



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 06:12 AM UTC

PDB ID : 4KTP / pdb_00004ktp
Title : Crystal structure of 2-O-alpha-glucosylglycerol phosphorylase in complex with glucose
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Deposited on : 2013-05-21
Resolution : 1.90 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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

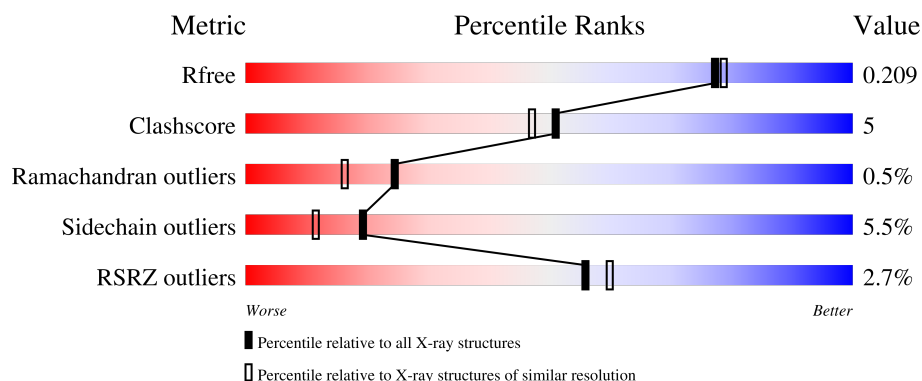
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 ≥ 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	769	2% 83% 14% .
1	B	769	4% 79% 16% ...

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13120 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 Glycoside hydrolase family 65 central catalytic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	767	Total	C	N	O	S	0	0	0
			6143	3881	1048	1192	22			
1	B	761	Total	C	N	O	S	0	0	0
			6086	3846	1034	1184	22			

There are 18 discrepancies between the modelled and reference sequences:

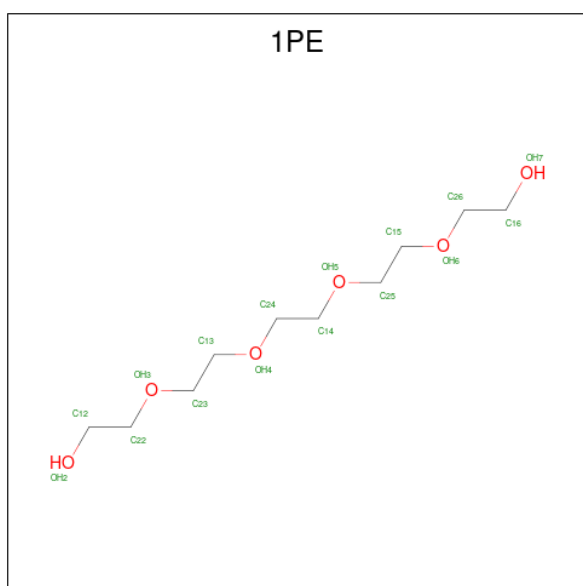
Chain	Residue	Modelled	Actual	Comment	Reference
A	226	PRO	SER	engineered mutation	UNP D6XZ22
A	762	LEU	-	expression tag	UNP D6XZ22
A	763	GLU	-	expression tag	UNP D6XZ22
A	764	HIS	-	expression tag	UNP D6XZ22
A	765	HIS	-	expression tag	UNP D6XZ22
A	766	HIS	-	expression tag	UNP D6XZ22
A	767	HIS	-	expression tag	UNP D6XZ22
A	768	HIS	-	expression tag	UNP D6XZ22
A	769	HIS	-	expression tag	UNP D6XZ22
B	226	PRO	SER	engineered mutation	UNP D6XZ22
B	762	LEU	-	expression tag	UNP D6XZ22
B	763	GLU	-	expression tag	UNP D6XZ22
B	764	HIS	-	expression tag	UNP D6XZ22
B	765	HIS	-	expression tag	UNP D6XZ22
B	766	HIS	-	expression tag	UNP D6XZ22
B	767	HIS	-	expression tag	UNP D6XZ22
B	768	HIS	-	expression tag	UNP D6XZ22
B	769	HIS	-	expression tag	UNP D6XZ22

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Ca	0	0
			2	2		

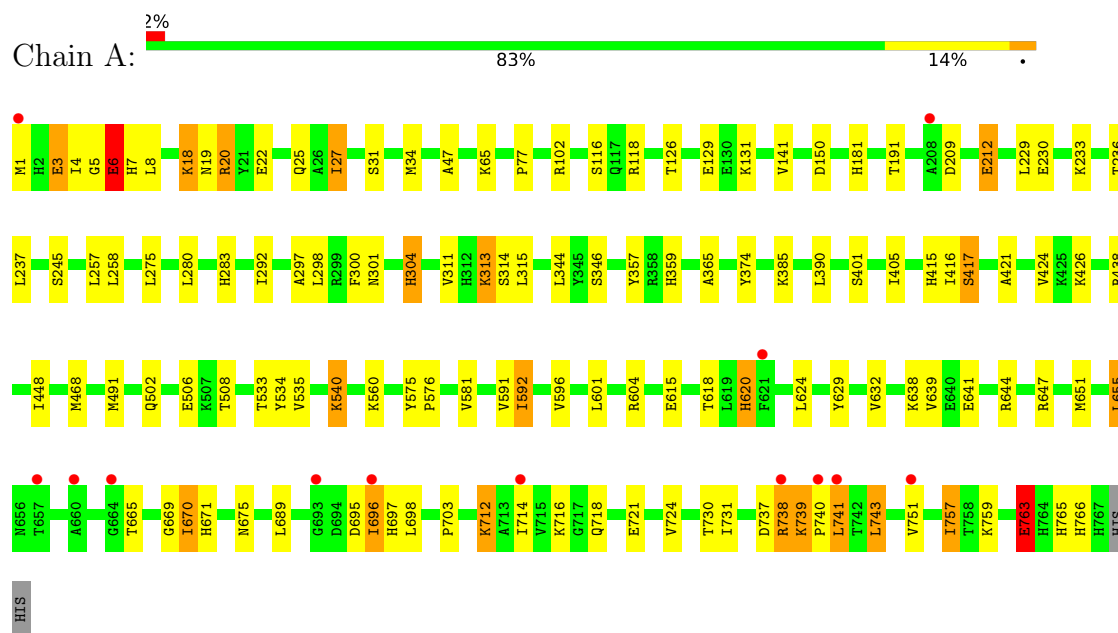
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	424	Total	O	0	0
			424	424		
6	B	412	Total	O	0	0
			412	412		

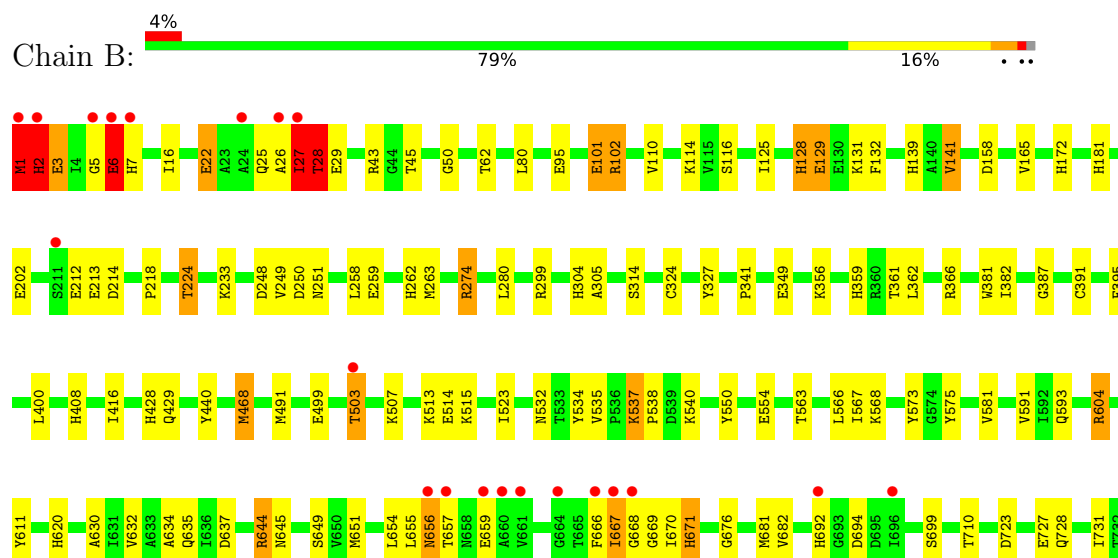
3 Residue-property plots

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: Glycoside hydrolase family 65 central catalytic



- Molecule 1: Glycoside hydrolase family 65 central catalytic



N733	K734	S735	E736	D737	R738	K739	F740	L741	T742	L743	H744	E748	K749	S750	V751	L752	D753	S754	E755	R756	T757	T758	K759	S760	R761	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.08Å 76.96Å 145.77Å 90.00° 128.39° 90.00°	Depositor
Resolution (Å)	19.94 – 1.90 19.94 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.94-1.90) 76.0 (19.94-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.206 (Not available) , 0.209	Depositor DCC
R_{free} test set	7048 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13120	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, BGC, CA, PG4

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	1.64	47/6291 (0.7%)	1.38	40/8532 (0.5%)
1	B	1.62	48/6230 (0.8%)	1.42	40/8449 (0.5%)
All	All	1.63	95/12521 (0.8%)	1.40	80/16981 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	251	ASN	N-CA	9.06	1.57	1.46
1	A	591	VAL	N-CA	7.91	1.55	1.46
1	B	630	ALA	N-CA	7.55	1.55	1.46
1	A	766	HIS	CE1-NE2	7.30	1.39	1.32
1	A	671	HIS	ND1-CE1	7.15	1.39	1.32

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	ASP	CA-C-N	-15.34	104.29	123.16
1	B	250	ASP	C-N-CA	-15.34	104.29	123.16
1	A	102	ARG	NE-CZ-NH2	-11.25	109.07	119.20
1	B	28	THR	N-CA-C	-10.86	99.22	111.71
1	B	656	ASN	N-CA-C	9.68	124.81	111.74

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	MET	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6143	0	5889	53	0
1	B	6086	0	5844	76	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	16	0	22	0	0
4	B	13	0	18	1	0
5	B	2	0	0	0	0
6	A	424	0	0	5	0
6	B	412	0	0	9	0
All	All	13120	0	11797	125	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 5.

The worst 5 of 125 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:101:GLU:HG3	6:B:1204:HOH:O	1.51	1.11
1:A:468:MET:HB2	1:B:468:MET:HE1	1.32	1.10
1:A:731:ILE:HD13	1:A:743:LEU:HD21	1.39	1.04
1:A:468:MET:SD	1:B:468:MET:HE2	1.98	1.03
1:B:25:GLN:O	1:B:29:GLU:HG2	1.61	1.00

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	765/769 (100%)	735 (96%)	28 (4%)	2 (0%)	36	29
1	B	759/769 (99%)	714 (94%)	39 (5%)	6 (1%)	16	8
All	All	1524/1538 (99%)	1449 (95%)	67 (4%)	8 (0%)	24	16

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	B	6	GLU
1	B	735	SER
1	B	751	VAL
1	B	757	ILE

5.3.2 Protein sidechains

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	656/658 (100%)	625 (95%)	31 (5%)	23	15
1	B	650/658 (99%)	609 (94%)	41 (6%)	16	8
All	All	1306/1316 (99%)	1234 (94%)	72 (6%)	19	11

5 of 72 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	659	GLU

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Mol	Chain	Res	Type
1	B	761	ARG
1	B	667	ILE
1	B	748	GLU
1	A	716	LYS

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

Mol	Chain	Res	Type
1	B	684	ASN
1	B	656	ASN
1	B	328	GLN
1	B	593	GLN
1	B	289	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
2	BGC	B	801	-	12,12,12	1.27	1 (8%)	17,17,17	1.34	2 (11%)
3	1PE	A	802	-	15,15,15	0.55	0	14,14,14	1.36	2 (14%)
4	PG4	B	802	-	12,12,12	0.62	0	11,11,11	1.28	1 (9%)
2	BGC	A	801	-	12,12,12	0.83	0	17,17,17	1.57	6 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BGC	B	801	-	-	0/2/22/22	0/1/1/1
3	1PE	A	802	-	-	3/13/13/13	-
4	PG4	B	802	-	-	4/10/10/10	-
2	BGC	A	801	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	BGC	C4-C5	2.72	1.58	1.53

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	1PE	OH3-C22-C12	-2.94	97.16	110.11
2	A	801	BGC	O4-C4-C3	-2.66	104.10	110.38
2	A	801	BGC	C1-C2-C3	-2.48	105.30	110.36
3	A	802	1PE	OH3-C23-C13	-2.47	99.12	110.35
4	B	802	PG4	C5-O3-C4	2.45	123.98	113.26

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	802	PG4	C1-C2-O2-C3
3	A	802	1PE	OH2-C12-C22-OH3
4	B	802	PG4	O2-C3-C4-O3
4	B	802	PG4	O4-C7-C8-O5
3	A	802	1PE	C16-C26-OH6-C15

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	802	PG4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	767/769 (99%)	-0.17	13 (1%) 69 72	16, 25, 47, 100	0
1	B	761/769 (98%)	-0.07	29 (3%) 44 47	14, 24, 58, 104	0
All	All	1528/1538 (99%)	-0.12	42 (2%) 56 60	14, 25, 54, 104	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	666	PHE	4.2
1	B	660	ALA	4.2
1	A	1	MET	3.8
1	B	2	HIS	3.3
1	B	1	MET	3.3

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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PG4	B	802	13/13	0.90	0.12	31,36,47,53	0
3	1PE	A	802	16/16	0.91	0.12	35,47,62,64	0
5	CA	B	804	1/1	0.92	0.07	45,45,45,45	0
2	BGC	B	801	12/12	0.97	0.06	19,20,23,27	0
5	CA	B	803	1/1	0.98	0.07	29,29,29,29	0
2	BGC	A	801	12/12	0.98	0.05	18,21,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.