



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:41 PM GMT

PDB ID : 4FQU
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
<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

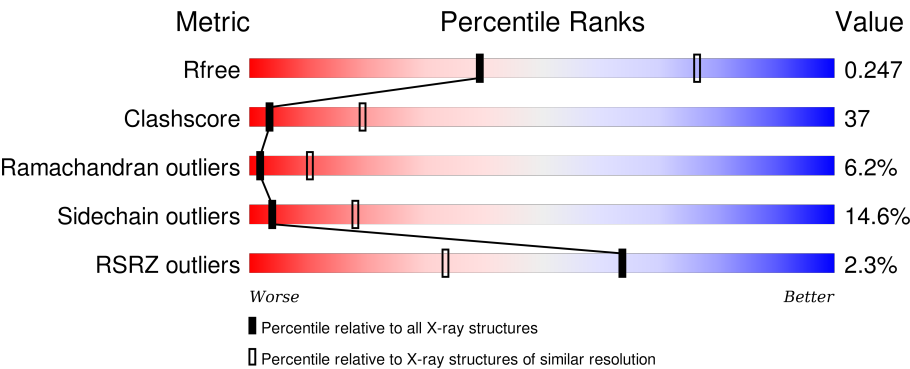
1 Overall quality at a glance ⓘ

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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 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	313	<div><div>3%</div><div>55%33%10% .</div></div>
1	B	313	<div><div>2%</div><div>52%35%8% . .</div></div>
1	C	313	<div><div>2%</div><div>45%43%9% .</div></div>
1	D	313	<div><div>3%</div><div>41%46%12% .</div></div>
1	E	313	<div><div>3%</div><div>45%40%13% .</div></div>

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Mol	Chain	Length	Quality of chain
1	F	313	<div><div></div><div>2%</div><div>55%</div><div>33%</div><div>7%</div><div></div><div></div></div>
1	G	313	<div><div></div><div>2%</div><div>46%</div><div>41%</div><div>9%</div><div></div><div></div></div>
1	H	313	<div><div></div><div>3%</div><div>38%</div><div>46%</div><div>13%</div><div></div><div></div></div>

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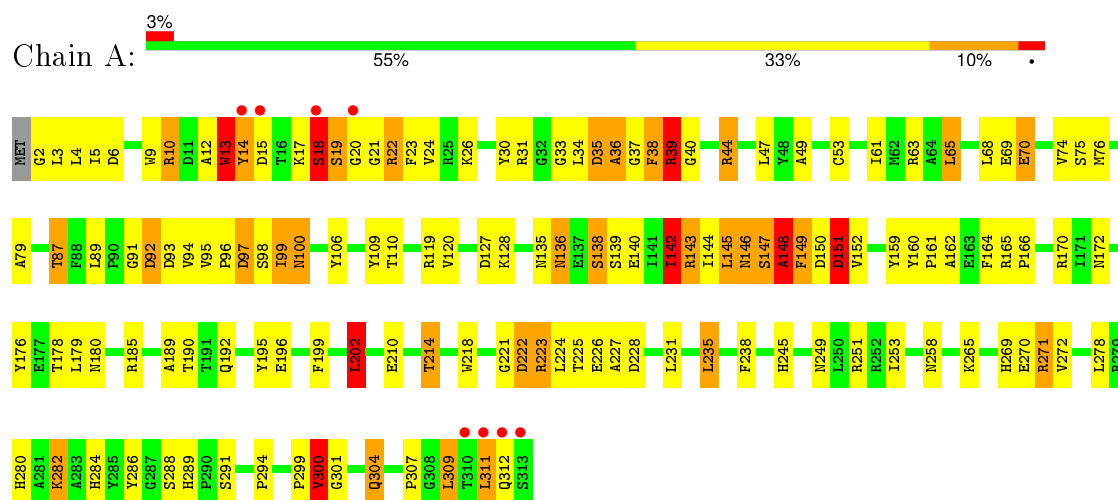
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	O	0	0
			2	2		
2	H	1	Total	O	0	0
			1	1		

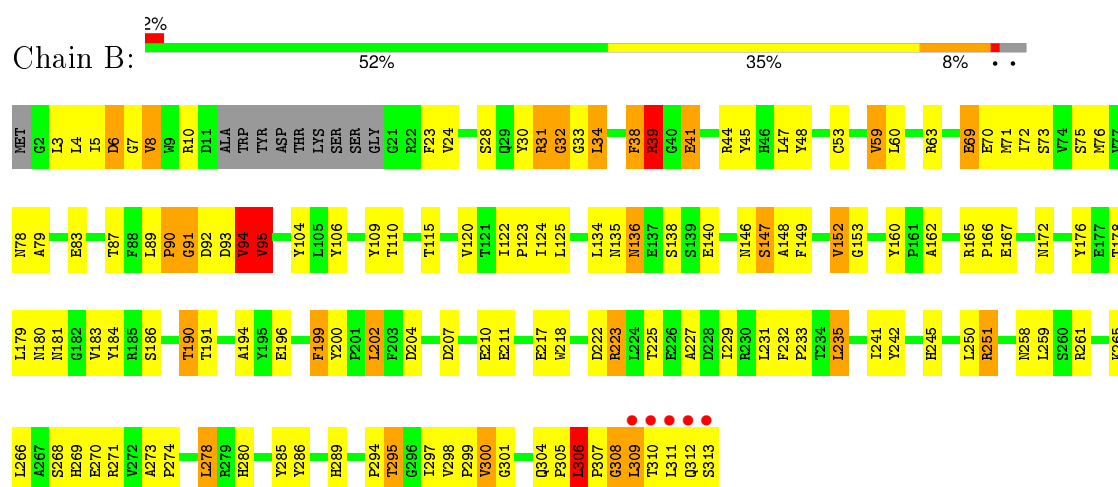
3 Residue-property plots

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 ($RSRZ > 2$). 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.

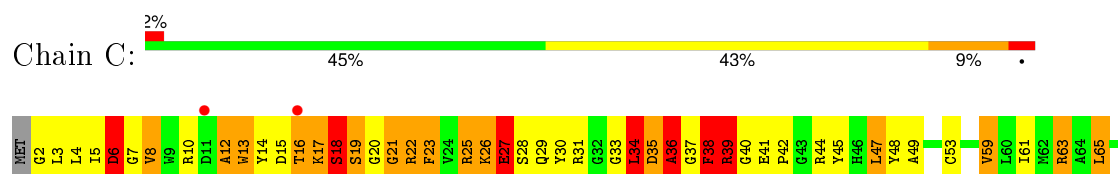
• Molecule 1: Putative glutathione transferase

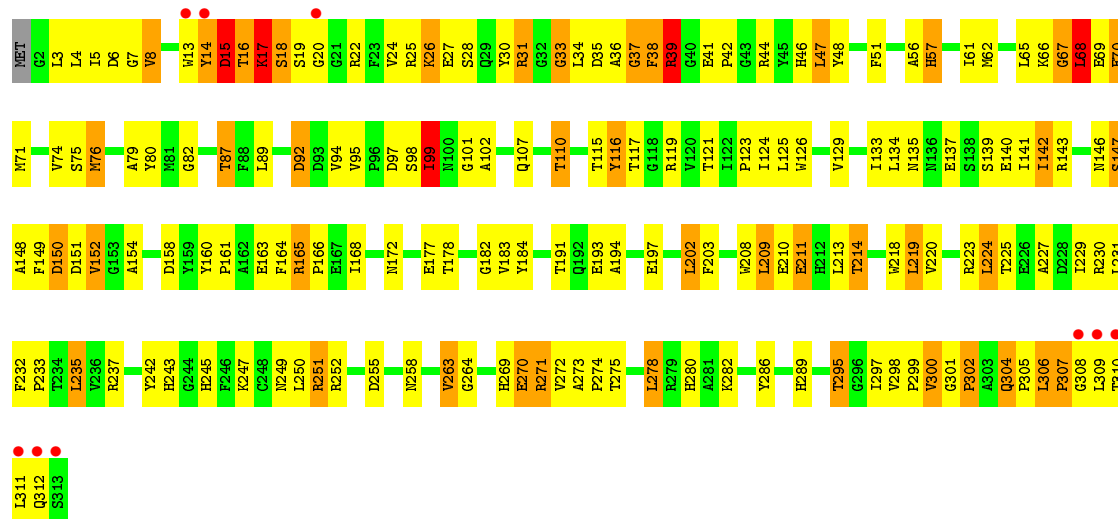


• Molecule 1: Putative glutathione transferase



• Molecule 1: Putative glutathione transferase





Chain F:

2% 55% 33% 7% 1%

MET G2 L3 L4 I5 I6 D6 G7 V8 D11 ALA TRP TYR ASP T16 S19 G20 G21 R22 F23 V24 R25 K26 E27 Y30 R31 G32 G33 L34 D35 A36 G37 F38 R39 G40 G41 P42 G43 R44 L47 Y48 A49 G53 R58 V59 L60 L68 E69 E70 V74 S75 M76 H77 N78 A79 R86 T87 F88 L89 P90 G91 V95 P96 D97 S98 R99 N100 Y106 T115 Y116 R119 I122 P123 I124 V129 N135 N136 S138 A137 F139 E140 I141 I142 R143 M146 S147 V152 A153 A154 Y160 P161 A162 E163 F164 R165 P166 E167 I171 N172 A173 E174 P175 V176 Y177 N180 T187 G187 E193 V208 L209 E210 E211 H212 L213 T214 G215 R216 E217 W218 L219 G221 D222 R223 L224 T225 E226 A227 D228 L235 H243 G244 H245 F246 N249 L250 R251 R252 I253 V256 P257 N258 L259 S260 V263 G264 K265 H269 E270 R271 V272 A273 P274

Chain G:

46% 41% 9%

• • •

Category	Value
Y171	1
G85	1
Y241	1
Y242	1
H245	1
H246	1
L250	1
R251	1
R252	1
L253	1
Y256	1
H257	1
L258	1
L259	1
Y263	1
H264	1
R265	1
L266	1
A267	1
R268	1
R269	1
E270	1
R271	1
V272	1
A273	1
P274	1
L278	1
R282	1
A283	1
H284	1
Y285	1
Y286	1
R289	1
P290	1
S291	1
T295	1
G296	1
V298	1
P299	1
V300	1
G301	1
P302	1
P305	1
L306	1
P307	1
G308	1
L309	1
T310	1
L311	1
Q312	1
S313	1
I171	1
R174	1
V175	1
Y176	1
E177	1
T178	1
L179	1
M180	1
G182	1
V183	1
S186	1
T190	1
T191	1
A194	1
Y195	1
E196	1
E197	1
A198	1
F199	1
Y200	1
L201	1
L202	1
F203	1
D204	1
T205	1
L206	1
D207	1
D208	1
L209	1
E210	1
E211	1
L212	1
L213	1
R216	1
E217	1
V218	1
L219	1
T220	1
G221	1
D222	1
E226	1
A227	1
D228	1
L231	1
T234	1
L235	1
T236	1
R237	1
F238	1
D239	1
A240	1
G86	1
T87	1
F88	1
L89	1
P90	1
G91	1
D92	1
D93	1
V94	1
D11	1
A12	1
V13	1
T14	1
Y109	1
T110	1
A111	1
T115	1
V120	1
L125	1
K128	1
V129	1
R132	1
L133	1
L134	1
R135	1
A136	1
E137	1
S138	1
S139	1
E140	1
I141	1
E142	1
R143	1
I144	1
L145	1
M146	1
S147	1
D150	1
A154	1
Y160	1
P161	1
A162	1
E163	1
F164	1
A165	1
P166	1
E167	1
I168	1
R169	1
P170	1
Y80	1
X81	1
G82	1
R83	1
P84	1
R25	1
Y30	1
R31	1
G32	1
G33	1
L34	1
R35	1
A36	1
G37	1
R38	1
R39	1
G40	1
E41	1
R42	1
R43	1
R44	1
L47	1
C53	1
R58	1
V59	1
L60	1
L61	1
X66	1
A67	1
L68	1
R65	1
Y80	1
X81	1
G82	1
R83	1
P84	1

Chain H:

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 – 2.83	Depositor EDS
% Data completeness (in resolution range)	87.9 (49.57-3.00) 84.0 (49.57-2.83)	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 0.197 , 0.247	Depositor DCC
R_{free} test set	1697 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.6	EDS
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 112629 reflections	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, 0.375 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	0.94	5/2562 (0.2%)	0.97	4/3490 (0.1%)
1	B	0.82	1/2488 (0.0%)	0.94	6/3387 (0.2%)
1	C	0.80	2/2552 (0.1%)	0.95	4/3476 (0.1%)
1	D	0.72	1/2552 (0.0%)	0.88	3/3478 (0.1%)
1	E	0.80	0/2554	0.92	4/3479 (0.1%)
1	F	0.93	2/2511 (0.1%)	0.95	2/3418 (0.1%)
1	G	0.68	0/2495	0.84	2/3397 (0.1%)
1	H	0.63	0/2511	0.79	0/3419
All	All	0.80	11/20225 (0.1%)	0.91	25/27544 (0.1%)

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 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	SER	CB-OG	6.75	1.51	1.42
1	B	53	CYS	CB-SG	-6.33	1.71	1.82
1	A	53	CYS	CB-SG	-6.18	1.71	1.82
1	F	70	GLU	CG-CD	6.14	1.61	1.51
1	A	70	GLU	CG-CD	5.71	1.60	1.51

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	39	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	E	76	MET	CG-SD-CE	-7.11	88.83	100.20
1	F	91	GLY	N-CA-C	6.47	129.29	113.10
1	C	91	GLY	N-CA-C	6.35	128.98	113.10
1	B	306	LEU	CA-CB-CG	6.27	129.72	115.30

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	178	0
1	B	2420	0	2340	152	0
1	C	2482	0	2392	196	0
1	D	2481	0	2383	236	0
1	E	2484	0	2385	189	0
1	F	2444	0	2354	147	0
1	G	2428	0	2344	153	0
1	H	2444	0	2351	207	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	1412	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 37.

The worst 5 of 1412 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	1.27
1:A:143:ARG:HH11	1:A:143:ARG:HG3	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
1:H:23:PHE:CB	1:H:24:VAL:HA	1.73	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%)	3	18
1	B	299/313 (96%)	252 (84%)	39 (13%)	8 (3%)	6	32
1	C	310/313 (99%)	238 (77%)	52 (17%)	20 (6%)	1	8
1	D	310/313 (99%)	238 (77%)	52 (17%)	20 (6%)	1	8
1	E	310/313 (99%)	247 (80%)	41 (13%)	22 (7%)	1	7
1	F	304/313 (97%)	262 (86%)	27 (9%)	15 (5%)	3	16
1	G	301/313 (96%)	241 (80%)	39 (13%)	21 (7%)	1	7
1	H	305/313 (97%)	213 (70%)	60 (20%)	32 (10%)	1	3
All	All	2449/2504 (98%)	1954 (80%)	343 (14%)	152 (6%)	2	10

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%)	223 (86%)	35 (14%)	5	20
1	B	250/260 (96%)	212 (85%)	38 (15%)	3	16
1	C	256/260 (98%)	221 (86%)	35 (14%)	4	20
1	D	255/260 (98%)	217 (85%)	38 (15%)	4	17
1	E	254/260 (98%)	216 (85%)	38 (15%)	3	17
1	F	252/260 (97%)	216 (86%)	36 (14%)	4	19
1	G	250/260 (96%)	214 (86%)	36 (14%)	4	18
1	H	249/260 (96%)	209 (84%)	40 (16%)	3	14
All	All	2024/2080 (97%)	1728 (85%)	296 (15%)	4	18

5 of 296 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	213	LEU
1	E	119	ARG
1	H	107	GLN
1	D	231	LEU
1	E	25	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	29	GLN

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Mol	Chain	Res	Type
1	E	304	GLN
1	H	245	HIS
1	E	172	ASN
1	E	243	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 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	312/313 (99%)	-0.56	8 (2%) 59 29	15, 25, 76, 137	0
1	B	303/313 (96%)	-0.51	5 (1%) 73 45	20, 38, 68, 147	0
1	C	312/313 (99%)	-0.54	7 (2%) 65 35	21, 36, 90, 132	0
1	D	312/313 (99%)	-0.42	8 (2%) 59 29	26, 45, 94, 153	0
1	E	312/313 (99%)	-0.44	9 (2%) 55 26	19, 41, 87, 146	0
1	F	308/313 (98%)	-0.59	6 (1%) 70 41	17, 29, 78, 139	0
1	G	305/313 (97%)	-0.40	5 (1%) 74 47	32, 49, 86, 154	0
1	H	309/313 (98%)	-0.13	10 (3%) 51 23	36, 63, 99, 164	0
All	All	2473/2504 (98%)	-0.45	58 (2%) 64 33	15, 41, 88, 164	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	310	THR	10.5
1	G	312	GLN	10.4
1	B	310	THR	8.6
1	F	310	THR	8.2
1	G	310	THR	8.0

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

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

6.3 Carbohydrates ⓘ

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.