



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 01:34 PM UTC

PDB ID : 4H5F / pdb_00004h5f
Title : Crystal structure of an amino acid ABC transporter substrate-binding protein from *Streptococcus pneumoniae* Canada MDR_19A bound to L-arginine, form 1
Authors : Stogios, P.J.; Wawrzak, Z.; Kudritska, M.; Minasov, G.; Yim, V.; Savchenko, A.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-09-18
Resolution : 1.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

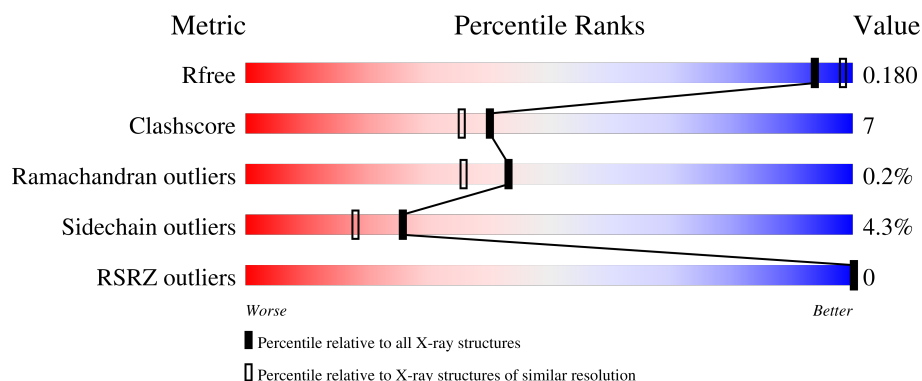
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	243	 85% 13% ..
1	B	243	 88% 11% .
1	C	243	 79% 20% .
1	D	243	 77% 20% ..

Validation Pipeline (wwPDB-VP) : 2.49

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
4	PEG	B	305	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 8142 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 Amino acid ABC superfamily ATP binding cassette transporter, binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	9	0
			1855	1167	300	381	7			
1	B	240	Total	C	N	O	S	0	2	0
			1824	1148	297	373	6			
1	C	240	Total	C	N	O	S	0	0	0
			1812	1140	295	371	6			
1	D	239	Total	C	N	O	S	0	0	0
			1803	1135	293	369	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	GLY	-	expression tag	UNP D6ZRZ2
A	136	HIS	ARG	SEE REMARK 999	UNP D6ZRZ2
B	29	GLY	-	expression tag	UNP D6ZRZ2
B	136	HIS	ARG	SEE REMARK 999	UNP D6ZRZ2
C	29	GLY	-	expression tag	UNP D6ZRZ2
C	136	HIS	ARG	SEE REMARK 999	UNP D6ZRZ2
D	29	GLY	-	expression tag	UNP D6ZRZ2
D	136	HIS	ARG	SEE REMARK 999	UNP D6ZRZ2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



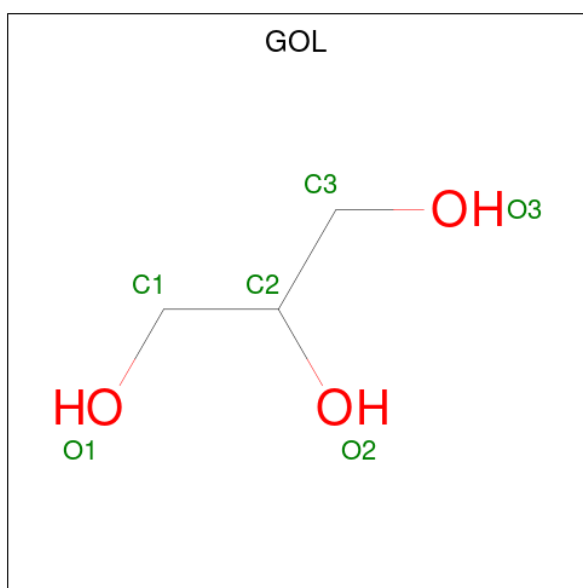
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total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

Continued on next page...

Continued from previous page...

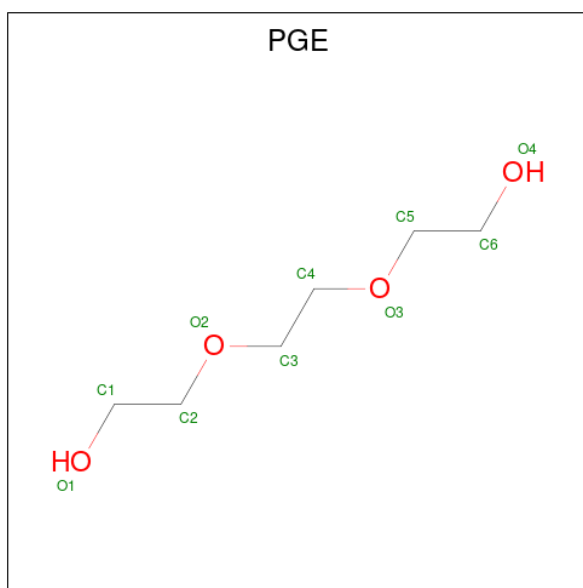
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		
4	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



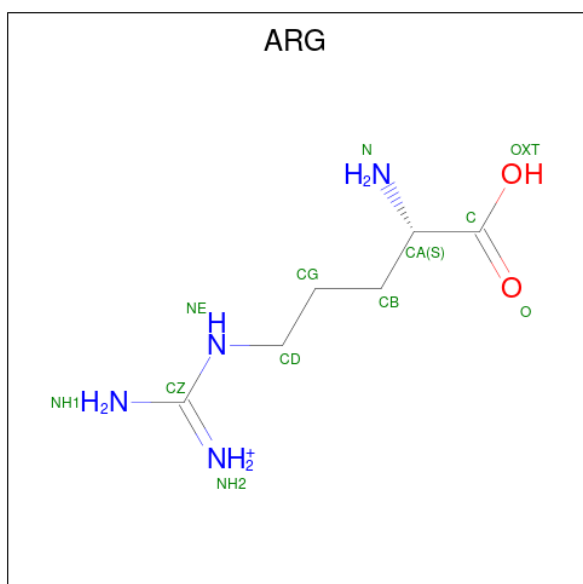
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



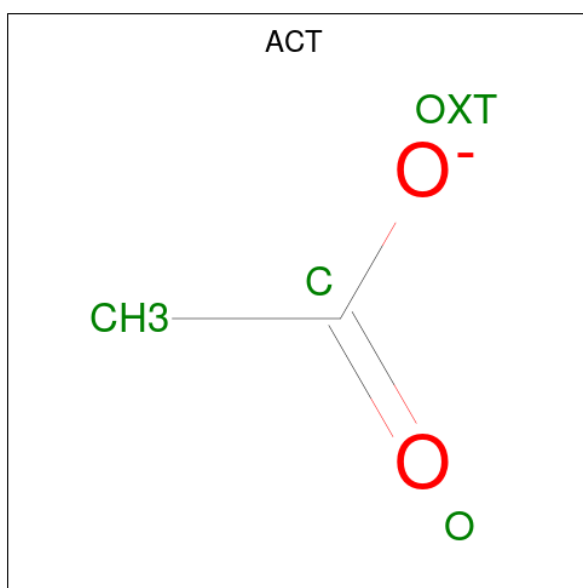
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	B	1	Total	C	O	0	0
			10	6	4		
6	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is ARGinine (CCD ID: ARG) (formula: $C_6H_{15}N_4O_2$).



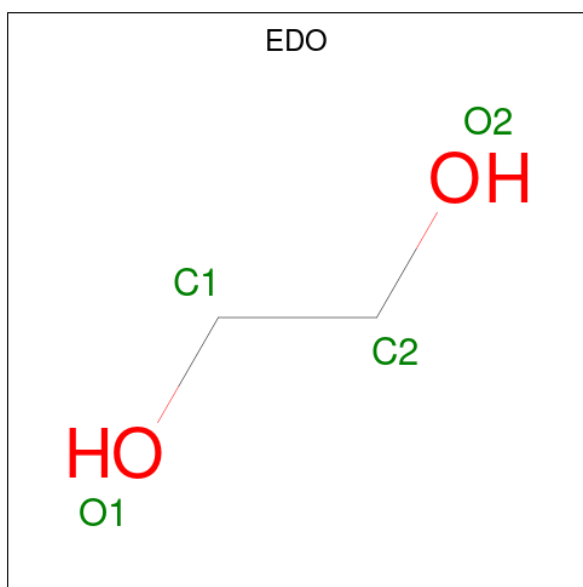
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			12	6	4	2		
7	B	1	Total	C	N	O	0	0
			12	6	4	2		
7	C	1	Total	C	N	O	0	0
			12	6	4	2		
7	D	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 8 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

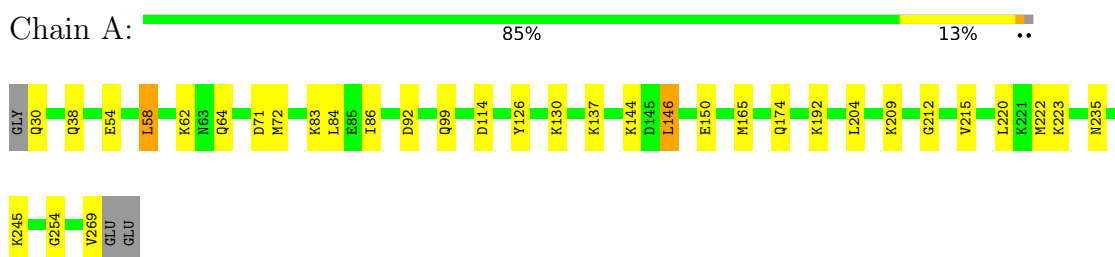
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	157	Total	O	0	14
			171	171		
10	B	138	Total	O	0	13
			151	151		
10	C	114	Total	O	0	4
			118	118		
10	D	89	Total	O	0	5
			93	93		

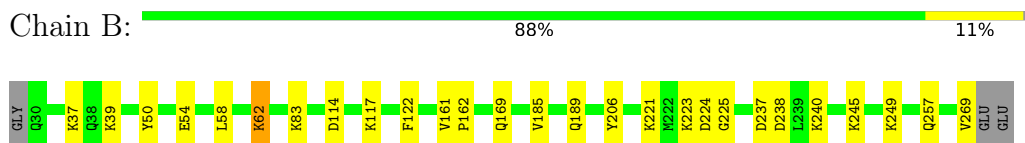
3 Residue-property plots

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.

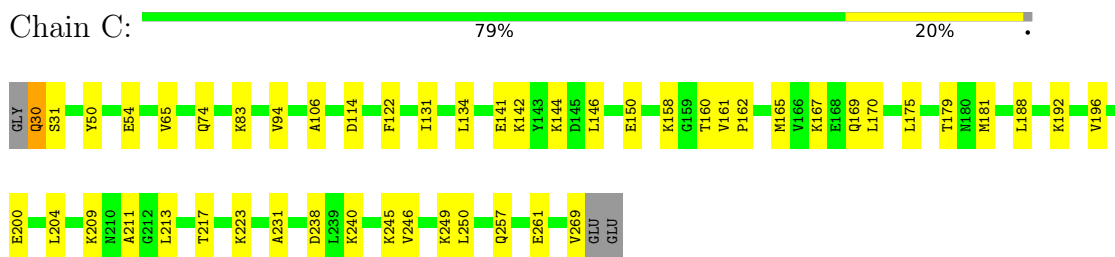
- Molecule 1: Amino acid ABC superfamily ATP binding cassette transporter, binding protein



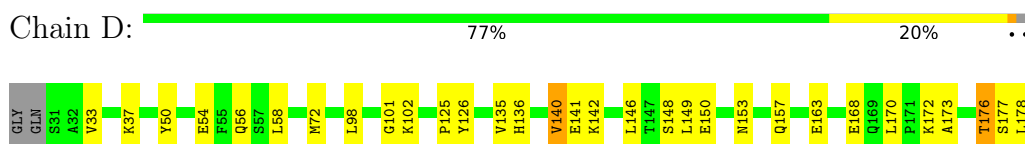
- Molecule 1: Amino acid ABC superfamily ATP binding cassette transporter, binding protein



- Molecule 1: Amino acid ABC superfamily ATP binding cassette transporter, binding protein



- Molecule 1: Amino acid ABC superfamily ATP binding cassette transporter, binding protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	99.37Å 61.70Å 103.63Å 90.00° 118.04° 90.00°	Depositor
Resolution (Å)	91.46 – 1.90 91.46 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.8 (91.46-1.90) 86.4 (91.46-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.164 , 0.200 0.162 , 0.180	Depositor DCC
R_{free} test set	4283 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.248 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8142	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.02% 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, SO4, EDO, ACT, PGE, CL, GOL

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	0.56	0/1887	0.81	0/2548
1	B	0.58	0/1847	0.82	1/2494 (0.0%)
1	C	0.51	0/1832	0.83	2/2475 (0.1%)
1	D	0.53	0/1823	0.84	1/2463 (0.0%)
All	All	0.54	0/7389	0.82	4/9980 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	ASP	N-CA-C	-5.72	104.68	111.03
1	C	94	VAL	N-CA-C	5.64	115.84	110.42
1	C	211	ALA	N-CA-C	-5.34	103.08	110.35
1	D	142	LYS	N-CA-C	-5.24	103.96	110.41

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	1855	0	1884	19	0
1	B	1824	0	1852	20	0
1	C	1812	0	1835	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1803	0	1827	27	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	1	0	0	0	0
4	A	56	0	71	3	0
4	B	28	0	36	6	0
4	C	35	0	41	2	0
4	D	14	0	16	2	0
5	A	18	0	24	0	0
5	C	12	0	16	3	0
5	D	6	0	8	0	0
6	A	10	0	14	1	0
6	B	20	0	28	0	0
6	C	10	0	14	2	0
7	A	12	0	12	0	0
7	B	12	0	12	0	0
7	C	12	0	12	0	0
7	D	12	0	12	0	0
8	B	16	0	12	0	0
8	C	8	0	6	0	0
8	D	4	0	3	0	0
9	B	4	0	6	1	0
10	A	171	0	0	8	0
10	B	151	0	0	5	0
10	C	118	0	0	6	0
10	D	93	0	0	3	0
All	All	8142	0	7741	101	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 7.

All (101) 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:189:GLN:HE22	4:B:306:PEG:H42	1.38	0.89
1:C:161:VAL:HG12	1:C:165:MET:HE2	1.65	0.78
1:B:114:ASP:HB2	9:B:303:EDO:H21	1.69	0.74
1:D:149:LEU:HD13	1:D:170:LEU:HD11	1.71	0.72
1:B:245:LYS:NZ	10:B:531:HOH:O	2.20	0.70
1:D:153:ASN:ND2	10:D:483:HOH:O	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HE2	4:B:305:PEG:H22	1.75	0.67
1:C:162:PRO:HA	1:C:165:MET:HE3	1.75	0.67
1:C:209:LYS:NZ	5:C:307:GOL:O1	2.27	0.66
1:C:131:ILE:HG21	1:C:165:MET:HE1	1.76	0.66
1:A:83:LYS:NZ	10:A:494:HOH:O	2.27	0.66
1:C:65:VAL:H	4:C:302:PEG:H11	1.62	0.64
1:C:245:LYS:NZ	10:C:500:HOH:O	2.25	0.62
1:B:83[B]:LYS:NZ	10:B:536:HOH:O	2.30	0.61
1:C:245:LYS:HE3	1:C:249:LYS:HE3	1.82	0.60
1:C:131:ILE:HD13	1:C:165:MET:HE1	1.85	0.59
1:C:142:LYS:NZ	10:C:492:HOH:O	2.35	0.59
4:C:303:PEG:H31	6:C:311:PGE:O2	2.04	0.58
1:B:169:GLN:NE2	1:B:221:LYS:O	2.35	0.58
1:D:56:GLN:NE2	10:D:442:HOH:O	2.26	0.58
1:D:249:LYS:HD3	4:D:302:PEG:H22	1.85	0.58
1:A:92:ASP:HB2	4:A:310:PEG:H32	1.85	0.57
1:C:74:GLN:HB3	6:C:311:PGE:H62	1.88	0.56
1:D:150:GLU:HA	1:D:173:ALA:HB2	1.87	0.56
1:D:58:LEU:HD13	1:D:269:VAL:HG21	1.88	0.56
1:D:178:LEU:HD13	1:D:183:GLU:HG3	1.88	0.56
1:C:188:LEU:HD22	1:C:196:VAL:HG23	1.88	0.55
1:C:30:GLN:NE2	10:C:433:HOH:O	2.36	0.54
1:A:192:LYS:HA	4:A:308:PEG:H31	1.89	0.54
1:A:58:LEU:HA	1:A:62:LYS:HA	1.90	0.53
1:A:209:LYS:HD3	10:A:525:HOH:O	2.07	0.53
1:C:150:GLU:HG2	1:C:170:LEU:HD22	1.91	0.53
1:C:158:LYS:HE2	5:C:308:GOL:H2	1.91	0.52
1:B:62:LYS:HE3	1:B:62:LYS:HA	1.92	0.51
1:C:200:GLU:O	1:C:204:LEU:HG	2.11	0.50
1:D:180:ASN:HD21	4:D:301:PEG:H11	1.76	0.50
1:A:204:LEU:HD23	1:A:215:VAL:HG21	1.94	0.50
10:A:471:HOH:O	1:C:30:GLN:HG3	2.12	0.49
1:A:130:LYS:NZ	10:A:530:HOH:O	2.45	0.49
1:B:223:LYS:HE3	1:C:179:THR:OG1	2.12	0.49
1:C:257:GLN:O	1:C:261:GLU:HG3	2.13	0.49
1:D:136:HIS:NE2	1:D:188:LEU:O	2.44	0.49
1:B:117:LYS:CE	4:B:305:PEG:H22	2.40	0.48
1:C:238:ASP:OD1	10:C:455:HOH:O	2.20	0.48
1:D:197:HIS:CE1	1:D:220:LEU:HD12	2.48	0.48
1:C:131:ILE:HG21	1:C:165:MET:CE	2.42	0.48
1:A:235:ASN:OD1	10:A:431:HOH:O	2.20	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:LEU:HD23	1:D:149:LEU:HD12	1.95	0.47
1:B:117:LYS:CE	4:B:305:PEG:H42	2.45	0.47
1:D:72:MET:HE1	1:D:126:TYR:CE2	2.49	0.47
1:D:177:SER:O	1:D:178:LEU:HD23	2.15	0.47
1:C:169:GLN:O	1:C:170:LEU:HD23	2.14	0.47
1:D:136:HIS:CE1	1:D:188:LEU:HG	2.49	0.47
1:B:237:ASP:HA	1:B:240:LYS:HB3	1.97	0.46
1:C:50:TYR:HE1	1:C:181:MET:HE3	1.79	0.46
1:A:71:ASP:OD2	10:A:555:HOH:O	2.20	0.46
1:D:135:VAL:HA	1:D:188:LEU:HD11	1.97	0.46
1:D:257:GLN:O	1:D:261:GLU:HG3	2.17	0.45
1:D:157:GLN:HB2	1:D:181:MET:HE2	1.99	0.45
1:C:141:GLU:HG2	1:C:144:LYS:NZ	2.32	0.44
1:C:167:LYS:HG3	1:C:175:LEU:CD2	2.48	0.44
1:B:83[A]:LYS:NZ	10:B:503:HOH:O	2.51	0.44
1:A:150:GLU:OE1	10:A:539:HOH:O	2.21	0.44
1:C:122:PHE:O	1:C:240:LYS:HE2	2.18	0.44
1:C:146:LEU:O	1:C:150:GLU:HG3	2.18	0.44
1:B:161:VAL:HB	1:B:162:PRO:HD3	2.00	0.43
1:D:140:VAL:HG13	1:D:216:ALA:HA	2.00	0.43
1:C:134:LEU:HD21	1:C:213:LEU:HD13	1.99	0.43
1:D:176:THR:HG21	1:D:193:ILE:HD11	2.00	0.43
1:D:227:ALA:HA	10:D:427:HOH:O	2.17	0.43
1:D:163:GLU:OE1	1:D:177:SER:OG	2.23	0.43
1:B:224:ASP:CG	1:B:225:GLY:HA2	2.45	0.42
1:C:83:LYS:HE3	10:C:423:HOH:O	2.18	0.42
1:B:185:VAL:HG21	1:B:206:TYR:CZ	2.55	0.42
1:C:246:VAL:O	1:C:250:LEU:HG	2.20	0.42
1:A:137:LYS:N	1:A:212[B]:GLY:O	2.39	0.42
1:A:99:GLN:HG3	10:A:455:HOH:O	2.19	0.42
1:D:33:VAL:O	1:D:37:LYS:HG3	2.19	0.42
1:B:122:PHE:O	1:B:240:LYS:HE2	2.20	0.42
1:A:72:MET:HE1	1:A:126:TYR:CE2	2.55	0.42
1:C:106:ALA:HB3	1:C:231:ALA:HB3	2.02	0.42
1:D:102:LYS:HA	1:D:102:LYS:HD2	1.88	0.42
1:D:187:GLU:O	1:D:193:ILE:N	2.50	0.41
1:D:125:PRO:HB3	1:D:227:ALA:HB3	2.01	0.41
6:A:315:PGE:H52	6:A:315:PGE:H32	1.82	0.41
1:B:39:LYS:NZ	10:B:488[B]:HOH:O	2.53	0.41
1:C:167:LYS:HG3	1:C:175:LEU:HD23	2.03	0.41
1:C:192:LYS:NZ	10:C:444:HOH:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LYS:HE3	1:D:101:GLY:O	2.20	0.41
1:A:146:LEU:HD11	1:A:220:LEU:HD23	2.03	0.41
1:A:165:MET:HE1	1:A:222[A]:MET:HG2	2.02	0.41
1:B:117:LYS:NZ	4:B:305:PEG:H42	2.36	0.41
1:C:160:THR:HB	1:C:162:PRO:HD2	2.03	0.41
1:A:223:LYS:HB2	1:A:223:LYS:HE2	1.77	0.40
1:A:254:GLY:HA3	1:B:257:GLN:HE21	1.86	0.40
1:C:114:ASP:OD2	1:C:223:LYS:HE2	2.22	0.40
1:D:172:LYS:HA	1:D:172:LYS:HD2	1.87	0.40
1:A:84:LEU:HD21	1:A:86:ILE:HD11	2.04	0.40
1:A:245:LYS:HA	4:A:311:PEG:H22	2.03	0.40
4:B:305:PEG:H41	10:B:523:HOH:O	2.21	0.40
1:C:158:LYS:CE	5:C:308:GOL:H2	2.51	0.40

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	247/243 (102%)	241 (98%)	6 (2%)	0	100	100
1	B	240/243 (99%)	231 (96%)	9 (4%)	0	100	100
1	C	238/243 (98%)	233 (98%)	5 (2%)	0	100	100
1	D	237/243 (98%)	225 (95%)	10 (4%)	2 (1%)	16	8
All	All	962/972 (99%)	930 (97%)	30 (3%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	211	ALA
1	D	212	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	204/199 (102%)	194 (95%)	10 (5%)	22	14
1	B	199/199 (100%)	193 (97%)	6 (3%)	36	30
1	C	197/199 (99%)	192 (98%)	5 (2%)	42	37
1	D	196/199 (98%)	183 (93%)	13 (7%)	15	8
All	All	796/796 (100%)	762 (96%)	34 (4%)	26	18

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	38	GLN
1	A	54	GLU
1	A	58	LEU
1	A	64	GLN
1	A	114	ASP
1	A	144	LYS
1	A	146	LEU
1	A	174	GLN
1	A	269	VAL
1	B	50	TYR
1	B	54	GLU
1	B	58	LEU
1	B	62	LYS
1	B	249	LYS
1	B	269	VAL
1	C	30	GLN
1	C	31	SER
1	C	54	GLU
1	C	217	THR
1	C	269	VAL
1	D	50	TYR
1	D	54	GLU
1	D	98	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	140	VAL
1	D	141	GLU
1	D	148	SER
1	D	168	GLU
1	D	176	THR
1	D	193	ILE
1	D	210	ASN
1	D	224	ASP
1	D	232	LEU
1	D	236	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	257	GLN
1	B	38	GLN
1	B	189	GLN
1	B	228	ASN
1	B	257	GLN
1	C	189	GLN
1	C	228	ASN
1	D	38	GLN
1	D	180	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 47 ligands modelled in this entry, 1 is monoatomic - leaving 46 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
5	GOL	A	312	-	5,5,5	0.38	0	5,5,5	0.30	0
2	SO4	B	301	-	4,4,4	0.25	0	6,6,6	0.13	0
2	SO4	C	301	-	4,4,4	0.20	0	6,6,6	0.20	0
8	ACT	B	302	-	3,3,3	0.81	0	3,3,3	1.51	0
4	PEG	A	310	-	6,6,6	1.06	0	5,5,5	1.52	0
7	ARG	A	317	-	10,11,11	0.83	1 (10%)	9,13,13	1.03	1 (11%)
4	PEG	A	307	-	6,6,6	1.14	0	5,5,5	2.57	2 (40%)
8	ACT	B	309	-	3,3,3	0.84	0	3,3,3	1.36	0
4	PEG	B	307	-	6,6,6	0.98	0	5,5,5	1.98	2 (40%)
8	ACT	B	308	-	3,3,3	0.84	0	3,3,3	1.28	0
5	GOL	C	308	-	5,5,5	0.43	0	5,5,5	0.50	0
4	PEG	D	302	-	6,6,6	1.19	0	5,5,5	1.25	0
5	GOL	A	314	-	5,5,5	0.35	0	5,5,5	0.39	0
4	PEG	A	308	-	6,6,6	0.99	0	5,5,5	2.73	3 (60%)
4	PEG	B	304	-	6,6,6	1.01	0	5,5,5	1.97	2 (40%)
4	PEG	C	304	-	6,6,6	1.05	0	5,5,5	2.02	2 (40%)
8	ACT	C	310	-	3,3,3	0.84	0	3,3,3	1.41	0
9	EDO	B	303	-	3,3,3	0.39	0	2,2,2	0.50	0
4	PEG	C	306	-	6,6,6	1.08	0	5,5,5	1.76	1 (20%)
4	PEG	A	309	-	6,6,6	1.10	0	5,5,5	1.46	0
5	GOL	D	303	-	5,5,5	0.44	0	5,5,5	0.24	0
4	PEG	B	305	-	6,6,6	0.98	0	5,5,5	2.04	2 (40%)
4	PEG	B	306	-	6,6,6	1.15	0	5,5,5	1.41	0
7	ARG	C	312	-	10,11,11	0.77	1 (10%)	9,13,13	1.03	1 (11%)
7	ARG	D	305	-	10,11,11	0.80	1 (10%)	9,13,13	0.96	1 (11%)
5	GOL	C	307	-	5,5,5	0.36	0	5,5,5	0.38	0
6	PGE	C	311	-	9,9,9	0.66	0	8,8,8	0.37	0
8	ACT	D	304	-	3,3,3	0.84	0	3,3,3	1.34	0
7	ARG	B	313	-	10,11,11	0.87	1 (10%)	9,13,13	0.93	1 (11%)
2	SO4	A	301	-	4,4,4	0.23	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	313	-	5,5,5	0.30	0	5,5,5	0.43	0
4	PEG	D	301	-	6,6,6	1.19	0	5,5,5	1.55	2 (40%)
8	ACT	B	310	-	3,3,3	0.76	0	3,3,3	1.39	0
8	ACT	C	309	-	3,3,3	0.81	0	3,3,3	1.41	0
6	PGE	B	312	-	9,9,9	0.70	0	8,8,8	0.51	0
2	SO4	A	303	-	4,4,4	0.25	0	6,6,6	0.24	0
4	PEG	A	305	-	6,6,6	1.00	0	5,5,5	1.90	1 (20%)
4	PEG	A	306	-	6,6,6	1.01	0	5,5,5	1.86	2 (40%)
6	PGE	A	315	-	9,9,9	0.42	0	8,8,8	0.53	0
4	PEG	A	316	-	6,6,6	1.06	0	5,5,5	1.74	2 (40%)
2	SO4	A	302	-	4,4,4	0.25	0	6,6,6	0.28	0
6	PGE	B	311	-	9,9,9	0.58	0	8,8,8	0.62	0
4	PEG	A	311	-	6,6,6	1.11	0	5,5,5	2.66	3 (60%)
4	PEG	C	305	-	6,6,6	1.08	0	5,5,5	1.84	2 (40%)
4	PEG	C	303	-	6,6,6	1.06	0	5,5,5	1.87	2 (40%)
4	PEG	C	302	-	6,6,6	1.03	0	5,5,5	1.54	1 (20%)

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
5	GOL	A	312	-	-	2/4/4/4	-
4	PEG	A	310	-	-	1/4/4/4	-
7	ARG	A	317	-	-	0/11/11/11	-
4	PEG	A	307	-	-	2/4/4/4	-
4	PEG	B	307	-	-	1/4/4/4	-
5	GOL	C	308	-	-	2/4/4/4	-
4	PEG	D	302	-	-	0/4/4/4	-
5	GOL	A	314	-	-	3/4/4/4	-
4	PEG	A	308	-	-	0/4/4/4	-
4	PEG	B	304	-	-	1/4/4/4	-
4	PEG	C	304	-	-	2/4/4/4	-
9	EDO	B	303	-	-	1/1/1/1	-
4	PEG	C	306	-	-	1/4/4/4	-
4	PEG	A	309	-	-	1/4/4/4	-
5	GOL	D	303	-	-	2/4/4/4	-
4	PEG	B	305	-	-	1/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	306	-	-	2/4/4/4	-
7	ARG	C	312	-	-	0/11/11/11	-
7	ARG	D	305	-	-	0/11/11/11	-
5	GOL	C	307	-	-	0/4/4/4	-
6	PGE	C	311	-	-	3/7/7/7	-
7	ARG	B	313	-	-	0/11/11/11	-
5	GOL	A	313	-	-	2/4/4/4	-
4	PEG	D	301	-	-	0/4/4/4	-
6	PGE	B	312	-	-	2/7/7/7	-
4	PEG	A	305	-	-	2/4/4/4	-
4	PEG	A	306	-	-	2/4/4/4	-
6	PGE	A	315	-	-	3/7/7/7	-
4	PEG	A	316	-	-	2/4/4/4	-
6	PGE	B	311	-	-	2/7/7/7	-
4	PEG	A	311	-	-	2/4/4/4	-
4	PEG	C	305	-	-	1/4/4/4	-
4	PEG	C	303	-	-	2/4/4/4	-
4	PEG	C	302	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	317	ARG	OXT-C	-2.36	1.23	1.30
7	B	313	ARG	OXT-C	-2.35	1.23	1.30
7	D	305	ARG	OXT-C	-2.31	1.23	1.30
7	C	312	ARG	OXT-C	-2.19	1.23	1.30

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	311	PEG	O2-C2-C1	4.55	130.14	110.11
4	A	308	PEG	O2-C2-C1	3.68	126.31	110.11
4	A	308	PEG	O2-C3-C4	3.57	125.86	110.11
4	A	307	PEG	O2-C2-C1	3.52	125.61	110.11
4	A	307	PEG	O2-C3-C4	3.26	124.48	110.11
4	A	305	PEG	O2-C2-C1	3.05	123.55	110.11
4	C	306	PEG	O2-C2-C1	3.00	123.32	110.11
7	C	312	ARG	OXT-C-O	-2.98	117.31	124.08
4	A	308	PEG	C3-O2-C2	-2.94	100.37	113.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	317	ARG	OXT-C-O	-2.94	117.41	124.08
4	B	304	PEG	O2-C3-C4	2.90	122.91	110.11
4	C	303	PEG	O2-C2-C1	2.81	122.48	110.11
4	B	305	PEG	O2-C2-C1	2.79	122.43	110.11
4	B	305	PEG	O2-C3-C4	2.77	122.33	110.11
4	C	305	PEG	O2-C2-C1	2.69	121.98	110.11
7	D	305	ARG	OXT-C-O	-2.68	117.99	124.08
4	A	311	PEG	O1-C1-C2	2.68	127.60	111.82
4	C	304	PEG	O2-C3-C4	2.66	121.85	110.11
4	B	307	PEG	O2-C2-C1	2.62	121.65	110.11
4	B	307	PEG	O2-C3-C4	2.62	121.64	110.11
4	C	304	PEG	O2-C2-C1	2.61	121.61	110.11
4	A	306	PEG	O2-C2-C1	2.57	121.44	110.11
7	B	313	ARG	OXT-C-O	-2.53	118.35	124.08
4	A	311	PEG	O2-C3-C4	2.49	121.07	110.11
4	C	305	PEG	O2-C3-C4	2.47	120.99	110.11
4	B	304	PEG	O2-C2-C1	2.39	120.64	110.11
4	A	306	PEG	O2-C3-C4	2.38	120.61	110.11
4	A	316	PEG	O2-C3-C4	2.37	120.58	110.11
4	C	303	PEG	O2-C3-C4	2.36	120.52	110.11
4	C	302	PEG	O2-C2-C1	2.20	119.82	110.11
4	D	301	PEG	O1-C1-C2	2.17	124.61	111.82
4	A	316	PEG	O2-C2-C1	2.13	119.51	110.11
4	D	301	PEG	C3-O2-C2	2.07	122.32	113.26

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	312	GOL	O1-C1-C2-C3
5	A	313	GOL	O1-C1-C2-O2
5	A	314	GOL	O1-C1-C2-C3
5	C	308	GOL	C1-C2-C3-O3
5	D	303	GOL	O1-C1-C2-O2
5	D	303	GOL	O1-C1-C2-C3
4	A	305	PEG	C4-C3-O2-C2
4	A	306	PEG	C4-C3-O2-C2
4	A	311	PEG	C1-C2-O2-C3
4	B	304	PEG	C4-C3-O2-C2
4	B	305	PEG	C4-C3-O2-C2
4	B	307	PEG	C1-C2-O2-C3
4	C	303	PEG	C1-C2-O2-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	305	PEG	C1-C2-O2-C3
4	C	306	PEG	C1-C2-O2-C3
6	B	312	PGE	C3-C4-O3-C5
4	A	305	PEG	O1-C1-C2-O2
4	A	306	PEG	O1-C1-C2-O2
4	A	307	PEG	O1-C1-C2-O2
4	A	309	PEG	O1-C1-C2-O2
4	A	310	PEG	O1-C1-C2-O2
4	A	316	PEG	O1-C1-C2-O2
4	A	316	PEG	O2-C3-C4-O4
4	B	306	PEG	O1-C1-C2-O2
4	B	306	PEG	O2-C3-C4-O4
4	C	302	PEG	O2-C3-C4-O4
4	C	303	PEG	O2-C3-C4-O4
4	C	304	PEG	O1-C1-C2-O2
4	C	304	PEG	O2-C3-C4-O4
4	A	311	PEG	O1-C1-C2-O2
4	A	307	PEG	O2-C3-C4-O4
5	A	313	GOL	O1-C1-C2-C3
5	A	312	GOL	O1-C1-C2-O2
5	A	314	GOL	O1-C1-C2-O2
5	C	308	GOL	O2-C2-C3-O3
6	C	311	PGE	C3-C4-O3-C5
5	A	314	GOL	O2-C2-C3-O3
6	B	311	PGE	C3-C4-O3-C5
6	C	311	PGE	C4-C3-O2-C2
6	A	315	PGE	C4-C3-O2-C2
6	A	315	PGE	C3-C4-O3-C5
9	B	303	EDO	O1-C1-C2-O2
6	B	312	PGE	C4-C3-O2-C2
6	B	311	PGE	O2-C3-C4-O3
6	A	315	PGE	O2-C3-C4-O3
6	C	311	PGE	O2-C3-C4-O3

There are no ring outliers.

14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	310	PEG	1	0
5	C	308	GOL	2	0
4	D	302	PEG	1	0
4	A	308	PEG	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	303	EDO	1	0
4	B	305	PEG	5	0
4	B	306	PEG	1	0
5	C	307	GOL	1	0
6	C	311	PGE	2	0
4	D	301	PEG	1	0
6	A	315	PGE	1	0
4	A	311	PEG	1	0
4	C	303	PEG	1	0
4	C	302	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	240/243 (98%)	-1.43	0 100 100	12, 23, 59, 89	9 (3%)
1	B	240/243 (98%)	-1.41	0 100 100	11, 25, 63, 102	2 (0%)
1	C	240/243 (98%)	-1.20	0 100 100	19, 33, 78, 93	0
1	D	239/243 (98%)	-1.08	0 100 100	19, 36, 90, 118	0
All	All	959/972 (98%)	-1.28	0 100 100	11, 28, 76, 118	11 (1%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
8	ACT	D	304	4/4	0.93	0.08	81,81,82,84	0
5	GOL	C	307	6/6	0.95	0.06	66,70,75,78	0
8	ACT	B	309	4/4	0.96	0.07	70,71,72,74	0
8	ACT	B	310	4/4	0.96	0.07	63,66,67,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ACT	C	310	4/4	0.96	0.06	60,61,62,62	0
4	PEG	C	303	7/7	0.96	0.10	65,72,78,78	0
8	ACT	B	308	4/4	0.97	0.07	67,68,69,70	0
5	GOL	A	313	6/6	0.98	0.04	61,63,66,66	0
5	GOL	A	314	6/6	0.98	0.05	47,53,55,57	0
4	PEG	B	305	7/7	0.98	0.04	39,41,44,45	0
4	PEG	C	302	7/7	0.98	0.05	43,47,51,51	0
4	PEG	A	306	7/7	0.98	0.05	47,48,50,50	0
4	PEG	C	304	7/7	0.98	0.06	51,53,55,56	0
8	ACT	C	309	4/4	0.98	0.04	51,53,53,53	0
4	PEG	C	305	7/7	0.98	0.05	45,46,48,52	0
4	PEG	D	302	7/7	0.98	0.07	56,61,70,73	0
4	PEG	A	305	7/7	0.99	0.04	30,33,39,44	0
2	SO4	A	301	5/5	0.99	0.04	41,42,44,44	0
4	PEG	A	307	7/7	0.99	0.04	39,41,45,46	0
4	PEG	C	306	7/7	0.99	0.04	51,55,63,63	0
4	PEG	D	301	7/7	0.99	0.05	45,48,55,59	0
4	PEG	A	308	7/7	0.99	0.06	47,54,56,57	0
5	GOL	A	312	6/6	0.99	0.04	44,47,50,50	0
4	PEG	A	309	7/7	0.99	0.03	36,39,51,55	0
4	PEG	A	310	7/7	0.99	0.05	47,55,59,59	0
4	PEG	A	311	7/7	0.99	0.05	43,50,53,56	0
5	GOL	C	308	6/6	0.99	0.04	30,48,50,52	0
5	GOL	D	303	6/6	0.99	0.05	52,54,57,60	0
6	PGE	A	315	10/10	0.99	0.05	45,51,53,54	0
6	PGE	B	311	10/10	0.99	0.04	38,47,51,52	0
6	PGE	B	312	10/10	0.99	0.05	32,47,59,59	0
6	PGE	C	311	10/10	0.99	0.05	46,52,60,61	0
7	ARG	C	312	12/12	0.99	0.03	19,22,29,30	0
7	ARG	D	305	12/12	0.99	0.02	21,25,29,31	0
8	ACT	B	302	4/4	0.99	0.04	39,41,43,44	0
4	PEG	A	316	7/7	0.99	0.05	54,62,62,62	0
4	PEG	B	304	7/7	0.99	0.04	39,42,51,51	0
2	SO4	A	302	5/5	0.99	0.04	65,70,71,71	0
4	PEG	B	306	7/7	0.99	0.04	45,46,48,48	0
4	PEG	B	307	7/7	0.99	0.04	44,49,52,55	0
2	SO4	C	301	5/5	0.99	0.03	43,47,49,52	0
9	EDO	B	303	4/4	0.99	0.05	39,39,40,46	0
3	CL	A	304	1/1	1.00	0.05	40,40,40,40	0
2	SO4	B	301	5/5	1.00	0.03	38,41,46,47	0
2	SO4	A	303	5/5	1.00	0.02	43,48,52,53	0
7	ARG	A	317	12/12	1.00	0.02	16,16,18,19	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	ARG	B	313	12/12	1.00	0.02	16,17,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.