WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:39 AM GMT

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PDB ID	:	2RKI
Title	:	Crystal Structure of HIV-1 Reverse Transcriptase (RT) in Complex with a triazole derived NNRTI
Authors	:	Lansdon, E.B.; Kirschberg, T.A.
Deposited on	:	2007-10-16
Resolution	:	2.30 Å(reported)

1　Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
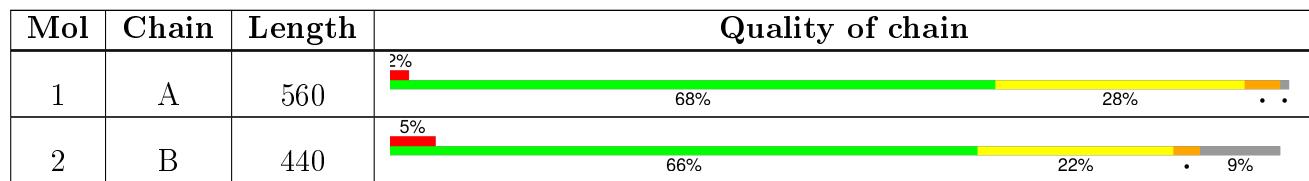
The reported resolution of this entry is 2.30 Å.

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	Percentile Ranks	Value
Rfree		0.269
Clashscore		14
Ramachandran outliers		0.3%
Sidechain outliers		6.9%
RSRZ outliers		3.3%

Worse　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	560	2% · 68% · 28% · ·
2	B	440	5% · 66% · 22% · 9%

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	GOL	A	569	-	-	-	X
5	SO4	A	563	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8224 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.
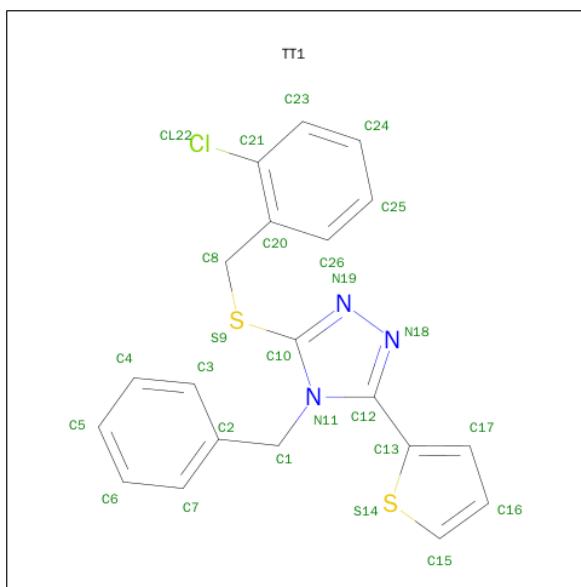
- Molecule 1 is a protein called HIV-1 reverse transcriptase (RT) p66.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	0	0	0
			4536	2931	759	838	8			

- Molecule 2 is a protein called HIV-1 reverse transcriptase (RT) p51.
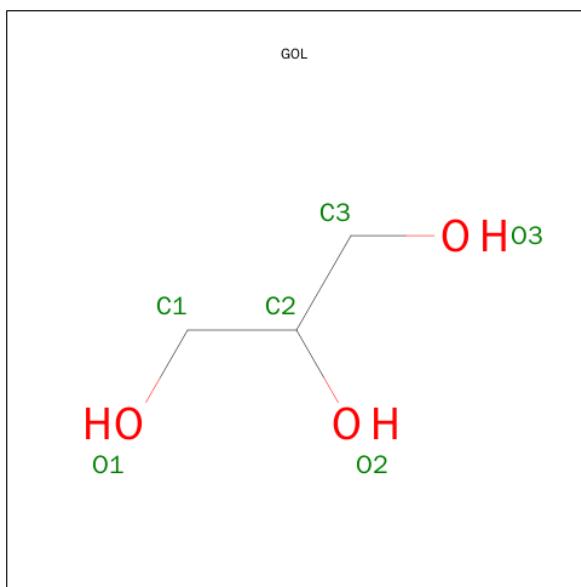
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			3328	2168	549	605	6			

- Molecule 3 is 4-BENZYL-3-[(2-CHLOROBENZYL)SULFANYL]-5-THIOPHEN-2-YL-4H-1 ,2,4-TRIAZOLE (three-letter code: TT1) (formula: $C_{20}H_{16}ClN_3S_2$).
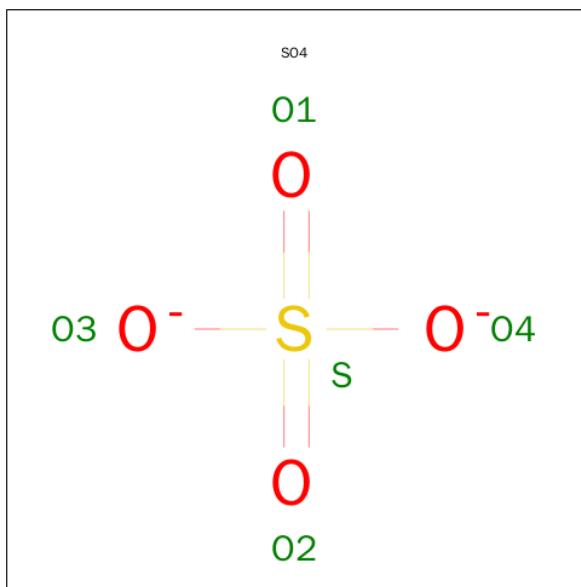
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	S	0	0
			26	20	1	3	2		

• Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total 4	Cl 4	0	0
6	A	1	Total 1	Cl 1	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	Mg 1	0	0
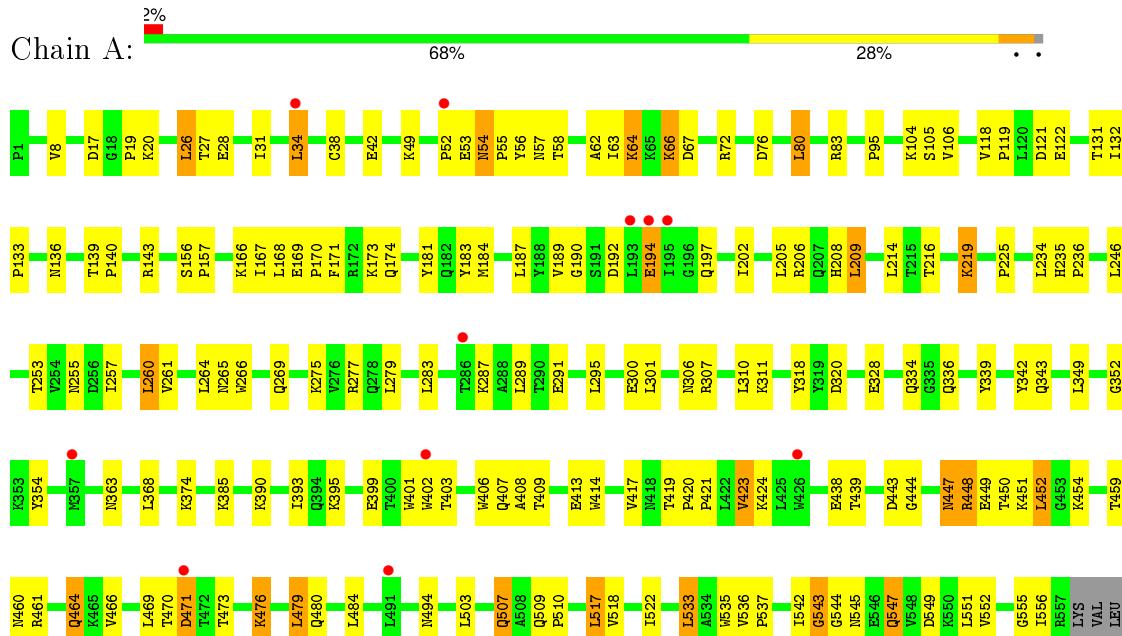
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	186	Total 186	O 186	0	0
8	B	111	Total 111	O 111	0	0
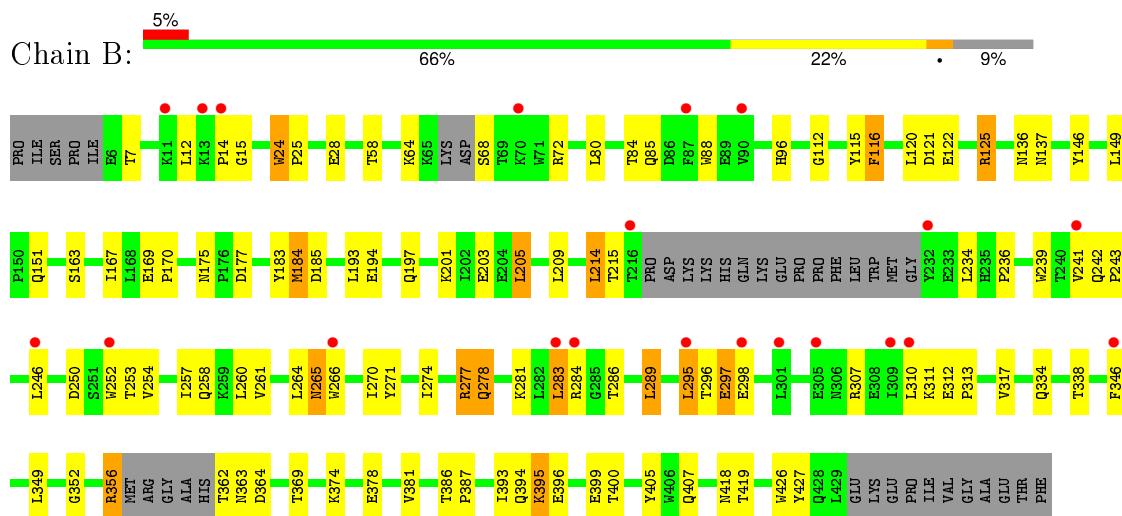
3 Residue-property plots (i)

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: HIV-1 reverse transcriptase (RT) p66

- Molecule 2: HIV-1 reverse transcriptase (RT) p51

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	118.39Å 154.17Å 154.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 2.30 47.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.0 (29.88-2.30) 90.1 (47.14-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.81 (at 2.32Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.216 , 0.270 0.212 , 0.269	Depositor DCC
R_{free} test set	2860 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.4	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 60748 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8224	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, MG, TT1, 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	0.33	0/4653	0.50	0/6321
2	B	0.33	0/3420	0.50	0/4647
All	All	0.33	0/8073	0.50	0/10968

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	4536	0	4590	143	0
2	B	3328	0	3359	88	0
3	A	26	0	16	2	0
4	A	6	0	8	2	0
5	A	25	0	0	0	0
6	A	1	0	0	0	0
6	B	4	0	0	0	0
7	A	1	0	0	0	0
8	A	186	0	0	7	0
8	B	111	0	0	7	0
All	All	8224	0	7973	222	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 14.

All (222) 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:459:THR:HG22	1:A:461:ARG:H	1.07	1.11
1:A:131:THR:HG22	1:A:143:ARG:HD2	1.30	1.06
1:A:459:THR:HG22	1:A:461:ARG:N	1.82	0.94
1:A:320:ASP:H	1:A:343:GLN:HE22	1.18	0.92
1:A:469:LEU:HD11	1:A:480:GLN:HG2	1.52	0.91
1:A:547:GLN:HE21	1:A:547:GLN:H	1.21	0.88
1:A:275:LYS:H	1:A:306:ASN:HD21	1.20	0.87
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.59	0.85
1:A:547:GLN:HE21	1:A:547:GLN:N	1.77	0.83
1:A:131:THR:CG2	1:A:143:ARG:HD2	2.09	0.80
1:A:131:THR:CG2	1:A:143:ARG:HH11	1.97	0.78
1:A:194:GLU:H	1:A:194:GLU:CD	1.86	0.78
1:A:555:GLY:N	1:A:556:ILE:HA	1.99	0.77
1:A:459:THR:CG2	1:A:461:ARG:H	1.91	0.77
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.66	0.75
2:B:278:GLN:HG2	2:B:298:GLU:HB2	1.69	0.74
2:B:58:THR:HG23	8:B:480:HOH:O	1.86	0.74
1:A:450:THR:HG22	1:A:452:LEU:HB3	1.68	0.74
1:A:438:GLU:OE2	1:A:459:THR:HG21	1.86	0.73
2:B:24:TRP:CE3	2:B:25:PRO:HD2	2.24	0.73
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.70	0.73
1:A:277:ARG:HH11	1:A:277:ARG:HG2	1.54	0.73
1:A:406:TRP:HD1	1:A:407:GLN:HE21	1.38	0.71
2:B:12:LEU:O	2:B:14:PRO:HD3	1.92	0.70
1:A:555:GLY:H	1:A:556:ILE:HA	1.54	0.70
1:A:277:ARG:NH1	1:A:334:GLN:HB3	2.06	0.69
2:B:394:GLN:HG2	2:B:396:GLU:OE1	1.93	0.69
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.74	0.68
2:B:395:LYS:O	2:B:399:GLU:HG2	1.92	0.68
1:A:54:ASN:ND2	1:A:56:TYR:H	1.91	0.68
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.74	0.68
1:A:401:TRP:HD1	1:A:402:TRP:CD1	2.11	0.68
1:A:57:ASN:OD1	1:A:131:THR:HG23	1.95	0.67
2:B:120:LEU:O	2:B:125:ARG:HD3	1.94	0.66
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.11	0.66
1:A:66:LYS:O	1:A:67:ASP:HB3	1.96	0.65
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:ND2	1:A:450:THR:H	1.95	0.65
2:B:369:THR:HG21	2:B:405:TYR:HB2	1.77	0.65
1:A:205:LEU:HD13	1:A:209:LEU:HD22	1.80	0.64
1:A:265:ASN:HD21	4:A:569:GOL:H32	1.62	0.64
1:A:342:TYR:HA	1:A:349:LEU:HD12	1.80	0.64
1:A:202:ILE:O	1:A:206:ARG:HG3	1.98	0.63
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.80	0.63
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.81	0.63
2:B:116:PHE:C	2:B:116:PHE:HD1	2.01	0.63
2:B:116:PHE:CD1	2:B:116:PHE:C	2.73	0.62
2:B:296:THR:CG2	2:B:298:GLU:HG2	2.29	0.62
2:B:24:TRP:CD2	2:B:25:PRO:HD2	2.35	0.61
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.66	0.61
2:B:84:THR:O	2:B:84:THR:HG22	2.00	0.61
2:B:72:ARG:NH2	8:B:552:HOH:O	2.36	0.59
1:A:450:THR:CG2	1:A:452:LEU:HB3	2.33	0.59
2:B:374:LYS:HE2	2:B:378:GLU:OE1	2.03	0.59
1:A:536:VAL:HG13	1:A:537:PRO:HD2	1.85	0.59
1:A:473:THR:OG1	1:A:476:LYS:HD3	2.02	0.58
2:B:253:THR:O	2:B:257:ILE:HG12	2.04	0.58
1:A:277:ARG:NH1	1:A:277:ARG:HG2	2.18	0.58
1:A:122:GLU:HG3	8:A:608:HOH:O	2.03	0.58
2:B:177:ASP:HB2	8:B:462:HOH:O	2.03	0.57
2:B:295:LEU:HD23	2:B:295:LEU:N	2.19	0.57
2:B:241:VAL:O	2:B:243:PRO:HD3	2.04	0.57
1:A:406:TRP:HZ3	1:A:507:GLN:HG2	1.69	0.56
2:B:296:THR:HG21	2:B:298:GLU:HG2	1.87	0.56
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.87	0.56
1:A:287:LYS:HB2	8:A:702:HOH:O	2.06	0.56
1:A:328:GLU:HG2	1:A:390:LYS:HB2	1.88	0.56
1:A:473:THR:HG23	1:A:476:LYS:NZ	2.20	0.56
1:A:209:LEU:HD23	1:A:216:THR:HG21	1.88	0.56
2:B:307:ARG:O	2:B:311:LYS:HG3	2.06	0.56
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.86	0.56
1:A:54:ASN:HD22	1:A:54:ASN:C	2.10	0.55
1:A:407:GLN:HE22	2:B:419:THR:H	1.54	0.55
2:B:175:ASN:HD21	2:B:201:LYS:NZ	2.05	0.55
1:A:54:ASN:HD22	1:A:56:TYR:H	1.54	0.54
2:B:296:THR:HG22	2:B:297:GLU:N	2.22	0.54
1:A:536:VAL:HG11	1:A:542:ILE:HG21	1.89	0.54
1:A:277:ARG:HH12	1:A:334:GLN:HB3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TYR:OH	3:A:568:TT1:H8	2.07	0.53
1:A:53:GLU:CD	1:A:53:GLU:H	2.12	0.53
1:A:447:ASN:HB3	1:A:450:THR:HB	1.90	0.53
2:B:64:LYS:HD3	2:B:68:SER:O	2.09	0.53
1:A:544:GLY:CA	2:B:286:THR:HG22	2.38	0.53
1:A:295:LEU:HD12	1:A:300:GLU:OE2	2.08	0.53
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.39	0.53
2:B:257:ILE:HB	2:B:283:LEU:HD11	1.91	0.52
1:A:518:VAL:O	1:A:522:ILE:HG13	2.09	0.52
1:A:173:LYS:HZ2	1:A:174:GLN:HG3	1.73	0.52
1:A:470:THR:O	1:A:471:ASP:OD1	2.27	0.52
2:B:214:LEU:HG	2:B:215:THR:N	2.24	0.52
2:B:236:PRO:HA	2:B:239:TRP:CD2	2.44	0.52
1:A:503:LEU:CD1	1:A:533:LEU:HD13	2.34	0.52
1:A:63:ILE:HG12	1:A:64:LYS:N	2.25	0.52
2:B:252:TRP:HD1	2:B:295:LEU:HD22	1.73	0.52
1:A:459:THR:CG2	1:A:460:ASN:N	2.73	0.51
1:A:27:THR:HG22	1:A:28:GLU:N	2.26	0.51
1:A:167:ILE:O	1:A:208:HIS:HE1	1.92	0.51
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.92	0.51
1:A:406:TRP:CZ3	1:A:507:GLN:HG2	2.45	0.51
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.46	0.51
1:A:447:ASN:ND2	1:A:449:GLU:H	2.09	0.51
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.92	0.51
1:A:34:LEU:HD13	1:A:62:ALA:HB2	1.93	0.51
1:A:260:LEU:HD13	1:A:279:LEU:HD13	1.94	0.50
2:B:266:TRP:HH2	2:B:427:TYR:OH	1.95	0.50
2:B:266:TRP:CD1	2:B:426:TRP:CZ3	3.00	0.50
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.94	0.50
2:B:125:ARG:HB3	2:B:146:TYR:O	2.12	0.49
2:B:297:GLU:HG2	2:B:298:GLU:N	2.26	0.49
1:A:277:ARG:NH1	1:A:334:GLN:CB	2.75	0.49
2:B:356:ARG:N	2:B:356:ARG:HD2	2.28	0.49
1:A:266:TRP:O	1:A:269:GLN:HG2	2.13	0.49
2:B:296:THR:HG22	2:B:298:GLU:H	1.78	0.49
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.95	0.48
2:B:254:VAL:O	2:B:258:GLN:HG3	2.12	0.48
2:B:151:GLN:HB3	2:B:185:ASP:OD2	2.13	0.48
1:A:27:THR:O	1:A:31:ILE:HG13	2.12	0.48
1:A:420:PRO:HA	1:A:421:PRO:C	2.33	0.48
1:A:354:TYR:HD1	1:A:374:LYS:HD2	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:HD21	1:A:56:TYR:HB2	1.78	0.48
2:B:312:GLU:HB3	2:B:313:PRO:HD2	1.94	0.48
2:B:246:LEU:HD22	2:B:260:LEU:HD11	1.95	0.48
1:A:64:LYS:HA	1:A:64:LYS:HD2	1.69	0.48
1:A:76:ASP:HA	8:A:692:HOH:O	2.14	0.48
1:A:17:ASP:O	1:A:83:ARG:NE	2.37	0.48
1:A:139:THR:HB	1:A:140:PRO:HD2	1.96	0.47
1:A:363:ASN:ND2	1:A:401:TRP:CH2	2.79	0.47
1:A:118:VAL:HG13	1:A:119:PRO:HD2	1.96	0.47
2:B:250:ASP:OD2	2:B:250:ASP:N	2.43	0.47
2:B:205:LEU:HD22	2:B:209:LEU:CD2	2.44	0.47
1:A:443:ASP:OD2	1:A:444:GLY:N	2.45	0.47
2:B:356:ARG:HH11	2:B:356:ARG:HG2	1.80	0.47
2:B:112:GLY:HA3	2:B:151:GLN:HE21	1.80	0.47
1:A:464:GLN:NE2	8:A:648:HOH:O	2.47	0.47
2:B:14:PRO:HA	2:B:15:GLY:HA2	1.55	0.47
1:A:354:TYR:CD1	1:A:374:LYS:HD2	2.49	0.47
1:A:26:LEU:HD22	1:A:133:PRO:HG3	1.97	0.47
1:A:542:ILE:O	1:A:543:GLY:O	2.33	0.46
2:B:356:ARG:HG3	8:B:514:HOH:O	2.16	0.46
2:B:296:THR:CG2	2:B:297:GLU:OE1	2.63	0.46
1:A:184:MET:HE1	8:A:753:HOH:O	2.15	0.46
2:B:214:LEU:HG	2:B:215:THR:H	1.80	0.46
1:A:95:PRO:HA	2:B:136:ASN:O	2.16	0.46
1:A:413:GLU:HA	8:A:737:HOH:O	2.14	0.46
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.56	0.46
1:A:336:GLN:NE2	8:A:644:HOH:O	2.43	0.46
1:A:542:ILE:O	1:A:543:GLY:C	2.55	0.45
2:B:64:LYS:O	2:B:407:GLN:NE2	2.49	0.45
2:B:183:TYR:CE2	2:B:184:MET:HG3	2.50	0.45
1:A:459:THR:HG22	1:A:460:ASN:N	2.30	0.45
1:A:194:GLU:OE1	1:A:197:GLN:HG3	2.16	0.45
1:A:395:LYS:HA	1:A:414:TRP:CH2	2.51	0.45
1:A:466:VAL:HG21	1:A:551:LEU:HG	1.98	0.45
2:B:175:ASN:HD21	2:B:201:LYS:HZ2	1.65	0.45
2:B:7:THR:HG23	2:B:7:THR:O	2.16	0.45
2:B:270:ILE:HG12	2:B:346:PHE:O	2.17	0.45
1:A:58:THR:HG23	1:A:76:ASP:O	2.16	0.45
1:A:393:ILE:CB	1:A:423:VAL:HG13	2.46	0.45
1:A:106:VAL:HA	1:A:189:VAL:O	2.16	0.45
2:B:393:ILE:HG12	2:B:394:GLN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ARG:O	1:A:451:LYS:HD2	2.16	0.44
1:A:407:GLN:NE2	2:B:419:THR:H	2.15	0.44
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.44
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.82	0.44
2:B:7:THR:HG21	8:B:506:HOH:O	2.17	0.44
1:A:52:PRO:HD2	1:A:53:GLU:OE1	2.18	0.44
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.99	0.44
1:A:67:ASP:CG	1:A:67:ASP:O	2.56	0.44
1:A:257:ILE:O	1:A:261:VAL:HG23	2.18	0.44
1:A:105:SER:O	1:A:190:GLY:HA2	2.18	0.44
1:A:26:LEU:CD2	1:A:133:PRO:HG3	2.48	0.44
2:B:266:TRP:HH2	2:B:427:TYR:HH	1.59	0.44
2:B:277:ARG:O	2:B:281:LYS:HG3	2.18	0.44
1:A:545:ASN:O	1:A:549:ASP:HB2	2.18	0.43
1:A:173:LYS:NZ	1:A:174:GLN:HG3	2.33	0.43
2:B:24:TRP:CH2	2:B:400:THR:HG22	2.53	0.43
2:B:163:SER:O	2:B:167:ILE:HG13	2.18	0.43
2:B:242:GLN:HB2	2:B:352:GLY:HA2	2.00	0.43
2:B:296:THR:HG22	2:B:297:GLU:OE1	2.19	0.43
2:B:96:HIS:HE1	2:B:381:VAL:O	2.01	0.43
1:A:409:THR:O	2:B:364:ASP:HB2	2.18	0.43
2:B:295:LEU:H	2:B:295:LEU:HD23	1.81	0.43
1:A:169:GLU:N	1:A:170:PRO:HD2	2.33	0.43
1:A:454:LYS:CB	1:A:552:VAL:HG13	2.49	0.43
1:A:473:THR:HG23	1:A:476:LYS:HZ3	1.83	0.42
1:A:509:GLN:N	1:A:510:PRO:CD	2.82	0.42
1:A:42:GLU:OE2	1:A:49:LYS:HE3	2.19	0.42
2:B:205:LEU:HD22	2:B:209:LEU:HD23	2.01	0.42
1:A:104:LYS:HB2	1:A:192:ASP:HA	2.01	0.42
2:B:194:GLU:HG3	2:B:197:GLN:HG3	2.01	0.42
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.55	0.42
1:A:27:THR:CG2	1:A:28:GLU:N	2.83	0.42
2:B:24:TRP:CZ3	2:B:400:THR:HG22	2.55	0.42
1:A:447:ASN:C	1:A:447:ASN:HD22	2.22	0.42
1:A:402:TRP:CD2	1:A:409:THR:HG21	2.55	0.42
2:B:122:GLU:HA	2:B:125:ARG:CG	2.50	0.42
2:B:137:ASN:ND2	8:B:540:HOH:O	2.53	0.42
1:A:54:ASN:ND2	1:A:54:ASN:C	2.73	0.42
2:B:271:TYR:O	2:B:274:ILE:HG12	2.20	0.42
1:A:171:PHE:CG	1:A:205:LEU:HD23	2.55	0.41
2:B:362:THR:OG1	2:B:363:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:THR:HG21	2:B:427:TYR:O	2.20	0.41
2:B:85:GLN:HA	2:B:88:TRP:NE1	2.35	0.41
2:B:116:PHE:HB3	8:B:520:HOH:O	2.20	0.41
1:A:399:GLU:O	1:A:403:THR:HG23	2.19	0.41
1:A:253:THR:HA	1:A:291:GLU:O	2.21	0.41
2:B:125:ARG:H	2:B:125:ARG:HG2	1.59	0.41
1:A:265:ASN:ND2	4:A:569:GOL:H32	2.31	0.41
1:A:34:LEU:HD12	1:A:34:LEU:HA	1.79	0.41
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.02	0.41
1:A:484:LEU:HD23	1:A:484:LEU:HA	1.78	0.41
1:A:225:PRO:CG	3:A:568:TT1:H25	2.50	0.41
2:B:7:THR:OG1	2:B:121:ASP:HA	2.21	0.41
2:B:261:VAL:O	2:B:265:ASN:HB3	2.21	0.41
1:A:194:GLU:N	1:A:194:GLU:CD	2.62	0.41
1:A:447:ASN:HD22	1:A:449:GLU:N	2.18	0.41
2:B:257:ILE:HG22	2:B:283:LEU:HD21	2.03	0.41
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.02	0.40
1:A:19:PRO:HD3	1:A:80:LEU:HD23	2.04	0.40
2:B:386:THR:HA	2:B:387:PRO:HD3	1.88	0.40
1:A:219:LYS:HB3	1:A:219:LYS:HE3	1.89	0.40
1:A:479:LEU:HB3	1:A:517:LEU:HD13	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	555/560 (99%)	531 (96%)	22 (4%)	2 (0%)	39	48
2	B	394/440 (90%)	380 (96%)	13 (3%)	1 (0%)	46	57
All	All	949/1000 (95%)	911 (96%)	35 (4%)	3 (0%)	46	57

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	ASN
1	A	543	GLY
2	B	284	ARG

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	497/500 (99%)	461 (93%)	36 (7%)	18	22
2	B	367/400 (92%)	343 (94%)	24 (6%)	21	27
All	All	864/900 (96%)	804 (93%)	60 (7%)	19	24

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	34	LEU
1	A	54	ASN
1	A	64	LYS
1	A	66	LYS
1	A	72	ARG
1	A	80	LEU
1	A	166	LYS
1	A	168	LEU
1	A	187	LEU
1	A	194	GLU
1	A	209	LEU
1	A	214	LEU
1	A	219	LYS
1	A	234	LEU
1	A	260	LEU
1	A	264	LEU
1	A	283	LEU
1	A	301	LEU
1	A	307	ARG

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Mol	Chain	Res	Type
1	A	311	LYS
1	A	368	LEU
1	A	385	LYS
1	A	423	VAL
1	A	424	LYS
1	A	447	ASN
1	A	448	ARG
1	A	452	LEU
1	A	464	GLN
1	A	471	ASP
1	A	476	LYS
1	A	479	LEU
1	A	507	GLN
1	A	517	LEU
1	A	533	LEU
1	A	547	GLN
2	B	24	TRP
2	B	28	GLU
2	B	80	LEU
2	B	116	PHE
2	B	125	ARG
2	B	184	MET
2	B	193	LEU
2	B	203	GLU
2	B	205	LEU
2	B	214	LEU
2	B	234	LEU
2	B	264	LEU
2	B	265	ASN
2	B	277	ARG
2	B	278	GLN
2	B	283	LEU
2	B	289	LEU
2	B	295	LEU
2	B	297	GLU
2	B	310	LEU
2	B	334	GLN
2	B	356	ARG
2	B	395	LYS
2	B	418	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	136	ASN
1	A	207	GLN
1	A	208	HIS
1	A	242	GLN
1	A	258	GLN
1	A	306	ASN
1	A	336	GLN
1	A	343	GLN
1	A	373	GLN
1	A	407	GLN
1	A	447	ASN
1	A	464	GLN
1	A	474	ASN
1	A	480	GLN
1	A	524	GLN
1	A	547	GLN
2	B	96	HIS
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	175	ASN
2	B	182	GLN
2	B	255	ASN
2	B	278	GLN
2	B	348	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	SO4	A	561	-	4,4,4	0.21	0	6,6,6	0.15	0
5	SO4	A	562	-	4,4,4	0.21	0	6,6,6	0.14	0
5	SO4	A	563	-	4,4,4	0.21	0	6,6,6	0.09	0
5	SO4	A	564	-	4,4,4	0.22	0	6,6,6	0.09	0
5	SO4	A	565	-	4,4,4	0.27	0	6,6,6	0.10	0
3	TT1	A	568	-	25,29,29	3.14	13 (52%)	24,39,39	1.07	1 (4%)
4	GOL	A	569	-	5,5,5	0.27	0	5,5,5	0.26	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	SO4	A	561	-	-	0/0/0/0	0/0/0/0
5	SO4	A	562	-	-	0/0/0/0	0/0/0/0
5	SO4	A	563	-	-	0/0/0/0	0/0/0/0
5	SO4	A	564	-	-	0/0/0/0	0/0/0/0
5	SO4	A	565	-	-	0/0/0/0	0/0/0/0
3	TT1	A	568	-	-	0/7/13/13	0/4/4/4
4	GOL	A	569	-	-	0/4/4/4	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	568	TT1	C12-N18	-4.37	1.27	1.33
3	A	568	TT1	C23-C21	2.28	1.44	1.39
3	A	568	TT1	C16-C17	2.31	1.47	1.39
3	A	568	TT1	C4-C3	2.55	1.44	1.38
3	A	568	TT1	C4-C5	2.70	1.44	1.38
3	A	568	TT1	C7-C2	2.78	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	568	TT1	C6-C7	2.91	1.44	1.38
3	A	568	TT1	C5-C6	3.07	1.45	1.38
3	A	568	TT1	C3-C2	3.50	1.46	1.38
3	A	568	TT1	C21-C20	4.11	1.46	1.39
3	A	568	TT1	C8-C20	5.55	1.58	1.51
3	A	568	TT1	C13-S14	6.22	1.79	1.72
3	A	568	TT1	C25-C26	7.79	1.54	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	568	TT1	C8-S9-C10	-3.61	98.57	101.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	568	TT1	2	0
4	A	569	GOL	2	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	557/560 (99%)	0.19	11 (1%)	68	75	33, 57, 88, 117	0
2	B	402/440 (91%)	0.34	21 (5%)	31	39	34, 55, 101, 127	0
All	All	959/1000 (95%)	0.25	32 (3%)	50	59	33, 56, 95, 127	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	346	PHE	5.2
2	B	295	LEU	4.4
1	A	286	THR	4.1
2	B	284	ARG	3.9
1	A	193	LEU	3.5
2	B	13	LYS	3.2
1	A	194	GLU	3.2
2	B	14	PRO	3.1
1	A	52	PRO	2.9
2	B	87	PHE	2.8
1	A	426	TRP	2.8
2	B	301	LEU	2.6
1	A	357	MET	2.5
2	B	309	ILE	2.5
1	A	471	ASP	2.4
2	B	216	THR	2.4
1	A	491	LEU	2.4
2	B	283	LEU	2.4
2	B	252	TRP	2.4
2	B	266	TRP	2.4
2	B	232	TYR	2.3
2	B	305	GLU	2.2
2	B	298	GLU	2.2
2	B	11	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	241	VAL	2.2
2	B	90	VAL	2.1
1	A	34	LEU	2.1
1	A	195	ILE	2.1
2	B	246	LEU	2.1
2	B	70	LYS	2.1
2	B	310	LEU	2.0
1	A	402	TRP	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 carbohydrates 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. 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, 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	LLDF	B-factors($Å^2$)	Q<0.9
4	GOL	A	569	6/6	0.60	0.28	4.44	98,100,101,101	0
5	SO4	A	563	5/5	0.85	0.23	3.17	159,159,159,159	0
3	TT1	A	568	26/26	0.84	0.18	2.00	39,44,58,59	0
5	SO4	A	561	5/5	0.90	0.15	1.09	95,95,96,98	0
5	SO4	A	562	5/5	0.96	0.11	-0.60	81,82,83,84	0
6	CL	B	443	1/1	0.95	0.11	-0.77	86,86,86,86	0
5	SO4	A	565	5/5	0.95	0.12	-1.12	90,91,91,92	0
7	MG	A	567	1/1	0.93	0.39	-	82,82,82,82	0
6	CL	B	441	1/1	0.91	0.23	-	73,73,73,73	0
6	CL	B	442	1/1	0.87	0.21	-	96,96,96,96	0
5	SO4	A	564	5/5	0.91	0.12	-	117,118,118,118	0
6	CL	A	566	1/1	0.96	0.21	-	83,83,83,83	0
6	CL	B	444	1/1	0.90	0.20	-	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.