Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2024 – 10:44 PM EST

PDB ID	:	1Y10
Title	:	Mycobacterial adenylyl cyclase Rv1264, holoenzyme, inhibited state
Authors	:	Tews, I.; Findeisen, F.; Sinning, I.; Schultz, A.; Schultz, J.E.; Linder, J.U.
Deposited on	:	2004-11-16
Resolution	:	2.30 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 (1)) were used in the production of this report:

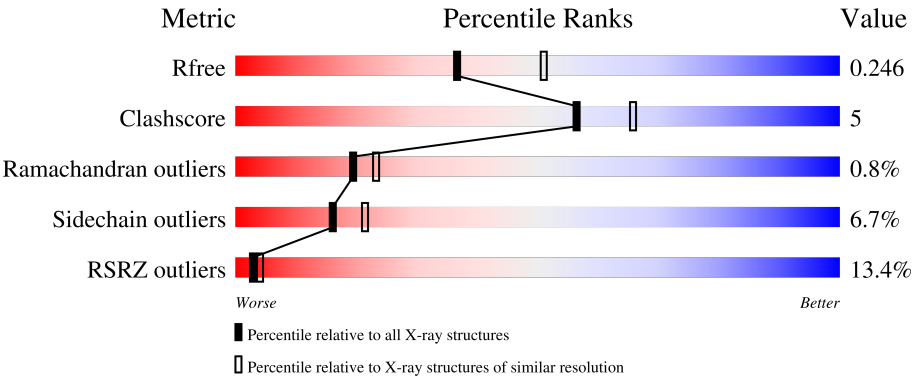
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	407	11% 79% 8% • 12%
1	B	407	13% 72% 13% • 12%
1	C	407	14% 75% 12% • 11%
1	D	407	10% 73% 13% • 13%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11381 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 Hypothetical protein Rv1264/MT1302.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2708	1699	497	501	11			
1	B	357	Total	C	N	O	S	0	0	0
			2689	1688	494	496	11			
1	C	363	Total	C	N	O	S	0	0	0
			2728	1711	500	506	11			
1	D	356	Total	C	N	O	S	0	0	0
			2678	1682	492	493	11			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	GLY	-	expression tag	UNP Q11055
A	399	SER	-	expression tag	UNP Q11055
A	400	ARG	-	expression tag	UNP Q11055
A	401	SER	-	expression tag	UNP Q11055
A	402	HIS	-	expression tag	UNP Q11055
A	403	HIS	-	expression tag	UNP Q11055
A	404	HIS	-	expression tag	UNP Q11055
A	405	HIS	-	expression tag	UNP Q11055
A	406	HIS	-	expression tag	UNP Q11055
A	407	HIS	-	expression tag	UNP Q11055
B	398	GLY	-	expression tag	UNP Q11055
B	399	SER	-	expression tag	UNP Q11055
B	400	ARG	-	expression tag	UNP Q11055
B	401	SER	-	expression tag	UNP Q11055
B	402	HIS	-	expression tag	UNP Q11055
B	403	HIS	-	expression tag	UNP Q11055
B	404	HIS	-	expression tag	UNP Q11055
B	405	HIS	-	expression tag	UNP Q11055
B	406	HIS	-	expression tag	UNP Q11055
B	407	HIS	-	expression tag	UNP Q11055
C	398	GLY	-	expression tag	UNP Q11055

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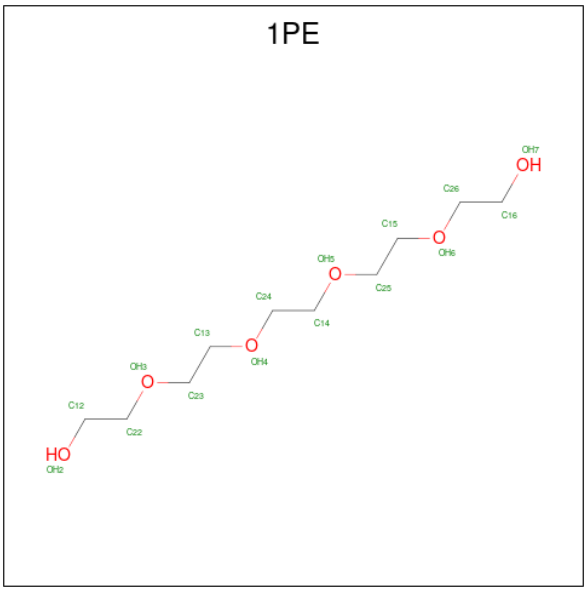
Chain	Residue	Modelled	Actual	Comment	Reference
C	399	SER	-	expression tag	UNP Q11055
C	400	ARG	-	expression tag	UNP Q11055
C	401	SER	-	expression tag	UNP Q11055
C	402	HIS	-	expression tag	UNP Q11055
C	403	HIS	-	expression tag	UNP Q11055
C	404	HIS	-	expression tag	UNP Q11055
C	405	HIS	-	expression tag	UNP Q11055
C	406	HIS	-	expression tag	UNP Q11055
C	407	HIS	-	expression tag	UNP Q11055
D	398	GLY	-	expression tag	UNP Q11055
D	399	SER	-	expression tag	UNP Q11055
D	400	ARG	-	expression tag	UNP Q11055
D	401	SER	-	expression tag	UNP Q11055
D	402	HIS	-	expression tag	UNP Q11055
D	403	HIS	-	expression tag	UNP Q11055
D	404	HIS	-	expression tag	UNP Q11055
D	405	HIS	-	expression tag	UNP Q11055
D	406	HIS	-	expression tag	UNP Q11055
D	407	HIS	-	expression tag	UNP Q11055

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Ca 3 3	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	3	Total Ca 3 3	0	0

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	B	1	Total C O 16 10 6	0	0
3	D	1	Total C O 16 10 6	0	0

- Molecule 4 is water.

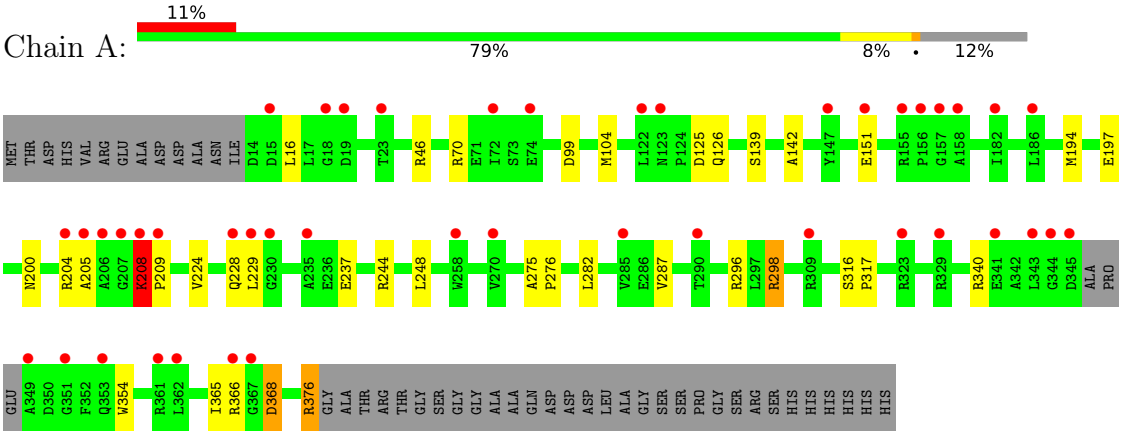
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	122	Total O 122 122	0	0
4	B	122	Total O 122 122	0	0
4	C	143	Total O 143 143	0	0
4	D	135	Total O 135 135	0	0

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.

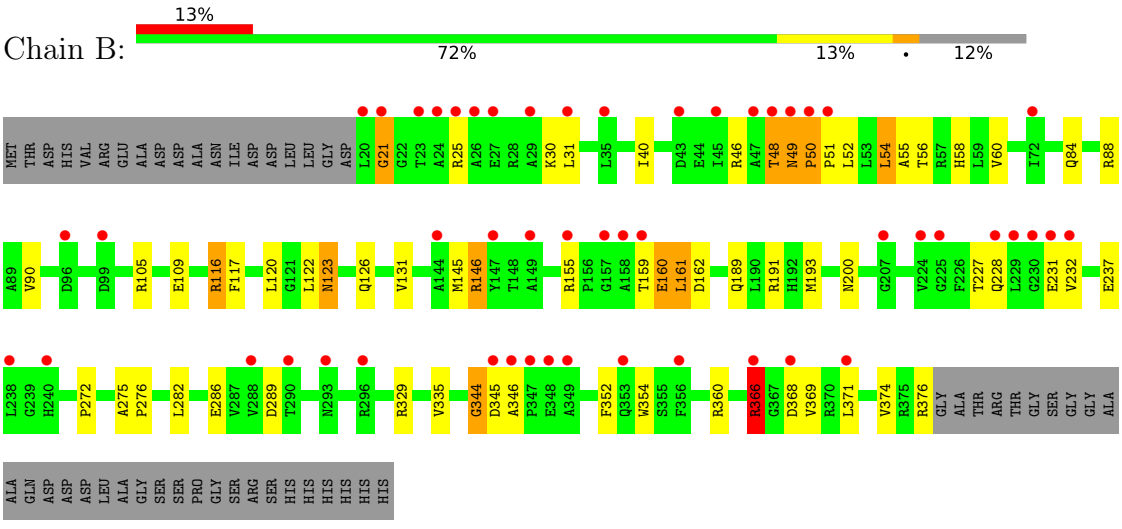
• Molecule 1: Hypothetical protein Rv1264/MT1302

Chain A:



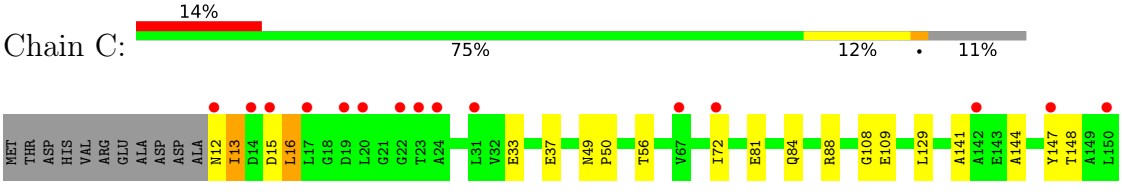
• Molecule 1: Hypothetical protein Rv1264/MT1302

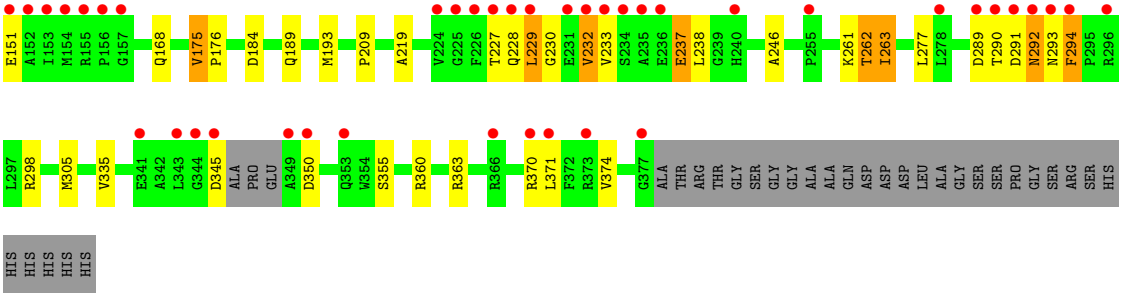
Chain B:



• Molecule 1: Hypothetical protein Rv1264/MT1302

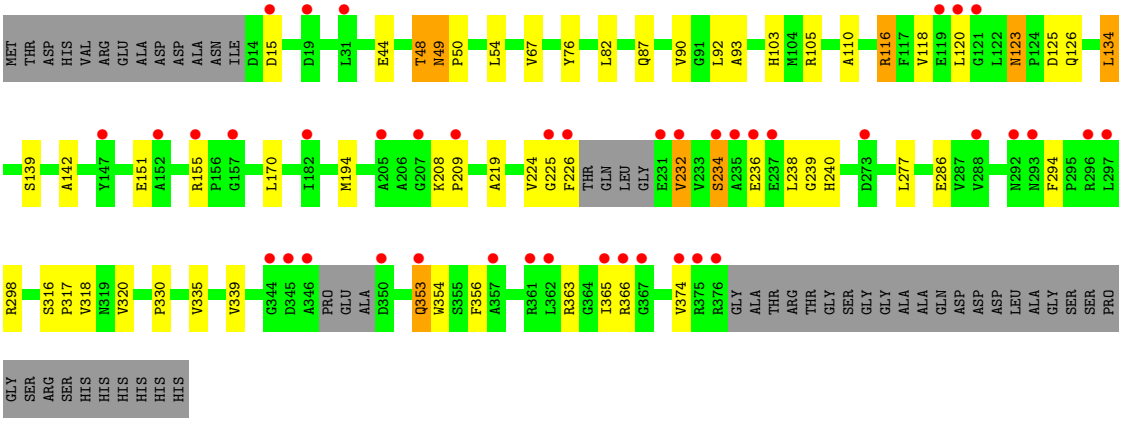
Chain C:





• Molecule 1: Hypothetical protein Rv1264/MT1302

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	61.94Å 146.83Å 84.85Å 90.00° 105.26° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 14.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-2.30) 98.0 (14.98-2.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.190 , 0.242 0.195 , 0.246	Depositor DCC
R_{free} test set	3191 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 50.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11381	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, 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	0.60	0/2751	0.64	0/3737
1	B	0.65	0/2734	0.65	0/3717
1	C	0.65	0/2771	0.67	0/3765
1	D	0.65	0/2720	0.64	0/3694
All	All	0.64	0/10976	0.65	0/14913

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	49	ASN	Peptide
1	C	292	ASN	Peptide

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	2708	0	2747	24	0
1	B	2689	0	2732	34	0
1	C	2728	0	2764	35	0
1	D	2678	0	2716	35	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	3	0	0	0	0
3	A	16	0	22	0	0
3	B	16	0	22	1	0
3	D	16	0	22	0	0
4	A	122	0	0	0	0
4	B	122	0	0	2	0
4	C	143	0	0	2	0
4	D	135	0	0	2	0
All	All	11381	0	11025	109	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 5.

All (109) 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:208:LYS:HB2	1:A:209:PRO:CD	1.95	0.96
1:C:12:ASN:HD21	1:C:15:ASP:HB2	1.34	0.92
1:A:208:LYS:HB2	1:A:209:PRO:HD2	1.62	0.78
1:D:226:PHE:HZ	1:D:330:PRO:CG	2.00	0.75
1:C:227:THR:HG22	1:C:228:GLN:H	1.52	0.74
1:B:31:LEU:HB2	1:B:160:GLU:OE1	1.89	0.72
1:A:139:SER:HA	1:B:189:GLN:HE22	1.56	0.70
1:A:248:LEU:HD11	1:A:287:VAL:HG21	1.72	0.70
1:D:226:PHE:HZ	1:D:330:PRO:HG2	1.57	0.68
1:B:344:GLY:O	1:B:346:ALA:N	2.27	0.67
1:D:87:GLN:HB2	1:D:92:LEU:HD12	1.75	0.67
1:D:123:ASN:HD21	1:D:125:ASP:HB2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:VAL:HG12	1:C:176:PRO:HD3	1.80	0.64
1:C:189:GLN:HE22	1:D:139:SER:HA	1.62	0.63
1:D:234:SER:O	1:D:238:LEU:HG	1.99	0.62
1:C:144:ALA:HA	1:C:147:TYR:CE2	2.34	0.62
1:C:141:ALA:HB2	1:D:134:LEU:HD13	1.80	0.62
1:A:151:GLU:OE1	1:B:126:GLN:NE2	2.33	0.62
1:C:12:ASN:ND2	1:C:15:ASP:HB2	2.13	0.61
1:C:232:VAL:HG12	1:C:233:VAL:H	1.66	0.60
1:C:246:ALA:HB2	1:C:262:THR:HG21	1.83	0.60
1:D:48:THR:HG21	1:D:54:LEU:HD13	1.83	0.60
1:A:208:LYS:HB2	1:A:209:PRO:HD3	1.79	0.59
1:D:208:LYS:HB2	1:D:209:PRO:HD2	1.85	0.58
1:D:67:VAL:HG22	1:D:105:ARG:HA	1.86	0.58
1:B:159:THR:HG22	1:B:162:ASP:OD2	2.05	0.57
1:A:340:ARG:HB3	1:A:354:TRP:CZ3	2.39	0.56
1:B:49:ASN:HB3	1:B:50:PRO:HD2	1.88	0.56
1:B:48:THR:HG21	1:B:54:LEU:HD11	1.88	0.56
1:D:224:VAL:HG23	1:D:225:GLY:O	2.05	0.56
1:D:353:GLN:HE21	1:D:353:GLN:N	2.03	0.55
1:D:82:LEU:HD21	1:D:118:VAL:HG21	1.89	0.55
1:C:56:THR:HB	1:D:194:MET:HE1	1.89	0.55
1:D:226:PHE:HZ	1:D:330:PRO:HG3	1.73	0.53
1:B:123:ASN:C	1:B:123:ASN:HD22	2.12	0.53
1:C:219:ALA:HB2	1:C:277:LEU:HD21	1.91	0.53
1:B:117:PHE:HB3	1:B:122:LEU:HD12	1.90	0.53
1:C:209:PRO:HB3	1:C:305:MET:HB2	1.90	0.52
1:D:76:TYR:HE1	4:D:707:HOH:O	1.92	0.52
1:A:70:ARG:HD2	1:A:99:ASP:OD2	2.11	0.50
1:A:194:MET:CE	1:B:60:VAL:HG21	2.42	0.50
1:B:21:GLY:HA2	1:B:25:ARG:HD2	1.94	0.50
1:C:12:ASN:OD1	1:C:13:ILE:N	2.45	0.50
1:C:72:ILE:HD13	1:C:108:GLY:HA3	1.94	0.50
1:D:226:PHE:CZ	1:D:330:PRO:HG2	2.44	0.49
1:C:175:VAL:N	1:C:176:PRO:HD2	2.27	0.49
1:A:224:VAL:HG12	1:A:298:ARG:HE	1.77	0.49
1:A:275:ALA:HB3	1:A:276:PRO:HD3	1.95	0.49
1:B:366:ARG:NH1	4:B:707:HOH:O	2.44	0.49
1:C:298:ARG:HH22	1:D:232:VAL:HG13	1.77	0.49
1:C:261:LYS:HE3	1:C:263:ILE:HG12	1.95	0.48
1:B:145:MET:HG2	3:B:602:1PE:H152	1.96	0.47
1:A:197:GLU:OE1	1:B:146:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HG21	1:B:354:TRP:CZ3	2.48	0.47
1:D:123:ASN:H	1:D:126:GLN:HE21	1.61	0.47
1:A:16:LEU:HD23	1:A:46:ARG:HG3	1.97	0.47
1:A:248:LEU:HD11	1:A:287:VAL:CG2	2.43	0.47
1:C:189:GLN:NE2	1:D:139:SER:HA	2.28	0.47
1:C:263:ILE:HG23	4:D:675:HOH:O	2.15	0.47
1:A:229:LEU:O	1:B:329:ARG:NH2	2.48	0.46
1:B:286:GLU:OE2	1:B:376:ARG:HD2	2.14	0.46
1:B:275:ALA:HB3	1:B:276:PRO:HD3	1.97	0.46
1:D:93:ALA:O	1:D:103:HIS:HE1	1.98	0.46
1:D:87:GLN:HA	1:D:90:VAL:HG22	1.97	0.46
1:C:129:LEU:HD13	1:D:239:GLY:HA3	1.97	0.46
1:B:344:GLY:C	1:B:346:ALA:H	2.20	0.45
1:A:194:MET:HE1	1:B:60:VAL:HG21	1.97	0.45
1:B:227:THR:HG22	1:B:228:GLN:H	1.81	0.45
1:A:205:ALA:HB3	1:B:50:PRO:HG2	1.99	0.45
1:B:40:ILE:HD11	1:B:55:ALA:HB2	1.98	0.45
1:B:84:GLN:O	1:B:88:ARG:HG3	2.16	0.45
1:C:141:ALA:HB2	1:D:134:LEU:CD1	2.47	0.44
1:C:233:VAL:HG13	1:C:237:GLU:HB3	1.99	0.44
1:D:44:GLU:O	1:D:48:THR:HG22	2.17	0.44
1:A:16:LEU:CD2	1:A:46:ARG:HG3	2.47	0.44
1:C:229:LEU:N	4:C:721:HOH:O	2.50	0.44
1:D:49:ASN:HD22	1:D:50:PRO:HA	1.83	0.44
1:D:335:VAL:CG1	1:D:339:VAL:HB	2.48	0.44
1:D:219:ALA:HB2	1:D:277:LEU:HD21	2.00	0.43
1:B:116:ARG:O	1:B:120:LEU:HG	2.19	0.43
1:D:224:VAL:HG12	1:D:298:ARG:HH11	1.83	0.43
1:B:50:PRO:HA	1:B:51:PRO:HD3	1.79	0.43
1:A:282:LEU:HD13	1:A:376:ARG:HD3	2.00	0.43
1:D:320:VAL:HG22	1:D:365:ILE:HG12	2.01	0.43
1:A:365:ILE:HG22	1:A:366:ARG:N	2.34	0.43
1:D:354:TRP:CE3	1:D:374:VAL:HG22	2.54	0.43
1:C:12:ASN:OD1	1:C:16:LEU:HD22	2.18	0.42
1:C:84:GLN:O	1:C:88:ARG:HG3	2.19	0.42
1:B:352:PHE:HB3	1:B:374:VAL:HG13	2.00	0.42
1:A:316:SER:N	1:A:317:PRO:HD2	2.34	0.42
1:B:90:VAL:CG1	1:B:131:VAL:HG13	2.49	0.42
1:C:12:ASN:ND2	1:C:15:ASP:OD2	2.52	0.42
1:C:184:ASP:HB3	1:D:110:ALA:HB1	2.02	0.42
1:D:316:SER:N	1:D:317:PRO:HD2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:TYR:HA	1:C:151:GLU:HB2	2.01	0.42
1:C:229:LEU:HG	4:C:721:HOH:O	2.20	0.42
1:B:58:HIS:HE1	1:C:109:GLU:OE1	2.01	0.42
1:D:116:ARG:O	1:D:120:LEU:HD13	2.20	0.42
1:A:104:MET:HE2	1:B:191:ARG:HD2	2.02	0.42
1:C:291:ASP:O	1:C:294:PHE:HB2	2.21	0.41
1:A:142:ALA:HB1	1:B:193:MET:CE	2.50	0.41
1:B:344:GLY:C	1:B:346:ALA:N	2.74	0.41
1:C:49:ASN:HA	1:C:50:PRO:HA	1.92	0.41
1:C:193:MET:HE1	1:D:142:ALA:O	2.21	0.41
1:C:335:VAL:HG21	1:C:374:VAL:HG21	2.02	0.41
1:A:228:GLN:HE21	1:A:296:ARG:HD2	1.86	0.41
1:B:272:PRO:O	4:B:610:HOH:O	2.20	0.41
1:B:30:LYS:HB3	1:B:161:LEU:HD12	2.03	0.40
1:C:33:GLU:O	1:C:37:GLU:HB2	2.22	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	356/407 (88%)	349 (98%)	5 (1%)	2 (1%)	25 31
1	B	355/407 (87%)	340 (96%)	9 (2%)	6 (2%)	9 8
1	C	359/407 (88%)	344 (96%)	11 (3%)	4 (1%)	14 15
1	D	350/407 (86%)	339 (97%)	11 (3%)	0	100 100
All	All	1420/1628 (87%)	1372 (97%)	36 (2%)	12 (1%)	19 23

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	48	THR
1	B	50	PRO
1	B	345	ASP
1	B	366	ARG
1	C	13	ILE
1	C	232	VAL
1	A	208	LYS
1	A	368	ASP
1	B	344	GLY
1	C	148	THR
1	C	230	GLY
1	B	21	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	277/312 (89%)	267 (96%)	10 (4%)	35	49
1	B	275/312 (88%)	252 (92%)	23 (8%)	11	13
1	C	279/312 (89%)	258 (92%)	21 (8%)	13	17
1	D	273/312 (88%)	253 (93%)	20 (7%)	14	18
All	All	1104/1248 (88%)	1030 (93%)	74 (7%)	16	21

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125	ASP
1	A	126	GLN
1	A	200	ASN
1	A	204	ARG
1	A	208	LYS
1	A	237	GLU
1	A	244	ARG
1	A	298	ARG
1	A	368	ASP
1	A	376	ARG

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Mol	Chain	Res	Type
1	B	46	ARG
1	B	52	LEU
1	B	54	LEU
1	B	56	THR
1	B	105	ARG
1	B	109	GLU
1	B	116	ARG
1	B	123	ASN
1	B	146	ARG
1	B	155	ARG
1	B	160	GLU
1	B	161	LEU
1	B	200	ASN
1	B	231	GLU
1	B	232	VAL
1	B	237	GLU
1	B	282	LEU
1	B	289	ASP
1	B	360	ARG
1	B	366	ARG
1	B	368	ASP
1	B	369	VAL
1	B	371	LEU
1	C	16	LEU
1	C	81	GLU
1	C	168	GLN
1	C	175	VAL
1	C	229	LEU
1	C	237	GLU
1	C	238	LEU
1	C	262	THR
1	C	263	ILE
1	C	289	ASP
1	C	290	THR
1	C	292	ASN
1	C	293	ASN
1	C	294	PHE
1	C	345	ASP
1	C	350	ASP
1	C	355	SER
1	C	360	ARG
1	C	363	ARG

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Mol	Chain	Res	Type
1	C	370	ARG
1	C	371	LEU
1	D	15	ASP
1	D	48	THR
1	D	49	ASN
1	D	116	ARG
1	D	123	ASN
1	D	134	LEU
1	D	151	GLU
1	D	155	ARG
1	D	170	LEU
1	D	232	VAL
1	D	234	SER
1	D	236	GLU
1	D	240	HIS
1	D	286	GLU
1	D	294	PHE
1	D	318	VAL
1	D	353	GLN
1	D	356	PHE
1	D	363	ARG
1	D	366	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	B	38	GLN
1	B	58	HIS
1	B	103	HIS
1	B	123	ASN
1	B	126	GLN
1	B	189	GLN
1	B	200	ASN
1	C	75	ASN
1	C	87	GLN
1	C	168	GLN
1	C	189	GLN
1	C	200	ASN
1	C	240	HIS
1	C	292	ASN
1	C	293	ASN

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Mol	Chain	Res	Type
1	C	319	ASN
1	D	38	GLN
1	D	49	ASN
1	D	87	GLN
1	D	103	HIS
1	D	126	GLN
1	D	240	HIS
1	D	353	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 11 ligands modelled in this entry, 8 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	1PE	D	603	-	15,15,15	0.57	0	14,14,14	0.28	0
3	1PE	A	601	-	15,15,15	0.63	0	14,14,14	0.21	0
3	1PE	B	602	-	15,15,15	0.57	0	14,14,14	0.22	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
3	1PE	D	603	-	-	9/13/13/13	-
3	1PE	A	601	-	-	6/13/13/13	-
3	1PE	B	602	-	-	6/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	1PE	OH2-C12-C22-OH3
3	A	601	1PE	OH4-C13-C23-OH3
3	B	602	1PE	OH4-C13-C23-OH3
3	A	601	1PE	OH5-C14-C24-OH4
3	D	603	1PE	OH6-C15-C25-OH5
3	D	603	1PE	OH2-C12-C22-OH3
3	D	603	1PE	OH7-C16-C26-OH6
3	D	603	1PE	C13-C23-OH3-C22
3	A	601	1PE	C24-C14-OH5-C25
3	D	603	1PE	C16-C26-OH6-C15
3	D	603	1PE	OH5-C14-C24-OH4
3	B	602	1PE	C23-C13-OH4-C24
3	D	603	1PE	C12-C22-OH3-C23
3	D	603	1PE	C24-C14-OH5-C25
3	A	601	1PE	C23-C13-OH4-C24
3	B	602	1PE	C24-C14-OH5-C25
3	D	603	1PE	OH4-C13-C23-OH3
3	A	601	1PE	OH6-C15-C25-OH5
3	B	602	1PE	OH2-C12-C22-OH3
3	B	602	1PE	OH7-C16-C26-OH6
3	B	602	1PE	OH6-C15-C25-OH5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	1PE	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	360/407 (88%)	0.76	44 (12%)	4 6	37, 48, 59, 70	0
1	B	357/407 (87%)	0.96	51 (14%)	2 3	38, 48, 62, 77	0
1	C	363/407 (89%)	0.87	56 (15%)	2 3	37, 48, 64, 70	0
1	D	356/407 (87%)	0.83	42 (11%)	4 6	34, 48, 62, 72	0
All	All	1436/1628 (88%)	0.85	193 (13%)	3 4	34, 48, 62, 77	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	345	ASP	11.5
1	B	20	LEU	9.8
1	D	226	PHE	9.2
1	A	207	GLY	7.9
1	D	344	GLY	7.7
1	D	234	SER	7.3
1	A	206	ALA	7.1
1	D	231	GLU	7.1
1	D	293	ASN	6.9
1	B	21	GLY	6.8
1	B	47	ALA	6.5
1	D	225	GLY	6.2
1	D	345	ASP	6.2
1	D	346	ALA	6.0
1	C	236	GLU	6.0
1	B	229	LEU	5.9
1	B	26	ALA	5.9
1	C	226	PHE	5.8
1	B	346	ALA	5.8
1	B	147	TYR	5.4
1	C	290	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	232	VAL	5.1
1	C	289	ASP	5.1
1	C	229	LEU	5.0
1	A	344	GLY	5.0
1	B	232	VAL	4.9
1	B	23	THR	4.9
1	C	12	ASN	4.9
1	A	228	GLN	4.9
1	B	96	ASP	4.9
1	B	348	GLU	4.9
1	C	344	GLY	4.8
1	D	235	ALA	4.8
1	C	147	TYR	4.8
1	D	292	ASN	4.7
1	B	49	ASN	4.5
1	C	345	ASP	4.5
1	B	48	THR	4.5
1	B	293	ASN	4.5
1	C	22	GLY	4.4
1	C	19	ASP	4.4
1	B	230	GLY	4.3
1	B	31	LEU	4.2
1	A	367	GLY	4.2
1	B	228	GLN	4.2
1	D	236	GLU	4.2
1	A	19	ASP	4.2
1	A	156	PRO	4.2
1	D	366	ARG	4.1
1	C	366	ARG	4.1
1	D	367	GLY	4.1
1	B	25	ARG	4.1
1	C	292	ASN	4.1
1	A	345	ASP	4.0
1	B	225	GLY	4.0
1	B	366	ARG	4.0
1	A	209	PRO	3.9
1	C	234	SER	3.9
1	C	150	LEU	3.9
1	C	156	PRO	3.9
1	A	151	GLU	3.8
1	B	368	ASP	3.8
1	A	157	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	147	TYR	3.8
1	B	27	GLU	3.7
1	B	207	GLY	3.7
1	B	24	ALA	3.7
1	C	225	GLY	3.7
1	D	361	ARG	3.6
1	A	290	THR	3.6
1	C	155	ARG	3.6
1	C	228	GLN	3.6
1	B	347	PRO	3.5
1	B	371	LEU	3.4
1	D	365	ILE	3.4
1	A	208	LYS	3.4
1	D	15	ASP	3.4
1	A	361	ARG	3.4
1	C	224	VAL	3.4
1	A	205	ALA	3.4
1	C	350	ASP	3.4
1	B	349	ALA	3.3
1	C	235	ALA	3.3
1	C	231	GLU	3.3
1	D	376	ARG	3.3
1	D	120	LEU	3.2
1	B	155	ARG	3.2
1	B	159	THR	3.2
1	B	231	GLU	3.2
1	D	157	GLY	3.2
1	C	294	PHE	3.1
1	D	121	GLY	3.1
1	C	151	GLU	3.1
1	C	20	LEU	3.1
1	C	23	THR	3.0
1	B	353	GLN	3.0
1	C	232	VAL	3.0
1	C	240	HIS	3.0
1	C	343	LEU	3.0
1	C	291	ASP	3.0
1	B	224	VAL	2.9
1	D	297	LEU	2.9
1	A	229	LEU	2.9
1	C	296	ARG	2.9
1	A	341	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	153	ILE	2.8
1	C	15	ASP	2.8
1	B	149	ALA	2.8
1	C	227	THR	2.8
1	A	158	ALA	2.8
1	C	17	LEU	2.8
1	A	74	GLU	2.8
1	D	31	LEU	2.8
1	C	31	LEU	2.7
1	A	366	ARG	2.7
1	C	152	ALA	2.7
1	A	204	ARG	2.6
1	D	357	ALA	2.6
1	D	207	GLY	2.6
1	B	50	PRO	2.6
1	D	205	ALA	2.6
1	A	309	ARG	2.6
1	D	119	GLU	2.6
1	B	72	ILE	2.6
1	B	99	ASP	2.6
1	A	349	ALA	2.6
1	A	351	GLY	2.6
1	D	19	ASP	2.6
1	B	288	VAL	2.5
1	A	155	ARG	2.5
1	A	343	LEU	2.5
1	A	362	LEU	2.5
1	C	24	ALA	2.5
1	D	147	TYR	2.5
1	D	155	ARG	2.5
1	C	353	GLN	2.4
1	A	323	ARG	2.4
1	D	374	VAL	2.4
1	B	296	ARG	2.4
1	C	293	ASN	2.4
1	A	230	GLY	2.4
1	B	240	HIS	2.4
1	A	258	TRP	2.4
1	D	350	ASP	2.4
1	A	23	THR	2.4
1	D	288	VAL	2.4
1	B	45	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	43	ASP	2.3
1	C	14	ASP	2.3
1	B	290	THR	2.3
1	A	15	ASP	2.3
1	C	377	GLY	2.3
1	C	373	ARG	2.3
1	D	375	ARG	2.3
1	D	273	ASP	2.3
1	A	18	GLY	2.3
1	A	122	LEU	2.2
1	B	35	LEU	2.2
1	C	371	LEU	2.2
1	B	51	PRO	2.2
1	B	29	ALA	2.2
1	C	72	ILE	2.2
1	C	154	MET	2.2
1	A	186	LEU	2.2
1	A	329	ARG	2.2
1	D	152	ALA	2.2
1	A	123	ASN	2.2
1	D	296	ARG	2.2
1	B	157	GLY	2.2
1	A	353	GLN	2.2
1	C	157	GLY	2.2
1	D	353	GLN	2.2
1	B	158	ALA	2.1
1	A	72	ILE	2.1
1	A	235	ALA	2.1
1	D	209	PRO	2.1
1	C	370	ARG	2.1
1	D	362	LEU	2.1
1	C	142	ALA	2.1
1	A	270	VAL	2.1
1	C	233	VAL	2.1
1	B	356	PHE	2.1
1	C	255	PRO	2.1
1	D	182	ILE	2.1
1	C	341	GLU	2.1
1	A	285	VAL	2.1
1	D	237	GLU	2.0
1	B	238	LEU	2.0
1	C	349	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	67	VAL	2.0
1	A	182	ILE	2.0
1	C	278	LEU	2.0
1	B	144	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)

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, 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	B-factors(Å^2)	Q<0.9
2	CA	A	608	1/1	0.80	0.12	70,70,70,70	0
2	CA	C	604	1/1	0.81	0.20	86,86,86,86	0
2	CA	A	607	1/1	0.82	0.22	76,76,76,76	0
2	CA	D	605	1/1	0.83	0.21	85,85,85,85	0
2	CA	A	609	1/1	0.84	0.14	65,65,65,65	0
3	1PE	B	602	16/16	0.88	0.15	60,64,74,74	0
3	1PE	D	603	16/16	0.88	0.15	65,71,77,77	0
3	1PE	A	601	16/16	0.89	0.15	57,66,71,71	0
2	CA	B	606	1/1	0.94	0.06	62,62,62,62	0
2	CA	D	611	1/1	0.95	0.17	70,70,70,70	0
2	CA	D	610	1/1	0.95	0.10	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.