



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 8, 2021 – 02:06 PM EDT

PDB ID : 7JQ6  
Title : The Phi-28 gp11 DNA packaging Motor  
Authors : Morais, M.C.; White, M.A.; Dill, E.  
Deposited on : 2020-08-10  
Resolution : 2.90 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.20  
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) : 2.20

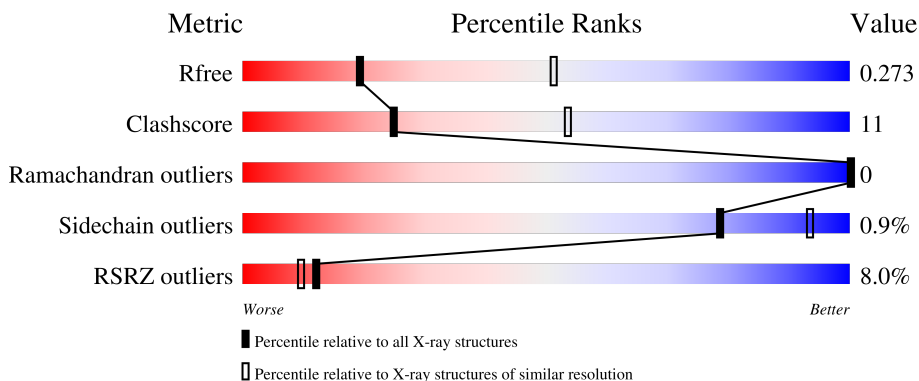
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	374	 2% 73% 25%
1	B	374	 6% 76% 22%
1	C	374	 14% 70% 27%
1	D	374	 13% 74% 24%
1	E	374	 3% 73% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	SO4	B	401	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30556 atoms, of which 15104 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 Encapsidation protein.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S	Se			
1	A	367	6123	2001	3031	516	565	2	8	0	0	0
1	B	366	6106	1995	3024	513	564	2	8	0	0	0
1	C	364	6060	1981	3001	506	562	2	8	0	0	0
1	D	368	6140	2007	3038	519	566	2	8	0	0	0
1	E	364	6072	1983	3010	507	562	2	8	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

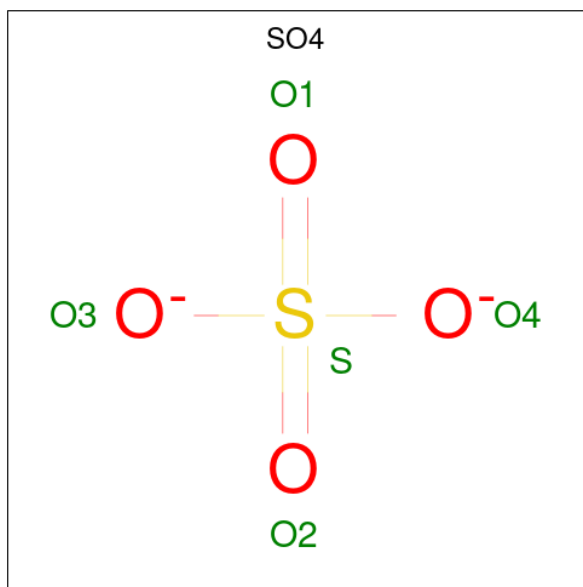
Chain	Residue	Modelled	Actual	Comment	Reference
A	367	LEU	-	expression tag	UNP B1ABI1
A	368	GLU	-	expression tag	UNP B1ABI1
A	369	HIS	-	expression tag	UNP B1ABI1
A	370	HIS	-	expression tag	UNP B1ABI1
A	371	HIS	-	expression tag	UNP B1ABI1
A	372	HIS	-	expression tag	UNP B1ABI1
A	373	HIS	-	expression tag	UNP B1ABI1
A	374	HIS	-	expression tag	UNP B1ABI1
B	367	LEU	-	expression tag	UNP B1ABI1
B	368	GLU	-	expression tag	UNP B1ABI1
B	369	HIS	-	expression tag	UNP B1ABI1
B	370	HIS	-	expression tag	UNP B1ABI1
B	371	HIS	-	expression tag	UNP B1ABI1
B	372	HIS	-	expression tag	UNP B1ABI1
B	373	HIS	-	expression tag	UNP B1ABI1
B	374	HIS	-	expression tag	UNP B1ABI1
C	367	LEU	-	expression tag	UNP B1ABI1
C	368	GLU	-	expression tag	UNP B1ABI1
C	369	HIS	-	expression tag	UNP B1ABI1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	370	HIS	-	expression tag	UNP B1ABI1
C	371	HIS	-	expression tag	UNP B1ABI1
C	372	HIS	-	expression tag	UNP B1ABI1
C	373	HIS	-	expression tag	UNP B1ABI1
C	374	HIS	-	expression tag	UNP B1ABI1
D	367	LEU	-	expression tag	UNP B1ABI1
D	368	GLU	-	expression tag	UNP B1ABI1
D	369	HIS	-	expression tag	UNP B1ABI1
D	370	HIS	-	expression tag	UNP B1ABI1
D	371	HIS	-	expression tag	UNP B1ABI1
D	372	HIS	-	expression tag	UNP B1ABI1
D	373	HIS	-	expression tag	UNP B1ABI1
D	374	HIS	-	expression tag	UNP B1ABI1
E	367	LEU	-	expression tag	UNP B1ABI1
E	368	GLU	-	expression tag	UNP B1ABI1
E	369	HIS	-	expression tag	UNP B1ABI1
E	370	HIS	-	expression tag	UNP B1ABI1
E	371	HIS	-	expression tag	UNP B1ABI1
E	372	HIS	-	expression tag	UNP B1ABI1
E	373	HIS	-	expression tag	UNP B1ABI1
E	374	HIS	-	expression tag	UNP B1ABI1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

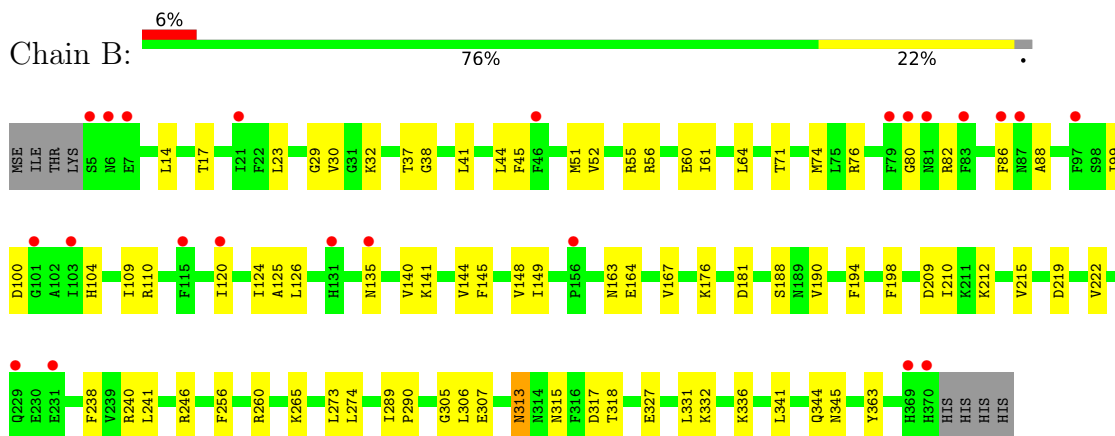
### 3 Residue-property plots [i](#)

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.

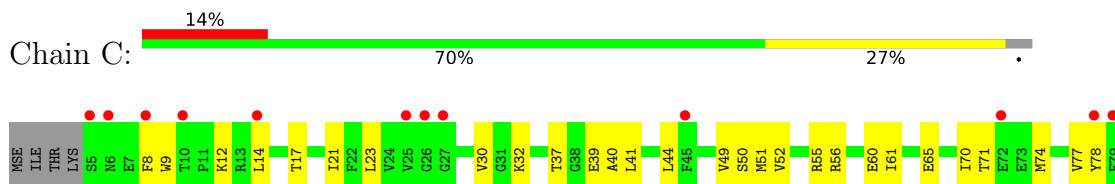
- Molecule 1: Encapsidation protein

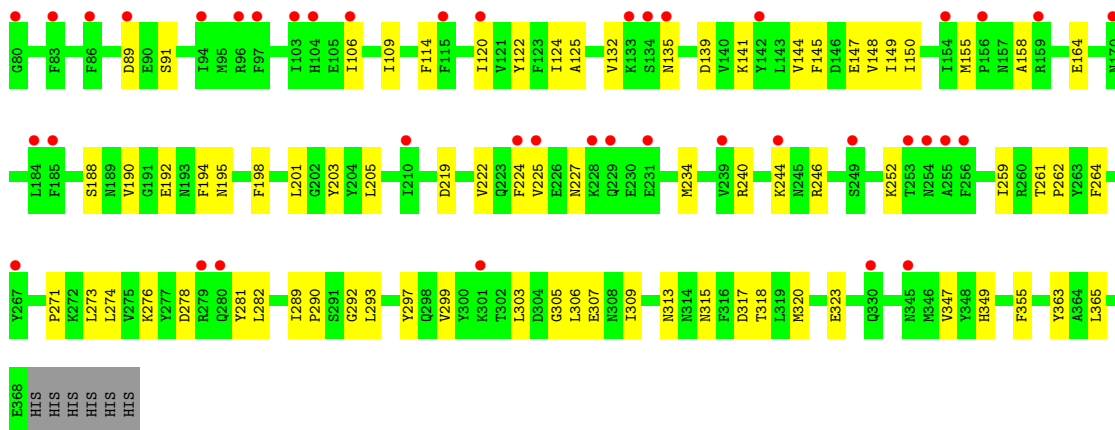


- Molecule 1: Encapsidation protein

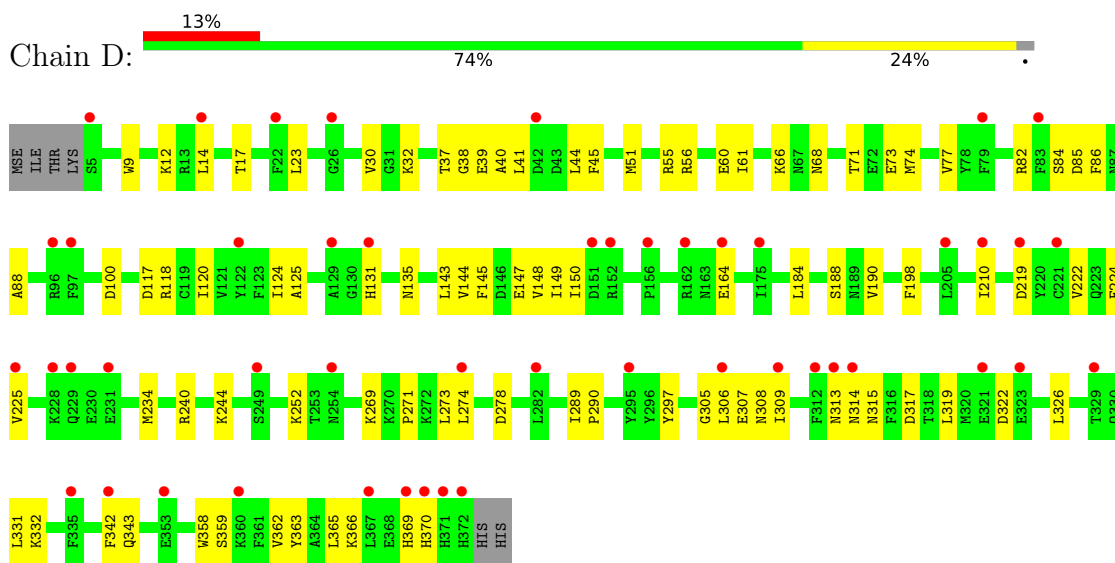


- Molecule 1: Encapsidation protein

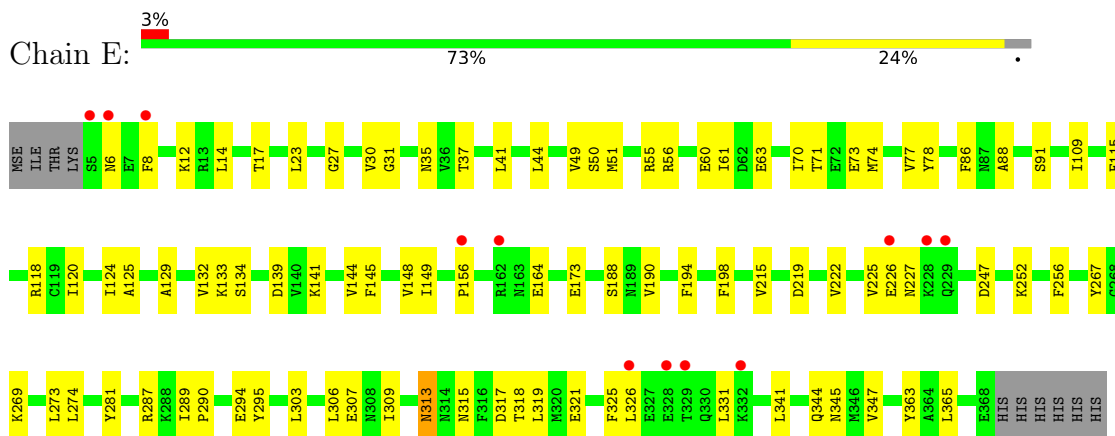




• Molecule 1: Encapsidation protein



• Molecule 1: Encapsidation protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	135.00Å 135.00Å 276.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.38 – 2.90 49.38 – 2.90	Depositor EDS
% Data completeness (in resolution range)	64.0 (49.38-2.90) 58.9 (49.38-2.90)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.52 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.13rc2_2986	Depositor
R, $R_{free}$	0.241 , 0.274 0.241 , 0.273	Depositor DCC
$R_{free}$ test set	1909 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.2	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	30556	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	101.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 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	0.29	0/3158	0.46	0/4240
1	B	0.28	0/3147	0.47	0/4225
1	C	0.27	0/3122	0.44	0/4192
1	D	0.27	0/3169	0.43	0/4255
1	E	0.30	0/3125	0.47	0/4195
All	All	0.28	0/15721	0.45	0/21107

There are no bond length outliers.

There are no bond angle outliers.

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	3092	3031	3031	73	0
1	B	3082	3024	3024	66	1
1	C	3059	3001	3001	77	1
1	D	3102	3038	3038	65	4
1	E	3062	3010	3010	77	1
2	A	10	0	0	0	0
2	B	15	0	0	3	0
2	C	10	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	5	0	0	1	0
2	E	15	0	0	0	1
All	All	15452	15104	15104	331	6

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 11.

The worst 5 of 331 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:A:240:ARG:NH1	1:B:219:ASP:OD1	1.77	1.16
1:E:41:LEU:HD11	1:E:74:MSE:HE3	1.44	0.96
1:E:56:ARG:NH2	1:E:148:VAL:O	2.03	0.92
1:A:73:GLU:OE1	1:B:135:ASN:ND2	2.03	0.92
1:B:240:ARG:NH1	1:C:219:ASP:OD1	2.05	0.89

The worst 5 of 6 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:D:308:ASN:CB	1:D:308:ASN:HB2[5_555]	1.04	0.56
1:C:317:ASP:OD1	1:E:12:LYS:NZ[3_665]	2.08	0.12
1:D:308:ASN:CB	1:D:308:ASN:CB[5_555]	2.08	0.12
1:D:269:LYS:HZ2	1:D:322:ASP:OD2[5_555]	1.58	0.02
1:D:269:LYS:NZ	1:D:322:ASP:OD2[5_555]	2.18	0.02

## 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	365/374 (98%)	359 (98%)	6 (2%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	364/374 (97%)	355 (98%)	9 (2%)	0	100	100
1	C	362/374 (97%)	354 (98%)	8 (2%)	0	100	100
1	D	366/374 (98%)	358 (98%)	8 (2%)	0	100	100
1	E	362/374 (97%)	353 (98%)	9 (2%)	0	100	100
All	All	1819/1870 (97%)	1779 (98%)	40 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	337/335 (101%)	334 (99%)	3 (1%)	78	93
1	B	336/335 (100%)	333 (99%)	3 (1%)	78	93
1	C	333/335 (99%)	331 (99%)	2 (1%)	86	96
1	D	338/335 (101%)	335 (99%)	3 (1%)	78	93
1	E	334/335 (100%)	330 (99%)	4 (1%)	71	91
All	All	1678/1675 (100%)	1663 (99%)	15 (1%)	78	93

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	313	ASN
1	E	313	ASN
1	D	145	PHE
1	E	345	ASN
1	E	134	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	ASN
1	D	67	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

11 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	401	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	A	402	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	401	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	E	401	-	4,4,4	0.12	0	6,6,6	0.09	0
2	SO4	C	401	-	4,4,4	0.14	0	6,6,6	0.10	0
2	SO4	B	402	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	C	402	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	E	402	-	4,4,4	0.13	0	6,6,6	0.11	0
2	SO4	D	401	-	4,4,4	0.15	0	6,6,6	0.10	0
2	SO4	E	403	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	403	-	4,4,4	0.14	0	6,6,6	0.08	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.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SO4	2	0
2	C	401	SO4	1	0
2	B	402	SO4	1	0
2	E	402	SO4	0	1
2	D	401	SO4	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	359/374 (95%)	0.25	7 (1%) 66 65	27, 67, 128, 176	0
1	B	358/374 (95%)	0.50	23 (6%) 19 15	33, 83, 143, 178	0
1	C	356/374 (95%)	0.97	53 (14%) 2 1	72, 115, 171, 213	0
1	D	360/374 (96%)	0.89	48 (13%) 3 2	41, 116, 170, 207	0
1	E	356/374 (95%)	0.22	12 (3%) 45 40	24, 59, 132, 167	0
All	All	1789/1870 (95%)	0.57	143 (7%) 12 9	24, 91, 155, 213	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	SER	8.2
1	A	5	SER	6.8
1	B	87	ASN	5.6
1	E	5	SER	5.5
1	C	27	GLY	5.4

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	B	402	5/5	0.83	0.33	97,114,117,118	0
2	SO4	A	402	5/5	0.84	0.25	104,105,106,107	0
2	SO4	B	403	5/5	0.85	0.29	137,138,139,139	0
2	SO4	C	402	5/5	0.86	0.18	131,131,132,133	0
2	SO4	E	403	5/5	0.87	0.18	109,110,110,111	0
2	SO4	C	401	5/5	0.89	0.24	123,124,124,124	0
2	SO4	B	401	5/5	0.92	0.26	84,86,89,91	0
2	SO4	D	401	5/5	0.94	0.20	102,106,107,108	0
2	SO4	E	402	5/5	0.96	0.13	73,75,78,80	0
2	SO4	A	401	5/5	0.98	0.21	56,60,63,64	0
2	SO4	E	401	5/5	0.98	0.27	55,59,61,61	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.