



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 10:59 AM UTC

PDB ID : 5AWF / pdb_00005awf
Title : Crystal structure of SufB-SufC-SufD complex from Escherichia coli
Authors : Hirabayashi, K.; Wada, K.
Deposited on : 2015-07-03
Resolution : 2.96 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

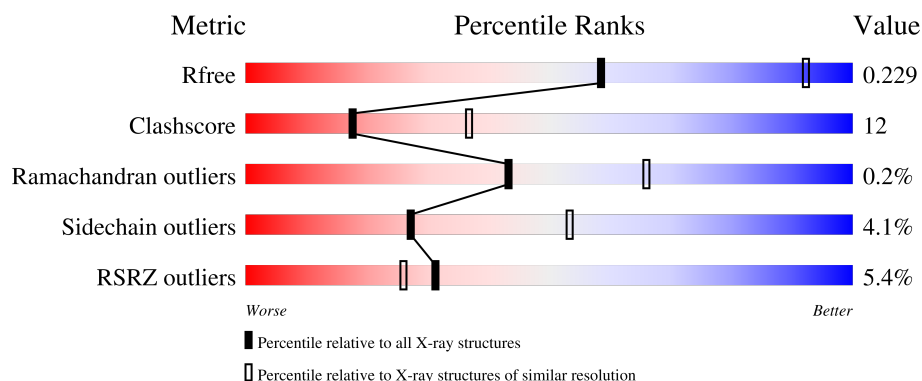
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	5% 58%18%22%
1	E	495	5% 52%23%23%
2	B	423	% 81%16%
2	F	423	4% 76%20%
3	C	248	6% 74%21%

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Mol	Chain	Length	Quality of chain
3	D	248	6% 64% 24% 6% 5%
3	G	248	4% 76% 19%
3	H	248	11% 56% 31% 6% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19914 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.

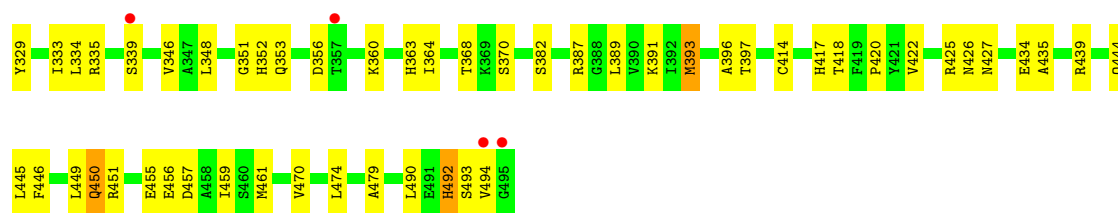
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	385	Total	C	N	O	S	0	0	0
			3004	1892	517	577	18			
1	E	381	Total	C	N	O	S	0	0	0
			2972	1872	511	571	18			

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

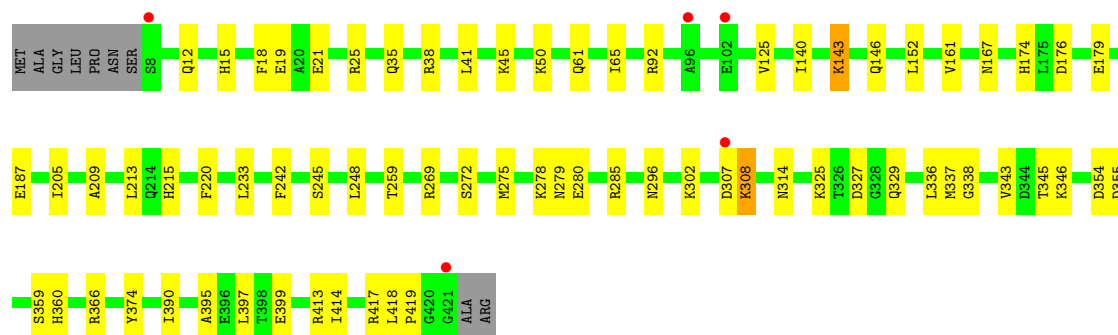
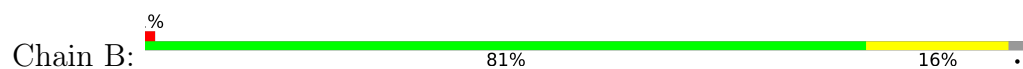
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	414	Total	C	N	O	S	0	0	0
			3238	2019	599	612	8			
2	F	414	Total	C	N	O	S	0	0	0
			3238	2019	599	612	8			

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

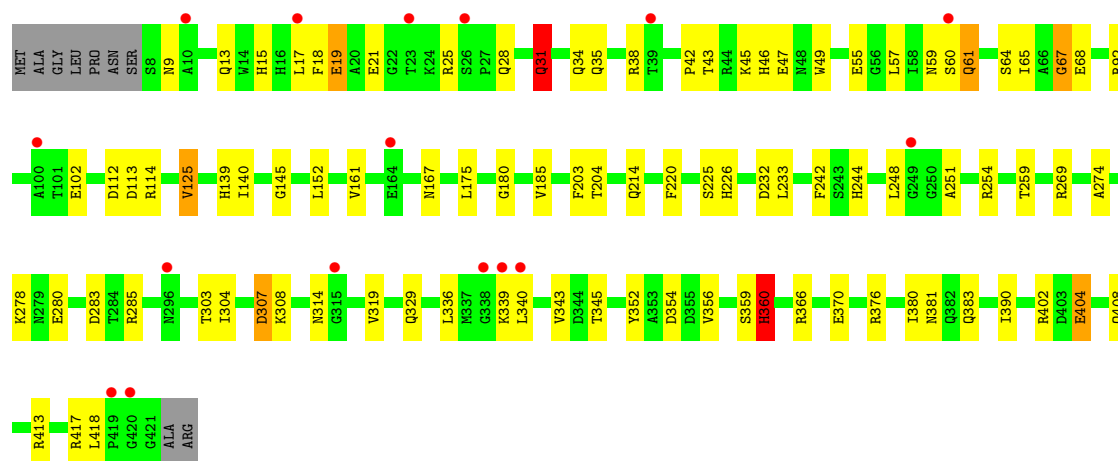
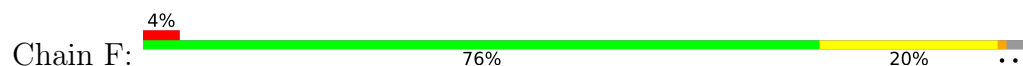
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	243	Total	C	N	O	S	0	0	0
			1898	1203	320	368	7			
3	D	235	Total	C	N	O	S	0	0	0
			1829	1158	310	354	7			
3	G	243	Total	C	N	O	S	0	0	0
			1898	1203	320	368	7			
3	H	236	Total	C	N	O	S	0	0	0
			1837	1164	311	355	7			



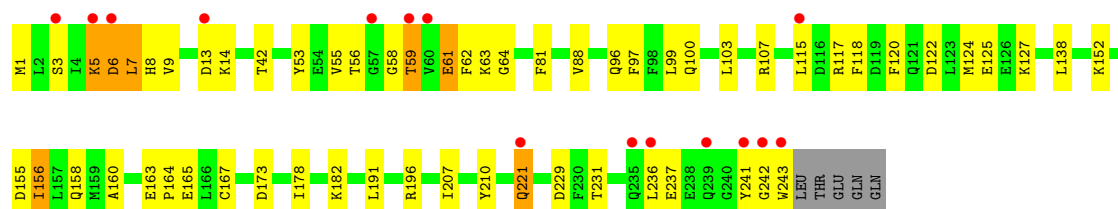
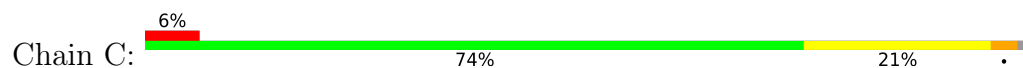
• Molecule 2: FeS cluster assembly protein SufD



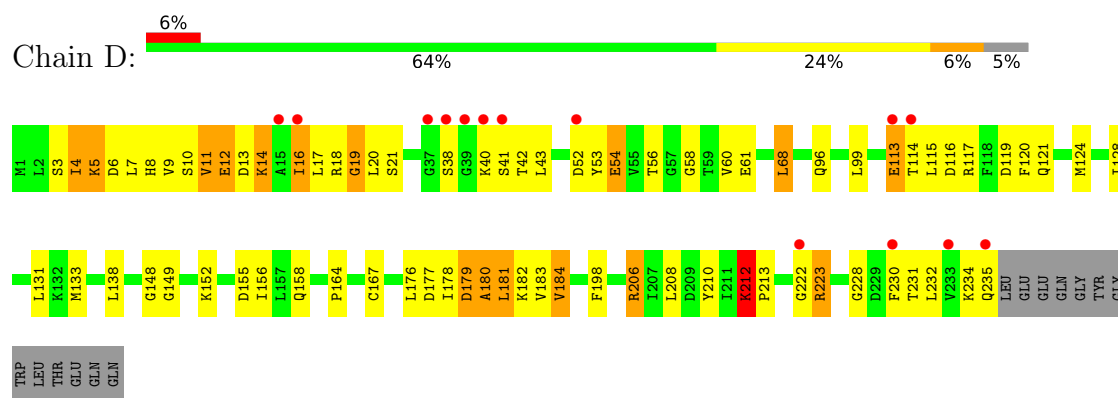
• Molecule 2: FeS cluster assembly protein SufD



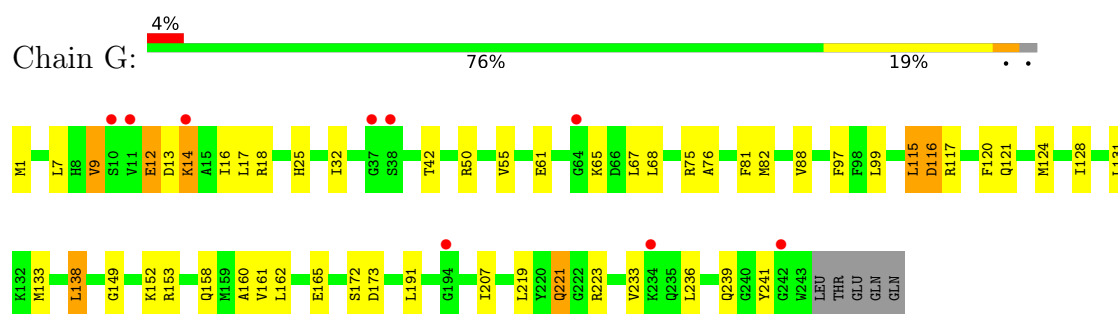
• Molecule 3: Probable ATP-dependent transporter SufC



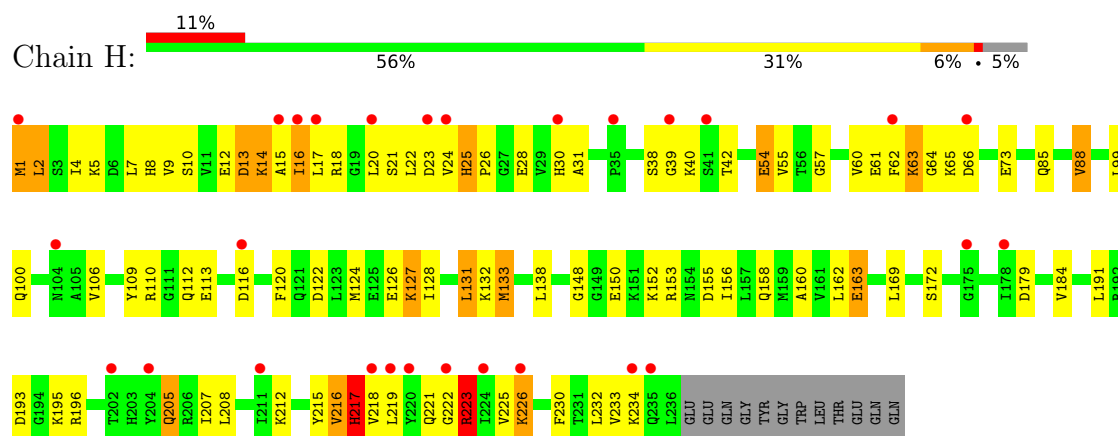
• Molecule 3: Probable ATP-dependent transporter SufC



• Molecule 3: Probable ATP-dependent transporter SufC



• Molecule 3: Probable ATP-dependent transporter SufC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.47Å 139.56Å 124.68Å 90.00° 113.10° 90.00°	Depositor
Resolution (Å)	41.11 – 2.96 41.11 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.2 (41.11-2.96) 94.7 (41.11-2.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.187 , 0.226 0.192 , 0.229	Depositor DCC
R_{free} test set	1995 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	63.4	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19914	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.41	1/3068 (0.0%)	0.92	9/4153 (0.2%)
1	E	0.40	0/3035	0.92	11/4108 (0.3%)
2	B	0.34	0/3300	0.79	0/4473
2	F	0.38	0/3300	0.87	5/4473 (0.1%)
3	C	0.42	0/1930	0.89	4/2604 (0.2%)
3	D	0.45	0/1858	0.97	6/2506 (0.2%)
3	G	0.39	0/1930	0.86	2/2604 (0.1%)
3	H	0.64	2/1866 (0.1%)	1.26	21/2517 (0.8%)
All	All	0.42	3/20287 (0.0%)	0.93	58/27438 (0.2%)

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	2
1	E	0	3
3	D	0	3
3	G	0	1
3	H	0	2
All	All	0	11

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	217	HIS	CA-CB	5.65	1.62	1.53
3	H	217	HIS	CA-C	5.60	1.59	1.52
1	A	294	THR	CA-C	5.22	1.59	1.52

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	14	LYS	CA-C-N	-12.13	106.28	122.42
3	H	14	LYS	C-N-CA	-12.13	106.28	122.42
1	A	288	PHE	CA-C-N	9.23	131.37	119.84
1	A	288	PHE	C-N-CA	9.23	131.37	119.84
3	H	131	LEU	N-CA-C	9.18	124.21	112.92

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	294	THR	Peptide
1	A	308	GLU	Peptide
3	D	113	GLU	Peptide
3	D	12	GLU	Peptide
3	D	14	LYS	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	3004	0	2916	64	0
1	E	2972	0	2887	88	0
2	B	3238	0	3184	43	0
2	F	3238	0	3184	64	0
3	C	1898	0	1896	44	0
3	D	1829	0	1840	83	0
3	G	1898	0	1896	37	0
3	H	1837	0	1851	95	0
All	All	19914	0	19654	489	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 12.

The worst 5 of 489 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:492:HIS:CE1	1:E:493:SER:HB3	1.82	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:30:HIS:HD1	3:H:215:TYR:HB2	1.22	1.03
3:H:61:GLU:OE2	3:H:64:GLY:N	1.96	0.97
3:D:12:GLU:HG3	3:D:14:LYS:HG3	1.42	0.97
2:F:381:ASN:HA	3:H:73:GLU:HG2	1.49	0.95

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	381/495 (77%)	364 (96%)	15 (4%)	2 (0%)	24	49
1	E	377/495 (76%)	367 (97%)	10 (3%)	0	100	100
2	B	412/423 (97%)	408 (99%)	4 (1%)	0	100	100
2	F	412/423 (97%)	402 (98%)	9 (2%)	1 (0%)	43	66
3	C	241/248 (97%)	235 (98%)	6 (2%)	0	100	100
3	D	233/248 (94%)	223 (96%)	10 (4%)	0	100	100
3	G	241/248 (97%)	232 (96%)	8 (3%)	1 (0%)	30	53
3	H	234/248 (94%)	226 (97%)	8 (3%)	0	100	100
All	All	2531/2828 (90%)	2457 (97%)	70 (3%)	4 (0%)	43	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	VAL
1	A	289	PRO
2	F	60	SER
3	G	12	GLU

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	323/413 (78%)	310 (96%)	13 (4%)	28	53
1	E	320/413 (78%)	303 (95%)	17 (5%)	20	45
2	B	344/350 (98%)	337 (98%)	7 (2%)	48	71
2	F	344/350 (98%)	334 (97%)	10 (3%)	37	61
3	C	207/212 (98%)	200 (97%)	7 (3%)	32	58
3	D	201/212 (95%)	189 (94%)	12 (6%)	17	40
3	G	207/212 (98%)	197 (95%)	10 (5%)	23	48
3	H	202/212 (95%)	189 (94%)	13 (6%)	16	38
All	All	2148/2374 (90%)	2059 (96%)	89 (4%)	27	53

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	21	GLU
3	G	131	LEU
2	F	35	GLN
2	F	404	GLU
3	G	223	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	318	GLN
2	F	210	ASN
3	H	25	HIS
2	F	122	GLN
2	F	214	GLN

5.3.3 RNA ⓘ

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	385/495 (77%)	0.17	26 (6%)	23 20	29, 63, 127, 184	0
1	E	381/495 (76%)	0.41	24 (6%)	26 22	43, 81, 140, 198	0
2	B	414/423 (97%)	-0.12	5 (1%)	76 71	28, 61, 100, 154	0
2	F	414/423 (97%)	0.26	16 (3%)	43 35	44, 78, 123, 176	0
3	C	243/248 (97%)	0.34	15 (6%)	26 22	43, 80, 140, 174	0
3	D	235/248 (94%)	0.47	14 (5%)	27 23	44, 90, 153, 194	0
3	G	243/248 (97%)	0.33	9 (3%)	45 37	46, 80, 128, 163	0
3	H	236/248 (95%)	0.78	28 (11%)	9 8	47, 114, 176, 266	0
All	All	2551/2828 (90%)	0.29	137 (5%)	31 26	28, 78, 143, 266	0

The worst 5 of 137 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	222	GLY	7.3
1	A	296	GLY	5.9
1	A	35	ALA	5.0
1	A	295	GLY	4.7
2	F	296	ASN	4.6

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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.