Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 06:27 AM EDT

PDB ID	:	4H5F
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 (i) 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 (i)) were used in the production of this report:

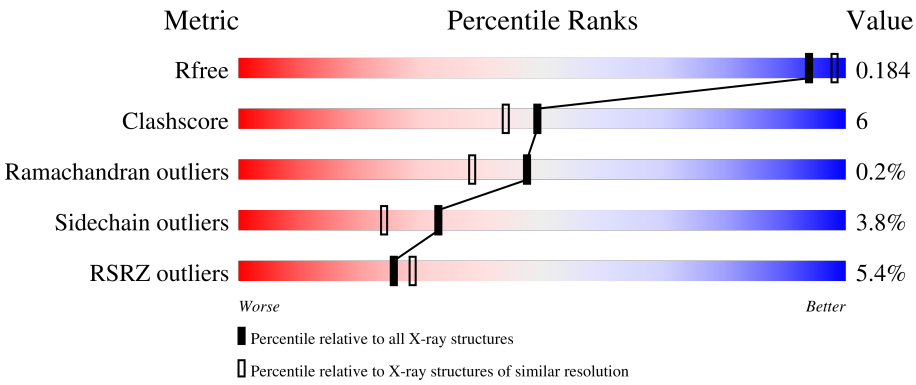
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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	87% 11%
1	B	243	2% 91% 8%
1	C	243	7% 80% 19%
1	D	243	11% 80% 18%

Validation Pipeline (wwPDB-VP) : 2.35.1

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 (i)

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.

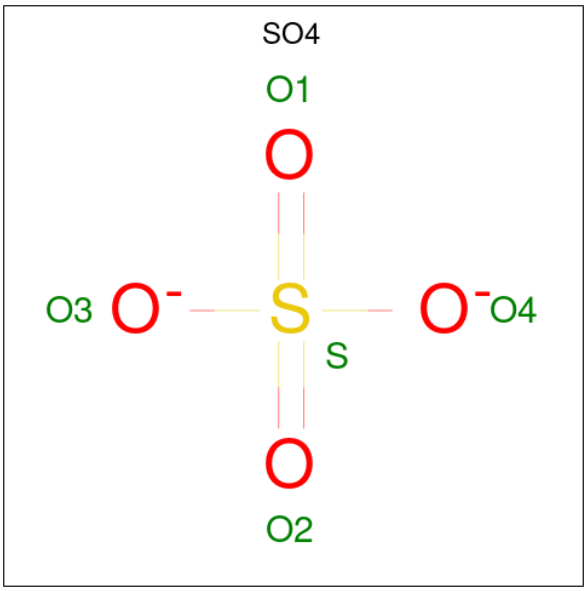
- Molecule 1 is a protein called Amino acid ABC superfamily ATP binding cassette transporter, binding protein.

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

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 (three-letter code: SO4) (formula: O_4S).

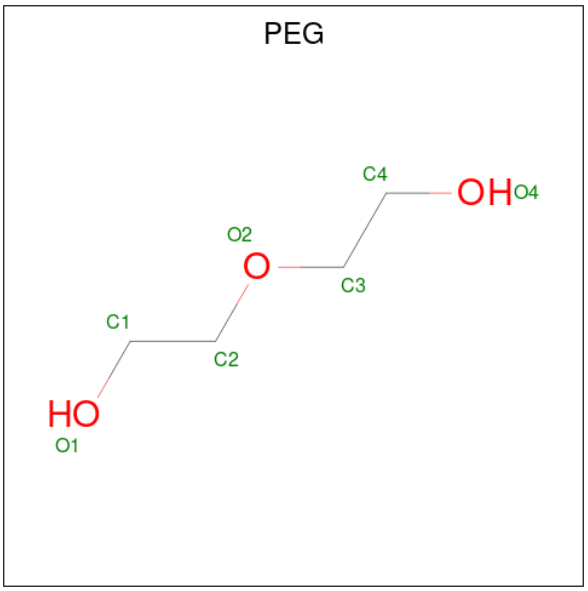


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

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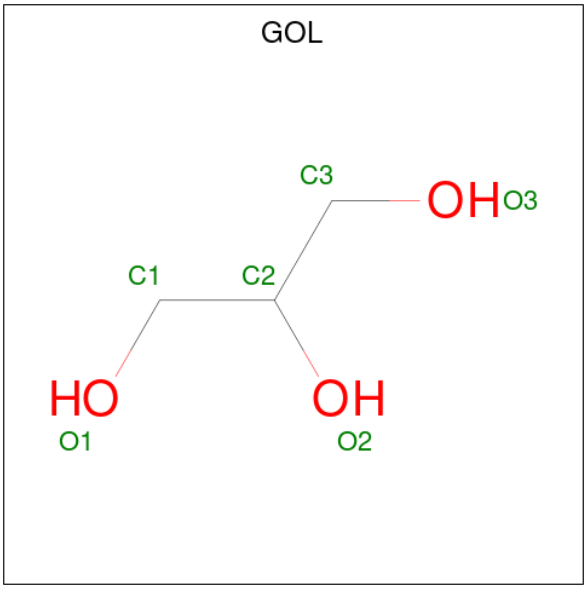
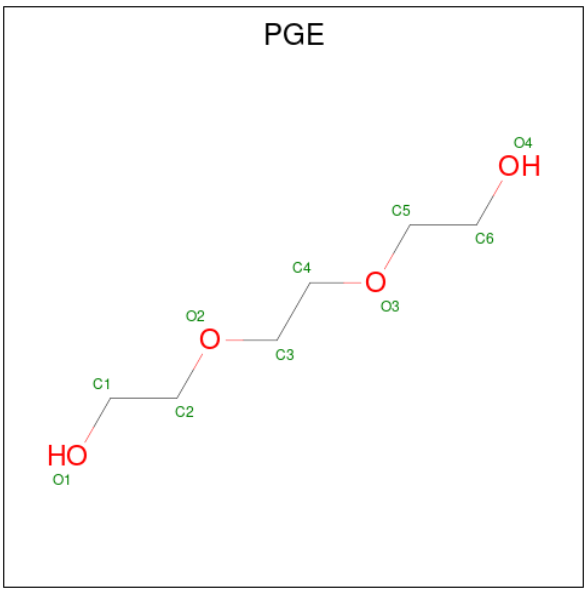
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
4	C	1	7	4	3		0	0
			Total	C	O			
4	C	1	7	4	3		0	0
			Total	C	O			
4	C	1	7	4	3		0	0
			Total	C	O			
4	D	1	7	4	3		0	0
			Total	C	O			
4	D	1	7	4	3		0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



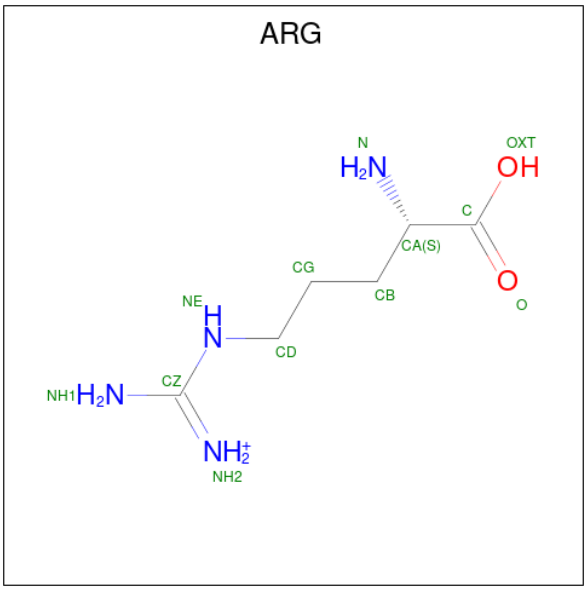
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	6	3	3		0	0
			Total	C	O			
5	A	1	6	3	3		0	0
			Total	C	O			
5	A	1	6	3	3		0	0
			Total	C	O			
5	C	1	6	3	3		0	0
			Total	C	O			
5	C	1	6	3	3		0	0
			Total	C	O			
5	D	1	6	3	3		0	0

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



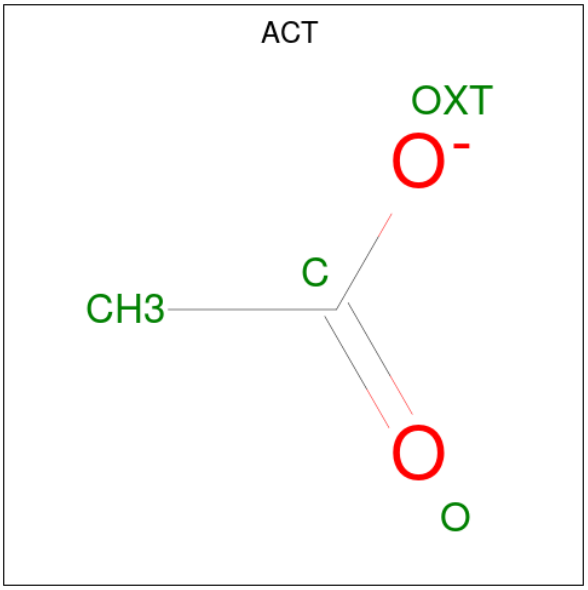
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O		0	0
			10	6	4			
6	B	1	Total	C	O		0	0
			10	6	4			
6	B	1	Total	C	O		0	0
			10	6	4			
6	C	1	Total	C	O		0	0
			10	6	4			

- Molecule 7 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



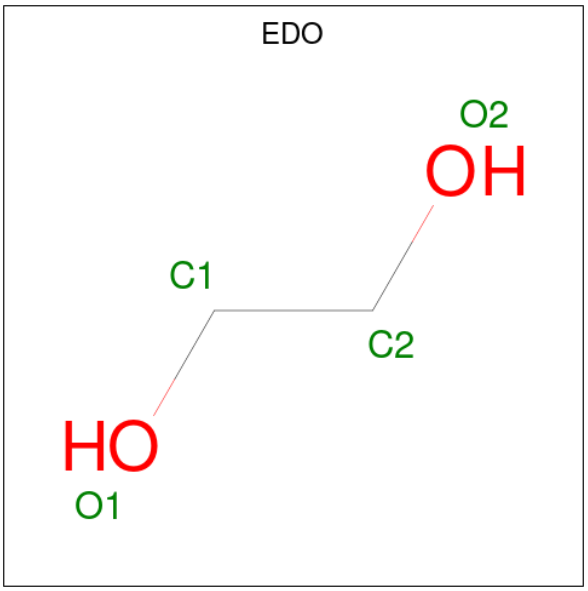
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
7	A	1	12	6	4	2	0	0
7	B	1	12	6	4	2	0	0
7	C	1	12	6	4	2	0	0
7	D	1	12	6	4	2	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 10 is water.

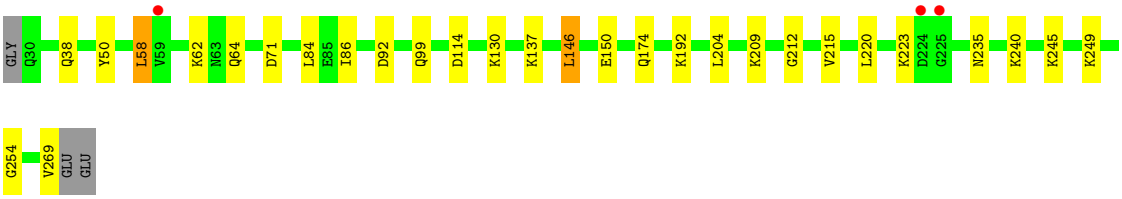
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	157	171	171	0	14
			Total	O		
10	B	138	151	151	0	13
			Total	O		
10	C	114	118	118	0	4
			Total	O		
10	D	89	93	93	0	5

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.

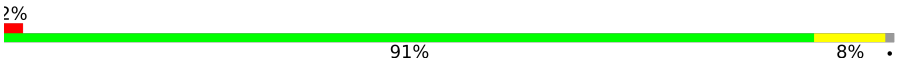
• Molecule 1: Amino acid ABC superfamily ATP binding cassette transporter, binding protein

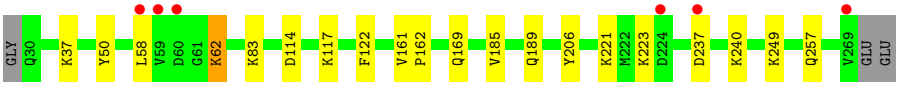
Chain A:



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

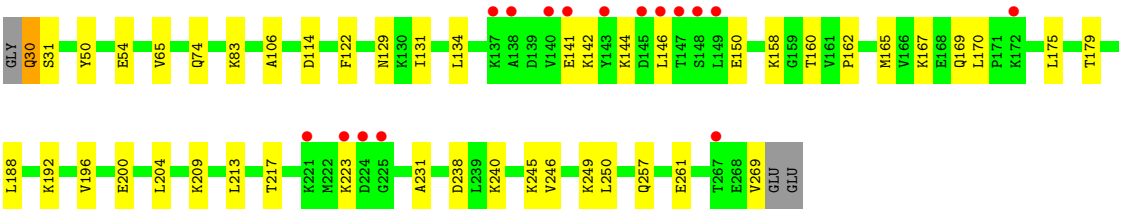
Chain B:





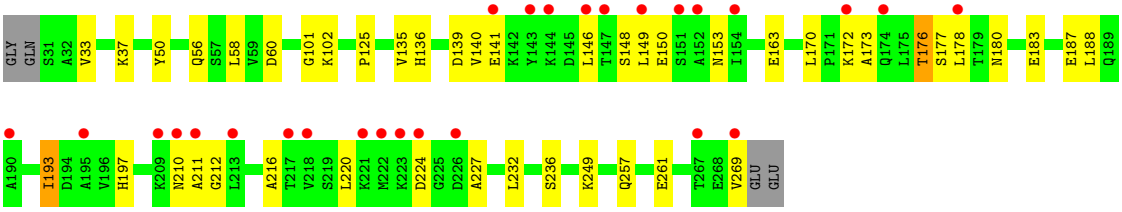
• Molecule 1: Amino acid ABC superfamily ATP binding cassette transporter, binding protein

Chain C:



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

Chain D:


GLY
GLN
S31
A32
V33
K37
Y50
Q56
S57
L58
V59
D60
G101
K102
P125
V135
H136
D139
V140
E141
K142
Y143
K144
D145
L146
T147
S148
L149
E150
S151
A152
N153
I154
E163
L170
P171
K172
A173
Q174
L175
T176
S177
L178
T179
N180
E183
E187
L188
Q189
A190
I193
D194
A195
V196
H197
K209
N210
A211
G212
L213
A216
T217
V218
S219
L220
K221
M222
K223
D224
G225
D226
A227
L232
S236
K249
Q257
E261
T267
E268
V269
GLU
GLU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 0.184	Depositor DCC
R_{free} test set	4107 reflections (5.00%)	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 , 67.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.248 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.96	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, EDO, PGE, GOL, PEG, ACT, 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	0.43	0/1887	0.55	0/2548
1	B	0.44	0/1847	0.55	0/2494
1	C	0.39	0/1832	0.53	0/2475
1	D	0.40	0/1823	0.56	0/2463
All	All	0.41	0/7389	0.55	0/9980

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 (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	18	0
1	B	1824	0	1852	16	0
1	C	1812	0	1835	32	0
1	D	1803	0	1827	25	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	9	0
10	B	151	0	0	2	0
10	C	118	0	0	6	0
10	D	93	0	0	3	0
All	All	8142	0	7741	91	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 (91) 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:131:ILE:HG21	1:C:165:MET:HE3	1.53	0.89
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:C:245:LYS:NZ	10:C:500:HOH:O	2.25	0.69
1:D:153:ASN:ND2	10:D:483:HOH:O	2.26	0.68
1:B:117:LYS:HE2	4:B:305:PEG:H22	1.75	0.67
1:C:209:LYS:NZ	5:C:307:GOL:O1	2.27	0.66
1:C:65:VAL:H	4:C:302:PEG:H11	1.62	0.64
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:142:LYS:NZ	10:C:492:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ILE:HD13	1:C:165:MET:HE1	1.86	0.58
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:A:249:LYS:NZ	10:A:478:HOH:O	2.36	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:A:240:LYS:NZ	10:A:503:HOH:O	2.41	0.53
1:C:158:LYS:HE2	5:C:308:GOL:H2	1.91	0.52
1:C:162:PRO:HA	1:C:165:MET:HE2	1.92	0.51
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: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:A:235:ASN:OD1	10:A:431:HOH:O	2.20	0.47
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: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:A:130:LYS:NZ	10:A:530:HOH:O	2.45	0.46
1:B:237:ASP:HA	1:B:240:LYS:HB3	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:GLN:O	1:D:261:GLU:HG3	2.17	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: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: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: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: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
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: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%)	19	9
All	All	962/972 (99%)	930 (97%)	30 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	211	ALA
1	D	212	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/199 (102%)	196 (96%)	8 (4%)	32	23
1	B	199/199 (100%)	195 (98%)	4 (2%)	55	51
1	C	197/199 (99%)	190 (96%)	7 (4%)	35	26
1	D	196/199 (98%)	185 (94%)	11 (6%)	21	11
All	All	796/796 (100%)	766 (96%)	30 (4%)	33	24

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	50	TYR
1	A	58	LEU
1	A	64	GLN
1	A	114	ASP
1	A	146	LEU
1	A	174	GLN
1	A	269	VAL
1	B	50	TYR
1	B	58	LEU
1	B	62	LYS
1	B	249	LYS
1	C	30	GLN
1	C	31	SER
1	C	50	TYR
1	C	54	GLU
1	C	129	ASN
1	C	217	THR
1	C	269	VAL
1	D	50	TYR
1	D	60	ASP
1	D	139	ASP
1	D	141	GLU
1	D	148	SER
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	257	GLN
1	B	189	GLN
1	B	257	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
6	PGE	A	315	-	9,9,9	0.41	0	8,8,8	0.54	0
7	ARG	C	312	-	10,11,11	0.74	1 (10%)	11,13,13	1.07	1 (9%)
4	PEG	C	303	-	6,6,6	1.05	0	5,5,5	1.88	2 (40%)
8	ACT	B	308	-	3,3,3	0.79	0	3,3,3	1.29	0
4	PEG	C	305	-	6,6,6	1.06	0	5,5,5	1.86	2 (40%)
7	ARG	B	313	-	10,11,11	0.84	1 (10%)	11,13,13	0.99	1 (9%)
5	GOL	C	308	-	5,5,5	0.42	0	5,5,5	0.46	0
7	ARG	D	305	-	10,11,11	0.78	1 (10%)	11,13,13	1.06	2 (18%)
7	ARG	A	317	-	10,11,11	0.81	1 (10%)	11,13,13	1.22	2 (18%)
8	ACT	B	309	-	3,3,3	0.79	0	3,3,3	1.37	0
4	PEG	B	304	-	6,6,6	1.00	0	5,5,5	1.99	2 (40%)
9	EDO	B	303	-	3,3,3	0.42	0	2,2,2	0.46	0
8	ACT	B	302	-	3,3,3	0.76	0	3,3,3	1.52	0
2	SO4	A	301	-	4,4,4	0.15	0	6,6,6	0.28	0
4	PEG	A	311	-	6,6,6	1.09	0	5,5,5	2.68	3 (60%)
4	PEG	A	306	-	6,6,6	0.99	0	5,5,5	1.88	2 (40%)
5	GOL	A	312	-	5,5,5	0.37	0	5,5,5	0.28	0
2	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.16	0
4	PEG	A	308	-	6,6,6	0.97	0	5,5,5	2.75	3 (60%)
5	GOL	A	313	-	5,5,5	0.29	0	5,5,5	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	PEG	C	306	-	6,6,6	1.07	0	5,5,5	1.78	1 (20%)
4	PEG	B	306	-	6,6,6	1.14	0	5,5,5	1.42	0
6	PGE	B	312	-	9,9,9	0.70	0	8,8,8	0.51	0
8	ACT	C	310	-	3,3,3	0.79	0	3,3,3	1.42	0
4	PEG	A	305	-	6,6,6	0.99	0	5,5,5	1.92	1 (20%)
4	PEG	B	307	-	6,6,6	0.96	0	5,5,5	2.00	2 (40%)
4	PEG	B	305	-	6,6,6	0.96	0	5,5,5	2.05	2 (40%)
4	PEG	A	310	-	6,6,6	1.04	0	5,5,5	1.54	0
4	PEG	C	302	-	6,6,6	1.01	0	5,5,5	1.56	1 (20%)
5	GOL	C	307	-	5,5,5	0.36	0	5,5,5	0.34	0
4	PEG	A	307	-	6,6,6	1.12	0	5,5,5	2.60	3 (60%)
4	PEG	A	316	-	6,6,6	1.05	0	5,5,5	1.76	2 (40%)
8	ACT	B	310	-	3,3,3	0.72	0	3,3,3	1.39	0
6	PGE	B	311	-	9,9,9	0.57	0	8,8,8	0.63	0
2	SO4	A	302	-	4,4,4	0.16	0	6,6,6	0.25	0
2	SO4	C	301	-	4,4,4	0.13	0	6,6,6	0.18	0
4	PEG	D	301	-	6,6,6	1.17	0	5,5,5	1.57	2 (40%)
6	PGE	C	311	-	9,9,9	0.65	0	8,8,8	0.37	0
5	GOL	A	314	-	5,5,5	0.34	0	5,5,5	0.35	0
4	PEG	C	304	-	6,6,6	1.04	0	5,5,5	2.04	2 (40%)
5	GOL	D	303	-	5,5,5	0.43	0	5,5,5	0.21	0
4	PEG	D	302	-	6,6,6	1.17	0	5,5,5	1.26	0
8	ACT	C	309	-	3,3,3	0.77	0	3,3,3	1.41	0
4	PEG	A	309	-	6,6,6	1.09	0	5,5,5	1.48	0
2	SO4	A	303	-	4,4,4	0.16	0	6,6,6	0.27	0
8	ACT	D	304	-	3,3,3	0.79	0	3,3,3	1.34	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
6	PGE	A	315	-	-	3/7/7/7	-
4	PEG	C	303	-	-	2/4/4/4	-
4	PEG	C	305	-	-	1/4/4/4	-
7	ARG	B	313	-	-	0/11/11/11	-
5	GOL	C	308	-	-	2/4/4/4	-
7	ARG	D	305	-	-	0/11/11/11	-
7	ARG	A	317	-	-	0/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	304	-	-	1/4/4/4	-
9	EDO	B	303	-	-	1/1/1/1	-
4	PEG	A	311	-	-	2/4/4/4	-
4	PEG	A	306	-	-	2/4/4/4	-
5	GOL	A	312	-	-	2/4/4/4	-
4	PEG	A	308	-	-	0/4/4/4	-
5	GOL	A	313	-	-	2/4/4/4	-
4	PEG	C	306	-	-	1/4/4/4	-
4	PEG	B	306	-	-	2/4/4/4	-
6	PGE	B	312	-	-	2/7/7/7	-
4	PEG	A	305	-	-	2/4/4/4	-
4	PEG	B	307	-	-	1/4/4/4	-
4	PEG	B	305	-	-	1/4/4/4	-
4	PEG	A	310	-	-	1/4/4/4	-
4	PEG	C	302	-	-	1/4/4/4	-
5	GOL	C	307	-	-	0/4/4/4	-
4	PEG	A	307	-	-	2/4/4/4	-
4	PEG	A	316	-	-	2/4/4/4	-
6	PGE	B	311	-	-	2/7/7/7	-
4	PEG	D	301	-	-	0/4/4/4	-
6	PGE	C	311	-	-	3/7/7/7	-
5	GOL	A	314	-	-	4/4/4/4	-
4	PEG	C	304	-	-	2/4/4/4	-
5	GOL	D	303	-	-	2/4/4/4	-
4	PEG	D	302	-	-	0/4/4/4	-
4	PEG	A	309	-	-	1/4/4/4	-
7	ARG	C	312	-	-	0/11/11/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	317	ARG	OXT-C	-2.27	1.23	1.30
7	B	313	ARG	OXT-C	-2.25	1.23	1.30
7	D	305	ARG	OXT-C	-2.21	1.23	1.30
7	C	312	ARG	OXT-C	-2.10	1.23	1.30

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	311	PEG	O2-C2-C1	4.57	130.14	110.07
4	A	308	PEG	O2-C2-C1	3.70	126.31	110.07
4	A	308	PEG	O2-C3-C4	3.59	125.86	110.07
4	A	307	PEG	O2-C2-C1	3.54	125.61	110.07
4	A	307	PEG	O2-C3-C4	3.28	124.48	110.07
4	A	305	PEG	O2-C2-C1	3.07	123.55	110.07
4	C	306	PEG	O2-C2-C1	3.02	123.32	110.07
7	C	312	ARG	OXT-C-O	-2.98	117.31	124.09
4	A	308	PEG	C3-O2-C2	-2.98	100.37	113.29
7	A	317	ARG	OXT-C-O	-2.94	117.41	124.09
4	B	304	PEG	O2-C3-C4	2.92	122.91	110.07
4	C	303	PEG	O2-C2-C1	2.83	122.48	110.07
4	B	305	PEG	O2-C2-C1	2.81	122.43	110.07
4	B	305	PEG	O2-C3-C4	2.79	122.33	110.07
4	A	311	PEG	O1-C1-C2	2.72	127.60	111.81
4	C	305	PEG	O2-C2-C1	2.71	121.98	110.07
7	D	305	ARG	OXT-C-O	-2.68	117.99	124.09
4	C	304	PEG	O2-C3-C4	2.68	121.85	110.07
4	B	307	PEG	O2-C2-C1	2.64	121.65	110.07
4	B	307	PEG	O2-C3-C4	2.63	121.64	110.07
4	C	304	PEG	O2-C2-C1	2.63	121.61	110.07
4	A	306	PEG	O2-C2-C1	2.59	121.44	110.07
7	A	317	ARG	OXT-C-CA	2.57	122.14	113.38
7	B	313	ARG	OXT-C-O	-2.53	118.35	124.09
4	A	311	PEG	O2-C3-C4	2.50	121.07	110.07
4	C	305	PEG	O2-C3-C4	2.49	120.99	110.07
4	B	304	PEG	O2-C2-C1	2.41	120.64	110.07
4	A	306	PEG	O2-C3-C4	2.40	120.61	110.07
4	A	316	PEG	O2-C3-C4	2.39	120.58	110.07
4	C	303	PEG	O2-C3-C4	2.38	120.52	110.07
4	C	302	PEG	O2-C2-C1	2.22	119.82	110.07
4	D	301	PEG	O1-C1-C2	2.21	124.61	111.81
4	A	316	PEG	O2-C2-C1	2.15	119.51	110.07
4	D	301	PEG	C3-O2-C2	2.09	122.32	113.29
7	D	305	ARG	OXT-C-CA	2.05	120.37	113.38
4	A	307	PEG	O4-C4-C3	2.01	123.48	111.81

There are no chirality outliers.

All (47) 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

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Mol	Chain	Res	Type	Atoms
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
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
5	A	314	GOL	C1-C2-C3-O3
6	B	312	PGE	C4-C3-O2-C2
6	B	311	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
6	A	315	PGE	O2-C3-C4-O3
6	C	311	PGE	O2-C3-C4-O3
9	B	303	EDO	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	315	PGE	1	0
4	C	303	PEG	1	0
5	C	308	GOL	2	0
9	B	303	EDO	1	0
4	A	311	PEG	1	0
4	A	308	PEG	1	0
4	B	306	PEG	1	0
4	B	305	PEG	5	0
4	A	310	PEG	1	0
4	C	302	PEG	1	0
5	C	307	GOL	1	0
4	D	301	PEG	1	0
6	C	311	PGE	2	0
4	D	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%)	-0.44	3 (1%)	77	79	16, 23, 59, 89	0
1	B	240/243 (98%)	-0.36	6 (2%)	57	60	17, 25, 63, 102	0
1	C	240/243 (98%)	-0.05	16 (6%)	17	20	19, 33, 78, 93	0
1	D	239/243 (98%)	0.18	27 (11%)	5	5	19, 36, 90, 118	0
All	All	959/972 (98%)	-0.17	52 (5%)	25	29	16, 28, 76, 118	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	211	ALA	7.4
1	D	147	THR	7.4
1	D	210	ASN	6.8
1	D	143	TYR	6.1
1	D	209	LYS	5.1
1	D	149	LEU	4.6
1	C	224	ASP	3.8
1	C	146	LEU	3.8
1	D	224	ASP	3.8
1	C	141	GLU	3.7
1	C	138	ALA	3.4
1	B	269	VAL	3.3
1	C	149	LEU	3.3
1	B	224	ASP	3.3
1	D	151	SER	3.1
1	D	144	LYS	3.1
1	D	195	ALA	3.1
1	D	172	LYS	3.0
1	D	190	ALA	3.0
1	D	213	LEU	2.8
1	D	141	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	152	ALA	2.8
1	C	143	TYR	2.8
1	A	59	VAL	2.8
1	D	146	LEU	2.7
1	B	59	VAL	2.7
1	C	225	GLY	2.6
1	C	137	LYS	2.5
1	D	174	GLN	2.5
1	B	60	ASP	2.5
1	D	218	VAL	2.5
1	C	172	LYS	2.5
1	A	224	ASP	2.5
1	D	267	THR	2.4
1	C	223	LYS	2.4
1	D	221	LYS	2.4
1	C	140	VAL	2.4
1	C	267	THR	2.3
1	D	154	ILE	2.3
1	D	226	ASP	2.2
1	C	147	THR	2.2
1	A	225	GLY	2.1
1	C	145	ASP	2.1
1	B	58	LEU	2.1
1	C	148	SER	2.1
1	D	178	LEU	2.1
1	D	269	VAL	2.1
1	B	237	ASP	2.1
1	C	221	LYS	2.1
1	D	222	MET	2.0
1	D	223	LYS	2.0
1	D	217	THR	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(Å^2)	Q<0.9
8	ACT	B	309	4/4	0.32	0.23	70,71,72,74	0
8	ACT	B	310	4/4	0.57	0.24	63,66,67,71	0
5	GOL	A	313	6/6	0.58	0.18	61,63,66,66	0
4	PEG	D	302	7/7	0.59	0.21	56,61,70,73	0
8	ACT	D	304	4/4	0.67	0.26	81,81,82,84	0
4	PEG	C	303	7/7	0.69	0.33	65,72,78,78	0
4	PEG	C	304	7/7	0.73	0.17	51,53,55,56	0
4	PEG	B	307	7/7	0.74	0.20	44,49,52,55	0
5	GOL	C	307	6/6	0.75	0.13	66,70,75,78	0
4	PEG	A	316	7/7	0.76	0.19	54,62,62,62	0
4	PEG	C	306	7/7	0.78	0.19	51,55,63,63	0
8	ACT	B	308	4/4	0.79	0.23	67,68,69,70	0
6	PGE	C	311	10/10	0.79	0.14	46,52,60,61	0
4	PEG	D	301	7/7	0.80	0.14	45,48,55,59	0
4	PEG	C	302	7/7	0.80	0.18	43,47,51,51	0
4	PEG	A	308	7/7	0.80	0.17	47,54,56,57	0
4	PEG	A	310	7/7	0.82	0.15	47,55,59,59	0
6	PGE	B	312	10/10	0.83	0.16	32,47,59,59	0
9	EDO	B	303	4/4	0.83	0.13	39,39,40,46	0
8	ACT	C	309	4/4	0.84	0.13	51,53,53,53	0
4	PEG	C	305	7/7	0.85	0.18	45,46,48,52	0
4	PEG	A	311	7/7	0.86	0.14	43,50,53,56	0
4	PEG	A	306	7/7	0.86	0.11	47,48,50,50	0
4	PEG	A	309	7/7	0.87	0.11	36,39,51,55	0
4	PEG	B	304	7/7	0.87	0.12	39,42,51,51	0
6	PGE	A	315	10/10	0.88	0.21	45,51,53,54	0
4	PEG	A	305	7/7	0.89	0.12	30,33,39,44	0
5	GOL	A	312	6/6	0.89	0.20	44,47,50,50	0
5	GOL	C	308	6/6	0.89	0.14	30,48,50,52	0
5	GOL	D	303	6/6	0.90	0.15	52,54,57,60	0
4	PEG	A	307	7/7	0.90	0.12	39,41,45,46	0
4	PEG	B	305	7/7	0.92	0.12	39,41,44,45	0
4	PEG	B	306	7/7	0.92	0.10	45,46,48,48	0
5	GOL	A	314	6/6	0.92	0.11	47,53,55,57	0
8	ACT	C	310	4/4	0.93	0.08	60,61,62,62	0
2	SO4	A	302	5/5	0.93	0.12	65,70,71,71	0
6	PGE	B	311	10/10	0.93	0.12	38,47,51,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	ARG	C	312	12/12	0.95	0.07	19,22,29,30	0
3	CL	A	304	1/1	0.96	0.04	40,40,40,40	0
7	ARG	D	305	12/12	0.97	0.07	21,25,29,31	0
8	ACT	B	302	4/4	0.97	0.09	39,41,43,44	0
2	SO4	A	303	5/5	0.97	0.10	43,48,52,53	0
7	ARG	A	317	12/12	0.98	0.09	16,16,18,19	0
7	ARG	B	313	12/12	0.98	0.08	16,17,21,21	0
2	SO4	A	301	5/5	0.98	0.09	41,42,44,44	0
2	SO4	C	301	5/5	0.98	0.07	43,47,49,52	0
2	SO4	B	301	5/5	0.99	0.11	38,41,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.