



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:38 PM GMT

PDB ID : 2H2E
Title : Structure of Rubisco LSMT bound to AzaAdoMet and Lysine
Authors : Couture, J.F.; Hauk, G.; Trievel, R.C.
Deposited on : 2006-05-18
Resolution : 2.60 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>

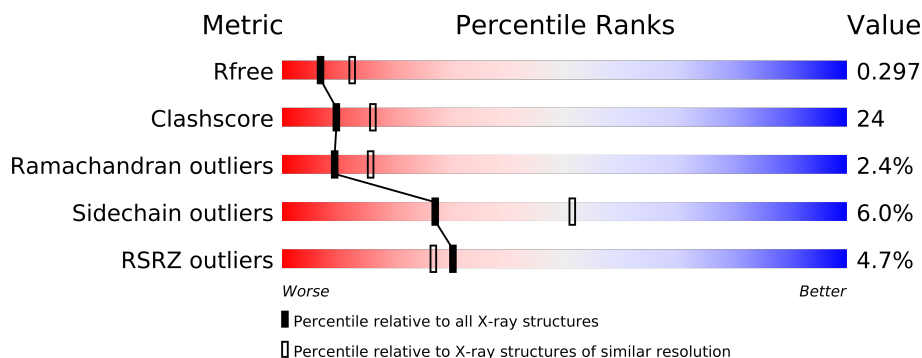
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	440	
1	B	440	
1	C	440	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SA8	A	800	-	X
2	SA8	B	801	-	X
2	SA8	C	802	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10977 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.

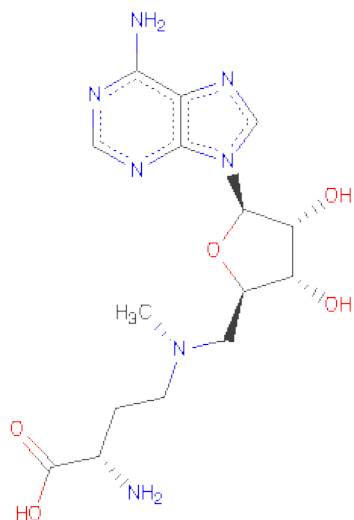
- Molecule 1 is a protein called Ribulose-1,5 bisphosphate carboxylase/oxygenase large subunit N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3413	2189	562	655	7			
1	B	440	Total	C	N	O	S	0	0	0
			3542	2270	585	680	7			
1	C	438	Total	C	N	O	S	0	0	0
			3526	2262	582	675	7			

There are 18 discrepancies between the modelled and reference sequences:

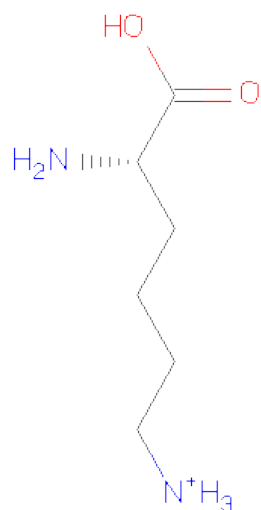
Chain	Residue	Modelled	Actual	Comment	Reference
A	483	GLU	-	CLONING ARTIFACT	UNP Q43088
A	484	ASN	-	CLONING ARTIFACT	UNP Q43088
A	485	LEU	-	CLONING ARTIFACT	UNP Q43088
A	486	TYR	-	CLONING ARTIFACT	UNP Q43088
A	487	PHE	-	CLONING ARTIFACT	UNP Q43088
A	488	GLN	-	CLONING ARTIFACT	UNP Q43088
B	483	GLU	-	CLONING ARTIFACT	UNP Q43088
B	484	ASN	-	CLONING ARTIFACT	UNP Q43088
B	485	LEU	-	CLONING ARTIFACT	UNP Q43088
B	486	TYR	-	CLONING ARTIFACT	UNP Q43088
B	487	PHE	-	CLONING ARTIFACT	UNP Q43088
B	488	GLN	-	CLONING ARTIFACT	UNP Q43088
C	483	GLU	-	CLONING ARTIFACT	UNP Q43088
C	484	ASN	-	CLONING ARTIFACT	UNP Q43088
C	485	LEU	-	CLONING ARTIFACT	UNP Q43088
C	486	TYR	-	CLONING ARTIFACT	UNP Q43088
C	487	PHE	-	CLONING ARTIFACT	UNP Q43088
C	488	GLN	-	CLONING ARTIFACT	UNP Q43088

- Molecule 2 is S-5'-AZAMETHIONINE-5'-DEOXYADENOSINE (three-letter code: SA8) (formula: C₁₅H₂₃N₇O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			27	15	7	5		
2	B	1	Total	C	N	O	0	0
			27	15	7	5		
2	C	1	Total	C	N	O	0	0
			27	15	7	5		

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			10	6	2	2		

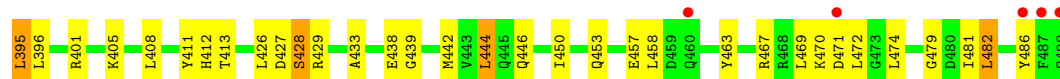
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			10	6	2	2		
3	A	1	Total	C	N	O	0	0
			10	6	2	2		

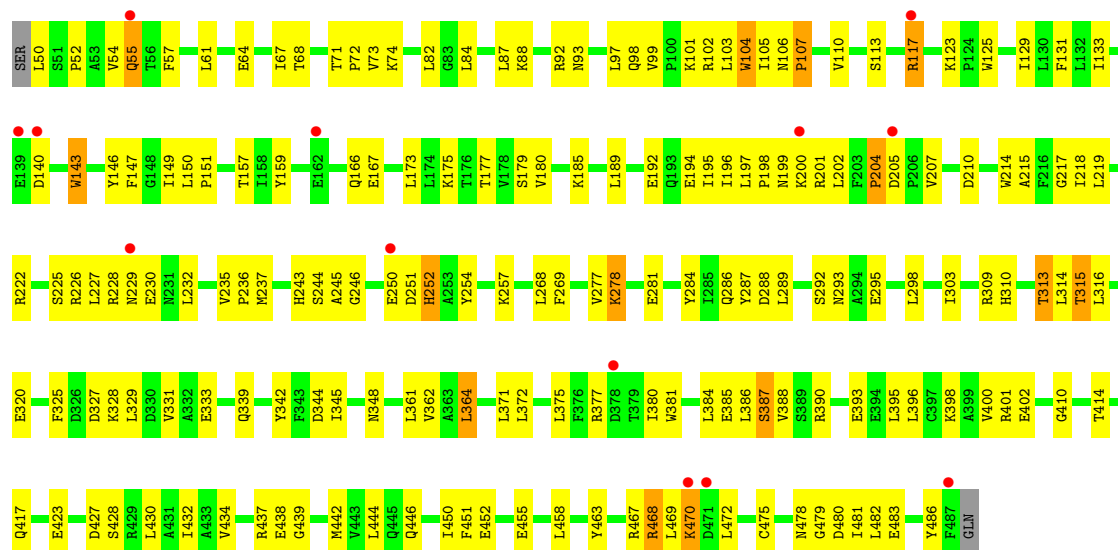
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	127	Total	O	0	0
			127	127		
4	C	141	Total	O	0	0
			141	141		



- Molecule 1: Ribulose-1,5 bisphosphate carboxylase/oxygenase large subunit N-methyltransferase

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	132.63Å 159.49Å 267.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.73 – 2.60 16.73 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.2 (16.73-2.60) 97.6 (16.73-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.59Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.298 0.262 , 0.297	Depositor DCC
R_{free} test set	4320 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	8 of 85610 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10977	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: SA8

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	0.40	0/3482	0.60	0/4723
1	B	0.40	0/3617	0.63	1/4906 (0.0%)
1	C	0.40	0/3601	0.62	0/4886
All	All	0.40	0/10700	0.61	1/14515 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	ILE	N-CA-C	-5.67	95.69	111.00

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	3413	0	3384	189	0
1	B	3542	0	3501	165	0
1	C	3526	0	3488	171	0
2	A	27	0	22	7	0
2	B	27	0	22	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	27	0	22	6	0
3	A	10	0	12	4	0
3	B	10	0	12	0	0
3	C	10	0	12	5	0
4	A	117	0	0	14	0
4	B	127	0	0	12	0
4	C	141	0	0	21	0
All	All	10977	0	10475	513	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 24.

All (513) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:78:VAL:HG11	1:B:282:GLN:HE22	1.19	1.05
1:C:177:THR:HG22	1:C:298:LEU:HD13	1.43	0.96
1:C:50:LEU:HD22	1:C:54:VAL:HG11	1.46	0.96
1:B:367:THR:HA	4:B:905:HOH:O	1.66	0.94
1:A:395:LEU:HD22	1:B:469:LEU:HD12	1.49	0.93
1:B:286:GLN:HE21	1:B:288:ASP:H	0.97	0.91
1:A:238:ALA:HB1	1:A:271:LEU:HD22	1.50	0.91
1:C:219:LEU:HD11	1:C:232:LEU:HD21	1.56	0.86
1:A:226:ARG:O	1:A:227:LEU:HD13	1.80	0.82
1:C:482:LEU:HG	4:C:1016:HOH:O	1.80	0.81
1:B:472:LEU:HD13	1:B:474:LEU:HD21	1.61	0.81
1:C:102:ARG:HB2	4:C:906:HOH:O	1.81	0.80
1:A:192:GLU:HA	1:A:196:ILE:HB	1.62	0.79
1:A:130:LEU:HD11	1:A:191:LEU:HD22	1.66	0.78
1:B:78:VAL:HG11	1:B:282:GLN:NE2	1.99	0.77
1:C:315:THR:HG21	4:C:921:HOH:O	1.83	0.77
1:B:286:GLN:HE21	1:B:288:ASP:N	1.78	0.77
1:A:227:LEU:HD23	1:A:231:ASN:HA	1.67	0.77
1:A:73:VAL:HG21	1:A:84:LEU:HB3	1.66	0.77
1:B:395:LEU:HD22	1:C:469:LEU:HD12	1.68	0.76
1:C:227:LEU:HB2	4:C:917:HOH:O	1.86	0.75
1:B:286:GLN:NE2	1:B:288:ASP:H	1.80	0.75
1:A:238:ALA:CB	1:A:271:LEU:HD22	2.15	0.75
1:C:97:LEU:HB2	1:C:237:MET:HE1	1.67	0.75
1:C:73:VAL:HG21	1:C:84:LEU:HB3	1.67	0.74
1:A:117:ARG:H	1:A:117:ARG:HD2	1.51	0.74
1:A:98:GLN:HA	1:A:269:PHE:O	1.88	0.74
1:C:287:TYR:OH	2:C:802:SA8:HE3	1.88	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:92:ARG:HB2	1:B:92:ARG:NH1	2.04	0.73
1:B:202:LEU:H	1:B:202:LEU:HD12	1.54	0.73
1:A:97:LEU:HD22	1:A:237:MET:SD	2.29	0.73
1:A:286:GLN:HG2	1:A:289:LEU:HG	1.69	0.73
1:C:157:THR:OG1	1:C:177:THR:HG21	1.90	0.72
1:B:199:ASN:HB3	1:B:202:LEU:HD13	1.71	0.72
1:A:100:PRO:HD2	1:A:103:LEU:HD12	1.70	0.72
1:B:179:SER:OG	1:C:482:LEU:HD11	1.91	0.71
1:C:250:GLU:HA	4:C:907:HOH:O	1.89	0.71
1:B:107:PRO:O	1:B:110:VAL:HG22	1.91	0.70
1:A:482:LEU:HD21	1:C:180:VAL:HA	1.73	0.70
1:B:329:LEU:O	1:B:333:GLU:HG3	1.90	0.70
1:B:264:SER:HA	1:B:267:TYR:CZ	2.27	0.70
1:A:101:LYS:HA	1:A:104:TRP:CD2	2.27	0.70
1:C:286:GLN:HG2	1:C:289:LEU:HG	1.75	0.69
1:B:157:THR:OG1	1:B:177:THR:HG21	1.91	0.69
1:B:174:LEU:O	1:B:178:VAL:HG23	1.93	0.68
1:B:348:ASN:H	1:B:446:GLN:HE22	1.40	0.68
1:C:286:GLN:HE21	1:C:288:ASP:H	1.41	0.68
1:B:241:ILE:HG12	1:B:285:ILE:HG23	1.75	0.68
1:A:118:VAL:HG13	4:A:910:HOH:O	1.92	0.68
1:B:394:GLU:HB2	1:B:458:LEU:HD21	1.75	0.68
1:A:96:ILE:HD11	1:A:273:SER:HB2	1.75	0.68
1:B:97:LEU:HB2	1:B:237:MET:HE1	1.74	0.68
1:A:97:LEU:HD22	1:A:237:MET:CG	2.23	0.68
1:A:256:VAL:H	1:A:268:LEU:HD11	1.58	0.68
1:A:466:GLU:HB2	4:A:909:HOH:O	1.93	0.68
1:B:117:ARG:H	1:B:117:ARG:HD2	1.59	0.67
1:B:381:TRP:O	1:B:385:GLU:HG3	1.94	0.67
1:B:92:ARG:CB	1:B:92:ARG:HH11	2.08	0.67
1:B:104:TRP:NE1	4:B:910:HOH:O	2.14	0.67
1:C:398:LYS:O	1:C:402:GLU:HG2	1.95	0.67
1:A:314:LEU:HG	1:A:345:ILE:HD12	1.77	0.67
1:B:226:ARG:HD3	4:B:967:HOH:O	1.94	0.67
1:C:254:TYR:HH	3:C:901:LYS:N	1.93	0.67
1:B:197:LEU:HB2	1:B:198:PRO:HD3	1.77	0.66
1:C:92:ARG:O	1:C:93:ASN:HB2	1.95	0.66
1:A:104:TRP:CH2	1:A:269:PHE:HB2	2.31	0.66
1:B:73:VAL:HG21	1:B:84:LEU:HB3	1.76	0.66
1:A:107:PRO:O	1:A:110:VAL:HG22	1.96	0.66
1:B:101:LYS:HA	1:B:104:TRP:CD2	2.31	0.66
1:B:101:LYS:HA	1:B:104:TRP:CE2	2.31	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:226:ARG:HH22	1:B:288:ASP:HA	1.60	0.65
1:C:97:LEU:HD13	1:C:237:MET:HE3	1.77	0.65
1:C:99:VAL:O	1:C:104:TRP:HH2	1.79	0.65
1:B:91:SER:HB2	1:B:94:ASP:OD1	1.97	0.65
1:A:157:THR:OG1	1:A:177:THR:HG21	1.96	0.65
1:C:244:SER:C	1:C:246:GLY:H	2.00	0.65
1:B:67:ILE:HD11	1:B:237:MET:SD	2.37	0.65
1:C:201:ARG:HB3	1:C:201:ARG:HH11	1.62	0.65
1:A:219:LEU:HD11	1:A:232:LEU:HD21	1.79	0.64
1:A:54:VAL:HA	1:A:149:ILE:HD11	1.77	0.64
1:A:286:GLN:NE2	1:A:288:ASP:H	1.95	0.64
1:B:202:LEU:N	1:B:202:LEU:HD12	2.12	0.64
1:A:197:LEU:HB2	1:A:198:PRO:HD3	1.78	0.64
2:C:802:SA8:H3'	4:C:983:HOH:O	1.97	0.64
1:B:99:VAL:O	1:B:104:TRP:HH2	1.81	0.64
1:A:358:TYR:O	1:A:362:VAL:HG23	1.98	0.63
1:A:97:LEU:HD11	1:A:238:ALA:HB2	1.79	0.63
1:C:479:GLY:O	1:C:483:GLU:HG2	1.99	0.63
1:A:249:THR:HG22	4:A:904:HOH:O	1.98	0.63
1:C:320:GLU:HA	1:C:325:PHE:CD1	2.34	0.63
1:C:117:ARG:H	1:C:117:ARG:HD2	1.63	0.63
1:B:61:LEU:HB3	1:B:67:ILE:HG12	1.81	0.63
1:B:401:ARG:O	1:B:405:LYS:HG3	1.99	0.63
1:C:278:LYS:H	1:C:278:LYS:HE3	1.64	0.62
1:C:104:TRP:CH2	1:C:269:PHE:HB2	2.34	0.62
1:A:286:GLN:HE21	1:A:288:ASP:C	2.02	0.62
1:A:117:ARG:HG2	4:A:910:HOH:O	1.98	0.62
1:A:486:TYR:HB2	1:C:123:LYS:NZ	2.15	0.62
1:A:62:GLN:HA	1:A:67:ILE:HG23	1.82	0.62
1:C:99:VAL:O	1:C:104:TRP:CH2	2.53	0.62
1:B:110:VAL:HG12	1:B:131:PHE:CG	2.34	0.61
1:B:73:VAL:CG2	1:B:84:LEU:HB3	2.31	0.61
1:B:59:LYS:HB2	1:B:59:LYS:NZ	2.14	0.61
1:B:243:HIS:HB3	2:B:801:SA8:N7	2.16	0.61
1:A:287:TYR:OH	2:A:800:SA8:HE3	2.00	0.61
1:B:395:LEU:CD2	1:C:469:LEU:HD12	2.29	0.61
1:B:201:ARG:HB3	1:B:201:ARG:NH1	2.15	0.61
1:A:300:TYR:HB3	4:A:975:HOH:O	1.99	0.61
1:A:482:LEU:HD11	1:C:179:SER:OG	2.00	0.61
1:B:201:ARG:HB3	1:B:201:ARG:HH11	1.66	0.61
1:A:82:LEU:O	2:A:800:SA8:N	2.33	0.61
1:A:202:LEU:C	1:A:204:PRO:HD3	2.22	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:251:ASP:O	1:C:252:HIS:O	2.18	0.60
1:A:176:THR:O	1:A:180:VAL:HG23	2.01	0.60
1:C:103:LEU:O	1:C:143:TRP:CZ3	2.54	0.60
1:C:159:TYR:OH	1:C:217:GLY:HA3	2.02	0.60
1:B:408:LEU:HD21	1:B:444:LEU:HB3	1.82	0.60
1:C:286:GLN:HE21	1:C:288:ASP:N	1.99	0.60
1:C:313:THR:HB	1:C:344:ASP:OD1	2.02	0.60
1:C:74:LYS:HB3	1:C:87:LEU:HD21	1.83	0.60
1:B:176:THR:HG21	1:C:481:ILE:HD12	1.82	0.60
1:B:157:THR:OG1	1:B:177:THR:CG2	2.50	0.60
1:C:327:ASP:O	1:C:331:VAL:HG23	2.02	0.60
1:B:92:ARG:HB2	1:B:92:ARG:HH11	1.66	0.59
1:C:388:VAL:O	1:C:463:TYR:HB3	2.02	0.59
1:B:78:VAL:HG12	1:B:79:THR:N	2.18	0.59
1:C:97:LEU:HB2	1:C:237:MET:CE	2.33	0.59
1:A:342:TYR:CZ	1:B:479:GLY:HA3	2.38	0.59
1:A:60:TRP:O	1:A:64:GLU:HG2	2.02	0.59
1:A:176:THR:HG21	1:B:481:ILE:HD12	1.85	0.59
1:B:244:SER:HB2	1:B:284:TYR:CG	2.37	0.59
1:A:474:LEU:HD22	1:C:316:LEU:CD2	2.33	0.59
1:A:286:GLN:HE21	1:A:288:ASP:H	1.50	0.59
1:A:99:VAL:HG21	1:A:237:MET:HB3	1.85	0.58
1:C:470:LYS:HA	1:C:470:LYS:HE2	1.85	0.58
1:A:252:HIS:NE2	1:A:285:ILE:HB	2.18	0.58
1:A:370:PHE:HB3	4:A:923:HOH:O	2.03	0.58
1:C:225:SER:HA	4:C:917:HOH:O	2.02	0.58
1:C:129:ILE:O	1:C:133:ILE:HG13	2.04	0.58
1:B:262:LEU:HD23	4:B:911:HOH:O	2.02	0.58
1:C:199:ASN:HB3	1:C:202:LEU:HD13	1.86	0.58
1:A:99:VAL:CG2	1:A:237:MET:HB3	2.33	0.58
1:C:278:LYS:HE3	1:C:281:GLU:OE1	2.04	0.58
1:C:103:LEU:HA	1:C:143:TRP:CH2	2.39	0.57
1:A:129:ILE:O	1:A:133:ILE:HG13	2.04	0.57
1:C:438:GLU:OE2	1:C:442:MET:HE2	2.05	0.57
1:C:348:ASN:H	1:C:446:GLN:HE22	1.50	0.57
1:B:393:GLU:O	1:B:396:LEU:HG	2.04	0.57
1:A:157:THR:CB	1:A:177:THR:HG21	2.34	0.57
1:C:194:GLU:C	1:C:195:ILE:HD12	2.24	0.57
1:A:329:LEU:O	1:A:333:GLU:HG3	2.04	0.57
1:A:366:GLY:HA3	4:A:977:HOH:O	2.04	0.57
1:A:99:VAL:O	1:A:104:TRP:HH2	1.86	0.57
1:B:348:ASN:N	1:B:446:GLN:HE22	2.02	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:103:LEU:O	1:B:143:TRP:HZ3	1.87	0.57
1:B:323:PRO:HG2	1:B:324:PHE:CD1	2.39	0.57
1:A:99:VAL:O	1:A:104:TRP:CH2	2.58	0.57
1:B:438:GLU:HG2	1:B:442:MET:HE2	1.87	0.57
1:C:129:ILE:HG23	1:C:215:ALA:HB3	1.87	0.57
1:C:428:SER:O	1:C:432:ILE:HG13	2.04	0.57
1:B:292:SER:OG	1:B:295:GLU:HG3	2.05	0.57
1:C:286:GLN:NE2	1:C:288:ASP:H	2.02	0.56
1:A:177:THR:HG22	1:A:298:LEU:HG	1.86	0.56
1:C:202:LEU:C	1:C:204:PRO:HD3	2.25	0.56
1:A:320:GLU:HA	1:A:325:PHE:CD1	2.39	0.56
1:A:101:LYS:HA	1:A:104:TRP:CE2	2.40	0.56
1:C:235:VAL:HG12	4:C:902:HOH:O	2.06	0.56
1:C:104:TRP:CZ2	4:C:990:HOH:O	2.52	0.56
1:C:106:ASN:HB2	1:C:107:PRO:HD2	1.87	0.56
1:B:192:GLU:HA	1:B:196:ILE:HB	1.88	0.56
1:C:196:ILE:HD13	1:C:207:VAL:HG21	1.87	0.56
1:B:97:LEU:HD22	1:B:237:MET:HE3	1.88	0.56
1:C:146:TYR:CE1	1:C:236:PRO:HA	2.41	0.56
1:B:185:LYS:O	1:B:189:LEU:HG	2.05	0.56
1:B:327:ASP:O	1:B:331:VAL:HG23	2.06	0.56
1:C:310:HIS:CD2	1:C:439:GLY:HA3	2.41	0.56
1:A:394:GLU:HB2	1:A:458:LEU:HD21	1.89	0.55
1:A:418:ASP:O	1:A:422:LYS:HG3	2.06	0.55
1:B:313:THR:HB	1:B:344:ASP:OD1	2.06	0.55
1:B:241:ILE:HG12	1:B:285:ILE:CG2	2.35	0.55
1:C:73:VAL:CG2	1:C:84:LEU:HB3	2.37	0.55
1:C:104:TRP:HH2	1:C:269:PHE:H	1.55	0.55
1:C:244:SER:C	1:C:246:GLY:N	2.59	0.55
1:B:227:LEU:HD22	1:B:255:GLU:OE1	2.06	0.55
1:C:50:LEU:HD22	1:C:54:VAL:CG1	2.28	0.55
1:B:467:ARG:HA	1:B:470:LYS:HG3	1.88	0.54
1:A:416:GLU:HB2	4:A:971:HOH:O	2.05	0.54
1:C:228:ARG:O	1:C:229:ASN:HB2	2.08	0.54
1:C:97:LEU:HD22	1:C:237:MET:HE3	1.88	0.54
1:C:202:LEU:H	1:C:202:LEU:HD12	1.71	0.54
1:B:467:ARG:HA	1:B:470:LYS:CG	2.36	0.54
1:B:103:LEU:O	1:B:143:TRP:CZ3	2.60	0.54
1:A:97:LEU:HD22	1:A:237:MET:HG3	1.88	0.54
1:C:104:TRP:HZ2	4:C:990:HOH:O	1.89	0.54
1:A:199:ASN:HB3	1:A:202:LEU:HD13	1.88	0.54
1:B:239:ASP:HB3	4:B:907:HOH:O	2.08	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:243:HIS:HE1	1:A:286:GLN:OE1	1.90	0.54
1:A:313:THR:HB	1:A:344:ASP:OD1	2.08	0.54
1:B:286:GLN:HE22	1:B:309:ARG:HH22	1.54	0.53
1:B:288:ASP:HB3	1:B:291:LYS:HG3	1.88	0.53
1:B:264:SER:HA	1:B:267:TYR:CE2	2.43	0.53
1:B:228:ARG:HA	4:B:923:HOH:O	2.08	0.53
1:C:329:LEU:O	1:C:333:GLU:HG3	2.08	0.53
1:A:155:ASP:OD2	1:A:428:SER:HB3	2.08	0.53
1:A:348:ASN:H	1:A:446:GLN:HE22	1.57	0.53
1:B:97:LEU:HB2	1:B:237:MET:CE	2.37	0.53
1:C:110:VAL:HG12	1:C:131:PHE:CG	2.43	0.53
1:A:167:GLU:HG3	1:A:437:ARG:NH1	2.22	0.53
1:C:157:THR:OG1	1:C:177:THR:CG2	2.57	0.53
1:C:455:GLU:O	1:C:458:LEU:HB2	2.08	0.53
1:A:247:VAL:HG21	1:A:285:ILE:HA	1.91	0.53
1:A:325:PHE:CZ	1:A:329:LEU:HD22	2.44	0.53
1:A:360:ARG:HG2	1:A:392:ASN:OD1	2.08	0.53
1:A:428:SER:HB2	4:A:936:HOH:O	2.09	0.53
1:C:430:LEU:O	1:C:434:VAL:HG23	2.09	0.53
1:B:264:SER:HA	1:B:267:TYR:CE1	2.44	0.52
1:A:484:ASN:HB3	4:A:980:HOH:O	2.09	0.52
1:B:124:PRO:HG2	4:C:1009:HOH:O	2.07	0.52
1:A:286:GLN:HE22	1:A:309:ARG:HH22	1.57	0.52
1:B:411:TYR:HB3	4:B:903:HOH:O	2.08	0.52
1:A:103:LEU:HA	1:A:143:TRP:CH2	2.44	0.52
1:A:486:TYR:HB2	1:C:123:LYS:HZ2	1.75	0.52
1:B:287:TYR:O	1:B:288:ASP:HB2	2.09	0.52
1:C:293:ASN:OD1	1:C:303:ILE:HB	2.09	0.52
1:C:250:GLU:HG2	1:C:289:LEU:HD12	1.92	0.52
1:A:255:GLU:HB2	1:A:268:LEU:HD12	1.91	0.52
1:A:466:GLU:HG2	1:A:470:LYS:HE2	1.92	0.52
1:A:286:GLN:HE21	1:A:288:ASP:N	2.08	0.52
1:B:99:VAL:O	1:B:104:TRP:CH2	2.63	0.52
1:C:104:TRP:NE1	4:C:990:HOH:O	2.41	0.52
1:B:342:TYR:CZ	1:C:479:GLY:HA3	2.45	0.52
1:A:408:LEU:HD21	1:A:444:LEU:HB3	1.92	0.52
1:B:201:ARG:HH12	1:B:202:LEU:HD11	1.75	0.52
1:A:78:VAL:HG23	1:A:80:GLU:HG2	1.92	0.52
1:A:244:SER:HB2	1:A:284:TYR:CG	2.45	0.52
1:A:174:LEU:O	1:A:178:VAL:HG23	2.09	0.52
1:C:151:PRO:HD3	1:C:222:ARG:HH21	1.75	0.52
1:C:54:VAL:HA	1:C:149:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:104:TRP:O	1:A:105:ILE:HG13	2.10	0.51
1:A:287:TYR:O	3:A:902:LYS:HA	2.11	0.51
1:B:104:TRP:O	1:B:105:ILE:HG13	2.10	0.51
1:C:201:ARG:NH1	1:C:201:ARG:HB3	2.25	0.51
1:A:96:ILE:HD13	1:A:283:VAL:HG11	1.92	0.51
1:A:103:LEU:O	1:A:143:TRP:CZ3	2.64	0.51
1:C:98:GLN:HA	1:C:269:PHE:O	2.10	0.51
1:A:60:TRP:CE3	1:A:61:LEU:HG	2.46	0.51
1:B:58:TRP:O	1:B:62:GLN:HG3	2.10	0.51
1:A:105:ILE:O	1:A:105:ILE:HG22	2.11	0.51
1:C:192:GLU:HA	1:C:196:ILE:HB	1.93	0.50
1:C:97:LEU:HD22	1:C:237:MET:CE	2.42	0.50
1:B:241:ILE:CG1	1:B:285:ILE:HG23	2.39	0.50
1:A:386:LEU:O	1:A:387:SER:CB	2.59	0.50
1:A:277:VAL:HG13	1:A:281:GLU:HB2	1.92	0.50
2:B:801:SA8:H3'	4:B:981:HOH:O	2.12	0.50
1:A:114:GLU:OE1	1:A:134:ARG:NH2	2.45	0.50
1:A:119:CYS:HA	1:A:122:LEU:HD12	1.93	0.50
1:B:226:ARG:NH2	1:B:288:ASP:HA	2.26	0.50
1:A:101:LYS:HG3	1:A:104:TRP:CD1	2.47	0.50
2:A:800:SA8:HE2	3:A:902:LYS:NZ	2.27	0.50
2:A:800:SA8:H3'	4:A:975:HOH:O	2.10	0.50
1:B:228:ARG:O	1:B:229:ASN:HB2	2.12	0.50
1:C:167:GLU:HG3	1:C:437:ARG:NH1	2.27	0.50
1:A:157:THR:HA	1:A:160:TRP:CD1	2.47	0.50
1:A:118:VAL:HG22	4:A:910:HOH:O	2.11	0.49
1:C:82:LEU:O	2:C:802:SA8:N	2.45	0.49
1:B:360:ARG:HG2	1:B:392:ASN:OD1	2.12	0.49
1:A:201:ARG:HH11	1:A:201:ARG:HB3	1.77	0.49
1:A:428:SER:O	1:A:432:ILE:HG13	2.12	0.49
1:B:202:LEU:C	1:B:204:PRO:HD3	2.32	0.49
1:B:333:GLU:HA	1:B:337:PHE:O	2.12	0.49
1:C:446:GLN:O	1:C:450:ILE:HG13	2.12	0.49
1:A:110:VAL:HG12	1:A:131:PHE:CG	2.48	0.49
1:C:410:GLY:HA3	4:C:937:HOH:O	2.12	0.49
1:C:371:LEU:HB3	1:C:380:ILE:HD13	1.93	0.49
1:B:176:THR:O	1:B:180:VAL:HG23	2.13	0.49
1:B:155:ASP:OD2	1:B:428:SER:HB3	2.13	0.49
1:C:222:ARG:O	3:C:901:LYS:HE3	2.13	0.49
1:A:98:GLN:HE21	1:A:270:SER:HG	1.57	0.48
1:C:481:ILE:HD11	4:C:1026:HOH:O	2.11	0.48
1:B:323:PRO:HG2	1:B:324:PHE:HD1	1.78	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:160:TRP:CD1	1:B:429:ARG:HD3	2.48	0.48
1:C:314:LEU:HG	1:C:345:ILE:HD12	1.95	0.48
1:B:49:SER:O	1:B:52:PRO:HG2	2.13	0.48
1:A:159:TYR:OH	1:A:217:GLY:HA3	2.13	0.48
1:C:167:GLU:HG3	1:C:437:ARG:HH12	1.78	0.48
1:B:376:PHE:O	1:B:378:ASP:N	2.46	0.48
1:C:483:GLU:HA	1:C:486:TYR:HD2	1.77	0.48
1:B:300:TYR:HA	4:B:981:HOH:O	2.12	0.48
1:A:256:VAL:H	1:A:268:LEU:CD1	2.25	0.48
1:B:104:TRP:CH2	1:B:269:PHE:HB2	2.49	0.48
1:C:173:LEU:O	1:C:177:THR:HG23	2.14	0.48
1:C:469:LEU:HD22	1:C:472:LEU:HD21	1.96	0.48
1:C:103:LEU:HA	1:C:143:TRP:HH2	1.77	0.48
1:A:476:GLY:O	1:C:175:LYS:HD2	2.13	0.48
1:B:226:ARG:NH2	1:B:250:GLU:CD	2.66	0.48
1:C:463:TYR:O	1:C:467:ARG:HG3	2.14	0.48
1:A:316:LEU:CD2	1:B:474:LEU:HD22	2.43	0.48
1:C:73:VAL:HG22	1:C:74:LYS:N	2.28	0.48
1:C:286:GLN:HE22	1:C:309:ARG:HH22	1.61	0.48
1:C:286:GLN:HE21	1:C:288:ASP:C	2.17	0.48
1:A:401:ARG:NH1	1:A:452:GLU:HG3	2.29	0.48
1:B:388:VAL:O	1:B:463:TYR:HB3	2.14	0.48
1:C:57:PHE:CE2	1:C:61:LEU:HD11	2.49	0.48
1:B:100:PRO:O	1:B:104:TRP:CZ3	2.66	0.48
1:C:72:PRO:HB3	1:C:88:LYS:HE3	1.95	0.48
1:B:274:PRO:O	1:B:275:LEU:HD23	2.14	0.48
1:C:292:SER:OG	1:C:295:GLU:HG3	2.14	0.48
1:A:356:LEU:N	1:A:357:PRO:HD2	2.28	0.47
1:C:244:SER:O	1:C:246:GLY:N	2.46	0.47
1:C:104:TRP:HE3	1:C:104:TRP:N	2.12	0.47
1:A:167:GLU:HG2	1:A:430:LEU:CD1	2.44	0.47
1:C:468:ARG:HB3	1:C:468:ARG:HH11	1.79	0.47
1:C:390:ARG:HH11	1:C:390:ARG:HG2	1.78	0.47
1:B:88:LYS:HD3	1:B:88:LYS:O	2.15	0.47
1:C:64:GLU:OE1	1:C:102:ARG:NH1	2.48	0.47
1:A:106:ASN:HB2	1:A:107:PRO:HD2	1.96	0.47
1:B:439:GLY:O	1:B:442:MET:HB2	2.14	0.47
1:B:390:ARG:HH11	1:B:390:ARG:HG2	1.80	0.47
1:B:194:GLU:C	1:B:195:ILE:HD12	2.35	0.47
1:A:163:GLU:H	1:A:163:GLU:CD	2.17	0.47
1:C:327:ASP:OD1	1:C:377:ARG:NH2	2.48	0.47
1:B:482:LEU:HD22	1:B:486:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:113:SER:HB2	4:C:979:HOH:O	2.15	0.47
1:B:320:GLU:HA	1:B:325:PHE:CD1	2.49	0.47
1:C:50:LEU:N	4:C:933:HOH:O	2.48	0.46
1:A:348:ASN:N	1:A:446:GLN:HE22	2.14	0.46
1:A:115:ILE:HG22	1:A:202:LEU:HD22	1.98	0.46
1:B:88:LYS:O	1:B:90:ILE:HG13	2.15	0.46
1:A:188:CYS:HB3	1:A:212:PHE:CD1	2.49	0.46
1:B:51:SER:N	1:B:52:PRO:HD2	2.30	0.46
1:A:136:ARG:HA	1:A:147:PHE:CD1	2.51	0.46
1:C:252:HIS:C	1:C:254:TYR:H	2.18	0.46
1:B:92:ARG:CB	1:B:92:ARG:NH1	2.69	0.46
1:C:386:LEU:O	1:C:387:SER:CB	2.63	0.46
1:A:310:HIS:CD2	1:A:439:GLY:HA3	2.51	0.46
1:B:227:LEU:HB3	1:B:228:ARG:H	1.56	0.46
1:C:67:ILE:CD1	1:C:71:THR:HG21	2.46	0.46
1:A:96:ILE:HD11	1:A:273:SER:CB	2.42	0.46
1:B:160:TRP:HA	1:B:429:ARG:NH1	2.31	0.46
1:A:103:LEU:HA	1:A:143:TRP:HH2	1.81	0.46
1:B:363:ALA:O	1:B:364:LEU:C	2.53	0.46
1:B:117:ARG:N	1:B:117:ARG:HD2	2.30	0.46
1:B:273:SER:OG	1:B:275:LEU:O	2.33	0.46
1:B:226:ARG:NH2	1:B:250:GLU:OE2	2.49	0.46
1:B:394:GLU:CB	1:B:458:LEU:HD21	2.46	0.46
1:A:199:ASN:HB3	1:A:202:LEU:CD1	2.45	0.46
1:A:214:TRP:O	1:A:218:ILE:HG12	2.15	0.46
1:B:250:GLU:OE2	1:B:288:ASP:HA	2.16	0.45
2:C:802:SA8:HE2	3:C:901:LYS:NZ	2.31	0.45
1:A:96:ILE:HD11	1:A:273:SER:CA	2.46	0.45
1:C:361:LEU:HD13	1:C:384:LEU:HD11	1.97	0.45
1:C:244:SER:HB2	1:C:284:TYR:CG	2.51	0.45
1:B:386:LEU:O	1:B:387:SER:CB	2.63	0.45
1:B:202:LEU:O	1:B:204:PRO:HD3	2.17	0.45
1:A:201:ARG:NH1	1:A:201:ARG:HB3	2.31	0.45
1:A:146:TYR:CE1	1:A:236:PRO:HA	2.52	0.45
1:A:427:ASP:O	1:A:428:SER:C	2.55	0.45
1:B:59:LYS:HZ2	1:B:59:LYS:HB2	1.77	0.45
1:A:100:PRO:C	1:A:102:ARG:N	2.70	0.45
1:A:101:LYS:HA	1:A:104:TRP:CE3	2.51	0.45
1:A:472:LEU:HD21	1:C:362:VAL:HG11	1.99	0.45
1:C:73:VAL:HG22	1:C:74:LYS:H	1.82	0.45
1:C:107:PRO:HB2	4:C:939:HOH:O	2.15	0.45
1:B:82:LEU:O	2:B:801:SA8:N	2.48	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:310:HIS:HE1	4:A:919:HOH:O	2.00	0.45
1:B:104:TRP:CZ2	1:B:269:PHE:HB2	2.52	0.44
1:A:465:GLN:O	1:A:468:ARG:HB3	2.16	0.44
1:A:59:LYS:O	1:A:63:GLU:HG3	2.17	0.44
1:C:364:LEU:HD23	1:C:372:LEU:HD11	1.99	0.44
1:A:243:HIS:HB3	2:A:800:SA8:N7	2.32	0.44
1:B:103:LEU:HA	1:B:143:TRP:CH2	2.52	0.44
1:A:78:VAL:CG2	1:A:80:GLU:HG2	2.47	0.44
1:C:381:TRP:O	1:C:385:GLU:HG3	2.17	0.44
1:A:222:ARG:O	3:A:902:LYS:HE3	2.18	0.44
1:C:386:LEU:O	1:C:387:SER:HB3	2.17	0.44
3:C:901:LYS:N	4:C:948:HOH:O	2.50	0.44
1:B:104:TRP:O	1:B:143:TRP:CH2	2.69	0.44
1:A:209:LEU:O	1:A:212:PHE:HB2	2.18	0.44
1:B:177:THR:HG22	1:B:298:LEU:HD13	1.98	0.44
1:A:96:ILE:CD1	1:A:283:VAL:HG11	2.47	0.44
1:A:255:GLU:HB3	1:A:268:LEU:O	2.17	0.44
1:B:129:ILE:O	1:B:133:ILE:HG13	2.18	0.44
1:A:104:TRP:HE3	1:A:104:TRP:N	2.16	0.44
1:B:363:ALA:HB1	1:B:395:LEU:HD13	1.99	0.44
1:A:390:ARG:HG2	1:A:390:ARG:HH11	1.83	0.44
1:C:401:ARG:NH1	1:C:452:GLU:HG3	2.33	0.44
1:C:377:ARG:HD3	1:C:377:ARG:HA	1.82	0.44
1:A:167:GLU:HG3	1:A:437:ARG:HH12	1.83	0.44
1:C:475:CYS:HB2	4:C:1020:HOH:O	2.17	0.44
1:B:219:LEU:HD11	1:B:232:LEU:CD2	2.48	0.44
1:A:238:ALA:O	1:A:241:ILE:HG22	2.18	0.44
1:A:202:LEU:H	1:A:202:LEU:HD12	1.81	0.44
1:B:54:VAL:O	1:B:57:PHE:HB3	2.18	0.44
1:B:97:LEU:HD22	1:B:237:MET:CE	2.48	0.43
1:B:243:HIS:H	2:B:801:SA8:C8	2.31	0.43
1:A:315:THR:HB	1:A:342:TYR:CD2	2.53	0.43
1:B:49:SER:N	4:B:1005:HOH:O	2.51	0.43
1:A:388:VAL:O	1:A:463:TYR:HB3	2.18	0.43
1:A:311:ALA:HB2	1:A:346:PHE:CD2	2.53	0.43
1:A:150:LEU:HA	1:A:151:PRO:HD3	1.86	0.43
1:B:253:ALA:HA	1:B:270:SER:O	2.17	0.43
1:C:104:TRP:CE2	4:C:990:HOH:O	2.71	0.43
1:B:173:LEU:HD12	1:B:177:THR:HG23	2.00	0.43
1:A:157:THR:OG1	1:A:177:THR:CG2	2.65	0.43
1:C:107:PRO:O	1:C:110:VAL:HG22	2.18	0.43
1:C:214:TRP:O	1:C:218:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:226:ARG:HD2	3:C:901:LYS:N	2.33	0.43
1:C:293:ASN:ND2	1:C:309:ARG:HB2	2.33	0.43
1:A:466:GLU:O	1:A:470:LYS:HG2	2.19	0.43
1:A:58:TRP:CE2	1:A:67:ILE:HD12	2.54	0.43
1:C:125:TRP:O	1:C:129:ILE:HG13	2.19	0.43
1:B:356:LEU:N	1:B:357:PRO:HD2	2.33	0.43
1:B:78:VAL:CG1	1:B:79:THR:N	2.80	0.43
1:C:67:ILE:HD11	1:C:237:MET:SD	2.59	0.43
1:A:243:HIS:CE1	1:A:286:GLN:OE1	2.71	0.43
1:A:255:GLU:N	1:A:255:GLU:OE1	2.52	0.43
1:A:61:LEU:HB3	1:A:67:ILE:HG22	2.00	0.43
1:A:194:GLU:C	1:A:195:ILE:HD12	2.39	0.43
1:A:104:TRP:O	1:A:105:ILE:CG1	2.67	0.43
1:A:221:SER:O	2:A:800:SA8:HE1	2.18	0.43
1:A:99:VAL:HG21	1:A:235:VAL:HG12	2.01	0.43
1:A:235:VAL:HG21	1:A:269:PHE:CD1	2.53	0.43
1:C:104:TRP:CE3	1:C:104:TRP:N	2.86	0.43
1:B:151:PRO:HD3	1:B:222:ARG:HH21	1.83	0.43
1:C:151:PRO:CD	1:C:222:ARG:HH21	2.32	0.42
1:B:262:LEU:HD22	1:B:266:ASP:HB2	2.01	0.42
1:B:168:LEU:HD21	1:B:433:ALA:HA	2.00	0.42
1:C:185:LYS:O	1:C:189:LEU:HG	2.18	0.42
1:A:104:TRP:CE3	1:A:104:TRP:N	2.87	0.42
1:B:364:LEU:HD23	1:B:372:LEU:HD11	2.01	0.42
1:C:226:ARG:HB3	1:C:252:HIS:CE1	2.54	0.42
1:C:226:ARG:HD3	1:C:252:HIS:CD2	2.54	0.42
1:A:247:VAL:HG21	1:A:285:ILE:CA	2.49	0.42
1:C:147:PHE:HD2	1:C:150:LEU:HD12	1.84	0.42
1:B:313:THR:HG21	1:C:478:ASN:OD1	2.18	0.42
1:A:172:GLN:OE1	1:A:313:THR:HG23	2.19	0.42
1:C:364:LEU:HD12	1:C:364:LEU:HA	1.84	0.42
1:B:88:LYS:HD3	1:B:88:LYS:C	2.39	0.42
1:B:453:GLN:O	1:B:457:GLU:HG3	2.20	0.42
1:B:97:LEU:CB	1:B:237:MET:HE1	2.47	0.42
1:B:192:GLU:O	1:B:197:LEU:HG	2.19	0.42
1:C:202:LEU:N	1:C:202:LEU:HD12	2.34	0.42
1:B:323:PRO:HB3	1:C:375:LEU:HD21	2.01	0.42
1:B:482:LEU:HB2	4:B:975:HOH:O	2.19	0.42
1:C:315:THR:C	1:C:316:LEU:HD23	2.39	0.42
1:A:370:PHE:CD1	1:A:370:PHE:C	2.93	0.42
1:A:319:SER:O	1:A:325:PHE:HD1	2.02	0.42
1:C:106:ASN:HB2	1:C:107:PRO:CD	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:458:LEU:HD12	1:C:458:LEU:HA	1.74	0.42
1:C:243:HIS:HB3	2:C:802:SA8:N7	2.35	0.42
1:A:337:PHE:HB3	1:A:358:TYR:HE1	1.85	0.42
1:A:57:PHE:CD1	1:A:146:TYR:HA	2.54	0.42
1:B:257:LYS:HB3	1:B:258:GLY:H	1.60	0.42
1:A:222:ARG:HD3	1:A:239:ASP:OD2	2.20	0.42
1:B:101:LYS:HG3	1:B:104:TRP:CD1	2.55	0.42
1:C:400:VAL:HG11	1:C:451:PHE:CD1	2.55	0.42
1:C:277:VAL:HG13	1:C:281:GLU:HB2	2.02	0.42
1:A:199:ASN:ND2	1:A:199:ASN:N	2.68	0.42
1:B:350:THR:HG23	4:B:1019:HOH:O	2.19	0.42
1:A:73:VAL:CG2	1:A:84:LEU:HB3	2.44	0.41
1:C:243:HIS:HB2	1:C:287:TYR:CD2	2.55	0.41
1:A:486:TYR:HB2	1:C:123:LYS:HZ3	1.85	0.41
1:A:202:LEU:O	1:A:204:PRO:HD3	2.19	0.41
1:A:377:ARG:HA	1:A:377:ARG:HD3	1.90	0.41
1:C:315:THR:HB	1:C:342:TYR:CD2	2.55	0.41
1:A:199:ASN:HD22	1:A:199:ASN:N	2.18	0.41
1:C:414:THR:OG1	1:C:417:GLN:HG3	2.20	0.41
1:A:220:ARG:HG3	4:A:994:HOH:O	2.21	0.41
1:B:130:LEU:HD21	1:B:191:LEU:HD13	2.02	0.41
1:A:151:PRO:CD	1:A:222:ARG:HH21	2.33	0.41
1:A:88:LYS:HA	1:A:88:LYS:HD2	1.89	0.41
1:A:384:LEU:HD23	1:A:384:LEU:HA	1.85	0.41
1:A:227:LEU:HD22	1:A:227:LEU:N	2.35	0.41
1:A:316:LEU:HD23	1:B:474:LEU:HD22	2.03	0.41
1:B:364:LEU:HD12	1:B:364:LEU:HA	1.87	0.41
1:A:105:ILE:HD11	1:A:143:TRP:CD2	2.55	0.41
1:A:404:CYS:O	1:A:408:LEU:HG	2.20	0.41
1:A:219:LEU:HD11	1:A:232:LEU:CD2	2.49	0.41
1:C:103:LEU:O	1:C:143:TRP:HZ3	1.99	0.41
1:B:313:THR:HG21	1:C:478:ASN:CG	2.41	0.41
1:C:328:LYS:HE2	1:C:364:LEU:HB3	2.02	0.41
1:A:225:SER:OG	1:A:231:ASN:HB3	2.21	0.41
1:A:126:LEU:HD22	1:A:191:LEU:HD11	2.02	0.41
1:B:446:GLN:O	1:B:450:ILE:HG13	2.21	0.41
1:A:157:THR:HB	1:A:177:THR:HG21	2.03	0.41
1:A:62:GLN:CA	1:A:67:ILE:HG23	2.49	0.41
1:C:390:ARG:NH1	1:C:390:ARG:HG2	2.36	0.41
1:B:412:HIS:CD2	1:B:413:THR:HG23	2.55	0.41
1:B:370:PHE:C	1:B:370:PHE:CD1	2.94	0.41
1:B:225:SER:HB2	1:B:226:ARG:H	1.64	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:ARG:C	1:A:227:LEU:HD13	2.41	0.41
2:C:802:SA8:HB1	2:C:802:SA8:H4'	2.03	0.41
1:A:472:LEU:HD23	1:A:472:LEU:HA	1.94	0.41
1:C:146:TYR:CZ	1:C:150:LEU:HD21	2.56	0.40
1:B:376:PHE:C	1:B:378:ASP:H	2.25	0.40
1:A:380:ILE:HG23	1:A:381:TRP:N	2.36	0.40
2:A:800:SA8:HE2	3:A:902:LYS:HZ3	1.84	0.40
1:C:101:LYS:HA	1:C:104:TRP:CD2	2.56	0.40
2:B:801:SA8:H4'	2:B:801:SA8:HA	2.03	0.40
1:C:393:GLU:O	1:C:396:LEU:HG	2.20	0.40
1:A:100:PRO:C	1:A:102:ARG:H	2.24	0.40
1:B:98:GLN:HA	1:B:269:PHE:O	2.21	0.40
1:C:143:TRP:O	1:C:147:PHE:CD1	2.75	0.40
1:B:310:HIS:CD2	1:B:439:GLY:HA3	2.55	0.40
1:C:197:LEU:HB2	1:C:198:PRO:CD	2.51	0.40
1:C:482:LEU:HD23	1:C:482:LEU:HA	1.87	0.40
1:A:106:ASN:HB2	1:A:107:PRO:CD	2.51	0.40
1:A:99:VAL:HA	1:A:100:PRO:HD3	1.89	0.40
1:C:310:HIS:HD2	4:C:984:HOH:O	2.05	0.40
1:C:228:ARG:C	1:C:230:GLU:H	2.24	0.40
1:A:480:ASP:O	1:A:484:ASN:HB2	2.22	0.40
1:C:396:LEU:C	1:C:396:LEU:HD12	2.42	0.40
1:C:52:PRO:O	1:C:55:GLN:HB3	2.21	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	418/440 (95%)	360 (86%)	47 (11%)	11 (3%)	8	13
1	B	438/440 (100%)	381 (87%)	45 (10%)	12 (3%)	8	13
1	C	436/440 (99%)	392 (90%)	36 (8%)	8 (2%)	13	25
All	All	1292/1320 (98%)	1133 (88%)	128 (10%)	31 (2%)	9	16

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	105	ILE
1	A	387	SER
1	B	226	ARG
1	B	364	LEU
1	C	252	HIS
1	C	387	SER
1	A	104	TRP
1	A	232	LEU
1	A	236	PRO
1	B	204	PRO
1	B	288	ASP
1	B	366	GLY
1	B	387	SER
1	C	140	ASP
1	A	204	PRO
1	A	428	SER
1	B	377	ARG
1	B	428	SER
1	C	200	LYS
1	C	364	LEU
1	B	105	ILE
1	C	245	ALA
1	A	469	LEU
1	C	204	PRO
1	A	241	ILE
1	B	231	ASN
1	B	236	PRO
1	A	479	GLY
1	B	261	GLY
1	A	365	GLY
1	C	105	ILE

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	374/386 (97%)	348 (93%)	26 (7%)	21 41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	386/386 (100%)	365 (95%)	21 (5%)	31	57
1	C	384/386 (100%)	362 (94%)	22 (6%)	29	54
All	All	1144/1158 (99%)	1075 (94%)	69 (6%)	27	51

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	58	TRP
1	A	89	ASP
1	A	94	ASP
1	A	104	TRP
1	A	117	ARG
1	A	143	TRP
1	A	157	THR
1	A	199	ASN
1	A	205	ASP
1	A	236	PRO
1	A	237	MET
1	A	252	HIS
1	A	267	TYR
1	A	268	LEU
1	A	298	LEU
1	A	299	ASP
1	A	300	TYR
1	A	313	THR
1	A	315	THR
1	A	321	SER
1	A	339	GLN
1	A	395	LEU
1	A	426	LEU
1	A	427	ASP
1	A	444	LEU
1	A	486	TYR
1	B	72	PRO
1	B	88	LYS
1	B	94	ASP
1	B	102	ARG
1	B	104	TRP
1	B	117	ARG
1	B	143	TRP
1	B	166	GLN

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Mol	Chain	Res	Type
1	B	205	ASP
1	B	232	LEU
1	B	236	PRO
1	B	249	THR
1	B	313	THR
1	B	315	THR
1	B	339	GLN
1	B	395	LEU
1	B	426	LEU
1	B	427	ASP
1	B	444	LEU
1	B	471	ASP
1	B	482	LEU
1	C	55	GLN
1	C	68	THR
1	C	104	TRP
1	C	107	PRO
1	C	117	ARG
1	C	143	TRP
1	C	166	GLN
1	C	205	ASP
1	C	210	ASP
1	C	257	LYS
1	C	268	LEU
1	C	278	LYS
1	C	313	THR
1	C	315	THR
1	C	339	GLN
1	C	395	LEU
1	C	423	GLU
1	C	427	ASP
1	C	444	LEU
1	C	468	ARG
1	C	470	LYS
1	C	480	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	145	HIS
1	A	169	GLN

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Mol	Chain	Res	Type
1	A	193	GLN
1	A	199	ASN
1	A	243	HIS
1	A	286	GLN
1	A	348	ASN
1	A	446	GLN
1	B	98	GLN
1	B	152	GLN
1	B	169	GLN
1	B	286	GLN
1	B	310	HIS
1	B	412	HIS
1	B	446	GLN
1	B	484	ASN
1	B	488	GLN
1	C	55	GLN
1	C	145	HIS
1	C	152	GLN
1	C	169	GLN
1	C	193	GLN
1	C	252	HIS
1	C	286	GLN
1	C	310	HIS
1	C	446	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 ⓘ

6 ligands 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	$\# Z > 2$
2	SA8	A	800	-	29,29,29	1.51	5 (17%)	42,42,42	1.55	7 (16%)
3	LYS	A	902	-	9,9,9	0.56	0	10,10,10	0.76	1 (10%)
2	SA8	B	801	-	29,29,29	1.52	5 (17%)	42,42,42	1.67	6 (14%)
3	LYS	B	900	-	9,9,9	0.60	0	10,10,10	0.62	0
2	SA8	C	802	-	29,29,29	1.30	4 (13%)	42,42,42	1.73	7 (16%)
3	LYS	C	901	-	9,9,9	0.51	0	10,10,10	0.71	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	SA8	A	800	-	-	0/17/33/33	0/1/3/3
3	LYS	A	902	-	-	0/9/9/9	0/0/0/0
2	SA8	B	801	-	-	0/17/33/33	0/1/3/3
3	LYS	B	900	-	-	0/9/9/9	0/0/0/0
2	SA8	C	802	-	-	0/17/33/33	0/1/3/3
3	LYS	C	901	-	-	0/9/9/9	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	SA8	C5'-ND	4.04	1.57	1.47
2	A	800	SA8	C5'-ND	3.89	1.57	1.47
2	A	800	SA8	CG-ND	3.70	1.56	1.46
2	C	802	SA8	C5'-ND	3.62	1.56	1.47
2	B	801	SA8	CG-ND	3.60	1.56	1.46
2	A	800	SA8	C4-N3	3.34	1.40	1.35
2	C	802	SA8	CG-ND	3.25	1.55	1.46
2	B	801	SA8	C4-N9	3.00	1.42	1.37
2	B	801	SA8	C4-N3	2.74	1.39	1.35
2	A	800	SA8	C4-N9	2.65	1.41	1.37
2	C	802	SA8	C4-N3	2.49	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	SA8	C8-N7	-2.24	1.30	1.34
2	A	800	SA8	C8-N7	-2.15	1.30	1.34
2	C	802	SA8	C8-N7	-2.12	1.30	1.34

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	SA8	O4'-C4'-C5'	5.27	116.43	108.62
2	C	802	SA8	C4'-C5'-ND	5.18	121.25	112.06
2	B	801	SA8	C4'-C5'-ND	4.72	120.44	112.06
2	A	800	SA8	C4'-C5'-ND	4.55	120.13	112.06
2	A	800	SA8	C8-N9-C4	-4.46	103.50	106.90
2	C	802	SA8	O4'-C4'-C5'	4.42	115.18	108.62
2	A	800	SA8	O4'-C4'-C5'	4.25	114.92	108.62
2	B	801	SA8	C8-N9-C4	-4.23	103.67	106.90
2	C	802	SA8	C8-N9-C4	-3.93	103.90	106.90
2	C	802	SA8	CE-ND-C5'	-3.77	105.01	111.22
2	B	801	SA8	C4'-O4'-C1'	-3.37	106.08	109.75
2	C	802	SA8	O4'-C1'-N9	3.36	111.56	108.44
2	B	801	SA8	O4'-C1'-N9	3.22	111.44	108.44
2	C	802	SA8	C4'-O4'-C1'	-2.86	106.64	109.75
2	A	800	SA8	CE-ND-C5'	-2.59	106.95	111.22
2	C	802	SA8	C3'-C2'-C1'	2.35	104.59	100.91
2	A	800	SA8	C4'-O4'-C1'	-2.31	107.24	109.75
2	A	800	SA8	C3'-C2'-C1'	2.27	104.45	100.91
2	B	801	SA8	CE-ND-C5'	-2.15	107.67	111.22
2	A	800	SA8	O4'-C1'-N9	2.10	110.40	108.44
3	A	902	LYS	C-CA-N	2.00	112.68	109.36

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	424/440 (96%)	0.27	27 (6%)	19 16	47, 71, 110, 127	0
1	B	440/440 (100%)	0.15	21 (4%)	29 26	39, 66, 103, 129	0
1	C	438/440 (99%)	0.06	13 (2%)	48 45	44, 66, 99, 112	0
All	All	1302/1320 (98%)	0.16	61 (4%)	30 27	39, 68, 105, 129	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	ASP	5.9
1	B	486	TYR	5.3
1	A	267	TYR	5.2
1	C	250	GLU	4.9
1	A	254	TYR	4.8
1	A	256	VAL	4.6
1	C	487	PHE	4.4
1	B	488	GLN	4.4
1	B	139	GLU	4.3
1	A	59	LYS	4.0
1	A	144	LYS	4.0
1	A	117	ARG	3.9
1	A	70	LYS	3.9
1	A	139	GLU	3.6
1	B	375	LEU	3.5
1	A	112	ALA	3.5
1	C	117	ARG	3.4
1	C	229	ASN	3.4
1	C	139	GLU	3.3
1	B	229	ASN	3.3
1	A	250	GLU	3.2
1	B	121	GLU	3.2
1	A	50	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	226	ARG	3.2
1	C	200	LYS	3.2
1	A	486	TYR	3.2
1	B	205	ASP	3.1
1	C	378	ASP	3.1
1	B	259	ALA	3.0
1	A	145	HIS	3.0
1	A	197	LEU	2.9
1	C	471	ASP	2.9
1	A	137	SER	2.9
1	C	205	ASP	2.9
1	A	121	GLU	2.7
1	B	378	ASP	2.7
1	B	144	LYS	2.7
1	A	111	ALA	2.7
1	B	254	TYR	2.6
1	A	253	ALA	2.5
1	C	470	LYS	2.5
1	B	117	ARG	2.5
1	B	228	ARG	2.5
1	A	201	ARG	2.4
1	B	112	ALA	2.4
1	B	204	PRO	2.4
1	A	138	ARG	2.4
1	B	193	GLN	2.3
1	B	460	GLN	2.3
1	B	130	LEU	2.3
1	B	471	ASP	2.3
1	C	162	GLU	2.2
1	B	487	PHE	2.2
1	C	55	GLN	2.1
1	A	69	ALA	2.1
1	A	471	ASP	2.1
1	A	166	GLN	2.1
1	A	460	GLN	2.1
1	A	55	GLN	2.0
1	B	140	ASP	2.0
1	C	140	ASP	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
2	SA8	B	801	27/27	0.32	5.96	85,97,100,103	0
2	SA8	A	800	27/27	0.26	4.71	100,103,107,107	0
2	SA8	C	802	27/27	0.25	3.47	90,98,102,105	0
3	LYS	B	900	10/10	0.24	0.96	69,79,84,84	0
3	LYS	A	902	10/10	0.24	0.78	81,91,96,96	0
3	LYS	C	901	10/10	0.14	-0.45	52,61,64,64	0

6.5 Other polymers ⓘ

There are no such residues in this entry.