



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:31 PM GMT

PDB ID : 1TW9
Title : Glutathione Transferase-2, apo form, from the nematode Heligmosomoides polygyrus
Authors : Schuller, D.J.; Liu, Q.; Kriksunov, I.A.; Campbell, A.M.; Barrett, J.; Brophy, P.M.; Hao, Q.
Deposited on : 2004-06-30
Resolution : 1.71 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

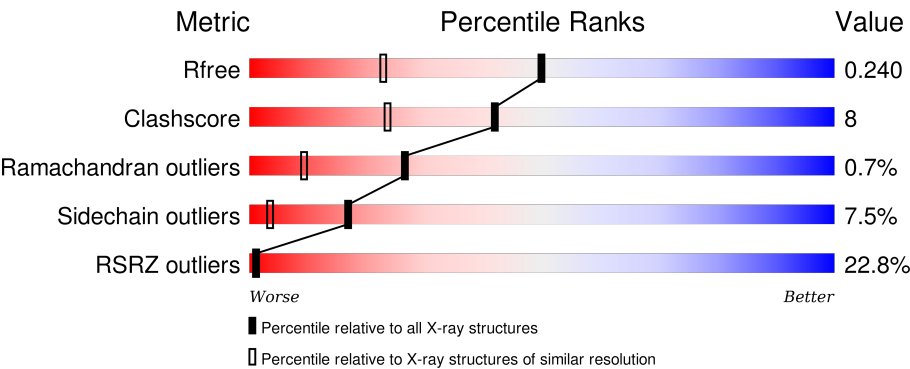
MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

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 1.71 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}	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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. 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	206	<div><div>18%</div><div><div></div><div>75%</div><div>16%</div><div>•</div><div>7%</div></div></div>
1	B	206	<div><div>18%</div><div><div></div><div>74%</div><div>13%</div><div>• •</div><div>9%</div></div></div>
1	C	206	<div><div>17%</div><div><div></div><div>80%</div><div>13%</div><div>•</div><div>6%</div></div></div>
1	D	206	<div><div>20%</div><div><div></div><div>77%</div><div>15%</div><div>• •</div><div>6%</div></div></div>
1	E	206	<div><div>24%</div><div><div></div><div>73%</div><div>17%</div><div>• •</div><div>6%</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	206	<div><div></div><div>30%</div><div></div><div>77%</div><div></div><div>18%</div><div></div><div></div></div>
1	G	206	<div><div></div><div>17%</div><div></div><div>75%</div><div></div><div>15%</div><div></div><div>8%</div></div>
1	H	206	<div><div></div><div>27%</div><div></div><div>71%</div><div></div><div>16%</div><div></div><div>5%</div><div>7%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14254 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 glutathione S-transferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	191	Total	C	N	O	S	0	0	0
			1531	989	256	280	6			
1	B	188	Total	C	N	O	S	0	0	0
			1507	974	252	275	6			
1	C	194	Total	C	N	O	S	0	0	0
			1563	1013	260	284	6			
1	D	194	Total	C	N	O	S	0	0	0
			1559	1008	260	285	6			
1	E	193	Total	C	N	O	S	0	0	0
			1542	997	257	282	6			
1	F	205	Total	C	N	O	S	0	0	0
			1645	1066	271	301	7			
1	G	189	Total	C	N	O	S	0	0	0
			1516	980	254	276	6			
1	H	191	Total	C	N	O	S	0	0	0
			1531	989	256	280	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	CLONING ARTIFACT	UNP Q9NJJQ6
A	2	VAL	-	CLONING ARTIFACT	UNP Q9NJJQ6
A	21	VAL	ILE	CONFLICT	UNP Q9NJJQ6
A	40	VAL	ALA	CONFLICT	UNP Q9NJJQ6
A	91	LEU	PRO	CONFLICT	UNP Q9NJJQ6
A	108	THR	MET	CONFLICT	UNP Q9NJJQ6
A	120	PRO	LEU	CONFLICT	UNP Q9NJJQ6
A	140	LEU	PRO	CONFLICT	UNP Q9NJJQ6
B	1	MET	-	CLONING ARTIFACT	UNP Q9NJJQ6
B	2	VAL	-	CLONING ARTIFACT	UNP Q9NJJQ6
B	21	VAL	ILE	CONFLICT	UNP Q9NJJQ6
B	40	VAL	ALA	CONFLICT	UNP Q9NJJQ6
B	91	LEU	PRO	CONFLICT	UNP Q9NJJQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	108	THR	MET	CONFLICT	UNP Q9NJJQ6
B	120	PRO	LEU	CONFLICT	UNP Q9NJJQ6
B	140	LEU	PRO	CONFLICT	UNP Q9NJJQ6
C	1	MET	-	CLONING ARTIFACT	UNP Q9NJJQ6
C	2	VAL	-	CLONING ARTIFACT	UNP Q9NJJQ6
C	21	VAL	ILE	CONFLICT	UNP Q9NJJQ6
C	40	VAL	ALA	CONFLICT	UNP Q9NJJQ6
C	91	LEU	PRO	CONFLICT	UNP Q9NJJQ6
C	108	THR	MET	CONFLICT	UNP Q9NJJQ6
C	120	PRO	LEU	CONFLICT	UNP Q9NJJQ6
C	140	LEU	PRO	CONFLICT	UNP Q9NJJQ6
D	1	MET	-	CLONING ARTIFACT	UNP Q9NJJQ6
D	2	VAL	-	CLONING ARTIFACT	UNP Q9NJJQ6
D	21	VAL	ILE	CONFLICT	UNP Q9NJJQ6
D	40	VAL	ALA	CONFLICT	UNP Q9NJJQ6
D	91	LEU	PRO	CONFLICT	UNP Q9NJJQ6
D	108	THR	MET	CONFLICT	UNP Q9NJJQ6
D	120	PRO	LEU	CONFLICT	UNP Q9NJJQ6
D	140	LEU	PRO	CONFLICT	UNP Q9NJJQ6
E	1	MET	-	CLONING ARTIFACT	UNP Q9NJJQ6
E	2	VAL	-	CLONING ARTIFACT	UNP Q9NJJQ6
E	21	VAL	ILE	CONFLICT	UNP Q9NJJQ6
E	40	VAL	ALA	CONFLICT	UNP Q9NJJQ6
E	91	LEU	PRO	CONFLICT	UNP Q9NJJQ6
E	108	THR	MET	CONFLICT	UNP Q9NJJQ6
E	120	PRO	LEU	CONFLICT	UNP Q9NJJQ6
E	140	LEU	PRO	CONFLICT	UNP Q9NJJQ6
F	1	MET	-	CLONING ARTIFACT	UNP Q9NJJQ6
F	2	VAL	-	CLONING ARTIFACT	UNP Q9NJJQ6
F	21	VAL	ILE	CONFLICT	UNP Q9NJJQ6
F	40	VAL	ALA	CONFLICT	UNP Q9NJJQ6
F	91	LEU	PRO	CONFLICT	UNP Q9NJJQ6
F	108	THR	MET	CONFLICT	UNP Q9NJJQ6
F	120	PRO	LEU	CONFLICT	UNP Q9NJJQ6
F	140	LEU	PRO	CONFLICT	UNP Q9NJJQ6
G	1	MET	-	CLONING ARTIFACT	UNP Q9NJJQ6
G	2	VAL	-	CLONING ARTIFACT	UNP Q9NJJQ6
G	21	VAL	ILE	CONFLICT	UNP Q9NJJQ6
G	40	VAL	ALA	CONFLICT	UNP Q9NJJQ6
G	91	LEU	PRO	CONFLICT	UNP Q9NJJQ6
G	108	THR	MET	CONFLICT	UNP Q9NJJQ6
G	120	PRO	LEU	CONFLICT	UNP Q9NJJQ6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	140	LEU	PRO	CONFLICT	UNP Q9NJJQ6
H	1	MET	-	CLONING ARTIFACT	UNP Q9NJJQ6
H	2	VAL	-	CLONING ARTIFACT	UNP Q9NJJQ6
H	21	VAL	ILE	CONFLICT	UNP Q9NJJQ6
H	40	VAL	ALA	CONFLICT	UNP Q9NJJQ6
H	91	LEU	PRO	CONFLICT	UNP Q9NJJQ6
H	108	THR	MET	CONFLICT	UNP Q9NJJQ6
H	120	PRO	LEU	CONFLICT	UNP Q9NJJQ6
H	140	LEU	PRO	CONFLICT	UNP Q9NJJQ6

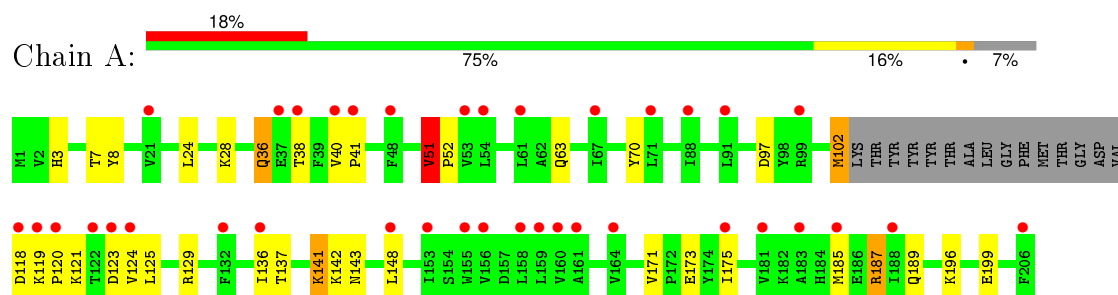
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	384	Total O 384 384	0	0
2	B	220	Total O 220 220	0	0
2	C	285	Total O 285 285	0	0
2	D	251	Total O 251 251	0	0
2	E	149	Total O 149 149	0	0
2	F	186	Total O 186 186	0	0
2	G	216	Total O 216 216	0	0
2	H	169	Total O 169 169	0	0

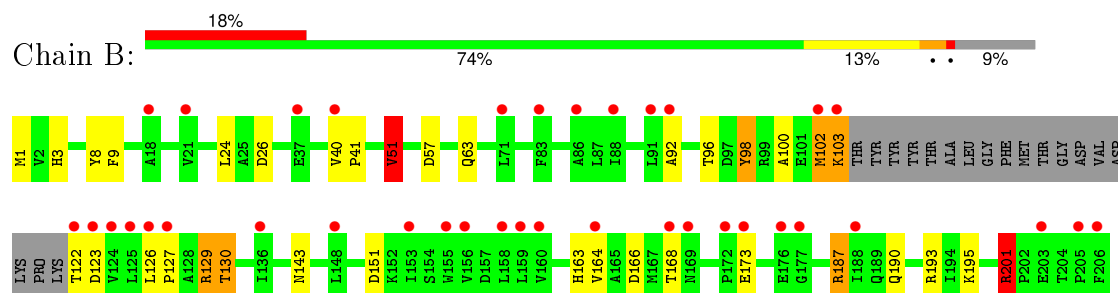
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

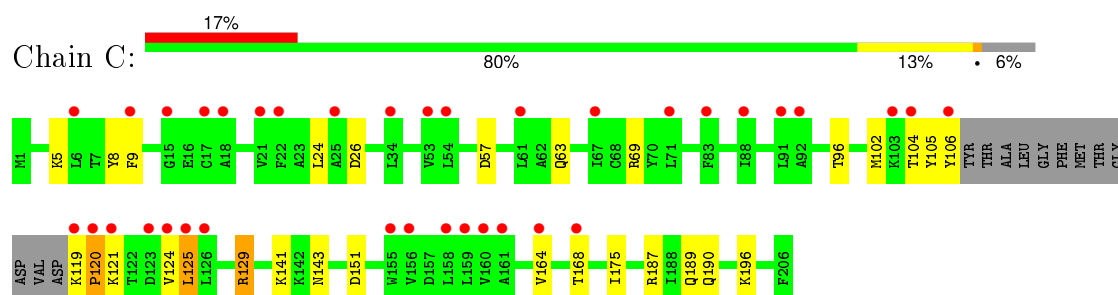
- Molecule 1: glutathione S-transferase 2



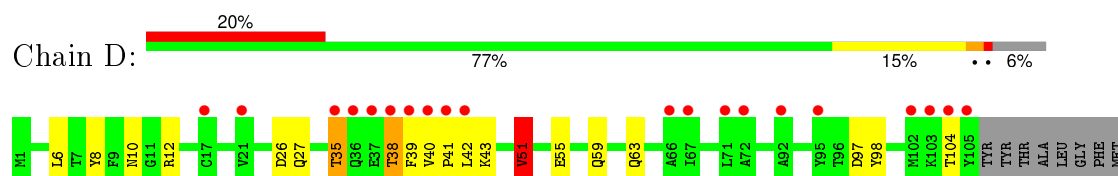
- Molecule 1: glutathione S-transferase 2

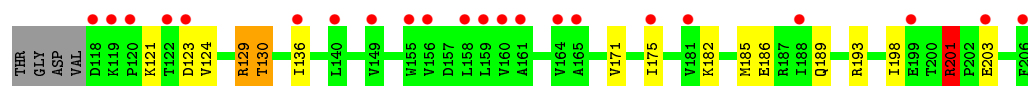


- Molecule 1: glutathione S-transferase 2



- Molecule 1: glutathione S-transferase 2

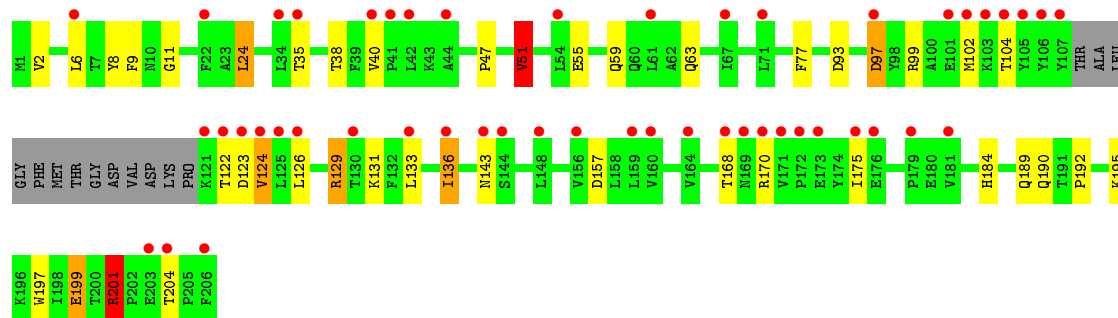




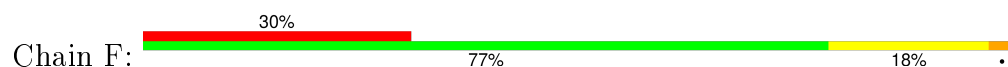
- Molecule 1: glutathione S-transferase 2



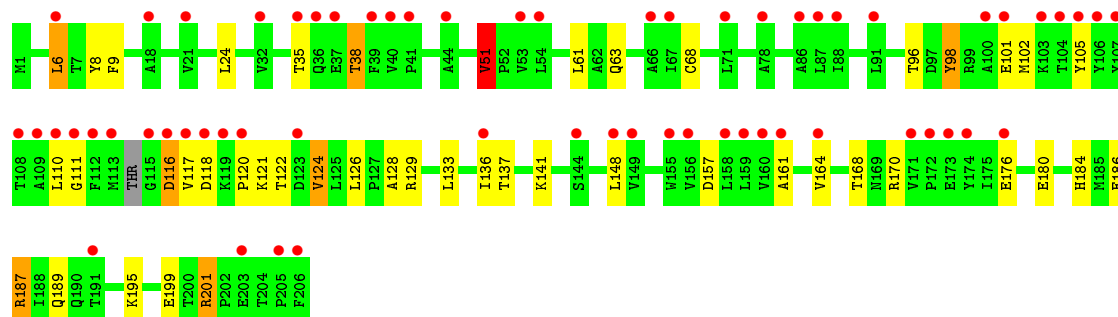
Chain E:



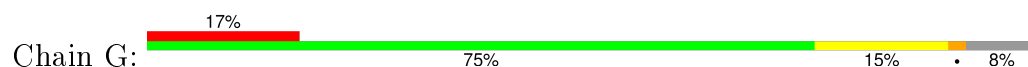
- Molecule 1: glutathione S-transferase 2



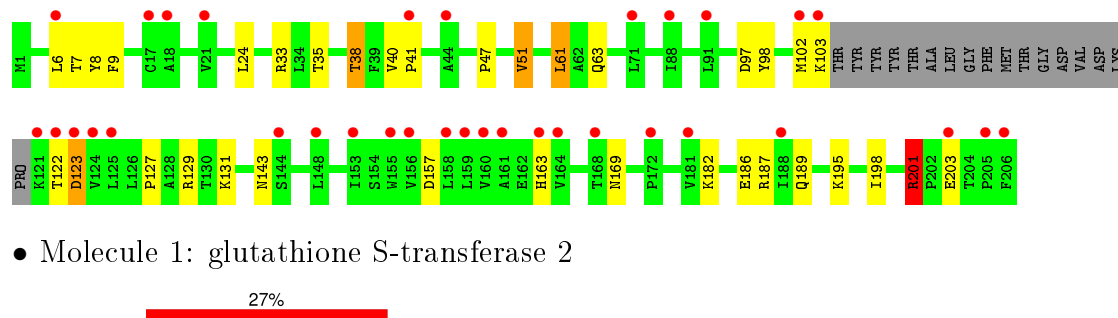
Chain F:



- Molecule 1: glutathione S-transferase 2



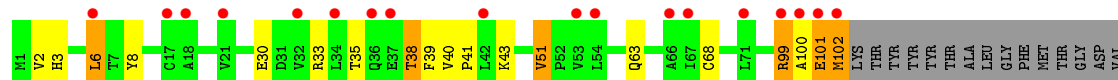
Chain G:

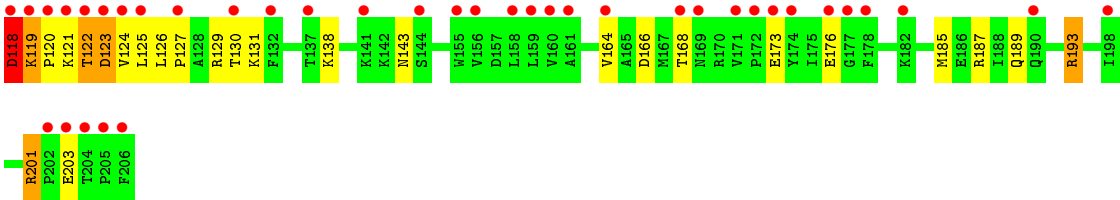


- Molecule 1: glutathione S-transferase 2



Chain H:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	72.68Å 74.03Å 88.57Å 79.09° 80.08° 81.55°	Depositor
Resolution (Å)	25.00 – 1.71 24.26 – 1.71	Depositor EDS
% Data completeness (in resolution range)	95.2 (25.00-1.71) 91.0 (24.26-1.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.71Å)	Xtriage
Refinement program	REFMAC 5.1.9999	Depositor
R, R_{free}	0.180 , 0.232 0.189 , 0.240	Depositor DCC
R_{free} test set	4565 reflections (2.55%)	DCC
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.9	EDS
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 184047 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14254	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.82% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	1.05	2/1568 (0.1%)	1.11	6/2120 (0.3%)
1	B	0.88	0/1543	1.00	8/2086 (0.4%)
1	C	0.96	0/1602	1.01	6/2166 (0.3%)
1	D	0.95	0/1597	0.99	5/2159 (0.2%)
1	E	0.94	2/1579 (0.1%)	0.98	8/2136 (0.4%)
1	F	0.97	2/1686 (0.1%)	1.04	6/2280 (0.3%)
1	G	0.88	0/1552	1.06	8/2097 (0.4%)
1	H	0.87	1/1568 (0.1%)	1.02	7/2120 (0.3%)
All	All	0.94	7/12695 (0.1%)	1.03	54/17164 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	199	GLU	CD-OE2	17.71	1.45	1.25
1	E	199	GLU	CD-OE1	8.35	1.34	1.25
1	H	68	CYS	CB-SG	-5.76	1.72	1.81
1	A	70	TYR	CD2-CE2	-5.55	1.31	1.39
1	A	70	TYR	CD1-CE1	-5.39	1.31	1.39
1	F	68	CYS	CB-SG	-5.06	1.73	1.81
1	F	161	ALA	CA-CB	5.01	1.62	1.52

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	201	ARG	NE-CZ-NH1	14.00	127.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	187	ARG	NE-CZ-NH1	13.65	127.13	120.30
1	B	201	ARG	NE-CZ-NH1	11.89	126.24	120.30
1	A	187	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	F	201	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	G	201	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	A	187	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	F	201	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	A	185	MET	CG-SD-CE	-9.25	85.40	100.20
1	C	187	ARG	NE-CZ-NH2	-9.03	115.79	120.30
1	A	51	VAL	CG1-CB-CG2	7.44	122.81	110.90
1	E	201	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	H	123	ASP	CB-CG-OD2	6.99	124.59	118.30
1	E	97	ASP	CB-CG-OD2	6.93	124.54	118.30
1	B	201	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	H	118	ASP	CB-CG-OD2	6.64	124.28	118.30
1	F	187	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	201	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	G	187	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	E	201	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	123	ASP	CB-CG-OD2	6.32	123.98	118.30
1	E	51	VAL	CG1-CB-CG2	6.24	120.88	110.90
1	B	51	VAL	CG1-CB-CG2	6.18	120.80	110.90
1	B	51	VAL	CB-CA-C	6.11	123.01	111.40
1	G	201	ARG	CD-NE-CZ	6.08	132.11	123.60
1	F	116	ASP	CB-CG-OD2	6.07	123.76	118.30
1	D	185	MET	CG-SD-CE	-6.03	90.55	100.20
1	D	123	ASP	CB-CG-OD2	5.91	123.62	118.30
1	F	6	LEU	CB-CG-CD2	5.77	120.81	111.00
1	B	151	ASP	CB-CG-OD2	5.62	123.36	118.30
1	F	51	VAL	CB-CA-C	5.61	122.06	111.40
1	C	69	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	26	ASP	CB-CG-OD1	5.56	123.30	118.30
1	G	97	ASP	CB-CG-OD2	5.53	123.28	118.30
1	G	61	LEU	CB-CG-CD2	5.50	120.34	111.00
1	H	6	LEU	CB-CG-CD2	5.48	120.32	111.00
1	B	187	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	129	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	H	201	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	G	157	ASP	CB-CG-OD1	5.39	123.16	118.30
1	A	51	VAL	CB-CA-C	5.36	121.58	111.40
1	E	51	VAL	N-CA-CB	-5.33	99.77	111.50
1	D	97	ASP	CB-CG-OD2	5.26	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	93	ASP	CB-CG-OD2	5.22	123.00	118.30
1	H	33	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	G	33	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	57	ASP	CB-CG-OD2	5.18	122.96	118.30
1	H	166	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	123	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	51	VAL	CB-CA-C	5.12	121.12	111.40
1	E	199	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	B	166	ASP	CB-CG-OD2	5.07	122.86	118.30
1	C	5	LYS	CD-CE-NZ	-5.05	100.07	111.70
1	H	193	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	102	MET	Peptide

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	1531	0	1527	26	0
1	B	1507	0	1503	27	0
1	C	1563	0	1561	20	0
1	D	1559	0	1556	28	0
1	E	1542	0	1527	29	0
1	F	1645	0	1634	36	1
1	G	1516	0	1516	16	0
1	H	1531	0	1527	27	0
2	A	384	0	0	12	1
2	B	220	0	0	10	0
2	C	285	0	0	8	0
2	D	251	0	0	8	1
2	E	149	0	0	11	1
2	F	186	0	0	8	0
2	G	216	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	169	0	0	4	0
All	All	14254	0	12351	207	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (207) 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:G:195:LYS:NZ	2:G:268:HOH:O	1.73	1.18
1:E:2:VAL:HB	2:E:1781:HOH:O	0.96	1.12
1:C:106:TYR:C	2:C:1685:HOH:O	1.88	1.10
1:B:96:THR:HG22	2:B:337:HOH:O	1.52	1.08
1:E:143:ASN:CG	2:E:1376:HOH:O	1.95	1.03
1:A:196:LYS:HD2	2:A:400:HOH:O	1.59	1.00
1:F:187:ARG:HB2	2:F:318:HOH:O	1.69	0.91
1:E:143:ASN:ND2	2:E:1376:HOH:O	2.02	0.90
1:D:186:GLU:OE2	2:D:220:HOH:O	1.95	0.83
1:B:190:GLN:HE22	1:B:195:LYS:HE2	1.44	0.82
1:B:193:ARG:NE	2:B:343:HOH:O	2.12	0.82
2:G:240:HOH:O	1:H:138:LYS:HE3	1.78	0.82
1:D:104:THR:HG21	2:D:426:HOH:O	1.79	0.81
1:F:176:GLU:OE1	2:F:351:HOH:O	1.97	0.81
1:E:40:VAL:HG23	2:E:1569:HOH:O	1.79	0.81
1:G:195:LYS:HD3	2:G:412:HOH:O	1.79	0.79
1:B:26:ASP:HB2	1:B:193:ARG:NH1	1.98	0.79
1:B:98:TYR:OH	1:B:163:HIS:HE1	1.66	0.79
1:A:38:THR:HG21	2:A:257:HOH:O	1.82	0.78
1:F:133:LEU:HA	1:F:136:ILE:HG22	1.64	0.78
1:E:47:PRO:O	2:E:1716:HOH:O	2.03	0.77
1:D:193:ARG:CZ	2:D:447:HOH:O	2.32	0.76
1:C:151:ASP:OD2	2:C:638:HOH:O	2.03	0.76
1:B:193:ARG:CZ	2:B:343:HOH:O	2.32	0.76
1:A:199:GLU:OE2	2:A:403:HOH:O	2.05	0.74
2:G:240:HOH:O	1:H:138:LYS:CE	2.33	0.74
1:F:116:ASP:OD1	1:F:118:ASP:HB2	1.88	0.73
1:D:182:LYS:NZ	1:D:186:GLU:OE1	2.22	0.72
1:H:164:VAL:HG12	1:H:185:MET:CE	2.20	0.72
1:E:97:ASP:HB2	2:E:1473:HOH:O	1.90	0.72
1:B:201:ARG:HD3	2:B:283:HOH:O	1.91	0.71
1:G:47:PRO:O	2:G:240:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:THR:HG21	2:B:251:HOH:O	1.89	0.71
1:F:164:VAL:O	1:F:168:THR:HG23	1.90	0.70
1:H:120:PRO:O	1:H:124:VAL:HG12	1.92	0.70
1:D:175:ILE:HG12	1:D:182:LYS:HB2	1.74	0.70
1:G:201:ARG:HD3	2:G:208:HOH:O	1.91	0.69
1:D:129:ARG:HH11	1:D:130:THR:HG22	1.57	0.69
1:D:10:ASN:OD1	2:D:405:HOH:O	2.10	0.68
1:C:164:VAL:O	1:C:168:THR:HG23	1.94	0.67
1:B:190:GLN:NE2	1:B:195:LYS:HE2	2.08	0.67
1:E:97:ASP:OD2	2:E:1486:HOH:O	2.12	0.67
1:D:193:ARG:NE	2:D:447:HOH:O	2.27	0.67
1:H:101:GLU:OE1	1:H:101:GLU:N	2.28	0.67
1:F:102:MET:HA	1:F:124:VAL:HG23	1.78	0.65
1:F:133:LEU:HA	1:F:136:ILE:CG2	2.27	0.65
1:H:3:HIS:HE1	1:H:30:GLU:OE2	1.78	0.65
1:H:164:VAL:O	1:H:168:THR:HG23	1.97	0.65
1:H:8:TYR:CD1	1:H:51:VAL:HG13	2.32	0.65
1:A:199:GLU:OE1	2:A:405:HOH:O	2.14	0.65
1:A:3:HIS:HD2	2:A:277:HOH:O	1.79	0.65
1:D:26:ASP:OD1	2:D:241:HOH:O	2.14	0.64
1:B:187:ARG:HD3	2:B:489:HOH:O	1.97	0.64
1:E:133:LEU:O	1:E:136:ILE:HG22	1.96	0.64
1:F:157:ASP:OD1	1:F:184:HIS:HE1	1.81	0.64
1:D:104:THR:HG23	1:D:104:THR:O	1.97	0.63
1:C:119:LYS:NZ	2:C:854:HOH:O	2.31	0.63
1:F:186:GLU:OE2	2:F:334:HOH:O	2.15	0.62
1:C:119:LYS:CE	2:H:893:HOH:O	2.47	0.62
1:H:35:THR:OG1	1:H:38:THR:HG23	2.00	0.61
1:E:195:LYS:O	1:E:199:GLU:HG3	2.01	0.61
1:A:97:ASP:OD2	2:A:263:HOH:O	2.16	0.61
1:D:8:TYR:CD1	1:D:51:VAL:HG13	2.36	0.61
1:E:157:ASP:OD1	1:E:184:HIS:HE1	1.84	0.61
1:F:133:LEU:CA	1:F:136:ILE:HG22	2.31	0.60
1:A:40:VAL:HB	1:A:41:PRO:HD3	1.83	0.60
1:D:26:ASP:HB2	1:D:193:ARG:NH1	2.16	0.60
1:D:38:THR:O	1:D:42:LEU:HD13	2.02	0.60
1:A:36:GLN:O	1:A:40:VAL:HG23	2.02	0.59
1:F:195:LYS:NZ	1:F:199:GLU:OE2	2.35	0.59
1:H:187:ARG:O	2:H:918:HOH:O	2.16	0.58
1:C:119:LYS:HE2	2:H:893:HOH:O	2.04	0.58
1:F:133:LEU:O	1:F:136:ILE:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:THR:HG22	1:E:38:THR:HG22	1.86	0.57
1:E:2:VAL:HG22	1:H:2:VAL:HB	1.85	0.57
1:F:133:LEU:C	1:F:136:ILE:HG22	2.25	0.57
1:E:143:ASN:CB	2:E:1376:HOH:O	2.46	0.57
1:D:121:LYS:HD2	1:D:171:VAL:HG13	1.86	0.56
1:E:104:THR:HG22	1:E:124:VAL:HG21	1.87	0.56
1:A:142:LYS:NZ	2:A:443:HOH:O	2.38	0.55
1:F:120:PRO:HA	1:F:124:VAL:HG13	1.88	0.55
1:H:173:GLU:HA	1:H:176:GLU:HG3	1.89	0.55
1:G:98:TYR:OH	1:G:163:HIS:HE1	1.90	0.54
1:F:96:THR:HG21	2:F:330:HOH:O	2.07	0.54
1:E:40:VAL:O	2:E:1564:HOH:O	2.19	0.53
1:F:35:THR:H	1:F:38:THR:CG2	2.21	0.53
1:H:127:PRO:O	1:H:130:THR:HG22	2.09	0.53
1:F:136:ILE:HD11	1:F:148:LEU:HD21	1.90	0.53
1:F:98:TYR:O	1:F:101:GLU:HG2	2.09	0.53
1:B:103:LYS:N	2:B:497:HOH:O	2.25	0.52
1:F:35:THR:OG1	1:F:38:THR:HG22	2.09	0.52
1:A:187:ARG:HD3	2:A:409:HOH:O	2.09	0.52
1:D:129:ARG:NH1	1:D:130:THR:HG22	2.23	0.52
1:F:102:MET:HA	1:F:124:VAL:CG2	2.40	0.52
1:H:125:LEU:C	1:H:125:LEU:HD13	2.29	0.52
1:B:126:LEU:HB2	1:B:127:PRO:HD3	1.92	0.51
1:E:126:LEU:O	1:E:129:ARG:HG3	2.11	0.51
1:F:136:ILE:HG23	1:F:137:THR:N	2.24	0.51
1:B:96:THR:HG21	2:B:361:HOH:O	2.10	0.50
1:B:8:TYR:CD1	1:B:51:VAL:HG13	2.46	0.50
1:H:8:TYR:HD1	1:H:51:VAL:HG13	1.75	0.50
1:C:120:PRO:HD2	2:C:1264:HOH:O	2.11	0.50
1:D:175:ILE:CG1	1:D:182:LYS:HB2	2.40	0.50
1:B:8:TYR:HA	1:B:51:VAL:HG13	1.94	0.50
1:E:197:TRP:O	1:E:201:ARG:HB3	2.11	0.49
1:A:8:TYR:CD1	1:A:51:VAL:HG13	2.47	0.49
1:B:126:LEU:O	1:B:129:ARG:HG3	2.13	0.49
1:H:164:VAL:HG12	1:H:185:MET:HE2	1.93	0.49
1:D:104:THR:HG22	2:D:431:HOH:O	2.11	0.49
1:C:104:THR:HG22	2:C:763:HOH:O	2.13	0.49
1:A:196:LYS:CD	2:A:400:HOH:O	2.38	0.48
1:F:120:PRO:CA	1:F:124:VAL:HG13	2.43	0.48
1:F:35:THR:H	1:F:38:THR:HG22	1.77	0.48
1:H:120:PRO:HA	1:H:124:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:THR:H	1:G:38:THR:CG2	2.26	0.48
1:F:184:HIS:HD2	2:F:328:HOH:O	1.96	0.48
1:D:40:VAL:HB	1:D:41:PRO:HD3	1.95	0.48
1:H:102:MET:HA	1:H:124:VAL:HG22	1.96	0.48
1:E:11:GLY:HA2	1:E:204:THR:HG21	1.96	0.48
1:B:98:TYR:OH	1:B:163:HIS:CE1	2.57	0.47
1:E:104:THR:CG2	1:E:124:VAL:HG21	2.45	0.47
1:F:187:ARG:O	2:F:289:HOH:O	2.21	0.47
1:D:198:ILE:HA	1:D:201:ARG:HD2	1.96	0.47
1:F:136:ILE:CD1	1:F:148:LEU:HD21	2.44	0.46
1:D:8:TYR:HD1	1:D:51:VAL:HG13	1.76	0.46
1:C:190:GLN:NE2	2:C:813:HOH:O	2.43	0.46
1:G:8:TYR:CD1	1:G:51:VAL:HG13	2.50	0.46
1:B:92:ALA:O	1:B:96:THR:HG23	2.14	0.46
1:F:8:TYR:CD1	1:F:51:VAL:HG13	2.50	0.46
1:D:12:ARG:HD2	1:D:201:ARG:NH2	2.29	0.46
1:H:39:PHE:CZ	1:H:43:LYS:HG2	2.50	0.46
1:G:35:THR:H	1:G:38:THR:HG22	1.80	0.46
1:A:136:ILE:HG23	1:A:148:LEU:HD21	1.98	0.46
1:A:102:MET:C	1:A:102:MET:SD	2.94	0.46
1:A:137:THR:HG22	1:A:141:LYS:HD2	1.98	0.46
1:D:55:GLU:HA	1:D:59:GLN:O	2.16	0.45
1:B:100:ALA:O	1:B:103:LYS:HB2	2.17	0.45
1:F:133:LEU:O	1:F:136:ILE:CG2	2.65	0.45
1:C:105:TYR:HB2	1:C:120:PRO:O	2.16	0.45
1:E:104:THR:CG2	1:E:124:VAL:HG11	2.47	0.45
1:E:8:TYR:CG	1:E:9:PHE:N	2.84	0.45
1:E:99:ARG:HD2	1:E:102:MET:SD	2.57	0.45
1:D:35:THR:CG2	1:D:38:THR:HG22	2.47	0.45
1:B:164:VAL:O	1:B:168:THR:HG23	2.17	0.45
1:F:101:GLU:HG3	1:F:128:ALA:CB	2.47	0.44
1:G:198:ILE:HA	1:G:201:ARG:HD2	1.99	0.44
1:F:105:TYR:C	1:F:105:TYR:CD1	2.90	0.44
1:B:193:ARG:NH2	2:B:343:HOH:O	2.48	0.44
1:D:35:THR:HG23	1:D:38:THR:HG22	1.98	0.44
1:A:36:GLN:NE2	1:A:36:GLN:O	2.51	0.43
1:E:55:GLU:HA	1:E:59:GLN:O	2.18	0.43
1:E:168:THR:HG22	1:E:175:ILE:HB	2.01	0.43
1:F:121:LYS:HE2	1:F:126:LEU:HD11	2.01	0.43
1:D:175:ILE:HG12	1:D:182:LYS:CB	2.47	0.43
1:C:196:LYS:HD3	2:C:1183:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:THR:HA	1:H:126:LEU:HD12	2.00	0.43
1:C:96:THR:HG21	2:C:613:HOH:O	2.17	0.43
1:F:121:LYS:CE	1:F:126:LEU:HD11	2.49	0.42
1:E:40:VAL:CG2	2:E:1569:HOH:O	2.51	0.42
1:C:105:TYR:CD1	1:C:120:PRO:O	2.72	0.42
1:E:170:ARG:HB3	2:E:1730:HOH:O	2.19	0.42
1:G:40:VAL:HB	1:G:41:PRO:HD3	2.00	0.42
1:H:127:PRO:HA	1:H:130:THR:HG22	2.00	0.42
1:F:8:TYR:CG	1:F:9:PHE:N	2.87	0.42
1:A:141:LYS:CE	2:A:447:HOH:O	2.66	0.42
1:G:103:LYS:NZ	2:G:422:HOH:O	2.52	0.42
1:H:99:ARG:O	1:H:101:GLU:N	2.53	0.42
1:G:123:ASP:O	1:G:127:PRO:HG2	2.18	0.42
1:E:8:TYR:CD1	1:E:51:VAL:HG13	2.54	0.42
1:H:101:GLU:CD	1:H:101:GLU:N	2.73	0.42
1:C:105:TYR:HD1	1:C:120:PRO:O	2.02	0.42
1:F:141:LYS:HD2	2:F:348:HOH:O	2.19	0.42
1:H:119:LYS:HE2	1:H:123:ASP:HB2	2.01	0.42
1:H:118:ASP:O	1:H:121:LYS:HB3	2.19	0.42
1:A:121:LYS:NZ	1:A:173:GLU:OE1	2.53	0.42
1:A:7:THR:O	1:A:52:PRO:HA	2.20	0.41
1:E:35:THR:H	1:E:38:THR:HG22	1.85	0.41
1:G:8:TYR:CG	1:G:9:PHE:N	2.89	0.41
1:D:39:PHE:CE2	1:D:43:LYS:HG3	2.55	0.41
1:G:182:LYS:NZ	1:G:186:GLU:OE2	2.50	0.41
1:A:119:LYS:HB3	1:A:120:PRO:CD	2.50	0.41
1:B:1:MET:HA	1:C:57:ASP:OD1	2.20	0.41
1:B:40:VAL:N	1:B:41:PRO:CD	2.84	0.41
1:F:110:LEU:HD11	1:F:170:ARG:HH22	1.86	0.41
1:A:8:TYR:HD1	1:A:51:VAL:HG13	1.86	0.41
1:G:7:THR:O	1:G:51:VAL:HG22	2.21	0.41
1:A:119:LYS:HB3	1:A:120:PRO:HD3	2.02	0.41
1:B:3:HIS:HD2	2:B:403:HOH:O	2.02	0.41
1:H:40:VAL:N	1:H:41:PRO:HD2	2.35	0.41
1:C:8:TYR:CG	1:C:9:PHE:N	2.89	0.41
1:E:24:LEU:HD13	1:E:77:PHE:CE2	2.55	0.41
1:F:187:ARG:HD3	2:F:299:HOH:O	2.20	0.41
1:B:98:TYR:CE2	1:B:163:HIS:CE1	3.09	0.41
1:C:119:LYS:N	1:C:120:PRO:CD	2.84	0.41
1:A:121:LYS:HE2	1:A:171:VAL:HG13	2.03	0.41
1:B:8:TYR:CG	1:B:9:PHE:N	2.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:163:HIS:HD2	2:G:390:HOH:O	2.03	0.40
1:B:8:TYR:HD1	1:B:51:VAL:HG13	1.85	0.40
1:A:141:LYS:NZ	2:A:447:HOH:O	2.17	0.40
1:A:175:ILE:HD12	1:A:175:ILE:HA	1.78	0.40
1:D:129:ARG:HD2	1:D:130:THR:N	2.37	0.40
1:H:120:PRO:HD2	2:H:754:HOH:O	2.19	0.40
1:C:105:TYR:CD2	1:C:125:LEU:HG	2.56	0.40
1:A:118:ASP:N	2:A:427:HOH:O	2.53	0.40
1:C:104:THR:HG23	1:C:124:VAL:HG11	2.03	0.40
1:C:175:ILE:HD12	1:C:175:ILE:HA	1.96	0.40
1:D:27:GLN:NE2	2:D:389:HOH:O	2.53	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:240:HOH:O	2:E:1566:HOH:O[1_444]	1.76	0.44
1:F:180:GLU:OE1	2:D:367:HOH:O[1_665]	2.07	0.13

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	187/206 (91%)	184 (98%)	2 (1%)	1 (0%)	34	15
1	B	184/206 (89%)	180 (98%)	3 (2%)	1 (0%)	34	15
1	C	190/206 (92%)	186 (98%)	2 (1%)	2 (1%)	17	4
1	D	190/206 (92%)	187 (98%)	2 (1%)	1 (0%)	34	15
1	E	189/206 (92%)	185 (98%)	3 (2%)	1 (0%)	34	15
1	F	201/206 (98%)	197 (98%)	2 (1%)	2 (1%)	19	5
1	G	185/206 (90%)	181 (98%)	3 (2%)	1 (0%)	34	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	187/206 (91%)	180 (96%)	5 (3%)	2 (1%)	17	4
All	All	1513/1648 (92%)	1480 (98%)	22 (2%)	11 (1%)	26	9

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	111	GLY
1	H	63	GLN
1	B	63	GLN
1	C	63	GLN
1	E	63	GLN
1	F	63	GLN
1	D	63	GLN
1	G	63	GLN
1	H	100	ALA
1	A	63	GLN
1	C	120	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	162/174 (93%)	151 (93%)	11 (7%)	20	4
1	B	159/174 (91%)	147 (92%)	12 (8%)	17	3
1	C	165/174 (95%)	157 (95%)	8 (5%)	31	11
1	D	165/174 (95%)	153 (93%)	12 (7%)	17	4
1	E	161/174 (92%)	149 (92%)	12 (8%)	17	3
1	F	173/174 (99%)	161 (93%)	12 (7%)	19	4
1	G	160/174 (92%)	145 (91%)	15 (9%)	11	2
1	H	162/174 (93%)	146 (90%)	16 (10%)	10	2
All	All	1307/1392 (94%)	1209 (92%)	98 (8%)	17	3

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	28	LYS
1	A	36	GLN
1	A	51	VAL
1	A	102	MET
1	A	124	VAL
1	A	125	LEU
1	A	129	ARG
1	A	141	LYS
1	A	143	ASN
1	A	189	GLN
1	B	24	LEU
1	B	51	VAL
1	B	98	TYR
1	B	102	MET
1	B	103	LYS
1	B	122	THR
1	B	123	ASP
1	B	129	ARG
1	B	130	THR
1	B	143	ASN
1	B	173	GLU
1	B	201	ARG
1	C	24	LEU
1	C	102	MET
1	C	121	LYS
1	C	125	LEU
1	C	129	ARG
1	C	141	LYS
1	C	143	ASN
1	C	189	GLN
1	D	6	LEU
1	D	35	THR
1	D	38	THR
1	D	51	VAL
1	D	98	TYR
1	D	124	VAL
1	D	129	ARG
1	D	130	THR
1	D	136	ILE
1	D	189	GLN
1	D	201	ARG
1	D	203	GLU

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Mol	Chain	Res	Type
1	E	6	LEU
1	E	24	LEU
1	E	51	VAL
1	E	122	THR
1	E	124	VAL
1	E	129	ARG
1	E	131	LYS
1	E	136	ILE
1	E	189	GLN
1	E	190	GLN
1	E	192	PRO
1	E	201	ARG
1	F	6	LEU
1	F	24	LEU
1	F	38	THR
1	F	51	VAL
1	F	61	LEU
1	F	98	TYR
1	F	117	VAL
1	F	122	THR
1	F	124	VAL
1	F	129	ARG
1	F	189	GLN
1	F	201	ARG
1	G	6	LEU
1	G	24	LEU
1	G	38	THR
1	G	51	VAL
1	G	61	LEU
1	G	102	MET
1	G	122	THR
1	G	123	ASP
1	G	129	ARG
1	G	131	LYS
1	G	143	ASN
1	G	169	ASN
1	G	189	GLN
1	G	201	ARG
1	G	203	GLU
1	H	6	LEU
1	H	38	THR
1	H	51	VAL

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Mol	Chain	Res	Type
1	H	99	ARG
1	H	101	GLU
1	H	102	MET
1	H	118	ASP
1	H	119	LYS
1	H	122	THR
1	H	129	ARG
1	H	131	LYS
1	H	143	ASN
1	H	189	GLN
1	H	193	ARG
1	H	201	ARG
1	H	203	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	36	GLN
1	A	63	GLN
1	A	143	ASN
1	A	190	GLN
1	B	3	HIS
1	B	63	GLN
1	B	143	ASN
1	B	163	HIS
1	B	190	GLN
1	C	143	ASN
1	D	27	GLN
1	D	63	GLN
1	D	190	GLN
1	E	63	GLN
1	E	184	HIS
1	E	190	GLN
1	F	63	GLN
1	F	184	HIS
1	G	63	GLN
1	G	143	ASN
1	G	163	HIS
1	H	3	HIS
1	H	27	GLN
1	H	143	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/206 (92%)	1.14	37 (19%) 1 1	29, 33, 37, 41	0
1	B	188/206 (91%)	1.22	37 (19%) 1 1	28, 33, 39, 42	0
1	C	194/206 (94%)	1.16	36 (18%) 2 2	29, 33, 38, 40	0
1	D	194/206 (94%)	1.25	42 (21%) 1 1	29, 33, 39, 43	0
1	E	193/206 (93%)	1.47	49 (25%) 1 1	29, 34, 39, 41	0
1	F	205/206 (99%)	1.44	61 (29%) 1 1	29, 33, 39, 43	0
1	G	189/206 (91%)	1.23	34 (17%) 2 2	29, 33, 38, 41	0
1	H	191/206 (92%)	1.45	56 (29%) 1 1	29, 34, 38, 41	0
All	All	1545/1648 (93%)	1.30	352 (22%) 1 1	28, 33, 39, 43	0

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	107	TYR	12.1
1	C	120	PRO	9.9
1	B	124	VAL	8.0
1	F	112	PHE	7.8
1	D	206	PHE	7.5
1	D	40	VAL	7.5
1	F	111	GLY	7.1
1	E	106	TYR	6.7
1	B	122	THR	6.6
1	G	124	VAL	6.6
1	G	160	VAL	6.4
1	F	104	THR	6.1
1	E	104	THR	6.0
1	A	160	VAL	6.0
1	C	160	VAL	6.0
1	A	120	PRO	5.9

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Mol	Chain	Res	Type	RSRZ
1	G	103	LYS	5.9
1	D	120	PRO	5.9
1	E	105	TYR	5.9
1	D	38	THR	5.9
1	D	118	ASP	5.8
1	H	160	VAL	5.7
1	H	118	ASP	5.7
1	F	109	ALA	5.5
1	F	206	PHE	5.4
1	H	206	PHE	5.4
1	H	120	PRO	5.4
1	B	125	LEU	5.4
1	H	158	LEU	5.3
1	D	119	LYS	5.3
1	G	164	VAL	5.3
1	E	203	GLU	5.3
1	F	113	MET	5.2
1	B	123	ASP	5.2
1	E	107	TYR	5.1
1	G	205	PRO	5.1
1	H	159	LEU	5.1
1	C	124	VAL	5.0
1	E	172	PRO	5.0
1	A	158	LEU	4.9
1	B	40	VAL	4.9
1	D	105	TYR	4.9
1	E	173	GLU	4.9
1	B	126	LEU	4.8
1	F	106	TYR	4.8
1	G	159	LEU	4.8
1	E	103	LYS	4.8
1	D	41	PRO	4.8
1	G	123	ASP	4.7
1	E	159	LEU	4.7
1	F	110	LEU	4.7
1	D	35	THR	4.7
1	C	159	LEU	4.7
1	B	127	PRO	4.6
1	F	117	VAL	4.6
1	E	169	ASN	4.5
1	H	161	ALA	4.4
1	B	159	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	164	VAL	4.4
1	B	160	VAL	4.3
1	F	161	ALA	4.3
1	F	159	LEU	4.2
1	E	160	VAL	4.2
1	D	104	THR	4.2
1	D	164	VAL	4.2
1	A	188	ILE	4.2
1	C	106	TYR	4.2
1	G	122	THR	4.2
1	H	177	GLY	4.2
1	A	122	THR	4.2
1	F	123	ASP	4.2
1	A	164	VAL	4.1
1	G	206	PHE	4.1
1	E	122	THR	4.1
1	E	176	GLU	4.1
1	F	172	PRO	4.1
1	G	156	VAL	4.1
1	F	118	ASP	4.1
1	D	67	ILE	4.1
1	H	127	PRO	4.0
1	B	158	LEU	4.0
1	G	203	GLU	4.0
1	F	115	GLY	3.9
1	H	155	TRP	3.9
1	A	67	ILE	3.9
1	D	39	PHE	3.9
1	H	171	VAL	3.8
1	G	161	ALA	3.8
1	E	168	THR	3.8
1	E	125	LEU	3.8
1	A	175	ILE	3.8
1	G	158	LEU	3.8
1	E	6	LEU	3.7
1	G	41	PRO	3.7
1	G	125	LEU	3.7
1	A	41	PRO	3.7
1	C	161	ALA	3.6
1	D	160	VAL	3.6
1	B	103	LYS	3.6
1	E	136	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	118	ASP	3.5
1	F	103	LYS	3.5
1	D	159	LEU	3.5
1	E	35	THR	3.5
1	C	21	VAL	3.5
1	E	121	LYS	3.5
1	A	181	VAL	3.5
1	C	126	LEU	3.5
1	H	21	VAL	3.5
1	C	71	LEU	3.4
1	D	103	LYS	3.4
1	D	37	GLU	3.4
1	A	119	LYS	3.4
1	H	101	GLU	3.4
1	E	97	ASP	3.3
1	E	123	ASP	3.3
1	E	144	SER	3.3
1	H	172	PRO	3.3
1	F	116	ASP	3.3
1	A	159	LEU	3.3
1	C	6	LEU	3.3
1	D	71	LEU	3.3
1	G	102	MET	3.3
1	H	102	MET	3.3
1	F	164	VAL	3.3
1	G	144	SER	3.3
1	H	205	PRO	3.3
1	C	119	LYS	3.3
1	B	37	GLU	3.2
1	A	71	LEU	3.2
1	C	158	LEU	3.2
1	D	203	GLU	3.2
1	A	54	LEU	3.2
1	C	104	THR	3.2
1	H	119	LYS	3.2
1	F	160	VAL	3.2
1	A	61	LEU	3.2
1	A	123	ASP	3.2
1	E	126	LEU	3.2
1	H	198	ILE	3.2
1	F	156	VAL	3.1
1	E	42	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	6	LEU	3.1
1	B	71	LEU	3.1
1	C	168	THR	3.1
1	D	21	VAL	3.1
1	E	71	LEU	3.1
1	G	71	LEU	3.1
1	F	205	PRO	3.0
1	E	156	VAL	3.0
1	H	124	VAL	3.0
1	H	144	SER	3.0
1	G	155	TRP	3.0
1	D	122	THR	3.0
1	C	67	ILE	3.0
1	D	181	VAL	3.0
1	E	206	PHE	3.0
1	B	91	LEU	3.0
1	B	168	THR	3.0
1	H	173	GLU	3.0
1	B	164	VAL	3.0
1	F	91	LEU	3.0
1	D	123	ASP	3.0
1	F	86	ALA	3.0
1	F	119	LYS	3.0
1	C	22	PHE	3.0
1	H	132	PHE	3.0
1	C	54	LEU	2.9
1	C	125	LEU	2.9
1	E	170	ARG	2.9
1	A	136	ILE	2.9
1	H	37	GLU	2.9
1	C	164	VAL	2.9
1	F	40	VAL	2.9
1	H	169	ASN	2.9
1	C	121	LYS	2.9
1	D	158	LEU	2.9
1	B	173	GLU	2.9
1	C	18	ALA	2.9
1	A	21	VAL	2.9
1	C	53	VAL	2.9
1	C	17	CYS	2.8
1	H	182	LYS	2.8
1	B	156	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	124	VAL	2.8
1	B	155	TRP	2.8
1	H	204	THR	2.8
1	B	136	ILE	2.8
1	F	88	ILE	2.8
1	E	61	LEU	2.8
1	H	125	LEU	2.8
1	F	171	VAL	2.8
1	F	136	ILE	2.8
1	H	99	ARG	2.8
1	F	71	LEU	2.8
1	H	54	LEU	2.8
1	C	155	TRP	2.8
1	H	164	VAL	2.8
1	E	34	LEU	2.7
1	E	148	LEU	2.7
1	B	203	GLU	2.7
1	E	41	PRO	2.7
1	G	6	LEU	2.7
1	G	44	ALA	2.7
1	H	122	THR	2.7
1	E	181	VAL	2.7
1	G	21	VAL	2.7
1	G	188	ILE	2.7
1	B	148	LEU	2.7
1	D	36	GLN	2.7
1	D	161	ALA	2.7
1	A	148	LEU	2.7
1	G	18	ALA	2.7
1	H	17	CYS	2.6
1	H	130	THR	2.6
1	B	18	ALA	2.6
1	C	15	GLY	2.6
1	A	38	THR	2.6
1	D	175	ILE	2.6
1	F	158	LEU	2.6
1	G	148	LEU	2.6
1	F	176	GLU	2.6
1	G	168	THR	2.6
1	H	202	PRO	2.6
1	E	40	VAL	2.6
1	D	42	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	36	GLN	2.5
1	F	108	THR	2.5
1	B	92	ALA	2.5
1	E	102	MET	2.5
1	E	204	THR	2.5
1	E	44	ALA	2.5
1	H	18	ALA	2.5
1	A	156	VAL	2.5
1	C	156	VAL	2.5
1	H	190	GLN	2.5
1	D	155	TRP	2.5
1	D	188	ILE	2.5
1	H	71	LEU	2.5
1	F	41	PRO	2.5
1	F	101	GLU	2.5
1	A	40	VAL	2.5
1	A	124	VAL	2.5
1	G	181	VAL	2.5
1	F	35	THR	2.5
1	A	91	LEU	2.5
1	D	136	ILE	2.5
1	E	175	ILE	2.5
1	E	130	THR	2.4
1	E	143	ASN	2.4
1	H	137	THR	2.4
1	A	161	ALA	2.4
1	B	86	ALA	2.4
1	H	176	GLU	2.4
1	H	203	GLU	2.4
1	F	149	VAL	2.4
1	H	32	VAL	2.4
1	B	102	MET	2.4
1	C	91	LEU	2.4
1	E	67	ILE	2.4
1	F	87	LEU	2.4
1	B	206	PHE	2.4
1	A	183	ALA	2.4
1	H	100	ALA	2.4
1	B	205	PRO	2.4
1	G	17	CYS	2.3
1	H	174	TYR	2.3
1	A	48	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	39	PHE	2.3
1	H	53	VAL	2.3
1	H	121	LYS	2.3
1	F	148	LEU	2.3
1	G	91	LEU	2.3
1	B	88	ILE	2.3
1	D	199	GLU	2.3
1	F	37	GLU	2.3
1	G	88	ILE	2.3
1	B	21	VAL	2.3
1	F	21	VAL	2.3
1	F	155	TRP	2.3
1	A	153	ILE	2.3
1	B	172	PRO	2.3
1	C	92	ALA	2.3
1	F	44	ALA	2.3
1	H	123	ASP	2.3
1	A	185	MET	2.3
1	C	123	ASP	2.3
1	C	88	ILE	2.3
1	D	149	VAL	2.3
1	F	53	VAL	2.3
1	G	121	LYS	2.2
1	D	66	ALA	2.2
1	E	54	LEU	2.2
1	F	54	LEU	2.2
1	A	155	TRP	2.2
1	D	102	MET	2.2
1	F	120	PRO	2.2
1	A	37	GLU	2.2
1	C	103	LYS	2.2
1	D	72	ALA	2.2
1	F	191	THR	2.2
1	B	188	ILE	2.2
1	A	206	PHE	2.2
1	B	83	PHE	2.2
1	E	179	PRO	2.2
1	C	34	LEU	2.1
1	D	17	CYS	2.1
1	H	36	GLN	2.1
1	F	78	ALA	2.1
1	D	156	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	141	LYS	2.1
1	H	156	VAL	2.1
1	C	83	PHE	2.1
1	E	22	PHE	2.1
1	H	34	LEU	2.1
1	F	18	ALA	2.1
1	H	66	ALA	2.1
1	F	144	SER	2.1
1	B	176	GLU	2.1
1	F	105	TYR	2.1
1	G	163	HIS	2.1
1	A	132	PHE	2.1
1	C	61	LEU	2.1
1	F	6	LEU	2.1
1	G	153	ILE	2.1
1	A	99	ARG	2.1
1	D	92	ALA	2.1
1	E	133	LEU	2.1
1	E	101	GLU	2.1
1	A	88	ILE	2.1
1	F	67	ILE	2.1
1	E	171	VAL	2.0
1	B	169	ASN	2.0
1	D	95	TYR	2.0
1	F	174	TYR	2.0
1	C	25	ALA	2.0
1	D	165	ALA	2.0
1	F	100	ALA	2.0
1	F	203	GLU	2.0
1	H	178	PHE	2.0
1	H	42	LEU	2.0
1	B	153	ILE	2.0
1	H	67	ILE	2.0
1	A	53	VAL	2.0
1	F	32	VAL	2.0
1	B	177	GLY	2.0
1	F	66	ALA	2.0
1	F	173	GLU	2.0
1	C	9	PHE	2.0
1	D	140	LEU	2.0
1	G	172	PRO	2.0
1	H	168	THR	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 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.