WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 14, 2023 – 10:58 PM JST

|		
PDB ID	:	6AKF
Title	:	Crystal structure of mouse claudin-3 P134A mutant in complex with C-terminal fragment of Clostridium perfringens enterotoxin
Authors	:	Nakamura, S.; Irie, K.; Fujiyoshi, Y.
Deposited on	:	2018-08-31
Resolution	:	3.90 Å(reported)

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 3.90 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.
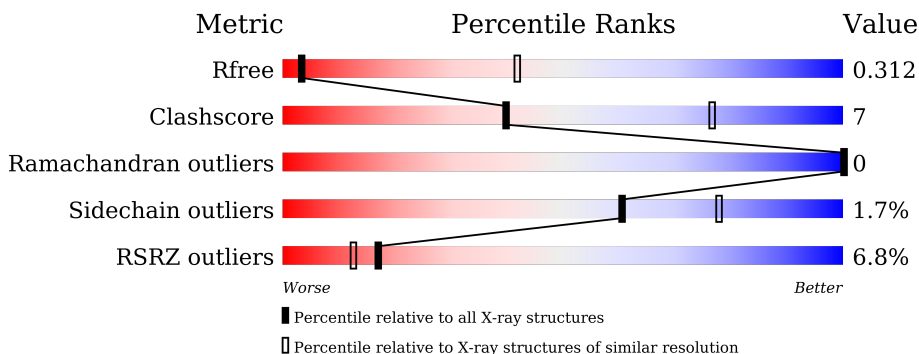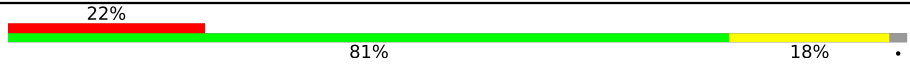

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1002 (4.14-3.66)
Clashscore	141614	1004 (4.12-3.68)
Ramachandran outliers	138981	1021 (4.14-3.66)
Sidechain outliers	138945	1014 (4.14-3.66)
RSRZ outliers	127900	1275 (4.20-3.60)

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 <=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	190	6% — 81% / 16% · ·
1	C	190	3% — 82% / 16% · ·
1	E	190	6% — 80% / 11% · 8%
1	G	190	3% — 77% / 12% · 11%
2	B	119	4% — 77% / 21% ·
2	D	119	% — 73% / 25% ·

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Mol	Chain	Length	Quality of chain
2	F	119	22% 81% 18%
2	H	119	12% 83% 15%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 8888 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 Claudin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total 1335	C 869	N 217	O 237	S 12	0	0	0
1	C	186	Total 1350	C 876	N 220	O 242	S 12	0	0	0
1	E	174	Total 1264	C 825	N 206	O 221	S 12	0	0	0
1	G	169	Total 1222	C 800	N 198	O 213	S 11	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	see sequence details	UNP Q9Z0G9
A	-5	HIS	-	see sequence details	UNP Q9Z0G9
A	-4	MET	-	see sequence details	UNP Q9Z0G9
A	-3	ALA	-	see sequence details	UNP Q9Z0G9
A	-2	SER	-	see sequence details	UNP Q9Z0G9
A	-1	GLY	-	see sequence details	UNP Q9Z0G9
A	0	SER	-	see sequence details	UNP Q9Z0G9
A	103	ALA	CYS	engineered mutation	UNP Q9Z0G9
A	106	ALA	CYS	engineered mutation	UNP Q9Z0G9
A	134	ALA	PRO	engineered mutation	UNP Q9Z0G9
A	181	ALA	CYS	engineered mutation	UNP Q9Z0G9
A	182	ALA	CYS	engineered mutation	UNP Q9Z0G9
C	-6	GLY	-	see sequence details	UNP Q9Z0G9
C	-5	HIS	-	see sequence details	UNP Q9Z0G9
C	-4	MET	-	see sequence details	UNP Q9Z0G9
C	-3	ALA	-	see sequence details	UNP Q9Z0G9
C	-2	SER	-	see sequence details	UNP Q9Z0G9
C	-1	GLY	-	see sequence details	UNP Q9Z0G9
C	0	SER	-	see sequence details	UNP Q9Z0G9
C	103	ALA	CYS	engineered mutation	UNP Q9Z0G9
C	106	ALA	CYS	engineered mutation	UNP Q9Z0G9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	134	ALA	PRO	engineered mutation	UNP Q9Z0G9
C	181	ALA	CYS	engineered mutation	UNP Q9Z0G9
C	182	ALA	CYS	engineered mutation	UNP Q9Z0G9
E	-6	GLY	-	see sequence details	UNP Q9Z0G9
E	-5	HIS	-	see sequence details	UNP Q9Z0G9
E	-4	MET	-	see sequence details	UNP Q9Z0G9
E	-3	ALA	-	see sequence details	UNP Q9Z0G9
E	-2	SER	-	see sequence details	UNP Q9Z0G9
E	-1	GLY	-	see sequence details	UNP Q9Z0G9
E	0	SER	-	see sequence details	UNP Q9Z0G9
E	103	ALA	CYS	engineered mutation	UNP Q9Z0G9
E	106	ALA	CYS	engineered mutation	UNP Q9Z0G9
E	134	ALA	PRO	engineered mutation	UNP Q9Z0G9
E	181	ALA	CYS	engineered mutation	UNP Q9Z0G9
E	182	ALA	CYS	engineered mutation	UNP Q9Z0G9
G	-6	GLY	-	see sequence details	UNP Q9Z0G9
G	-5	HIS	-	see sequence details	UNP Q9Z0G9
G	-4	MET	-	see sequence details	UNP Q9Z0G9
G	-3	ALA	-	see sequence details	UNP Q9Z0G9
G	-2	SER	-	see sequence details	UNP Q9Z0G9
G	-1	GLY	-	see sequence details	UNP Q9Z0G9
G	0	SER	-	see sequence details	UNP Q9Z0G9
G	103	ALA	CYS	engineered mutation	UNP Q9Z0G9
G	106	ALA	CYS	engineered mutation	UNP Q9Z0G9
G	134	ALA	PRO	engineered mutation	UNP Q9Z0G9
G	181	ALA	CYS	engineered mutation	UNP Q9Z0G9
G	182	ALA	CYS	engineered mutation	UNP Q9Z0G9

- Molecule 2 is a protein called Heat-labile enterotoxin B chain.

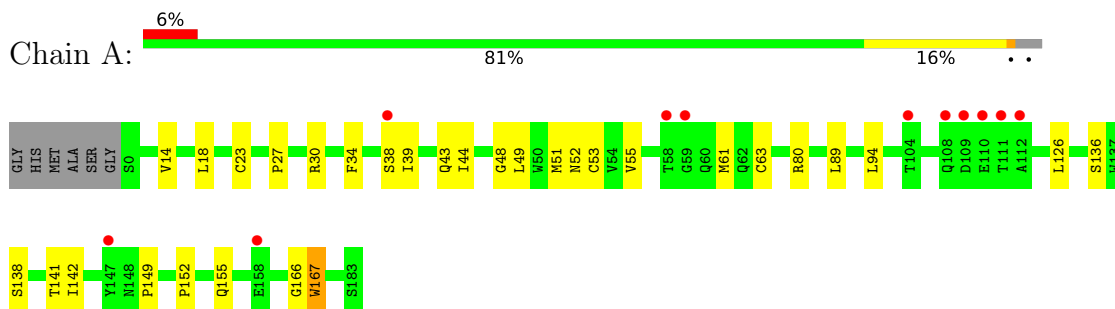| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	117	Total 925	C 591	N 155	O 178	S 1	0	0	0
2	D	117	Total 932	C 595	N 157	O 179	S 1	0	0	0
2	F	117	Total 928	C 592	N 156	O 179	S 1	0	0	0
2	H	117	Total 932	C 595	N 157	O 179	S 1	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

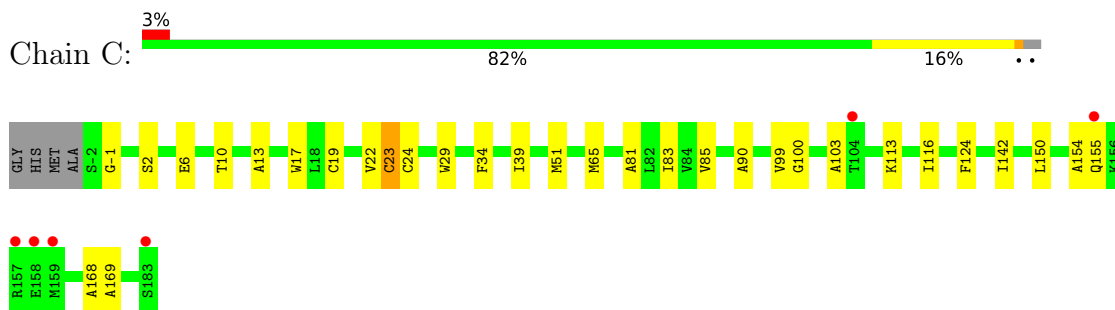| Chain	Residue	Modelled	Actual	Comment	Reference
B	201	GLY	-	see sequence details	UNP P01558
B	202	SER	-	see sequence details	UNP P01558
B	313	ALA	SER	engineered mutation	UNP P01558
D	201	GLY	-	see sequence details	UNP P01558
D	202	SER	-	see sequence details	UNP P01558
D	313	ALA	SER	engineered mutation	UNP P01558
F	201	GLY	-	see sequence details	UNP P01558
F	202	SER	-	see sequence details	UNP P01558
F	313	ALA	SER	engineered mutation	UNP P01558
H	201	GLY	-	see sequence details	UNP P01558
H	202	SER	-	see sequence details	UNP P01558
H	313	ALA	SER	engineered mutation	UNP P01558

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.
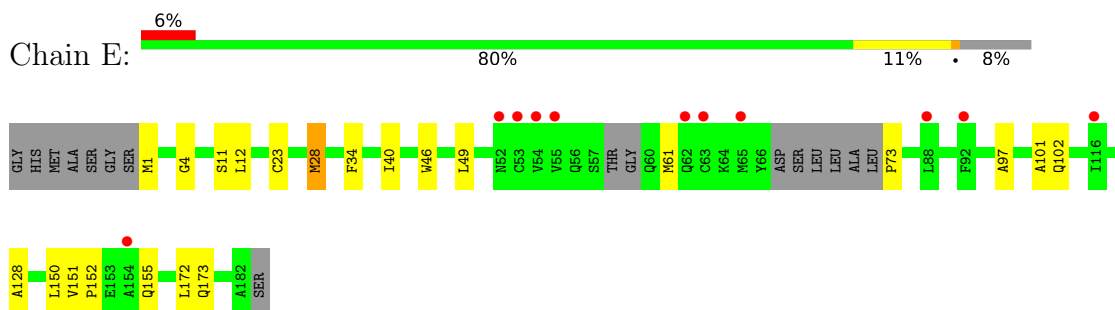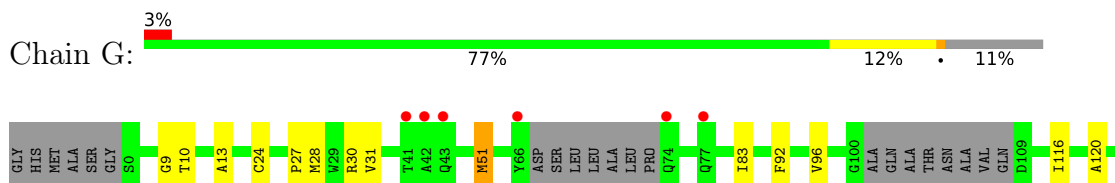
- Molecule 1: Claudin-3

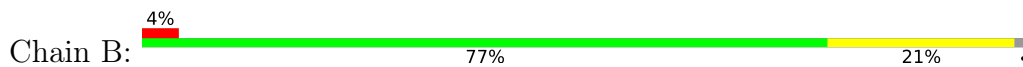- Molecule 1: Claudin-3

- Molecule 1: Claudin-3

- Molecule 1: Claudin-3

F124 L132 I142 P152 E153 R157 W167 A170 L179 S183

• Molecule 2: Heat-labile enterotoxin B chain

4%

Chain B:

77% 21%

GLY SER A203 A204 A205 R208 L211 T212 D213 A214 L223 Y224 Y232 L238 T243 I244 T245 A246 A255 D260 L278 D284 D288 L291 D292 A293 Y296 N303 S304 S307 Y310 P311 I314 Q317 K318 F319

• Molecule 2: Heat-labile enterotoxin B chain

%

Chain D:

73% 25%

GLY SER A203 A204 A205 R208 A214 L223 Y224 D225 Q236 K237 L238 H241 L242 T243 I244 T245 Q249 K250 Y251 R252 I253 L254 K257 F261 N262 S277 G281 D288 I289 S290 L291 D292 Q295 Y296 V297 L298 V299 Y306 L315 F316 Q317 K318 F319

• Molecule 2: Heat-labile enterotoxin B chain

22%

Chain F:

81% 18%

GLY SER A203 A204 A205 T206 E207 P219 L223 R227 W234 K237 L238 N239 L240 H241 L242 K250 Y251 R252 I253 I258 F261 N262 I263 Y264 L271 V272 K273 L274 E275 Q276 S277 V282 K283 D288 I289 Y296 V299 M300 K301 S304 S307 Y312
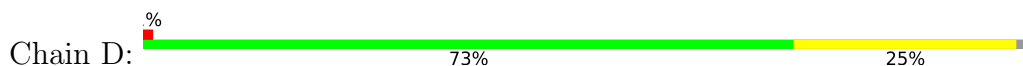
A313 Q317 K318 F319

• Molecule 2: Heat-labile enterotoxin B chain

12%

Chain H:

83% 15%

GLY SER A203 A204 E207 R208 L209 L215 N216 S217 N218 L223 Y224 D225 Q236 R227 W234 T235 Q236 K237 L238 N239 L240 H241 L242 T243 I244 L254 A255 S256 E275 D284 Q294 Q295 Y296 S305 L315 F316 F319

4 Data and refinement statistics ⓘ

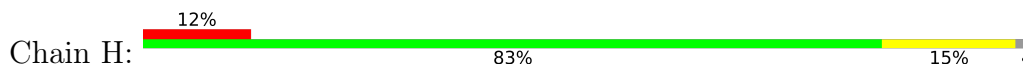| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.54Å 127.45Å 165.70Å 90.00° 104.53° 90.00°	Depositor
Resolution (Å)	46.66 – 3.90 48.16 – 3.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.66-3.90) 98.6 (48.16-3.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.80 (at 3.88Å)	Xtriage
Refinement program	PHENIX 1.13_2998, REFMAC 5	Depositor
R, R_{free}	0.274 , 0.312 0.274 , 0.312	Depositor DCC
R_{free} test set	1314 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å^2)	95.6	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.22 , 48.9	EDS
L-test for twinning[2]	$< |L| > = 0.41, < L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.81	EDS
Total number of atoms	8888	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.58	1/1357 (0.1%)	0.73	0/1855
1	C	0.55	0/1372	0.78	1/1875 (0.1%)
1	E	0.55	0/1284	0.75	1/1753 (0.1%)
1	G	0.65	1/1241 (0.1%)	0.72	1/1694 (0.1%)
2	B	0.58	0/946	0.83	0/1288
2	D	0.52	0/953	0.76	0/1296
2	F	0.51	0/949	0.75	0/1292
2	H	0.51	0/953	0.74	0/1296
All	All	0.56	2/9055 (0.0%)	0.76	3/12349 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	27	PRO	N-CD	-13.52	1.28	1.47
1	A	167	TRP	CB-CG	6.37	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	-1	GLY	N-CA-C	6.39	129.08	113.10
1	G	27	PRO	CA-N-CD	6.27	120.48	111.70
1	E	28	MET	N-CA-C	-5.23	96.88	111.00

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1335	0	1387	21	0
1	C	1350	0	1404	21	0
1	E	1264	0	1306	25	0
1	G	1222	0	1262	16	0
2	B	925	0	892	25	0
2	D	932	0	907	17	0
2	F	928	0	896	16	0
2	H	932	0	907	10	0
All	All	8888	0	8961	130	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 7.

The worst 5 of 130 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)
2:B:211:LEU:HB3	2:B:244:ILE:HD11	1.21	1.14
2:B:205:ALA:HB3	2:B:238:LEU:HA	1.30	1.09
2:B:211:LEU:HB3	2:B:244:ILE:CD1	1.91	0.98
1:E:97:ALA:O	1:E:101:ALA:HB2	1.74	0.88
1:E:97:ALA:O	1:E:101:ALA:CB	2.30	0.79

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	182/190 (96%)	178 (98%)	4 (2%)	0	100	100
1	C	184/190 (97%)	181 (98%)	3 (2%)	0	100	100
1	E	168/190 (88%)	165 (98%)	3 (2%)	0	100	100
1	G	163/190 (86%)	159 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	115/119 (97%)	113 (98%)	2 (2%)	0	100	100
2	D	115/119 (97%)	112 (97%)	3 (3%)	0	100	100
2	F	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
2	H	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
All	All	1157/1236 (94%)	1136 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	135/143 (94%)	133 (98%)	2 (2%)	65	80
1	C	138/143 (96%)	137 (99%)	1 (1%)	84	90
1	E	126/143 (88%)	124 (98%)	2 (2%)	62	79
1	G	121/143 (85%)	118 (98%)	3 (2%)	47	69
2	B	99/102 (97%)	97 (98%)	2 (2%)	55	74
2	D	101/102 (99%)	99 (98%)	2 (2%)	55	74
2	F	100/102 (98%)	99 (99%)	1 (1%)	76	86
2	H	101/102 (99%)	98 (97%)	3 (3%)	41	64
All	All	921/980 (94%)	905 (98%)	16 (2%)	60	78

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	239	ASN
2	H	225	ASP
2	B	208	ARG
2	F	227	ARG
1	G	92	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	285	HIS
2	D	295	GLN
2	H	295	GLN
2	H	216	ASN
2	H	249	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	184/190 (96%)	-0.09	11 (5%)	21	16	53, 91, 142, 171	0
1	C	186/190 (97%)	-0.25	6 (3%)	47	37	55, 97, 167, 258	0
1	E	174/190 (91%)	0.02	11 (6%)	20	14	84, 147, 232, 357	0
1	G	169/190 (88%)	-0.19	6 (3%)	42	33	87, 149, 208, 247	0
2	B	117/119 (98%)	-0.27	5 (4%)	35	28	42, 83, 133, 192	0
2	D	117/119 (98%)	-0.18	1 (0%)	84	77	51, 91, 130, 183	0
2	F	117/119 (98%)	1.12	26 (22%)	0	0	86, 138, 198, 228	0
2	H	117/119 (98%)	0.51	14 (11%)	4	4	73, 121, 154, 182	0
All	All	1181/1236 (95%)	0.04	80 (6%)	17	12	42, 115, 193, 357	0

The worst 5 of 80 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	204	ALA	9.9
2	F	205	ALA	9.7
2	B	204	ALA	9.7
2	F	206	THR	9.7
2	F	203	ALA	9.1

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 monosaccharides 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.