



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 03:49 pm BST

PDB ID : 6EMI
Title : Crystal structure of a variant of human butyrylcholinesterase expressed in bacteria.
Authors : Brazzolotto, X.; Igert, A.; Guillon, V.; Santoni, G.; Nachon, F.
Deposited on : 2017-10-02
Resolution : 2.48 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

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

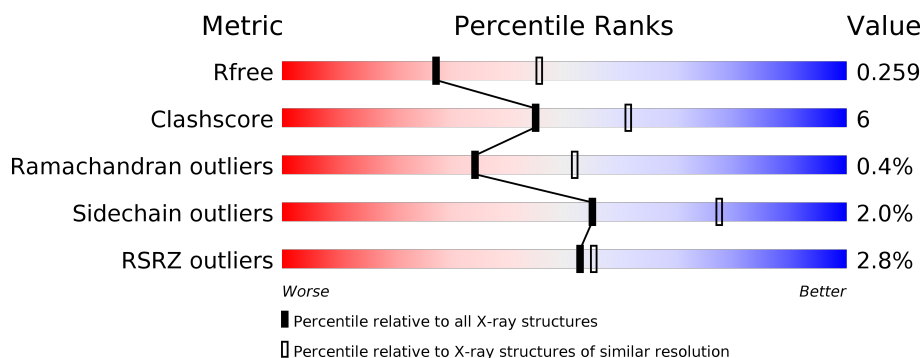
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	532	 3% 83% 16% •
1	B	532	 2% 84% 14% ••

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
2	EDO	B	611	-	-	-	X
2	EDO	B	612	-	-	-	X
2	EDO	B	613	-	-	-	X
3	PEG	B	617	-	-	-	X
5	PGE	A	610	-	-	X	-
5	PGE	B	621	-	-	-	X
6	PG4	B	623	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9018 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 Cholinesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	1	1	0
			4213	2711	708	775	19			
1	B	527	Total	C	N	O	S	12	0	0
			4210	2709	708	775	18			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P06276
A	-1	ALA	-	expression tag	UNP P06276
A	0	MET	-	expression tag	UNP P06276
A	7	THR	ALA	engineered mutation	UNP P06276
A	48	PRO	SER	engineered mutation	UNP P06276
A	54	GLY	ASP	engineered mutation	UNP P06276
A	66	MET	CYS	engineered mutation	UNP P06276
A	71	THR	GLN	engineered mutation	UNP P06276
A	110	MET	LEU	engineered mutation	UNP P06276
A	111	VAL	ILE	engineered mutation	UNP P06276
A	126	PRO	HIS	engineered mutation	UNP P06276
A	176	LYS	GLN	engineered mutation	UNP P06276
A	180	ASP	LYS	engineered mutation	UNP P06276
A	188	ASP	ASN	engineered mutation	UNP P06276
A	190	ASN	LYS	engineered mutation	UNP P06276
A	191	ARG	SER	engineered mutation	UNP P06276
A	215	PRO	SER	engineered mutation	UNP P06276
A	227	ALA	PHE	engineered mutation	UNP P06276
A	234	MET	THR	engineered mutation	UNP P06276
A	236	PRO	LEU	engineered mutation	UNP P06276
A	237	GLU	TYR	engineered mutation	UNP P06276
A	250	LEU	THR	engineered mutation	UNP P06276
A	274	ASP	LEU	engineered mutation	UNP P06276
A	283	SER	GLY	engineered mutation	UNP P06276
A	305	THR	ILE	engineered mutation	UNP P06276

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Chain	Residue	Modelled	Actual	Comment	Reference
A	342	ASP	ASN	engineered mutation	UNP P06276
A	356	VAL	ILE	engineered mutation	UNP P06276
A	360	ASN	GLY	engineered mutation	UNP P06276
A	377	GLU	VAL	engineered mutation	UNP P06276
A	379	GLU	ASP	engineered mutation	UNP P06276
A	380	ASP	GLN	engineered mutation	UNP P06276
A	387	ASP	GLU	engineered mutation	UNP P06276
A	390	ALA	GLY	engineered mutation	UNP P06276
A	391	GLU	ASP	engineered mutation	UNP P06276
A	397	PHE	ASN	engineered mutation	UNP P06276
A	406	ALA	THR	engineered mutation	UNP P06276
A	409	TYR	PHE	engineered mutation	UNP P06276
A	410	ALA	SER	engineered mutation	UNP P06276
A	412	HIS	TRP	engineered mutation	UNP P06276
A	417	TYR	PHE	engineered mutation	UNP P06276
A	454	LEU	ASP	engineered mutation	UNP P06276
A	459	GLU	ALA	engineered mutation	UNP P06276
A	466	GLU	SER	engineered mutation	UNP P06276
A	468	MET	VAL	engineered mutation	UNP P06276
A	469	ARG	LYS	engineered mutation	UNP P06276
A	489	GLN	SER	engineered mutation	UNP P06276
A	495	PRO	SER	engineered mutation	UNP P06276
A	508	SER	THR	engineered mutation	UNP P06276
A	518	HIS	GLN	engineered mutation	UNP P06276
A	523	ASN	THR	engineered mutation	UNP P06276
B	-2	GLY	-	expression tag	UNP P06276
B	-1	ALA	-	expression tag	UNP P06276
B	0	MET	-	expression tag	UNP P06276
B	7	THR	ALA	engineered mutation	UNP P06276
B	48	PRO	SER	engineered mutation	UNP P06276
B	54	GLY	ASP	engineered mutation	UNP P06276
B	66	MET	CYS	engineered mutation	UNP P06276
B	71	THR	GLN	engineered mutation	UNP P06276
B	110	MET	LEU	engineered mutation	UNP P06276
B	111	VAL	ILE	engineered mutation	UNP P06276
B	126	PRO	HIS	engineered mutation	UNP P06276
B	176	LYS	GLN	engineered mutation	UNP P06276
B	180	ASP	LYS	engineered mutation	UNP P06276
B	188	ASP	ASN	engineered mutation	UNP P06276
B	190	ASN	LYS	engineered mutation	UNP P06276
B	191	ARG	SER	engineered mutation	UNP P06276
B	215	PRO	SER	engineered mutation	UNP P06276

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Chain	Residue	Modelled	Actual	Comment	Reference
B	227	ALA	PHE	engineered mutation	UNP P06276
B	234	MET	THR	engineered mutation	UNP P06276
B	236	PRO	LEU	engineered mutation	UNP P06276
B	237	GLU	TYR	engineered mutation	UNP P06276
B	250	LEU	THR	engineered mutation	UNP P06276
B	274	ASP	LEU	engineered mutation	UNP P06276
B	283	SER	GLY	engineered mutation	UNP P06276
B	305	THR	ILE	engineered mutation	UNP P06276
B	342	ASP	ASN	engineered mutation	UNP P06276
B	356	VAL	ILE	engineered mutation	UNP P06276
B	360	ASN	GLY	engineered mutation	UNP P06276
B	377	GLU	VAL	engineered mutation	UNP P06276
B	379	GLU	ASP	engineered mutation	UNP P06276
B	380	ASP	GLN	engineered mutation	UNP P06276
B	387	ASP	GLU	engineered mutation	UNP P06276
B	390	ALA	GLY	engineered mutation	UNP P06276
B	391	GLU	ASP	engineered mutation	UNP P06276
B	397	PHE	ASN	engineered mutation	UNP P06276
B	406	ALA	THR	engineered mutation	UNP P06276
B	409	TYR	PHE	engineered mutation	UNP P06276
B	410	ALA	SER	engineered mutation	UNP P06276
B	412	HIS	TRP	engineered mutation	UNP P06276
B	417	TYR	PHE	engineered mutation	UNP P06276
B	454	LEU	ASP	engineered mutation	UNP P06276
B	459	GLU	ALA	engineered mutation	UNP P06276
B	466	GLU	SER	engineered mutation	UNP P06276
B	468	MET	VAL	engineered mutation	UNP P06276
B	469	ARG	LYS	engineered mutation	UNP P06276
B	489	GLN	SER	engineered mutation	UNP P06276
B	495	PRO	SER	engineered mutation	UNP P06276
B	508	SER	THR	engineered mutation	UNP P06276
B	518	HIS	GLN	engineered mutation	UNP P06276
B	523	ASN	THR	engineered mutation	UNP P06276

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



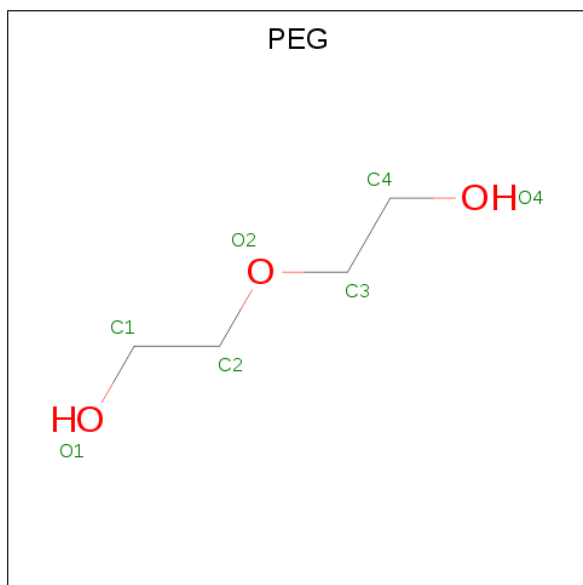
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total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

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

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

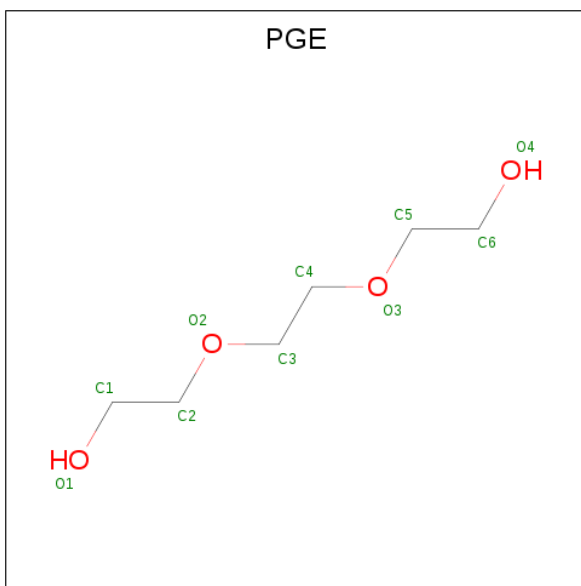


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

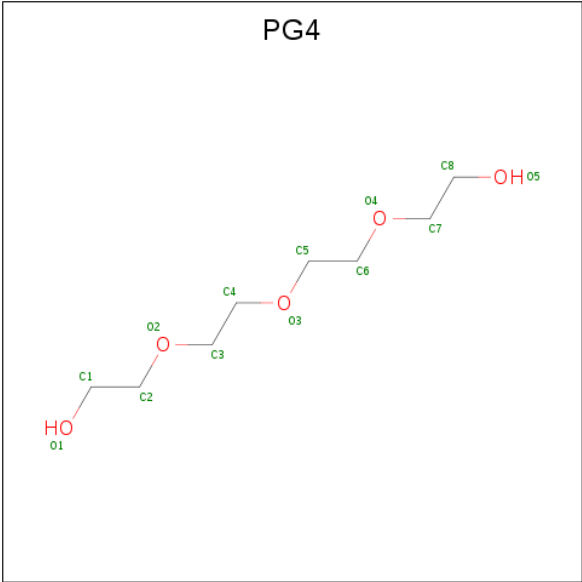
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Cl	0	0
			2	2		
4	A	5	Total	Cl	0	0
			5	5		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

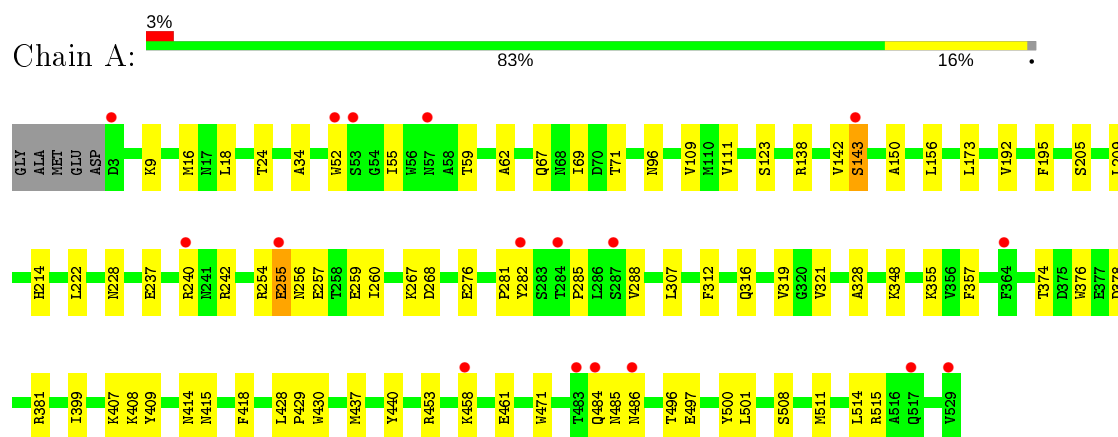
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	186	Total	O	0	0
			186	186		
7	B	190	Total	O	0	0
			190	190		

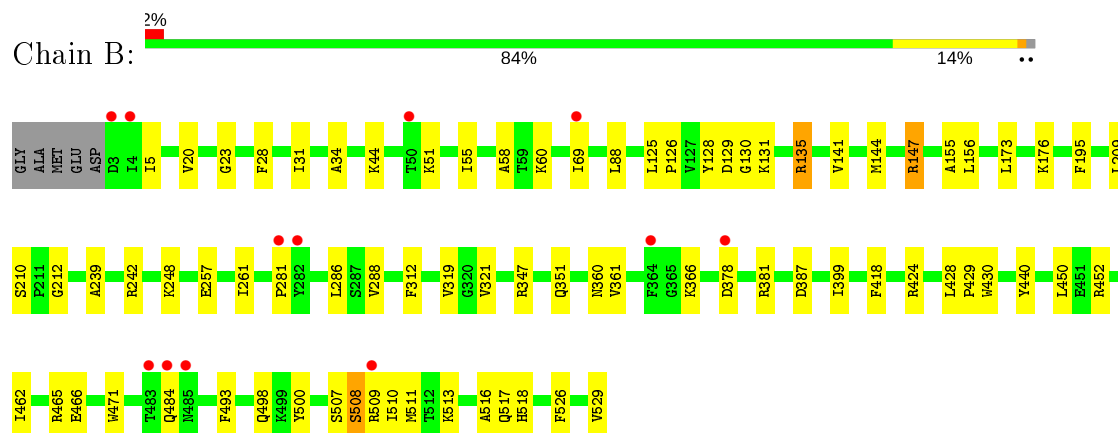
3 Residue-property plots [i](#)

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: Cholinesterase



• Molecule 1: Cholinesterase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	159.84Å 75.17Å 122.07Å 90.00° 93.37° 90.00°	Depositor
Resolution (Å)	65.02 – 2.48 121.86 – 2.48	Depositor EDS
% Data completeness (in resolution range)	98.4 (65.02-2.48) 98.6 (121.86-2.48)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.222 , 0.255 0.227 , 0.259	Depositor DCC
R_{free} test set	2586 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9018	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5176e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PG4, PGE, EDO, CL

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	0.25	0/4338	0.43	0/5893
1	B	0.27	0/4332	0.44	0/5885
All	All	0.26	0/8670	0.44	0/11778

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

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	4213	0	4093	54	0
1	B	4210	0	4090	52	0
2	A	12	0	18	1	0
2	B	56	0	84	4	0
3	A	7	0	10	0	0
3	B	21	0	30	2	0
4	A	5	0	0	1	0
4	B	2	0	0	1	0
5	A	60	0	84	13	0
5	B	30	0	42	1	0
6	B	26	0	36	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	186	0	0	6	0
7	B	190	0	0	7	0
All	All	9018	0	8487	111	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 6.

All (111) 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:501:LEU:HD11	1:A:508:SER:HB3	1.64	0.78
1:A:156:LEU:HD13	1:A:257:GLU:HG2	1.68	0.76
1:B:510:ILE:H	6:B:624:PG4:H11	1.54	0.72
1:A:453:ARG:NH2	7:A:701:HOH:O	2.23	0.72
1:B:361:VAL:HB	1:B:366:LYS:HE3	1.72	0.71
1:B:507:SER:HB3	1:B:509:ARG:HG3	1.72	0.71
1:B:126:PRO:HD2	2:B:612:EDO:H11	1.73	0.70
1:B:484:GLN:NE2	7:B:703:HOH:O	2.25	0.69
1:A:316:GLN:HE22	5:A:610:PGE:H2	1.59	0.67
1:A:96:ASN:HD22	1:A:143:SER:HB3	1.60	0.67
1:B:44:LYS:O	1:B:147:ARG:NH1	2.27	0.65
1:A:205:SER:HB3	1:A:222:LEU:HD21	1.79	0.65
1:B:381:ARG:NH1	1:B:387:ASP:OD1	2.30	0.64
1:B:242:ARG:NH1	1:B:288:VAL:O	2.31	0.63
1:A:407:LYS:NZ	7:A:708:HOH:O	2.34	0.61
1:A:242:ARG:NH1	1:A:288:VAL:O	2.34	0.60
1:A:123:SER:HB2	1:A:143:SER:OG	2.01	0.60
1:A:415:ASN:H	5:A:610:PGE:H62	1.67	0.59
1:A:316:GLN:HE21	5:A:610:PGE:H6	1.67	0.59
1:B:484:GLN:HG2	2:B:611:EDO:H12	1.84	0.59
1:B:378:ASP:OD2	7:B:701:HOH:O	2.17	0.59
1:A:255:GLU:CD	1:A:255:GLU:H	2.06	0.58
1:A:378:ASP:HB3	1:A:381:ARG:HG3	1.85	0.58
1:A:62:ALA:HA	5:A:614:PGE:H3	1.86	0.58
1:B:429:PRO:HG3	2:B:614:EDO:H12	1.85	0.57
1:A:307:LEU:HB3	1:A:408:LYS:HG2	1.87	0.57
1:B:360:ASN:ND2	7:B:713:HOH:O	2.38	0.56
1:A:138:ARG:NH1	4:A:606:CL:CL	2.68	0.56
1:A:267:LYS:NZ	7:A:713:HOH:O	2.38	0.55
1:A:240:ARG:NH1	7:A:706:HOH:O	2.38	0.55
1:B:286:LEU:HD23	5:B:622:PGE:H32	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:GLN:HE21	1:B:518:HIS:CD2	2.26	0.54
1:A:500:TYR:CZ	1:A:511:MET:HB2	2.43	0.54
1:A:111:VAL:HG22	1:A:142:VAL:HB	1.90	0.53
1:A:414:ASN:HA	5:A:610:PGE:H5	1.90	0.53
1:A:209:LEU:HD23	1:A:312:PHE:HB3	1.90	0.52
1:A:319:VAL:O	1:A:418:PHE:HA	2.10	0.52
2:B:606:EDO:H11	2:B:613:EDO:H11	1.91	0.52
1:B:321:VAL:HG11	1:B:399:ILE:HA	1.92	0.52
4:B:619:CL:CL	7:B:874:HOH:O	2.56	0.52
1:B:424:ARG:NH2	1:B:430:TRP:O	2.43	0.51
1:B:517:GLN:HE21	1:B:518:HIS:HD2	1.57	0.51
1:A:55:ILE:H	5:A:613:PGE:H6	1.75	0.51
1:B:526:PHE:O	1:B:529:VAL:HG22	2.10	0.51
1:A:496:THR:OG1	1:A:497:GLU:N	2.44	0.51
1:B:156:LEU:HD13	1:B:257:GLU:HB2	1.94	0.50
1:B:28:PHE:HB3	1:B:31:ILE:HD11	1.93	0.50
1:A:355:LYS:NZ	7:A:702:HOH:O	2.33	0.50
1:A:321:VAL:HG11	1:A:399:ILE:HA	1.94	0.50
1:B:500:TYR:CZ	1:B:511:MET:HB2	2.47	0.50
1:A:355:LYS:HG2	5:A:615:PGE:H12	1.93	0.49
1:B:212:GLY:HA3	3:B:616:PEG:H41	1.95	0.49
1:B:450:LEU:HD11	1:B:465:ARG:HG3	1.94	0.49
1:B:23:GLY:HA3	1:B:135:ARG:HH11	1.77	0.49
1:B:321:VAL:HG21	1:B:399:ILE:HG12	1.94	0.49
1:A:458:LYS:NZ	1:A:461:GLU:OE2	2.40	0.48
1:A:430:TRP:HE1	1:A:440:TYR:HH	1.61	0.47
1:B:319:VAL:O	1:B:418:PHE:HA	2.15	0.47
1:B:510:ILE:HB	6:B:624:PG4:H32	1.96	0.47
1:A:150:ALA:N	1:A:276:GLU:OE1	2.36	0.47
1:B:176:LYS:NZ	7:B:721:HOH:O	2.45	0.47
5:A:612:PGE:H42	5:A:612:PGE:H22	1.46	0.47
1:B:513:LYS:HB3	1:B:516:ALA:HB2	1.95	0.47
1:A:52:TRP:HB2	5:A:613:PGE:H22	1.97	0.47
1:B:129:ASP:OD1	1:B:131:LYS:NZ	2.45	0.47
1:B:60:LYS:O	6:B:623:PG4:H11	2.15	0.47
1:B:209:LEU:HD23	1:B:312:PHE:HB3	1.96	0.46
1:A:255:GLU:OE2	1:A:259:GLU:HG2	2.15	0.46
1:B:23:GLY:HA3	1:B:135:ARG:NH1	2.29	0.46
1:A:348:LYS:HA	1:A:348:LYS:HD3	1.75	0.46
5:A:612:PGE:H6	5:A:612:PGE:H42	1.54	0.46
1:A:514:LEU:HG	1:A:515:ARG:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HB	1:A:192:VAL:HG22	1.97	0.46
1:B:58:ALA:HA	6:B:623:PG4:H12	1.97	0.46
1:B:493:PHE:CE2	1:B:498:GLN:HG3	2.51	0.46
1:B:130:GLY:HA3	1:B:141:VAL:HG11	1.97	0.45
1:A:16:MET:HG3	1:A:59:THR:HG22	1.99	0.45
1:B:34:ALA:HB2	1:B:173:LEU:HD23	1.98	0.45
1:B:428:LEU:HD21	1:B:440:TYR:CG	2.51	0.45
1:B:69:ILE:HD11	1:B:88:LEU:HD11	1.99	0.45
1:A:34:ALA:HB2	1:A:173:LEU:HD23	1.98	0.45
1:B:462:ILE:O	1:B:466:GLU:HG3	2.16	0.45
1:B:210:SER:HA	3:B:616:PEG:H11	1.98	0.45
1:B:20:VAL:O	1:B:135:ARG:HD3	2.17	0.45
1:A:316:GLN:NE2	5:A:610:PGE:H2	2.31	0.45
1:A:18:LEU:O	1:A:24:THR:HA	2.17	0.44
1:A:408:LYS:HE2	1:A:408:LYS:HB2	1.69	0.44
1:A:228:ASN:HA	2:A:601:EDO:H21	2.00	0.44
1:A:500:TYR:CE1	1:A:514:LEU:HB2	2.53	0.44
5:A:615:PGE:H4	5:A:615:PGE:H62	1.56	0.43
1:A:237:GLU:H	1:A:237:GLU:CD	2.20	0.43
1:B:5:ILE:HD13	1:B:55:ILE:HD13	2.00	0.43
1:A:256:ASN:ND2	7:A:719:HOH:O	2.41	0.42
1:A:428:LEU:HD12	1:A:429:PRO:HD2	2.02	0.42
1:A:484:GLN:C	1:A:486:ASN:H	2.23	0.42
1:B:465:ARG:NH1	7:B:710:HOH:O	2.34	0.42
1:A:69:ILE:HG22	1:A:71:THR:HG23	2.02	0.42
1:B:510:ILE:O	6:B:624:PG4:H41	2.20	0.42
1:A:316:GLN:NE2	5:A:610:PGE:H3	2.35	0.42
1:B:125:LEU:HB2	1:B:128:TYR:CD2	2.55	0.42
1:B:257:GLU:O	1:B:261:ILE:HG12	2.20	0.42
1:B:424:ARG:HG3	1:B:428:LEU:HD12	2.03	0.41
1:B:155:ALA:HB3	1:B:239:ALA:HB1	2.02	0.41
1:B:248:LYS:HB3	1:B:248:LYS:HE2	1.90	0.41
1:A:285:PRO:HG2	1:A:357:PHE:CE1	2.56	0.41
1:A:374:THR:HG22	1:A:376:TRP:CZ2	2.56	0.41
1:A:254:ARG:HB2	1:A:260:ILE:HG13	2.03	0.41
1:B:176:LYS:NZ	7:B:737:HOH:O	2.54	0.40
1:B:347:ARG:O	1:B:351:GLN:HG3	2.21	0.40
1:A:328:ALA:HB2	1:A:437:MET:HE3	2.04	0.40
1:A:321:VAL:HG21	1:A:399:ILE:HG12	2.04	0.40

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	526/532 (99%)	505 (96%)	19 (4%)	2 (0%)	34	52
1	B	525/532 (99%)	500 (95%)	23 (4%)	2 (0%)	34	52
All	All	1051/1064 (99%)	1005 (96%)	42 (4%)	4 (0%)	34	52

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	508	SER
1	B	281	PRO
1	A	281	PRO
1	A	485	ASN

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	453/455 (100%)	443 (98%)	10 (2%)	52	75
1	B	452/455 (99%)	444 (98%)	8 (2%)	59	80
All	All	905/910 (100%)	887 (98%)	18 (2%)	55	77

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	67	GLN

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Mol	Chain	Res	Type
1	A	143	SER
1	A	195	PHE
1	A	214	HIS
1	A	255	GLU
1	A	268	ASP
1	A	282	TYR
1	A	409	TYR
1	A	471	TRP
1	B	51	LYS
1	B	135	ARG
1	B	144	MET
1	B	147	ARG
1	B	195	PHE
1	B	452	ARG
1	B	471	TRP
1	B	508	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	316	GLN
1	B	518	HIS

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 39 ligands modelled in this entry, 7 are monoatomic - leaving 32 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	EDO	B	608	-	3,3,3	0.46	0	2,2,2	0.29	0
5	PGE	B	620	-	9,9,9	0.75	0	8,8,8	0.76	0
2	EDO	B	613	-	3,3,3	0.47	0	2,2,2	0.28	0
2	EDO	B	612	-	3,3,3	0.45	0	2,2,2	0.28	0
5	PGE	A	612	-	9,9,9	0.88	0	8,8,8	0.72	0
3	PEG	B	615	-	6,6,6	0.48	0	5,5,5	0.24	0
2	EDO	B	614	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	B	610	-	3,3,3	0.46	0	2,2,2	0.34	0
3	PEG	B	616	-	6,6,6	0.48	0	5,5,5	0.22	0
3	PEG	B	617	-	6,6,6	0.49	0	5,5,5	0.28	0
5	PGE	A	611	-	9,9,9	0.72	0	8,8,8	0.79	0
5	PGE	A	615	-	9,9,9	0.85	0	8,8,8	0.73	0
2	EDO	A	602	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	A	601	-	3,3,3	0.48	0	2,2,2	0.30	0
2	EDO	B	603	-	3,3,3	0.46	0	2,2,2	0.34	0
2	EDO	B	607	-	3,3,3	0.45	0	2,2,2	0.34	0
5	PGE	B	621	-	9,9,9	0.77	0	8,8,8	0.75	0
5	PGE	A	614	-	9,9,9	0.76	0	8,8,8	0.78	0
2	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	B	611	-	3,3,3	0.47	0	2,2,2	0.30	0
2	EDO	B	602	-	3,3,3	0.47	0	2,2,2	0.35	0
5	PGE	A	613	-	9,9,9	0.76	0	8,8,8	0.75	0
2	EDO	B	606	-	3,3,3	0.46	0	2,2,2	0.36	0
2	EDO	B	609	-	3,3,3	0.46	0	2,2,2	0.34	0
6	PG4	B	623	-	12,12,12	0.82	0	11,11,11	0.57	0
3	PEG	A	604	-	6,6,6	0.49	0	5,5,5	0.28	0
2	EDO	B	601	-	3,3,3	0.45	0	2,2,2	0.42	0
2	EDO	B	604	-	3,3,3	0.45	0	2,2,2	0.33	0
5	PGE	B	622	-	9,9,9	0.72	0	8,8,8	0.79	0
2	EDO	B	605	-	3,3,3	0.46	0	2,2,2	0.33	0
6	PG4	B	624	-	12,12,12	0.90	0	11,11,11	0.56	0
5	PGE	A	610	-	9,9,9	0.79	0	8,8,8	0.77	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
2	EDO	B	608	-	-	0/1/1/1	-
5	PGE	B	620	-	-	5/7/7/7	-
2	EDO	B	613	-	-	0/1/1/1	-
2	EDO	B	612	-	-	0/1/1/1	-
5	PGE	A	612	-	-	6/7/7/7	-
3	PEG	B	615	-	-	1/4/4/4	-
2	EDO	B	614	-	-	0/1/1/1	-
2	EDO	B	610	-	-	0/1/1/1	-
3	PEG	B	616	-	-	3/4/4/4	-
3	PEG	B	617	-	-	3/4/4/4	-
5	PGE	A	611	-	-	4/7/7/7	-
5	PGE	A	615	-	-	6/7/7/7	-
2	EDO	A	602	-	-	0/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	B	603	-	-	0/1/1/1	-
2	EDO	B	607	-	-	0/1/1/1	-
5	PGE	B	621	-	-	6/7/7/7	-
5	PGE	A	614	-	-	5/7/7/7	-
2	EDO	A	603	-	-	0/1/1/1	-
2	EDO	B	611	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-
5	PGE	A	613	-	-	3/7/7/7	-
2	EDO	B	606	-	-	0/1/1/1	-
2	EDO	B	609	-	-	0/1/1/1	-
6	PG4	B	623	-	-	6/10/10/10	-
3	PEG	A	604	-	-	3/4/4/4	-
2	EDO	B	601	-	-	0/1/1/1	-
2	EDO	B	604	-	-	0/1/1/1	-
5	PGE	B	622	-	-	4/7/7/7	-
2	EDO	B	605	-	-	0/1/1/1	-
6	PG4	B	624	-	-	4/10/10/10	-
5	PGE	A	610	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	612	PGE	C4-C3-O2-C2
6	B	624	PG4	C6-C5-O3-C4
5	A	615	PGE	C6-C5-O3-C4
5	A	615	PGE	C4-C3-O2-C2
6	B	623	PG4	O2-C3-C4-O3
5	A	610	PGE	O2-C3-C4-O3
5	B	621	PGE	O2-C3-C4-O3
5	B	622	PGE	O2-C3-C4-O3
5	A	612	PGE	C6-C5-O3-C4
5	B	620	PGE	O3-C5-C6-O4
5	B	621	PGE	O3-C5-C6-O4
3	B	616	PEG	O1-C1-C2-O2
3	A	604	PEG	O1-C1-C2-O2
5	B	620	PGE	O2-C3-C4-O3
5	A	611	PGE	O1-C1-C2-O2
5	A	611	PGE	O3-C5-C6-O4
6	B	623	PG4	O4-C7-C8-O5
5	B	622	PGE	O3-C5-C6-O4
3	B	615	PEG	O2-C3-C4-O4
5	B	621	PGE	O1-C1-C2-O2
5	B	622	PGE	O1-C1-C2-O2
6	B	623	PG4	C6-C5-O3-C4
5	A	615	PGE	O2-C3-C4-O3
5	A	610	PGE	O1-C1-C2-O2
5	B	621	PGE	C4-C3-O2-C2
5	B	620	PGE	O1-C1-C2-O2
3	B	617	PEG	O2-C3-C4-O4
3	B	616	PEG	O2-C3-C4-O4
6	B	623	PG4	O1-C1-C2-O2
3	A	604	PEG	O2-C3-C4-O4
6	B	624	PG4	O1-C1-C2-O2
5	B	620	PGE	C6-C5-O3-C4
5	A	614	PGE	O3-C5-C6-O4
5	B	622	PGE	C6-C5-O3-C4
5	A	610	PGE	C6-C5-O3-C4
5	A	610	PGE	C1-C2-O2-C3
6	B	623	PG4	C8-C7-O4-C6
5	A	615	PGE	C3-C4-O3-C5
5	A	614	PGE	C1-C2-O2-C3
3	A	604	PEG	C1-C2-O2-C3
5	A	610	PGE	C4-C3-O2-C2
3	B	616	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
6	B	623	PG4	C3-C4-O3-C5
5	B	621	PGE	C6-C5-O3-C4
5	A	612	PGE	C1-C2-O2-C3
5	A	612	PGE	O1-C1-C2-O2
5	A	614	PGE	C6-C5-O3-C4
5	A	615	PGE	O3-C5-C6-O4
6	B	624	PG4	O3-C5-C6-O4
5	A	612	PGE	O2-C3-C4-O3
5	A	611	PGE	O2-C3-C4-O3
5	B	621	PGE	C3-C4-O3-C5
3	B	617	PEG	C1-C2-O2-C3
5	A	614	PGE	O1-C1-C2-O2
3	B	617	PEG	C4-C3-O2-C2
5	A	611	PGE	C6-C5-O3-C4
6	B	624	PG4	O2-C3-C4-O3
5	B	620	PGE	C3-C4-O3-C5
5	A	613	PGE	C6-C5-O3-C4
5	A	612	PGE	O3-C5-C6-O4
5	A	615	PGE	O1-C1-C2-O2
5	A	613	PGE	C3-C4-O3-C5
5	A	613	PGE	O2-C3-C4-O3
5	A	614	PGE	O2-C3-C4-O3

There are no ring outliers.

15 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	613	EDO	1	0
2	B	612	EDO	1	0
5	A	612	PGE	2	0
2	B	614	EDO	1	0
3	B	616	PEG	2	0
5	A	615	PGE	2	0
2	A	601	EDO	1	0
5	A	614	PGE	1	0
2	B	611	EDO	1	0
5	A	613	PGE	2	0
2	B	606	EDO	1	0
6	B	623	PG4	2	0
5	B	622	PGE	1	0
6	B	624	PG4	3	0
5	A	610	PGE	6	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 ⓘ

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, 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	527/532 (99%)	0.40	17 (3%)	47 50	22, 39, 60, 80	1 (0%)
1	B	527/532 (99%)	0.36	12 (2%)	60 62	24, 39, 60, 84	4 (0%)
All	All	1054/1064 (99%)	0.38	29 (2%)	53 55	22, 39, 60, 84	5 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	TYR	5.7
1	A	484	GLN	4.4
1	A	3	ASP	4.3
1	B	484	GLN	4.2
1	B	483	THR	4.2
1	A	282	TYR	3.7
1	B	69	ILE	3.6
1	A	483	THR	3.5
1	B	3	ASP	3.5
1	B	364	PHE	3.3
1	A	517	GLN	3.1
1	A	53	SER	3.1
1	B	4	ILE	3.0
1	A	255	GLU	3.0
1	A	143	SER	2.9
1	B	378	ASP	2.8
1	A	364	PHE	2.7
1	B	50	THR	2.6
1	A	57	ASN	2.5
1	B	509	ARG	2.4
1	A	486	ASN	2.4
1	A	240	ARG	2.4
1	A	284	THR	2.3
1	B	281	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	287	SER	2.2
1	A	529	VAL	2.1
1	A	458	LYS	2.1
1	A	52	TRP	2.1
1	B	485	ASN	2.1

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(Å ²)	Q<0.9
2	EDO	B	613	4/4	0.40	0.71	48,52,55,57	0
4	CL	B	618	1/1	0.53	0.14	86,86,86,86	0
2	EDO	B	611	4/4	0.53	0.61	58,59,73,74	0
5	PGE	B	621	10/10	0.59	0.41	55,60,71,75	0
2	EDO	B	606	4/4	0.62	0.29	46,47,51,56	0
4	CL	A	609	1/1	0.62	0.19	77,77,77,77	0
5	PGE	A	615	10/10	0.65	0.37	67,77,79,80	0
2	EDO	B	612	4/4	0.66	0.43	47,54,55,65	0
2	EDO	B	607	4/4	0.69	0.27	47,52,59,67	0
5	PGE	A	614	10/10	0.70	0.24	53,58,67,68	0
5	PGE	A	613	10/10	0.71	0.23	61,69,73,76	0
5	PGE	A	612	10/10	0.72	0.28	47,50,54,56	0
2	EDO	A	603	4/4	0.72	0.37	50,55,58,64	0
3	PEG	B	615	7/7	0.73	0.31	33,45,49,51	0
5	PGE	A	610	10/10	0.73	0.37	37,47,50,64	0
6	PG4	B	624	13/13	0.74	0.37	52,59,63,65	0
3	PEG	B	617	7/7	0.75	0.44	52,57,64,68	0
3	PEG	B	616	7/7	0.75	0.40	37,41,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	B	604	4/4	0.76	0.18	55,56,58,68	0
5	PGE	B	620	10/10	0.77	0.25	55,61,64,69	0
2	EDO	B	605	4/4	0.78	0.20	52,56,58,60	0
2	EDO	B	609	4/4	0.78	0.16	50,51,52,56	0
6	PG4	B	623	13/13	0.79	0.50	49,54,64,68	0
5	PGE	B	622	10/10	0.79	0.37	39,48,56,60	0
5	PGE	A	611	10/10	0.81	0.39	44,54,62,63	0
4	CL	B	619	1/1	0.81	0.13	64,64,64,64	0
2	EDO	B	614	4/4	0.83	0.32	54,55,57,62	0
4	CL	A	606	1/1	0.84	0.13	74,74,74,74	0
2	EDO	B	602	4/4	0.85	0.16	39,41,42,44	0
2	EDO	A	602	4/4	0.86	0.17	36,42,53,63	0
2	EDO	A	601	4/4	0.86	0.23	36,39,40,43	0
2	EDO	B	608	4/4	0.87	0.22	54,55,59,61	0
2	EDO	B	603	4/4	0.87	0.21	53,54,55,55	0
3	PEG	A	604	7/7	0.87	0.18	45,48,50,53	0
4	CL	A	605	1/1	0.90	0.10	67,67,67,67	0
2	EDO	B	601	4/4	0.90	0.18	30,31,31,33	0
4	CL	A	608	1/1	0.91	0.15	66,66,66,66	0
2	EDO	B	610	4/4	0.94	0.12	44,46,46,52	0
4	CL	A	607	1/1	0.95	0.08	67,67,67,67	0

6.5 Other polymers ⓘ

There are no such residues in this entry.