



wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 26, 2017 – 02:50 PM EDT

PDB ID : 4E2L
Title : Crystal Structure of the periplasmic domain of mutant FepE LPS O-antigen chain length regulator protein
Authors : Kalynych, S.; Yao, D.; Magee, J.D.; Cygler, M.
Deposited on : unknown
Resolution : 2.80 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

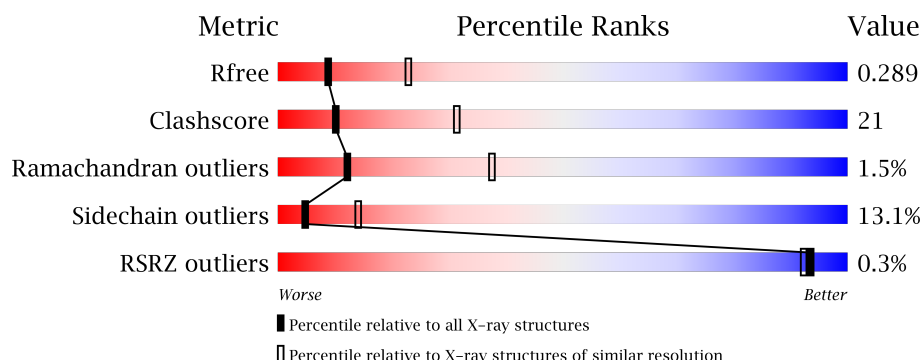
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	271	
1	B	271	
1	C	271	
1	D	271	
1	E	271	

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Mol	Chain	Length	Quality of chain
1	F	271	 53% 32% 5% 10%
1	G	271	 60% 23% 6% 11%
1	H	271	 59% 25% 5% 11%
1	I	271	 55% 28% 6% 11%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16883 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 Ferric enterobactin (Enterochelin) transport.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1881	1204	306	368	3			
1	B	240	Total	C	N	O	S	0	0	0
			1903	1213	317	370	3			
1	C	246	Total	C	N	O	S	0	0	0
			1893	1209	314	367	3			
1	D	240	Total	C	N	O	S	0	0	0
			1869	1195	309	362	3			
1	E	241	Total	C	N	O	S	0	0	0
			1848	1178	301	366	3			
1	F	244	Total	C	N	O	S	0	0	0
			1898	1214	314	367	3			
1	G	240	Total	C	N	O	S	0	0	0
			1859	1193	303	360	3			
1	H	242	Total	C	N	O	S	0	0	0
			1858	1190	306	359	3			
1	I	242	Total	C	N	O	S	0	0	0
			1874	1198	314	359	3			

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
A	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
A	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
A	262	GLY	-	LINKER	UNP Q8XBV8
A	263	SER	-	LINKER	UNP Q8XBV8
A	264	GLY	-	LINKER	UNP Q8XBV8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
B	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
B	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
B	262	GLY	-	LINKER	UNP Q8XBV8
B	263	SER	-	LINKER	UNP Q8XBV8
B	264	GLY	-	LINKER	UNP Q8XBV8
C	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
C	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
C	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
C	262	GLY	-	LINKER	UNP Q8XBV8
C	263	SER	-	LINKER	UNP Q8XBV8
C	264	GLY	-	LINKER	UNP Q8XBV8
D	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
D	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
D	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
D	262	GLY	-	LINKER	UNP Q8XBV8
D	263	SER	-	LINKER	UNP Q8XBV8
D	264	GLY	-	LINKER	UNP Q8XBV8
E	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
E	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
E	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
E	262	GLY	-	LINKER	UNP Q8XBV8

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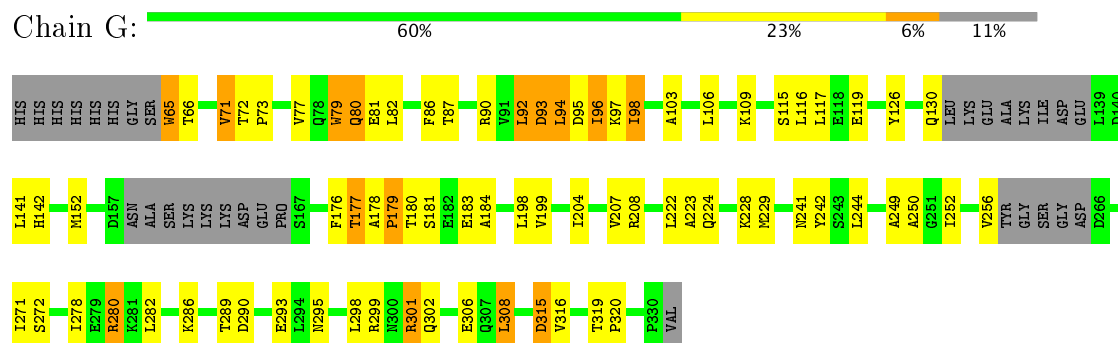
Chain	Residue	Modelled	Actual	Comment	Reference
E	263	SER	-	LINKER	UNP Q8XBV8
E	264	GLY	-	LINKER	UNP Q8XBV8
F	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
F	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
F	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
F	262	GLY	-	LINKER	UNP Q8XBV8
F	263	SER	-	LINKER	UNP Q8XBV8
F	264	GLY	-	LINKER	UNP Q8XBV8
G	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
G	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
G	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
G	262	GLY	-	LINKER	UNP Q8XBV8
G	263	SER	-	LINKER	UNP Q8XBV8
G	264	GLY	-	LINKER	UNP Q8XBV8
H	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
H	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8
H	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
H	262	GLY	-	LINKER	UNP Q8XBV8
H	263	SER	-	LINKER	UNP Q8XBV8
H	264	GLY	-	LINKER	UNP Q8XBV8
I	57	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	58	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	59	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	60	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	61	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	62	HIS	-	EXPRESSION TAG	UNP Q8XBV8
I	63	GLY	-	EXPRESSION TAG	UNP Q8XBV8

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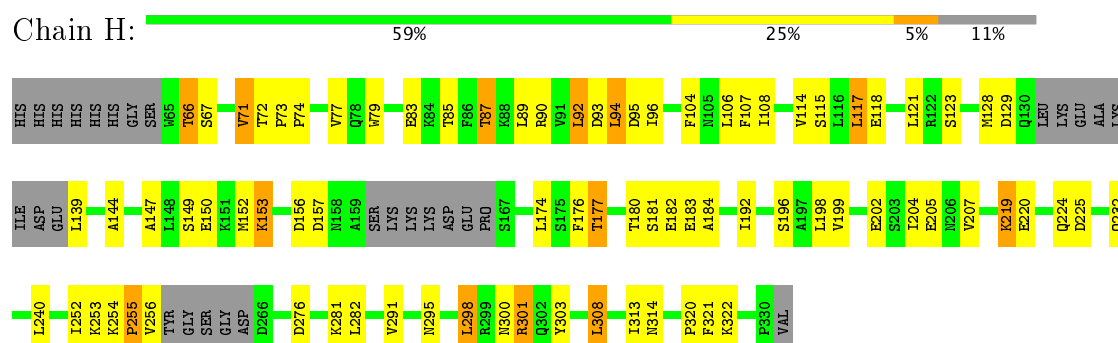
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Chain	Residue	Modelled	Actual	Comment	Reference
I	64	SER	-	EXPRESSION TAG	UNP Q8XBV8
I	262	GLY	-	LINKER	UNP Q8XBV8
I	263	SER	-	LINKER	UNP Q8XBV8
I	264	GLY	-	LINKER	UNP Q8XBV8

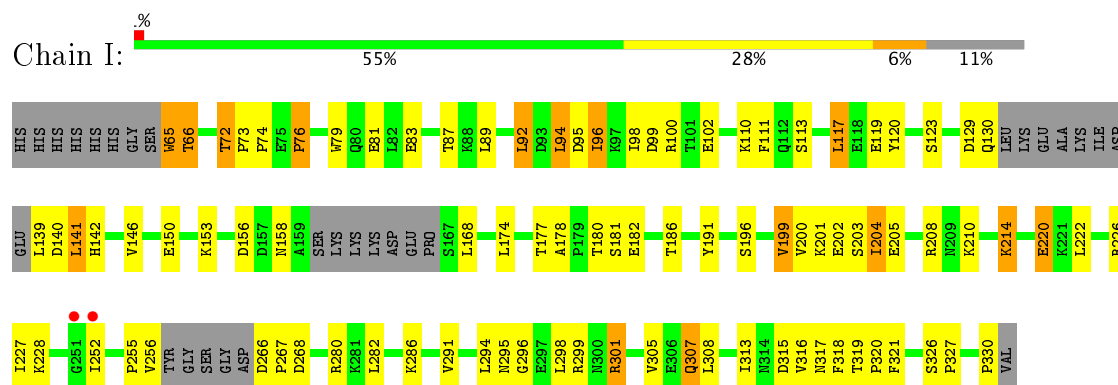
- Molecule 1: Ferric enterobactin (Enterochelin) transport



- Molecule 1: Ferric enterobactin (Enterochelin) transport



- Molecule 1: Ferric enterobactin (Enterochelin) transport



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	208.31Å 141.26Å 136.89Å 90.00° 107.03° 90.00°	Depositor
Resolution (Å)	49.72 – 2.80 49.71 – 2.79	Depositor EDS
% Data completeness (in resolution range)	86.8 (49.72-2.80) 98.0 (49.71-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	11.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.15 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.242 , 0.289 0.238 , 0.289	Depositor DCC
R_{free} test set	4618 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16883	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% 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	0.50	0/1911	0.63	0/2594
1	B	0.43	0/1932	0.60	1/2617 (0.0%)
1	C	0.44	0/1923	0.63	1/2617 (0.0%)
1	D	0.44	0/1899	0.57	0/2577
1	E	0.47	0/1877	0.60	0/2557
1	F	0.47	0/1928	0.59	0/2618
1	G	0.46	0/1889	0.58	0/2566
1	H	0.43	0/1887	0.59	0/2565
1	I	0.44	0/1903	0.60	0/2585
All	All	0.45	0/17149	0.60	2/23296 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	LEU	CA-CB-CG	6.11	129.35	115.30
1	B	222	LEU	CA-CB-CG	5.41	127.75	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	THR	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	1881	0	1854	113	0
1	B	1903	0	1909	86	0
1	C	1893	0	1832	101	0
1	D	1869	0	1830	80	0
1	E	1848	0	1780	83	0
1	F	1898	0	1862	101	0
1	G	1859	0	1827	73	0
1	H	1858	0	1823	64	0
1	I	1874	0	1856	79	0
All	All	16883	0	16573	702	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 21.

The worst 5 of 702 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:79:TRP:CZ2	1:G:98:ILE:HD11	1.80	1.16
1:A:222:LEU:HD13	1:A:301:ARG:HG2	1.27	1.15
1:I:301:ARG:HH21	1:I:301:ARG:HG2	1.06	1.11
1:G:280:ARG:HH11	1:G:280:ARG:HG3	1.08	1.11
1:B:301:ARG:HH11	1:B:301:ARG:HG2	1.10	1.08

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	232/271 (86%)	211 (91%)	17 (7%)	4 (2%)	11	34
1	B	232/271 (86%)	212 (91%)	14 (6%)	6 (3%)	6	21
1	C	238/271 (88%)	214 (90%)	18 (8%)	6 (2%)	6	22
1	D	232/271 (86%)	215 (93%)	14 (6%)	3 (1%)	14	41
1	E	233/271 (86%)	212 (91%)	18 (8%)	3 (1%)	14	41
1	F	236/271 (87%)	212 (90%)	23 (10%)	1 (0%)	38	72
1	G	232/271 (86%)	214 (92%)	15 (6%)	3 (1%)	14	41
1	H	234/271 (86%)	219 (94%)	14 (6%)	1 (0%)	38	72
1	I	234/271 (86%)	214 (92%)	16 (7%)	4 (2%)	11	34
All	All	2103/2439 (86%)	1923 (91%)	149 (7%)	31 (2%)	12	37

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	PRO
1	C	139	LEU
1	C	140	ASP
1	D	112	GLN
1	D	255	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	204/243 (84%)	172 (84%)	32 (16%)	3	9
1	B	210/243 (86%)	184 (88%)	26 (12%)	5	16
1	C	197/243 (81%)	166 (84%)	31 (16%)	3	9
1	D	198/243 (82%)	173 (87%)	25 (13%)	5	16
1	E	196/243 (81%)	170 (87%)	26 (13%)	4	13
1	F	201/243 (83%)	181 (90%)	20 (10%)	9	26
1	G	198/243 (82%)	172 (87%)	26 (13%)	5	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	196/243 (81%)	170 (87%)	26 (13%)	4	13
1	I	200/243 (82%)	176 (88%)	24 (12%)	6	18
All	All	1800/2187 (82%)	1564 (87%)	236 (13%)	5	14

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	216	GLN
1	E	203	SER
1	I	94	LEU
1	D	241	ASN
1	E	91	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	224	GLN
1	I	314	ASN
1	I	158	ASN
1	F	307	GLN
1	I	307	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 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 [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	240/271 (88%)	-0.07	1 (0%) 92 90	41, 56, 74, 88	0
1	B	240/271 (88%)	-0.10	0 100 100	44, 60, 77, 89	0
1	C	246/271 (90%)	-0.01	1 (0%) 92 90	44, 64, 80, 89	0
1	D	240/271 (88%)	0.01	2 (0%) 86 81	43, 62, 82, 95	0
1	E	241/271 (88%)	-0.08	1 (0%) 92 90	41, 61, 80, 94	0
1	F	244/271 (90%)	-0.10	0 100 100	38, 58, 78, 89	0
1	G	240/271 (88%)	-0.13	0 100 100	40, 56, 76, 94	0
1	H	242/271 (89%)	-0.09	0 100 100	42, 56, 75, 97	0
1	I	242/271 (89%)	-0.07	2 (0%) 86 81	39, 58, 75, 89	0
All	All	2175/2439 (89%)	-0.07	7 (0%) 93 92	38, 59, 79, 97	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	252	ILE	4.6
1	I	251	GLY	3.6
1	D	252	ILE	3.2
1	A	250	ALA	3.0
1	D	251	GLY	2.9

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.