



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 12:31 am GMT

PDB ID : 5DCB
Title : Neisseria meningitidis 3-deoxy-D-arabino-heptulosonate 7-phosphate synthase regulated and complexed with PEP
Authors : Heyes, L.C.; Parker, E.J.
Deposited on : 2015-08-23
Resolution : 2.05 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28683
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

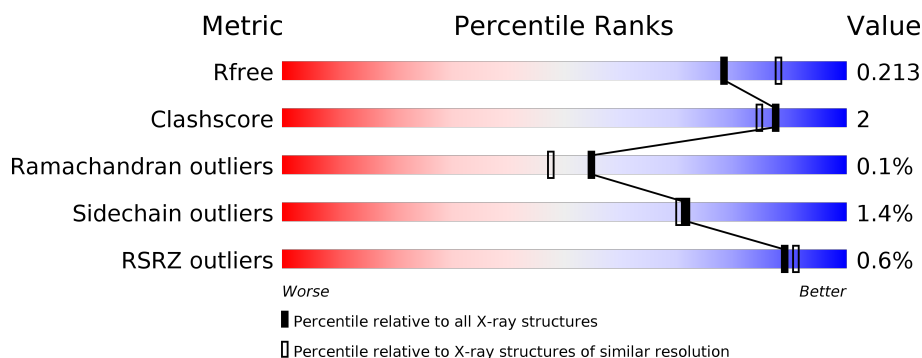
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (2.04-2.04)

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. 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	351	94% . .
1	B	351	92% 7% .
1	C	351	2% 93% 6% .
1	D	351	92% 6% . .

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	404	-	-	-	X
4	EDO	B	402	-	-	-	X
5	PEG	A	405	-	-	-	X
5	PEG	D	403	-	-	-	X
6	PGE	A	406	-	-	X	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 11505 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 Phospho-2-dehydro-3-deoxyheptonate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	2	0
			2669	1669	480	506	14			
1	B	346	Total	C	N	O	S	0	1	0
			2652	1660	479	499	14			
1	C	348	Total	C	N	O	S	0	0	0
			2633	1649	472	498	14			
1	D	345	Total	C	N	O	S	0	1	0
			2666	1670	481	501	14			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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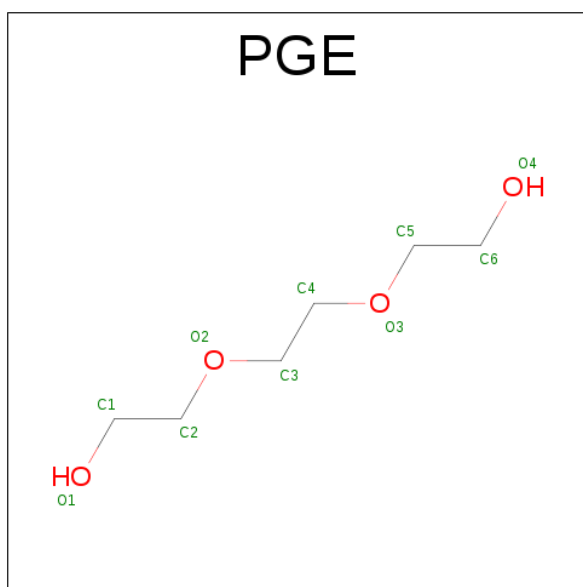
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



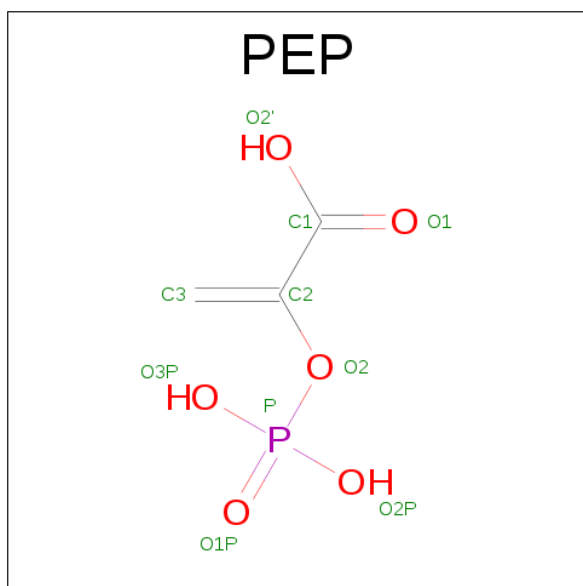
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 7 is PHOSPHOENOLPYRUVATE (three-letter code: PEP) (formula: $C_3H_5O_6P$).



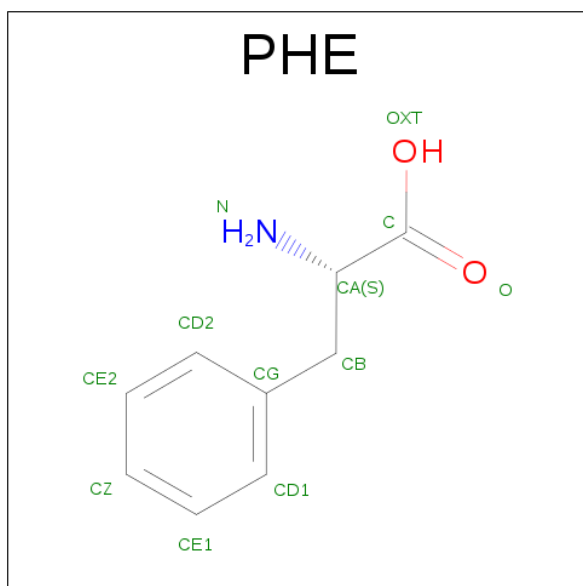
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			10	3	6	1		
7	B	1	Total	C	O	P	0	0
			10	3	6	1		
7	C	1	Total	C	O	P	0	0
			10	3	6	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 8 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			12	9	1	2		
8	B	1	Total	C	N	O	0	0
			12	9	1	2		
8	C	1	Total	C	N	O	0	0
			12	9	1	2		
8	D	1	Total	C	N	O	0	0
			12	9	1	2		

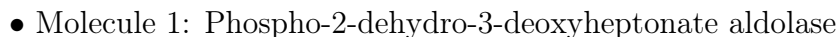
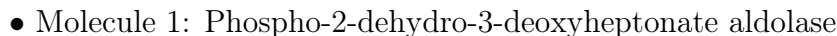
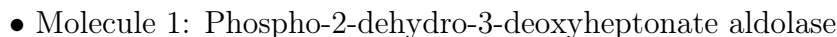
- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Cl	0	0
			1	1		
9	A	1	Total	Cl	0	0
			1	1		
9	D	1	Total	Cl	0	0
			1	1		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	209	Total 209	O 209	0	0
10	B	201	Total 201	O 201	0	0
10	C	121	Total 121	O 121	0	0
10	D	214	Total 214	O 214	0	0

- Molecule 1: Phospho-2-dehydro-3-deoxyheptonate aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.46Å 140.31Å 75.50Å 90.00° 96.89° 90.00°	Depositor
Resolution (Å)	74.96 – 2.05 40.75 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.8 (74.96-2.05) 99.9 (40.75-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.169 , 0.212 0.176 , 0.213	Depositor DCC
R_{free} test set	6047 reflections (6.62%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11505	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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: PGE, CL, MN, PEP, EDO, SO4, 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	0.50	0/2720	0.66	0/3684
1	B	0.51	0/2703	0.68	0/3662
1	C	0.44	0/2684	0.63	0/3642
1	D	0.53	0/2716	0.67	1/3673 (0.0%)
All	All	0.50	0/10823	0.66	1/14661 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	267	ASP	CB-CG-OD1	5.01	122.81	118.30

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	2669	0	2625	10	0
1	B	2652	0	2612	13	0
1	C	2633	0	2567	13	0
1	D	2666	0	2659	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	0	0	0
4	A	8	0	12	0	0
4	B	4	0	6	0	0
4	D	4	0	6	0	0
5	A	7	0	10	0	0
5	D	7	0	10	2	0
6	A	10	0	14	10	0
7	A	10	0	2	0	0
7	B	10	0	2	0	0
7	C	10	0	2	0	0
7	D	10	0	2	0	0
8	A	12	0	8	0	0
8	B	12	0	8	0	0
8	C	12	0	8	0	0
8	D	12	0	8	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
9	D	1	0	0	1	0
10	A	209	0	0	4	0
10	B	201	0	0	0	0
10	C	121	0	0	1	0
10	D	214	0	0	2	0
All	All	11505	0	10561	52	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.

The worst 5 of 52 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)
6:A:406:PGE:H6	10:A:645:HOH:O	1.73	0.88
6:A:406:PGE:C6	10:A:645:HOH:O	2.34	0.74
1:A:209:HIS:CE1	6:A:406:PGE:H5	2.30	0.66
6:A:406:PGE:H42	1:B:102:THR:O	1.97	0.62
1:D:219:HIS:HD2	1:D:220:SER:O	1.83	0.62

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	346/351 (99%)	338 (98%)	7 (2%)	1 (0%)	44	35
1	B	345/351 (98%)	334 (97%)	11 (3%)	0	100	100
1	C	346/351 (99%)	334 (96%)	12 (4%)	0	100	100
1	D	344/351 (98%)	337 (98%)	6 (2%)	1 (0%)	44	35
All	All	1381/1404 (98%)	1343 (97%)	36 (3%)	2 (0%)	55	47

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	ASP
1	D	294	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	280/289 (97%)	277 (99%)	3 (1%)	78	77
1	B	277/289 (96%)	274 (99%)	3 (1%)	78	77
1	C	272/289 (94%)	268 (98%)	4 (2%)	70	68
1	D	282/289 (98%)	276 (98%)	6 (2%)	59	54
All	All	1111/1156 (96%)	1095 (99%)	16 (1%)	71	70

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	189	ASN
1	C	236	ARG
1	D	189	ASN
1	C	18	LEU
1	D	233	VAL

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

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 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	A	402	-	4,4,4	0.48	0	6,6,6	0.24	0
4	EDO	A	403	-	3,3,3	0.29	0	2,2,2	0.58	0
4	EDO	A	404	-	3,3,3	0.59	0	2,2,2	0.27	0
5	PEG	A	405	-	6,6,6	0.41	0	5,5,5	0.30	0
6	PGE	A	406	-	9,9,9	0.46	0	8,8,8	0.78	0
7	PEP	A	407	-	6,9,9	1.21	1 (16%)	9,13,13	1.29	1 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PHE	A	408	-	8,12,12	0.55	0	10,15,15	0.45	0
4	EDO	B	402	-	3,3,3	0.48	0	2,2,2	0.19	0
7	PEP	B	403	-	6,9,9	1.12	0	9,13,13	1.21	0
8	PHE	B	404	-	8,12,12	0.48	0	10,15,15	0.37	0
7	PEP	C	402	-	6,9,9	1.26	1 (16%)	9,13,13	1.29	0
8	PHE	C	403	-	8,12,12	0.39	0	10,15,15	0.36	0
4	EDO	D	402	-	3,3,3	0.55	0	2,2,2	0.12	0
5	PEG	D	403	-	6,6,6	0.40	0	5,5,5	0.53	0
7	PEP	D	404	-	6,9,9	1.13	0	9,13,13	1.32	0
8	PHE	D	405	-	8,12,12	0.66	0	10,15,15	0.52	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
3	SO4	A	402	-	-	0/0/0/0	0/0/0/0
4	EDO	A	403	-	-	0/1/1/1	0/0/0/0
4	EDO	A	404	-	-	0/1/1/1	0/0/0/0
5	PEG	A	405	-	-	0/4/4/4	0/0/0/0
6	PGE	A	406	-	-	0/7/7/7	0/0/0/0
7	PEP	A	407	-	-	0/5/9/9	0/0/0/0
8	PHE	A	408	-	-	0/4/8/8	0/1/1/1
4	EDO	B	402	-	-	0/1/1/1	0/0/0/0
7	PEP	B	403	-	-	0/5/9/9	0/0/0/0
8	PHE	B	404	-	-	0/4/8/8	0/1/1/1
7	PEP	C	402	-	-	0/5/9/9	0/0/0/0
8	PHE	C	403	-	-	0/4/8/8	0/1/1/1
4	EDO	D	402	-	-	0/1/1/1	0/0/0/0
5	PEG	D	403	-	-	0/4/4/4	0/0/0/0
7	PEP	D	404	-	-	0/5/9/9	0/0/0/0
8	PHE	D	405	-	-	0/4/8/8	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	402	PEP	O2-C2	2.36	1.45	1.39
7	A	407	PEP	O2-C2	2.61	1.46	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
7	A	407	PEP	O3P-P-O2P	2.51	117.75	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	406	PGE	10	0
5	D	403	PEG	2	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(Å²)	Q<0.9	
1	A	346/351 (98%)	-0.59	0	100	100	16, 24, 36, 49	0
1	B	346/351 (98%)	-0.52	0	100	100	16, 24, 36, 51	0
1	C	348/351 (99%)	-0.19	7 (2%)	65	70	18, 38, 57, 74	0
1	D	345/351 (98%)	-0.56	1 (0%)	93	94	15, 23, 36, 52	0
All	All	1385/1404 (98%)	-0.46	8 (0%)	89	91	15, 26, 49, 74	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	4	HIS	3.2
1	C	294	ASP	2.8
1	C	115	LEU	2.7
1	D	5	TYR	2.5
1	C	3	HIS	2.4

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	EDO	A	404	4/4	0.55	0.45	17.35	57,63,64,69	0
6	PGE	A	406	10/10	0.83	0.34	6.80	38,41,45,46	0
4	EDO	B	402	4/4	0.88	0.27	4.27	53,54,54,55	0
5	PEG	A	405	7/7	0.91	0.20	3.01	50,51,51,54	0
5	PEG	D	403	7/7	0.79	0.20	2.83	47,49,53,53	0
8	PHE	C	403	12/12	0.95	0.10	0.12	22,22,24,25	0
8	PHE	B	404	12/12	0.96	0.10	-0.03	17,18,21,21	0
8	PHE	A	408	12/12	0.97	0.09	-0.38	18,21,22,23	0
7	PEP	A	407	10/10	0.98	0.08	-0.52	28,30,32,33	0
7	PEP	D	404	10/10	0.97	0.09	-0.65	20,27,28,29	0
2	MN	D	401	1/1	1.00	0.08	-0.69	19,19,19,19	0
8	PHE	D	405	12/12	0.97	0.07	-0.80	18,19,19,20	0
7	PEP	B	403	10/10	0.98	0.09	-0.83	23,26,27,29	0
2	MN	B	401	1/1	1.00	0.08	-0.85	21,21,21,21	0
2	MN	A	401	1/1	1.00	0.06	-1.09	22,22,22,22	0
7	PEP	C	402	10/10	0.96	0.09	-1.39	35,40,41,41	0
2	MN	C	401	1/1	0.96	0.08	-1.40	40,40,40,40	0
9	CL	D	406	1/1	0.98	0.04	-1.74	55,55,55,55	0
9	CL	B	405	1/1	1.00	0.04	-	23,23,23,23	0
3	SO4	A	402	5/5	0.91	0.32	-	60,66,70,72	0
4	EDO	A	403	4/4	0.93	0.14	-	44,45,46,48	0
9	CL	A	409	1/1	0.99	0.05	-	33,33,33,33	0
4	EDO	D	402	4/4	0.84	0.32	-	41,44,44,47	0

6.5 Other polymers ⓘ

There are no such residues in this entry.