



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 12:01 PM UTC

PDB ID : 4FQU / pdb_00004fqu
Title : Glutathionyl-Hydroquinone Reductase PcpF of *Sphingobium chlorophenolicum*
Authors : Green, A.R.; Hayes, R.P.; Xun, L.; Kang, C.
Deposited on : 2012-06-25
Resolution : 3.00 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

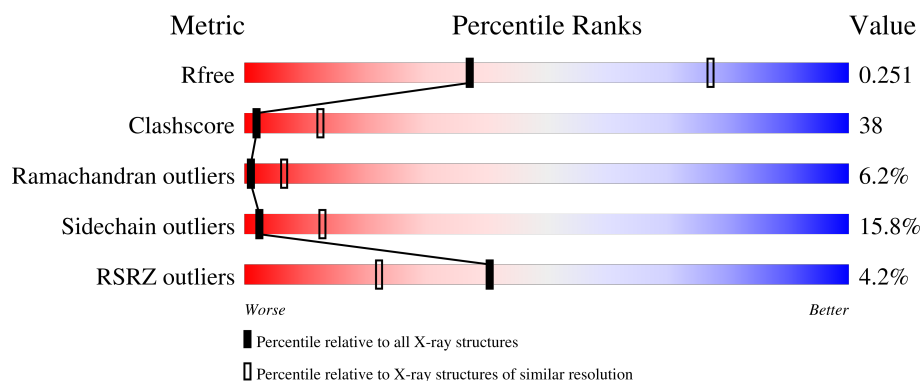
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	313	4% 50% 35% 12% .
1	B	313	3% 50% 35% 11% ..
1	C	313	4% 40% 44% 12% .
1	D	313	4% 37% 45% 16% .
1	E	313	4% 41% 42% 14% .

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Mol	Chain	Length	Quality of chain
1	F	313	3% 50% 35% 9% • •
1	G	313	4% 42% 42% 11% • •
1	H	313	5% 33% 49% 16% ••

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19729 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 Putative glutathione transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2491	1592	435	458	6			
1	B	303	Total	C	N	O	S	0	0	0
			2420	1549	424	441	6			
1	C	312	Total	C	N	O	S	0	0	0
			2482	1584	435	457	6			
1	D	312	Total	C	N	O	S	0	0	0
			2481	1586	432	457	6			
1	E	312	Total	C	N	O	S	0	0	0
			2484	1587	435	456	6			
1	F	308	Total	C	N	O	S	0	0	0
			2444	1559	429	450	6			
1	G	305	Total	C	N	O	S	0	0	0
			2428	1551	426	445	6			
1	H	309	Total	C	N	O	S	0	0	0
			2444	1561	430	447	6			

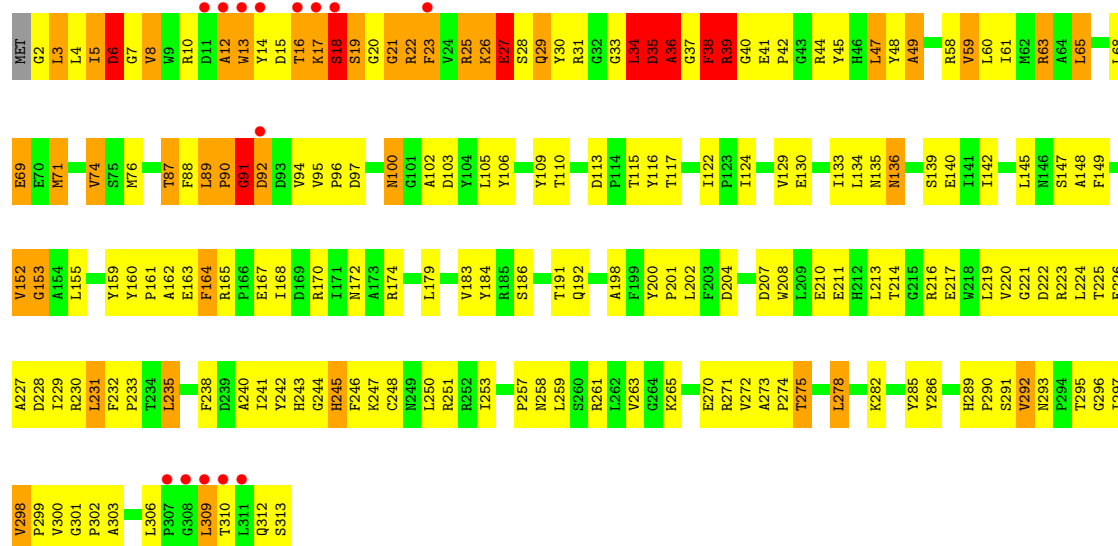
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	5	Total	O	0	0
			5	5		
2	C	9	Total	O	0	0
			9	9		
2	D	3	Total	O	0	0
			3	3		
2	E	1	Total	O	0	0
			1	1		
2	F	13	Total	O	0	0
			13	13		

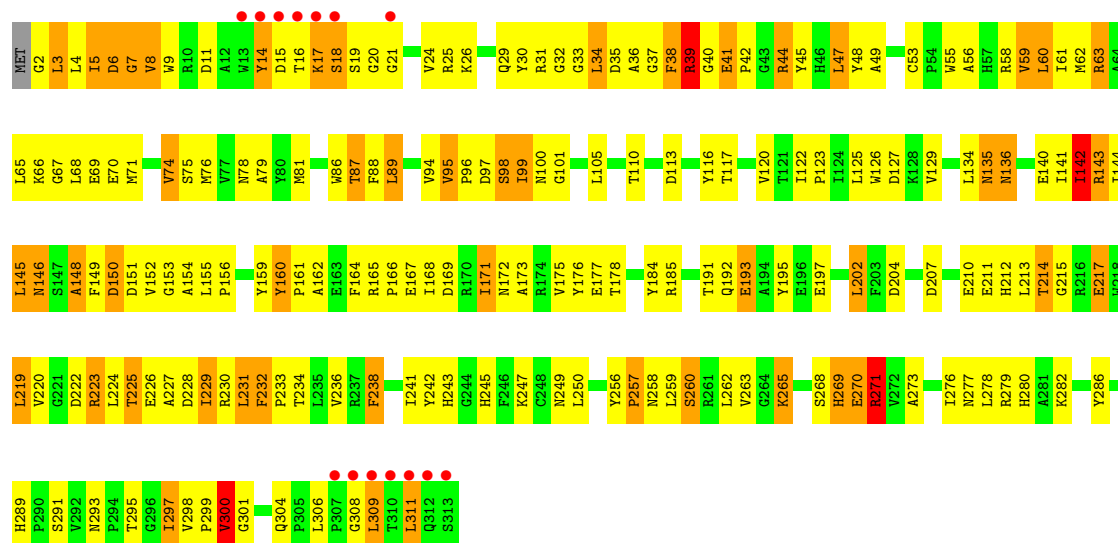
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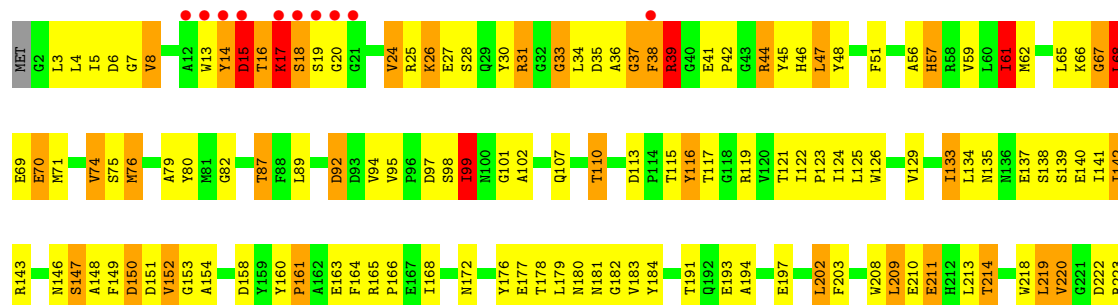
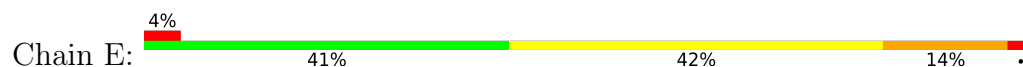
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	O	0	0
			2	2		
2	H	1	Total	O	0	0
			1	1		

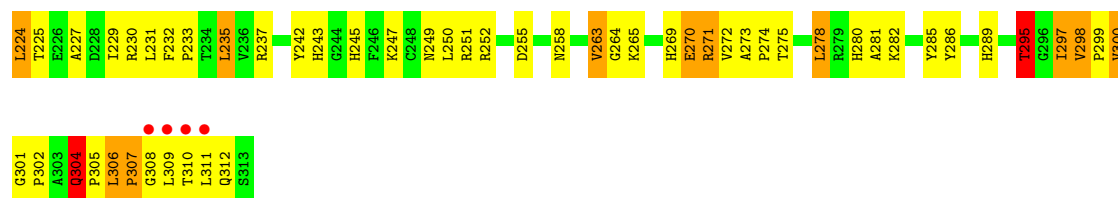


• Molecule 1: Putative glutathione transferase

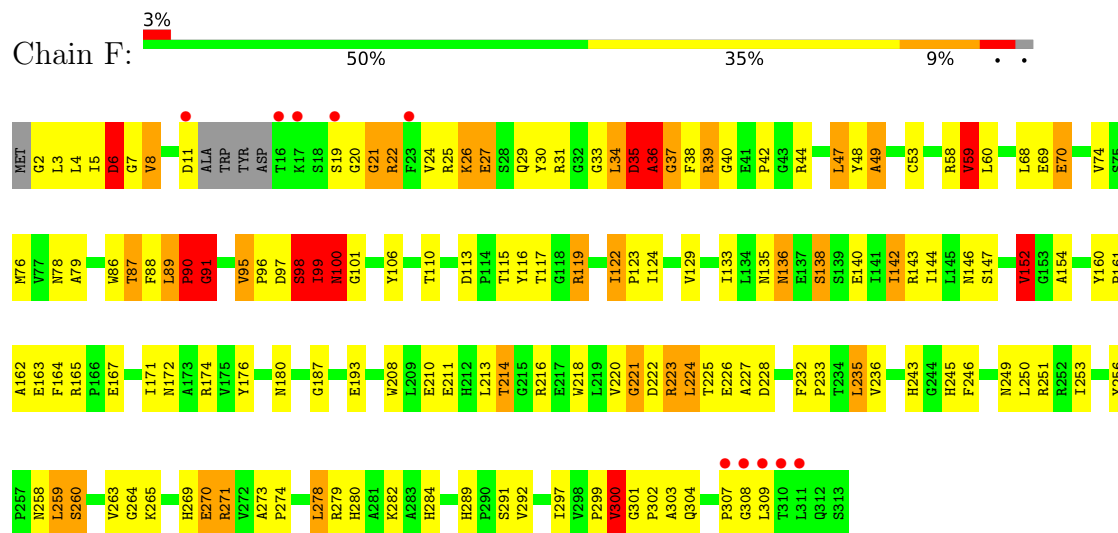


• Molecule 1: Putative glutathione transferase

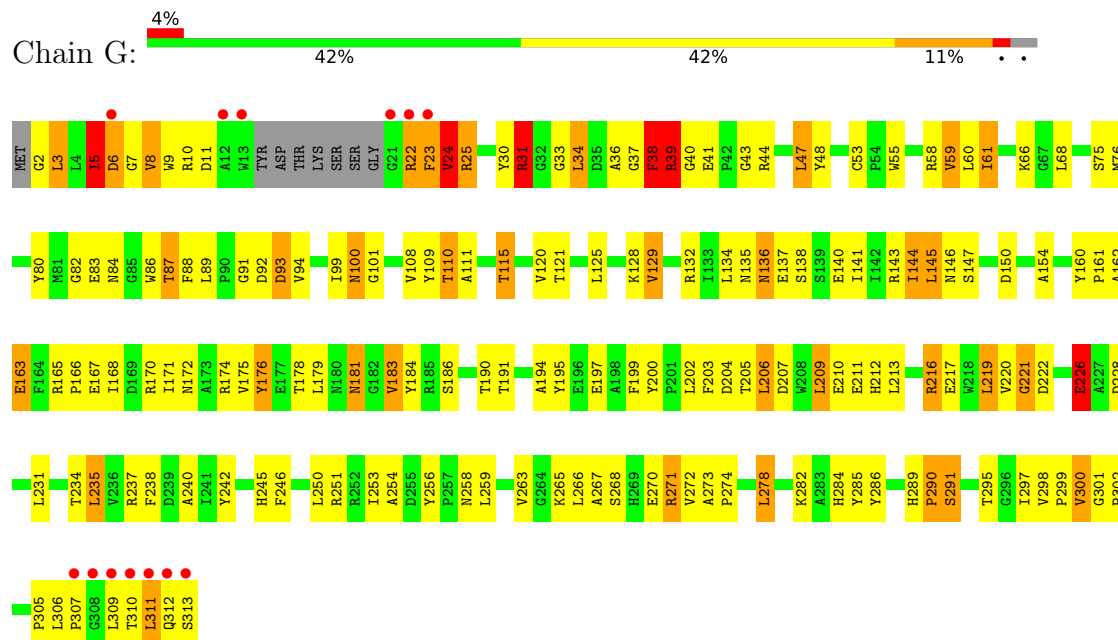




• Molecule 1: Putative glutathione transferase

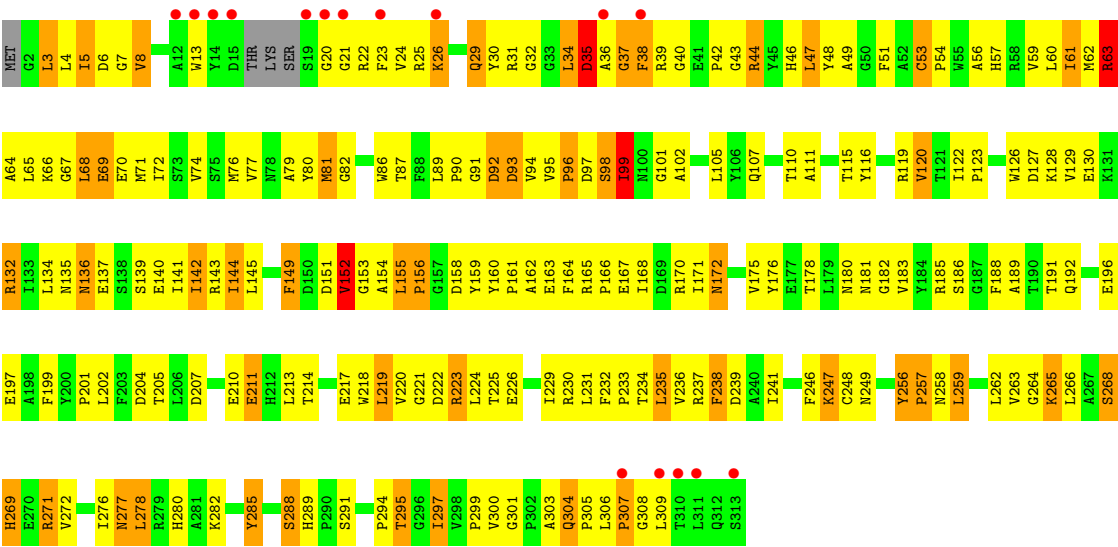


• Molecule 1: Putative glutathione transferase



• Molecule 1: Putative glutathione transferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	242.84Å 242.84Å 242.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.00 49.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.9 (49.57-3.00) 87.5 (49.57-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.36 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, R_{free}	0.202 , 0.256 0.195 , 0.251	Depositor DCC
R_{free} test set	2007 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19729	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.17	10/2562 (0.4%)	1.34	27/3490 (0.8%)
1	B	1.00	3/2488 (0.1%)	1.27	21/3387 (0.6%)
1	C	0.98	0/2552	1.28	20/3476 (0.6%)
1	D	0.90	2/2552 (0.1%)	1.25	26/3478 (0.7%)
1	E	1.01	2/2554 (0.1%)	1.27	18/3479 (0.5%)
1	F	1.13	7/2511 (0.3%)	1.30	23/3418 (0.7%)
1	G	0.84	0/2495	1.19	13/3397 (0.4%)
1	H	0.78	0/2511	1.11	15/3419 (0.4%)
All	All	0.99	24/20225 (0.1%)	1.25	163/27544 (0.6%)

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	A	0	3
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	9

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	ALA	CA-CB	7.79	1.64	1.52
1	F	99	ILE	CA-CB	7.77	1.65	1.54
1	A	148	ALA	CA-C	7.27	1.61	1.53
1	A	283	ALA	CA-CB	-7.26	1.42	1.53
1	A	310	THR	CA-CB	7.15	1.58	1.53

The worst 5 of 163 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	6	ASP	N-CA-C	-12.47	96.78	114.12
1	A	149	PHE	N-CA-C	-12.36	96.94	112.88
1	G	24	VAL	N-CA-C	11.52	121.23	111.90
1	A	95	VAL	CA-C-N	10.37	131.01	119.92
1	A	95	VAL	C-N-CA	10.37	131.01	119.92

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	ALA	Peptide
1	A	39	ARG	Peptide
1	A	40	GLY	Peptide
1	C	36	ALA	Peptide
1	C	6	ASP	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	2491	0	2406	185	0
1	B	2420	0	2340	158	0
1	C	2482	0	2392	211	0
1	D	2481	0	2383	241	0
1	E	2484	0	2385	200	0
1	F	2444	0	2354	150	0
1	G	2428	0	2344	162	0
1	H	2444	0	2351	222	0
2	A	21	0	0	3	0
2	B	5	0	0	0	0
2	C	9	0	0	4	0
2	D	3	0	0	1	0
2	E	1	0	0	0	0
2	F	13	0	0	1	0
2	G	2	0	0	0	0
2	H	1	0	0	0	0
All	All	19729	0	18955	1483	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 38.

The worst 5 of 1483 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:A:39:ARG:HE	1:A:148:ALA:C	1.39	1.31
1:C:49:ALA:HB3	1:C:76:MET:HE1	1.26	1.18
1:A:143:ARG:HG3	1:A:143:ARG:HH11	1.06	1.14
1:A:221:GLY:HA3	2:A:401:HOH:O	1.46	1.12
1:C:213:LEU:HD21	1:C:219:LEU:HD23	1.29	1.12

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	310/313 (99%)	263 (85%)	33 (11%)	14 (4%)	2	12
1	B	299/313 (96%)	252 (84%)	39 (13%)	8 (3%)	4	22
1	C	310/313 (99%)	238 (77%)	52 (17%)	20 (6%)	1	5
1	D	310/313 (99%)	238 (77%)	52 (17%)	20 (6%)	1	5
1	E	310/313 (99%)	247 (80%)	41 (13%)	22 (7%)	1	4
1	F	304/313 (97%)	262 (86%)	27 (9%)	15 (5%)	1	10
1	G	301/313 (96%)	241 (80%)	39 (13%)	21 (7%)	1	4
1	H	305/313 (97%)	213 (70%)	60 (20%)	32 (10%)	0	2
All	All	2449/2504 (98%)	1954 (80%)	343 (14%)	152 (6%)	1	6

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	TRP

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Mol	Chain	Res	Type
1	A	36	ALA
1	A	38	PHE
1	A	147	SER
1	A	307	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	258/260 (99%)	219 (85%)	39 (15%)	3	14
1	B	250/260 (96%)	211 (84%)	39 (16%)	2	13
1	C	256/260 (98%)	216 (84%)	40 (16%)	2	13
1	D	255/260 (98%)	212 (83%)	43 (17%)	2	11
1	E	254/260 (98%)	212 (84%)	42 (16%)	2	12
1	F	252/260 (97%)	214 (85%)	38 (15%)	3	14
1	G	250/260 (96%)	213 (85%)	37 (15%)	3	15
1	H	249/260 (96%)	207 (83%)	42 (17%)	2	11
All	All	2024/2080 (97%)	1704 (84%)	320 (16%)	2	13

5 of 320 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	223	ARG
1	H	70	GLU
1	F	279	ARG
1	G	144	ILE
1	H	149	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	293	ASN

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Mol	Chain	Res	Type
1	H	136	ASN
1	E	304	GLN
1	H	100	ASN
1	H	280	HIS

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	312/313 (99%)	-0.59	14 (4%)	38	20	15, 25, 76, 137	0
1	B	303/313 (96%)	-0.35	8 (2%)	57	34	20, 38, 68, 147	0
1	C	312/313 (99%)	-0.31	14 (4%)	38	20	21, 36, 90, 132	0
1	D	312/313 (99%)	-0.15	14 (4%)	38	20	26, 45, 94, 153	0
1	E	312/313 (99%)	-0.19	14 (4%)	38	20	19, 41, 87, 146	0
1	F	308/313 (98%)	-0.51	10 (3%)	50	29	17, 29, 78, 139	0
1	G	305/313 (97%)	-0.11	13 (4%)	40	21	32, 49, 86, 154	0
1	H	309/313 (98%)	0.23	16 (5%)	33	17	36, 63, 99, 164	0
All	All	2473/2504 (98%)	-0.25	103 (4%)	40	22	15, 41, 88, 164	0

The worst 5 of 103 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	13	TRP	8.7
1	H	15	ASP	8.3
1	B	11	ASP	7.3
1	H	309	LEU	6.8
1	G	311	LEU	6.6

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.