



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 21, 2025 – 04:48 pm BST

PDB ID : 9H4U / pdb_00009h4u
Title : Deacetylase FI8 utilizes unconventional variant of a catalytic triad: the diluted triad
Authors : Palm, G.J.; Lammers, M.
Deposited on : 2024-10-21
Resolution : 1.54 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 Phenix2.0rc1
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.45.1

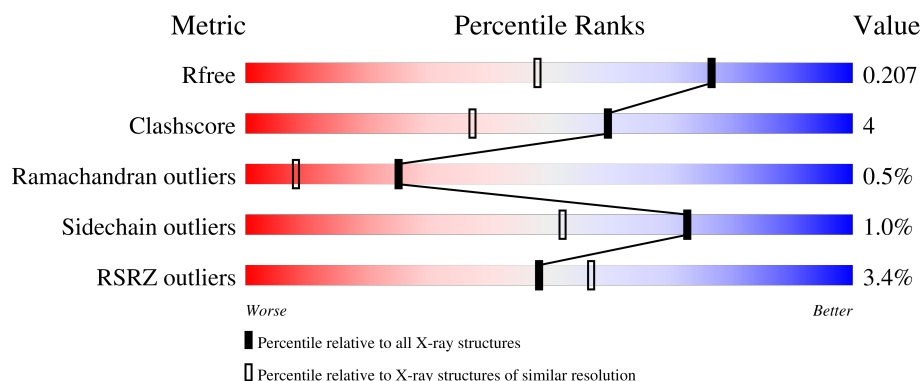
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.54 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}	164625	3511 (1.56-1.52)
Clashscore	180529	3784 (1.56-1.52)
Ramachandran outliers	177936	3720 (1.56-1.52)
Sidechain outliers	177891	3717 (1.56-1.52)
RSRZ outliers	164620	3510 (1.56-1.52)

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	641	<div> <div>2%</div> <div>89%</div> <div>8%</div> <div>.</div> </div>
1	B	641	<div> <div>5%</div> <div>88%</div> <div>8%</div> <div>..</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	PEG	B	703	-	-	X	-
3	PEG	B	704	-	-	X	-

2 Entry composition [i](#)

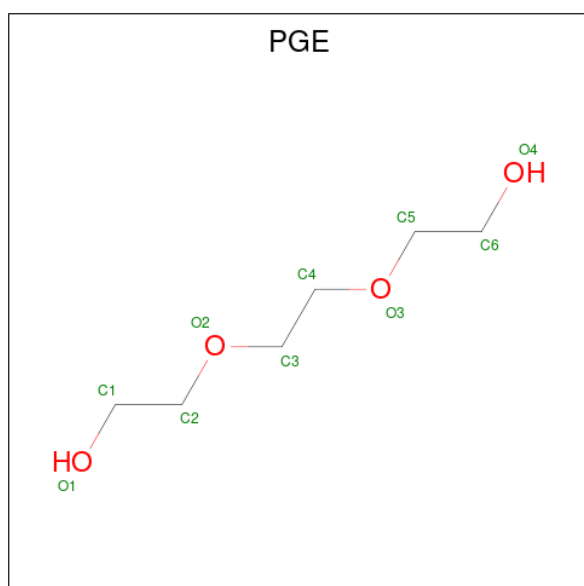
There are 6 unique types of molecules in this entry. The entry contains 21523 atoms, of which 10137 are hydrogens and 0 are deuteriums.

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 Carbohydrate esterase FI8.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	622	Total	As	C	H	N	O	S	114	23	0
			10075	1	3254	4995	844	966	15			
1	B	622	Total	As	C	H	N	O	S	112	26	0
			10132	1	3276	5022	849	969	15			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



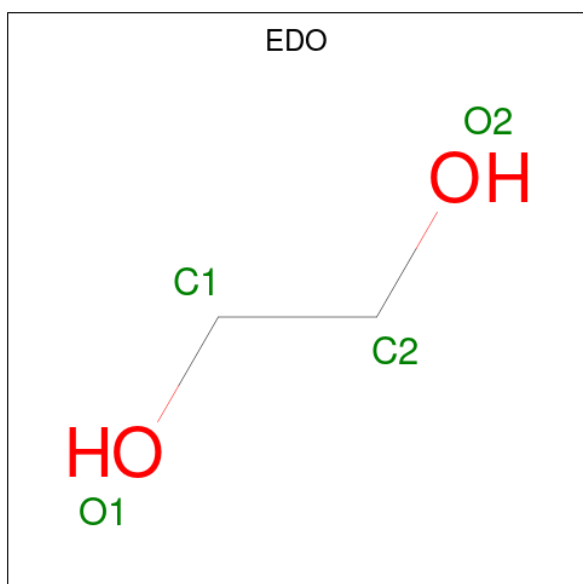
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	2	0
			24	6	14	4		
2	B	1	Total	C	H	O	2	0
			24	6	14	4		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	2	0
			17	4	10	3		
3	A	1	Total	C	H	O	2	0
			17	4	10	3		
3	B	1	Total	C	H	O	2	0
			17	4	10	3		
3	B	1	Total	C	H	O	2	0
			17	4	10	3		
3	B	1	Total	C	H	O	2	0
			17	4	10	3		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H O 10 2 6 2	2	0
4	A	1	Total C H O 10 2 6 2	2	0
4	B	1	Total C H O 10 2 6 2	2	0
4	B	1	Total C H O 10 2 6 2	2	0
4	B	1	Total C H O 10 2 6 2	2	0
4	B	1	Total C H O 10 2 6 2	2	0
4	B	1	Total C H O 10 2 6 2	2	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Ca 4 4	0	0
5	B	4	Total Ca 4 4	0	0

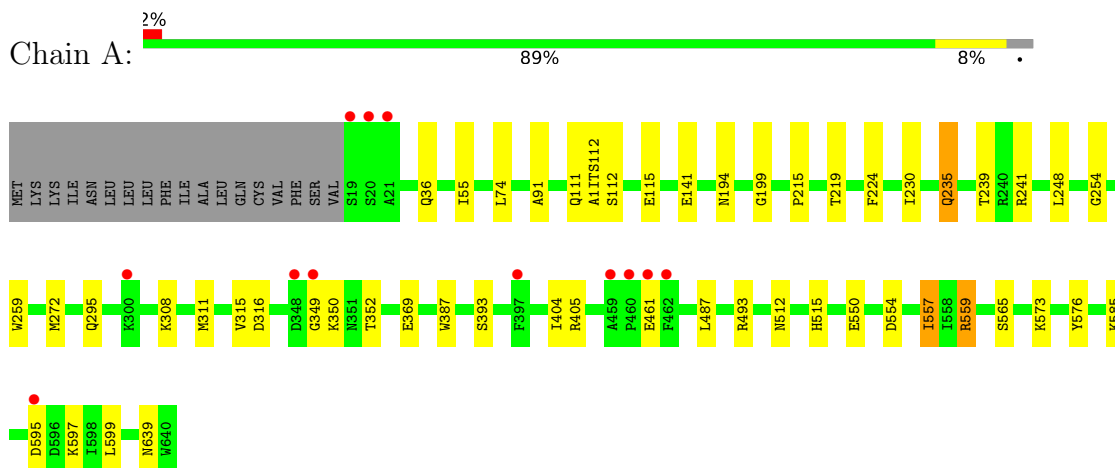
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	571	Total O 574 574	0	4
6	B	524	Total O 531 531	0	7

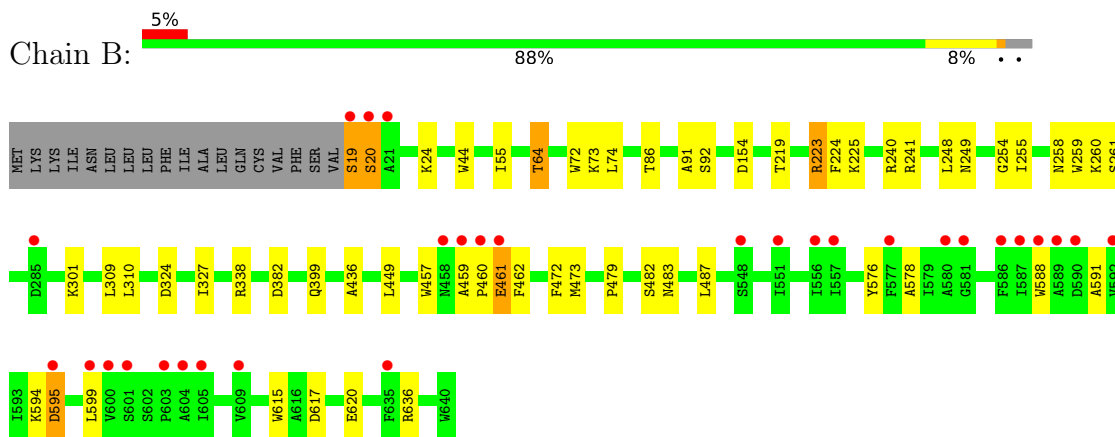
3 Residue-property plots [i](#)

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: Carbohydrate esterase FI8



• Molecule 1: Carbohydrate esterase FI8



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.66Å 120.04Å 141.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.38 – 1.54 48.38 – 1.54	Depositor EDS
% Data completeness (in resolution range)	96.0 (48.38-1.54) 95.9 (48.38-1.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.70 (at 1.54Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.170 , 0.201 0.176 , 0.207	Depositor DCC
R_{free} test set	11964 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	21523	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: CA, PGE, EDO, A1ITS, 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	0.67	0/5279	1.04	8/7165 (0.1%)
1	B	0.67	0/5308	1.08	9/7204 (0.1%)
All	All	0.67	0/10587	1.06	17/14369 (0.1%)

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	3
All	All	0	5

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ARG	NE-CZ-NH2	-9.62	110.54	119.20
1	B	86	THR	CA-CB-OG1	-6.59	99.71	109.60
1	A	141	GLU	CB-CG-CD	6.25	123.23	112.60
1	A	224	PHE	CA-CB-CG	-6.19	107.61	113.80
1	B	224	PHE	CA-CB-CG	-5.89	107.91	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	559	ARG	Sidechain
1	B	223	ARG	Sidechain
1	B	241[A]	ARG	Sidechain
1	B	241[B]	ARG	Sidechain

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	5080	4995	4932	32	0
1	B	5110	5022	4957	49	0
2	A	10	14	14	0	0
2	B	10	14	14	0	0
3	A	14	20	20	5	0
3	B	21	30	30	13	0
4	A	8	12	12	1	0
4	B	20	30	29	6	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	574	0	0	7	0
6	B	531	0	0	7	0
All	All	11386	10137	10008	85	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 85 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:55[B]:ILE:HD13	1:B:74[B]:LEU:HD21	1.28	1.14
1:A:55:ILE:HD12	1:A:74[B]:LEU:HD21	1.60	0.84
3:B:704:PEG:H21	6:B:878:HOH:O	1.75	0.84
1:B:324:ASP:O	4:B:702:EDO:H12	1.82	0.80
3:A:703:PEG:H21	6:A:925:HOH:O	1.82	0.80

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	641/641 (100%)	625 (98%)	14 (2%)	2 (0%)	37	19
1	B	644/641 (100%)	624 (97%)	15 (2%)	5 (1%)	16	3
All	All	1285/1282 (100%)	1249 (97%)	29 (2%)	7 (0%)	25	8

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	595	ASP
1	A	595	ASP
1	A	91	ALA
1	B	91	ALA
1	B	20	SER

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	550/545 (101%)	541 (98%)	9 (2%)	58	30
1	B	552/545 (101%)	549 (100%)	3 (0%)	86	76
All	All	1102/1090 (101%)	1090 (99%)	12 (1%)	73	48

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	573	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	576	TYR
1	B	576	TYR
1	B	19	SER
1	A	461	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	42	ASN
1	B	359	ASN
1	B	235	GLN
1	B	499	HIS
1	B	287	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 8 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
4	EDO	A	704	-	3,3,3	0.18	0	2,2,2	0.19	0
4	EDO	A	705	-	3,3,3	0.16	0	2,2,2	0.54	0
3	PEG	A	702	-	6,6,6	0.16	0	5,5,5	0.18	0
3	PEG	B	704	-	6,6,6	0.58	0	5,5,5	0.81	0
3	PEG	B	701	-	6,6,6	0.96	0	5,5,5	0.77	0
2	PGE	B	705	-	9,9,9	0.32	0	8,8,8	0.21	0
3	PEG	A	703	-	6,6,6	0.38	0	5,5,5	0.21	0
4	EDO	B	702	-	3,3,3	0.90	0	2,2,2	1.47	0
4	EDO	B	706	-	3,3,3	0.81	0	2,2,2	1.18	0
4	EDO	B	707	-	3,3,3	0.50	0	2,2,2	0.98	0
4	EDO	B	709	-	3,3,3	0.20	0	2,2,2	0.41	0
4	EDO	B	708	-	3,3,3	0.19	0	2,2,2	0.11	0
3	PEG	B	703	-	6,6,6	0.39	0	5,5,5	0.36	0
2	PGE	A	701	-	9,9,9	0.30	0	8,8,8	0.15	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
4	EDO	A	704	-	-	0/1/1/1	-
4	EDO	A	705	-	-	0/1/1/1	-
3	PEG	A	702	-	-	3/4/4/4	-
3	PEG	B	704	-	-	2/4/4/4	-
3	PEG	B	701	-	-	1/4/4/4	-
2	PGE	B	705	-	-	3/7/7/7	-
3	PEG	A	703	-	-	2/4/4/4	-
4	EDO	B	702	-	-	1/1/1/1	-
4	EDO	B	706	-	-	1/1/1/1	-
4	EDO	B	707	-	-	1/1/1/1	-
4	EDO	B	709	-	-	1/1/1/1	-
4	EDO	B	708	-	-	1/1/1/1	-
3	PEG	B	703	-	-	1/4/4/4	-
2	PGE	A	701	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	705	PGE	O1-C1-C2-O2
3	B	703	PEG	O1-C1-C2-O2
3	B	704	PEG	O2-C3-C4-O4
3	A	702	PEG	O2-C3-C4-O4
3	A	702	PEG	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	EDO	1	0
3	A	702	PEG	2	0
3	B	704	PEG	5	0
3	B	701	PEG	1	0
3	A	703	PEG	3	0
4	B	702	EDO	2	0
4	B	706	EDO	1	0
4	B	707	EDO	2	0
4	B	708	EDO	1	0
3	B	703	PEG	7	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	621/641 (96%)	-0.23	12 (1%)	66 75	9, 26, 52, 77	18 (2%)
1	B	621/641 (96%)	-0.04	30 (4%)	36 45	11, 26, 57, 103	22 (3%)
All	All	1242/1282 (96%)	-0.14	42 (3%)	48 57	9, 26, 54, 103	40 (3%)

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460[A]	PRO	6.2
1	B	19	SER	5.1
1	B	461[A]	GLU	4.7
1	A	19	SER	4.4
1	A	460	PRO	4.2

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(\AA^2)	Q<0.9
2	PGE	A	701	10/10	0.76	0.18	56,67,76,77	2
2	PGE	B	705	10/10	0.76	0.21	59,74,86,86	2
3	PEG	B	701	7/7	0.79	0.20	41,46,57,57	2
4	EDO	B	709	4/4	0.80	0.27	42,44,49,49	10
3	PEG	A	703	7/7	0.82	0.17	45,51,62,68	2
5	CA	A	708	1/1	0.82	0.23	47,47,47,47	1
4	EDO	B	702	4/4	0.83	0.16	39,43,44,44	2
3	PEG	A	702	7/7	0.84	0.16	63,66,74,74	2
4	EDO	B	707	4/4	0.84	0.19	42,49,50,54	2
4	EDO	A	704	4/4	0.85	0.14	51,51,53,53	2
4	EDO	B	708	4/4	0.85	0.15	57,59,60,60	2
3	PEG	B	704	7/7	0.87	0.15	27,39,55,58	2
4	EDO	B	706	4/4	0.88	0.22	23,27,30,30	10
3	PEG	B	703	7/7	0.89	0.10	40,43,50,50	2
5	CA	B	712	1/1	0.90	0.11	28,28,28,28	1
5	CA	B	713	1/1	0.93	0.09	37,37,37,37	1
4	EDO	A	705	4/4	0.96	0.08	22,24,25,25	10
5	CA	B	710	1/1	0.96	0.08	31,31,31,31	1
5	CA	A	709	1/1	0.98	0.10	27,27,27,27	1
5	CA	A	706	1/1	0.98	0.05	32,32,32,32	1
5	CA	A	707	1/1	0.99	0.03	27,27,27,27	0
5	CA	B	711	1/1	0.99	0.04	25,25,25,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.