Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 05:57 AM EDT

PDB ID	:	2WY6
Title	:	Clostridium perfringens alpha-toxin strain NCTC8237 mutant T74I
Authors	:	Vachieri, S.G.; Naylor, C.E.; Basak, A.K.
Deposited on	:	2009-11-12
Resolution	:	3.20 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:

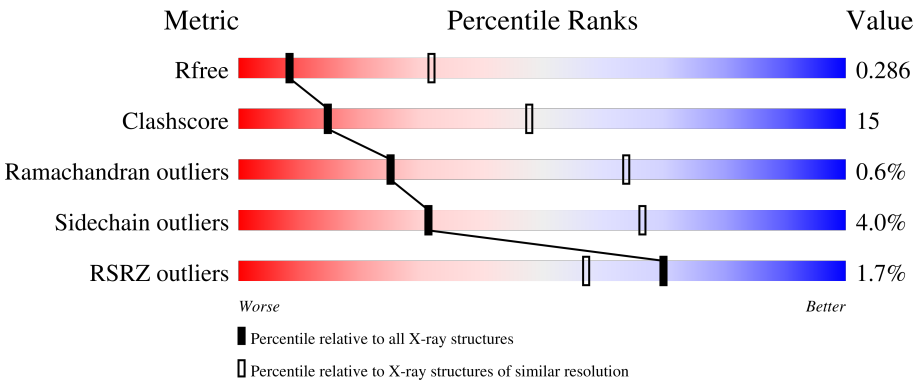
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	370	2% 70% 26% • •
1	B	370	% 68% 28% • •
1	C	370	2% 67% 28% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8429 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 PHOSPHOLIPASE C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	361	2798	1767	457	565	9	0	0	0
1	B	365	2807	1780	455	563	9	0	0	0
1	C	358	2790	1760	456	565	9	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	ILE	THR	engineered mutation	UNP Q0TV31
A	335	PRO	SER	conflict	UNP Q0TV31
B	74	ILE	THR	engineered mutation	UNP Q0TV31
B	335	PRO	SER	conflict	UNP Q0TV31
C	74	ILE	THR	engineered mutation	UNP Q0TV31
C	335	PRO	SER	conflict	UNP Q0TV31

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
3	A	3	3	3	0	0

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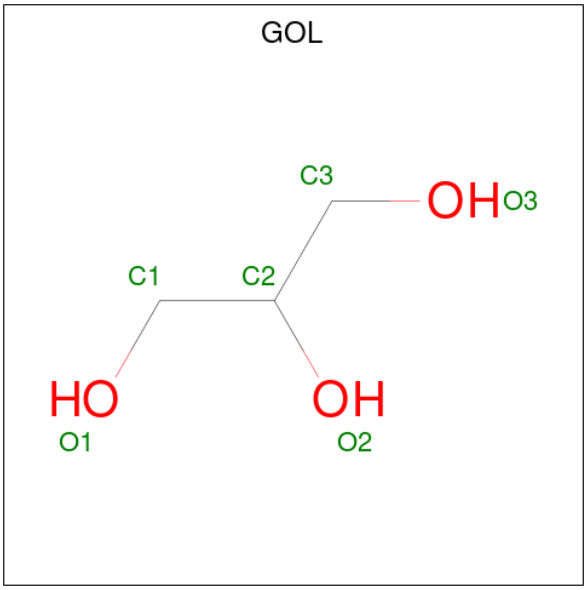
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	7	Total Cd 7 7	0	0
3	C	5	Total Cd 5 5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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



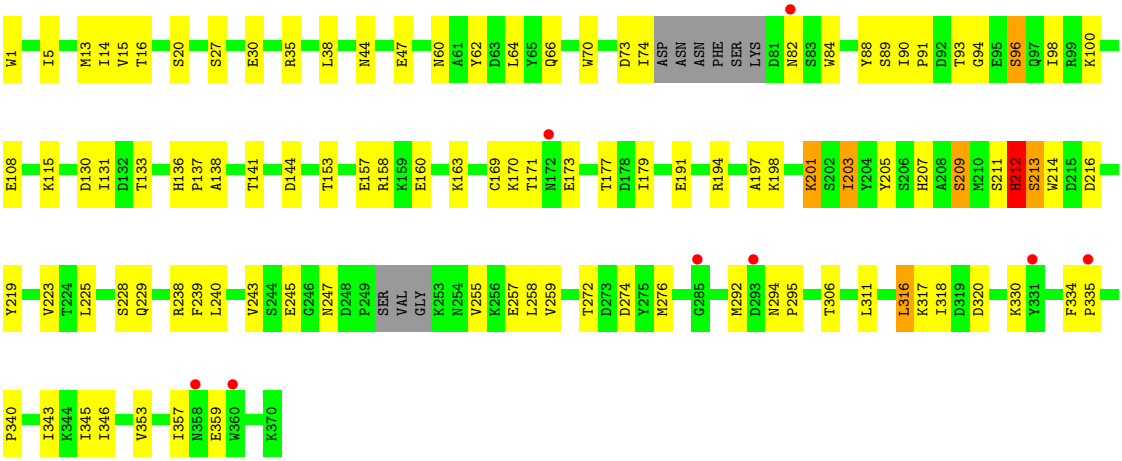
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

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.

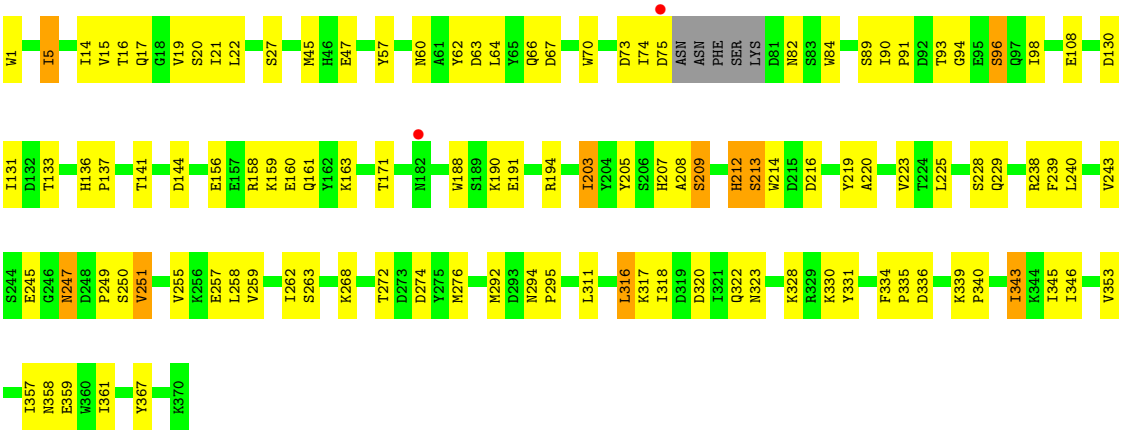
• Molecule 1: PHOSPHOLIPASE C

Chain A:



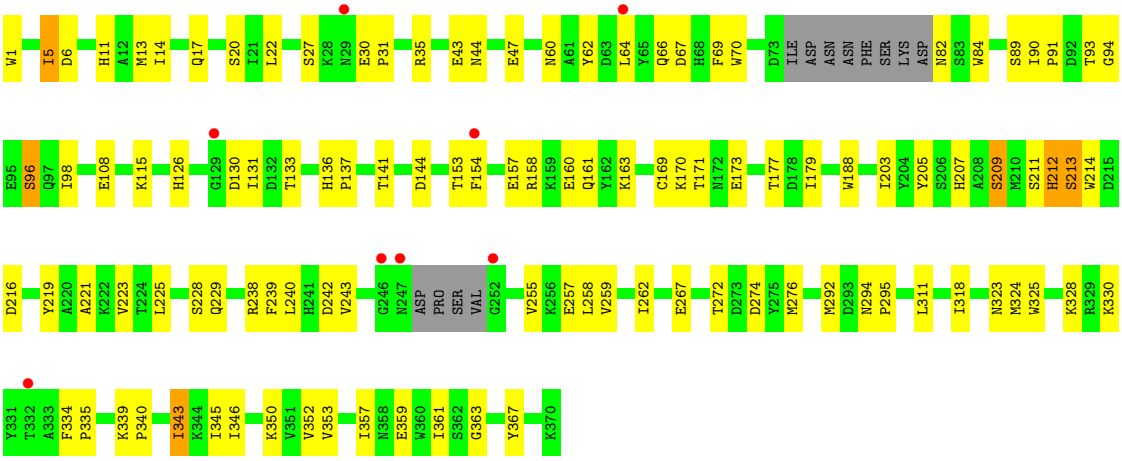
• Molecule 1: PHOSPHOLIPASE C

Chain B:



• Molecule 1: PHOSPHOLIPASE C

Chain C:


W1 I5 D6 H11 A12 M13 I14 Q17 S20 I21 L22 S27 K28 N29 E30 P31 R35 E43 N44 E47 N60 A61 Y62 D63 L64 Y65 Q66 D67 H68 F69 W70 D73 ILE ASP ASN ASN PHE SER LYS ASP N82 S83 W84 S89 I90 P91 D92 T93 G94
E95 S96 Q97 I98 E108 K115 H126 G129 D130 I131 D132 T133 H136 P137 T141 D144 T153 F154 E157 R158 K159 E160 Q161 Y162 K163 C169 K170 T171 M172 E173 T177 D178 I179 W188 I203 Y204 Y205 S206 H207 A208 S209 M210 S211 H212 S213 W214 D215
D216 Y219 A220 A221 K222 V223 T224 L225 S228 Q229 R238 F239 L240 H241 D242 V243 G246 N247 ASP PRO SER VAL G252 V255 K256 E257 L258 V259 I262 E267 T272 D273 D274 Y275 M276 M292 D293 N294 P295 L311 I318 N323 M324 W325 K328 R329 K330
Y331 T332 A333 F334 P335 K339 P340 I343 K344 I345 I346 K350 V351 V352 V353 I357 N358 E359 W360 I361 S362 G363 Y367 K370

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.24Å 107.24Å 225.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.91 – 3.20 24.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.91-3.20) 100.0 (24.91-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 3.17Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.219 , 0.281 0.217 , 0.286	Depositor DCC
R_{free} test set	1088 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	89.0	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 65.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8429	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: ZN, CD, GOL, CA

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	0.53	2/2872 (0.1%)	0.61	2/3918 (0.1%)
1	B	0.48	0/2884	0.60	0/3940
1	C	0.45	0/2864	0.58	0/3905
All	All	0.48	2/8620 (0.0%)	0.60	2/11763 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	LYS	CD-CE	5.45	1.64	1.51
1	A	212	HIS	CB-CG	5.05	1.59	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	LYS	CD-CE-NZ	6.93	127.64	111.70
1	A	212	HIS	CB-CA-C	5.94	122.29	110.40

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	2798	0	2456	74	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2807	0	2455	86	3
1	C	2790	0	2448	84	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	3	0	0	0	0
3	B	7	0	0	0	0
3	C	5	0	0	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
5	A	6	0	8	1	0
5	C	6	0	8	3	0
All	All	8429	0	7375	242	3

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 15.

All (242) 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:205:TYR:O	1:A:212:HIS:CE1	2.08	1.06
1:C:205:TYR:O	1:C:212:HIS:CE1	2.25	0.89
1:B:205:TYR:O	1:B:212:HIS:CE1	2.34	0.81
1:A:205:TYR:O	1:A:212:HIS:NE2	2.17	0.78
1:B:316:LEU:HD12	1:B:317:LYS:H	1.50	0.76
1:C:207:HIS:CE1	5:C:1371:GOL:O2	2.41	0.73
1:A:47:GLU:HG2	1:A:115:LYS:HG3	1.70	0.73
1:C:169:CYS:HB3	1:C:173:GLU:HB2	1.71	0.72
1:B:274:ASP:OD2	1:B:330:LYS:HD2	1.89	0.71
1:A:169:CYS:HB3	1:A:173:GLU:HB2	1.73	0.70
1:A:294:ASN:HB3	1:A:295:PRO:HD2	1.74	0.70
1:C:239:PHE:O	1:C:243:VAL:HG22	1.93	0.69
1:C:30:GLU:OE1	1:C:171:THR:HG21	1.93	0.69
1:C:47:GLU:HG2	1:C:115:LYS:HG3	1.75	0.68
1:B:294:ASN:HB3	1:B:295:PRO:HD2	1.76	0.67
1:C:44:ASN:OD1	1:C:115:LYS:HE3	1.94	0.67
1:A:44:ASN:OD1	1:A:115:LYS:HE3	1.94	0.66
1:A:316:LEU:HD12	1:A:317:LYS:H	1.61	0.66
1:B:158:ARG:HG3	1:B:158:ARG:HH11	1.60	0.66
1:C:340:PRO:HG2	1:C:357:ILE:HG21	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:OD1	1:A:198:LYS:NZ	2.29	0.66
1:C:93:THR:H	1:C:96:SER:HB3	1.62	0.65
1:A:90:ILE:HG23	1:A:91:PRO:HD2	1.79	0.65
1:C:294:ASN:HB3	1:C:295:PRO:HD2	1.79	0.65
1:A:340:PRO:HG2	1:A:357:ILE:HG21	1.79	0.64
1:A:44:ASN:OD1	1:A:115:LYS:CE	2.45	0.64
1:B:316:LEU:HD12	1:B:317:LYS:N	2.12	0.64
1:C:90:ILE:HG23	1:C:91:PRO:HD2	1.80	0.64
1:C:225:LEU:O	1:C:229:GLN:HG3	1.98	0.64
1:A:316:LEU:HD11	1:A:320:ASP:CB	2.29	0.63
1:B:316:LEU:HD11	1:B:320:ASP:CB	2.28	0.63
1:B:131:ILE:O	1:B:137:PRO:HG3	1.99	0.63
1:C:27:SER:CB	1:C:171:THR:HB	2.28	0.63
1:C:205:TYR:O	1:C:212:HIS:NE2	2.32	0.63
1:B:340:PRO:HG2	1:B:357:ILE:HG21	1.80	0.62
1:A:30:GLU:OE1	1:A:171:THR:HG21	2.00	0.62
1:B:93:THR:H	1:B:96:SER:HB3	1.65	0.61
1:B:90:ILE:HG23	1:B:91:PRO:HD2	1.82	0.61
1:C:131:ILE:O	1:C:137:PRO:HG3	2.00	0.60
1:B:130:ASP:O	1:B:136:HIS:HB2	2.02	0.60
1:A:316:LEU:HD11	1:A:320:ASP:HB3	1.84	0.59
1:B:255:VAL:HG23	1:B:318:ILE:HG12	1.84	0.59
1:B:27:SER:CB	1:B:171:THR:HB	2.33	0.59
1:C:27:SER:HB2	1:C:171:THR:HB	1.84	0.59
1:C:158:ARG:HG3	1:C:158:ARG:HH11	1.68	0.59
1:B:94:GLY:O	1:B:98:ILE:HG13	2.02	0.59
1:B:225:LEU:O	1:B:229:GLN:HG3	2.03	0.59
1:C:357:ILE:HG22	1:C:359:GLU:H	1.67	0.59
1:C:255:VAL:HG23	1:C:318:ILE:HG12	1.85	0.58
1:A:27:SER:CB	1:A:171:THR:HB	2.33	0.58
1:B:339:LYS:HE2	1:B:358:ASN:O	2.03	0.58
1:A:131:ILE:O	1:A:137:PRO:HG3	2.03	0.58
1:B:316:LEU:HD11	1:B:320:ASP:HB3	1.84	0.58
1:A:357:ILE:HG22	1:A:359:GLU:H	1.68	0.58
1:B:239:PHE:O	1:B:243:VAL:HG22	2.03	0.58
1:B:255:VAL:HG12	1:B:311:LEU:HD22	1.85	0.58
1:A:294:ASN:HB3	1:A:295:PRO:CD	2.34	0.57
1:B:160:GLU:O	1:B:163:LYS:HG3	2.02	0.57
1:C:130:ASP:O	1:C:136:HIS:HB2	2.04	0.57
1:B:251:VAL:HG12	1:B:251:VAL:O	2.04	0.57
1:B:330:LYS:HZ1	1:B:336:ASP:H	1.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:ASN:OD1	1:C:115:LYS:CE	2.52	0.57
1:A:27:SER:HB2	1:A:171:THR:HB	1.85	0.57
1:B:272:THR:OG1	1:B:274:ASP:HB2	2.05	0.57
1:B:294:ASN:HB3	1:B:295:PRO:CD	2.34	0.56
1:A:93:THR:H	1:A:96:SER:HB3	1.69	0.56
1:A:255:VAL:HG23	1:A:318:ILE:HG12	1.87	0.56
1:A:213:SER:OG	1:A:214:TRP:N	2.36	0.56
1:B:361:ILE:HD13	1:B:367:TYR:HB2	1.88	0.56
1:C:267:GLU:OE1	1:C:339:LYS:NZ	2.33	0.55
1:A:14:ILE:HD13	1:A:228:SER:HB3	1.88	0.55
1:C:30:GLU:CD	1:C:171:THR:HG21	2.27	0.55
1:C:94:GLY:O	1:C:98:ILE:HG13	2.06	0.55
1:B:274:ASP:HB2	1:B:328:LYS:HD2	1.89	0.55
1:C:213:SER:OG	1:C:214:TRP:N	2.40	0.55
1:B:357:ILE:HG22	1:B:359:GLU:H	1.71	0.55
1:B:205:TYR:O	1:B:212:HIS:NE2	2.38	0.55
1:C:255:VAL:HG12	1:C:311:LEU:HD22	1.89	0.55
1:A:239:PHE:O	1:A:243:VAL:HG22	2.06	0.55
1:B:255:VAL:HG12	1:B:255:VAL:O	2.07	0.55
1:A:30:GLU:HB3	1:A:35:ARG:NH2	2.22	0.54
1:A:272:THR:OG1	1:A:274:ASP:HB2	2.07	0.54
1:A:316:LEU:HD12	1:A:317:LYS:N	2.22	0.54
1:B:67:ASP:OD1	1:B:67:ASP:N	2.38	0.54
1:C:294:ASN:HB3	1:C:295:PRO:CD	2.36	0.54
1:C:255:VAL:CG2	1:C:318:ILE:HG12	2.38	0.54
1:B:1:TRP:CE2	1:B:133:THR:HG22	2.44	0.53
1:C:170:LYS:HB2	1:C:173:GLU:HG3	1.89	0.53
1:A:90:ILE:CG2	1:A:91:PRO:HD2	2.38	0.53
1:B:27:SER:HB2	1:B:171:THR:HB	1.89	0.53
1:B:255:VAL:CG2	1:B:318:ILE:HG12	2.38	0.53
1:A:170:LYS:HB2	1:A:173:GLU:HG3	1.89	0.53
1:C:328:LYS:HE3	1:C:363:GLY:O	2.07	0.53
1:B:330:LYS:HZ1	1:B:336:ASP:N	2.06	0.53
1:A:94:GLY:O	1:A:98:ILE:HG13	2.09	0.53
1:A:141:THR:N	1:A:144:ASP:HB2	2.24	0.53
1:B:158:ARG:HG3	1:B:158:ARG:NH1	2.24	0.53
1:B:14:ILE:HD13	1:B:228:SER:HB3	1.91	0.52
1:B:141:THR:N	1:B:144:ASP:HB2	2.24	0.52
1:C:209:SER:OG	1:C:212:HIS:HD2	1.92	0.52
1:A:138:ALA:HA	1:A:201:LYS:HG3	1.90	0.52
1:A:153:THR:O	1:A:157:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:THR:O	1:C:157:GLU:HG3	2.10	0.52
1:A:207:HIS:NE2	5:A:1376:GOL:H32	2.24	0.52
1:C:30:GLU:HB3	1:C:35:ARG:NH2	2.25	0.52
1:B:60:ASN:HB3	1:B:62:TYR:H	1.75	0.52
1:C:272:THR:OG1	1:C:274:ASP:HB2	2.09	0.52
1:B:188:TRP:CZ3	1:B:238:ARG:HG2	2.45	0.52
1:A:30:GLU:CD	1:A:171:THR:HG21	2.30	0.52
1:B:212:HIS:H	1:B:212:HIS:CD2	2.26	0.52
1:A:141:THR:H	1:A:144:ASP:HB2	1.75	0.51
1:B:209:SER:OG	1:B:212:HIS:HD2	1.93	0.51
1:B:250:SER:O	1:B:251:VAL:C	2.48	0.51
1:C:90:ILE:CG2	1:C:91:PRO:HD2	2.40	0.51
1:B:160:GLU:HB3	1:C:219:TYR:CZ	2.45	0.51
1:B:345:ILE:HB	1:B:353:VAL:HB	1.93	0.51
1:A:88:TYR:OH	1:B:47:GLU:OE2	2.28	0.51
1:C:141:THR:N	1:C:144:ASP:HB2	2.26	0.51
1:C:212:HIS:CD2	1:C:212:HIS:H	2.29	0.51
1:A:1:TRP:CE2	1:A:133:THR:HG22	2.46	0.50
1:C:14:ILE:HD13	1:C:228:SER:HB3	1.93	0.50
1:C:219:TYR:O	1:C:223:VAL:HG23	2.11	0.50
1:A:130:ASP:O	1:A:136:HIS:HB2	2.11	0.50
1:A:255:VAL:HG12	1:A:311:LEU:HD22	1.92	0.50
1:C:257:GLU:O	1:C:258:LEU:HD23	2.12	0.50
1:A:225:LEU:O	1:A:229:GLN:HG3	2.11	0.50
1:A:257:GLU:O	1:A:258:LEU:HD23	2.12	0.50
1:C:179:ILE:CG2	1:C:238:ARG:HB2	2.41	0.50
1:C:361:ILE:HD13	1:C:367:TYR:HB2	1.94	0.50
1:A:345:ILE:HB	1:A:353:VAL:HB	1.94	0.50
1:A:60:ASN:HB3	1:A:62:TYR:H	1.76	0.49
1:B:74:ILE:CG2	1:B:75:ASP:N	2.75	0.49
1:A:245:GLU:HB3	1:A:247:ASN:OD1	2.13	0.49
1:C:345:ILE:HB	1:C:353:VAL:HB	1.94	0.49
1:A:255:VAL:CG2	1:A:318:ILE:HG12	2.43	0.49
1:B:213:SER:OG	1:B:214:TRP:N	2.46	0.49
1:C:82:ASN:OD1	1:C:84:TRP:HB3	2.13	0.49
1:A:259:VAL:HB	1:A:346:ILE:HB	1.95	0.48
1:B:219:TYR:O	1:B:223:VAL:HG23	2.12	0.48
1:C:350:LYS:O	1:C:352:VAL:HG13	2.13	0.48
1:A:158:ARG:HG3	1:A:158:ARG:HH11	1.75	0.48
1:C:1:TRP:CE2	1:C:133:THR:HG22	2.49	0.48
1:A:276:MET:HB3	1:A:292:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:THR:H	1:B:144:ASP:HB2	1.78	0.47
1:C:67:ASP:N	1:C:67:ASP:OD1	2.39	0.47
1:C:60:ASN:HB3	1:C:62:TYR:H	1.79	0.47
1:B:90:ILE:CG2	1:B:91:PRO:HD2	2.43	0.47
1:C:160:GLU:O	1:C:163:LYS:HG3	2.14	0.47
1:A:64:LEU:HB2	1:A:66:GLN:NE2	2.30	0.47
1:B:330:LYS:HZ1	1:B:335:PRO:HA	1.79	0.47
1:C:203:ILE:HD11	1:C:223:VAL:HG11	1.96	0.47
1:A:179:ILE:CG2	1:A:238:ARG:HB2	2.44	0.47
1:B:64:LEU:HB2	1:B:66:GLN:NE2	2.30	0.47
1:B:208:ALA:HB2	1:B:220:ALA:HB1	1.97	0.47
1:B:203:ILE:HD11	1:B:223:VAL:HG11	1.97	0.47
1:B:250:SER:OG	1:B:318:ILE:HD11	2.14	0.47
1:A:15:VAL:HG23	1:A:16:THR:N	2.30	0.46
1:C:340:PRO:HG2	1:C:357:ILE:CG2	2.45	0.46
1:B:274:ASP:CB	1:B:328:LYS:HD2	2.45	0.46
1:C:259:VAL:HB	1:C:346:ILE:HB	1.97	0.46
1:A:274:ASP:OD2	1:A:330:LYS:HA	2.14	0.46
1:B:74:ILE:HG23	1:B:75:ASP:N	2.30	0.46
1:A:219:TYR:O	1:A:223:VAL:HG23	2.15	0.46
1:B:82:ASN:OD1	1:B:84:TRP:HB3	2.16	0.46
1:A:70:TRP:O	1:A:137:PRO:HA	2.15	0.46
1:A:160:GLU:O	1:A:163:LYS:HG3	2.15	0.46
1:B:73:ASP:O	1:B:74:ILE:C	2.53	0.46
1:B:158:ARG:O	1:B:161:GLN:HG2	2.16	0.46
1:B:330:LYS:CE	1:B:334:PHE:O	2.64	0.45
1:B:322:GLN:HG2	1:B:323:ASN:OD1	2.17	0.45
1:C:255:VAL:HG12	1:C:255:VAL:O	2.16	0.45
1:B:316:LEU:HD11	1:B:320:ASP:HB2	1.97	0.45
1:C:323:ASN:O	1:C:324:MET:HG3	2.16	0.45
1:B:257:GLU:O	1:B:258:LEU:HD23	2.16	0.45
1:B:245:GLU:C	1:B:247:ASN:N	2.70	0.45
1:C:70:TRP:O	1:C:137:PRO:HA	2.17	0.45
1:C:108:GLU:OE1	1:C:108:GLU:HA	2.16	0.45
1:C:207:HIS:HE1	5:C:1371:GOL:O2	1.94	0.45
1:B:259:VAL:HB	1:B:346:ILE:HB	1.98	0.45
1:C:11:HIS:HE1	1:C:126:HIS:O	1.99	0.45
1:C:211:SER:O	1:C:212:HIS:O	2.35	0.45
1:A:100:LYS:HD3	1:A:306:THR:HG21	1.99	0.45
1:A:108:GLU:OE1	1:A:108:GLU:HA	2.17	0.45
1:A:340:PRO:HG2	1:A:357:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:PRO:HG2	1:B:357:ILE:CG2	2.46	0.44
1:C:158:ARG:O	1:C:161:GLN:HG2	2.17	0.44
1:C:158:ARG:HG3	1:C:158:ARG:NH1	2.31	0.44
1:C:30:GLU:OE1	1:C:171:THR:CG2	2.65	0.44
1:C:47:GLU:OE1	1:C:115:LYS:HE2	2.17	0.44
1:A:316:LEU:CD1	1:A:320:ASP:HB2	2.48	0.43
1:B:268:LYS:HB2	1:B:268:LYS:HE3	1.67	0.43
1:C:209:SER:HB3	1:C:212:HIS:CD2	2.54	0.43
1:A:316:LEU:HD11	1:A:320:ASP:HB2	1.99	0.43
1:B:316:LEU:CD1	1:B:320:ASP:HB2	2.48	0.43
1:C:188:TRP:CZ3	1:C:238:ARG:HG2	2.53	0.43
1:C:27:SER:HB3	1:C:171:THR:HB	2.01	0.43
1:A:209:SER:OG	1:A:212:HIS:HD2	2.02	0.43
1:C:141:THR:H	1:C:144:ASP:HB2	1.83	0.43
1:C:262:ILE:HG12	1:C:343:ILE:HD12	2.00	0.43
1:C:238:ARG:NE	1:C:242:ASP:OD2	2.44	0.43
1:A:38:LEU:HB2	1:A:240:LEU:HD13	2.01	0.42
1:B:70:TRP:O	1:B:137:PRO:HA	2.19	0.42
1:B:276:MET:HB3	1:B:292:MET:HE3	2.00	0.42
1:C:69:PHE:O	1:C:70:TRP:HB2	2.19	0.42
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.82	0.42
1:A:211:SER:O	1:A:212:HIS:O	2.37	0.42
1:B:64:LEU:HD23	1:B:64:LEU:HA	1.78	0.42
1:C:274:ASP:OD2	1:C:330:LYS:HA	2.19	0.42
1:B:156:GLU:O	1:B:159:LYS:HG2	2.20	0.42
1:A:255:VAL:HG12	1:A:255:VAL:O	2.19	0.42
1:B:17:GLN:O	1:B:21:ILE:HG13	2.20	0.42
1:B:190:LYS:NZ	1:B:194:ARG:HH22	2.18	0.42
1:B:191:GLU:OE1	1:B:194:ARG:NH1	2.53	0.42
1:B:274:ASP:HA	1:B:331:TYR:HB2	2.01	0.42
1:C:276:MET:HB3	1:C:292:MET:HE3	2.01	0.42
1:A:334:PHE:HA	1:A:335:PRO:HD3	1.79	0.42
1:B:75:ASP:HB2	1:B:194:ARG:HH21	1.84	0.42
1:B:22:LEU:HD21	1:B:240:LEU:HD12	2.02	0.42
1:C:64:LEU:HB2	1:C:66:GLN:NE2	2.35	0.42
1:C:334:PHE:HA	1:C:335:PRO:HD3	1.79	0.42
1:A:82:ASN:OD1	1:A:84:TRP:HB3	2.19	0.42
1:B:5:ILE:HG12	1:B:57:TYR:CD1	2.55	0.42
1:B:330:LYS:NZ	1:B:335:PRO:HA	2.34	0.42
1:C:22:LEU:HD21	1:C:240:LEU:HD12	2.02	0.42
1:A:191:GLU:OE1	1:A:194:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:MET:O	1:C:17:GLN:HG2	2.20	0.41
1:C:221:ALA:O	1:C:225:LEU:HB2	2.19	0.41
1:C:211:SER:O	1:C:212:HIS:C	2.57	0.41
1:B:15:VAL:HG23	1:B:16:THR:N	2.35	0.41
1:C:207:HIS:HE1	5:C:1371:GOL:O3	2.04	0.41
1:A:158:ARG:HG3	1:A:158:ARG:NH1	2.35	0.41
1:B:108:GLU:OE1	1:B:108:GLU:HA	2.21	0.41
1:B:19:VAL:HG11	1:B:45:MET:HE1	2.03	0.41
1:A:131:ILE:O	1:A:197:ALA:HA	2.21	0.41
1:C:30:GLU:HA	1:C:31:PRO:HD3	1.95	0.41
1:C:5:ILE:HG22	1:C:6:ASP:N	2.35	0.41
1:B:262:ILE:HG12	1:B:343:ILE:HD12	2.02	0.41
1:C:325:TRP:HB2	1:C:367:TYR:O	2.22	0.40
1:A:130:ASP:HA	1:A:133:THR:HG23	2.04	0.40
1:A:203:ILE:HD11	1:A:223:VAL:HG11	2.03	0.40
1:A:73:ASP:O	1:A:74:ILE:C	2.60	0.40
1:C:130:ASP:HA	1:C:133:THR:HG23	2.03	0.40

All (3) 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:A:212:HIS:CE1	1:B:207:HIS:CE1[4_445]	2.07	0.13
1:B:63:ASP:OD2	1:C:43:GLU:OE2[7_455]	2.12	0.08
1:A:212:HIS:NE2	1:B:207:HIS:NE2[4_445]	2.19	0.01

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	355/370 (96%)	329 (93%)	25 (7%)	1 (0%)	41 74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	361/370 (98%)	328 (91%)	29 (8%)	4 (1%)	14	51
1	C	352/370 (95%)	321 (91%)	30 (8%)	1 (0%)	41	74
All	All	1068/1110 (96%)	978 (92%)	84 (8%)	6 (1%)	25	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	247	ASN
1	B	251	VAL
1	A	212	HIS
1	B	212	HIS
1	C	212	HIS
1	B	249	PRO

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	276/319 (86%)	264 (96%)	12 (4%)	29	64
1	B	274/319 (86%)	263 (96%)	11 (4%)	31	66
1	C	276/319 (86%)	266 (96%)	10 (4%)	35	69
All	All	826/957 (86%)	793 (96%)	33 (4%)	31	66

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	13	MET
1	A	20	SER
1	A	89	SER
1	A	96	SER
1	A	177	THR
1	A	203	ILE
1	A	209	SER

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Mol	Chain	Res	Type
1	A	213	SER
1	A	216	ASP
1	A	316	LEU
1	A	343	ILE
1	B	5	ILE
1	B	20	SER
1	B	89	SER
1	B	96	SER
1	B	203	ILE
1	B	209	SER
1	B	213	SER
1	B	216	ASP
1	B	263	SER
1	B	316	LEU
1	B	343	ILE
1	C	5	ILE
1	C	20	SER
1	C	89	SER
1	C	96	SER
1	C	154	PHE
1	C	177	THR
1	C	209	SER
1	C	213	SER
1	C	216	ASP
1	C	343	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	212	HIS
1	A	294	ASN
1	B	212	HIS
1	B	294	ASN
1	C	37	ASN
1	C	207	HIS
1	C	212	HIS
1	C	294	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 22 are monoatomic - leaving 2 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	1376	-	5,5,5	0.45	0	5,5,5	0.50	0
5	GOL	C	1371	-	5,5,5	0.50	0	5,5,5	0.16	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
5	GOL	A	1376	-	-	3/4/4/4	-
5	GOL	C	1371	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1376	GOL	C1-C2-C3-O3
5	C	1371	GOL	O1-C1-C2-O2
5	C	1371	GOL	O1-C1-C2-C3
5	C	1371	GOL	C1-C2-C3-O3
5	A	1376	GOL	O2-C2-C3-O3
5	C	1371	GOL	O2-C2-C3-O3
5	A	1376	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1376	GOL	1	0
5	C	1371	GOL	3	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	361/370 (97%)	-0.08	8 (2%)	62	48	46, 85, 138, 250	0
1	B	365/370 (98%)	-0.17	2 (0%)	91	86	48, 83, 124, 195	0
1	C	358/370 (96%)	-0.01	8 (2%)	62	48	56, 95, 149, 208	0
All	All	1084/1110 (97%)	-0.09	18 (1%)	70	57	46, 88, 140, 250	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	GLY	4.1
1	C	252	GLY	3.2
1	A	335	PRO	3.1
1	A	360	TRP	3.1
1	C	332	THR	2.9
1	C	64	LEU	2.8
1	B	182	ASN	2.7
1	C	246	GLY	2.7
1	A	331	TYR	2.7
1	C	154	PHE	2.6
1	B	75	ASP	2.4
1	A	358	ASN	2.4
1	C	247	ASN	2.3
1	C	29	ASN	2.2
1	C	129	GLY	2.2
1	A	172	ASN	2.1
1	A	82	ASN	2.1
1	A	293	ASP	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
4	CA	C	1377	1/1	0.78	0.13	111,111,111,111	0
5	GOL	A	1376	6/6	0.79	0.39	66,72,79,83	0
4	CA	A	1375	1/1	0.81	0.38	110,110,110,110	0
4	CA	B	1377	1/1	0.88	0.22	127,127,127,127	0
3	CD	B	1380	1/1	0.95	0.18	110,110,110,110	0
3	CD	C	1375	1/1	0.95	0.14	122,122,122,122	0
2	ZN	B	1372	1/1	0.95	0.23	74,74,74,74	0
5	GOL	C	1371	6/6	0.95	0.13	83,88,98,99	0
4	CA	B	1378	1/1	0.96	0.05	99,99,99,99	0
3	CD	B	1371	1/1	0.96	0.17	92,92,92,92	0
3	CD	B	1373	1/1	0.97	0.15	70,70,70,70	0
3	CD	B	1374	1/1	0.97	0.21	81,81,81,81	0
3	CD	C	1378	1/1	0.97	0.19	123,123,123,123	0
3	CD	A	1374	1/1	0.98	0.08	96,96,96,96	0
3	CD	C	1374	1/1	0.98	0.17	88,88,88,88	0
3	CD	C	1376	1/1	0.99	0.17	84,84,84,84	0
3	CD	A	1373	1/1	0.99	0.19	80,80,80,80	0
3	CD	B	1375	1/1	0.99	0.12	110,110,110,110	0
3	CD	B	1379	1/1	0.99	0.05	119,119,119,119	0
2	ZN	A	1371	1/1	0.99	0.22	61,61,61,61	0
3	CD	C	1373	1/1	0.99	0.18	76,76,76,76	0
2	ZN	C	1372	1/1	0.99	0.21	66,66,66,66	0
3	CD	A	1372	1/1	0.99	0.19	68,68,68,68	0
3	CD	B	1376	1/1	1.00	0.14	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.