



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 02:01 AM UTC

PDB ID : 1TW9 / pdb_00001tw9
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 wwPDB X-ray Structure Validation Summary 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

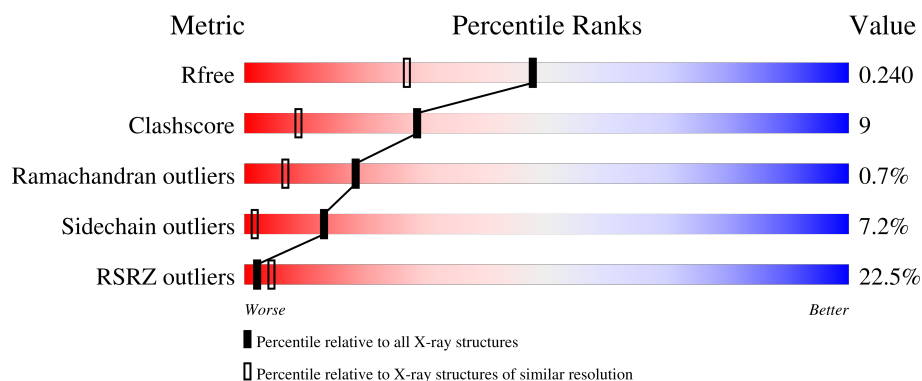
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	206	10% 76% 15% • 7%
1	B	206	25% 75% 13% • 9%
1	C	206	18% 82% 11% • 6%
1	D	206	20% 75% 16% •• 6%
1	E	206	25% 71% 18% • 6%

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Mol	Chain	Length	Quality of chain
1	F	206	21% 74% 24%
1	G	206	16% 77% 13% 8%
1	H	206	34% 71% 16% 5% 7%

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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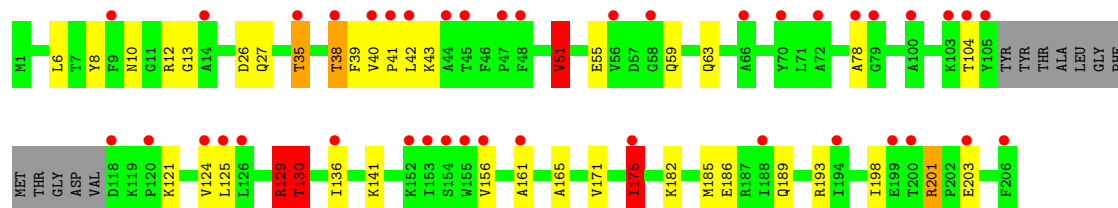
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Chain	Residue	Modelled	Actual	Comment	Reference
G	140	LEU	PRO	conflict	UNP Q9NJJQ6
H	1	MET	-	cloning artifact	UNP Q9NJJQ6
H	2	VAL	-	cloning artifact	UNP Q9NJJQ6
H	21	VAL	ILE	conflict	UNP Q9NJJQ6
H	40	VAL	ALA	conflict	UNP Q9NJJQ6
H	91	LEU	PRO	conflict	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.

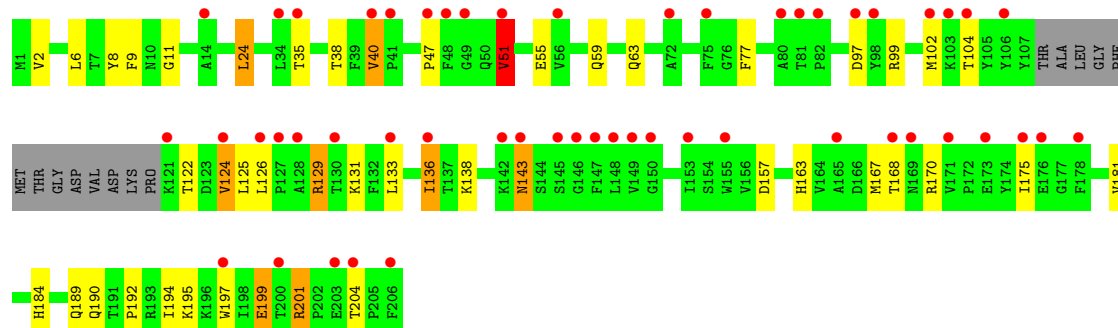
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	384	Total O 384 384	0	0
2	B	220	Total O 220 220	0	0
2	C	285	Total O 285 285	0	0
2	D	251	Total O 251 251	0	0
2	E	149	Total O 149 149	0	0
2	F	186	Total O 186 186	0	0
2	G	216	Total O 216 216	0	0
2	H	169	Total O 169 169	0	0

Chain D: 



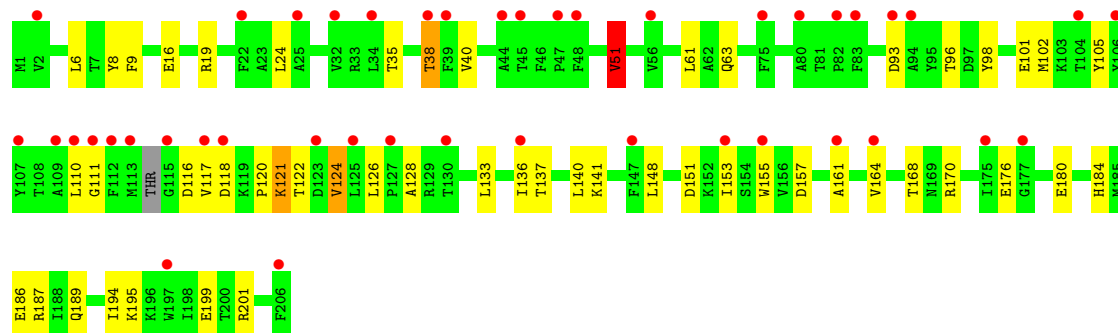
• Molecule 1: glutathione S-transferase 2

Chain E: 



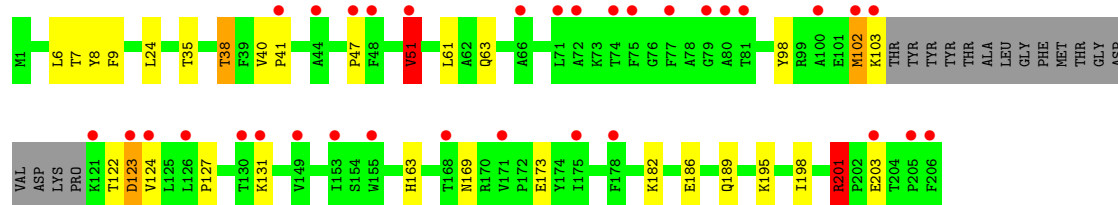
• Molecule 1: glutathione S-transferase 2

Chain F: 

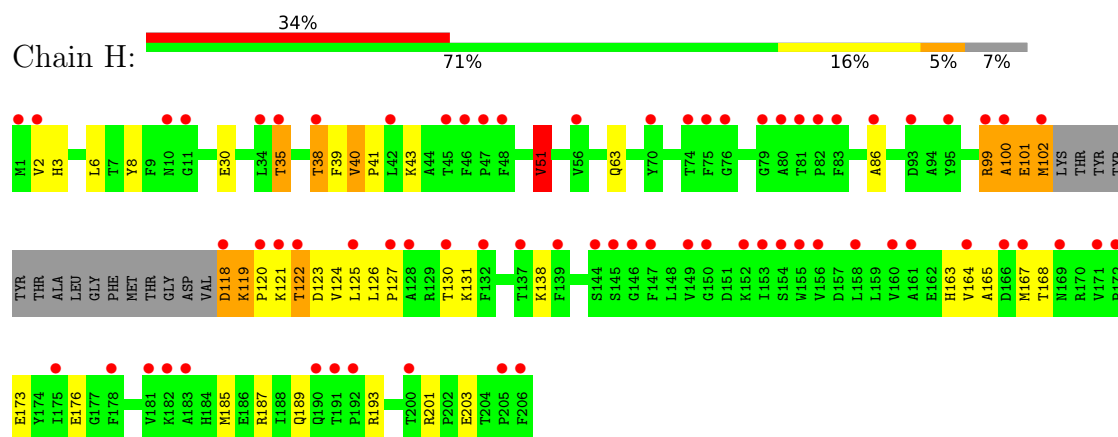


• Molecule 1: glutathione S-transferase 2

Chain G: 



• Molecule 1: glutathione S-transferase 2



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 25.00 – 1.71	Depositor EDS
% Data completeness (in resolution range)	95.2 (25.00-1.71) 95.8 (25.00-1.71)	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	4568 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	1.24	1/1568 (0.1%)	1.14	4/2120 (0.2%)
1	B	1.11	1/1543 (0.1%)	1.06	4/2086 (0.2%)
1	C	1.18	3/1602 (0.2%)	1.05	1/2166 (0.0%)
1	D	1.17	4/1597 (0.3%)	1.12	6/2159 (0.3%)
1	E	1.07	2/1579 (0.1%)	1.10	4/2136 (0.2%)
1	F	1.17	4/1686 (0.2%)	1.16	8/2280 (0.4%)
1	G	1.11	1/1552 (0.1%)	1.09	3/2097 (0.1%)
1	H	1.10	2/1568 (0.1%)	1.13	2/2120 (0.1%)
All	All	1.15	18/12695 (0.1%)	1.11	32/17164 (0.2%)

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

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	199	GLU	CD-OE2	10.41	1.45	1.25
1	H	40	VAL	CA-CB	6.96	1.57	1.54
1	A	78	ALA	CA-CB	-6.76	1.43	1.53
1	C	18	ALA	CA-CB	-6.50	1.43	1.53
1	F	161	ALA	CA-CB	6.20	1.62	1.53

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	51	VAL	N-CA-CB	-8.18	99.77	111.21
1	F	51	VAL	N-CA-CB	-7.13	101.22	111.21
1	A	51	VAL	N-CA-CB	-7.07	101.32	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	MET	CG-SD-CE	-7.05	85.40	100.90
1	D	175	ILE	N-CA-C	6.49	120.26	112.80

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	19	0
1	D	1559	0	1556	31	0
1	E	1542	0	1527	30	0
1	F	1645	0	1634	36	1
1	G	1516	0	1516	17	0
1	H	1531	0	1527	33	0
2	A	384	0	0	12	1
2	B	220	0	0	10	0
2	C	285	0	0	7	0
2	D	251	0	0	9	1
2	E	149	0	0	11	1
2	F	186	0	0	8	0
2	G	216	0	0	8	0
2	H	169	0	0	5	0
All	All	14254	0	12351	217	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 9.

The worst 5 of 217 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:C:106:TYR:C	2:C:1685:HOH:O	1.88	1.14
1:E:2:VAL:HB	2:E:1781:HOH:O	0.96	1.12
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	1.07

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%)	24	11
1	B	184/206 (89%)	180 (98%)	3 (2%)	1 (0%)	24	11
1	C	190/206 (92%)	186 (98%)	2 (1%)	2 (1%)	11	3
1	D	190/206 (92%)	187 (98%)	2 (1%)	1 (0%)	24	11
1	E	189/206 (92%)	185 (98%)	3 (2%)	1 (0%)	24	11
1	F	201/206 (98%)	197 (98%)	2 (1%)	2 (1%)	12	4
1	G	185/206 (90%)	181 (98%)	3 (2%)	1 (0%)	24	11
1	H	187/206 (91%)	180 (96%)	5 (3%)	2 (1%)	11	3
All	All	1513/1648 (92%)	1480 (98%)	22 (2%)	11 (1%)	18	7

5 of 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

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%)	14	2
1	B	159/174 (91%)	150 (94%)	9 (6%)	18	3
1	C	165/174 (95%)	159 (96%)	6 (4%)	31	8
1	D	165/174 (95%)	152 (92%)	13 (8%)	11	1
1	E	161/174 (92%)	147 (91%)	14 (9%)	9	1
1	F	173/174 (99%)	161 (93%)	12 (7%)	14	2
1	G	160/174 (92%)	145 (91%)	15 (9%)	8	1
1	H	162/174 (93%)	148 (91%)	14 (9%)	10	1
All	All	1307/1392 (94%)	1213 (93%)	94 (7%)	13	2

5 of 94 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	51	VAL
1	G	122	THR
1	F	117	VAL
1	G	6	LEU
1	G	169	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	3	HIS

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Mol	Chain	Res	Type
1	H	27	GLN
1	H	189	GLN
1	C	143	ASN
1	C	63	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	191/206 (92%)	1.07	20 (10%) 11 16	29, 33, 37, 41	0
1	B	188/206 (91%)	1.51	51 (27%) 1 3	28, 33, 39, 42	0
1	C	194/206 (94%)	1.26	37 (19%) 3 5	29, 33, 38, 40	0
1	D	194/206 (94%)	1.34	41 (21%) 2 5	29, 33, 39, 43	0
1	E	193/206 (93%)	1.53	52 (26%) 1 3	29, 34, 39, 41	0
1	F	205/206 (99%)	1.45	43 (20%) 2 5	29, 33, 39, 43	0
1	G	189/206 (91%)	1.40	33 (17%) 4 6	29, 33, 38, 41	0
1	H	191/206 (92%)	1.68	70 (36%) 1 1	29, 34, 38, 41	0
All	All	1545/1648 (93%)	1.40	347 (22%) 2 4	28, 33, 39, 43	0

The worst 5 of 347 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	120	PRO	5.8
1	B	127	PRO	5.1
1	B	124	VAL	4.9
1	E	147	PHE	4.8
1	A	122	THR	4.7

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.