



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 12:43 AM EST

PDB ID : 3OM7  
Title : Crystal structure of B. megaterium levansucrase mutant Y247W  
Authors : Strube, C.P.; Homann, A.; Gamer, M.; Jahn, D.; Seibel, J.; Heinz, D.W.  
Deposited on : 2010-08-26  
Resolution : 1.86 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

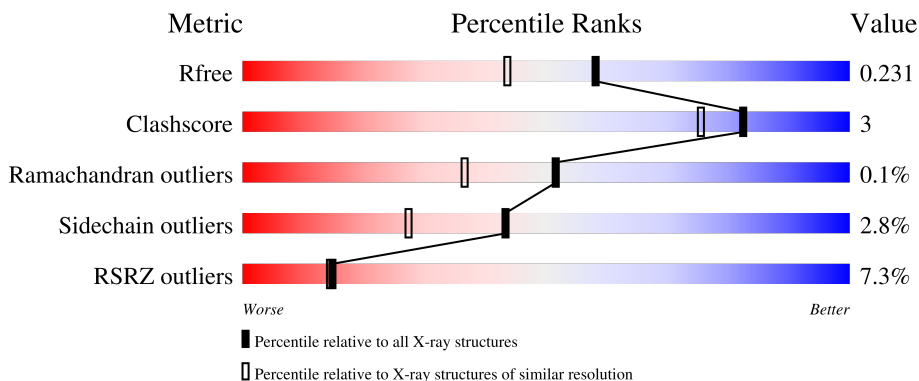
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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	 8% 91% 6% ..
1	B	456	 9% 92% 6% .
1	C	456	 5% 90% 7% ..
1	D	456	 7% 90% 8% ..

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15429 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	C	448	3550	2230	593	720	7	0	2	0
1	A	448	3569	2239	600	723	7	0	3	0
1	B	448	3564	2238	595	724	7	0	3	0
1	D	448	3552	2230	595	720	7	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



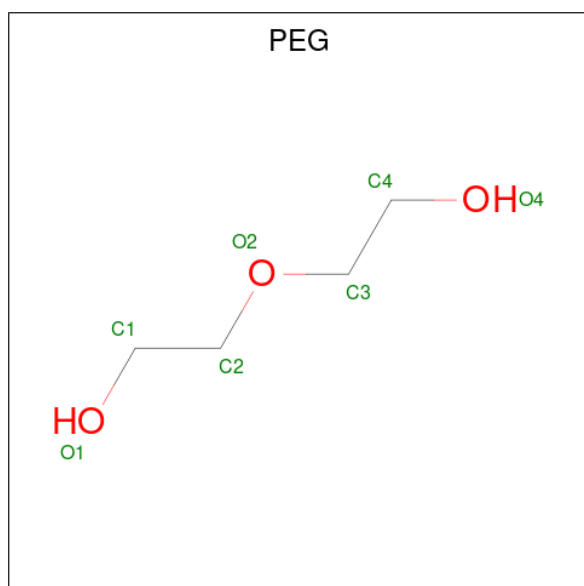
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		

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



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

- Molecule 5 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
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	D	1	Total C O 7 4 3	0	0

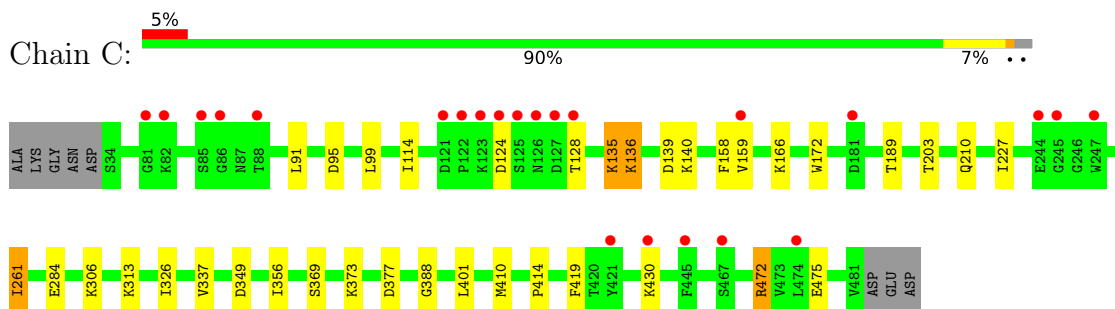
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	320	Total 320	O 320	0	0
6	A	281	Total 281	O 281	0	0
6	B	209	Total 209	O 209	0	0
6	D	284	Total 284	O 284	0	0

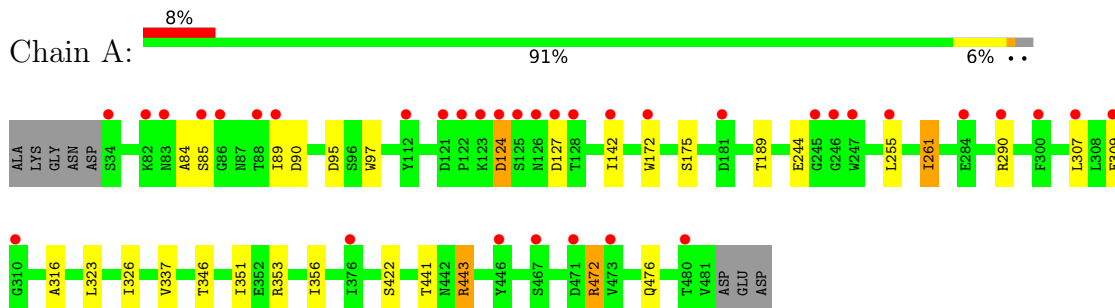
### 3 Residue-property plots [i](#)

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.

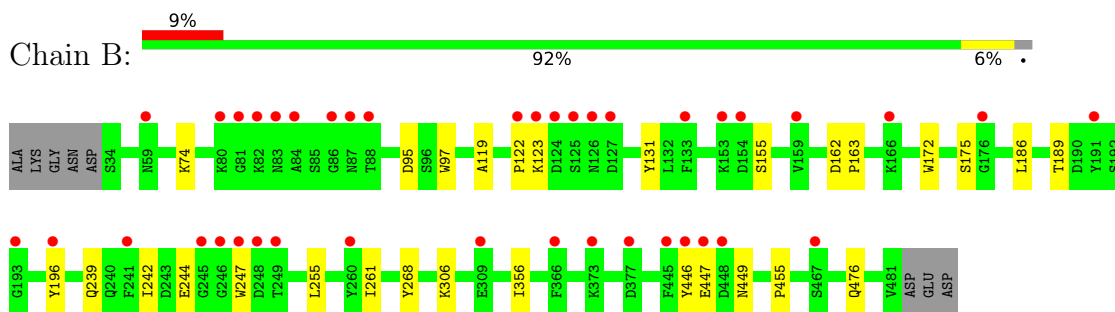
- Molecule 1: Levansucrase



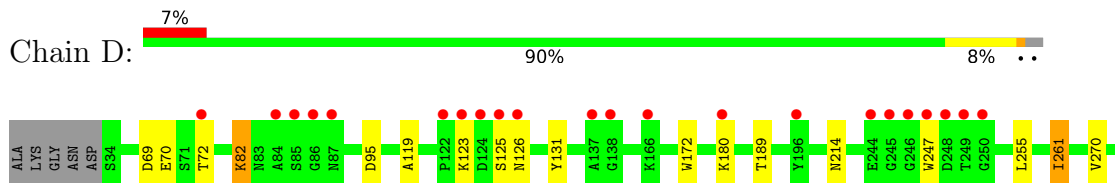
- Molecule 1: Levansucrase

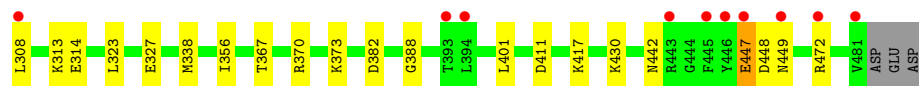


- Molecule 1: Levansucrase



- Molecule 1: Levansucrase







## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.53Å 100.05Å 95.45Å 90.00° 90.51° 90.00°	Depositor
Resolution (Å)	50.01 – 1.86 47.72 – 1.86	Depositor EDS
% Data completeness (in resolution range)	91.8 (50.01-1.86) 94.5 (47.72-1.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.53 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.201 , 0.216 0.217 , 0.231	Depositor DCC
$R_{free}$ test set	7005 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.1	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.022 for h,-k,-l 0.058 for l,-k,h	Xtriage
Reported twinning fraction	0.711 for H, K, L 0.157 for -h,-k,l 0.131 for -L, K, H	Depositor
Outliers	0 of 139985 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	15429	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: PEG, 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	0.35	0/3647	0.52	0/4936
1	B	0.35	0/3648	0.52	0/4938
1	C	0.35	0/3634	0.52	0/4919
1	D	0.35	0/3630	0.51	0/4914
All	All	0.35	0/14559	0.52	0/19707

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	3569	0	3400	19	0
1	B	3564	0	3396	13	0
1	C	3550	0	3389	19	0
1	D	3552	0	3384	22	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	10	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	10	0	14	0	0
3	C	10	0	14	0	0
3	D	10	0	14	0	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	D	5	0	0	0	0
5	A	7	0	10	0	0
5	B	7	0	10	0	0
5	D	7	0	10	0	0
6	A	281	0	0	0	0
6	B	209	0	0	0	0
6	C	320	0	0	0	0
6	D	284	0	0	2	0
All	All	15429	0	13655	71	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 (71) 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:472:ARG:HH11	1:A:472:ARG:HG2	1.43	0.83
1:C:472:ARG:HG2	1:C:472:ARG:HH11	1.43	0.82
1:C:306:LYS:HE2	1:C:377:ASP:OD2	1.87	0.73
1:D:327:GLU:HB2	1:D:338:MET:HE1	1.74	0.69
1:A:353:ARG:HD2	1:A:422:SER:OG	1.92	0.69
1:A:261:ILE:HG21	1:A:356:ILE:HG23	1.77	0.66
1:D:472:ARG:HG2	1:D:472:ARG:HH11	1.60	0.66
1:B:196:TYR:HD1	1:B:247:TRP:HZ3	1.45	0.64
1:A:443:ARG:HH11	1:A:443:ARG:HG2	1.61	0.64
1:B:196:TYR:HD1	1:B:247:TRP:CZ3	2.17	0.63
1:C:261:ILE:HG21	1:C:356:ILE:HG23	1.83	0.61
1:D:261:ILE:HG21	1:D:356:ILE:HG23	1.83	0.59
1:A:443:ARG:HG2	1:A:443:ARG:NH1	2.17	0.58
1:C:136:LYS:H	1:C:136:LYS:HD3	1.69	0.58
1:A:472:ARG:HG2	1:A:472:ARG:NH1	2.14	0.58
1:B:196:TYR:CD1	1:B:247:TRP:HZ3	2.22	0.57
1:C:172:TRP:HB2	1:C:189:THR:HB	1.87	0.57
1:C:136:LYS:H	1:C:136:LYS:CD	2.19	0.56
1:D:70:GLU:CG	1:D:417:LYS:HD3	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:327:GLU:HB2	1:D:338:MET:CE	2.35	0.54
1:A:441:THR:HB	1:A:443:ARG:HD2	1.90	0.54
1:B:261:ILE:HG21	1:B:356:ILE:HG23	1.90	0.54
1:D:172:TRP:HB2	1:D:189:THR:HB	1.90	0.53
1:D:126:ASN:O	1:D:126:ASN:CG	2.48	0.53
1:D:308:LEU:O	1:D:313:LYS:HD3	2.09	0.52
1:D:447:GLU:HG3	1:D:448:ASP:HA	1.92	0.51
1:A:172:TRP:HB2	1:A:189:THR:HB	1.92	0.51
1:A:124:ASP:N	1:A:124:ASP:OD1	2.44	0.51
1:A:326:ILE:HG22	1:A:337:VAL:HA	1.93	0.50
1:D:69:ASP:O	1:D:72:THR:HG22	2.12	0.50
1:A:89:ILE:HG22	1:A:90:ASP:N	2.27	0.49
1:B:172:TRP:HB2	1:B:189:THR:HB	1.94	0.49
1:C:472:ARG:HG2	1:C:472:ARG:NH1	2.18	0.49
1:A:323:LEU:HG	1:A:351:ILE:HD12	1.93	0.49
1:A:142:ILE:HD12	1:A:476:GLN:HB3	1.95	0.48
1:D:370:ARG:HH21	1:D:373:LYS:HE3	1.79	0.47
1:D:125:SER:OG	1:D:126:ASN:N	2.46	0.47
1:C:159:VAL:HG22	1:A:85:SER:HB2	1.98	0.46
1:B:196:TYR:CD1	1:B:247:TRP:CZ3	2.99	0.46
1:B:239:GLN:HA	1:B:242:ILE:HD12	1.98	0.46
1:D:323:LEU:HD11	1:D:367:THR:HB	1.98	0.46
1:D:442:ASN:O	1:D:449:ASN:HA	2.16	0.46
1:D:388:GLY:HA3	1:D:401:LEU:HD12	1.98	0.45
1:C:135:LYS:HE2	1:C:139:ASP:O	2.16	0.44
1:D:472:ARG:HG2	1:D:472:ARG:NH1	2.29	0.44
1:A:290[B]:ARG:O	1:A:290[B]:ARG:HD2	2.18	0.43
1:B:162:ASP:HA	1:B:163:PRO:HD3	1.93	0.43
1:D:119:ALA:HB3	1:D:131:TYR:CD1	2.53	0.43
1:A:316:ALA:O	1:A:346:THR:HA	2.19	0.43
1:A:353:ARG:CD	1:A:422:SER:OG	2.66	0.43
1:D:261:ILE:HD11	1:D:270:VAL:HG23	2.01	0.43
1:C:388:GLY:HA3	1:C:401:LEU:HD12	2.01	0.42
1:C:410:MET:HE1	1:C:419:PHE:CE1	2.54	0.42
1:B:306:LYS:HD3	1:B:306:LYS:C	2.39	0.42
1:C:414:PRO:HA	1:C:419:PHE:CD1	2.54	0.42
1:B:455:PRO:HA	1:B:476:GLN:HA	2.00	0.42
1:C:472:ARG:HH11	1:C:472:ARG:CG	2.22	0.42
1:B:97:TRP:CD1	1:B:175:SER:HA	2.54	0.42
1:C:284:GLU:OE1	1:C:313:LYS:HE2	2.19	0.42
1:C:140:LYS:O	1:C:475:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ILE:HG13	1:B:268:TYR:HB2	2.02	0.41
1:A:97:TRP:CD1	1:A:175:SER:HA	2.56	0.41
1:D:82:LYS:N	1:D:82:LYS:HD2	2.36	0.41
1:D:180:LYS:HG3	6:D:498:HOH:O	2.20	0.41
1:B:119:ALA:HB3	1:B:131:TYR:CD1	2.56	0.41
1:C:99:LEU:HD22	1:C:114:ILE:HD12	2.03	0.41
1:D:370:ARG:HB2	6:D:605:HOH:O	2.20	0.40
1:C:158:PHE:CG	1:A:84:ALA:HB1	2.57	0.40
1:C:326:ILE:HG22	1:C:337:VAL:HA	2.03	0.40
1:D:382:ASP:O	1:D:411:ASP:HA	2.21	0.40
1:C:203:THR:HB	1:C:227:ILE:HD11	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	449/456 (98%)	435 (97%)	14 (3%)	0	100	100
1	B	449/456 (98%)	432 (96%)	16 (4%)	1 (0%)	47	33
1	C	448/456 (98%)	435 (97%)	13 (3%)	0	100	100
1	D	447/456 (98%)	428 (96%)	19 (4%)	0	100	100
All	All	1793/1824 (98%)	1730 (96%)	62 (4%)	1 (0%)	51	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	122	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	393/396 (99%)	383 (98%)	10 (2%)	47	31
1	B	393/396 (99%)	383 (98%)	10 (2%)	47	31
1	C	392/396 (99%)	378 (96%)	14 (4%)	35	18
1	D	391/396 (99%)	381 (97%)	10 (3%)	46	30
All	All	1569/1584 (99%)	1525 (97%)	44 (3%)	43	27

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	91	LEU
1	C	95	ASP
1	C	124	ASP
1	C	128	THR
1	C	135	LYS
1	C	136	LYS
1	C	166	LYS
1	C	210	GLN
1	C	261	ILE
1	C	349	ASP
1	C	369	SER
1	C	373	LYS
1	C	430	LYS
1	C	472	ARG
1	A	95	ASP
1	A	124	ASP
1	A	127	ASP
1	A	244	GLU
1	A	255	LEU
1	A	261	ILE
1	A	307	LEU
1	A	309	GLU
1	A	443	ARG
1	A	472	ARG

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Mol	Chain	Res	Type
1	B	74	LYS
1	B	95	ASP
1	B	123	LYS
1	B	155	SER
1	B	186	LEU
1	B	244	GLU
1	B	255	LEU
1	B	446	TYR
1	B	447	GLU
1	B	449	ASN
1	D	82	LYS
1	D	95	ASP
1	D	123	LYS
1	D	214	ASN
1	D	247	TRP
1	D	255	LEU
1	D	261	ILE
1	D	314	GLU
1	D	430	LYS
1	D	447	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	62	GLN
1	C	101	ASN
1	C	110	HIS
1	C	167	ASN
1	C	210	GLN
1	C	312	ASN
1	C	381	GLN
1	A	57	GLN
1	A	297	ASN
1	A	312	ASN
1	B	282	GLN
1	B	450	HIS
1	D	101	ASN
1	D	214	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 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z  > 2$
5	PEG	A	486	-	6,6,6	0.43	0	5,5,5	0.26	0
4	SO4	A	8	-	4,4,4	0.13	0	6,6,6	0.34	0
5	PEG	B	485	-	6,6,6	0.45	0	5,5,5	0.31	0
3	PGE	D	485	-	9,9,9	0.47	0	8,8,8	0.26	0
4	SO4	B	5	-	4,4,4	0.13	0	6,6,6	0.08	0
3	PGE	C	485	-	9,9,9	0.44	0	8,8,8	0.31	0
4	SO4	A	2	-	4,4,4	0.14	0	6,6,6	0.09	0
3	PGE	B	486	-	9,9,9	0.42	0	8,8,8	0.27	0
4	SO4	C	4	-	4,4,4	0.14	0	6,6,6	0.09	0
4	SO4	A	6	-	4,4,4	0.14	0	6,6,6	0.07	0
5	PEG	D	486	-	6,6,6	0.41	0	5,5,5	0.31	0
4	SO4	D	7	-	4,4,4	0.15	0	6,6,6	0.08	0
3	PGE	A	485	-	9,9,9	0.45	0	8,8,8	0.28	0
4	SO4	C	486	-	4,4,4	0.12	0	6,6,6	0.05	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
5	PEG	A	486	-	-	3/4/4/4	-
5	PEG	B	485	-	-	3/4/4/4	-
3	PGE	D	485	-	-	4/7/7/7	-
3	PGE	C	485	-	-	5/7/7/7	-
3	PGE	B	486	-	-	3/7/7/7	-
5	PEG	D	486	-	-	3/4/4/4	-
3	PGE	A	485	-	-	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
3	C	485	PGE	O2-C3-C4-O3
3	D	485	PGE	O3-C5-C6-O4
5	A	486	PEG	O1-C1-C2-O2
5	B	485	PEG	O1-C1-C2-O2
5	D	486	PEG	O2-C3-C4-O4
3	A	485	PGE	O2-C3-C4-O3
3	C	485	PGE	O1-C1-C2-O2
3	A	485	PGE	O1-C1-C2-O2
3	C	485	PGE	O3-C5-C6-O4
3	A	485	PGE	O3-C5-C6-O4
5	B	485	PEG	O2-C3-C4-O4
5	D	486	PEG	O1-C1-C2-O2
3	B	486	PGE	O2-C3-C4-O3
5	A	486	PEG	C4-C3-O2-C2
5	A	486	PEG	C1-C2-O2-C3
5	D	486	PEG	C1-C2-O2-C3
3	D	485	PGE	C1-C2-O2-C3
3	D	485	PGE	C4-C3-O2-C2
3	A	485	PGE	C3-C4-O3-C5
3	C	485	PGE	C6-C5-O3-C4
5	B	485	PEG	C4-C3-O2-C2
3	A	485	PGE	C6-C5-O3-C4
3	C	485	PGE	C4-C3-O2-C2
3	A	485	PGE	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	B	486	PGE	C6-C5-O3-C4
3	D	485	PGE	C3-C4-O3-C5
3	B	486	PGE	C3-C4-O3-C5

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

### 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%)	0.77	35 (7%) 13 13	9, 15, 25, 33	12 (2%)
1	B	448/456 (98%)	0.84	40 (8%) 9 9	8, 15, 28, 34	9 (2%)
1	C	448/456 (98%)	0.68	23 (5%) 28 26	9, 14, 24, 32	11 (2%)
1	D	448/456 (98%)	0.73	32 (7%) 16 15	9, 16, 27, 32	8 (1%)
All	All	1792/1824 (98%)	0.75	130 (7%) 15 14	8, 15, 27, 34	40 (2%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	125	SER	12.6
1	D	247	TRP	9.2
1	C	125	SER	7.8
1	B	82	LYS	7.4
1	A	82	LYS	7.4
1	A	86	GLY	7.4
1	A	126	ASN	6.7
1	C	126	ASN	6.7
1	A	34	SER	6.4
1	A	88	THR	6.3
1	B	249	THR	6.2
1	C	124	ASP	5.6
1	A	124	ASP	5.6
1	B	84	ALA	5.5
1	C	123	LYS	5.5
1	B	125	SER	5.4
1	D	446	TYR	5.4
1	C	121	ASP	5.4
1	B	247	TRP	5.2
1	B	83	ASN	5.2
1	B	246	GLY	5.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	447	GLU	5.0
1	B	196	TYR	5.0
1	A	127	ASP	5.0
1	A	85	SER	4.8
1	A	83	ASN	4.7
1	D	248	ASP	4.7
1	B	245	GLY	4.7
1	D	447	GLU	4.6
1	C	85	SER	4.6
1	D	246	GLY	4.6
1	B	248	ASP	4.5
1	C	122	PRO	4.5
1	B	87	ASN	4.5
1	B	86	GLY	4.4
1	B	81	GLY	4.4
1	C	86	GLY	4.3
1	C	88	THR	4.3
1	D	245	GLY	4.3
1	D	249	THR	4.2
1	D	125	SER	4.2
1	A	247	TRP	4.1
1	B	446	TYR	3.9
1	B	241	PHE	3.9
1	D	250	GLY	3.8
1	B	159	VAL	3.8
1	A	89	ILE	3.8
1	B	122	PRO	3.8
1	D	138	GLY	3.7
1	D	196	TYR	3.6
1	B	467	SER	3.6
1	D	123	LYS	3.6
1	D	445	PHE	3.5
1	A	471	ASP	3.5
1	C	430	LYS	3.5
1	D	126	ASN	3.5
1	B	448	ASP	3.5
1	B	127	ASP	3.2
1	B	445	PHE	3.2
1	A	112	TYR	3.1
1	B	193	GLY	3.1
1	C	159	VAL	3.1
1	B	126	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	245	GLY	3.1
1	A	128	THR	3.1
1	C	82	LYS	3.0
1	A	467	SER	3.0
1	A	309	GLU	3.0
1	D	481	VAL	3.0
1	D	308	LEU	2.9
1	B	154	ASP	2.9
1	D	137	ALA	2.9
1	D	124	ASP	2.9
1	A	142	ILE	2.9
1	D	443	ARG	2.9
1	B	153	LYS	2.9
1	B	88	THR	2.9
1	B	373	LYS	2.8
1	D	85	SER	2.8
1	D	449	ASN	2.7
1	C	245	GLY	2.7
1	A	181	ASP	2.6
1	A	307	LEU	2.6
1	D	394	LEU	2.6
1	A	246	GLY	2.6
1	B	123	LYS	2.6
1	D	244	GLU	2.6
1	A	255	LEU	2.5
1	A	121	ASP	2.5
1	A	172	TRP	2.5
1	B	124	ASP	2.5
1	B	176	GLY	2.4
1	D	84	ALA	2.4
1	A	122	PRO	2.4
1	C	247	TRP	2.4
1	A	446	TYR	2.4
1	C	181	ASP	2.4
1	A	300	PHE	2.4
1	D	122	PRO	2.4
1	C	474	LEU	2.3
1	C	421	TYR	2.3
1	B	166	LYS	2.3
1	B	260	TYR	2.3
1	A	290[A]	ARG	2.3
1	A	376	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	81	GLY	2.3
1	D	72	THR	2.3
1	D	472	ARG	2.3
1	D	87	ASN	2.3
1	A	123	LYS	2.3
1	A	473	VAL	2.2
1	D	180	LYS	2.2
1	B	133	PHE	2.2
1	C	467	SER	2.2
1	A	480	THR	2.2
1	C	244	GLU	2.2
1	C	445	PHE	2.2
1	D	166	LYS	2.1
1	B	191	TYR	2.1
1	C	127	ASP	2.1
1	B	59[A]	ASN	2.1
1	D	86	GLY	2.1
1	A	310	GLY	2.1
1	B	309[A]	GLU	2.0
1	B	377	ASP	2.0
1	B	80	LYS	2.0
1	A	284	GLU	2.0
1	C	128	THR	2.0
1	D	393	THR	2.0
1	B	366	PHE	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	PGE	A	485	10/10	0.72	0.25	35,36,37,37	0
5	PEG	A	486	7/7	0.72	0.17	34,34,34,35	0
5	PEG	D	486	7/7	0.75	0.19	30,31,32,32	0
3	PGE	D	485	10/10	0.76	0.22	36,36,36,37	0
4	SO4	A	2	5/5	0.77	0.25	50,50,50,50	0
5	PEG	B	485	7/7	0.78	0.17	36,36,36,36	0
4	SO4	D	7	5/5	0.79	0.19	37,37,38,38	0
3	PGE	C	485	10/10	0.80	0.18	32,33,34,34	0
3	PGE	B	486	10/10	0.84	0.23	34,35,35,35	0
4	SO4	A	6	5/5	0.89	0.17	43,43,43,43	0
4	SO4	B	5	5/5	0.90	0.17	37,37,38,38	0
4	SO4	C	4	5/5	0.94	0.13	33,34,34,34	0
4	SO4	A	8	5/5	0.95	0.09	31,31,31,31	0
4	SO4	C	486	5/5	0.95	0.14	29,30,30,30	0
2	CA	D	1	1/1	0.99	0.04	14,14,14,14	0
2	CA	C	1	1/1	0.99	0.10	11,11,11,11	0
2	CA	A	1	1/1	0.99	0.08	15,15,15,15	0
2	CA	B	1	1/1	1.00	0.05	15,15,15,15	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.