



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 10, 2022 – 04:05 PM EDT

PDB ID : 8DX4
Title : Clostridioides difficile R20291 minor pilin - PilW fused with Maltose Binding Protein
Authors : Ronish, L.A.; Piepenbrink, K.
Deposited on : 2022-08-02
Resolution : 2.49 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 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
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)	:	2.29

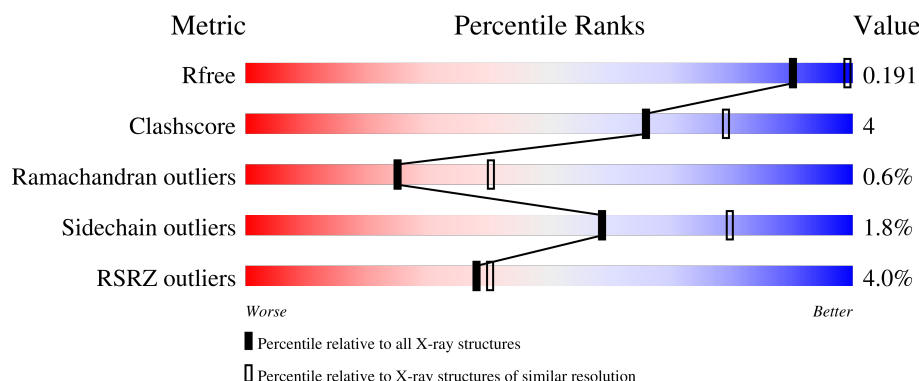
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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 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	512	 5% 87% 9% . .
1	B	512	 3% 88% 9% .
1	C	512	 4% 85% 12% .
1	D	512	 4% 87% 9% . .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15965 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 Maltodextrin-binding protein, Putative pilin protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	5	3	0
			3778	2427	610	731	10			
1	B	497	Total	C	N	O	S	0	5	0
			3818	2453	617	738	10			
1	C	497	Total	C	N	O	S	0	4	0
			3845	2471	622	743	9			
1	D	493	Total	C	N	O	S	0	9	0
			3795	2440	610	734	11			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP A0A4P1LXE0
A	82	ALA	ASP	conflict	UNP A0A4P1LXE0
A	83	ALA	LYS	conflict	UNP A0A4P1LXE0
A	172	ALA	GLU	conflict	UNP A0A4P1LXE0
A	173	ALA	ASN	conflict	UNP A0A4P1LXE0
A	239	ALA	LYS	conflict	UNP A0A4P1LXE0
A	359	ALA	GLU	conflict	UNP A0A4P1LXE0
A	362	ALA	LYS	conflict	UNP A0A4P1LXE0
A	363	ALA	ASP	conflict	UNP A0A4P1LXE0
A	1159	LEU	-	expression tag	UNP A0A0H3N4W9
A	1160	GLU	-	expression tag	UNP A0A0H3N4W9
A	1161	HIS	-	expression tag	UNP A0A0H3N4W9
A	1162	HIS	-	expression tag	UNP A0A0H3N4W9
A	1163	HIS	-	expression tag	UNP A0A0H3N4W9
A	1164	HIS	-	expression tag	UNP A0A0H3N4W9
A	1165	HIS	-	expression tag	UNP A0A0H3N4W9
A	1166	HIS	-	expression tag	UNP A0A0H3N4W9
B	0	MET	-	initiating methionine	UNP A0A4P1LXE0
B	82	ALA	ASP	conflict	UNP A0A4P1LXE0
B	83	ALA	LYS	conflict	UNP A0A4P1LXE0
B	172	ALA	GLU	conflict	UNP A0A4P1LXE0

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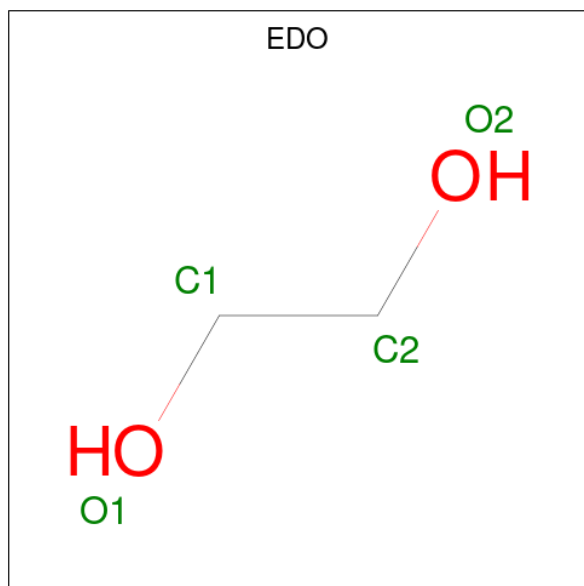
Chain	Residue	Modelled	Actual	Comment	Reference
B	173	ALA	ASN	conflict	UNP A0A4P1LXE0
B	239	ALA	LYS	conflict	UNP A0A4P1LXE0
B	359	ALA	GLU	conflict	UNP A0A4P1LXE0
B	362	ALA	LYS	conflict	UNP A0A4P1LXE0
B	363	ALA	ASP	conflict	UNP A0A4P1LXE0
B	1159	LEU	-	expression tag	UNP A0A0H3N4W9
B	1160	GLU	-	expression tag	UNP A0A0H3N4W9
B	1161	HIS	-	expression tag	UNP A0A0H3N4W9
B	1162	HIS	-	expression tag	UNP A0A0H3N4W9
B	1163	HIS	-	expression tag	UNP A0A0H3N4W9
B	1164	HIS	-	expression tag	UNP A0A0H3N4W9
B	1165	HIS	-	expression tag	UNP A0A0H3N4W9
B	1166	HIS	-	expression tag	UNP A0A0H3N4W9
C	0	MET	-	initiating methionine	UNP A0A4P1LXE0
C	82	ALA	ASP	conflict	UNP A0A4P1LXE0
C	83	ALA	LYS	conflict	UNP A0A4P1LXE0
C	172	ALA	GLU	conflict	UNP A0A4P1LXE0
C	173	ALA	ASN	conflict	UNP A0A4P1LXE0
C	239	ALA	LYS	conflict	UNP A0A4P1LXE0
C	359	ALA	GLU	conflict	UNP A0A4P1LXE0
C	362	ALA	LYS	conflict	UNP A0A4P1LXE0
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C	1159	LEU	-	expression tag	UNP A0A0H3N4W9
C	1160	GLU	-	expression tag	UNP A0A0H3N4W9
C	1161	HIS	-	expression tag	UNP A0A0H3N4W9
C	1162	HIS	-	expression tag	UNP A0A0H3N4W9
C	1163	HIS	-	expression tag	UNP A0A0H3N4W9
C	1164	HIS	-	expression tag	UNP A0A0H3N4W9
C	1165	HIS	-	expression tag	UNP A0A0H3N4W9
C	1166	HIS	-	expression tag	UNP A0A0H3N4W9
D	0	MET	-	initiating methionine	UNP A0A4P1LXE0
D	82	ALA	ASP	conflict	UNP A0A4P1LXE0
D	83	ALA	LYS	conflict	UNP A0A4P1LXE0
D	172	ALA	GLU	conflict	UNP A0A4P1LXE0
D	173	ALA	ASN	conflict	UNP A0A4P1LXE0
D	239	ALA	LYS	conflict	UNP A0A4P1LXE0
D	359	ALA	GLU	conflict	UNP A0A4P1LXE0
D	362	ALA	LYS	conflict	UNP A0A4P1LXE0
D	363	ALA	ASP	conflict	UNP A0A4P1LXE0
D	1159	LEU	-	expression tag	UNP A0A0H3N4W9
D	1160	GLU	-	expression tag	UNP A0A0H3N4W9
D	1161	HIS	-	expression tag	UNP A0A0H3N4W9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1162	HIS	-	expression tag	UNP A0A0H3N4W9
D	1163	HIS	-	expression tag	UNP A0A0H3N4W9
D	1164	HIS	-	expression tag	UNP A0A0H3N4W9
D	1165	HIS	-	expression tag	UNP A0A0H3N4W9
D	1166	HIS	-	expression tag	UNP A0A0H3N4W9

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



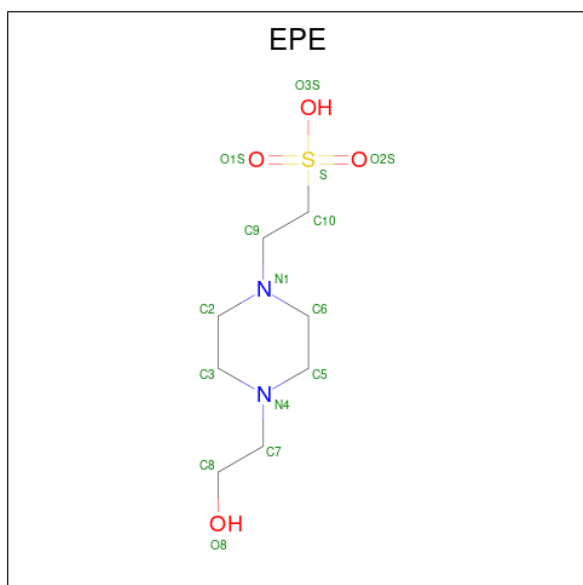
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



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

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



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

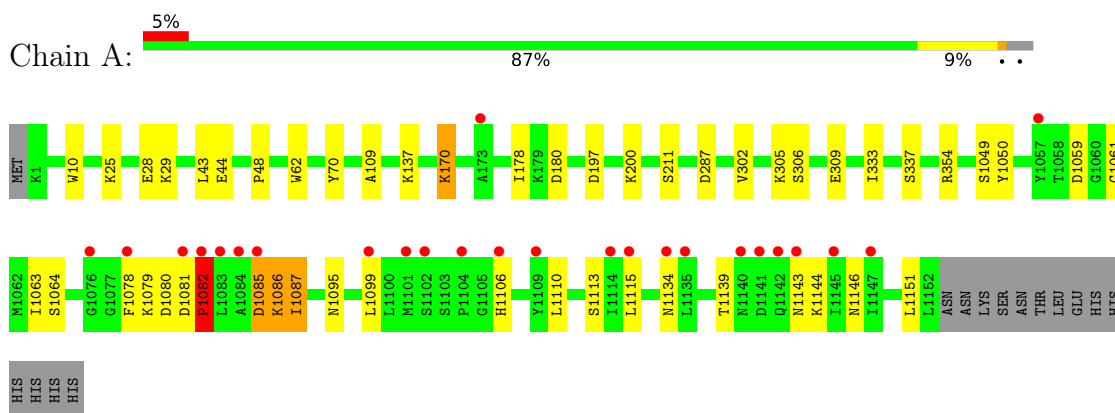
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	88	Total 88	O 88	0	0
6	B	201	Total 201	O 201	0	0
6	C	165	Total 165	O 165	0	0
6	D	171	Total 171	O 171	0	0

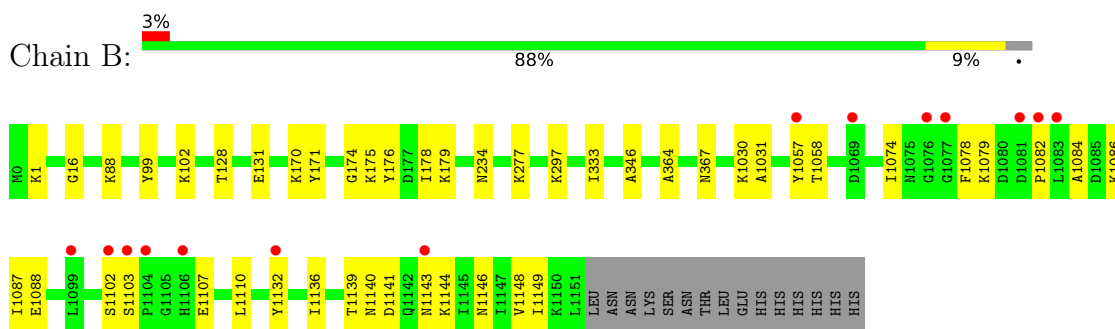
3 Residue-property plots [i](#)

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.

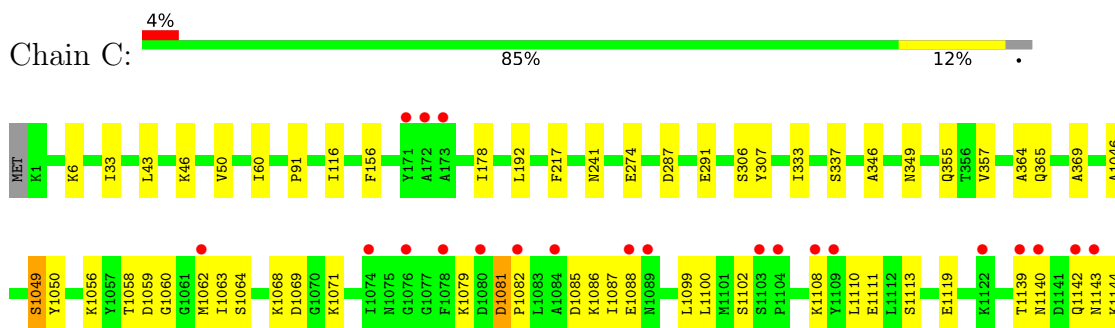
- Molecule 1: Maltodextrin-binding protein, Putative pilin protein



- Molecule 1: Maltodextrin-binding protein, Putative pilin protein



- Molecule 1: Maltodextrin-binding protein, Putative pilin protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.33Å 81.80Å 102.96Å 92.44° 90.95° 113.37°	Depositor
Resolution (Å)	39.73 – 2.49 102.80 – 2.49	Depositor EDS
% Data completeness (in resolution range)	93.5 (39.73-2.49) 91.1 (102.80-2.49)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.186 , 0.218 0.188 , 0.191	Depositor DCC
R_{free} test set	3179 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	39.0	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.207 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15965	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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: PEG, EDO, EPE, PGE

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	0.29	0/3871	0.52	1/5263 (0.0%)
1	B	0.29	0/3917	0.47	0/5316
1	C	0.29	0/3938	0.51	0/5339
1	D	0.31	0/3895	0.50	0/5287
All	All	0.30	0/15621	0.50	1/21205 (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	A	29	LYS	CD-CE-NZ	-10.53	87.49	111.70

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	3778	0	3708	29	0
1	B	3818	0	3785	30	0
1	C	3845	0	3839	31	1
1	D	3795	0	3749	34	1
2	A	16	0	24	1	0
2	B	16	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	12	0	18	3	0
2	D	28	0	42	0	0
3	C	15	0	17	2	0
4	D	10	0	14	1	0
5	D	7	0	10	0	0
6	A	88	0	0	0	0
6	B	201	0	0	3	0
6	C	165	0	0	3	0
6	D	171	0	0	0	0
All	All	15965	0	15230	123	1

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.

All (123) 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:1134:ASN:ND2	1:B:367:ASN:OD1	2.10	0.85
1:D:1094:TYR:CZ	1:D:1120:ILE:HD11	2.15	0.80
1:D:1094:TYR:CE1	1:D:1120:ILE:HD11	2.16	0.79
1:C:365:GLN:HG3	2:C:1202:EDO:H12	1.66	0.77
1:B:1078:PHE:HB3	1:B:1082:PRO:HD2	1.66	0.76
1:D:197:ASP:HA	1:D:200:LYS:HG2	1.70	0.74
1:D:197:ASP:OD1	1:D:200:LYS:NZ	2.21	0.72
1:A:1115:LEU:HD23	1:A:1144:LYS:HD2	1.74	0.69
1:C:274[B]:GLU:OE1	6:C:1301:HOH:O	2.10	0.68
1:C:1059:ASP:HB3	1:C:1079:LYS:HE3	1.76	0.68
1:A:354:ARG:NH2	1:B:1:LYS:O	2.28	0.67
1:B:99:TYR:O	1:B:102:LYS:HG2	1.96	0.64
1:A:1081:ASP:N	1:A:1082:PRO:HD3	2.12	0.64
1:A:197:ASP:HA	1:A:200:LYS:HG2	1.80	0.64
1:D:1056:LYS:HG2	1:D:1057:TYR:H	1.63	0.63
1:B:88:LYS:NZ	6:B:1302:HOH:O	2.31	0.63
1:A:287:ASP:OD1	1:A:306:SER:OG	2.17	0.62
1:B:1136:ILE:HG12	1:B:1149:ILE:HG12	1.81	0.62
1:A:1139:THR:HG23	1:A:1146:ASN:HB3	1.84	0.60
1:A:48:PRO:HG3	1:A:70:TYR:CE1	2.38	0.58
1:A:1050:TYR:CE2	1:A:1059:ASP:HB2	2.39	0.58
1:C:1050:TYR:OH	1:C:1059:ASP:HB2	2.04	0.57
1:A:1085:ASP:C	1:A:1087:ILE:H	2.07	0.57
1:B:1102:SER:OG	1:B:1110:LEU:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:VAL:HG22	4:D:1202:PGE:H5	1.88	0.56
1:D:1032:LYS:HB3	1:D:1094:TYR:CZ	2.40	0.56
1:B:1058:THR:HG22	1:B:1103:SER:HB2	1.87	0.56
1:D:178:ILE:HG22	1:D:333:ILE:HD12	1.88	0.56
1:A:1080:ASP:HB3	1:A:1082:PRO:HG3	1.87	0.55
1:B:16:GLY:H	1:B:297:LYS:HD2	1.72	0.55
1:C:1049:SER:HB3	1:C:1082:PRO:CG	2.37	0.54
1:A:305:LYS:O	1:A:309:GLU:HG2	2.06	0.54
1:C:287:ASP:OD1	1:C:306:SER:OG	2.24	0.54
1:C:349:ASN:HB3	1:C:355:GLN:HG2	1.90	0.53
1:D:146:ALA:O	1:D:224[B]:MET:HG3	2.09	0.53
1:A:1063:ILE:HG12	1:A:1079:LYS:HD3	1.88	0.53
1:B:234:ASN:HB2	6:B:1427:HOH:O	2.07	0.53
1:C:1069:ASP:O	1:C:1071:LYS:HG2	2.09	0.53
1:A:10:TRP:HB3	1:A:43:LEU:HD11	1.91	0.53
1:B:16:GLY:N	1:B:297:LYS:HD2	2.23	0.53
1:C:241:ASN:ND2	6:C:1307:HOH:O	2.42	0.52
1:C:1046:ALA:O	1:C:1082:PRO:HG2	2.08	0.52
1:C:369:ALA:HB3	2:C:1202:EDO:H11	1.91	0.52
1:D:1103:SER:O	1:D:1105:GLY:N	2.38	0.52
1:A:1139:THR:CG2	1:A:1146:ASN:HB3	2.40	0.52
1:A:25:LYS:O	1:A:28[A]:GLU:HG2	2.10	0.51
1:B:1078:PHE:HB3	1:B:1082:PRO:CD	2.40	0.51
1:A:1082:PRO:HD2	1:A:1086:LYS:HG2	1.92	0.51
1:C:1111:GLU:HG2	1:C:1150:LYS:HG2	1.93	0.50
1:D:1102:SER:HB2	1:D:1110:LEU:HD23	1.93	0.50
1:B:128:THR:OG1	1:B:131:GLU:OE2	2.23	0.50
1:D:1056:LYS:HG2	1:D:1057:TYR:N	2.27	0.50
1:D:48:PRO:HG3	1:D:70:TYR:CE1	2.48	0.48
1:A:170:LYS:HE2	1:A:180:ASP:OD2	2.13	0.48
1:A:1099:LEU:HB3	1:A:1113:SER:OG	2.12	0.48
1:C:1085:ASP:O	1:C:1087:ILE:HG12	2.13	0.48
1:B:1079:LYS:C	1:B:1082:PRO:HD3	2.34	0.48
1:B:179:LYS:HD3	1:B:1031:ALA:HB2	1.96	0.48
1:D:196:VAL:HG12	1:D:200:LYS:HZ2	1.79	0.47
1:D:1110:LEU:HB3	1:D:1151:LEU:HB2	1.97	0.47
1:A:1078:PHE:CE2	1:C:91:PRO:HB3	2.50	0.47
1:B:1132:TYR:CD2	1:B:1136:ILE:HD11	2.50	0.47
1:C:346:ALA:HB2	1:C:364:ALA:HB2	1.97	0.47
1:C:192:LEU:HD23	1:C:357:VAL:HG13	1.96	0.46
1:D:1120:ILE:HG23	1:D:1120:ILE:HD12	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:TYR:HE2	1:A:1059:ASP:HB2	1.79	0.46
1:D:171:TYR:OH	1:D:174:GLY:HA2	2.16	0.46
1:A:178:ILE:HG22	1:A:333:ILE:HD12	1.97	0.46
1:C:178:ILE:HG22	1:C:333:ILE:HD12	1.98	0.46
1:D:1056:LYS:HE3	1:D:1104:PRO:HD3	1.98	0.46
1:C:46:LYS:O	1:C:50:VAL:HG23	2.17	0.45
1:D:1127:LYS:O	1:D:1131:ASP:HB2	2.17	0.45
1:C:1058:THR:HG22	1:C:1102:SER:OG	2.16	0.45
1:A:1110:LEU:HD23	1:A:1110:LEU:HA	1.83	0.45
1:B:1139:THR:HG23	1:B:1146:ASN:OD1	2.17	0.45
1:D:1103:SER:OG	1:D:1104:PRO:HD2	2.17	0.45
1:D:1139:THR:OG1	1:D:1146:ASN:HB3	2.16	0.45
1:C:1056:LYS:NZ	1:C:1060:GLY:O	2.48	0.45
1:D:1125:LEU:HD11	1:D:1145:ILE:HD13	1.99	0.45
1:B:1074:ILE:HD12	1:B:1088:GLU:HG2	2.00	0.44
1:C:1063:ILE:O	1:C:1099:LEU:HD12	2.17	0.44
1:D:1063:ILE:CG2	1:D:1100:LEU:HB3	2.48	0.44
1:C:43:LEU:HD13	1:C:60:ILE:HD11	1.98	0.44
1:C:6:LYS:HA	1:C:33:ILE:HG23	2.00	0.44
1:B:179:LYS:HD3	1:B:1031:ALA:CB	2.48	0.44
1:D:1086:LYS:HG2	1:D:1087:ILE:H	1.83	0.43
1:A:44:GLU:HB3	1:A:62:TRP:CZ2	2.53	0.43
1:D:1120:ILE:HA	1:D:1120:ILE:HD13	1.46	0.43
1:B:171:TYR:OH	1:B:174:GLY:HA2	2.17	0.43
1:A:137:LYS:HD3	2:A:1201:EDO:H12	2.00	0.43
1:D:287:ASP:OD1	1:D:306:SER:OG	2.26	0.43
1:C:1110:LEU:HD12	1:C:1110:LEU:HA	1.78	0.43
2:C:1201:EDO:H11	6:C:1428:HOH:O	2.17	0.43
1:B:1136:ILE:HA	1:B:1148:VAL:O	2.19	0.43
1:A:1063:ILE:HG12	1:A:1079:LYS:CD	2.49	0.43
1:B:1078:PHE:HB2	1:B:1084:ALA:HB2	2.01	0.43
1:C:1139:THR:OG1	1:C:1140:ASN:N	2.48	0.43
3:C:1203:EPE:H81	3:C:1203:EPE:H32	1.85	0.42
1:B:346:ALA:HB2	1:B:364:ALA:HB2	2.00	0.42
1:B:1084:ALA:C	1:B:1086:LYS:H	2.22	0.42
1:D:1086:LYS:O	1:D:1088:GLU:N	2.51	0.42
1:C:156:PHE:HE1	3:C:1203:EPE:H22	1.85	0.42
1:D:1086:LYS:HE3	1:D:1086:LYS:HB3	1.81	0.42
1:B:1030:LYS:HB3	1:B:1030:LYS:HE3	1.77	0.42
1:D:349:ASN:HB3	1:D:355:GLN:HG2	2.02	0.42
1:D:1086:LYS:C	1:D:1088:GLU:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1143:ASN:O	1:B:1144:LYS:HG3	2.19	0.42
1:A:109:ALA:HA	1:A:302:VAL:HA	2.02	0.42
1:C:1062:MET:HA	1:C:1100:LEU:O	2.19	0.42
1:A:1063:ILE:O	1:A:1099:LEU:HD12	2.19	0.41
1:C:116:ILE:HG22	1:C:217:PHE:CZ	2.55	0.41
1:B:178:ILE:HG22	1:B:333:ILE:HD12	2.02	0.41
1:B:277:LYS:NZ	6:B:1324:HOH:O	2.53	0.41
1:C:1142:GLN:O	1:C:1143:ASN:HB2	2.21	0.41
1:D:346:ALA:HB2	1:D:364:ALA:HB2	2.02	0.41
1:A:1085:ASP:C	1:A:1087:ILE:N	2.74	0.41
1:B:175:LYS:HG3	1:B:176:TYR:N	2.36	0.41
1:C:291:GLU:HA	1:C:307:TYR:OH	2.21	0.41
1:C:1081:ASP:C	1:C:1085:ASP:HA	2.41	0.41
1:D:1138:ILE:HA	1:D:1146:ASN:O	2.21	0.41
1:D:1063:ILE:HG22	1:D:1100:LEU:HB3	2.03	0.40
1:B:1057:TYR:HB2	1:B:1103:SER:OG	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:SER:OG	1:D:41[B]:ASP:OD2[1_445]	2.17	0.03

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	498/512 (97%)	466 (94%)	25 (5%)	7 (1%)	11	18
1	B	500/512 (98%)	476 (95%)	24 (5%)	0	100	100
1	C	499/512 (98%)	480 (96%)	18 (4%)	1 (0%)	47	66
1	D	498/512 (97%)	478 (96%)	16 (3%)	4 (1%)	19	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1995/2048 (97%)	1900 (95%)	83 (4%)	12 (1%)	25 40

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1082	PRO
1	A	1087	ILE
1	A	1086	LYS
1	C	1108	LYS
1	D	1110	LEU
1	A	1143	ASN
1	A	1151	LEU
1	D	1104	PRO
1	A	1095	ASN
1	D	1108	LYS
1	D	1087	ILE
1	A	1061	GLY

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	383/410 (93%)	375 (98%)	8 (2%)	53 76
1	B	392/410 (96%)	387 (99%)	5 (1%)	69 86
1	C	398/410 (97%)	389 (98%)	9 (2%)	50 74
1	D	388/410 (95%)	383 (99%)	5 (1%)	69 86
All	All	1561/1640 (95%)	1534 (98%)	27 (2%)	59 81

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	211	SER
1	A	337	SER

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Mol	Chain	Res	Type
1	A	1049	SER
1	A	1064	SER
1	A	1082	PRO
1	A	1085	ASP
1	A	1106	HIS
1	B	170	LYS
1	B	1087	ILE
1	B	1107	GLU
1	B	1140	ASN
1	B	1141	ASP
1	C	1049	SER
1	C	1064	SER
1	C	1068	LYS
1	C	1081	ASP
1	C	1086	LYS
1	C	1088	GLU
1	C	1113	SER
1	C	1119	GLU
1	C	1144	LYS
1	D	1064	SER
1	D	1078	PHE
1	D	1086	LYS
1	D	1106	HIS
1	D	1137	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	241	ASN
1	D	1095	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 ligands are modelled in this entry.

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	D	1201	-	3,3,3	0.44	0	2,2,2	0.18	0
2	EDO	D	1204	-	3,3,3	0.44	0	2,2,2	0.27	0
2	EDO	A	1201	-	3,3,3	0.44	0	2,2,2	0.47	0
2	EDO	C	1202	-	3,3,3	0.50	0	2,2,2	0.36	0
5	PEG	D	1206	-	6,6,6	0.49	0	5,5,5	0.27	0
2	EDO	A	1202	-	3,3,3	0.45	0	2,2,2	0.35	0
2	EDO	B	1201	-	3,3,3	0.46	0	2,2,2	0.38	0
2	EDO	C	1201	-	3,3,3	0.45	0	2,2,2	0.33	0
2	EDO	B	1202	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	A	1204	-	3,3,3	0.44	0	2,2,2	0.37	0
2	EDO	A	1203	-	3,3,3	0.47	0	2,2,2	0.27	0
2	EDO	D	1205	-	3,3,3	0.45	0	2,2,2	0.33	0
2	EDO	B	1204	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	D	1203	-	3,3,3	0.45	0	2,2,2	0.43	0
2	EDO	D	1208	-	3,3,3	0.47	0	2,2,2	0.33	0
2	EDO	C	1204	-	3,3,3	0.76	0	2,2,2	0.42	0
4	PGE	D	1202	-	9,9,9	0.31	0	8,8,8	0.39	0
2	EDO	B	1203	-	3,3,3	0.45	0	2,2,2	0.34	0
2	EDO	D	1207	-	3,3,3	0.48	0	2,2,2	0.36	0
3	EPE	C	1203	-	15,15,15	0.91	1 (6%)	18,20,20	1.75	5 (27%)
2	EDO	D	1209	-	3,3,3	0.54	0	2,2,2	1.12	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	D	1201	-	-	1/1/1/1	-
2	EDO	D	1204	-	-	1/1/1/1	-
2	EDO	A	1201	-	-	1/1/1/1	-
2	EDO	C	1202	-	-	0/1/1/1	-
5	PEG	D	1206	-	-	2/4/4/4	-
2	EDO	A	1202	-	-	0/1/1/1	-
2	EDO	B	1201	-	-	1/1/1/1	-
2	EDO	C	1201	-	-	0/1/1/1	-
2	EDO	B	1202	-	-	0/1/1/1	-
2	EDO	A	1204	-	-	1/1/1/1	-
2	EDO	A	1203	-	-	0/1/1/1	-
2	EDO	D	1205	-	-	0/1/1/1	-
2	EDO	B	1204	-	-	1/1/1/1	-
2	EDO	D	1203	-	-	1/1/1/1	-
2	EDO	D	1208	-	-	0/1/1/1	-
2	EDO	C	1204	-	-	1/1/1/1	-
4	PGE	D	1202	-	-	3/7/7/7	-
2	EDO	B	1203	-	-	0/1/1/1	-
2	EDO	D	1207	-	-	1/1/1/1	-
3	EPE	C	1203	-	-	2/9/19/19	0/1/1/1
2	EDO	D	1209	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1203	EPE	C10-S	3.05	1.81	1.77

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1203	EPE	C5-N4-C3	3.36	116.40	108.83
3	C	1203	EPE	C7-N4-C3	3.22	119.47	111.23
3	C	1203	EPE	C7-N4-C5	3.04	119.00	111.23
3	C	1203	EPE	O2S-S-C10	2.76	110.24	106.92
3	C	1203	EPE	O3S-S-C10	2.07	109.11	105.77

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1203	EPE	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
3	C	1203	EPE	S-C10-C9-N1
4	D	1202	PGE	O2-C3-C4-O3
2	A	1201	EDO	O1-C1-C2-O2
5	D	1206	PEG	O2-C3-C4-O4
2	C	1204	EDO	O1-C1-C2-O2
2	D	1207	EDO	O1-C1-C2-O2
2	B	1204	EDO	O1-C1-C2-O2
2	D	1201	EDO	O1-C1-C2-O2
4	D	1202	PGE	C3-C4-O3-C5
5	D	1206	PEG	C1-C2-O2-C3
4	D	1202	PGE	C1-C2-O2-C3
2	D	1204	EDO	O1-C1-C2-O2
2	A	1204	EDO	O1-C1-C2-O2
2	B	1201	EDO	O1-C1-C2-O2
2	D	1203	EDO	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	EDO	1	0
2	C	1202	EDO	2	0
2	C	1201	EDO	1	0
4	D	1202	PGE	1	0
3	C	1203	EPE	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

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	497/512 (97%)	-0.09	25 (5%)	28 30	34, 67, 127, 163	0
1	B	497/512 (97%)	-0.32	14 (2%)	53 55	20, 48, 126, 155	0
1	C	497/512 (97%)	-0.33	22 (4%)	34 36	25, 48, 116, 142	0
1	D	493/512 (96%)	-0.28	18 (3%)	41 44	23, 48, 123, 174	0
All	All	1984/2048 (96%)	-0.25	79 (3%)	38 40	20, 54, 123, 174	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1102	SER	7.7
1	B	1083	LEU	7.2
1	B	1082	PRO	5.5
1	D	1075	ASN	4.9
1	A	1081	ASP	4.8
1	A	1104	PRO	4.7
1	B	1143	ASN	4.4
1	B	1104	PRO	4.4
1	B	1076	GLY	4.3
1	B	1103	SER	4.3
1	D	1101	MET	4.1
1	D	1128	LEU	3.9
1	C	1082	PRO	3.8
1	A	1140	ASN	3.7
1	D	1100	LEU	3.6
1	B	1106	HIS	3.6
1	C	173	ALA	3.6
1	B	1102	SER	3.5
1	A	1084	ALA	3.4
1	C	1078	PHE	3.4
1	A	1076	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	1140	ASN	3.3
1	C	1108	LYS	3.3
1	B	1099	LEU	3.2
1	C	1076	GLY	3.2
1	C	1143	ASN	3.2
1	D	1079	LYS	3.1
1	A	1082	PRO	3.0
1	C	1145	ILE	3.0
1	C	1104	PRO	3.0
1	D	1099	LEU	3.0
1	C	1080	ASP	2.9
1	D	1115	LEU	2.9
1	D	1132	TYR	2.9
1	C	1103	SER	2.9
1	D	1106	HIS	2.9
1	C	1142	GLN	2.8
1	B	1077	GLY	2.8
1	C	1089	ASN	2.8
1	D	1078	PHE	2.8
1	A	1135	LEU	2.7
1	A	1142	GLN	2.7
1	D	1104	PRO	2.6
1	A	1101	MET	2.6
1	C	1109	TYR	2.6
1	A	1115	LEU	2.6
1	A	1134	ASN	2.6
1	A	1085	ASP	2.5
1	A	1057	TYR	2.5
1	D	1088	GLU	2.5
1	A	1141	ASP	2.4
1	C	1139	THR	2.4
1	D	1062	MET	2.4
1	C	1084	ALA	2.4
1	A	1102	SER	2.4
1	B	1132	TYR	2.3
1	A	1099	LEU	2.3
1	C	1062	MET	2.3
1	A	1109	TYR	2.3
1	A	1083	LEU	2.3
1	A	1106	HIS	2.2
1	C	1122	LYS	2.2
1	A	1078	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1145	ILE	2.2
1	A	1143	ASN	2.2
1	B	1057	TYR	2.2
1	B	1081	ASP	2.2
1	B	1069	ASP	2.1
1	A	1114	ILE	2.1
1	D	1067	LYS	2.1
1	D	1103	SER	2.1
1	C	1088	GLU	2.1
1	A	173	ALA	2.1
1	C	171	TYR	2.1
1	D	1109	TYR	2.1
1	A	1147	ILE	2.1
1	C	1074	ILE	2.0
1	C	172	ALA	2.0
1	D	1110	LEU	2.0

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 monosaccharides 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
5	PEG	D	1206	7/7	0.58	0.23	74,80,82,83	0
2	EDO	C	1201	4/4	0.79	0.17	53,54,56,57	0
3	EPE	C	1203	15/15	0.82	0.23	86,89,108,108	0
2	EDO	A	1203	4/4	0.84	0.17	75,75,76,78	0
2	EDO	D	1203	4/4	0.85	0.14	88,89,89,89	0
2	EDO	C	1204	4/4	0.87	0.18	72,72,80,83	0
2	EDO	B	1201	4/4	0.88	0.15	65,67,71,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	B	1204	4/4	0.90	0.14	81,81,81,82	0
2	EDO	D	1207	4/4	0.90	0.11	66,67,67,68	0
2	EDO	D	1208	4/4	0.90	0.12	72,72,73,75	0
2	EDO	A	1204	4/4	0.90	0.13	71,71,72,73	0
4	PGE	D	1202	10/10	0.90	0.17	59,62,68,68	0
2	EDO	B	1203	4/4	0.90	0.18	45,50,50,51	0
2	EDO	D	1209	4/4	0.91	0.14	67,68,73,88	0
2	EDO	D	1205	4/4	0.91	0.14	68,70,72,73	0
2	EDO	D	1204	4/4	0.92	0.17	62,63,63,64	0
2	EDO	B	1202	4/4	0.92	0.21	60,62,65,69	0
2	EDO	C	1202	4/4	0.93	0.24	54,55,55,62	0
2	EDO	A	1202	4/4	0.93	0.23	65,65,67,68	0
2	EDO	D	1201	4/4	0.93	0.12	50,54,57,61	0
2	EDO	A	1201	4/4	0.93	0.18	54,55,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.