



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 4, 2021 – 08:42 PM JST

PDB ID : 5AWG
Title : Crystal structure of Hg-bound SufB-SufC-SufD complex from Escherichia coli
Authors : Hirabayashi, K.; Wada, K.
Deposited on : 2015-07-03
Resolution : 4.28 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.23.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

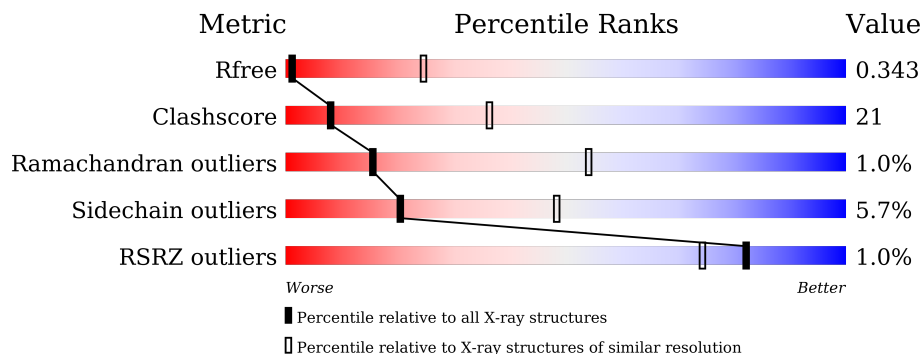
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.28 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.



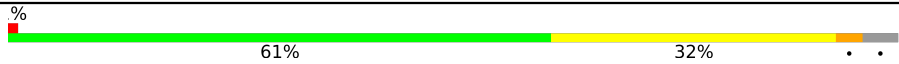

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1001 (4.76-3.80)
Clashscore	141614	1063 (4.76-3.80)
Ramachandran outliers	138981	1018 (4.76-3.80)
Sidechain outliers	138945	1002 (4.76-3.80)
RSRZ outliers	127900	1074 (4.84-3.70)

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	495	 41% 32% 23% 2%
1	E	495	 33% 37% 25% 5% 2%
2	B	423	 56% 27% 15% 2% 2%
2	F	423	 45% 35% 16% 2% 2%
3	C	248	 62% 29% 5% 4%
3	D	248	 62% 30% 5% 2%

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Mol	Chain	Length	Quality of chain
3	G	248	 <p>%</p> <p>61% 32% . .</p>
3	H	248	 <p>%</p> <p>58% 33% . . 5%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18808 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 FeS cluster assembly protein SufB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	380	Total	C	N	O	S	0	0	0
			2968	1869	509	572	18			
1	E	372	Total	C	N	O	S	0	0	0
			2910	1833	498	561	18			

- Molecule 2 is a protein called FeS cluster assembly protein SufD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	361	Total	C	N	O	S	0	0	0
			2798	1743	514	533	8			
2	F	355	Total	C	N	O	S	0	0	0
			2752	1712	507	525	8			

- Molecule 3 is a protein called Probable ATP-dependent transporter SufC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	237	Total	C	N	O	S	0	0	0
			1846	1169	312	358	7			
3	D	235	Total	C	N	O	S	0	0	0
			1829	1158	310	354	7			
3	G	239	Total	C	N	O	S	0	0	0
			1864	1179	315	363	7			
3	H	236	Total	C	N	O	S	0	0	0
			1837	1164	311	355	7			

- Molecule 4 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
4	A	1	Total	Hg	0	0
			1	1		
4	B	1	Total	Hg	0	0
			1	1		

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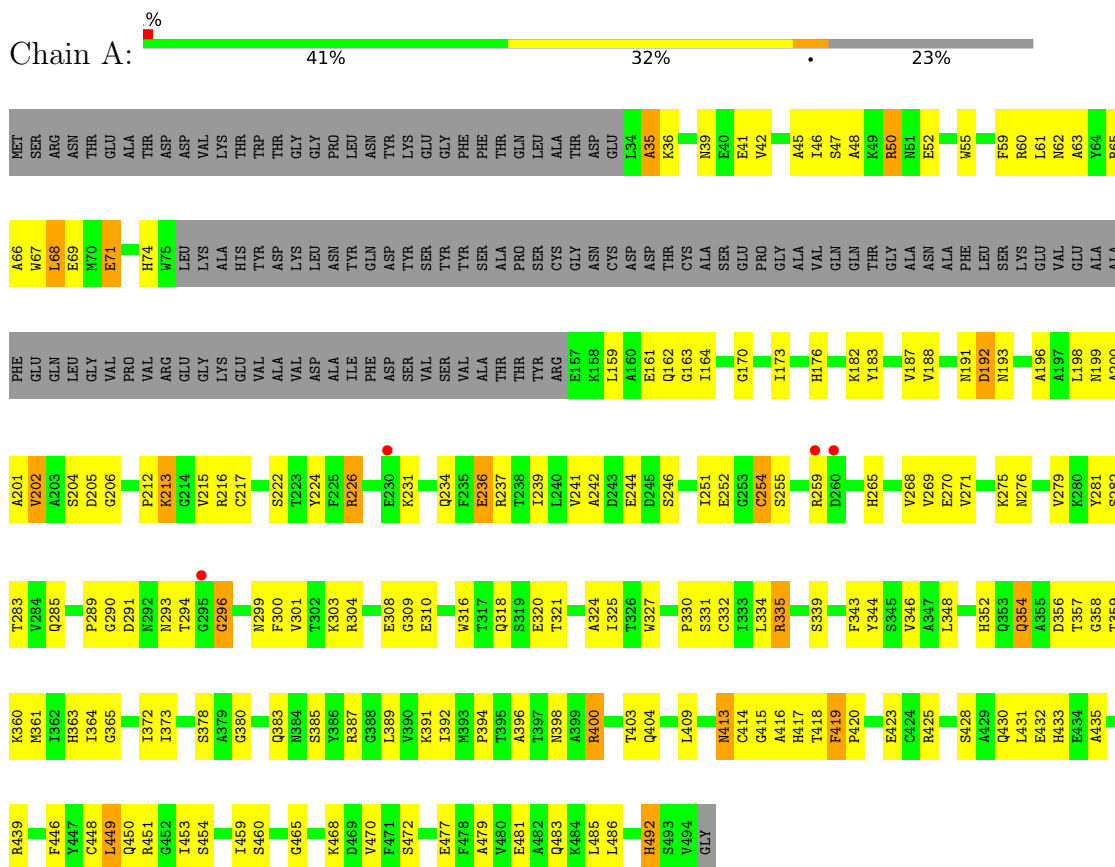
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total 1	Hg 1	0	0
4	F	1	Total 1	Hg 1	0	0

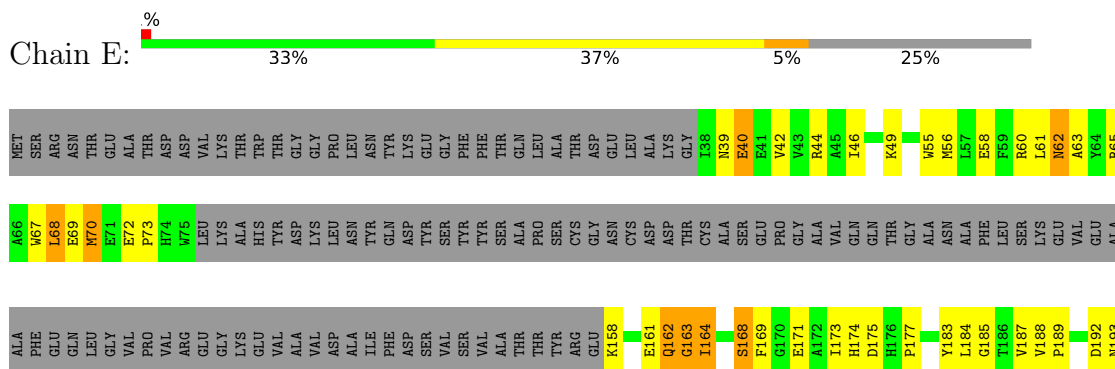
3 Residue-property plots

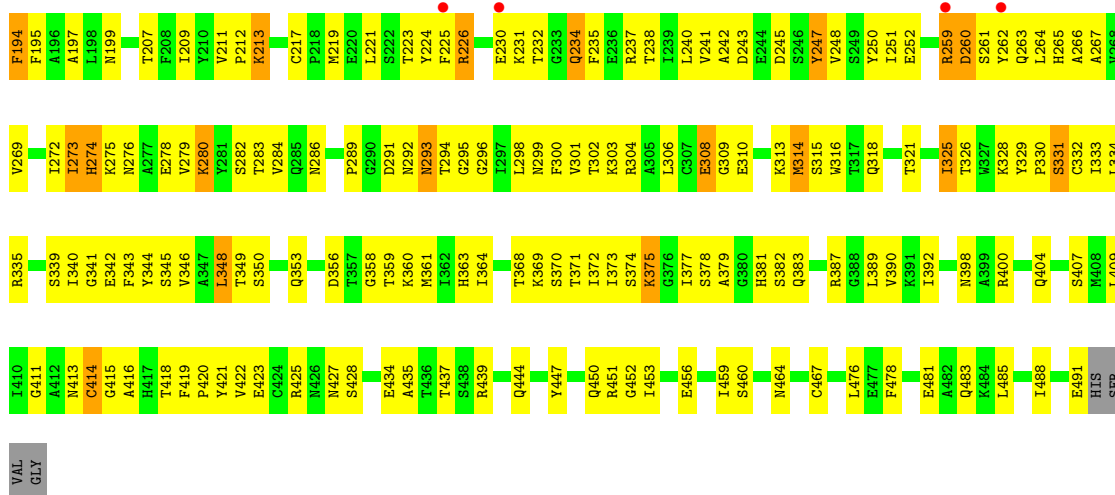
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: FeS cluster assembly protein SufB

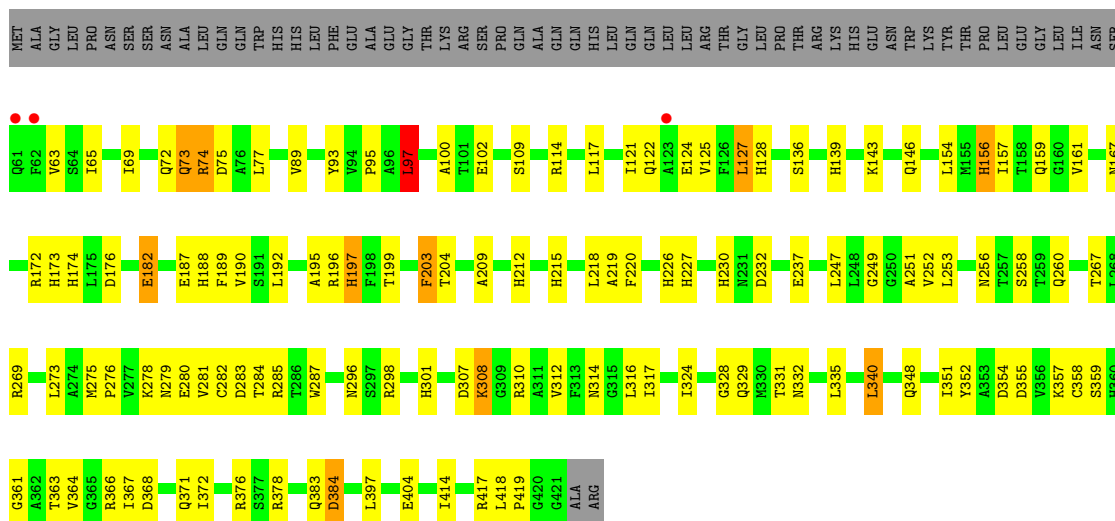


- Molecule 1: FeS cluster assembly protein SufB

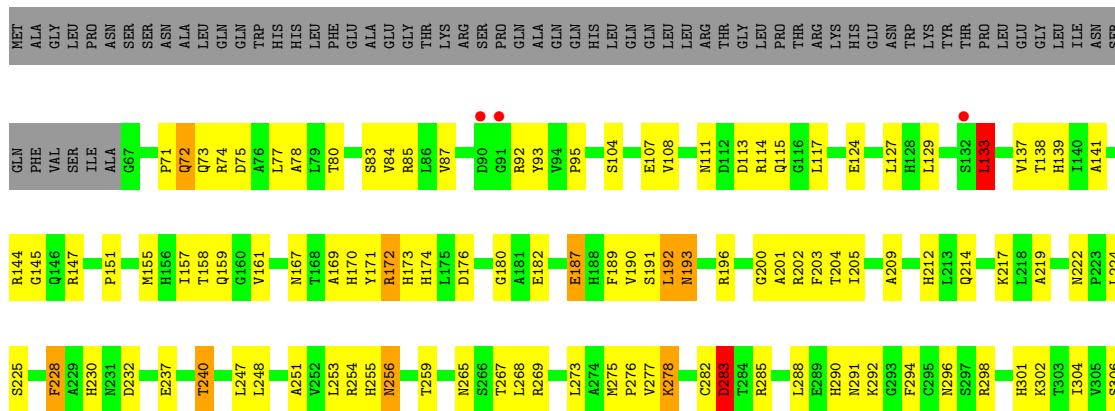
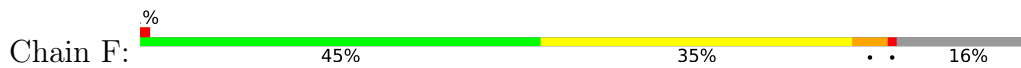




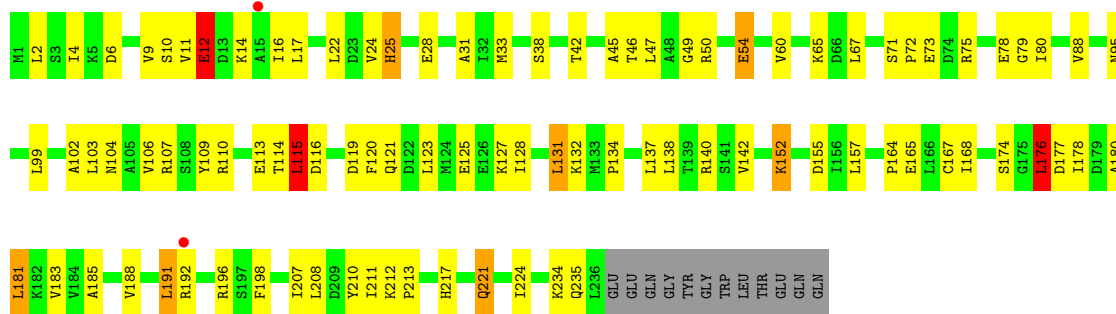
• Molecule 2: FeS cluster assembly protein SufD



• Molecule 2: FeS cluster assembly protein SufD



Chain H: %
58% 33% •• 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.85Å 139.38Å 124.41Å 90.00° 113.55° 90.00°	Depositor
Resolution (Å)	43.94 – 4.28 47.93 – 4.28	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.94-4.28) 92.9 (47.93-4.28)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 4.29Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.295 , 0.340 0.299 , 0.343	Depositor DCC
R_{free} test set	1286 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	94.9	Xtrriage
Anisotropy	0.390	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.025 for l,-k,h	Xtrriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	18808	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	0.37	0/3031	0.76	4/4104 (0.1%)
1	E	0.40	0/2972	0.84	2/4025 (0.0%)
2	B	0.31	0/2847	0.69	2/3858 (0.1%)
2	F	0.34	0/2800	0.82	5/3794 (0.1%)
3	C	0.34	0/1875	0.84	3/2529 (0.1%)
3	D	0.31	0/1858	0.76	0/2506
3	G	0.32	0/1893	0.69	2/2553 (0.1%)
3	H	0.33	0/1866	0.90	10/2517 (0.4%)
All	All	0.34	0/19142	0.79	28/25886 (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	E	0	2
2	F	0	1
3	D	0	1
3	G	0	2
3	H	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	LEU	CA-CB-CG	7.68	132.96	115.30
1	A	68	LEU	CB-CG-CD1	-7.41	98.41	111.00
2	B	97	LEU	CA-CB-CG	7.18	131.83	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	115	LEU	CA-CB-CG	7.01	131.42	115.30
2	F	192	LEU	CB-CA-C	-6.99	96.93	110.20

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	113	GLU	Peptide
1	E	231	LYS	Peptide
1	E	61	LEU	Peptide
2	F	321	GLN	Sidechain
3	G	115	LEU	Peptide

5.2 Too-close contacts [i](#)

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	2968	0	2876	150	0
1	E	2910	0	2816	184	0
2	B	2798	0	2754	89	0
2	F	2752	0	2707	150	0
3	C	1846	0	1857	73	0
3	D	1829	0	1840	57	0
3	G	1864	0	1871	59	0
3	H	1837	0	1851	80	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	18808	0	18572	798	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 798 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:E:161:GLU:HA	1:E:162:GLN:HG3	1.46	0.98
2:F:230:HIS:HA	2:F:256:ASN:ND2	1.81	0.95
1:E:314:MET:SD	1:E:314:MET:N	2.43	0.91
2:B:249:GLY:HA2	2:B:417:ARG:HH22	1.36	0.91
1:A:316:TRP:HB3	1:A:318:GLN:HE22	1.34	0.90

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	376/495 (76%)	350 (93%)	18 (5%)	8 (2%)	7	39
1	E	368/495 (74%)	339 (92%)	26 (7%)	3 (1%)	19	60
2	B	359/423 (85%)	344 (96%)	14 (4%)	1 (0%)	41	76
2	F	353/423 (84%)	337 (96%)	14 (4%)	2 (1%)	25	65
3	C	235/248 (95%)	221 (94%)	11 (5%)	3 (1%)	12	49
3	D	233/248 (94%)	222 (95%)	10 (4%)	1 (0%)	34	72
3	G	237/248 (96%)	222 (94%)	12 (5%)	3 (1%)	12	49
3	H	234/248 (94%)	222 (95%)	10 (4%)	2 (1%)	17	56
All	All	2395/2828 (85%)	2257 (94%)	115 (5%)	23 (1%)	15	54

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	163	GLY
1	A	202	VAL
1	A	259	ARG
1	A	289	PRO

5.3.2 Protein sidechains [i](#)

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	320/413 (78%)	304 (95%)	16 (5%)	24 51
1	E	314/413 (76%)	283 (90%)	31 (10%)	8 29
2	B	297/350 (85%)	282 (95%)	15 (5%)	24 51
2	F	292/350 (83%)	270 (92%)	22 (8%)	13 40
3	C	203/212 (96%)	194 (96%)	9 (4%)	28 54
3	D	201/212 (95%)	192 (96%)	9 (4%)	27 54
3	G	205/212 (97%)	198 (97%)	7 (3%)	37 61
3	H	202/212 (95%)	195 (96%)	7 (4%)	36 61
All	All	2034/2374 (86%)	1918 (94%)	116 (6%)	20 48

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	217	CYS
3	H	12	GLU
1	E	314	MET
3	H	6	ASP
2	F	349	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	293	ASN
1	E	381	HIS
2	F	360	HIS
1	E	353	GLN
1	E	404	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	380/495 (76%)	0.00	4 (1%) 80 72	62, 101, 137, 154	0
1	E	372/495 (75%)	0.03	4 (1%) 80 72	77, 111, 147, 178	0
2	B	361/423 (85%)	-0.14	3 (0%) 86 79	57, 96, 127, 142	0
2	F	355/423 (83%)	-0.14	3 (0%) 86 79	73, 104, 132, 149	0
3	C	237/248 (95%)	-0.13	1 (0%) 92 87	81, 110, 135, 156	0
3	D	235/248 (94%)	0.01	4 (1%) 70 61	74, 118, 149, 165	0
3	G	239/248 (96%)	-0.13	3 (1%) 77 68	77, 108, 142, 162	0
3	H	236/248 (95%)	0.06	2 (0%) 86 79	85, 137, 166, 171	0
All	All	2415/2828 (85%)	-0.06	24 (0%) 82 74	57, 108, 147, 178	0

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	91	GLY	3.6
1	E	262	TYR	3.5
2	B	61	GLN	3.4
2	F	132	SER	3.3
1	A	295	GLY	3.2

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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HG	B	600	1/1	0.88	0.11	172,172,172,172	0
4	HG	F	600	1/1	0.94	0.10	176,176,176,176	0
4	HG	A	600	1/1	0.97	0.14	128,128,128,128	0
4	HG	E	600	1/1	0.98	0.06	117,117,117,117	0

6.5 Other polymers [i](#)

There are no such residues in this entry.