



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 06:03 AM EST

PDB ID : 3OM6  
Title : Crystal structure of B. megaterium levansucrase mutant Y247A  
Authors : Strube, C.P.; Homann, A.; Gamer, M.; Jahn, D.; Seibel, J.; Heinz, D.W.  
Deposited on : 2010-08-26  
Resolution : 1.96 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.36  
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) : 2.36

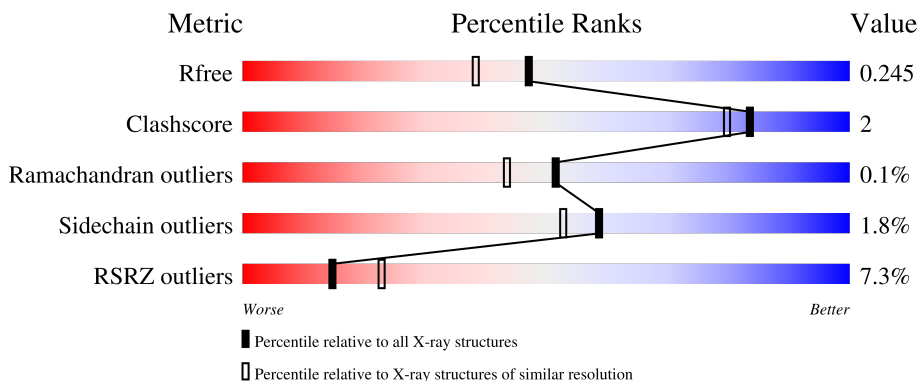
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	456	 6% 92% 6%
1	B	456	 10% 89% 9%
1	C	456	 4% 90% 8%
1	D	456	 9% 91% 7%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15500 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 Levansucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	448	3535	2218	592	718	7	0	0	0
1	B	448	3552	2229	594	722	7	0	2	0
1	C	448	3535	2218	592	718	7	0	0	0
1	D	448	3562	2234	596	725	7	0	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	247	ALA	TYR	engineered mutation	UNP D5DC07
B	247	ALA	TYR	engineered mutation	UNP D5DC07
C	247	ALA	TYR	engineered mutation	UNP D5DC07
D	247	ALA	TYR	engineered mutation	UNP D5DC07

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

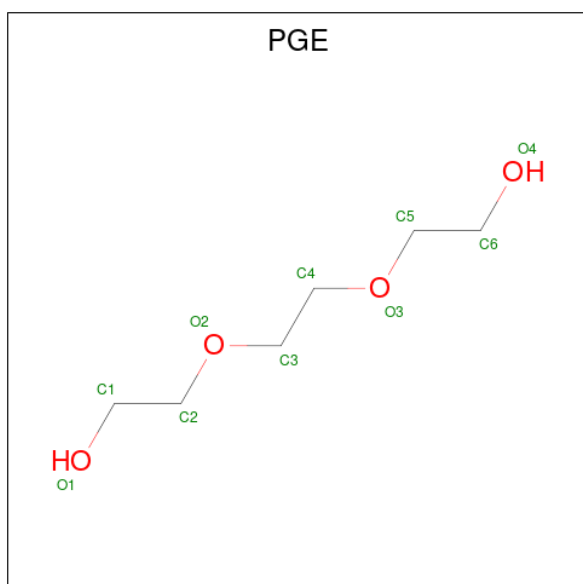
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			10	6	4		

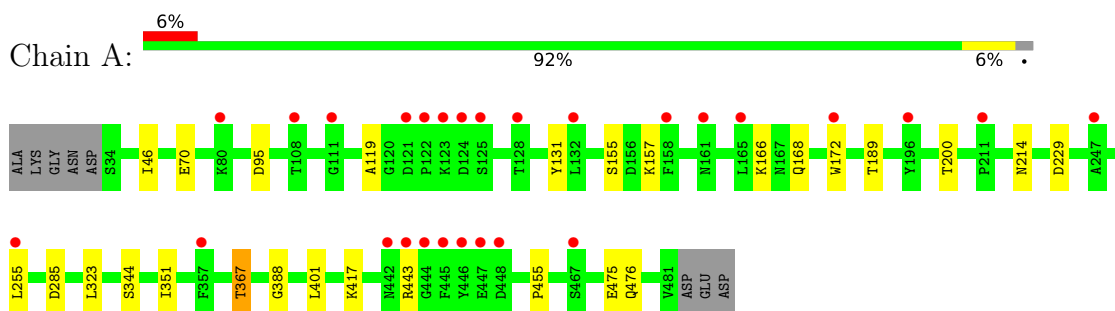
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	352	Total	O	0	0
			352	352		
5	B	347	Total	O	0	0
			347	347		
5	C	276	Total	O	0	0
			276	276		
5	D	302	Total	O	0	0
			302	302		

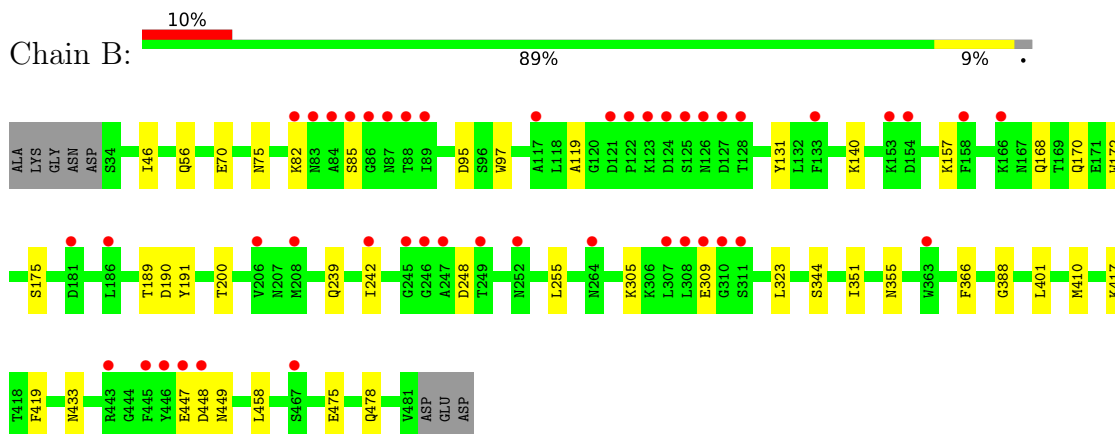
### 3 Residue-property plots [i](#)

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.

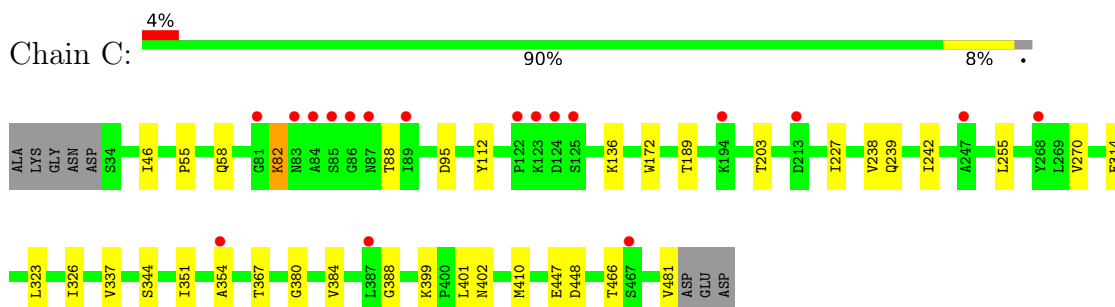
- Molecule 1: Levansucrase



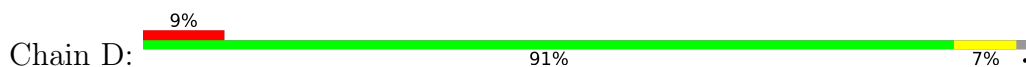
- Molecule 1: Levansucrase

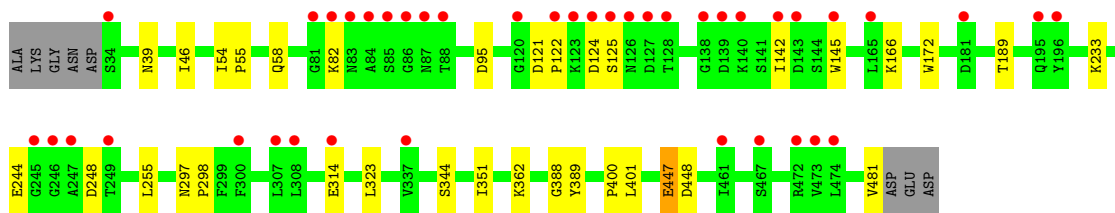


- Molecule 1: Levansucrase



- Molecule 1: Levansucrase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.79Å 100.02Å 95.54Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	50.01 – 1.96 47.77 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.5 (50.01-1.96) 95.2 (47.77-1.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 1.95Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.222 , 0.230 0.230 , 0.245	Depositor DCC
$R_{free}$ test set	6216 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	16.1	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 40.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.012 for l,k,-h 0.028 for h,-k,-l 0.019 for l,-k,h	Xtrriage
Reported twinning fraction	0.664 for H, K, L 0.116 for -h,-k,l 0.110 for L, -K, H 0.111 for -L, K, H	Depositor
Outliers	0 of 120932 reflections	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	15500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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: PGE, CA, 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	0.34	0/3611	0.48	0/4887
1	B	0.34	0/3628	0.48	0/4910
1	C	0.34	0/3611	0.48	0/4887
1	D	0.35	0/3647	0.48	0/4935
All	All	0.34	0/14497	0.48	0/19619

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	3535	0	3374	13	0
1	B	3552	0	3389	21	0
1	C	3535	0	3374	20	0
1	D	3562	0	3400	15	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	0	0
3	D	5	0	0	0	0
4	C	10	0	14	0	0
5	A	352	0	0	1	0
5	B	347	0	0	0	0
5	C	276	0	0	1	0
5	D	302	0	0	1	0
All	All	15500	0	13551	67	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 2.

All (67) 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:305:LYS:O	1:B:309[A]:GLU:HG3	1.77	0.85
1:C:402:ASN:HD21	1:C:466:THR:H	1.26	0.82
1:A:155:SER:HB2	1:B:85:SER:HA	1.68	0.76
1:A:351:ILE:HB	1:A:367:THR:HG21	1.73	0.69
1:D:314[B]:GLU:HA	1:D:314[B]:GLU:OE1	1.93	0.68
1:C:82:LYS:N	1:C:82:LYS:HE3	2.11	0.65
1:C:384:VAL:HG22	1:C:410:MET:HB3	1.83	0.60
1:B:46:ILE:HD12	1:B:344:SER:HB3	1.86	0.58
1:A:285:ASP:OD2	1:C:55:PRO:O	2.22	0.57
1:C:172:TRP:HB2	1:C:189:THR:HB	1.85	0.56
1:B:70:GLU:HG2	1:B:417:LYS:HD3	1.88	0.56
1:B:447:GLU:HA	1:B:448:ASP:C	2.27	0.55
1:C:380:GLY:HA2	5:C:898:HOH:O	2.07	0.54
1:B:475:GLU:HB2	1:B:478:GLN:HB2	1.89	0.54
1:D:46:ILE:HD12	1:D:344:SER:HB3	1.89	0.54
1:C:46:ILE:HD12	1:C:344:SER:HB3	1.90	0.53
1:C:447:GLU:HG2	1:C:448:ASP:HA	1.90	0.53
1:C:323:LEU:HG	1:C:351:ILE:HD12	1.91	0.52
1:A:172:TRP:HB2	1:A:189:THR:HB	1.92	0.51
1:D:55:PRO:O	1:D:58:GLN:HG2	2.10	0.51
1:D:172:TRP:HB2	1:D:189:THR:HB	1.93	0.51
1:B:388:GLY:HA3	1:B:401:LEU:HD12	1.92	0.50
1:B:323:LEU:HG	1:B:351:ILE:HD12	1.94	0.49
1:A:388:GLY:HA3	1:A:401:LEU:HD12	1.95	0.49
1:D:121:ASP:OD1	1:D:122:PRO:HD2	2.11	0.49
1:B:239:GLN:HA	1:B:242:ILE:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:362:LYS:HE2	5:D:560:HOH:O	2.13	0.48
1:C:112:TYR:CZ	1:C:136:LYS:HE3	2.49	0.48
1:D:323:LEU:HG	1:D:351:ILE:HD12	1.95	0.47
1:B:433:ASN:HB3	1:B:458:LEU:HD22	1.97	0.47
1:D:54:ILE:N	1:D:55:PRO:HD2	2.30	0.47
1:C:82:LYS:HE2	1:C:88:THR:HB	1.96	0.47
1:C:239:GLN:HA	1:C:242:ILE:HD12	1.97	0.47
1:A:70:GLU:HG2	1:A:417:LYS:HD3	1.97	0.46
1:A:157:LYS:HD3	1:A:168:GLN:HB3	1.97	0.46
1:B:75:ASN:HD21	1:B:449:ASN:H	1.65	0.45
1:A:46:ILE:HD12	1:A:344:SER:HB3	1.98	0.45
1:C:323:LEU:HD11	1:C:367:THR:HB	1.98	0.45
1:A:455:PRO:HA	1:A:476:GLN:HA	1.99	0.45
1:B:170:GLN:HB2	1:B:191:TYR:HD2	1.82	0.45
1:D:142:ILE:HA	1:D:145:TRP:HD1	1.82	0.44
1:A:119:ALA:HB3	1:A:131:TYR:CD2	2.52	0.44
1:A:200:THR:HG23	1:A:229:ASP:HB3	2.00	0.44
1:D:297:ASN:N	1:D:298:PRO:HD2	2.32	0.44
1:B:449:ASN:N	1:B:449:ASN:OD1	2.50	0.44
1:C:326:ILE:HG22	1:C:337:VAL:HA	1.99	0.44
1:D:388:GLY:HA3	1:D:401:LEU:HD12	2.00	0.44
1:D:447:GLU:HG3	1:D:448:ASP:OD1	2.18	0.43
1:C:55:PRO:O	1:C:58:GLN:HG2	2.19	0.43
1:C:238:VAL:O	1:C:242:ILE:HG13	2.19	0.42
1:B:119:ALA:HB3	1:B:131:TYR:CD2	2.55	0.42
1:B:70:GLU:CG	1:B:417:LYS:HD3	2.48	0.42
1:D:447:GLU:HG3	1:D:448:ASP:HA	2.01	0.42
1:B:157:LYS:HD3	1:B:168:GLN:HB3	2.00	0.42
1:B:172:TRP:HB2	1:B:189:THR:HB	2.01	0.42
1:B:355:ASN:HB3	1:B:366:PHE:HB2	2.01	0.42
1:C:203:THR:HB	1:C:227:ILE:HD11	2.01	0.42
1:D:54:ILE:N	1:D:55:PRO:CD	2.83	0.42
1:B:97:TRP:CD1	1:B:175:SER:HA	2.55	0.41
1:B:410:MET:HE1	1:B:419:PHE:CE1	2.55	0.41
1:D:389:TYR:CD1	1:D:400:PRO:HA	2.56	0.41
1:C:270:VAL:HG12	1:C:354:ALA:HB1	2.02	0.41
1:C:399:LYS:HA	1:C:399:LYS:HD2	1.86	0.41
1:A:323:LEU:HG	1:A:351:ILE:HD12	2.03	0.41
1:B:190:ASP:HB3	1:B:200:THR:HB	2.02	0.41
1:A:475:GLU:HB3	5:A:651:HOH:O	2.20	0.40
1:C:388:GLY:HA3	1:C:401:LEU:HD12	2.04	0.40

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	446/456 (98%)	428 (96%)	18 (4%)	0	100	100
1	B	448/456 (98%)	430 (96%)	18 (4%)	0	100	100
1	C	446/456 (98%)	429 (96%)	17 (4%)	0	100	100
1	D	450/456 (99%)	434 (96%)	15 (3%)	1 (0%)	47	38
All	All	1790/1824 (98%)	1721 (96%)	68 (4%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	125	SER

### 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	389/395 (98%)	383 (98%)	6 (2%)	65	60
1	B	391/395 (99%)	385 (98%)	6 (2%)	65	60
1	C	389/395 (98%)	384 (99%)	5 (1%)	69	65
1	D	393/395 (100%)	382 (97%)	11 (3%)	43	33
All	All	1562/1580 (99%)	1534 (98%)	28 (2%)	59	53

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
1	A	166	LYS
1	A	214	ASN
1	A	255	LEU
1	A	367	THR
1	A	443	ARG
1	B	56	GLN
1	B	82	LYS
1	B	95	ASP
1	B	140	LYS
1	B	248	ASP
1	B	255	LEU
1	C	82	LYS
1	C	95	ASP
1	C	255	LEU
1	C	314	GLU
1	C	481	VAL
1	D	39	ASN
1	D	82	LYS
1	D	95	ASP
1	D	124	ASP
1	D	166	LYS
1	D	233	LYS
1	D	244	GLU
1	D	248	ASP
1	D	255	LEU
1	D	447	GLU
1	D	481	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	50	ASN
1	C	402	ASN
1	D	39	ASN
1	D	126	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](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	SO4	B	3	-	4,4,4	0.21	0	6,6,6	0.47	0
3	SO4	A	485	-	4,4,4	0.27	0	6,6,6	0.31	0
3	SO4	B	5	-	4,4,4	0.22	0	6,6,6	0.22	0
3	SO4	D	2	-	4,4,4	0.29	0	6,6,6	0.30	0
3	SO4	B	4	-	4,4,4	0.26	0	6,6,6	0.35	0
4	PGE	C	485	-	9,9,9	0.33	0	8,8,8	0.50	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
4	PGE	C	485	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	485	PGE	O1-C1-C2-O2
4	C	485	PGE	O2-C3-C4-O3
4	C	485	PGE	O3-C5-C6-O4
4	C	485	PGE	C6-C5-O3-C4
4	C	485	PGE	C4-C3-O2-C2

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, 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	448/456 (98%)	0.88	27 (6%) 21 30	7, 13, 21, 26	5 (1%)
1	B	448/456 (98%)	0.92	45 (10%) 7 11	3, 13, 23, 26	5 (1%)
1	C	448/456 (98%)	0.82	18 (4%) 38 48	6, 13, 19, 24	5 (1%)
1	D	448/456 (98%)	0.91	41 (9%) 9 14	4, 13, 21, 26	5 (1%)
All	All	1792/1824 (98%)	0.88	131 (7%) 15 23	3, 13, 21, 26	20 (1%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	SER	8.0
1	D	84	ALA	7.5
1	D	81	GLY	7.1
1	B	84	ALA	6.8
1	A	446	TYR	6.1
1	B	125	SER	6.0
1	D	122	PRO	5.9
1	B	446	TYR	5.4
1	B	448	ASP	5.2
1	D	88	THR	5.1
1	A	444	GLY	5.0
1	D	85	SER	4.9
1	C	123	LYS	4.9
1	D	82	LYS	4.9
1	C	84	ALA	4.8
1	B	128	THR	4.7
1	A	447	GLU	4.7
1	C	122	PRO	4.6
1	D	125	SER	4.5
1	B	86	GLY	4.4
1	B	124	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	125	SER	4.3
1	D	83	ASN	4.3
1	D	87	ASN	4.3
1	C	247	ALA	4.2
1	A	445	PHE	4.2
1	A	196	TYR	4.2
1	D	196	TYR	4.0
1	D	138	GLY	4.0
1	A	443	ARG	4.0
1	B	85	SER	3.9
1	C	467	SER	3.9
1	B	310	GLY	3.9
1	D	123	LYS	3.8
1	B	445	PHE	3.8
1	B	88	THR	3.8
1	B	126	ASN	3.8
1	B	309[A]	GLU	3.7
1	B	87	ASN	3.7
1	D	86	GLY	3.7
1	D	246	GLY	3.6
1	B	447	GLU	3.5
1	B	249	THR	3.5
1	B	83	ASN	3.4
1	D	128	THR	3.4
1	A	122	PRO	3.3
1	B	127	ASP	3.2
1	A	211	PRO	3.2
1	D	142	ILE	3.2
1	C	87	ASN	3.2
1	D	34	SER	3.1
1	A	448	ASP	3.1
1	C	85	SER	3.1
1	B	158	PHE	3.1
1	D	120	GLY	3.0
1	B	467	SER	3.0
1	D	300	PHE	3.0
1	D	249	THR	2.9
1	D	245	GLY	2.9
1	B	363	TRP	2.9
1	C	124	ASP	2.9
1	B	242	ILE	2.9
1	B	247	ALA	2.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	140	LYS	2.9
1	A	121	ASP	2.8
1	D	307	LEU	2.8
1	A	128	THR	2.8
1	B	123	LYS	2.8
1	B	153	LYS	2.8
1	D	247	ALA	2.8
1	A	467	SER	2.8
1	D	467	SER	2.8
1	C	86	GLY	2.7
1	B	311	SER	2.7
1	B	89	ILE	2.7
1	B	121	ASP	2.6
1	B	245	GLY	2.6
1	D	126	ASN	2.6
1	C	83	ASN	2.6
1	C	81	GLY	2.6
1	A	123	LYS	2.5
1	B	133	PHE	2.5
1	A	357	PHE	2.5
1	D	143	ASP	2.5
1	D	473	VAL	2.4
1	B	186	LEU	2.4
1	D	308	LEU	2.4
1	B	122	PRO	2.4
1	A	132	LEU	2.4
1	D	145	TRP	2.4
1	A	108	THR	2.3
1	B	82	LYS	2.3
1	A	247	ALA	2.3
1	B	154	ASP	2.3
1	B	264	ASN	2.3
1	C	89	ILE	2.3
1	B	208	MET	2.3
1	D	181	ASP	2.3
1	B	166	LYS	2.3
1	D	337	VAL	2.3
1	A	442	ASN	2.3
1	C	268	TYR	2.3
1	A	124	ASP	2.3
1	B	252	ASN	2.3
1	B	206	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	307	LEU	2.2
1	D	127	ASP	2.2
1	D	139	ASP	2.2
1	D	314[A]	GLU	2.2
1	A	255	LEU	2.2
1	A	165	LEU	2.2
1	D	474	LEU	2.2
1	A	111	GLY	2.2
1	B	246	GLY	2.1
1	C	213	ASP	2.1
1	D	461	ILE	2.1
1	D	472	ARG	2.1
1	D	124	ASP	2.1
1	A	158	PHE	2.1
1	A	172	TRP	2.1
1	A	161	ASN	2.1
1	B	117	ALA	2.1
1	C	354	ALA	2.1
1	A	80	LYS	2.0
1	C	194	LYS	2.0
1	B	443	ARG	2.0
1	B	308	LEU	2.0
1	C	387	LEU	2.0
1	B	181	ASP	2.0
1	D	195	GLN	2.0
1	D	165	LEU	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
3	SO4	B	4	5/5	0.82	0.21	33,33,33,33	0
4	PGE	C	485	10/10	0.87	0.15	20,20,21,21	0
3	SO4	D	2	5/5	0.93	0.12	31,31,32,32	0
3	SO4	B	3	5/5	0.93	0.15	32,32,32,32	0
3	SO4	B	5	5/5	0.94	0.21	31,31,31,31	0
3	SO4	A	485	5/5	0.95	0.10	30,30,30,30	0
2	CA	C	1	1/1	0.97	0.08	10,10,10,10	0
2	CA	B	1	1/1	0.99	0.04	12,12,12,12	0
2	CA	A	1	1/1	0.99	0.05	13,13,13,13	0
2	CA	D	1	1/1	0.99	0.07	14,14,14,14	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.