Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:41 AM GMT

PDB ID	:	2XYD
Title	:	human Angiotenisn converting enzyme N-domain in complex with Phosphinic tripeptide
Authors	:	Akif, M.; Schwager, S.L.; Anthony, C.S.; Czarny, B.; Beau, F.; Dive, V.; Sturrock, E.D.; Acharya, K.R.
Deposited on	:	2010-11-17
Resolution	:	2.15 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

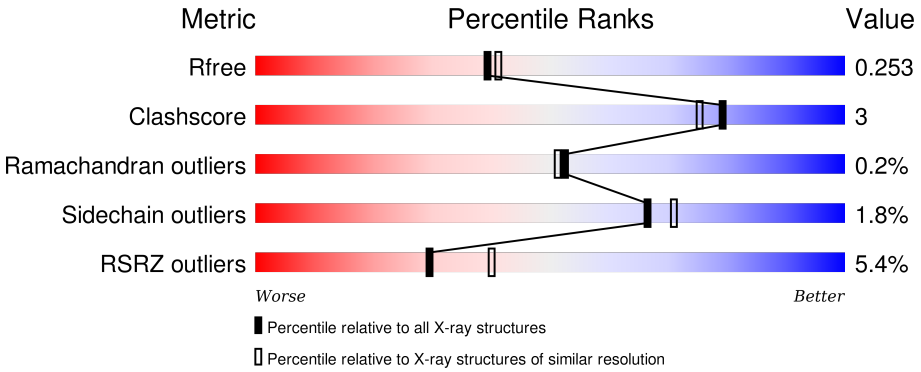
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	610	5% 91% 8%
1	B	610	6% 88% 10%

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
10	NAG	B	1616	-	-	-	X
11	P6G	B	1622	-	-	-	X
4	NAG	A	1614	-	-	-	X
8	PEG	A	1622	-	-	-	X
8	PEG	B	1623	-	-	-	X
9	PG4	B	1621	-	-	-	X

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 10490 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.

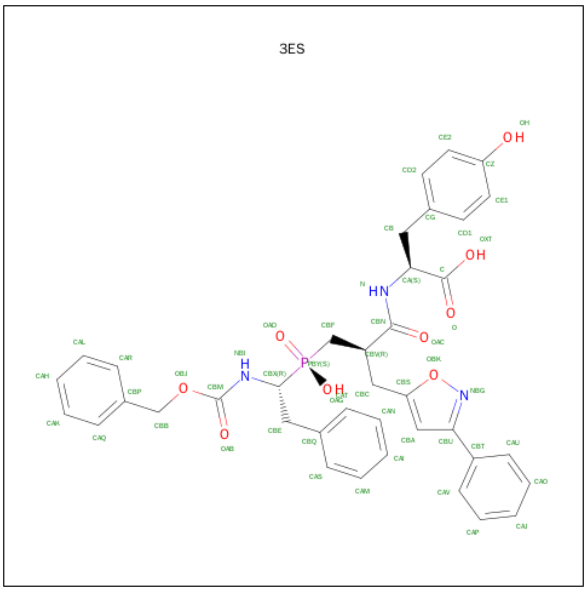
- Molecule 1 is a protein called ANGIOTENSIN-CONVERTING ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	607	Total	C	N	O	S	0	2	0
			4944	3178	849	898	19			
1	B	607	Total	C	N	O	S	0	2	0
			4937	3174	846	898	19			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
A	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
A	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821
B	9	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	25	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	82	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	117	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	289	GLN	ASN	ENGINEERED MUTATION	UNP P12821
B	545	ARG	GLN	ENGINEERED MUTATION	UNP P12821
B	576	LEU	PRO	ENGINEERED MUTATION	UNP P12821

- Molecule 2 is [(2S)-2-({3-[HYDROXYL(2-PHENYL-(1R)-1-{[(BENZYLOXY)[(2S)-2-({3-[HYDROXYL(2-PHENYL-(1R)-1-CARBONYL]-AMINO}ETHYL)PHOSPHINYL]-2-[(3-PHENYLISOXAZOL-5-YL)METHYL]-1-OXO-PROPYL}AMINO)-3-(4-HYDROXY-PHENYL) (three-letter code: 3ES) (formula: $C_{38}H_{38}N_3O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			51	38	3	9	1		
2	B	1	Total	C	N	O	P	0	0
			51	38	3	9	1		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			24	14	1	9		
3	B	2	Total	C	N	O	0	0
			24	14	1	9		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	4	Total	C	N	O	0	0
			49	28	2	19		

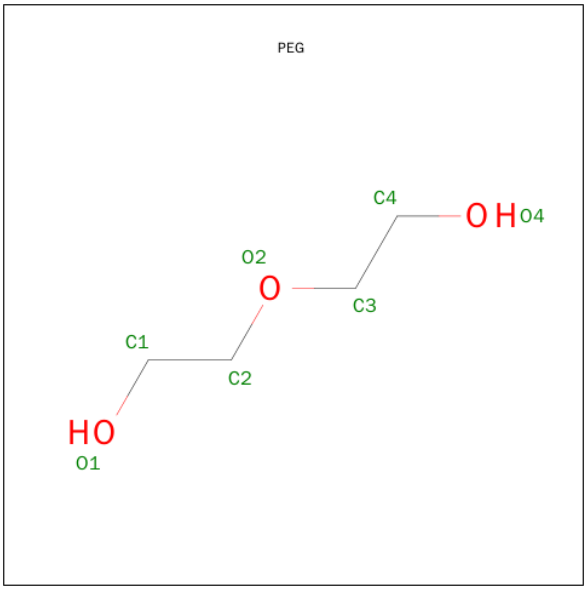
- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

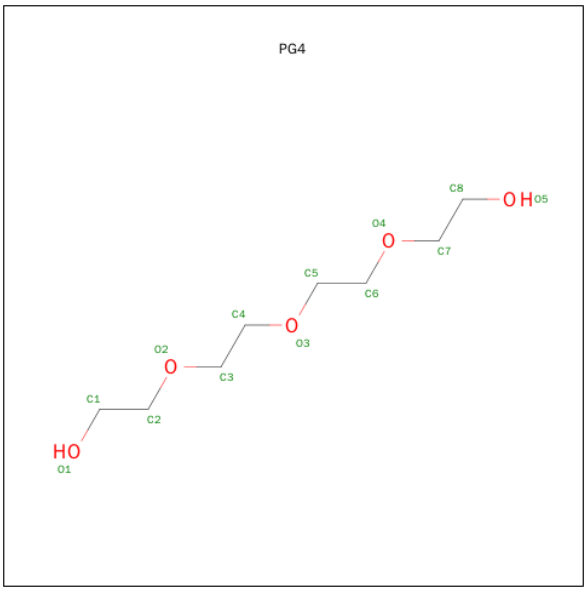
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total Cl 1 1	0	0
7	A	1	Total Cl 1 1	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

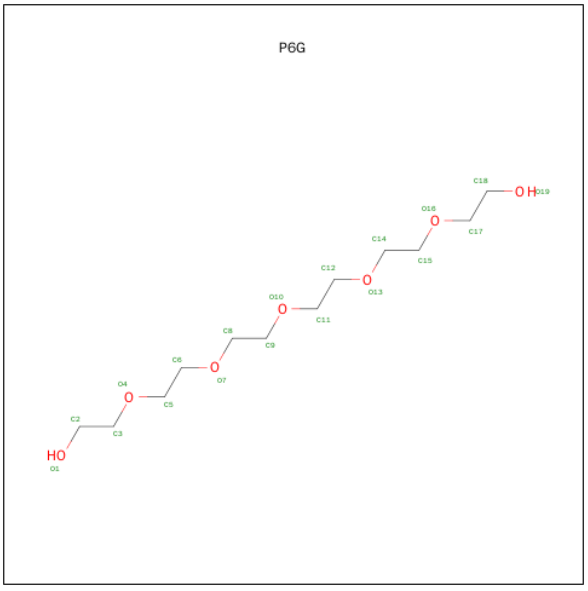


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		
9	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 10 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 11 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 12 is water.

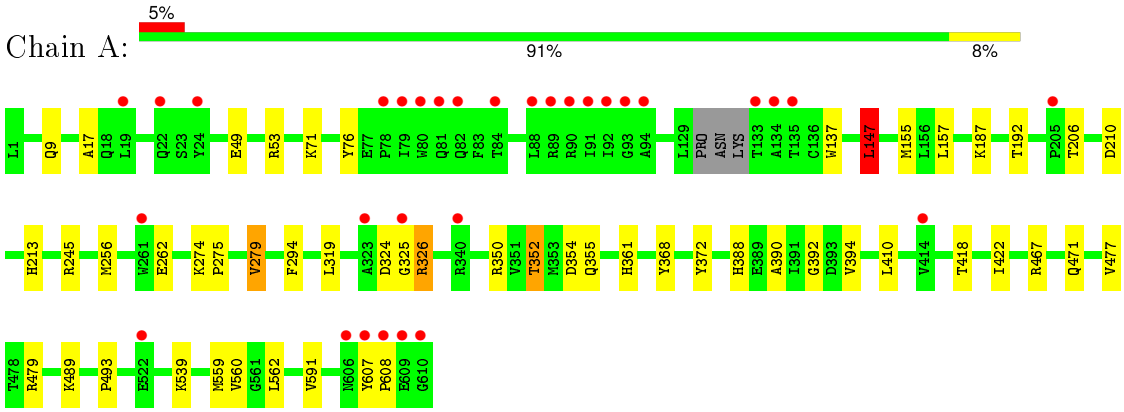
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	136	Total	O	0	0
			136	136		
12	B	105	Total	O	0	0
			105	105		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

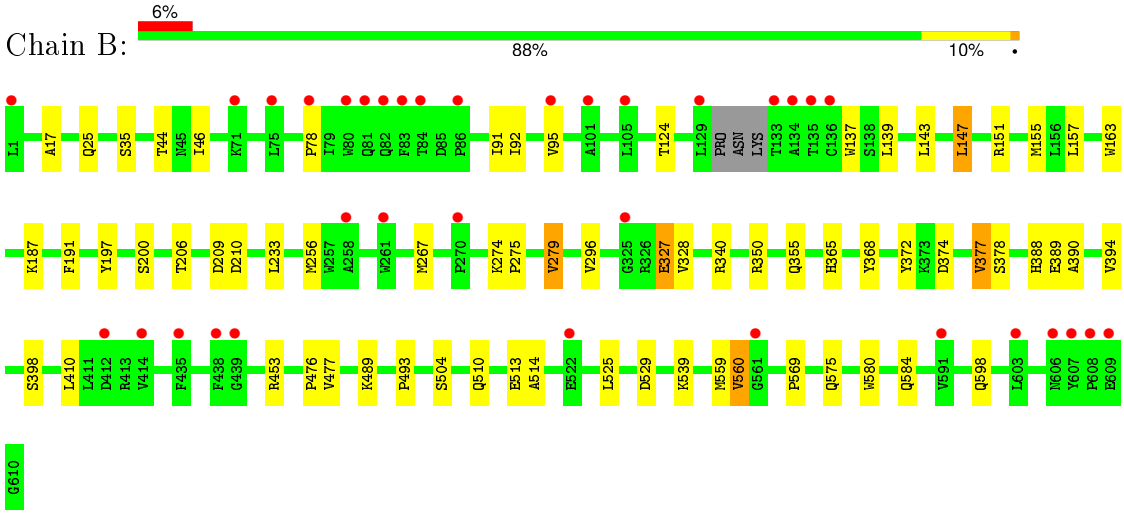
- Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

Chain A:



- Molecule 1: ANGIOTENSIN-CONVERTING ENZYME

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	72.84Å 76.44Å 82.95Å 89.11° 64.43° 75.87°	Depositor
Resolution (Å)	40.28 – 2.15 40.28 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.28-2.15) 88.3 (40.28-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.41 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.256 0.220 , 0.253	Depositor DCC
R_{free} test set	3876 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 77635 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10490	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.99% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, 3ES, NAG, CL, PG4, FUC, P6G, PEG

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	0.46	0/5106	0.55	1/6957 (0.0%)
1	B	0.43	0/5098	0.53	0/6947
All	All	0.44	0/10204	0.54	1/13904 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	LEU	CA-CB-CG	-5.64	102.33	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4944	0	4696	30	0
1	B	4937	0	4693	40	0
2	A	51	0	36	0	0
2	B	51	0	36	1	0
3	A	24	0	22	0	0
3	B	24	0	22	0	0
4	A	28	0	25	0	0
4	B	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	49	0	43	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	21	0	30	0	0
8	B	7	0	10	0	0
9	A	10	0	13	1	0
9	B	13	0	18	0	0
10	B	39	0	34	0	0
11	B	19	0	26	1	0
12	A	136	0	0	1	0
12	B	105	0	0	0	0
All	All	10490	0	9729	69	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 3.

All (69) 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:44:THR:O	1:B:328:VAL:HG12	1.62	0.99
1:B:124:THR:HG22	1:B:327:GLU:HG2	1.59	0.83
1:A:245:ARG:HG2	1:A:591:VAL:HG11	1.59	0.82
1:B:350:ARG:H	1:B:355:GLN:HE21	1.35	0.74
1:A:352:THR:HG21	1:A:354:ASP:OD1	1.88	0.74
1:A:467:ARG:HH11	1:A:471:GLN:HE22	1.37	0.72
1:A:352:THR:CG2	1:A:354:ASP:OD1	2.39	0.70
1:B:390:ALA:O	1:B:394:VAL:HG23	1.91	0.70
1:B:340:ARG:HH11	1:B:374:ASP:HA	1.58	0.69
1:A:352:THR:HG22	1:A:355:GLN:H	1.60	0.65
1:A:187:LYS:HE2	1:A:192:THR:O	1.97	0.64
1:B:25:GLN:HG2	1:B:377:VAL:HG12	1.79	0.64
1:A:324:ASP:O	1:A:326:ARG:N	2.30	0.64
1:B:296:VAL:HG22	11:B:1622:P6G:H51	1.81	0.63
1:B:157:LEU:HD11	1:B:477:VAL:HG13	1.80	0.63
1:B:46:ILE:HB	1:B:327:GLU:HB3	1.81	0.62
1:B:147:LEU:HD22	1:B:256:MET:HA	1.84	0.60
1:A:147:LEU:HD22	1:A:256:MET:HA	1.83	0.60
1:B:510:GLN:HG2	1:B:569:PRO:HG2	1.84	0.60
1:B:17:ALA:HB1	1:B:92:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HD11	1:A:477:VAL:HG13	1.84	0.58
9:A:1625:PG4:H32	1:B:453:ARG:HH21	1.69	0.58
1:B:151:ARG:NH1	1:B:267:MET:HG3	2.20	0.56
1:A:279:VAL:HG11	1:A:410:LEU:HD13	1.89	0.54
1:B:365:HIS:CE1	2:B:1611:3ES:HBB2	2.43	0.53
1:B:514:ALA:HB2	1:B:560:VAL:HG23	1.91	0.52
1:A:17:ALA:HA	1:A:76:TYR:CZ	2.46	0.51
1:B:233:LEU:HD23	1:B:267:MET:HE3	1.94	0.50
1:B:233:LEU:HD23	1:B:267:MET:CE	2.41	0.50
1:A:213[B]:HIS:HD2	12:A:2048:HOH:O	1.94	0.49
1:A:324:ASP:O	1:A:324:ASP:OD1	2.30	0.49
1:A:361:HIS:HA	1:A:392:GLY:HA3	1.94	0.49
1:A:245:ARG:HG2	1:A:591:VAL:CG1	2.37	0.48
1:B:25:GLN:HE21	1:B:378:SER:H	1.61	0.48
1:A:206:THR:HG23	1:A:210:ASP:OD2	2.13	0.48
1:B:197:TYR:O	1:B:200:SER:OG	2.27	0.48
1:A:294:PHE:CZ	1:A:319:LEU:HD22	2.48	0.47
1:B:25:GLN:CG	1:B:377:VAL:HG12	2.45	0.47
1:B:274:LYS:HB3	1:B:275:PRO:CD	2.45	0.47
1:B:340:ARG:NH1	1:B:374:ASP:HA	2.26	0.47
1:A:274:LYS:HB3	1:A:275:PRO:HD2	1.95	0.47
1:B:139:LEU:HD22	1:B:163:TRP:CZ2	2.50	0.46
1:B:539:LYS:HE3	1:B:559:MET:O	2.15	0.46
1:A:418:THR:O	1:A:422:ILE:HG12	2.15	0.46
1:A:137:TRP:CZ3	1:A:155:MET:HE1	2.51	0.45
1:B:350:ARG:H	1:B:355:GLN:NE2	2.08	0.45
1:B:513:GLU:HA	1:B:525:LEU:HD11	1.99	0.45
1:B:489:LYS:O	1:B:493:PRO:HD2	2.17	0.45
1:B:187:LYS:HA	1:B:191:PHE:O	2.17	0.45
1:B:206:THR:HG23	1:B:210:ASP:OD2	2.17	0.45
1:A:489:LYS:O	1:A:493:PRO:HD2	2.16	0.44
1:A:560:VAL:HG12	1:A:562:LEU:H	1.83	0.44
1:A:539:LYS:HE3	1:A:559:MET:O	2.17	0.44
1:B:46:ILE:HG13	1:B:327:GLU:O	2.18	0.44
1:A:479:ARG:H	1:B:598:GLN:NE2	2.17	0.43
1:A:49:GLU:HG3	1:A:53:ARG:NH1	2.33	0.43
1:B:279:VAL:HG11	1:B:410:LEU:HD13	2.01	0.43
1:B:91:ILE:O	1:B:95:VAL:HG23	2.19	0.43
1:B:137:TRP:CZ3	1:B:155:MET:HE1	2.54	0.42
1:B:139:LEU:HA	1:B:143:LEU:HD12	2.02	0.42
1:B:157:LEU:HD13	1:B:476:PRO:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:TYR:HA	1:A:608:PRO:HA	1.83	0.41
1:B:389:GLU:HB2	1:B:504:SER:HB2	2.03	0.41
1:B:398:SER:HB3	1:B:529:ASP:OD1	2.20	0.41
1:A:467:ARG:NH1	1:A:471:GLN:HE22	2.12	0.41
1:A:9:GLN:NE2	1:A:71:LYS:NZ	2.69	0.40
1:A:390:ALA:O	1:A:394:VAL:HG23	2.20	0.40
1:B:580:TRP:O	1:B:584:GLN:HG2	2.21	0.40
1:A:350:ARG:HB2	1:A:355:GLN:HG3	2.04	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	605/610 (99%)	595 (98%)	9 (2%)	1 (0%)	52	51
1	B	605/610 (99%)	588 (97%)	15 (2%)	2 (0%)	46	42
All	All	1210/1220 (99%)	1183 (98%)	24 (2%)	3 (0%)	52	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	GLY
1	B	575	GLN
1	B	78	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	514/524 (98%)	506 (98%)	8 (2%)	70	76
1	B	514/524 (98%)	504 (98%)	10 (2%)	65	69
All	All	1028/1048 (98%)	1010 (98%)	18 (2%)	66	71

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

Mol	Chain	Res	Type
1	A	147	LEU
1	A	262	GLU
1	A	279	VAL
1	A	326	ARG
1	A	352	THR
1	A	368	TYR
1	A	372	TYR
1	A	388	HIS
1	B	35	SER
1	B	147	LEU
1	B	209	ASP
1	B	279	VAL
1	B	327	GLU
1	B	368	TYR
1	B	372	TYR
1	B	377	VAL
1	B	388	HIS
1	B	560	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	25	GLN
1	A	371	GLN
1	A	471	GLN
1	A	491	HIS
1	A	582	GLN
1	B	25	GLN
1	B	188	GLN
1	B	355	GLN

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Mol	Chain	Res	Type
1	B	371	GLN
1	B	491	HIS
1	B	598	GLN

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

15 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	1612	1,3	14,14,15	0.52	0	15,19,21	0.97	1 (6%)
3	FUC	A	1613	3	10,10,11	0.71	0	14,14,16	1.53	3 (21%)
4	NAG	A	1614	1,4	14,14,15	0.55	0	15,19,21	0.94	1 (6%)
4	NAG	A	1615	4	14,14,15	0.50	0	15,19,21	0.96	1 (6%)
5	NAG	A	1616	1,5	14,14,15	0.51	0	15,19,21	0.85	0
5	NAG	A	1617	5	14,14,15	0.54	0	15,19,21	0.82	0
5	BMA	A	1618	5	11,11,12	0.42	0	14,15,17	0.75	0
5	FUC	A	1619	5	10,10,11	0.56	0	14,14,16	0.73	0
3	NAG	B	1612	1,3	14,14,15	0.54	0	15,19,21	1.19	2 (13%)
3	FUC	B	1613	3	10,10,11	0.59	0	14,14,16	1.29	2 (14%)
4	NAG	B	1614	1,4	14,14,15	0.57	0	15,19,21	0.80	0
4	NAG	B	1615	4	14,14,15	0.46	0	15,19,21	1.12	1 (6%)
10	NAG	B	1616	1,10	14,14,15	0.47	0	15,19,21	0.80	0
10	NAG	B	1617	10	14,14,15	0.54	0	15,19,21	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
10	BMA	B	1618	10	11,11,12	0.50	0	14,15,17	1.43	2 (14%)

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
3	NAG	A	1612	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	1613	3	-	0/0/17/20	0/1/1/1
4	NAG	A	1614	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1615	4	-	0/6/23/26	0/1/1/1
5	NAG	A	1616	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1617	5	-	0/6/23/26	0/1/1/1
5	BMA	A	1618	5	-	0/2/19/22	0/1/1/1
5	FUC	A	1619	5	-	0/0/17/20	0/1/1/1
3	NAG	B	1612	1,3	-	0/6/23/26	0/1/1/1
3	FUC	B	1613	3	-	0/0/17/20	0/1/1/1
4	NAG	B	1614	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	1615	4	-	0/6/23/26	0/1/1/1
10	NAG	B	1616	1,10	-	0/6/23/26	0/1/1/1
10	NAG	B	1617	10	-	0/6/23/26	0/1/1/1
10	BMA	B	1618	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1612	NAG	C2-N2-C7	-2.37	119.99	123.04
3	B	1612	NAG	O5-C5-C6	2.18	112.07	107.35
3	A	1613	FUC	C2-C3-C4	2.34	115.02	111.04
10	B	1617	NAG	C1-O5-C5	2.40	115.30	112.25
3	B	1612	NAG	C4-C3-C2	2.41	114.97	111.23
3	A	1613	FUC	O5-C5-C6	2.58	110.39	106.13
4	A	1614	NAG	C1-O5-C5	2.63	115.58	112.25
3	B	1613	FUC	C1-C2-C3	2.67	112.70	109.54
3	B	1613	FUC	O5-C5-C6	2.76	110.69	106.13
4	A	1615	NAG	C1-O5-C5	3.04	116.10	112.25
10	B	1618	BMA	C1-O5-C5	3.13	116.22	112.25
10	B	1618	BMA	C1-C2-C3	3.56	113.75	109.54
3	A	1613	FUC	C1-C2-C3	3.77	114.01	109.54
4	B	1615	NAG	C1-O5-C5	3.86	117.15	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	3ES	A	1611	6	46,55,55	1.61	8 (17%)	55,75,75	1.03	3 (5%)
8	PEG	A	1622	-	6,6,6	0.43	0	5,5,5	0.34	0
8	PEG	A	1623	-	6,6,6	0.46	0	5,5,5	0.29	0
8	PEG	A	1624	-	6,6,6	0.42	0	5,5,5	0.37	0
9	PG4	A	1625	-	9,9,12	0.46	0	8,8,11	0.33	0
2	3ES	B	1611	6	46,55,55	1.68	7 (15%)	55,75,75	1.49	8 (14%)
9	PG4	B	1621	-	12,12,12	0.50	0	11,11,11	0.25	0
11	P6G	B	1622	-	18,18,18	0.56	0	17,17,17	0.16	0
8	PEG	B	1623	-	6,6,6	0.43	0	5,5,5	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3ES	A	1611	6	-	0/37/48/48	0/4/5/5
8	PEG	A	1622	-	-	0/4/4/4	0/0/0/0
8	PEG	A	1623	-	-	0/4/4/4	0/0/0/0
8	PEG	A	1624	-	-	0/4/4/4	0/0/0/0
9	PG4	A	1625	-	-	0/7/7/10	0/0/0/0
2	3ES	B	1611	6	-	0/37/48/48	0/4/5/5
9	PG4	B	1621	-	-	0/10/10/10	0/0/0/0
11	P6G	B	1622	-	-	0/16/16/16	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	B	1623	-	-	0/4/4/4	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1611	3ES	CBT-CBU	-6.31	1.39	1.48
2	B	1611	3ES	CBT-CBU	-5.88	1.39	1.48
2	A	1611	3ES	CBB-CBP	-4.34	1.40	1.50
2	B	1611	3ES	CBB-CBP	-4.32	1.40	1.50
2	B	1611	3ES	CBA-CBU	-2.90	1.35	1.40
2	A	1611	3ES	CBA-CBU	-2.58	1.35	1.40
2	B	1611	3ES	CBA-CBS	-2.41	1.33	1.39
2	A	1611	3ES	CBA-CBS	-2.23	1.34	1.39
2	A	1611	3ES	CBV-CBN	2.07	1.55	1.51
2	A	1611	3ES	CBE-CBQ	2.19	1.56	1.51
2	B	1611	3ES	CBV-CBN	2.83	1.56	1.51
2	A	1611	3ES	CBC-CBS	2.91	1.54	1.50
2	A	1611	3ES	PBY-CBF	3.09	1.82	1.79
2	B	1611	3ES	CBC-CBS	3.64	1.55	1.50
2	B	1611	3ES	PBY-CBF	4.09	1.83	1.79

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1611	3ES	OBJ-CBM-OAB	-3.27	117.49	124.22
2	B	1611	3ES	CBA-CBU-CBT	-2.94	125.31	129.40
2	B	1611	3ES	OAG-PBY-OAD	-2.29	110.20	113.72
2	A	1611	3ES	CB-CA-N	2.05	114.31	108.23
2	B	1611	3ES	CB-CA-N	2.21	114.78	108.23
2	A	1611	3ES	CBU-CBA-CBS	2.49	108.82	105.43
2	A	1611	3ES	CBB-OBJ-CBM	2.78	122.53	115.91
2	B	1611	3ES	CBU-CBA-CBS	3.20	109.80	105.43
2	B	1611	3ES	OBJ-CBM-NBI	3.89	119.17	110.54
2	B	1611	3ES	CBT-CBU-NBG	4.15	125.69	120.81
2	B	1611	3ES	OBJ-CBB-CBP	4.29	120.15	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1625	PG4	1	0
2	B	1611	3ES	1	0
11	B	1622	P6G	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	607/610 (99%)	0.10	31 (5%)	32	42	19, 32, 52, 70	0
1	B	607/610 (99%)	0.40	35 (5%)	26	36	20, 38, 61, 68	0
All	All	1214/1220 (99%)	0.25	66 (5%)	29	40	19, 35, 57, 70	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	325	GLY	7.9
1	B	84	THR	4.8
1	B	1	LEU	4.7
1	A	78	PRO	4.6
1	B	325	GLY	4.5
1	A	607	TYR	4.5
1	B	135	THR	4.4
1	B	609	GLU	4.3
1	B	78	PRO	4.1
1	B	71	LYS	3.8
1	B	105	LEU	3.8
1	B	134	ALA	3.7
1	B	82	GLN	3.4
1	A	323	ALA	3.4
1	A	609	GLU	3.2
1	B	133	THR	3.1
1	A	606	ASN	3.1
1	A	80	TRP	3.0
1	B	80	TRP	2.9
1	B	561	GLY	2.8
1	A	133	THR	2.8
1	A	134	ALA	2.7
1	B	83	PHE	2.7
1	A	135	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	79	ILE	2.6
1	B	591	VAL	2.6
1	A	81	GLN	2.5
1	A	82	GLN	2.5
1	B	81	GLN	2.5
1	B	412	ASP	2.5
1	B	607	TYR	2.4
1	B	86	PRO	2.4
1	A	84	THR	2.4
1	B	435	PHE	2.4
1	A	88	LEU	2.4
1	A	414	VAL	2.4
1	B	439	GLY	2.4
1	A	608	PRO	2.3
1	A	19	LEU	2.3
1	B	261	TRP	2.3
1	B	522	GLU	2.3
1	A	89	ARG	2.3
1	B	438	PHE	2.3
1	B	606	ASN	2.3
1	B	608	PRO	2.3
1	A	22	GLN	2.3
1	A	261	TRP	2.3
1	A	92	ILE	2.3
1	B	101	ALA	2.3
1	B	75	LEU	2.2
1	B	603	LEU	2.2
1	B	95	VAL	2.2
1	A	205	PRO	2.2
1	B	414	VAL	2.1
1	A	24	TYR	2.1
1	A	91	ILE	2.1
1	B	270	PRO	2.1
1	A	93	GLY	2.1
1	A	90	ARG	2.1
1	B	129	LEU	2.1
1	A	610	GLY	2.1
1	B	136	CYS	2.1
1	A	522	GLU	2.0
1	A	340	ARG	2.0
1	A	94	ALA	2.0
1	B	258	ALA	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
10	NAG	B	1616	14/15	0.76	0.28	3.74	76,80,81,82	0
4	NAG	A	1614	14/15	0.90	0.21	2.40	50,53,54,56	0
4	NAG	B	1614	14/15	0.78	0.25	1.39	51,55,58,63	0
3	NAG	B	1612	14/15	0.88	0.14	0.95	49,53,58,62	0
3	NAG	A	1612	14/15	0.86	0.14	0.67	45,49,54,59	0
5	NAG	A	1616	14/15	0.95	0.12	-0.36	50,54,57,58	0
3	FUC	B	1613	10/11	0.66	0.29	-	65,67,68,69	0
3	FUC	A	1613	10/11	0.67	0.36	-	63,65,66,66	0
4	NAG	A	1615	14/15	0.83	0.29	-	58,58,61,61	0
5	BMA	A	1618	11/12	0.79	0.23	-	66,67,67,68	0
10	BMA	B	1618	11/12	0.70	0.38	-	88,89,89,89	0
10	NAG	B	1617	14/15	0.79	0.37	-	85,86,86,88	0
5	NAG	A	1617	14/15	0.90	0.24	-	60,63,65,65	0
5	FUC	A	1619	10/11	0.88	0.20	-	57,58,59,59	0
4	NAG	B	1615	14/15	0.79	0.54	-	67,70,71,71	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
8	PEG	B	1623	7/7	0.85	0.33	11.59	51,52,53,55	0
8	PEG	A	1622	7/7	0.92	0.22	4.78	49,49,49,50	0
11	P6G	B	1622	19/19	0.68	0.18	3.83	53,55,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
9	PG4	B	1621	13/13	0.71	0.17	3.29	56,59,61,61	0
2	3ES	B	1611	51/51	0.94	0.19	0.94	23,32,47,47	0
2	3ES	A	1611	51/51	0.94	0.17	0.71	22,30,43,43	0
8	PEG	A	1623	7/7	0.75	0.21	0.70	59,60,60,61	0
9	PG4	A	1625	10/13	0.91	0.15	0.70	50,51,52,52	0
8	PEG	A	1624	7/7	0.82	0.18	0.38	56,57,58,58	0
7	CL	B	1620	1/1	0.98	0.08	-3.24	31,31,31,31	0
7	CL	A	1621	1/1	1.00	0.06	-3.37	23,23,23,23	0
6	ZN	A	1620	1/1	1.00	0.13	-	25,25,25,25	0
6	ZN	B	1619	1/1	1.00	0.13	-	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.