



wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 11:37 pm BST

PDB ID : 6SCD
Title : Polyester hydrolase PE-H Y250S mutant of *Pseudomonas aestusnigri*
Authors : Bollinger, A.; Thies, S.; Kobus, S.; Hoepfner, A.; Smits, S.H.J.; Jaeger, K.-E.
Deposited on : 2019-07-24
Resolution : 1.35 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 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 : 2.11
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) : 2.11

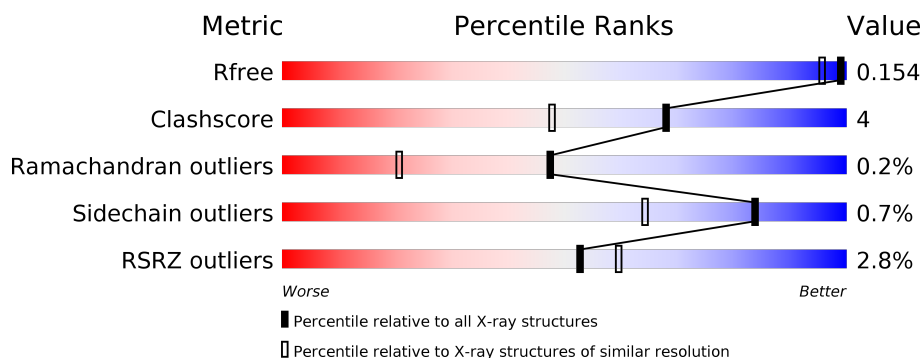
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 on 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	312	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, green 78%, yellow 7%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 78% 7% 15% </div> </div>
1	B	312	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, green 74%, yellow 10%, grey 15%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 4% 74% 10% 15% </div> </div>

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PO4	A	402	-	X	-	-
7	GOL	A	408	-	X	-	-
7	GOL	A	409	-	X	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4590 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 Polyester hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	9	0
			2043	1284	347	401	11			
1	B	266	Total	C	N	O	S	0	4	0
			2005	1260	340	394	11			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	SER	TYR	engineered mutation	UNP A0A1H6AD45
A	305	LEU	-	expression tag	UNP A0A1H6AD45
A	306	GLU	-	expression tag	UNP A0A1H6AD45
A	307	HIS	-	expression tag	UNP A0A1H6AD45
A	308	HIS	-	expression tag	UNP A0A1H6AD45
A	309	HIS	-	expression tag	UNP A0A1H6AD45
A	310	HIS	-	expression tag	UNP A0A1H6AD45
A	311	HIS	-	expression tag	UNP A0A1H6AD45
A	312	HIS	-	expression tag	UNP A0A1H6AD45
B	250	SER	TYR	engineered mutation	UNP A0A1H6AD45
B	305	LEU	-	expression tag	UNP A0A1H6AD45
B	306	GLU	-	expression tag	UNP A0A1H6AD45
B	307	HIS	-	expression tag	UNP A0A1H6AD45
B	308	HIS	-	expression tag	UNP A0A1H6AD45
B	309	HIS	-	expression tag	UNP A0A1H6AD45
B	310	HIS	-	expression tag	UNP A0A1H6AD45
B	311	HIS	-	expression tag	UNP A0A1H6AD45
B	312	HIS	-	expression tag	UNP A0A1H6AD45

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

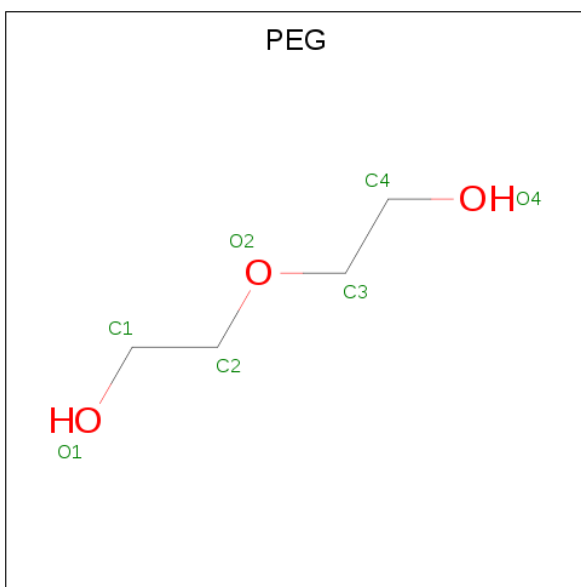
- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Na	0	0
			2	2		
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	2	Total	Cl	0	0
			2	2		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



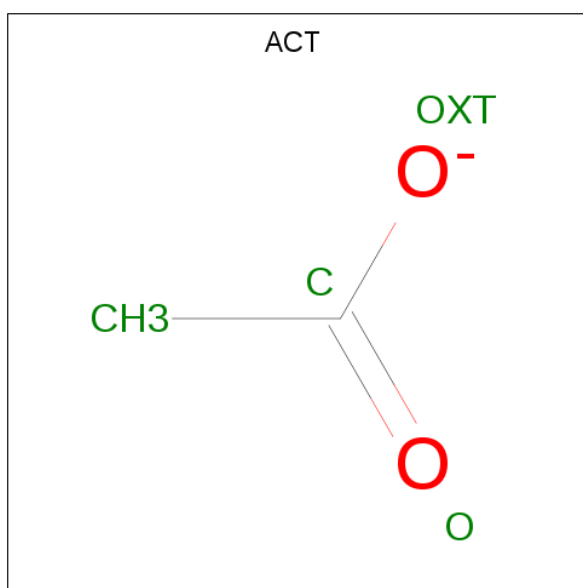
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		

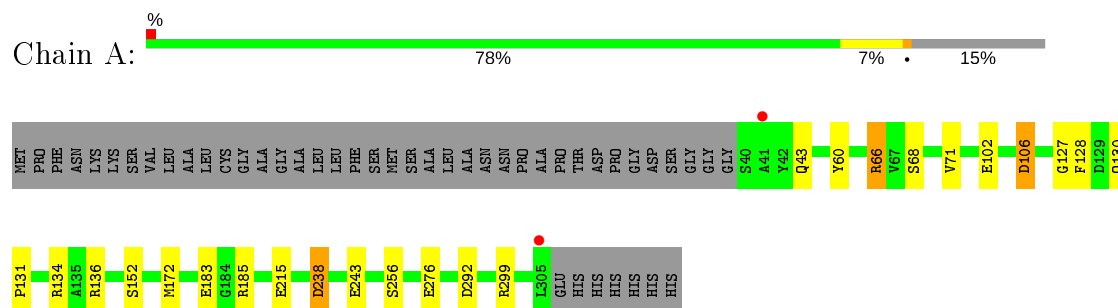
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	288	Total 288	O 288	0	0
9	B	205	Total 205	O 205	0	0

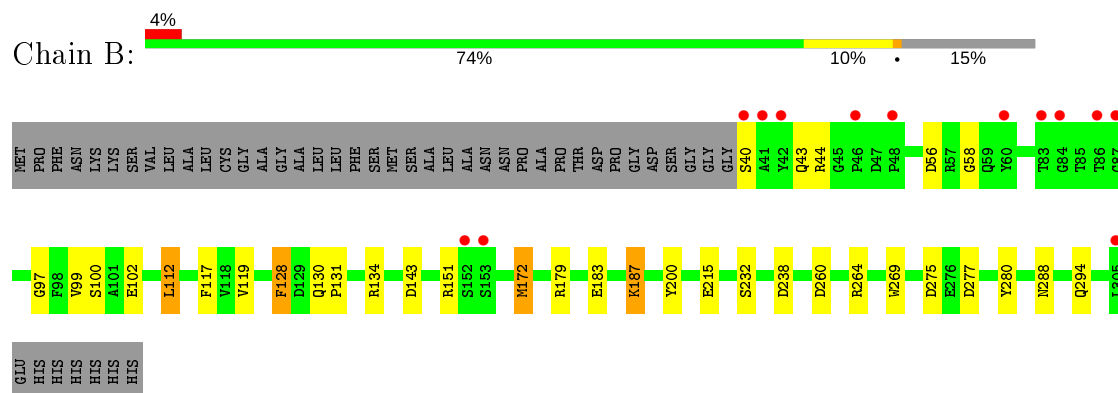
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Polyester hydrolase



• Molecule 1: Polyester hydrolase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	94.53Å 98.27Å 121.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.34 – 1.35 47.26 – 1.35	Depositor EDS
% Data completeness (in resolution range)	99.1 (76.34-1.35) 99.1 (47.26-1.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.35Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.113 , 0.152 0.115 , 0.154	Depositor DCC
R_{free} test set	6012 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	4590	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, NA, PO4, SO4, ACT, 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	1.31	11/2122 (0.5%)	1.21	14/2886 (0.5%)
1	B	1.36	11/2068 (0.5%)	1.30	23/2816 (0.8%)
All	All	1.34	22/4190 (0.5%)	1.26	37/5702 (0.6%)

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	A	0	2
1	B	0	2
All	All	0	4

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	256	SER	CB-OG	-16.30	1.21	1.42
1	B	40	SER	CA-CB	10.33	1.68	1.52
1	A	102	GLU	CD-OE2	-9.94	1.14	1.25
1	A	183	GLU	CD-OE1	8.57	1.35	1.25
1	B	102	GLU	CB-CG	-7.40	1.38	1.52

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	B	264	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	238	ASP	CB-CG-OD2	-8.74	110.43	118.30
1	B	112	LEU	CB-CG-CD1	8.00	124.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	ARG	NE-CZ-NH1	7.90	124.25	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ASP	Sidechain
1	A	134	ARG	Sidechain
1	B	134	ARG	Sidechain
1	B	58	GLY	Mainchain

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	2043	0	1964	20	0
1	B	2005	0	1910	11	0
2	A	5	0	0	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	2	0	0	1	0
5	B	1	0	0	0	0
6	A	7	0	10	1	0
7	A	12	0	16	0	0
8	A	4	0	3	1	0
9	A	288	0	0	3	0
9	B	205	0	0	3	0
All	All	4590	0	3903	30	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 4.

The worst 5 of 30 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:130[B]:GLN:OE1	1:A:172[B]:MET:HE1	1.42	1.20
1:A:130[B]:GLN:OE1	1:A:172[B]:MET:CE	2.06	1.03
1:A:130[B]:GLN:CD	1:A:172[B]:MET:HE1	1.80	1.02
1:A:130[B]:GLN:HA	1:A:172[B]:MET:HE2	1.40	1.00
1:A:130[B]:GLN:CD	1:A:172[B]:MET:CE	2.37	0.93

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	273/312 (88%)	264 (97%)	9 (3%)	0	100	100
1	B	268/312 (86%)	259 (97%)	8 (3%)	1 (0%)	34	12
All	All	541/624 (87%)	523 (97%)	17 (3%)	1 (0%)	47	21

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	99	VAL

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	227/254 (89%)	226 (100%)	1 (0%)	91	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	219/254 (86%)	217 (99%)	2 (1%)	78	53
All	All	446/508 (88%)	443 (99%)	3 (1%)	84	64

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ARG
1	B	151	ARG
1	B	187	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 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	PO4	A	403	-	4,4,4	1.47	1 (25%)	6,6,6	1.78	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	408	-	5,5,5	1.97	1 (20%)	5,5,5	1.96	3 (60%)
2	SO4	A	401	-	4,4,4	0.35	0	6,6,6	0.29	0
3	PO4	A	402	-	4,4,4	2.85	3 (75%)	6,6,6	5.19	5 (83%)
7	GOL	A	409	-	5,5,5	1.50	1 (20%)	5,5,5	3.44	3 (60%)
3	PO4	B	401	-	4,4,4	2.12	2 (50%)	6,6,6	0.86	0
6	PEG	A	407	-	6,6,6	1.71	1 (16%)	5,5,5	2.53	1 (20%)
8	ACT	A	410	-	1,3,3	1.56	0	0,3,3	0.00	-

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
7	GOL	A	409	-	-	4/4/4/4	-
7	GOL	A	408	-	-	3/4/4/4	-
6	PEG	A	407	-	-	3/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	PO4	P-O1	-3.93	1.41	1.50
7	A	408	GOL	O1-C1	3.34	1.56	1.42
3	A	402	PO4	P-O2	-3.18	1.45	1.54
7	A	409	GOL	O1-C1	3.08	1.55	1.42
3	B	401	PO4	P-O2	-3.00	1.45	1.54

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	PO4	O4-P-O3	-9.16	78.58	107.97
7	A	409	GOL	C3-C2-C1	5.76	134.09	111.70
3	A	402	PO4	O3-P-O1	-5.14	92.09	110.89
3	A	402	PO4	O3-P-O2	-4.99	91.94	107.97
6	A	407	PEG	O2-C2-C1	4.65	130.51	110.07

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	408	GOL	O1-C1-C2-C3
7	A	409	GOL	O1-C1-C2-C3
7	A	409	GOL	C1-C2-C3-O3
7	A	408	GOL	O1-C1-C2-O2
6	A	407	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	407	PEG	1	0
8	A	410	ACT	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	266/312 (85%)	-0.38	2 (0%) 86 89	12, 16, 29, 57	0
1	B	266/312 (85%)	-0.08	13 (4%) 29 33	13, 23, 38, 66	0
All	All	532/624 (85%)	-0.23	15 (2%) 53 59	12, 18, 36, 66	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	THR	5.3
1	B	41	ALA	5.3
1	B	305	LEU	3.8
1	B	42	TYR	3.6
1	B	153	SER	2.8

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 carbohydrates 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(\AA^2)	Q<0.9
7	GOL	A	409	6/6	0.84	0.24	26,30,35,40	6
8	ACT	A	410	4/4	0.84	0.10	28,29,30,30	4
6	PEG	A	407	7/7	0.87	0.08	35,36,52,65	0
7	GOL	A	408	6/6	0.90	0.10	33,41,50,54	0
3	PO4	A	402	5/5	0.97	0.09	28,35,41,49	5
3	PO4	A	403	5/5	0.97	0.06	26,31,34,39	5
3	PO4	B	401	5/5	0.98	0.11	29,32,44,45	5
2	SO4	A	401	5/5	0.99	0.04	15,15,15,16	0
4	NA	B	403	1/1	1.00	0.08	20,20,20,20	0
5	CL	B	404	1/1	1.00	0.05	17,17,17,17	0
5	CL	A	405	1/1	1.00	0.08	14,14,14,14	0
4	NA	B	402	1/1	1.00	0.08	17,17,17,17	0
5	CL	A	406	1/1	1.00	0.05	19,19,19,19	0
4	NA	A	404	1/1	1.00	0.07	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.