



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 02:54 AM EST

PDB ID : 3OM4  
Title : Crystal structure of B. megaterium levansucrase mutant K373A  
Authors : Strube, C.P.; Homann, A.; Gamer, M.; Jahn, D.; Seibel, J.; Heinz, D.W.  
Deposited on : 2010-08-26  
Resolution : 1.75 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>.

---

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

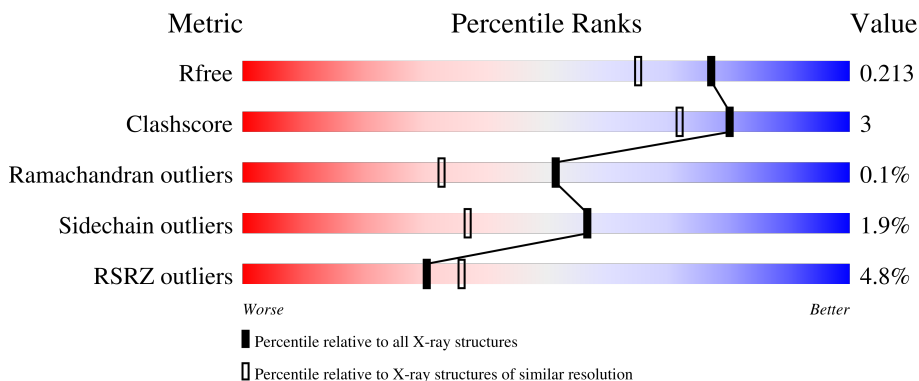
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

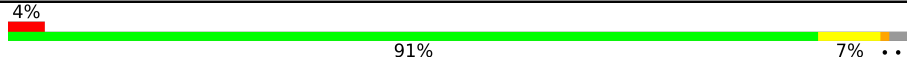
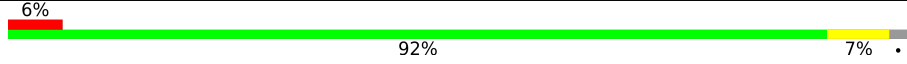
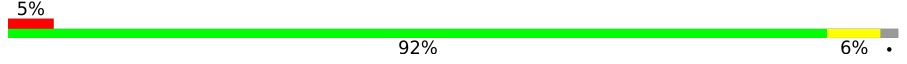
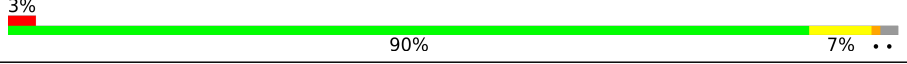
The reported resolution of this entry is 1.75 Å.

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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	 4% 91% 7% ..
1	B	456	 6% 92% 7% .
1	C	456	 5% 92% 6% .
1	D	456	 3% 90% 7% ..

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 15821 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	3558	2237	592	722	7	0	4	0
1	B	448	3553	2230	592	724	7	0	3	0
1	C	448	3572	2243	596	726	7	0	5	0
1	D	448	3577	2243	596	730	8	0	5	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	ALA	LYS	engineered mutation	UNP D5DC07
B	373	ALA	LYS	engineered mutation	UNP D5DC07
C	373	ALA	LYS	engineered mutation	UNP D5DC07
D	373	ALA	LYS	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 DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



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

*Continued on next page...*

Continued from previous page...

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	C O	0	0
			13	8 5		

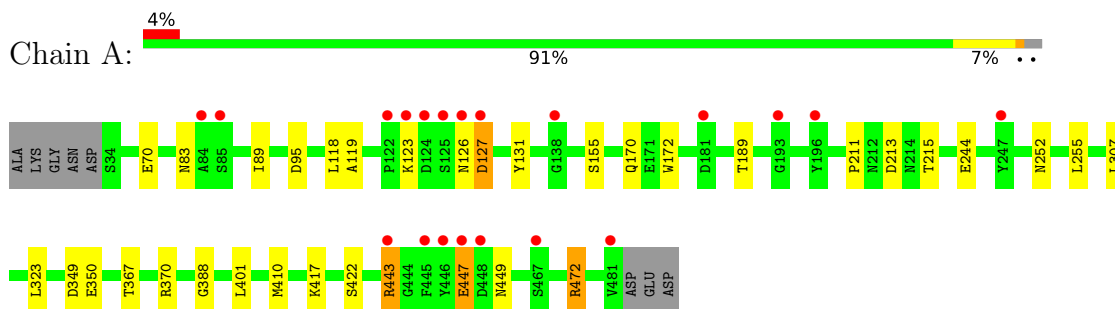
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	367	Total	O	0	0
			367	367		
7	B	370	Total	O	0	0
			370	370		
7	C	350	Total	O	0	0
			350	350		
7	D	370	Total	O	0	0
			370	370		

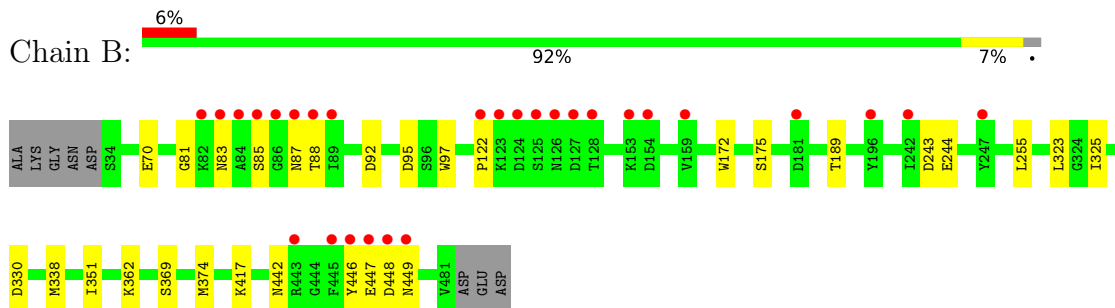
### 3 Residue-property plots [i](#)

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.

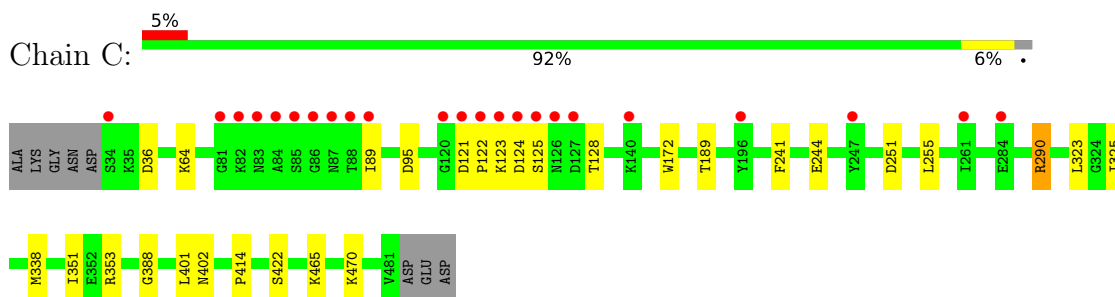
- Molecule 1: Levansucrase



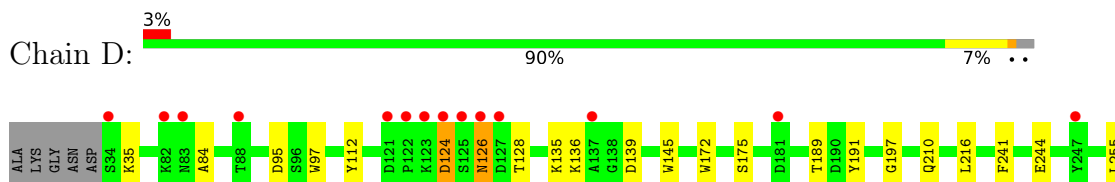
- Molecule 1: Levansucrase

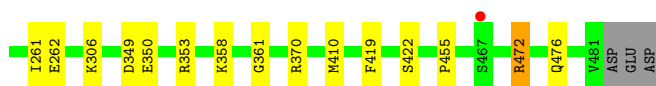


- Molecule 1: Levansucrase



- Molecule 1: Levansucrase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.58Å 100.08Å 95.54Å 90.00° 90.67° 90.00°	Depositor
Resolution (Å)	47.77 – 1.75 47.77 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.77-1.75) 98.8 (47.77-1.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.41 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.202 , 0.213 0.201 , 0.213	Depositor DCC
$R_{free}$ test set	8763 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.6	Xtriage
Anisotropy	0.089	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.059 for l,k,-h 0.058 for h,-k,-l 0.053 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	15821	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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, PG4, CA, PGE, PEG

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	0/3647	0.53	0/4938
1	B	0.34	0/3636	0.53	0/4922
1	C	0.34	0/3655	0.52	0/4947
1	D	0.36	0/3654	0.53	0/4946
All	All	0.35	0/14592	0.53	0/19753

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	3558	0	3402	23	0
1	B	3553	0	3385	18	0
1	C	3572	0	3408	19	0
1	D	3577	0	3398	19	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	7	0	10	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	10	0	14	1	0
4	B	20	0	28	0	0
4	C	10	0	14	1	0
4	D	10	0	14	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	10	0	0	0	0
5	D	10	0	0	0	0
6	C	13	0	18	0	0
7	A	367	0	0	2	0
7	B	370	0	0	2	0
7	C	350	0	0	1	0
7	D	370	0	0	1	0
All	All	15821	0	13691	77	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 3.

All (77) 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:D:353:ARG:HD2	1:D:422:SER:OG	1.67	0.94
1:A:472:ARG:HH11	1:A:472:ARG:HG2	1.36	0.90
1:D:472:ARG:HG2	1:D:472:ARG:HH11	1.40	0.87
1:C:290:ARG:HG2	1:C:290:ARG:HH11	1.48	0.79
1:C:353:ARG:HD2	1:C:422:SER:OG	1.82	0.79
1:A:127:ASP:O	1:A:127:ASP:CG	2.21	0.77
1:B:83:ASN:HB2	1:B:87:ASN:H	1.58	0.68
1:D:135:LYS:HE2	1:D:139:ASP:O	1.95	0.66
1:C:290:ARG:HG2	1:C:290:ARG:NH1	2.10	0.66
1:D:306:LYS:HD2	7:D:1405:HOH:O	1.95	0.66
1:C:64:LYS:NZ	7:C:1456:HOH:O	2.29	0.64
1:A:244:GLU:HG2	7:A:501:HOH:O	1.98	0.62
1:A:472:ARG:HG2	1:A:472:ARG:NH1	2.12	0.62
1:B:448:ASP:HB2	7:B:1442:HOH:O	2.01	0.61
1:A:126:ASN:HB2	1:A:170:GLN:HE22	1.70	0.57
1:C:36:ASP:HB3	1:C:290:ARG:HE	1.69	0.57
1:D:112:TYR:CE1	1:D:136:LYS:HD3	2.40	0.57
1:D:172:TRP:HB2	1:D:189:THR:HB	1.86	0.56
1:C:172:TRP:HB2	1:C:189:THR:HB	1.87	0.56
1:A:155:SER:HB2	1:B:85:SER:HA	1.87	0.55

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ASN:HB2	1:A:170:GLN:NE2	2.21	0.55
1:A:83:ASN:HB3	1:A:89:ILE:HG12	1.89	0.55
1:B:330:ASP:HB3	7:B:1373:HOH:O	2.08	0.54
1:A:172:TRP:HB2	1:A:189:THR:HB	1.90	0.54
1:C:89:ILE:HD11	1:C:122:PRO:HA	1.92	0.52
1:C:241:PHE:O	1:C:244:GLU:HG2	2.10	0.52
1:C:414:PRO:HB3	4:C:486:PGE:H42	1.92	0.52
1:D:353:ARG:CD	1:D:422:SER:OG	2.50	0.51
1:D:472:ARG:HG2	1:D:472:ARG:NH1	2.16	0.49
1:B:172:TRP:HB2	1:B:189:THR:HB	1.95	0.49
1:A:70:GLU:HG2	1:A:417:LYS:HD3	1.95	0.49
1:B:369:SER:HB3	1:B:374:MET:CE	2.43	0.48
1:B:81:GLY:O	1:B:88:THR:HA	2.14	0.48
1:C:402:ASN:OD1	1:C:465[A]:LYS:HE2	2.13	0.48
1:C:465[A]:LYS:HE2	1:C:465[A]:LYS:HA	1.96	0.48
1:A:447:GLU:H	1:A:447:GLU:CD	2.17	0.47
1:B:83:ASN:HB2	1:B:87:ASN:N	2.27	0.46
1:B:70:GLU:CG	1:B:417:LYS:HD3	2.46	0.46
1:B:92:ASP:OD2	1:B:122:PRO:HG2	2.16	0.46
1:B:442:ASN:O	1:B:449:ASN:HA	2.16	0.46
1:C:353:ARG:CD	1:C:422:SER:OG	2.60	0.46
1:A:119:ALA:HB3	1:A:131:TYR:CD2	2.51	0.46
1:D:84:ALA:HB2	1:D:124:ASP:OD1	2.16	0.46
1:A:252:ASN:HD22	1:A:350:GLU:HG3	1.81	0.45
1:D:97:TRP:CD1	1:D:175:SER:HA	2.52	0.45
1:A:323:LEU:HD11	1:A:367:THR:HB	1.98	0.45
1:C:244:GLU:OE1	1:C:251:ASP:OD2	2.35	0.45
1:A:449:ASN:OD1	1:A:449:ASN:N	2.49	0.45
1:D:410:MET:HE1	1:D:419:PHE:CE1	2.51	0.44
1:D:455:PRO:HA	1:D:476:GLN:HA	1.98	0.44
1:B:83:ASN:N	1:B:87:ASN:O	2.45	0.44
1:C:123:LYS:O	1:C:125:SER:N	2.51	0.44
1:B:323:LEU:HG	1:B:351:ILE:HD12	2.00	0.43
1:A:443:ARG:HG2	7:A:522:HOH:O	2.18	0.43
1:C:290:ARG:HH11	1:C:290:ARG:CG	2.25	0.43
1:D:210:GLN:HG2	1:D:216:LEU:HD23	2.00	0.43
1:A:350:GLU:OE2	1:A:370:ARG:NH2	2.45	0.43
1:C:323:LEU:HG	1:C:351:ILE:HD12	2.01	0.43
1:A:252:ASN:ND2	1:A:350:GLU:HG3	2.34	0.43
1:B:325:ILE:HG23	1:B:338:MET:HB2	2.01	0.43
1:B:83:ASN:HB3	1:B:85:SER:H	1.84	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ASP:HB3	1:C:470:LYS:HE2	2.01	0.42
1:D:358:LYS:HE2	1:D:361:GLY:HA2	2.01	0.42
1:C:388:GLY:HA3	1:C:401:LEU:HD12	2.02	0.42
1:D:241:PHE:O	1:D:244:GLU:HG2	2.19	0.42
1:D:191:TYR:CE1	1:D:197:GLY:HA2	2.54	0.42
1:D:350:GLU:OE2	1:D:370:ARG:NH1	2.51	0.42
1:B:97:TRP:CD1	1:B:175:SER:HA	2.55	0.42
1:D:135:LYS:HD3	1:D:145:TRP:CE2	2.55	0.42
1:D:261:ILE:HG13	1:D:262:GLU:N	2.35	0.41
1:A:118:LEU:HD12	4:A:486:PGE:H4	2.01	0.41
1:A:472:ARG:NH1	1:A:472:ARG:CG	2.82	0.41
1:A:388:GLY:HA3	1:A:401:LEU:HD12	2.02	0.41
1:B:447:GLU:HG3	1:B:449:ASN:OD1	2.20	0.41
1:A:211:PRO:HG2	1:A:215:THR:HB	2.02	0.41
1:A:410:MET:HE3	1:A:410:MET:HB3	1.92	0.40
1:C:325:ILE:HG23	1:C:338:MET:HB2	2.03	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	450/456 (99%)	436 (97%)	14 (3%)	0	100	100
1	B	449/456 (98%)	432 (96%)	17 (4%)	0	100	100
1	C	451/456 (99%)	437 (97%)	13 (3%)	1 (0%)	47	29
1	D	451/456 (99%)	439 (97%)	11 (2%)	1 (0%)	47	29
All	All	1801/1824 (99%)	1744 (97%)	55 (3%)	2 (0%)	51	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	126	ASN
1	C	124	ASP

### 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	393/395 (100%)	382 (97%)	11 (3%)	43	20
1	B	392/395 (99%)	387 (99%)	5 (1%)	69	54
1	C	394/395 (100%)	389 (99%)	5 (1%)	69	54
1	D	394/395 (100%)	386 (98%)	8 (2%)	55	34
All	All	1573/1580 (100%)	1544 (98%)	29 (2%)	57	40

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASP
1	A	123	LYS
1	A	127	ASP
1	A	213	ASP
1	A	255	LEU
1	A	307	LEU
1	A	349	ASP
1	A	422	SER
1	A	443	ARG
1	A	447	GLU
1	A	472	ARG
1	B	95	ASP
1	B	244	GLU
1	B	255	LEU
1	B	362	LYS
1	B	446	TYR
1	C	95	ASP
1	C	121	ASP
1	C	128	THR
1	C	255	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	290	ARG
1	D	35	LYS
1	D	95	ASP
1	D	124	ASP
1	D	126	ASN
1	D	128	THR
1	D	255	LEU
1	D	349	ASP
1	D	472	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	252	ASN
1	B	83	ASN
1	B	266	HIS
1	D	59	ASN
1	D	110	HIS

### 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 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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
6	PG4	C	485	-	12,12,12	0.56	0	11,11,11	0.46	0
4	PGE	B	486	-	9,9,9	0.46	0	8,8,8	0.37	0
3	PEG	A	485	-	6,6,6	0.64	0	5,5,5	0.56	0
4	PGE	B	485	-	9,9,9	0.54	0	8,8,8	0.38	0
4	PGE	A	486	-	9,9,9	0.52	0	8,8,8	0.48	0
5	SO4	A	6	-	4,4,4	0.18	0	6,6,6	0.12	0
4	PGE	D	485	-	9,9,9	0.50	0	8,8,8	0.47	0
5	SO4	C	4	-	4,4,4	0.15	0	6,6,6	0.12	0
5	SO4	B	7	-	4,4,4	0.27	0	6,6,6	0.26	0
4	PGE	C	486	-	9,9,9	0.52	0	8,8,8	0.45	0
5	SO4	D	486	-	4,4,4	0.14	0	6,6,6	0.08	0
5	SO4	D	5	-	4,4,4	0.15	0	6,6,6	0.04	0
5	SO4	C	2	-	4,4,4	0.14	0	6,6,6	0.20	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
6	PG4	C	485	-	-	4/10/10/10	-
4	PGE	B	486	-	-	2/7/7/7	-
3	PEG	A	485	-	-	3/4/4/4	-
4	PGE	B	485	-	-	4/7/7/7	-
4	PGE	A	486	-	-	4/7/7/7	-
4	PGE	D	485	-	-	4/7/7/7	-
4	PGE	C	486	-	-	6/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	485	PG4	O2-C3-C4-O3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	B	486	PGE	O1-C1-C2-O2
4	B	485	PGE	O2-C3-C4-O3
4	A	486	PGE	O1-C1-C2-O2
4	B	485	PGE	O1-C1-C2-O2
4	B	485	PGE	O3-C5-C6-O4
4	D	485	PGE	O1-C1-C2-O2
4	D	485	PGE	O3-C5-C6-O4
6	C	485	PG4	O1-C1-C2-O2
6	C	485	PG4	O4-C7-C8-O5
4	C	486	PGE	O3-C5-C6-O4
3	A	485	PEG	O1-C1-C2-O2
4	B	486	PGE	C6-C5-O3-C4
4	C	486	PGE	C6-C5-O3-C4
4	C	486	PGE	C1-C2-O2-C3
4	D	485	PGE	C6-C5-O3-C4
6	C	485	PG4	C3-C4-O3-C5
4	A	486	PGE	C4-C3-O2-C2
4	A	486	PGE	O2-C3-C4-O3
3	A	485	PEG	C4-C3-O2-C2
4	C	486	PGE	O2-C3-C4-O3
4	A	486	PGE	O3-C5-C6-O4
4	B	485	PGE	C1-C2-O2-C3
3	A	485	PEG	O2-C3-C4-O4
4	D	485	PGE	C4-C3-O2-C2
4	C	486	PGE	C4-C3-O2-C2
4	C	486	PGE	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	486	PGE	1	0
4	C	486	PGE	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

### 6.1 Protein, DNA and RNA chains

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%)	0.16	20 (4%) 33 39	5, 12, 22, 28	11 (2%)
1	B	448/456 (98%)	0.23	28 (6%) 20 25	6, 11, 23, 32	10 (2%)
1	C	448/456 (98%)	0.20	23 (5%) 28 34	5, 11, 22, 29	12 (2%)
1	D	448/456 (98%)	0.13	15 (3%) 46 53	5, 11, 20, 27	8 (1%)
All	All	1792/1824 (98%)	0.18	86 (4%) 30 36	5, 11, 22, 32	41 (2%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	TYR	8.9
1	B	84	ALA	8.1
1	C	124	ASP	7.8
1	B	125	SER	7.4
1	D	247	TYR	6.3
1	D	125	SER	6.2
1	A	122	PRO	6.2
1	C	247	TYR	6.0
1	B	85	SER	5.9
1	B	86	GLY	5.7
1	B	247	TYR	5.5
1	A	125	SER	5.5
1	D	126	ASN	5.3
1	A	447	GLU	5.1
1	C	84	ALA	5.1
1	B	126	ASN	5.1
1	C	121	ASP	5.0
1	C	125	SER	5.0
1	C	126	ASN	4.8
1	B	88	THR	4.8
1	B	82	LYS	4.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	126	ASN	4.3
1	D	123	LYS	4.2
1	B	87	ASN	4.0
1	D	127	ASP	4.0
1	D	88	THR	3.9
1	C	85	SER	3.9
1	B	123	LYS	3.8
1	B	83	ASN	3.8
1	C	123	LYS	3.7
1	D	467	SER	3.3
1	C	88	THR	3.3
1	D	122	PRO	3.3
1	C	82	LYS	3.3
1	A	196	TYR	3.2
1	D	124	ASP	3.2
1	C	34	SER	3.2
1	A	127	ASP	3.1
1	A	445	PHE	3.1
1	D	82	LYS	3.1
1	A	124	ASP	3.0
1	C	87	ASN	3.0
1	A	446	TYR	3.0
1	C	196	TYR	3.0
1	C	261	ILE	2.9
1	C	127	ASP	2.8
1	C	86	GLY	2.8
1	B	449	ASN	2.8
1	A	123	LYS	2.8
1	A	481	VAL	2.8
1	B	448	ASP	2.8
1	B	446	TYR	2.7
1	B	159	VAL	2.7
1	B	127	ASP	2.6
1	B	154	ASP	2.6
1	A	467	SER	2.5
1	D	121	ASP	2.5
1	A	84	ALA	2.5
1	A	181	ASP	2.5
1	A	138	GLY	2.4
1	D	83	ASN	2.4
1	B	443	ARG	2.4
1	D	34	SER	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	193	GLY	2.4
1	A	443	ARG	2.4
1	C	83	ASN	2.4
1	B	447	GLU	2.4
1	A	448	ASP	2.3
1	B	89	ILE	2.3
1	A	85	SER	2.3
1	D	181	ASP	2.3
1	C	284	GLU	2.2
1	B	122	PRO	2.2
1	B	445	PHE	2.2
1	B	196	TYR	2.2
1	C	122	PRO	2.2
1	C	89	ILE	2.2
1	B	242	ILE	2.1
1	B	181	ASP	2.1
1	C	81	GLY	2.1
1	B	128	THR	2.1
1	D	137	ALA	2.1
1	B	153	LYS	2.1
1	C	140	LYS	2.0
1	B	124	ASP	2.0
1	C	120	GLY	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.

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	PGE	C	486	10/10	0.85	0.14	22,22,23,23	0
4	PGE	B	486	10/10	0.86	0.17	22,23,23,23	0
3	PEG	A	485	7/7	0.86	0.15	30,30,30,30	0
4	PGE	B	485	10/10	0.88	0.14	21,22,22,23	0
4	PGE	D	485	10/10	0.88	0.15	22,22,23,23	0
6	PG4	C	485	13/13	0.88	0.14	27,28,29,30	0
4	PGE	A	486	10/10	0.89	0.13	22,22,22,23	0
5	SO4	D	5	5/5	0.94	0.16	31,31,32,32	0
5	SO4	B	7	5/5	0.95	0.17	30,31,31,31	0
5	SO4	D	486	5/5	0.96	0.16	30,30,30,30	0
5	SO4	C	2	5/5	0.96	0.15	29,29,29,29	0
5	SO4	C	4	5/5	0.96	0.15	31,31,31,31	0
5	SO4	A	6	5/5	0.97	0.17	32,32,32,32	0
2	CA	B	1	1/1	1.00	0.06	8,8,8,8	0
2	CA	C	1	1/1	1.00	0.06	7,7,7,7	0
2	CA	D	1	1/1	1.00	0.07	6,6,6,6	0
2	CA	A	1	1/1	1.00	0.05	8,8,8,8	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.