



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:28 PM GMT

PDB ID : 1P5Q
Title : Crystal Structure of FKBP52 C-terminal Domain
Authors : Wu, B.; Li, P.; Lou, Z.; Shu, C.; Ding, Y.; Shen, B.; Rao, Z.
Deposited on : 2003-04-28
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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

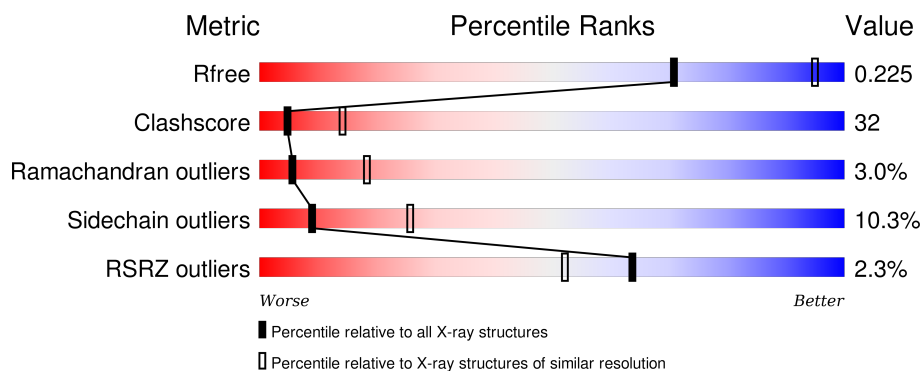
1 Overall quality at a glance ⓘ

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}	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	336	
1	B	336	
1	C	336	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7448 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 FK506-binding protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	Se	0	0	0
			2292	1446	405	434	5	2			
1	B	283	Total	C	N	O	S	Se	0	0	0
			2292	1446	405	434	5	2			
1	C	283	Total	C	N	O	S	Se	0	0	0
			2292	1446	405	434	5	2			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	124	MET	-	EXPRESSION TAG	UNP Q02790
A	125	GLY	-	EXPRESSION TAG	UNP Q02790
A	126	SER	-	EXPRESSION TAG	UNP Q02790
A	127	SER	-	EXPRESSION TAG	UNP Q02790
A	128	HIS	-	EXPRESSION TAG	UNP Q02790
A	129	HIS	-	EXPRESSION TAG	UNP Q02790
A	130	HIS	-	EXPRESSION TAG	UNP Q02790
A	131	HIS	-	EXPRESSION TAG	UNP Q02790
A	132	HIS	-	EXPRESSION TAG	UNP Q02790
A	133	HIS	-	EXPRESSION TAG	UNP Q02790
A	134	SER	-	EXPRESSION TAG	UNP Q02790
A	135	SER	-	EXPRESSION TAG	UNP Q02790
A	136	GLY	-	EXPRESSION TAG	UNP Q02790
A	137	LEU	-	EXPRESSION TAG	UNP Q02790
A	138	VAL	-	EXPRESSION TAG	UNP Q02790
A	139	PRO	-	EXPRESSION TAG	UNP Q02790
A	140	ARG	-	EXPRESSION TAG	UNP Q02790
A	141	GLY	-	EXPRESSION TAG	UNP Q02790
A	142	SER	-	EXPRESSION TAG	UNP Q02790
A	143	HIS	-	EXPRESSION TAG	UNP Q02790
A	144	MET	-	EXPRESSION TAG	UNP Q02790
A	145	GLU	-	EXPRESSION TAG	UNP Q02790
A	211	MSE	MET	MODIFIED RESIDUE	UNP Q02790

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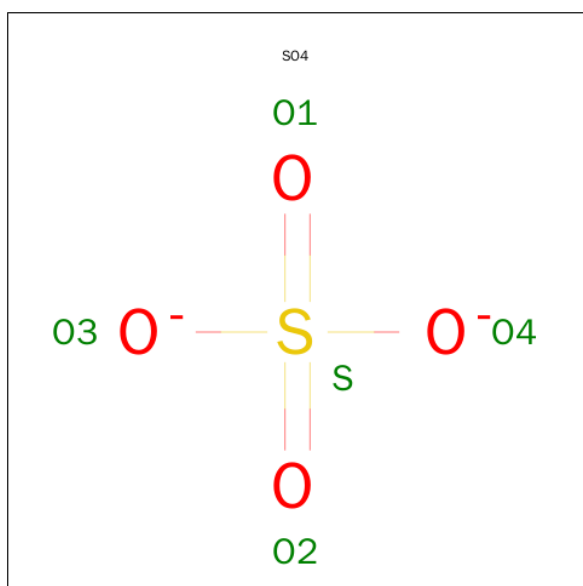
Chain	Residue	Modelled	Actual	Comment	Reference
A	261	MSE	MET	MODIFIED RESIDUE	UNP Q02790
A	357	SER	PHE	CONFLICT	UNP Q02790
B	124	MET	-	EXPRESSION TAG	UNP Q02790
B	125	GLY	-	EXPRESSION TAG	UNP Q02790
B	126	SER	-	EXPRESSION TAG	UNP Q02790
B	127	SER	-	EXPRESSION TAG	UNP Q02790
B	128	HIS	-	EXPRESSION TAG	UNP Q02790
B	129	HIS	-	EXPRESSION TAG	UNP Q02790
B	130	HIS	-	EXPRESSION TAG	UNP Q02790
B	131	HIS	-	EXPRESSION TAG	UNP Q02790
B	132	HIS	-	EXPRESSION TAG	UNP Q02790
B	133	HIS	-	EXPRESSION TAG	UNP Q02790
B	134	SER	-	EXPRESSION TAG	UNP Q02790
B	135	SER	-	EXPRESSION TAG	UNP Q02790
B	136	GLY	-	EXPRESSION TAG	UNP Q02790
B	137	LEU	-	EXPRESSION TAG	UNP Q02790
B	138	VAL	-	EXPRESSION TAG	UNP Q02790
B	139	PRO	-	EXPRESSION TAG	UNP Q02790
B	140	ARG	-	EXPRESSION TAG	UNP Q02790
B	141	GLY	-	EXPRESSION TAG	UNP Q02790
B	142	SER	-	EXPRESSION TAG	UNP Q02790
B	143	HIS	-	EXPRESSION TAG	UNP Q02790
B	144	MET	-	EXPRESSION TAG	UNP Q02790
B	145	GLU	-	EXPRESSION TAG	UNP Q02790
B	211	MSE	MET	MODIFIED RESIDUE	UNP Q02790
B	261	MSE	MET	MODIFIED RESIDUE	UNP Q02790
B	357	SER	PHE	CONFLICT	UNP Q02790
C	124	MET	-	EXPRESSION TAG	UNP Q02790
C	125	GLY	-	EXPRESSION TAG	UNP Q02790
C	126	SER	-	EXPRESSION TAG	UNP Q02790
C	127	SER	-	EXPRESSION TAG	UNP Q02790
C	128	HIS	-	EXPRESSION TAG	UNP Q02790
C	129	HIS	-	EXPRESSION TAG	UNP Q02790
C	130	HIS	-	EXPRESSION TAG	UNP Q02790
C	131	HIS	-	EXPRESSION TAG	UNP Q02790
C	132	HIS	-	EXPRESSION TAG	UNP Q02790
C	133	HIS	-	EXPRESSION TAG	UNP Q02790
C	134	SER	-	EXPRESSION TAG	UNP Q02790
C	135	SER	-	EXPRESSION TAG	UNP Q02790
C	136	GLY	-	EXPRESSION TAG	UNP Q02790
C	137	LEU	-	EXPRESSION TAG	UNP Q02790
C	138	VAL	-	EXPRESSION TAG	UNP Q02790

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Chain	Residue	Modelled	Actual	Comment	Reference
C	139	PRO	-	EXPRESSION TAG	UNP Q02790
C	140	ARG	-	EXPRESSION TAG	UNP Q02790
C	141	GLY	-	EXPRESSION TAG	UNP Q02790
C	142	SER	-	EXPRESSION TAG	UNP Q02790
C	143	HIS	-	EXPRESSION TAG	UNP Q02790
C	144	MET	-	EXPRESSION TAG	UNP Q02790
C	145	GLU	-	EXPRESSION TAG	UNP Q02790
C	211	MSE	MET	MODIFIED RESIDUE	UNP Q02790
C	261	MSE	MET	MODIFIED RESIDUE	UNP Q02790
C	357	SER	PHE	CONFLICT	UNP Q02790

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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

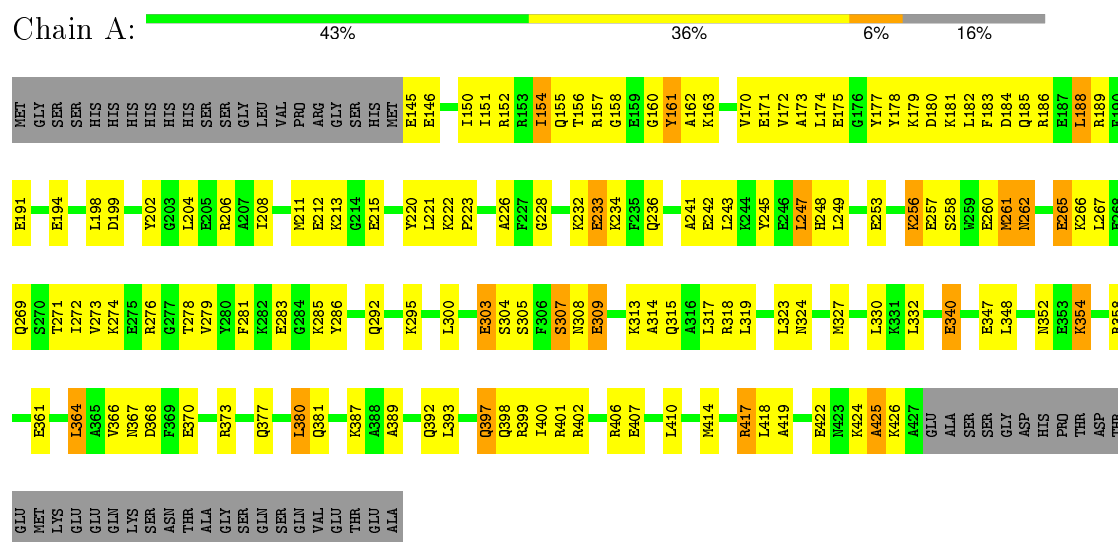
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total	O	0	0
			177	177		
3	B	174	Total	O	0	0
			174	174		
3	C	176	Total	O	0	0
			176	176		

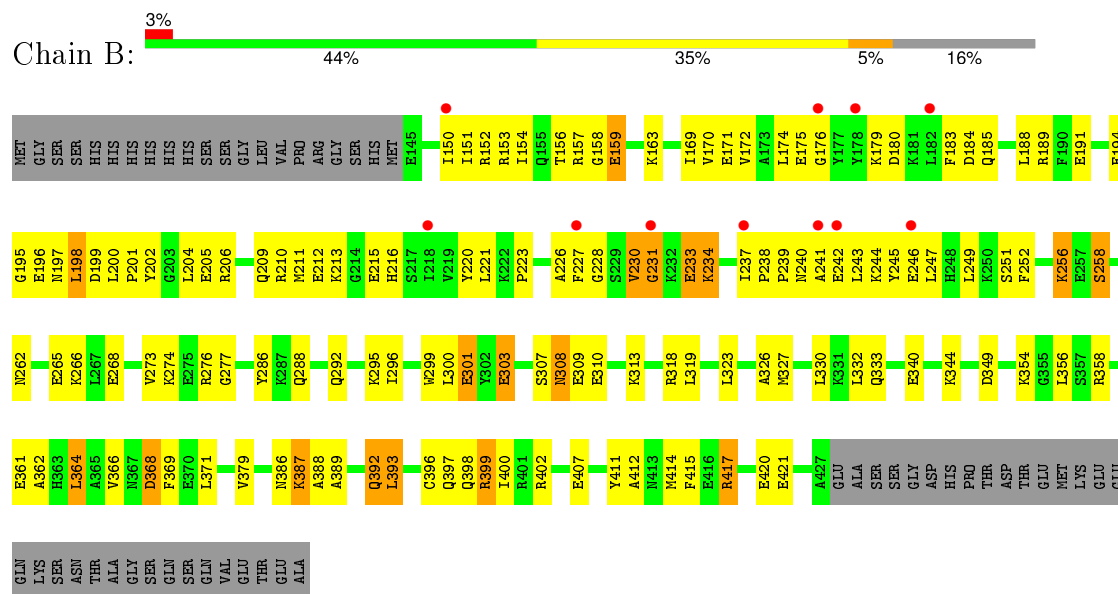
3 Residue-property plots

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.

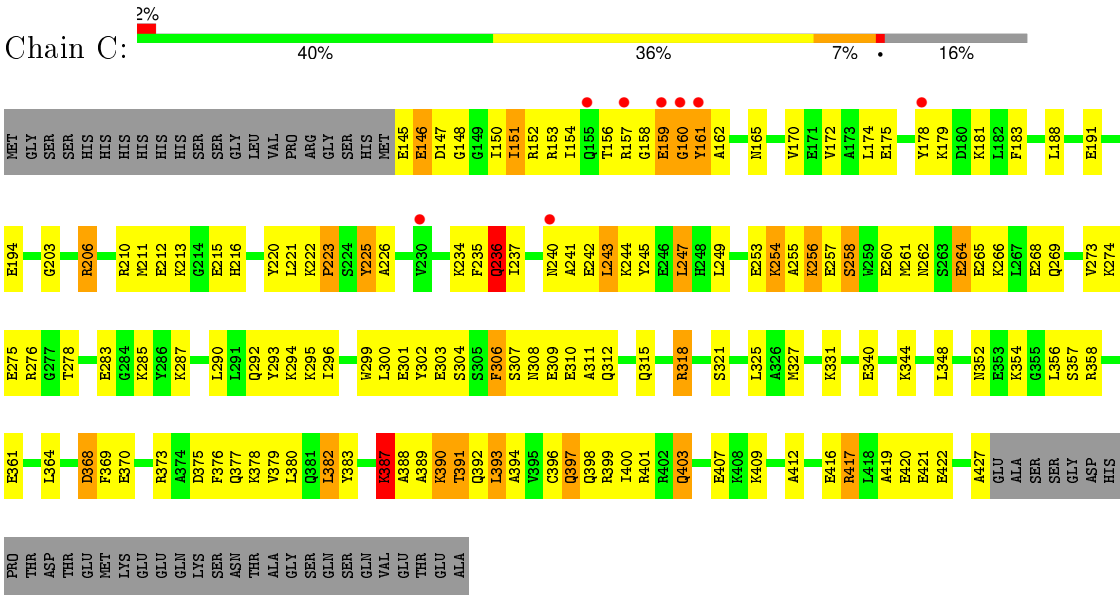
• Molecule 1: FK506-binding protein 4



• Molecule 1: FK506-binding protein 4



• Molecule 1: FK506-binding protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	114.27Å 142.93Å 170.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 48.02 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 97.9 (48.02-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.212 , 0.284 0.231 , 0.225	Depositor DCC
R_{free} test set	1685 reflections (4.94%)	DCC
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 66464 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7448	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4

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	0.61	0/2328	0.77	0/3113
1	B	0.62	0/2328	0.77	1/3113 (0.0%)
1	C	0.66	1/2328 (0.0%)	0.82	2/3113 (0.1%)
All	All	0.63	1/6984 (0.0%)	0.79	3/9339 (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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	268	GLU	CG-CD	5.61	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	318	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	C	318	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	B	231	GLY	N-CA-C	5.26	126.26	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	225	TYR	Sidechain

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	2292	0	2289	162	0
1	B	2292	0	2289	134	0
1	C	2292	0	2289	146	1
2	A	20	0	0	0	0
2	B	10	0	0	0	0
2	C	15	0	0	1	0
3	A	177	0	0	28	0
3	B	174	0	0	17	0
3	C	176	0	0	24	0
All	All	7448	0	6867	435	1

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 32.

The worst 5 of 435 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:B:414:MET:CE	1:B:414:MET:SD	2.02	1.47
1:C:387:LYS:HD2	1:C:388:ALA:H	0.96	1.13
1:B:387:LYS:HD2	1:B:388:ALA:N	1.64	1.11
1:C:397:GLN:HE21	1:C:397:GLN:HA	1.17	1.09
1:B:392:GLN:HA	1:B:392:GLN:HE21	1.18	1.04

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:GLU:OE1	1:C:283:GLU:OE1[4_565]	2.17	0.03

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	281/336 (84%)	250 (89%)	26 (9%)	5 (2%)	11	34
1	B	281/336 (84%)	244 (87%)	29 (10%)	8 (3%)	6	21
1	C	281/336 (84%)	232 (83%)	37 (13%)	12 (4%)	3	10
All	All	843/1008 (84%)	726 (86%)	92 (11%)	25 (3%)	5	18

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	301	GLU
1	B	308	ASN
1	C	159	GLU
1	C	161	TYR
1	C	223	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	237/281 (84%)	212 (90%)	25 (10%)	8	24
1	B	237/281 (84%)	213 (90%)	24 (10%)	9	27
1	C	237/281 (84%)	213 (90%)	24 (10%)	9	27
All	All	711/843 (84%)	638 (90%)	73 (10%)	9	26

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	268	GLU
1	B	361	GLU
1	C	393	LEU
1	B	319	LEU
1	B	366	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	HIS
1	B	315	GLN
1	C	381	GLN
1	B	209	GLN
1	C	392	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](#)

9 ligands are modelled in this entry.

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
2	SO4	A	1001	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	A	1002	-	4,4,4	0.46	0	6,6,6	0.14	0
2	SO4	A	1003	-	4,4,4	0.45	0	6,6,6	0.19	0
2	SO4	A	1004	-	4,4,4	0.32	0	6,6,6	0.10	0
2	SO4	B	1005	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	B	1006	-	4,4,4	0.44	0	6,6,6	0.10	0
2	SO4	C	1007	-	4,4,4	0.40	0	6,6,6	0.22	0
2	SO4	C	1008	-	4,4,4	0.36	0	6,6,6	0.17	0
2	SO4	C	1009	-	4,4,4	0.63	0	6,6,6	0.17	0

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
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1005	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1006	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1007	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1008	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1009	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1007	SO4	1	0

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 [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	281/336 (83%)	0.03	0 100 100	23, 52, 88, 127	0
1	B	281/336 (83%)	0.32	11 (3%) 43 31	21, 54, 90, 126	0
1	C	281/336 (83%)	0.23	8 (2%) 56 44	21, 53, 92, 137	0
All	All	843/1008 (83%)	0.19	19 (2%) 64 52	21, 53, 91, 137	0

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	ARG	4.2
1	C	155	GLN	3.6
1	B	227	PHE	3.4
1	C	161	TYR	3.3
1	B	150	ILE	3.1

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(\AA^2)	Q<0.9
2	SO4	A	1002	5/5	0.93	0.20	-0.53	68,69,76,80	0
2	SO4	A	1003	5/5	0.97	0.16	-0.53	73,74,75,79	0
2	SO4	B	1006	5/5	0.93	0.17	-0.60	76,80,83,85	0
2	SO4	B	1005	5/5	0.91	0.22	-0.94	105,106,113,115	0
2	SO4	C	1009	5/5	0.94	0.13	-1.22	70,71,84,89	0
2	SO4	C	1007	5/5	0.97	0.13	-2.37	71,73,81,81	0
2	SO4	C	1008	5/5	0.90	0.23	-	104,106,110,113	0
2	SO4	A	1001	5/5	0.93	0.13	-	112,113,115,116	0
2	SO4	A	1004	5/5	0.87	0.18	-	108,112,114,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.