



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 20, 2016 – 05:30 AM EST

PDB ID : 5IUN
Title : Crystal structure of the DesK-DesR complex in the phosphatase state
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Deposited on : 2016-03-18
Resolution : 2.79 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

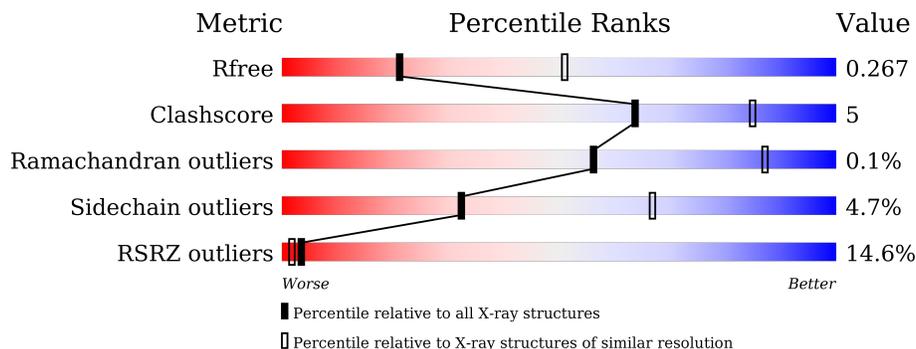
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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	224	 26% 82% 14% .
1	B	224	 12% 85% 10% . .
1	E	224	 11% 87% 10% . .
2	C	139	 % 79% 14% . 6%
2	D	139	 24% 81% 12% . 6%
2	F	139	 4% 79% 12% . . 7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8112 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 Sensor histidine kinase DesK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	Total 1689	C 1055	N 305	O 323	S 6	0	0	0
1	B	216	Total 1697	C 1061	N 301	O 329	S 6	0	0	0
1	E	220	Total 1707	C 1066	N 303	O 332	S 6	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLY	-	expression tag	UNP O34757
A	148	SER	-	expression tag	UNP O34757
A	149	GLY	-	expression tag	UNP O34757
A	150	ILE	SER	engineered mutation	UNP O34757
A	153	LEU	SER	engineered mutation	UNP O34757
A	157	ILE	ARG	engineered mutation	UNP O34757
B	147	GLY	-	expression tag	UNP O34757
B	148	SER	-	expression tag	UNP O34757
B	149	GLY	-	expression tag	UNP O34757
B	150	ILE	SER	engineered mutation	UNP O34757
B	153	LEU	SER	engineered mutation	UNP O34757
B	157	ILE	ARG	engineered mutation	UNP O34757
E	147	GLY	-	expression tag	UNP O34757
E	148	SER	-	expression tag	UNP O34757
E	149	GLY	-	expression tag	UNP O34757
E	150	ILE	SER	engineered mutation	UNP O34757
E	153	LEU	SER	engineered mutation	UNP O34757
E	157	ILE	ARG	engineered mutation	UNP O34757

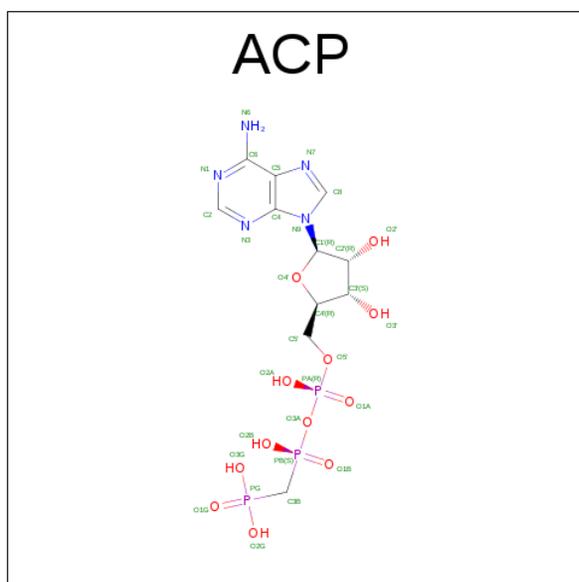
- Molecule 2 is a protein called Transcriptional regulatory protein DesR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	131	Total	C	N	O	S	0	0	0
			979	618	162	190	9			
2	D	130	Total	C	N	O	S	0	0	0
			946	600	154	184	8			
2	F	129	Total	C	N	O	S	0	0	0
			954	604	156	185	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	GLY	-	expression tag	UNP O34723
C	-2	SER	-	expression tag	UNP O34723
C	-1	GLY	-	expression tag	UNP O34723
C	0	SER	-	expression tag	UNP O34723
D	-3	GLY	-	expression tag	UNP O34723
D	-2	SER	-	expression tag	UNP O34723
D	-1	GLY	-	expression tag	UNP O34723
D	0	SER	-	expression tag	UNP O34723
F	-3	GLY	-	expression tag	UNP O34723
F	-2	SER	-	expression tag	UNP O34723
F	-1	GLY	-	expression tag	UNP O34723
F	0	SER	-	expression tag	UNP O34723

- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).

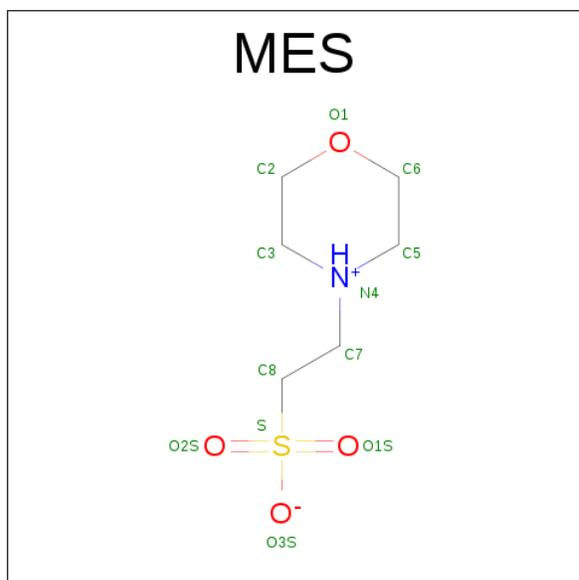


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	E	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

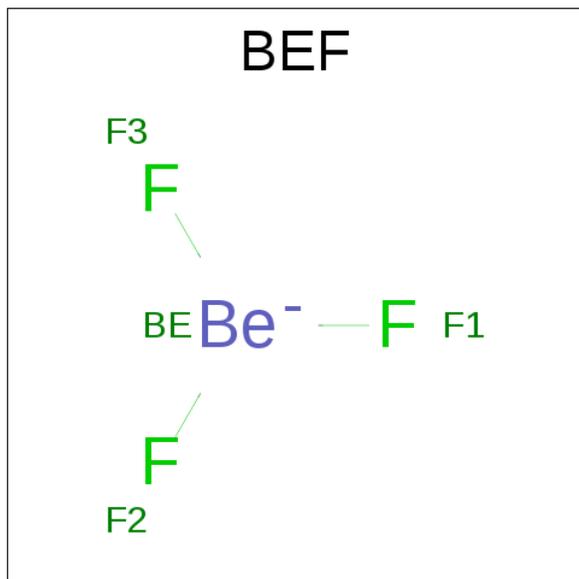
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



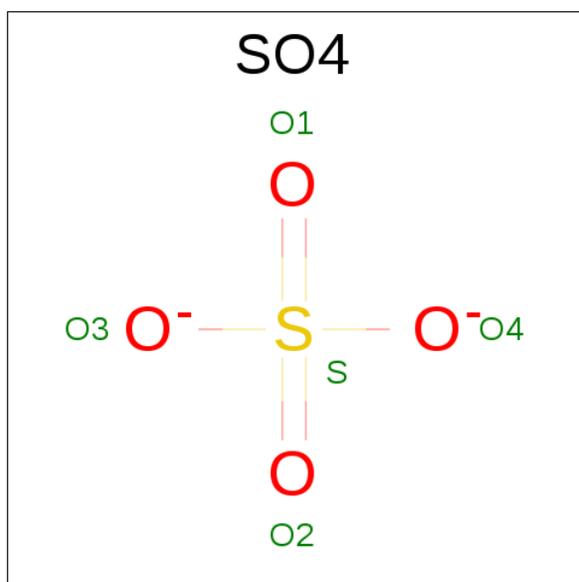
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	12	6	1	4	1	0	0

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
6	C	1	4	1	3	0	0
6	D	1	4	1	3	0	0
6	F	1	4	1	3	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	O	S	0	0
			5	4	1		

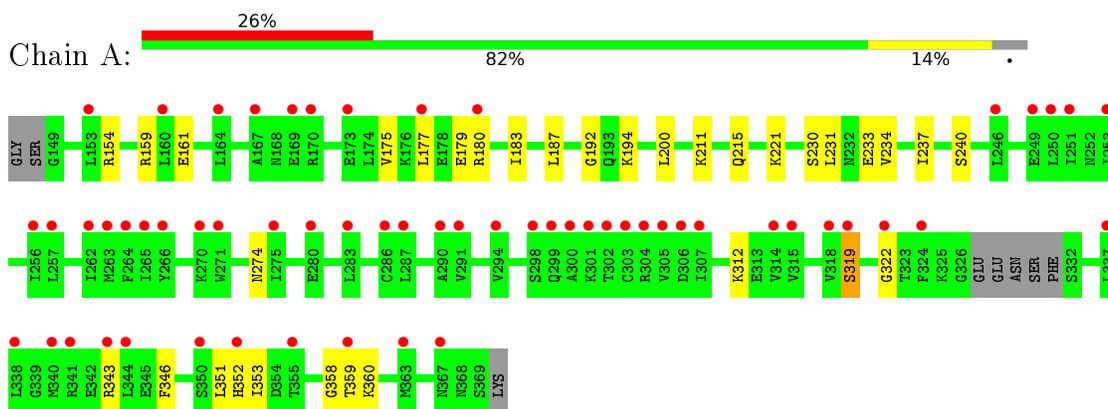
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	O	0	0
			2	2		
8	B	1	Total	O	0	0
			1	1		
8	C	3	Total	O	0	0
			3	3		
8	D	2	Total	O	0	0
			2	2		
8	E	2	Total	O	0	0
			2	2		
8	F	2	Total	O	0	0
			2	2		

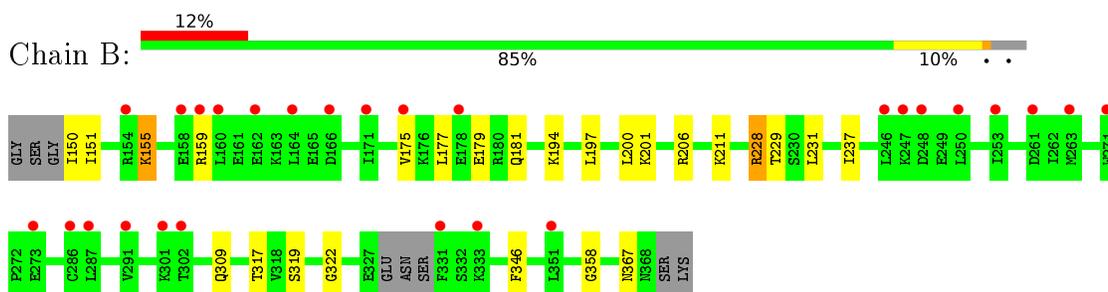
3 Residue-property plots [i](#)

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.

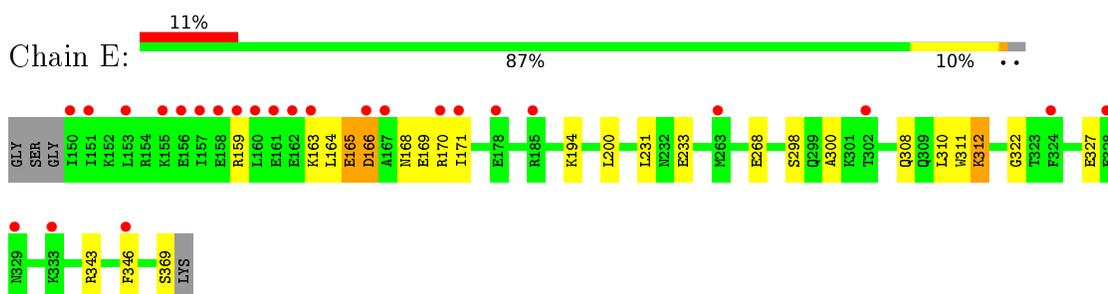
- Molecule 1: Sensor histidine kinase DesK



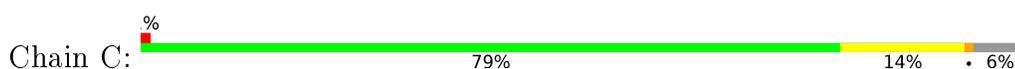
- Molecule 1: Sensor histidine kinase DesK

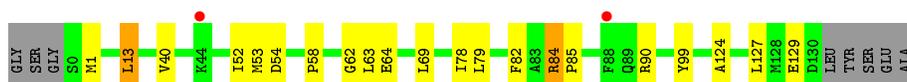


- Molecule 1: Sensor histidine kinase DesK

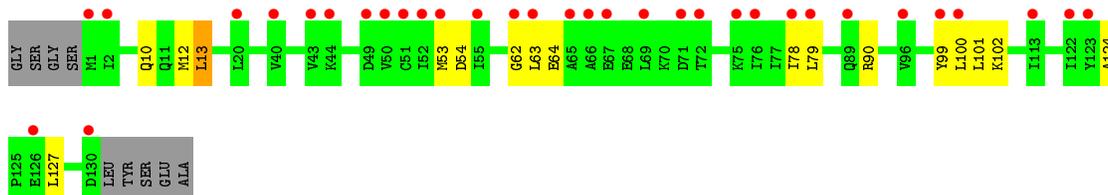
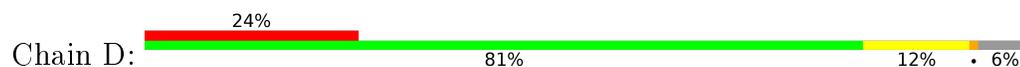


- Molecule 2: Transcriptional regulatory protein DesR

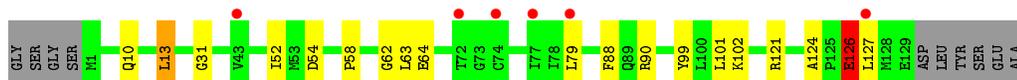
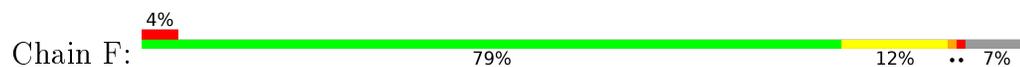




- Molecule 2: Transcriptional regulatory protein DesR



- Molecule 2: Transcriptional regulatory protein DesR



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	94.33Å 94.33Å 239.91Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.35 – 2.79 48.35 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.35-2.79) 99.5 (48.35-2.79)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.81Å)	Xtrriage
Refinement program	BUSTER-TNT 2.10.2	Depositor
R, R_{free}	0.213 , 0.248 0.230 , 0.267	Depositor DCC
R_{free} test set	1568 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	86.6	Xtrriage
Anisotropy	0.201	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 79.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8112	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: MG, ACP, BEF, SO4, MES

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	0.46	0/1703	0.71	0/2289
1	B	0.49	0/1710	0.71	0/2296
1	E	0.58	0/1723	0.76	0/2320
2	C	0.49	0/990	0.71	0/1333
2	D	0.45	0/957	0.66	0/1294
2	F	0.51	0/965	0.73	1/1302 (0.1%)
All	All	0.50	0/8048	0.72	1/10834 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	126	GLU	CA-CB-CG	5.25	124.94	113.40

There are no chirality outliers.

There are no planarity outliers.

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	1689	0	1730	17	0
1	B	1697	0	1737	17	0
1	E	1707	0	1716	12	0
2	C	979	0	990	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	946	0	937	20	0
2	F	954	0	957	14	0
3	A	31	0	14	0	0
3	B	31	0	14	0	0
3	E	31	0	14	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	12	0	13	2	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
6	F	4	0	0	0	0
7	C	5	0	0	0	0
8	A	2	0	0	0	0
8	B	1	0	0	0	0
8	C	3	0	0	0	0
8	D	2	0	0	0	0
8	E	2	0	0	0	0
8	F	2	0	0	0	0
All	All	8112	0	8122	84	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 5.

The worst 5 of 84 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:D:124:ALA:HB3	2:D:127:LEU:HD23	1.59	0.84
1:E:166:ASP:O	1:E:170:ARG:HB2	1.81	0.80
1:B:197:LEU:HD21	2:D:12:MET:HG2	1.69	0.74
2:C:124:ALA:HB3	2:C:127:LEU:HD12	1.69	0.74
1:A:353:ILE:HD11	1:A:359:THR:HG23	1.68	0.73

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	212/224 (95%)	209 (99%)	3 (1%)	0	100	100
1	B	212/224 (95%)	210 (99%)	2 (1%)	0	100	100
1	E	218/224 (97%)	213 (98%)	5 (2%)	0	100	100
2	C	129/139 (93%)	126 (98%)	2 (2%)	1 (1%)	24	58
2	D	128/139 (92%)	126 (98%)	2 (2%)	0	100	100
2	F	127/139 (91%)	125 (98%)	2 (2%)	0	100	100
All	All	1026/1089 (94%)	1009 (98%)	16 (2%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	129	GLU

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	183/199 (92%)	171 (93%)	12 (7%)	21	51
1	B	185/199 (93%)	177 (96%)	8 (4%)	35	70
1	E	183/199 (92%)	173 (94%)	10 (6%)	27	59
2	C	103/113 (91%)	100 (97%)	3 (3%)	50	83
2	D	96/113 (85%)	94 (98%)	2 (2%)	61	90
2	F	99/113 (88%)	94 (95%)	5 (5%)	29	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	849/936 (91%)	809 (95%)	40 (5%)	32 67

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	317	THR
2	C	85	PRO
2	F	13	LEU
2	C	13	LEU
2	D	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	368	ASN
2	C	10	GLN
1	E	255	GLN
1	B	367	ASN
1	E	279	ASN

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](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACP	A	401	4	29,33,33	0.86	1 (3%)	29,52,52	0.95	1 (3%)
5	MES	A	403	-	12,12,12	0.70	0	15,16,16	0.50	0
3	ACP	B	401	4	29,33,33	0.87	1 (3%)	29,52,52	0.73	0
6	BEF	C	202	2	0,3,3	0.00	-	0,3,3	0.00	-
7	SO4	C	203	-	4,4,4	0.20	0	6,6,6	0.14	0
6	BEF	D	202	2	0,3,3	0.00	-	0,3,3	0.00	-
3	ACP	E	401	4	29,33,33	0.90	1 (3%)	29,52,52	0.74	0
6	BEF	F	202	2	0,3,3	0.00	-	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ACP	A	401	4	-	0/15/38/38	0/3/3/3
5	MES	A	403	-	-	0/6/14/14	0/1/1/1
3	ACP	B	401	4	-	0/15/38/38	0/3/3/3
6	BEF	C	202	2	-	0/0/0/0	0/0/0/0
7	SO4	C	203	-	-	0/0/0/0	0/0/0/0
6	BEF	D	202	2	-	0/0/0/0	0/0/0/0
3	ACP	E	401	4	-	0/15/38/38	0/3/3/3
6	BEF	F	202	2	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	401	ACP	PB-O2B	-3.03	1.49	1.56
3	B	401	ACP	PB-O2B	-2.94	1.49	1.56
3	A	401	ACP	PG-O1G	2.03	1.54	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ACP	O1G-PG-C3B	-3.56	102.98	111.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	403	MES	2	0

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	216/224 (96%)	1.32	59 (27%) 1 0	72, 142, 193, 210	0
1	B	216/224 (96%)	0.84	27 (12%) 5 2	72, 114, 154, 175	0
1	E	220/224 (98%)	0.79	25 (11%) 7 3	58, 93, 156, 172	0
2	C	131/139 (94%)	0.38	2 (1%) 76 68	71, 93, 128, 145	0
2	D	130/139 (93%)	1.18	33 (25%) 1 0	114, 150, 177, 190	0
2	F	129/139 (92%)	0.57	6 (4%) 35 24	69, 95, 142, 173	0
All	All	1042/1089 (95%)	0.88	152 (14%) 3 2	58, 113, 175, 210	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	157	ILE	9.3
1	B	171	ILE	8.7
2	D	63	LEU	8.4
1	B	246	LEU	8.2
1	B	331	PHE	6.5

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 [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
7	SO4	C	203	5/5	0.80	0.20	1.48	173,173,174,174	0
5	MES	A	403	12/12	0.81	0.27	1.35	146,149,156,156	0
4	MG	C	201	1/1	0.99	0.20	1.17	101,101,101,101	0
4	MG	F	201	1/1	0.97	0.22	0.97	79,79,79,79	0
6	BEF	C	202	4/4	0.96	0.20	0.05	78,82,82,88	0
6	BEF	F	202	4/4	0.98	0.19	-0.38	79,81,82,89	0
4	MG	D	201	1/1	0.95	0.16	-0.38	142,142,142,142	0
3	ACP	B	401	31/31	0.95	0.18	-0.52	93,99,107,110	0
3	ACP	E	401	31/31	0.94	0.17	-0.55	89,100,114,117	0
6	BEF	D	202	4/4	0.98	0.14	-1.08	117,120,121,122	0
3	ACP	A	401	31/31	0.86	0.17	-1.35	153,161,177,180	0
4	MG	B	402	1/1	0.90	0.09	-	117,117,117,117	0
4	MG	E	402	1/1	0.95	0.16	-	99,99,99,99	0
4	MG	A	402	1/1	0.88	0.05	-	186,186,186,186	0

6.5 Other polymers [i](#)

There are no such residues in this entry.