD2	1:G:148:LEU:HD12	2.42	0.50
1:I:151:ILE:O	1:I:155:GLN:HG3	2.11	0.50
1:A:120:ALA:HA	1:A:134:GLU:O	2.12	0.50
3:F:1526:HOH:O	1:G:1:SER:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:31:ARG:HH22	1:H:64:GLY:HA2	1.77	0.50
1:B:17:ASN:HD21	1:B:92:LYS:CB	2.25	0.50
1:E:146:ASP:OD1	1:E:149:ARG:NH1	2.34	0.50
1:F:125:ASP:HB2	1:F:126:PRO:CD	2.42	0.50
1:H:51:GLY:O	1:H:54:ALA:HB3	2.13	0.49
1:I:156:TYR:CE1	1:I:160:HIS:CD2	3.00	0.49
1:J:125:ASP:HB2	1:J:126:PRO:HD2	1.93	0.49
1:C:85:SER:HB3	1:C:88:ILE:HG12	1.93	0.49
1:J:28:THR:HA	3:J:5545:HOH:O	2.12	0.49
1:J:109:ASN:HD21	1:J:118:ASP:HB2	1.77	0.49
1:J:125:ASP:HB2	1:J:126:PRO:CD	2.42	0.49
1:A:41:ASP:OD2	1:A:78:HIS:ND1	2.31	0.49
1:D:164:VAL:CG1	1:D:165:CYS:N	2.75	0.49
1:A:165:CYS:C	1:B:46:CYS:HG	2.21	0.48
1:C:38:TYR:CZ	1:C:71:SER:HB3	2.48	0.48
1:A:60:LEU:HD22	1:A:65:VAL:HG11	1.95	0.48
1:F:82:HIS:HA	1:F:88:ILE:HG22	1.95	0.48
1:J:32:TRP:CB	1:J:65:VAL:HG22	2.44	0.48
1:D:31:ARG:HD3	1:D:66:ASP:OD2	2.12	0.48
1:J:25:GLU:HG2	1:J:26:LYS:N	2.28	0.48
1:A:109:ASN:HD21	1:A:118:ASP:HB2	1.77	0.48
1:I:82:HIS:HD2	3:I:4808:HOH:O	1.96	0.47
1:I:120:ALA:HA	1:I:134:GLU:O	2.14	0.47
1:B:70:VAL:HG22	1:B:96:ILE:HB	1.95	0.47
1:G:125:ASP:HB2	1:G:126:PRO:CD	2.44	0.47
1:J:127:GLN:NE2	1:J:127:GLN:H	2.12	0.47
1:B:125:ASP:HB2	1:B:126:PRO:CD	2.44	0.47
1:C:32:TRP:CE2	1:C:126:PRO:HD3	2.50	0.47
3:A:1187:HOH:O	1:B:1:SER:HB3	2.13	0.47
1:J:57:TYR:CE1	1:J:93:TYR:HB3	2.49	0.47
1:J:15:PHE:HE2	1:J:82:HIS:CG	2.32	0.47
1:B:82:HIS:HA	1:B:88:ILE:HG22	1.97	0.47
1:B:17:ASN:HD21	1:B:92:LYS:HB3	1.79	0.47
1:C:109:ASN:HD21	1:C:118:ASP:HB2	1.79	0.47
1:D:164:VAL:HG12	1:D:165:CYS:H	1.80	0.47
1:I:71:SER:OG	1:I:78:HIS:HE1	1.97	0.47
1:A:10:PHE:O	1:A:24:THR:HA	2.15	0.47
1:B:40:ALA:O	1:B:43:THR:HG23	2.15	0.47
1:D:6:LYS:HA	1:D:128:GLY:O	2.14	0.47
1:J:46:CYS:HB3	1:J:48:THR:OG1	2.15	0.46
1:J:111:ARG:NH1	1:J:118:ASP:HA	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLU:N	1:B:19:GLU:OE1	2.48	0.46
1:E:17:ASN:OD1	1:E:92:LYS:HG3	2.15	0.46
1:F:32:TRP:CE2	1:F:126:PRO:HD3	2.50	0.46
1:E:46:CYS:C	1:E:48:THR:N	2.72	0.46
1:G:125:ASP:OD1	1:G:125:ASP:C	2.58	0.46
1:H:90:LYS:O	1:H:92:LYS:HE3	2.16	0.46
1:I:11:LYS:HE3	1:I:22:GLU:OE2	2.15	0.46
1:A:70:VAL:HG22	1:A:96:ILE:HB	1.96	0.46
1:D:160:HIS:N	1:D:161:PRO:HD3	2.30	0.46
1:J:82:HIS:HA	1:J:88:ILE:CG2	2.45	0.46
1:G:40:ALA:HB1	3:H:2597:HOH:O	2.15	0.46
1:I:17:ASN:HD21	1:I:92:LYS:HA	1.79	0.46
1:I:31:ARG:CD	1:I:66:ASP:OD2	2.64	0.46
1:H:147:LEU:O	1:H:151:ILE:HG13	2.14	0.46
1:A:165:CYS:C	1:B:46:CYS:SG	2.99	0.46
1:A:146:ASP:OD1	1:A:149:ARG:NH1	2.49	0.46
1:A:149:ARG:NH1	1:B:143:ASP:HB2	2.30	0.46
1:D:15:PHE:HD1	1:D:20:PHE:CE1	2.34	0.46
1:B:32:TRP:CE2	1:B:126:PRO:HD3	2.51	0.46
1:C:120:ALA:HB2	1:C:135:VAL:HG13	1.97	0.46
1:D:31:ARG:HH22	1:D:64:GLY:HA2	1.81	0.46
1:G:46:CYS:C	1:G:48:THR:H	2.24	0.46
1:H:146:ASP:OD1	1:H:149:ARG:NH1	2.43	0.46
1:C:57:TYR:CE1	1:C:93:TYR:HB3	2.50	0.45
1:D:120:ALA:HA	1:D:134:GLU:O	2.17	0.45
1:D:146:ASP:OD2	1:D:150:LYS:HE3	2.16	0.45
1:E:57:TYR:CZ	1:E:61:GLN:NE2	2.85	0.45
1:D:162:GLY:O	1:D:164:VAL:N	2.48	0.45
1:G:164:VAL:CG1	1:G:165:CYS:H	2.22	0.45
1:B:17:ASN:HD21	1:B:92:LYS:CA	2.30	0.45
1:C:52:ASP:HB3	1:C:144:ALA:CB	2.41	0.45
1:J:32:TRP:CE2	1:J:126:PRO:HD3	2.51	0.45
1:A:32:TRP:CE2	1:A:126:PRO:HD3	2.51	0.45
1:A:120:ALA:HB2	1:A:135:VAL:HG13	1.97	0.45
1:E:56:HIS:HD2	1:E:148:LEU:HD12	1.82	0.45
1:B:47:PRO:CB	1:B:88:ILE:HD11	2.47	0.45
1:G:121:THR:HG21	3:G:2626:HOH:O	2.15	0.45
1:D:123:VAL:HB	1:D:132:ALA:HB3	1.97	0.45
1:G:2:LEU:HD23	1:G:2:LEU:HA	1.82	0.45
1:H:9:PRO:HA	1:H:25:GLU:HB3	1.99	0.45
1:B:15:PHE:HE2	1:B:82:HIS:CG	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PRO:CG	1:B:88:ILE:HD11	2.47	0.44
1:J:57:TYR:OH	1:J:61:GLN:NE2	2.50	0.44
1:J:143:ASP:OD1	1:J:145:SER:N	2.50	0.44
1:J:82:HIS:CG	1:J:82:HIS:O	2.70	0.44
1:A:165:CYS:CB	1:B:46:CYS:SG	3.05	0.44
1:E:71:SER:OG	1:E:73:ASP:HB2	2.18	0.44
1:D:10:PHE:O	1:D:24:THR:HA	2.17	0.44
1:C:31:ARG:NH2	1:C:64:GLY:HA2	2.32	0.44
1:G:61:GLN:HA	1:G:61:GLN:HE21	1.82	0.44
1:B:86:GLU:O	1:B:89:ALA:HB3	2.17	0.44
1:J:81:TRP:C	1:J:83:SER:H	2.26	0.44
1:H:11:LYS:HE2	1:H:22:GLU:OE2	2.18	0.44
1:A:125:ASP:C	1:A:125:ASP:OD1	2.60	0.44
1:F:143:ASP:OD1	1:F:145:SER:HB2	2.17	0.44
1:E:111:ARG:HD3	1:E:114:GLU:OE1	2.16	0.43
1:E:41:ASP:OD2	1:E:78:HIS:ND1	2.42	0.43
1:F:125:ASP:HB2	1:F:126:PRO:HD2	1.99	0.43
1:B:164:VAL:O	1:B:165:CYS:CB	2.66	0.43
1:E:111:ARG:C	1:E:113:ASP:N	2.76	0.43
1:J:111:ARG:HE	1:J:111:ARG:HB2	1.69	0.43
1:D:36:PHE:O	1:D:69:SER:HA	2.18	0.43
1:D:78:HIS:HD2	1:D:95:MET:O	2.02	0.43
1:D:125:ASP:HB2	1:D:126:PRO:HD2	2.01	0.43
1:C:120:ALA:HA	1:C:134:GLU:O	2.18	0.43
3:C:3026:HOH:O	1:D:1:SER:HB3	2.19	0.43
1:D:65:VAL:HG21	1:D:151:ILE:HG21	2.01	0.43
1:G:23:VAL:HA	1:G:27:ASP:OD2	2.18	0.43
1:J:3:ILE:O	1:J:3:ILE:HG23	2.18	0.43
1:B:85:SER:CB	1:B:88:ILE:HG12	2.49	0.43
1:C:60:LEU:HB3	1:C:65:VAL:HB	2.01	0.43
1:F:56:HIS:HB3	1:F:148:LEU:HD11	2.00	0.43
1:J:163:GLU:O	1:J:164:VAL:O	2.36	0.43
1:A:107:PHE:O	1:A:108:ASP:C	2.61	0.43
1:D:71:SER:C	1:D:73:ASP:H	2.27	0.43
1:H:46:CYS:HA	1:H:47:PRO:HD3	1.77	0.43
1:H:52:ASP:HB3	1:H:144:ALA:HB2	2.00	0.43
1:E:56:HIS:HB3	1:E:148:LEU:HD11	2.00	0.43
1:H:1:SER:HB2	3:I:4526:HOH:O	2.18	0.43
1:E:49:GLU:OE1	1:E:141:GLY:HA2	2.19	0.42
1:F:151:ILE:O	1:F:155:GLN:HG3	2.18	0.42
3:G:3597:HOH:O	1:H:40:ALA:HB1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ARG:HB2	1:C:136:THR:O	2.19	0.42
1:H:119:ARG:NH2	1:H:138:GLU:OE1	2.43	0.42
1:B:98:ASP:HA	3:B:2019:HOH:O	2.18	0.42
1:C:39:PRO:O	1:C:116:LEU:HD22	2.19	0.42
1:D:85:SER:HB3	1:D:88:ILE:CG1	2.48	0.42
1:D:107:PHE:O	1:D:108:ASP:C	2.62	0.42
1:J:57:TYR:O	1:J:61:GLN:HB2	2.20	0.42
1:C:37:PHE:CD2	1:C:70:VAL:HB	2.54	0.42
1:H:11:LYS:NZ	1:H:22:GLU:OE2	2.50	0.42
1:I:146:ASP:OD1	1:I:149:ARG:NH1	2.52	0.42
1:J:4:ASN:CG	1:J:4:ASN:O	2.62	0.42
1:H:82:HIS:HA	1:H:88:ILE:HG22	2.01	0.42
1:E:32:TRP:NE1	1:E:126:PRO:HD3	2.35	0.42
1:E:127:GLN:N	1:E:127:GLN:CD	2.78	0.42
1:E:153:ALA:O	1:E:157:VAL:HG23	2.19	0.42
1:I:125:ASP:C	1:I:125:ASP:OD1	2.63	0.42
1:D:52:ASP:HB3	1:D:144:ALA:HB2	2.02	0.42
1:H:108:ASP:O	1:I:1:SER:HB3	2.20	0.42
1:B:159:ALA:C	1:B:161:PRO:HD3	2.45	0.42
1:G:120:ALA:HA	1:G:134:GLU:O	2.19	0.42
1:I:153:ALA:O	1:I:157:VAL:HG23	2.19	0.42
1:D:83:SER:HB3	3:D:4102:HOH:O	2.20	0.42
1:F:109:ASN:HD21	1:F:118:ASP:HB2	1.85	0.42
1:I:11:LYS:HE3	1:I:22:GLU:CD	2.45	0.42
1:A:148:LEU:O	1:A:152:LYS:HG3	2.20	0.41
1:H:159:ALA:O	1:H:160:HIS:ND1	2.53	0.41
1:D:2:LEU:HD23	1:D:2:LEU:HA	1.90	0.41
1:D:73:ASP:HB2	1:D:78:HIS:HE1	1.86	0.41
1:G:98:ASP:HA	3:G:2519:HOH:O	2.20	0.41
1:H:159:ALA:C	1:H:160:HIS:ND1	2.78	0.41
1:J:107:PHE:O	1:J:108:ASP:C	2.64	0.41
1:A:32:TRP:CB	1:A:65:VAL:HG22	2.51	0.41
1:A:125:ASP:HB2	1:A:126:PRO:CD	2.51	0.41
1:B:120:ALA:HA	1:B:134:GLU:O	2.21	0.41
1:B:82:HIS:HA	1:B:88:ILE:CG2	2.50	0.41
1:D:32:TRP:CE2	1:D:155:GLN:HG2	2.55	0.41
1:E:17:ASN:ND2	1:E:17:ASN:N	2.68	0.41
1:J:46:CYS:C	1:J:48:THR:N	2.77	0.41
1:C:28:THR:HA	3:C:3045:HOH:O	2.19	0.41
1:F:137:ALA:HB3	1:F:140:ILE:HD12	2.03	0.41
1:H:17:ASN:ND2	1:H:92:LYS:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LYS:HD2	1:A:22:GLU:CD	2.46	0.41
1:A:62:LYS:HE2	3:H:3761:HOH:O	2.21	0.41
1:A:165:CYS:HA	1:A:166:PRO:HD3	1.64	0.41
1:B:143:ASP:OD1	1:B:145:SER:HB2	2.21	0.41
1:D:32:TRP:CE3	1:D:125:ASP:HA	2.56	0.41
1:F:59:GLU:OE2	1:F:148:LEU:HD13	2.20	0.41
1:I:156:TYR:CZ	1:I:160:HIS:CD2	3.09	0.41
1:J:120:ALA:HA	1:J:134:GLU:O	2.21	0.41
1:D:53:VAL:HG12	1:D:93:TYR:CE2	2.56	0.41
1:D:164:VAL:CG1	1:D:165:CYS:H	2.33	0.41
1:G:66:ASP:HA	3:G:2583:HOH:O	2.20	0.41
1:I:67:VAL:O	1:I:93:TYR:HB2	2.21	0.41
1:D:78:HIS:CB	1:D:95:MET:HE2	2.51	0.40
1:F:139:GLY:HA3	1:G:157:VAL:HG21	2.03	0.40
1:J:111:ARG:O	1:J:113:ASP:N	2.54	0.40
1:B:17:ASN:ND2	1:B:92:LYS:CA	2.82	0.40
1:C:57:TYR:O	1:C:61:GLN:HG2	2.22	0.40
1:D:136:THR:HB	1:D:140:ILE:HB	2.03	0.40
1:J:32:TRP:HB3	1:J:65:VAL:HG22	2.03	0.40
1:D:96:ILE:HG22	1:D:97:GLY:N	2.35	0.40
1:J:91:ILE:HG23	1:J:93:TYR:CE1	2.56	0.40
1:D:46:CYS:HA	1:D:47:PRO:HD3	1.93	0.40
1:G:61:GLN:HE21	1:G:61:GLN:CA	2.34	0.40
1:E:45:VAL:O	1:E:47:PRO:HD3	2.21	0.40
1:F:119:ARG:HD2	1:F:138:GLU:HG2	2.04	0.40
1:F:164:VAL:HG11	1:G:44:PHE:HB3	2.03	0.40
1:I:47:PRO:HB2	1:I:87:THR:HG21	2.03	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	164/186 (88%)	158 (96%)	6 (4%)	0	100	100
1	B	163/186 (88%)	154 (94%)	6 (4%)	3 (2%)	6	14
1	C	161/186 (87%)	156 (97%)	5 (3%)	0	100	100
1	D	164/186 (88%)	152 (93%)	11 (7%)	1 (1%)	21	42
1	E	163/186 (88%)	144 (88%)	14 (9%)	5 (3%)	3	5
1	F	164/186 (88%)	157 (96%)	4 (2%)	3 (2%)	6	14
1	G	163/186 (88%)	156 (96%)	6 (4%)	1 (1%)	21	42
1	H	161/186 (87%)	153 (95%)	8 (5%)	0	100	100
1	I	164/186 (88%)	156 (95%)	6 (4%)	2 (1%)	10	23
1	J	163/186 (88%)	146 (90%)	15 (9%)	2 (1%)	10	23
All	All	1630/1860 (88%)	1532 (94%)	81 (5%)	17 (1%)	12	28

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	164	VAL
1	F	165	CYS
1	G	164	VAL
1	J	164	VAL
1	B	164	VAL
1	D	163	GLU
1	E	17	ASN
1	F	162	GLY
1	I	162	GLY
1	J	112	GLU
1	E	162	GLY
1	I	161	PRO
1	B	17	ASN
1	E	58	GLU
1	B	42	PHE
1	E	84	SER
1	E	47	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	139/154 (90%)	136 (98%)	3 (2%)	45	72
1	B	138/154 (90%)	136 (99%)	2 (1%)	59	81
1	C	136/154 (88%)	134 (98%)	2 (2%)	57	80
1	D	139/154 (90%)	134 (96%)	5 (4%)	31	58
1	E	138/154 (90%)	133 (96%)	5 (4%)	31	58
1	F	139/154 (90%)	134 (96%)	5 (4%)	31	58
1	G	138/154 (90%)	133 (96%)	5 (4%)	31	58
1	H	136/154 (88%)	131 (96%)	5 (4%)	30	57
1	I	139/154 (90%)	138 (99%)	1 (1%)	76	89
1	J	138/154 (90%)	131 (95%)	7 (5%)	21	45
All	All	1380/1540 (90%)	1340 (97%)	40 (3%)	37	65

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	CYS
1	A	52	ASP
1	A	148	LEU
1	B	4	ASN
1	B	138	GLU
1	C	52	ASP
1	C	59	GLU
1	D	4	ASN
1	D	33	SER
1	D	48	THR
1	D	71	SER
1	D	124	VAL
1	E	17	ASN
1	E	46	CYS
1	E	71	SER
1	E	87	THR
1	E	113	ASP
1	F	4	ASN
1	F	46	CYS
1	F	48	THR
1	F	86	GLU
1	F	165	CYS
1	G	4	ASN

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Mol	Chain	Res	Type
1	G	46	CYS
1	G	58	GLU
1	G	71	SER
1	G	165	CYS
1	H	4	ASN
1	H	8	LYS
1	H	22	GLU
1	H	52	ASP
1	H	71	SER
1	I	31	ARG
1	J	43	THR
1	J	61	GLN
1	J	86	GLU
1	J	87	THR
1	J	127	GLN
1	J	163	GLU
1	J	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	82	HIS
1	A	109	ASN
1	B	4	ASN
1	B	17	ASN
1	B	82	HIS
1	B	109	ASN
1	B	127	GLN
1	B	160	HIS
1	C	12	ASN
1	C	109	ASN
1	C	155	GLN
1	D	13	GLN
1	D	109	ASN
1	D	131	GLN
1	E	82	HIS
1	E	109	ASN
1	F	109	ASN
1	G	12	ASN
1	G	56	HIS
1	G	61	GLN

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Mol	Chain	Res	Type
1	G	82	HIS
1	G	109	ASN
1	H	82	HIS
1	H	109	ASN
1	H	127	GLN
1	I	4	ASN
1	I	17	ASN
1	I	82	HIS
1	I	109	ASN
1	I	127	GLN
1	I	160	HIS
1	J	61	GLN
1	J	109	ASN
1	J	127	GLN
1	J	155	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is 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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	166/186 (89%)	-0.54	5 (3%)	52	47	18, 34, 65, 106	0
1	B	165/186 (88%)	-0.43	2 (1%)	76	73	18, 35, 62, 115	0
1	C	163/186 (87%)	-0.41	4 (2%)	58	52	21, 38, 65, 88	0
1	D	166/186 (89%)	-0.04	1 (0%)	85	83	30, 50, 73, 101	0
1	E	165/186 (88%)	0.26	4 (2%)	59	54	36, 59, 95, 141	0
1	F	166/186 (89%)	-0.61	4 (2%)	59	54	18, 32, 62, 119	0
1	G	165/186 (88%)	-0.54	3 (1%)	67	63	21, 35, 67, 115	0
1	H	163/186 (87%)	-0.42	5 (3%)	51	45	21, 40, 66, 99	0
1	I	166/186 (89%)	-0.49	2 (1%)	76	73	24, 37, 60, 99	0
1	J	165/186 (88%)	-0.08	4 (2%)	59	54	30, 48, 82, 121	0
All	All	1650/1860 (88%)	-0.33	34 (2%)	63	58	18, 41, 76, 141	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	166	PRO	7.5
1	A	166	PRO	5.7
1	A	164	VAL	5.7
1	G	165	CYS	4.4
1	E	164	VAL	4.2
1	J	164	VAL	3.8
1	D	166	PRO	3.7
1	B	165	CYS	3.7
1	I	166	PRO	3.6
1	H	162	GLY	3.3
1	J	165	CYS	3.2
1	G	164	VAL	3.0
1	C	162	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	161	PRO	2.9
1	B	164	VAL	2.9
1	A	44	PHE	2.8
1	H	163	GLU	2.8
1	C	163	GLU	2.7
1	A	165	CYS	2.6
1	F	164	VAL	2.6
1	H	161	PRO	2.5
1	A	46	CYS	2.5
1	E	45	VAL	2.5
1	H	1	SER	2.5
1	F	165	CYS	2.4
1	J	86	GLU	2.4
1	I	162	GLY	2.3
1	E	162	GLY	2.2
1	E	44	PHE	2.2
1	F	46	CYS	2.2
1	J	163	GLU	2.1
1	H	156	TYR	2.1
1	G	46	CYS	2.0
1	C	1	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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	NA	A	6001	1/1	0.79	0.29	14,14,14,14	1

6.5 Other polymers ⓘ

There are no such residues in this entry.