



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:50 AM UTC

PDB ID : 3DER / pdb_00003der
Title : Crystal structure of dipeptide epimerase from *Thermotoga maritima* complexed with L-Ala-L-Lys dipeptide
Authors : Fedorov, A.A.; Fedorov, E.V.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.
Deposited on : 2008-06-10
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

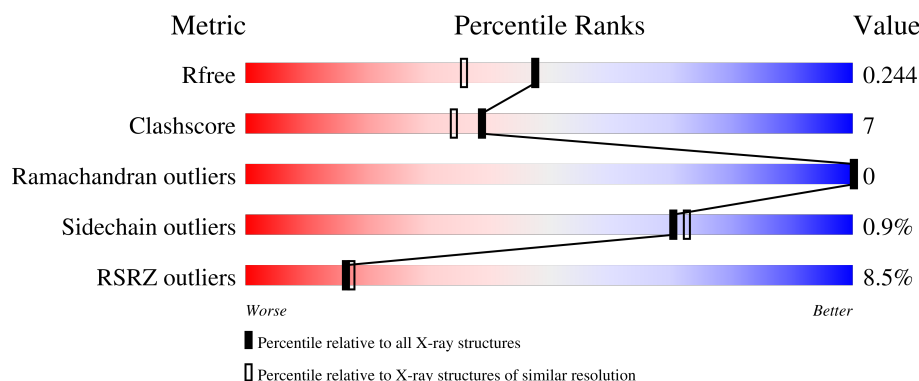
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	345	8% 82% 16% ..
1	B	345	9% 80% 18% ..
1	C	345	6% 82% 16% ..
1	D	345	11% 81% 17% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11531 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.

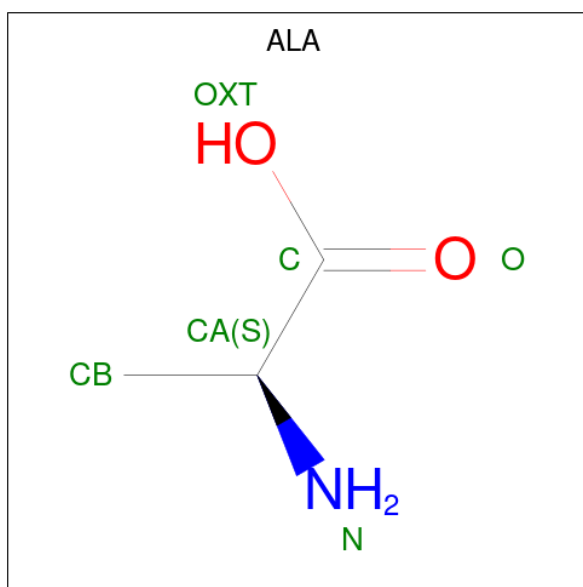
- Molecule 1 is a protein called Muconate cycloisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2687	1705	461	511	10			
1	B	341	Total	C	N	O	S	0	0	0
			2687	1705	461	511	10			
1	C	341	Total	C	N	O	S	0	0	0
			2687	1705	461	511	10			
1	D	341	Total	C	N	O	S	0	0	0
			2687	1705	461	511	10			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

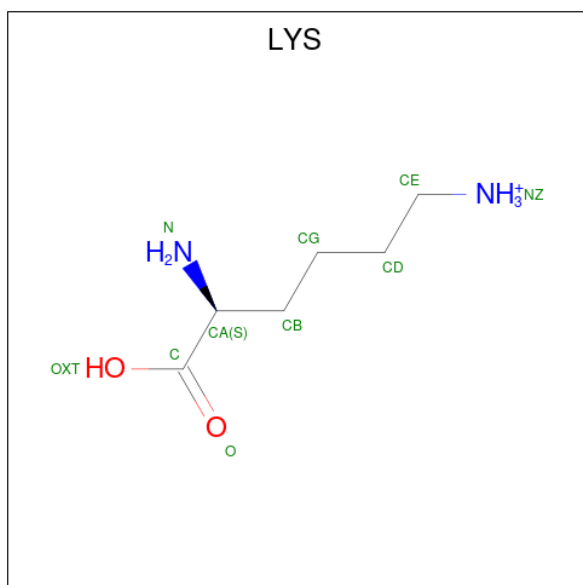
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ALANINE (CCD ID: ALA) (formula: C₃H₇NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			5	3	1	1		
3	B	1	Total	C	N	O	0	0
			5	3	1	1		
3	C	1	Total	C	N	O	0	0
			5	3	1	1		
3	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 4 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



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

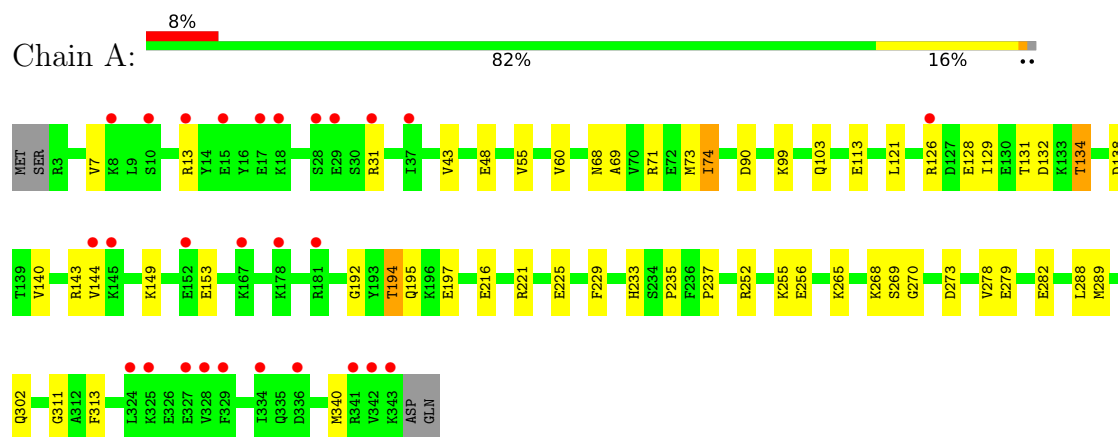
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	180	Total	O	0	0
			180	180		
5	B	170	Total	O	0	0
			170	170		
5	C	207	Total	O	0	0
			207	207		
5	D	162	Total	O	0	0
			162	162		

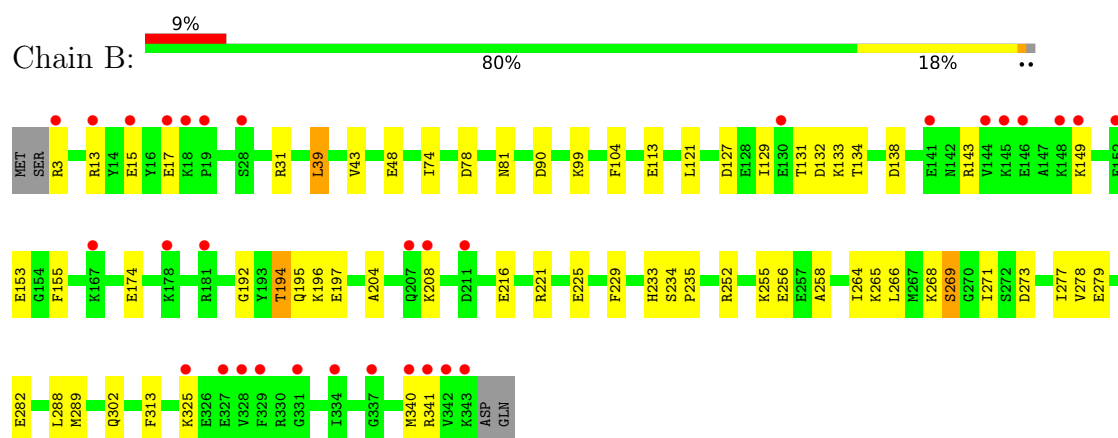
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

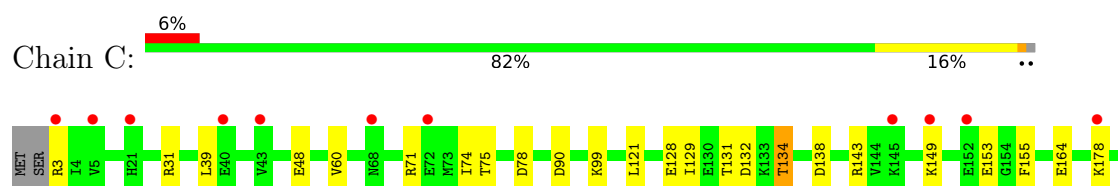
- Molecule 1: Muconate cycloisomerase



- Molecule 1: Muconate cycloisomerase

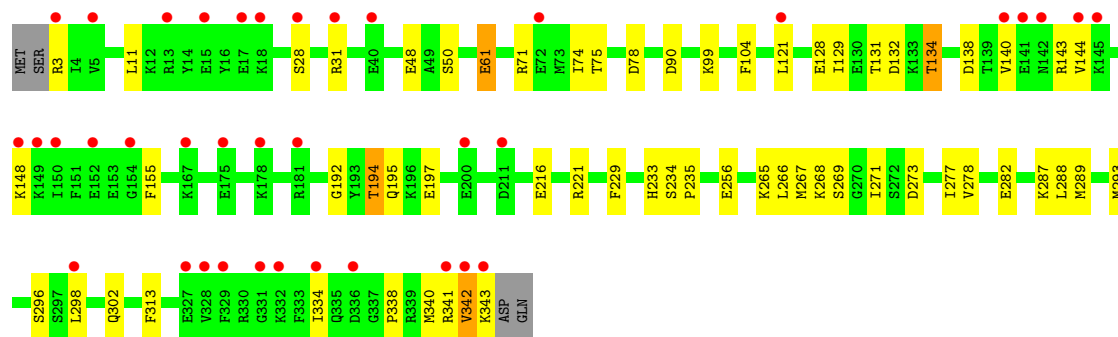
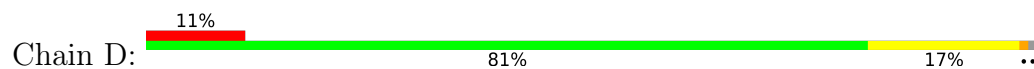


- Molecule 1: Muconate cycloisomerase





● Molecule 1: Muconate cycloisomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	190.69Å 190.69Å 283.11Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.99 – 1.90 24.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.8 (24.99-1.90) 97.9 (24.99-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.244 0.231 , 0.244	Depositor DCC
R_{free} test set	11570 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11531	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.36	0/2726	0.93	12/3662 (0.3%)
1	B	0.35	0/2726	0.92	15/3662 (0.4%)
1	C	0.37	0/2726	0.94	14/3662 (0.4%)
1	D	0.35	0/2726	0.93	14/3662 (0.4%)
All	All	0.35	0/10904	0.93	55/14648 (0.4%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	PRO	N-CA-C	8.94	125.03	114.03
1	C	235	PRO	N-CA-C	7.92	123.76	113.86
1	A	194	THR	N-CA-C	-7.64	100.67	110.53
1	D	235	PRO	N-CA-C	7.60	123.36	113.86
1	B	235	PRO	N-CA-C	7.22	123.23	113.84
1	D	221	ARG	N-CA-C	7.02	118.93	111.28
1	D	234	SER	CA-C-N	6.96	126.59	119.56
1	D	234	SER	C-N-CA	6.96	126.59	119.56
1	B	194	THR	N-CA-C	-6.94	100.53	110.59
1	C	234	SER	CA-C-N	6.66	126.28	119.56
1	C	234	SER	C-N-CA	6.66	126.28	119.56
1	A	74	ILE	N-CA-C	6.65	121.20	113.42
1	C	192	GLY	N-CA-C	6.62	122.17	114.16
1	B	216	GLU	N-CA-C	6.56	120.19	109.76
1	B	221	ARG	N-CA-C	6.53	118.40	111.28
1	C	221	ARG	N-CA-C	6.50	119.19	111.71
1	C	194	THR	N-CA-C	-6.48	101.19	110.59
1	B	74	ILE	N-CA-C	6.45	119.36	113.10
1	A	192	GLY	N-CA-C	6.44	121.95	114.16
1	D	194	THR	N-CA-C	-6.41	101.30	110.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	ARG	N-CA-C	6.30	118.95	111.71
1	C	313	PHE	N-CA-C	6.25	119.66	109.59
1	A	216	GLU	N-CA-C	6.17	119.58	109.76
1	A	313	PHE	N-CA-C	6.08	119.38	109.59
1	D	74	ILE	N-CA-C	5.98	119.51	113.47
1	C	134	THR	N-CA-C	5.94	119.50	109.76
1	D	216	GLU	N-CA-C	5.87	119.47	110.20
1	B	289	MET	N-CA-C	-5.83	100.43	109.24
1	A	270	GLY	N-CA-C	-5.82	103.30	112.61
1	D	313	PHE	N-CA-C	5.79	118.91	109.59
1	D	192	GLY	N-CA-C	5.79	121.16	114.16
1	C	216	GLU	N-CA-C	5.76	118.91	109.76
1	A	289	MET	N-CA-C	-5.74	100.57	109.24
1	C	74	ILE	N-CA-C	5.72	119.25	113.47
1	A	134	THR	N-CA-C	5.68	119.50	109.96
1	B	234	SER	CA-C-N	5.68	125.35	119.56
1	B	234	SER	C-N-CA	5.68	125.35	119.56
1	D	289	MET	N-CA-C	-5.67	100.45	109.23
1	B	313	PHE	N-CA-C	5.64	118.67	109.59
1	D	134	THR	N-CA-C	5.63	119.42	109.96
1	B	134	THR	N-CA-C	5.61	119.39	109.96
1	B	81	ASN	N-CA-C	-5.25	104.36	111.55
1	C	269	SER	N-CA-C	5.22	119.92	113.50
1	B	258	ALA	N-CA-C	5.19	117.83	111.82
1	C	288	LEU	N-CA-C	5.17	117.54	109.52
1	D	288	LEU	N-CA-C	5.14	117.48	109.52
1	C	258	ALA	N-CA-C	5.13	118.69	112.23
1	A	288	LEU	N-CA-C	5.11	117.44	109.52
1	A	55	VAL	N-CA-C	5.10	116.20	111.45
1	D	296	SER	N-CA-C	-5.07	102.50	110.36
1	B	192	GLY	N-CA-C	5.07	120.29	114.16
1	C	289	MET	N-CA-C	-5.06	101.39	109.23
1	B	269	SER	N-CA-C	5.02	119.68	113.50
1	D	28	SER	N-CA-C	-5.01	107.56	113.97
1	B	288	LEU	N-CA-C	5.00	117.27	109.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2687	0	2723	34	0
1	B	2687	0	2723	39	0
1	C	2687	0	2723	34	0
1	D	2687	0	2723	44	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	5	0	4	1	0
3	B	5	0	4	0	0
3	C	5	0	4	1	0
3	D	5	0	4	1	0
4	A	10	0	13	1	0
4	B	10	0	13	0	0
4	C	10	0	13	0	0
4	D	10	0	13	1	0
5	A	180	0	0	3	1
5	B	170	0	0	4	0
5	C	207	0	0	1	1
5	D	162	0	0	4	0
All	All	11531	0	10960	147	1

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 7.

All (147) 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:D:267:MET:HB3	1:D:293:MET:HE2	1.42	0.99
1:A:126:ARG:HD2	1:A:311:GLY:HA2	1.63	0.80
1:D:334:ILE:HD11	1:D:343:LYS:HB3	1.67	0.76
1:B:204:ALA:O	1:B:208:LYS:HD3	1.86	0.76
1:C:31:ARG:HH21	1:C:31:ARG:HG3	1.55	0.71
1:B:129:ILE:HG13	1:B:340:MET:HE3	1.71	0.71
1:B:138:ASP:O	1:B:143:ARG:HD2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:VAL:O	1:C:282:GLU:HG3	1.94	0.67
1:A:265:LYS:HB2	1:A:268:LYS:HE2	1.79	0.65
1:D:266:LEU:HD22	1:D:271:ILE:HD13	1.79	0.65
1:D:278:VAL:O	1:D:282:GLU:HG3	1.97	0.64
1:D:71:ARG:O	1:D:75:THR:HG23	1.98	0.63
1:B:149:LYS:O	1:B:153:GLU:HG3	1.98	0.63
1:C:149:LYS:O	1:C:153:GLU:HG3	1.97	0.63
1:D:48:GLU:HB2	1:D:298:LEU:HD12	1.82	0.62
1:D:134:THR:HG1	3:D:411:ALA:N	1.98	0.61
1:A:278:VAL:O	1:A:282:GLU:HG3	2.00	0.61
1:A:129:ILE:HG13	1:A:340:MET:HE3	1.81	0.60
1:D:195:GLN:NE2	5:D:569:HOH:O	2.33	0.60
1:C:129:ILE:HG13	1:C:340:MET:HE3	1.83	0.60
1:A:252:ARG:O	1:A:256:GLU:HG2	2.01	0.60
1:A:149:LYS:O	1:A:153:GLU:HG3	2.03	0.59
1:A:138:ASP:O	1:A:143:ARG:HD2	2.03	0.58
1:D:342:VAL:HA	5:D:564:HOH:O	2.03	0.58
1:B:13:ARG:NH1	1:B:31:ARG:HD3	2.19	0.58
1:B:194:THR:OG1	1:B:197:GLU:HG3	2.03	0.57
1:B:278:VAL:O	1:B:282:GLU:HG3	2.05	0.57
1:B:174:GLU:OE1	1:B:208:LYS:HE2	2.05	0.57
1:C:138:ASP:O	1:C:143:ARG:HD2	2.05	0.57
1:D:128:GLU:HB2	1:D:341:ARG:HG2	1.87	0.57
1:D:131:THR:HB	1:D:340:MET:HE1	1.87	0.57
1:A:7:VAL:HG21	1:A:74:ILE:HD11	1.86	0.57
1:A:128:GLU:HG2	1:A:129:ILE:N	2.20	0.55
1:A:225:GLU:HG3	5:A:425:HOH:O	2.07	0.55
1:D:342:VAL:HG23	5:D:564:HOH:O	2.05	0.55
1:B:252:ARG:O	1:B:256:GLU:HG2	2.07	0.55
1:D:48:GLU:H	1:D:302:GLN:NE2	2.04	0.55
1:D:267:MET:CB	1:D:293:MET:HE2	2.27	0.54
1:A:195:GLN:NE2	5:A:562:HOH:O	2.35	0.54
1:C:128:GLU:HG2	1:C:129:ILE:N	2.22	0.54
1:A:255:LYS:HE3	1:B:255:LYS:HG3	1.90	0.54
1:C:48:GLU:H	1:C:302:GLN:NE2	2.06	0.54
1:D:229:PHE:O	1:D:233:HIS:HD2	1.90	0.54
1:D:265:LYS:HB2	1:D:268:LYS:HE2	1.89	0.54
1:C:155:PHE:CD1	1:C:338:PRO:HB3	2.44	0.53
1:A:255:LYS:HD2	1:B:255:LYS:HE3	1.91	0.52
1:D:138:ASP:O	1:D:143:ARG:HD2	2.10	0.51
1:D:334:ILE:HD12	1:D:334:ILE:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:ARG:HD2	1:A:311:GLY:CA	2.38	0.50
1:B:48:GLU:H	1:B:302:GLN:NE2	2.10	0.50
1:D:129:ILE:HG13	1:D:340:MET:HE3	1.94	0.50
1:A:229:PHE:O	1:A:233:HIS:HD2	1.95	0.50
1:B:133:LYS:HD2	1:B:155:PHE:CE2	2.47	0.50
1:D:194:THR:OG1	1:D:197:GLU:HG3	2.12	0.50
1:A:134:THR:HG1	3:A:411:ALA:N	2.11	0.49
1:C:134:THR:HG1	3:C:411:ALA:N	2.10	0.49
1:B:13:ARG:HH12	1:B:31:ARG:HD3	1.76	0.49
1:B:195:GLN:NE2	5:B:571:HOH:O	2.45	0.49
1:D:269:SER:HB3	1:D:273:ASP:HB2	1.94	0.49
1:B:229:PHE:O	1:B:233:HIS:HD2	1.94	0.49
1:C:90:ASP:OD1	1:C:99:LYS:HE3	2.12	0.49
1:C:265:LYS:HB2	1:C:268:LYS:HE2	1.93	0.49
5:B:480:HOH:O	1:D:233:HIS:HE1	1.96	0.48
1:B:104:PHE:CE1	1:B:302:GLN:HA	2.49	0.48
1:B:265:LYS:HB2	1:B:268:LYS:HE2	1.94	0.48
1:C:31:ARG:NH1	1:C:60:VAL:CG1	2.77	0.47
1:B:225:GLU:HG3	5:B:430:HOH:O	2.14	0.47
1:B:17:GLU:HA	1:B:325:LYS:HE3	1.97	0.47
1:D:132:ASP:OD1	1:D:132:ASP:C	2.56	0.47
1:C:229:PHE:O	1:C:233:HIS:HD2	1.96	0.47
1:A:31:ARG:CZ	1:A:60:VAL:HG11	2.44	0.47
1:C:132:ASP:C	1:C:132:ASP:OD1	2.57	0.47
1:D:3:ARG:HA	1:D:78:ASP:HA	1.97	0.47
1:D:334:ILE:CD1	1:D:343:LYS:HB3	2.42	0.47
1:A:131:THR:HB	1:A:340:MET:HE1	1.97	0.47
1:B:15:GLU:HG3	1:B:325:LYS:HD2	1.97	0.47
1:C:252:ARG:O	1:C:256:GLU:HG2	2.16	0.46
1:D:104:PHE:CE1	1:D:302:GLN:HA	2.50	0.46
1:C:71:ARG:O	1:C:75:THR:HG23	2.15	0.46
1:A:69:ALA:O	1:A:73:MET:HG3	2.15	0.46
1:B:127:ASP:O	1:B:341:ARG:HG3	2.15	0.46
1:D:50:SER:O	1:D:293:MET:HE3	2.16	0.46
1:A:269:SER:HB3	1:A:273:ASP:HB2	1.98	0.46
1:A:48:GLU:H	1:A:302:GLN:NE2	2.13	0.46
1:A:194:THR:OG1	1:A:197:GLU:HG3	2.16	0.46
1:A:99:LYS:O	1:A:103:GLN:HG3	2.15	0.46
1:A:131:THR:HB	1:A:340:MET:CE	2.46	0.46
1:A:132:ASP:OD1	1:A:132:ASP:C	2.58	0.45
1:A:265:LYS:HZ3	4:A:412:LYS:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:GLU:HB2	1:C:341:ARG:HG2	1.99	0.45
1:D:273:ASP:O	1:D:277:ILE:HG13	2.15	0.45
1:B:132:ASP:OD1	1:B:132:ASP:C	2.59	0.45
1:C:269:SER:HB3	1:C:273:ASP:HB2	1.98	0.45
1:D:144:VAL:HG12	1:D:148:LYS:HE3	1.99	0.45
1:B:208:LYS:HD2	1:B:208:LYS:N	2.32	0.44
1:C:178:LYS:HB3	1:C:178:LYS:NZ	2.31	0.44
1:A:279:GLU:HG3	1:B:279:GLU:HG3	2.00	0.44
1:A:13:ARG:NH2	1:A:31:ARG:HH11	2.15	0.44
1:D:287:LYS:CE	5:D:466:HOH:O	2.66	0.44
1:C:48:GLU:H	1:C:302:GLN:HE22	1.65	0.44
1:B:39:LEU:HD23	1:B:113:GLU:CD	2.43	0.44
1:C:31:ARG:HG3	1:C:31:ARG:NH2	2.27	0.44
1:B:90:ASP:OD1	1:B:99:LYS:HE3	2.18	0.44
1:A:68:ASN:ND2	1:A:71:ARG:HH12	2.16	0.43
1:C:3:ARG:HA	1:C:78:ASP:HA	2.01	0.43
1:C:131:THR:HB	1:C:340:MET:HE1	1.99	0.43
1:D:155:PHE:CD1	1:D:338:PRO:HB3	2.54	0.43
1:C:216:GLU:O	1:C:217:GLN:C	2.62	0.43
5:A:590:HOH:O	1:C:233:HIS:HE1	2.01	0.43
1:D:90:ASP:OD1	1:D:99:LYS:HE3	2.19	0.43
1:B:43:VAL:HG21	1:B:113:GLU:HG2	2.00	0.42
1:B:196:LYS:HG2	5:B:440:HOH:O	2.18	0.42
1:C:240:ALA:HB2	1:C:259:VAL:HG11	2.01	0.42
1:D:11:LEU:HD21	1:D:31:ARG:HH21	1.85	0.42
1:C:269:SER:O	1:C:273:ASP:HB2	2.20	0.42
1:B:264:ILE:HD11	1:B:277:ILE:HG22	2.01	0.42
1:B:341:ARG:CZ	1:B:341:ARG:HB2	2.49	0.42
1:D:128:GLU:OE1	1:D:341:ARG:HD3	2.20	0.42
1:A:237:PRO:HG3	1:C:196:LYS:HG3	2.02	0.42
1:A:140:VAL:O	1:A:144:VAL:HG23	2.19	0.42
1:B:104:PHE:CD2	1:B:302:GLN:HG2	2.55	0.42
1:D:131:THR:HB	1:D:340:MET:CE	2.49	0.42
1:B:131:THR:HB	1:B:340:MET:HE1	2.01	0.41
1:B:208:LYS:N	1:B:208:LYS:CD	2.83	0.41
1:C:31:ARG:NH1	1:C:60:VAL:HG11	2.36	0.41
1:D:269:SER:HB3	1:D:273:ASP:CB	2.51	0.41
1:D:265:LYS:HZ3	4:D:412:LYS:HA	1.85	0.41
1:C:264:ILE:HD11	1:C:277:ILE:HG22	2.03	0.41
1:C:341:ARG:HB2	1:C:341:ARG:NH1	2.35	0.41
1:A:90:ASP:OD1	1:A:99:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:GLU:HB2	1:D:298:LEU:CD1	2.50	0.41
1:D:298:LEU:C	1:D:298:LEU:HD13	2.44	0.41
1:C:164:GLU:HG2	5:C:754:HOH:O	2.20	0.41
1:A:43:VAL:HG21	1:A:113:GLU:HG2	2.03	0.41
1:B:266:LEU:HD22	1:B:271:ILE:HD13	2.02	0.41
1:B:3:ARG:HA	1:B:78:ASP:HA	2.03	0.41
1:D:229:PHE:O	1:D:233:HIS:CD2	2.72	0.41
1:D:267:MET:HB2	1:D:293:MET:HG3	2.03	0.41
1:A:126:ARG:NH1	1:A:128:GLU:O	2.54	0.40
1:B:269:SER:HB3	1:B:273:ASP:HB2	2.03	0.40
1:D:61:GLU:CD	1:D:61:GLU:H	2.29	0.40
1:D:140:VAL:O	1:D:144:VAL:HG23	2.22	0.40
1:B:15:GLU:CG	1:B:325:LYS:HD2	2.51	0.40
1:B:13:ARG:NH1	1:B:31:ARG:CD	2.84	0.40
1:C:131:THR:HB	1:C:340:MET:CE	2.51	0.40
1:C:189:ALA:HB3	1:C:218:PRO:HA	2.02	0.40
1:D:48:GLU:H	1:D:302:GLN:HE22	1.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:482:HOH:O	5:C:741:HOH:O[12_545]	2.10	0.10

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	339/345 (98%)	327 (96%)	12 (4%)	0	100	100
1	B	339/345 (98%)	327 (96%)	12 (4%)	0	100	100
1	C	339/345 (98%)	328 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	339/345 (98%)	327 (96%)	12 (4%)	0	100	100
All	All	1356/1380 (98%)	1309 (96%)	47 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	288/292 (99%)	287 (100%)	1 (0%)	86	88
1	B	288/292 (99%)	286 (99%)	2 (1%)	76	78
1	C	288/292 (99%)	285 (99%)	3 (1%)	68	70
1	D	288/292 (99%)	284 (99%)	4 (1%)	59	59
All	All	1152/1168 (99%)	1142 (99%)	10 (1%)	70	73

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU
1	B	39	LEU
1	B	121	LEU
1	C	39	LEU
1	C	121	LEU
1	C	208	LYS
1	D	61	GLU
1	D	121	LEU
1	D	256	GLU
1	D	342	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN

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Mol	Chain	Res	Type
1	A	81	ASN
1	A	207	GLN
1	A	233	HIS
1	A	302	GLN
1	A	335	GLN
1	B	21	HIS
1	B	233	HIS
1	B	302	GLN
1	B	335	GLN
1	C	56	ASN
1	C	233	HIS
1	C	302	GLN
1	C	335	GLN
1	D	56	ASN
1	D	68	ASN
1	D	233	HIS
1	D	302	GLN
1	D	335	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ALA	D	411	4	3,4,5	0.58	0	2,4,6	0.78	0
3	ALA	C	411	4	3,4,5	0.71	0	2,4,6	0.82	0
4	LYS	C	412	3	8,9,9	0.78	0	7,10,10	0.31	0
3	ALA	A	411	4	3,4,5	0.69	0	2,4,6	0.75	0
4	LYS	A	412	3	8,9,9	0.81	0	7,10,10	0.27	0
4	LYS	D	412	3	8,9,9	0.73	0	7,10,10	0.21	0
3	ALA	B	411	4	3,4,5	0.69	0	2,4,6	0.82	0
4	LYS	B	412	2,3	8,9,9	0.75	0	7,10,10	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ALA	D	411	4	-	1/1/2/4	-
3	ALA	C	411	4	-	1/1/2/4	-
4	LYS	C	412	3	-	2/9/9/9	-
3	ALA	A	411	4	-	1/1/2/4	-
4	LYS	A	412	3	-	2/9/9/9	-
4	LYS	D	412	3	-	2/9/9/9	-
3	ALA	B	411	4	-	1/1/2/4	-
4	LYS	B	412	2,3	-	2/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	411	ALA	O-C-CA-CB
3	B	411	ALA	O-C-CA-CB
3	C	411	ALA	O-C-CA-CB
3	D	411	ALA	O-C-CA-CB
4	A	412	LYS	O-C-CA-CB
4	A	412	LYS	OXT-C-CA-CB
4	D	412	LYS	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
4	D	412	LYS	O-C-CA-CB
4	C	412	LYS	OXT-C-CA-CB
4	C	412	LYS	O-C-CA-CB
4	B	412	LYS	OXT-C-CA-CB
4	B	412	LYS	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	411	ALA	1	0
3	C	411	ALA	1	0
3	A	411	ALA	1	0
4	A	412	LYS	1	0
4	D	412	LYS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	341/345 (98%)	0.54	27 (7%)	18 20	20, 29, 46, 61	0
1	B	341/345 (98%)	0.47	32 (9%)	14 14	21, 29, 48, 61	0
1	C	341/345 (98%)	0.34	19 (5%)	30 32	20, 26, 44, 58	0
1	D	341/345 (98%)	0.78	38 (11%)	10 11	22, 31, 49, 61	0
All	All	1364/1380 (98%)	0.53	116 (8%)	16 17	20, 29, 47, 61	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	342	VAL	6.8
1	D	329	PHE	6.2
1	D	328	VAL	5.6
1	D	343	LYS	5.1
1	D	342	VAL	4.8
1	A	343	LYS	4.6
1	C	343	LYS	4.4
1	A	145	LYS	4.4
1	B	18	LYS	4.2
1	B	343	LYS	4.2
1	C	152	GLU	4.1
1	D	331	GLY	4.0
1	C	342	VAL	3.8
1	A	328	VAL	3.8
1	A	18	LYS	3.8
1	D	181	ARG	3.8
1	B	181	ARG	3.7
1	C	181	ARG	3.7
1	B	145	LYS	3.6
1	A	342	VAL	3.6
1	D	40	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	334	ILE	3.5
1	B	327	GLU	3.5
1	C	328	VAL	3.5
1	C	178	LYS	3.4
1	B	328	VAL	3.4
1	B	167	LYS	3.3
1	D	336	ASP	3.3
1	D	18	LYS	3.3
1	A	13	ARG	3.3
1	B	144	VAL	3.2
1	A	152	GLU	3.2
1	C	341	ARG	3.2
1	B	15	GLU	3.1
1	D	3	ARG	3.1
1	C	145	LYS	3.1
1	B	28	SER	3.1
1	A	336	ASP	3.0
1	A	341	ARG	3.0
1	B	341	ARG	3.0
1	A	181	ARG	3.0
1	D	341	ARG	3.0
1	B	146	GLU	2.9
1	A	15	GLU	2.9
1	D	145	LYS	2.9
1	B	152	GLU	2.8
1	A	28	SER	2.8
1	B	178	LYS	2.8
1	D	327	GLU	2.8
1	C	3	ARG	2.7
1	C	327	GLU	2.7
1	D	167	LYS	2.7
1	D	13	ARG	2.7
1	D	152	GLU	2.7
1	B	13	ARG	2.7
1	A	327	GLU	2.6
1	A	8	LYS	2.6
1	A	329	PHE	2.6
1	D	178	LYS	2.6
1	C	40	GLU	2.5
1	B	208	LYS	2.5
1	D	72	GLU	2.5
1	D	149	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	17	GLU	2.5
1	D	144	VAL	2.5
1	A	10	SER	2.4
1	D	211	ASP	2.4
1	D	150	ILE	2.4
1	D	141	GLU	2.3
1	C	68	ASN	2.3
1	D	142	ASN	2.3
1	C	72	GLU	2.3
1	B	329	PHE	2.3
1	C	21	HIS	2.3
1	A	334	ILE	2.3
1	A	325	LYS	2.3
1	B	211	ASP	2.3
1	C	5	VAL	2.3
1	D	298	LEU	2.3
1	D	332	LYS	2.3
1	D	154	GLY	2.3
1	D	15	GLU	2.3
1	A	29	GLU	2.2
1	B	149	LYS	2.2
1	B	340	MET	2.2
1	C	149	LYS	2.2
1	B	207	GLN	2.2
1	C	211	ASP	2.2
1	A	37	ILE	2.2
1	A	144	VAL	2.2
1	D	140	VAL	2.2
1	A	178	LYS	2.2
1	A	31	ARG	2.2
1	B	337	GLY	2.2
1	B	325	LYS	2.2
1	D	148	LYS	2.2
1	B	334	ILE	2.1
1	D	175	GLU	2.1
1	A	324	LEU	2.1
1	A	126	ARG	2.1
1	B	148	LYS	2.1
1	D	5	VAL	2.1
1	D	121	LEU	2.1
1	B	17	GLU	2.0
1	B	141	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	17	GLU	2.0
1	D	200	GLU	2.0
1	D	28	SER	2.0
1	B	19	PRO	2.0
1	B	130	GLU	2.0
1	A	167	LYS	2.0
1	C	334	ILE	2.0
1	B	331	GLY	2.0
1	B	3	ARG	2.0
1	C	43	VAL	2.0
1	D	31	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
2	MG	D	401	1/1	0.87	0.11	27,27,27,27	0
4	LYS	D	412	10/10	0.91	0.11	26,28,35,39	0
4	LYS	A	412	10/10	0.92	0.10	25,26,32,33	0
2	MG	C	401	1/1	0.93	0.07	27,27,27,27	0
3	ALA	B	411	5/6	0.93	0.09	26,27,29,29	0
4	LYS	C	412	10/10	0.94	0.09	22,23,28,29	0
4	LYS	B	412	10/10	0.94	0.09	28,30,35,38	0
3	ALA	A	411	5/6	0.95	0.08	25,26,27,27	0
2	MG	B	401	1/1	0.96	0.11	27,27,27,27	0
3	ALA	D	411	5/6	0.96	0.08	26,27,28,29	0
2	MG	A	401	1/1	0.96	0.05	26,26,26,26	0
3	ALA	C	411	5/6	0.97	0.06	22,22,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.