



Full wwPDB X-ray Structure Validation Report

Sep 3, 2014 – 08:11 PM EDT

PDB ID : 2P1R
Title : Crystal structure of Salmonella typhimurium YegS, a putative lipid kinase homologous to eukaryotic sphingosine and diacylglycerol kinases.
Authors : Nichols, C.E.; Lamb, H.K.; Lockyer, M.; Charles, I.G.; Pyne, S.; Hawkins, A.R.; Stammers, D.K.
Deposited on : 2007-03-06
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

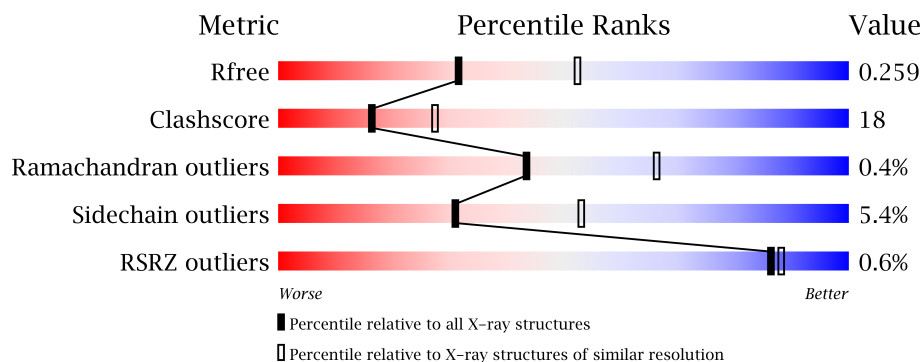
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23489
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	299	
1	B	299	
1	C	299	
1	D	299	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9044 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Lipid kinase yegS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	Se	2	0	0
			2180	1367	383	418	5	7			
1	B	290	Total	C	N	O	S	Se	2	0	0
			2180	1367	383	418	5	7			
1	C	283	Total	C	N	O	S	Se	2	0	0
			2128	1335	373	408	5	7			
1	D	283	Total	C	N	O	S	Se	2	0	0
			2128	1335	373	408	5	7			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0

- Molecule 5 is water.

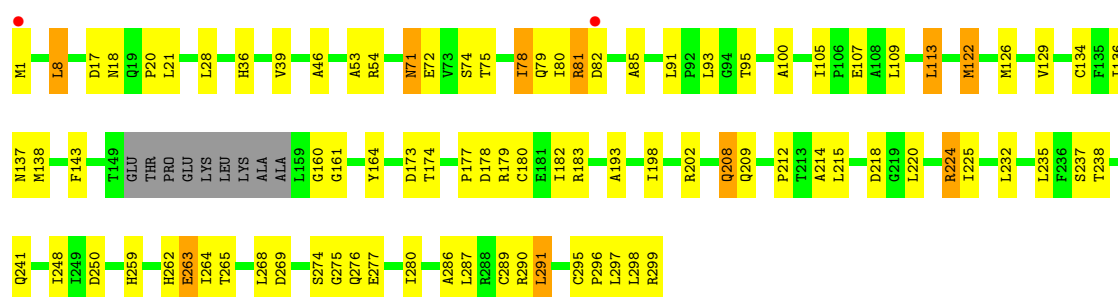
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	103	Total 103	O 103	0	0
5	B	110	Total 110	O 110	0	0
5	C	99	Total 99	O 99	0	0
5	D	102	Total 102	O 102	0	0

3 Residue-property plots

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.

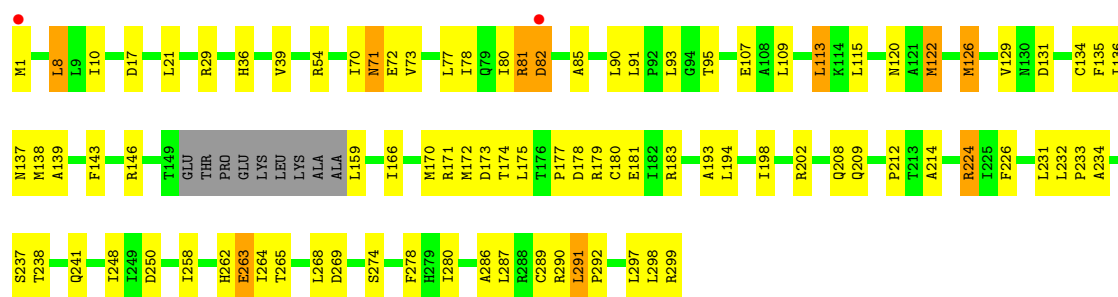
• Molecule 1: Lipid kinase yegS

Chain A: 



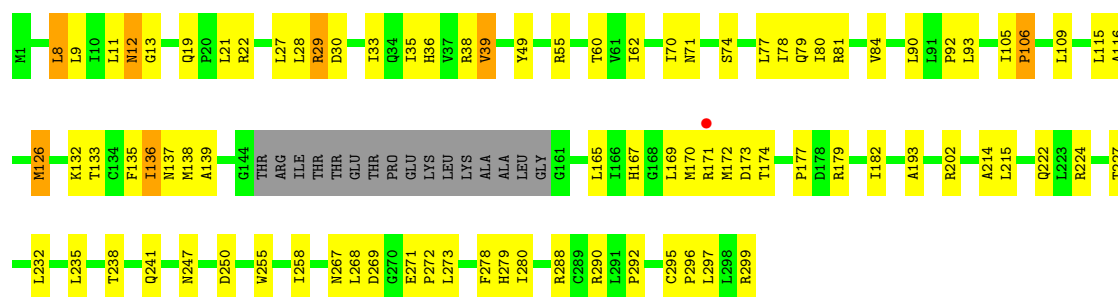
• Molecule 1: Lipid kinase yegS

Chain B: 



• Molecule 1: Lipid kinase yegS

Chain C: 



• Molecule 1: Lipid kinase yegS

I198	R202	A214	L215	D218	G219	L220	L221	Q222	L223	R224	T227	L232	L235	T238	L239	T240	Q241	N247	D250	L258	L268	D269	G270	E271	P272	H279	L280	L283	R288	C289	R290	L291	C295	P296	L297	L298	R299												
A116	G119	M120	A121	M122	M126	A127	M128	K132	T133	C134	F135	I136	M137	M139	G144	THR	ARG	ILE	THR	THR	GLU	THR	PRO	GLU	LYS	LEU	LYS	ALA	ALA	LEU	GLY	G161	L165	H166	G168	L169	M170	R171	M172	D173	T174	L175	T176	P177	D178	R179	I182	R183	A193
M1	L8	L11	M12	G13	K14	Q19	P20	L21	R22	L27	L28	E29	D30	E31	G32	I33	H36	V37	R38	V39	A46	Y49	V50	D51	E52	A53	T60	N71	E72	V73	S74	L77	I78	Q79	R81	V84	P92	L93	A100	T101	I105	T109							

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.00Å 70.99Å 102.16Å 90.00° 118.51° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 29.92 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-2.50) 97.7 (29.92-2.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.255 0.205 , 0.259	Depositor DCC
R_{free} test set	4620 reflections (10.08%)	DCC
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 27.6	EDS
Estimated twinning fraction	0.477 for -h-l,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 45843 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9044	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, 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	0.34	0/2211	0.62	0/2991
1	B	0.35	0/2211	0.61	0/2991
1	C	0.33	0/2159	0.62	0/2920
1	D	0.34	0/2159	0.62	0/2920
All	All	0.34	0/8740	0.62	0/11822

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2180	0	2171	70	0
1	B	2180	0	2171	75	0
1	C	2128	0	2112	83	0
1	D	2128	0	2112	93	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	103	0	0	5	0
5	B	110	0	0	5	0
5	C	99	0	0	4	0
5	D	102	0	0	1	0
All	All	9044	0	8566	311	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (311) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:71:ASN:HD21	1:C:135:PHE:HA	1.13	1.12
1:D:100:ALA:HB1	1:D:105:ILE:HD11	1.39	1.04
1:D:71:ASN:HD21	1:D:135:PHE:HA	1.23	1.02
1:A:54:ARG:HH22	1:A:82:ASP:HB2	1.33	0.91
1:D:128:MSE:HE3	1:D:283:LEU:HD11	1.56	0.86
1:A:100:ALA:HB1	1:A:105:ILE:HD11	1.58	0.84
1:D:92:PRO:HD3	1:D:105:ILE:HD12	1.61	0.81
1:C:167:HIS:NE2	1:C:173:ASP:HA	1.94	0.81
1:D:167:HIS:NE2	1:D:173:ASP:HA	1.97	0.79
1:C:71:ASN:ND2	1:C:135:PHE:HA	1.94	0.78
1:C:126:MSE:SE	1:C:136:ILE:HG23	2.33	0.78
1:C:136:ILE:H	1:C:136:ILE:HD12	1.50	0.76
1:D:71:ASN:ND2	1:D:135:PHE:HA	2.02	0.73
1:B:202:ARG:HD3	1:B:214:ALA:O	1.88	0.73
1:D:100:ALA:HB1	1:D:105:ILE:CD1	2.17	0.72
1:A:275:GLY:HA3	5:A:367:HOH:O	1.90	0.72
1:B:54:ARG:HH22	1:B:82:ASP:HB2	1.54	0.72
1:B:174:THR:HG22	5:B:388:HOH:O	1.89	0.71
1:C:90:LEU:HB2	1:C:105:ILE:CD1	2.21	0.70
1:D:126:MSE:SE	1:D:136:ILE:HG23	2.42	0.70
1:A:265:THR:HG22	1:A:274:SER:OG	1.92	0.69
1:A:160:GLY:HA3	1:D:128:MSE:HE1	1.72	0.69
1:C:224:ARG:HD2	1:C:250:ASP:OD2	1.91	0.69
1:D:171:ARG:HD3	1:D:272:PRO:HB3	1.75	0.69
1:D:202:ARG:HG2	1:D:214:ALA:HB3	1.74	0.68
1:D:171:ARG:HH11	1:D:272:PRO:HG3	1.58	0.68
1:D:136:ILE:H	1:D:136:ILE:HD12	1.59	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:171:ARG:HH11	1:C:272:PRO:HG3	1.59	0.67
1:D:295:CYS:HB3	1:D:298:LEU:HD12	1.75	0.67
1:B:265:THR:HG22	1:B:274:SER:OG	1.94	0.67
1:A:100:ALA:HB1	1:A:105:ILE:CD1	2.24	0.66
1:C:21:LEU:HB2	1:C:109:LEU:HD21	1.77	0.66
1:C:268:LEU:O	1:C:271:GLU:HG2	1.95	0.66
1:D:46:ALA:HB3	1:D:72:GLU:HG2	1.79	0.65
1:D:122:MSE:HE2	1:D:291:LEU:HB2	1.77	0.64
1:A:174:THR:HG22	5:A:388:HOH:O	1.98	0.64
1:C:90:LEU:HB2	1:C:105:ILE:HD13	1.79	0.64
1:C:93:LEU:HD21	1:C:109:LEU:HD11	1.80	0.64
1:C:19:GLN:HE22	1:C:22:ARG:HD2	1.63	0.64
1:D:135:PHE:CD2	1:D:268:LEU:HD12	2.32	0.63
1:D:93:LEU:HD21	1:D:109:LEU:HD11	1.80	0.63
1:B:95:THR:HG23	1:C:80:ILE:CG2	2.30	0.62
1:D:268:LEU:O	1:D:271:GLU:HG2	1.99	0.62
1:A:202:ARG:HG2	1:A:214:ALA:HB3	1.81	0.62
1:A:173:ASP:OD1	1:A:174:THR:HG23	2.00	0.61
1:D:92:PRO:HD3	1:D:105:ILE:CD1	2.30	0.61
1:B:166:ILE:HD11	1:B:231:LEU:HD23	1.81	0.61
1:A:143:PHE:CD2	1:A:178:ASP:HB3	2.35	0.61
1:A:8:LEU:HD22	1:A:36:HIS:HB2	1.81	0.61
1:A:122:MSE:HE2	1:A:298:LEU:HD11	1.82	0.61
1:A:177:PRO:HA	1:A:193:ALA:O	1.99	0.61
1:B:137:ASN:HB3	1:B:269:ASP:OD1	2.01	0.61
1:B:173:ASP:OD1	1:B:174:THR:HG23	2.01	0.61
1:D:268:LEU:N	1:D:268:LEU:HD22	2.17	0.60
1:B:126:MSE:SE	1:B:136:ILE:HG23	2.52	0.60
1:B:1:MSE:HE3	1:B:1:MSE:O	2.02	0.60
1:A:143:PHE:HD2	1:A:178:ASP:HB3	1.67	0.59
1:C:171:ARG:HD3	1:C:272:PRO:HB3	1.84	0.59
1:D:223:LEU:HD12	1:D:224:ARG:H	1.67	0.59
1:A:224:ARG:HD2	1:A:248:ILE:HG23	1.85	0.59
1:A:183:ARG:HD3	5:A:307:HOH:O	2.02	0.59
1:B:202:ARG:HG2	1:B:214:ALA:HB3	1.85	0.58
1:A:81:ARG:HG3	1:A:81:ARG:HH11	1.67	0.58
1:B:8:LEU:HD22	1:B:36:HIS:HB2	1.84	0.58
1:C:28:LEU:O	1:C:33:ILE:HB	2.03	0.58
1:B:138:MSE:HB3	5:B:387:HOH:O	2.03	0.58
1:D:172:MSE:HG3	1:D:175:LEU:HD21	1.85	0.58
1:C:202:ARG:HG2	1:C:214:ALA:HB3	1.85	0.58
1:D:100:ALA:CB	1:D:105:ILE:HD11	2.26	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:177:PRO:HA	1:B:193:ALA:O	2.04	0.58
1:B:202:ARG:HG3	1:B:297:LEU:CD2	2.34	0.58
1:D:19:GLN:HE22	1:D:22:ARG:HD2	1.68	0.58
1:B:232:LEU:HD11	1:C:279:HIS:CE1	2.39	0.57
1:D:136:ILE:HD12	1:D:269:ASP:OD2	2.05	0.57
1:C:171:ARG:NH1	1:C:272:PRO:HG3	2.19	0.57
1:D:27:LEU:O	1:D:30:ASP:HB2	2.05	0.57
1:B:120:ASN:O	1:B:290:ARG:HA	2.05	0.57
1:B:289:CYS:O	1:B:291:LEU:HD22	2.05	0.57
1:D:215:LEU:HB2	1:D:218:ASP:OD2	2.04	0.57
1:A:208:GLN:HG3	1:A:235:LEU:HD22	1.87	0.56
1:C:165:LEU:HD23	1:C:232:LEU:HD12	1.87	0.56
1:B:78:ILE:HD11	1:B:286:ALA:CB	2.35	0.56
1:D:12:ASN:HD22	1:D:14:LYS:HB2	1.71	0.56
1:A:28:LEU:HD12	1:A:113:LEU:CD1	2.36	0.56
1:A:1:MSE:HE3	1:A:1:MSE:O	2.05	0.56
1:C:182:ILE:HG12	1:C:258:ILE:HD12	1.89	0.55
1:C:268:LEU:HB2	1:C:271:GLU:HG3	1.88	0.55
1:B:232:LEU:C	1:B:232:LEU:HD23	2.26	0.55
1:B:136:ILE:HD12	1:B:137:ASN:N	2.21	0.55
1:B:10:ILE:HD12	1:B:73:VAL:HG22	1.89	0.55
1:A:289:CYS:O	1:A:291:LEU:HD22	2.07	0.55
1:A:74:SER:HB3	1:A:126:MSE:SE	2.57	0.54
1:D:28:LEU:O	1:D:33:ILE:HB	2.06	0.54
1:C:202:ARG:HG3	1:C:297:LEU:HD22	1.89	0.54
1:A:126:MSE:HE3	1:A:134:CYS:HB3	1.89	0.54
1:C:29:ARG:NH1	1:C:35:ILE:O	2.40	0.54
1:C:8:LEU:HD22	1:C:36:HIS:HB2	1.88	0.54
1:D:222:GLN:HA	1:D:222:GLN:NE2	2.22	0.54
1:B:143:PHE:CD2	1:B:178:ASP:HB3	2.43	0.54
1:D:223:LEU:HD12	1:D:224:ARG:N	2.23	0.54
1:A:198:ILE:HD13	1:A:280:ILE:HD12	1.90	0.54
1:D:38:ARG:HD2	1:D:49:TYR:CE2	2.43	0.54
1:D:232:LEU:HD23	1:D:235:LEU:HD12	1.89	0.53
1:A:95:THR:HG23	1:D:80:ILE:CG2	2.39	0.53
1:D:170:MSE:HE2	1:D:172:MSE:HG3	1.90	0.53
1:D:74:SER:HB3	1:D:126:MSE:HE1	1.89	0.53
1:B:81:ARG:HG3	1:B:81:ARG:HH11	1.73	0.53
1:D:224:ARG:HD2	1:D:250:ASP:OD2	2.09	0.53
1:C:19:GLN:NE2	1:C:22:ARG:HD2	2.24	0.53
1:B:290:ARG:O	1:B:291:LEU:HD13	2.09	0.53
1:C:8:LEU:HD13	1:C:9:LEU:N	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:224:ARG:HD3	1:A:250:ASP:OD2	2.09	0.52
1:A:81:ARG:HG3	1:A:81:ARG:NH1	2.25	0.52
1:B:71:ASN:OD1	1:B:269:ASP:HB2	2.09	0.52
1:D:136:ILE:CD1	1:D:136:ILE:H	2.20	0.52
1:D:177:PRO:HA	1:D:193:ALA:O	2.09	0.52
1:B:135:PHE:CE2	1:B:139:ALA:HB2	2.45	0.52
1:D:171:ARG:NH1	1:D:272:PRO:HG3	2.25	0.52
1:D:50:VAL:O	1:D:53:ALA:HB3	2.10	0.52
1:A:126:MSE:HE3	1:A:134:CYS:CB	2.40	0.52
1:A:179:ARG:HG2	1:A:179:ARG:HH21	1.74	0.52
1:A:8:LEU:HG	1:A:53:ALA:HB2	1.92	0.52
1:C:132:LYS:HG3	1:C:133:THR:N	2.25	0.52
1:C:202:ARG:HG3	1:C:297:LEU:CD2	2.40	0.52
1:C:27:LEU:O	1:C:30:ASP:HB2	2.09	0.52
1:D:8:LEU:HD22	1:D:36:HIS:HB2	1.92	0.52
1:A:8:LEU:HD22	1:A:36:HIS:CB	2.40	0.51
1:B:171:ARG:O	1:B:172:MSE:HE2	2.10	0.51
1:A:202:ARG:HG3	1:A:297:LEU:CD2	2.40	0.51
1:D:198:ILE:CD1	1:D:280:ILE:HD12	2.41	0.51
1:A:202:ARG:HD2	1:A:212:PRO:O	2.11	0.51
1:B:159:LEU:HD23	1:B:159:LEU:O	2.10	0.51
1:B:159:LEU:N	5:B:383:HOH:O	2.43	0.51
1:A:75:THR:HA	1:A:126:MSE:HE1	1.92	0.51
1:A:160:GLY:H	1:A:164:TYR:HB2	1.75	0.51
1:A:122:MSE:HE2	1:A:298:LEU:CD1	2.39	0.51
1:C:71:ASN:HD22	1:C:136:ILE:CD1	2.24	0.51
1:B:198:ILE:HD13	1:B:280:ILE:HD12	1.93	0.51
1:D:218:ASP:OD1	1:D:220:LEU:N	2.40	0.51
1:B:54:ARG:HH22	1:B:82:ASP:CB	2.21	0.51
1:D:268:LEU:HB2	1:D:271:GLU:HG3	1.93	0.50
1:C:78:ILE:HD13	1:C:126:MSE:HE2	1.93	0.50
1:D:132:LYS:HG3	1:D:133:THR:N	2.25	0.50
1:B:115:LEU:HD21	1:B:292:PRO:HD3	1.94	0.50
1:D:93:LEU:HD21	1:D:109:LEU:CD1	2.41	0.50
1:B:172:MSE:HA	1:B:172:MSE:HE2	1.94	0.50
1:B:72:GLU:HG2	5:B:304:HOH:O	2.12	0.50
1:C:12:ASN:HD22	1:C:13:GLY:N	2.10	0.50
1:C:232:LEU:HD13	1:C:235:LEU:HD12	1.94	0.50
1:D:173:ASP:OD1	1:D:174:THR:HG23	2.12	0.50
1:B:224:ARG:HG2	1:B:226:PHE:CZ	2.48	0.49
1:B:238:THR:OG1	1:B:241:GLN:HG3	2.13	0.49
1:C:169:LEU:C	1:C:170:MSE:HG3	2.31	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:165:LEU:HD23	1:C:232:LEU:CD1	2.42	0.49
1:B:70:ILE:HD13	1:B:90:LEU:HD22	1.94	0.49
1:B:126:MSE:HE3	1:B:134:CYS:CB	2.42	0.49
1:B:8:LEU:HD22	1:B:36:HIS:CB	2.43	0.49
1:B:81:ARG:HG3	1:B:81:ARG:NH1	2.28	0.48
1:C:173:ASP:CG	1:C:174:THR:H	2.16	0.48
1:D:132:LYS:HG3	1:D:133:THR:H	1.78	0.48
1:C:135:PHE:CD2	1:C:268:LEU:HD12	2.49	0.48
1:A:179:ARG:NH2	1:A:179:ARG:HG2	2.28	0.48
1:A:215:LEU:HD13	1:A:299:ARG:HB2	1.94	0.48
1:B:198:ILE:CD1	1:B:280:ILE:HD12	2.44	0.48
1:B:143:PHE:CZ	1:B:264:ILE:HD12	2.49	0.48
1:B:262:HIS:O	1:B:263:GLU:C	2.51	0.48
1:A:202:ARG:HD3	1:A:214:ALA:O	2.14	0.48
1:A:232:LEU:HD23	1:A:232:LEU:C	2.34	0.48
1:B:183:ARG:HD3	5:B:360:HOH:O	2.14	0.48
1:B:122:MSE:HE2	1:B:298:LEU:CD1	2.43	0.48
1:C:177:PRO:HA	1:C:193:ALA:O	2.13	0.48
1:D:81:ARG:HH11	1:D:81:ARG:HG3	1.78	0.48
1:A:262:HIS:O	1:A:263:GLU:C	2.52	0.48
1:C:8:LEU:HD22	1:C:36:HIS:CB	2.43	0.48
1:A:182:ILE:HD12	1:A:225:ILE:HD11	1.95	0.47
1:B:146:ARG:NE	1:B:265:THR:HG21	2.29	0.47
1:D:21:LEU:HB2	1:D:109:LEU:HD21	1.96	0.47
1:D:179:ARG:HH21	1:D:179:ARG:HG2	1.79	0.47
1:C:74:SER:HB3	1:C:126:MSE:HE1	1.96	0.47
1:C:137:ASN:HB3	1:C:269:ASP:OD1	2.13	0.47
1:D:121:ALA:HB1	1:D:288:ARG:HB3	1.97	0.47
1:C:222:GLN:NE2	1:C:222:GLN:HA	2.29	0.47
1:A:238:THR:OG1	1:A:241:GLN:HG3	2.14	0.47
1:D:165:LEU:HD23	1:D:232:LEU:HD22	1.97	0.47
1:D:8:LEU:HD22	1:D:36:HIS:CB	2.45	0.47
1:B:299:ARG:HH11	1:B:299:ARG:HG3	1.80	0.47
1:B:54:ARG:HD2	1:B:80:ILE:CD1	2.44	0.47
1:A:18:ASN:OD1	1:A:20:PRO:HD2	2.15	0.47
1:B:232:LEU:HD11	1:C:279:HIS:HE1	1.80	0.47
1:D:102:SER:OG	1:D:297:LEU:HD11	2.15	0.47
1:A:259:HIS:ND1	1:A:277:GLU:OE2	2.46	0.47
1:C:273:LEU:HG	1:C:278:PHE:HE2	1.80	0.47
1:C:11:LEU:O	1:C:39:VAL:HA	2.15	0.46
1:B:78:ILE:HD11	1:B:286:ALA:HB3	1.97	0.46
1:B:122:MSE:HE2	1:B:298:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:132:LYS:HG3	1:C:133:THR:H	1.80	0.46
1:D:183:ARG:HG3	1:D:183:ARG:HH11	1.79	0.46
1:D:116:ALA:O	1:D:290:ARG:HD2	2.16	0.46
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.80	0.46
1:C:70:ILE:CD1	1:C:90:LEU:HD22	2.46	0.46
1:D:215:LEU:HD12	5:D:367:HOH:O	2.15	0.46
1:B:175:LEU:HB3	1:B:194:LEU:HD11	1.97	0.46
1:D:132:LYS:HG3	1:D:133:THR:HG23	1.97	0.46
1:A:75:THR:O	1:A:79:GLN:HG3	2.17	0.45
1:C:172:MSE:HA	1:C:172:MSE:HE2	1.98	0.45
1:C:288:ARG:HH11	1:C:288:ARG:HG3	1.81	0.45
1:A:71:ASN:HD21	1:A:136:ILE:H	1.63	0.45
1:B:21:LEU:HD22	1:B:93:LEU:HD11	1.97	0.45
1:C:132:LYS:HG3	1:C:133:THR:HG23	1.97	0.45
1:B:159:LEU:HD13	1:C:79:GLN:HE22	1.81	0.45
1:C:92:PRO:O	1:C:93:LEU:HD23	2.16	0.45
1:D:172:MSE:CG	1:D:175:LEU:HD21	2.45	0.45
1:A:54:ARG:HD2	1:A:80:ILE:CD1	2.47	0.45
1:B:179:ARG:HG2	1:B:180:CYS:N	2.32	0.45
1:B:234:ALA:HB1	1:B:248:ILE:HD11	1.99	0.45
1:D:78:ILE:HD13	1:D:126:MSE:HE2	1.98	0.45
1:D:11:LEU:O	1:D:39:VAL:HA	2.17	0.45
1:A:109:LEU:O	1:A:113:LEU:HB2	2.17	0.45
1:A:78:ILE:CD1	1:A:287:LEU:HB3	2.47	0.45
1:D:183:ARG:HG3	1:D:183:ARG:NH1	2.32	0.45
1:D:222:GLN:HE21	1:D:222:GLN:HA	1.81	0.45
1:D:92:PRO:O	1:D:93:LEU:HD23	2.17	0.44
1:A:137:ASN:HB3	1:A:269:ASP:OD1	2.18	0.44
1:C:71:ASN:HD22	1:C:136:ILE:HD12	1.82	0.44
1:D:74:SER:C	1:D:126:MSE:HE1	2.38	0.44
1:B:202:ARG:HD2	1:B:212:PRO:O	2.18	0.44
1:D:182:ILE:HG23	1:D:258:ILE:CD1	2.48	0.44
1:D:179:ARG:NH2	1:D:179:ARG:HG2	2.33	0.44
1:A:107:GLU:O	1:D:84:VAL:HG21	2.17	0.44
1:B:54:ARG:HD2	1:B:80:ILE:HD13	2.00	0.44
1:C:78:ILE:HG21	1:C:126:MSE:HE2	1.98	0.44
1:D:227:THR:OG1	1:D:247:ASN:HA	2.18	0.44
1:B:109:LEU:O	1:B:113:LEU:HB2	2.18	0.44
1:D:19:GLN:NE2	1:D:22:ARG:HD2	2.33	0.43
1:A:218:ASP:OD1	1:A:220:LEU:N	2.46	0.43
1:B:232:LEU:HD13	5:C:323:HOH:O	2.17	0.43
1:D:238:THR:OG1	1:D:241:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:255:TRP:HA	1:C:280:ILE:O	2.19	0.43
1:C:9:LEU:HD12	1:C:62:ILE:O	2.18	0.43
1:C:81:ARG:HG3	1:C:81:ARG:HH11	1.81	0.43
1:D:60:THR:HG21	1:D:116:ALA:O	2.18	0.43
1:C:105:ILE:HA	1:C:106:PRO:HD3	1.92	0.43
1:C:93:LEU:HD21	1:C:109:LEU:CD1	2.47	0.43
1:D:169:LEU:C	1:D:170:MSE:HG3	2.38	0.43
1:B:78:ILE:CD1	1:B:287:LEU:HB3	2.48	0.43
1:D:182:ILE:HG23	1:D:258:ILE:HD13	2.00	0.43
1:D:71:ASN:HD22	1:D:136:ILE:CD1	2.31	0.43
1:C:70:ILE:HD13	1:C:90:LEU:HD22	2.01	0.43
1:A:237:SER:HB3	1:A:241:GLN:HB2	2.00	0.43
1:A:21:LEU:HD22	1:A:93:LEU:HD11	2.01	0.43
1:B:107:GLU:O	1:C:84:VAL:HG21	2.18	0.43
1:A:78:ILE:HD11	1:A:286:ALA:CB	2.49	0.43
1:B:126:MSE:HE3	1:B:134:CYS:HB2	2.01	0.43
1:D:239:LEU:HD23	1:D:239:LEU:N	2.34	0.43
1:C:299:ARG:HG3	1:C:299:ARG:HH11	1.83	0.42
1:A:138:MSE:HE2	1:A:138:MSE:HB2	1.95	0.42
1:B:179:ARG:HG2	1:B:179:ARG:NH2	2.34	0.42
1:C:38:ARG:HD2	1:C:49:TYR:CE2	2.54	0.42
1:A:161:GLY:O	1:A:164:TYR:N	2.49	0.42
1:D:268:LEU:CD2	1:D:268:LEU:N	2.81	0.42
1:D:295:CYS:HA	1:D:296:PRO:HD3	1.92	0.42
1:D:202:ARG:HG3	1:D:297:LEU:CD2	2.50	0.42
1:B:232:LEU:N	1:B:233:PRO:HD2	2.34	0.42
1:D:136:ILE:HD12	1:D:137:ASN:H	1.84	0.42
1:B:237:SER:HB3	1:B:241:GLN:HB2	2.00	0.42
1:C:271:GLU:HB3	5:C:369:HOH:O	2.20	0.42
1:D:138:MSE:HE2	1:D:138:MSE:HB2	1.94	0.42
1:A:198:ILE:CD1	1:A:280:ILE:HD12	2.49	0.42
1:A:46:ALA:HB3	5:A:309:HOH:O	2.19	0.42
1:D:38:ARG:HD2	1:D:49:TYR:CD2	2.55	0.42
1:B:224:ARG:HD3	1:B:250:ASP:OD2	2.18	0.42
1:D:172:MSE:CB	1:D:175:LEU:HD21	2.50	0.42
1:C:8:LEU:HA	1:C:36:HIS:HB2	2.02	0.42
1:D:198:ILE:HD13	1:D:280:ILE:HD12	2.02	0.42
1:C:33:ILE:HG22	1:C:35:ILE:HG13	2.02	0.41
1:D:51:ASP:OD1	1:D:81:ARG:NH1	2.53	0.41
1:A:295:CYS:HA	1:A:296:PRO:HD3	1.86	0.41
1:A:95:THR:HA	1:D:81:ARG:O	2.20	0.41
1:C:12:ASN:HD22	1:C:13:GLY:H	1.69	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:55:ARG:HD3	5:C:393:HOH:O	2.19	0.41
1:A:224:ARG:HD2	1:A:248:ILE:CG2	2.49	0.41
1:A:264:ILE:HG12	1:A:265:THR:N	2.35	0.41
1:A:80:ILE:HB	1:A:85:ALA:HB2	2.02	0.41
1:B:170:MSE:O	1:B:172:MSE:HE3	2.20	0.41
1:B:179:ARG:HH21	1:B:179:ARG:HG2	1.85	0.41
1:B:179:ARG:HH12	1:B:181:GLU:HB2	1.84	0.41
1:C:167:HIS:CD2	1:C:173:ASP:HA	2.54	0.41
1:C:268:LEU:HB2	1:C:271:GLU:CG	2.50	0.41
1:C:295:CYS:HA	1:C:296:PRO:HD3	1.85	0.41
1:C:60:THR:HG21	1:C:116:ALA:O	2.20	0.41
1:C:215:LEU:HD12	5:C:356:HOH:O	2.21	0.41
1:C:238:THR:OG1	1:C:241:GLN:HG3	2.20	0.41
1:C:171:ARG:HG3	1:C:267:ASN:ND2	2.35	0.41
1:D:239:LEU:CD2	1:D:239:LEU:H	2.33	0.41
1:C:227:THR:OG1	1:C:247:ASN:HA	2.21	0.41
1:A:232:LEU:HD11	1:D:279:HIS:CE1	2.55	0.41
1:B:126:MSE:HE3	1:B:134:CYS:HB3	2.02	0.41
1:C:182:ILE:HG12	1:C:258:ILE:CD1	2.50	0.41
1:A:263:GLU:HA	1:A:276:GLN:HG2	2.02	0.41
1:B:8:LEU:C	1:B:8:LEU:CD1	2.89	0.41
1:D:100:ALA:O	1:D:105:ILE:HG12	2.20	0.40
1:C:115:LEU:HD21	1:C:292:PRO:HD3	2.02	0.40
1:A:290:ARG:O	1:A:291:LEU:HD13	2.21	0.40
1:A:72:GLU:HG2	5:A:309:HOH:O	2.21	0.40
1:C:138:MSE:HG3	1:C:139:ALA:N	2.36	0.40
1:C:179:ARG:HH21	1:C:179:ARG:HG2	1.86	0.40
1:B:80:ILE:HB	1:B:85:ALA:HB2	2.03	0.40
1:C:179:ARG:NH2	1:C:179:ARG:HG2	2.37	0.40
1:C:116:ALA:O	1:C:290:ARG:HD2	2.22	0.40
1:D:239:LEU:HD23	1:D:239:LEU:H	1.86	0.40
1:B:258:ILE:HB	1:B:278:PHE:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	286/299 (96%)	262 (92%)	23 (8%)	1 (0%)	50	73
1	B	286/299 (96%)	265 (93%)	19 (7%)	2 (1%)	30	50
1	C	279/299 (93%)	260 (93%)	18 (6%)	1 (0%)	43	66
1	D	279/299 (93%)	263 (94%)	15 (5%)	1 (0%)	43	66
All	All	1130/1196 (94%)	1050 (93%)	75 (7%)	5 (0%)	43	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	GLU
1	B	263	GLU
1	B	82	ASP
1	D	119	GLY
1	C	106	PRO

5.3.2 Protein sidechains ⓘ

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	229/229 (100%)	213 (93%)	16 (7%)	21	38
1	B	229/229 (100%)	211 (92%)	18 (8%)	18	31
1	C	223/229 (97%)	216 (97%)	7 (3%)	52	79
1	D	223/229 (97%)	215 (96%)	8 (4%)	47	73
All	All	904/916 (99%)	855 (95%)	49 (5%)	31	53

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	17	ASP
1	A	39	VAL
1	A	71	ASN

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Mol	Chain	Res	Type
1	A	78	ILE
1	A	81	ARG
1	A	91	LEU
1	A	113	LEU
1	A	122	MSE
1	A	129	VAL
1	A	180	CYS
1	A	208	GLN
1	A	209	GLN
1	A	224	ARG
1	A	268	LEU
1	A	291	LEU
1	B	8	LEU
1	B	17	ASP
1	B	29	ARG
1	B	39	VAL
1	B	71	ASN
1	B	77	LEU
1	B	81	ARG
1	B	91	LEU
1	B	113	LEU
1	B	122	MSE
1	B	126	MSE
1	B	129	VAL
1	B	131	ASP
1	B	208	GLN
1	B	209	GLN
1	B	224	ARG
1	B	268	LEU
1	B	291	LEU
1	C	8	LEU
1	C	12	ASN
1	C	29	ARG
1	C	39	VAL
1	C	77	LEU
1	C	126	MSE
1	C	136	ILE
1	D	8	LEU
1	D	31	GLU
1	D	39	VAL
1	D	77	LEU
1	D	126	MSE

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Mol	Chain	Res	Type
1	D	136	ILE
1	D	224	ARG
1	D	299	ARG

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

Mol	Chain	Res	Type
1	A	190	GLN
1	A	209	GLN
1	A	222	GLN
1	A	262	HIS
1	B	71	ASN
1	B	209	GLN
1	B	222	GLN
1	B	262	HIS
1	C	12	ASN
1	C	19	GLN
1	C	47	GLN
1	C	71	ASN
1	C	79	GLN
1	C	186	ASN
1	C	222	GLN
1	C	259	HIS
1	C	267	ASN
1	C	279	HIS
1	D	12	ASN
1	D	19	GLN
1	D	71	ASN
1	D	79	GLN
1	D	186	ASN
1	D	222	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 14 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	290/299 (96%)	-0.48	2 (0%) 84 86	16, 34, 67, 118	1 (0%)
1	B	290/299 (96%)	-0.48	2 (0%) 84 86	13, 34, 71, 122	1 (0%)
1	C	283/299 (94%)	-0.38	1 (0%) 90 92	19, 40, 79, 128	1 (0%)
1	D	283/299 (94%)	-0.39	2 (0%) 84 86	16, 38, 76, 130	1 (0%)
All	All	1146/1196 (95%)	-0.44	7 (0%) 86 88	13, 37, 74, 130	4 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	171	ARG	4.8
1	B	1	MSE	3.2
1	D	171	ARG	2.9
1	B	82	ASP	2.5
1	A	1	MSE	2.4
1	A	82	ASP	2.2
1	D	169	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	CL	D	303	1/1	0.12	0.37	48,48,48,48	0
3	CA	B	301	1/1	0.11	0.28	39,39,39,39	0
2	NA	B	300	1/1	0.10	-0.08	34,34,34,34	0
3	CA	D	302	1/1	0.11	-0.50	79,79,79,79	0
3	CA	C	302	1/1	0.09	-0.75	72,72,72,72	0
3	CA	C	301	1/1	0.10	-1.05	51,51,51,51	0
3	CA	B	302	1/1	0.11	-1.07	44,44,44,44	0
2	NA	A	300	1/1	0.08	-1.21	23,23,23,23	0
3	CA	D	301	1/1	0.09	-1.30	49,49,49,49	0
3	CA	A	301	1/1	0.09	-1.46	39,39,39,39	0
3	CA	C	300	1/1	0.08	-2.08	38,38,38,38	0
4	CL	C	303	1/1	0.06	-2.23	49,49,49,49	0
3	CA	D	300	1/1	0.07	-2.41	41,41,41,41	0
3	CA	A	302	1/1	0.06	-4.19	48,48,48,48	0

6.5 Other polymers

There are no such residues in this entry.