



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 02:50 AM GMT

PDB ID : 2D33
Title : Crystal Structure of gamma-Glutamylcysteine Synthetase Complexed with Aluminum Fluoride
Authors : Hibi, T.; Nakayama, M.; Nii, H.; Kurokawa, Y.; Katano, H.; Oda, J.
Deposited on : 2005-09-25
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>

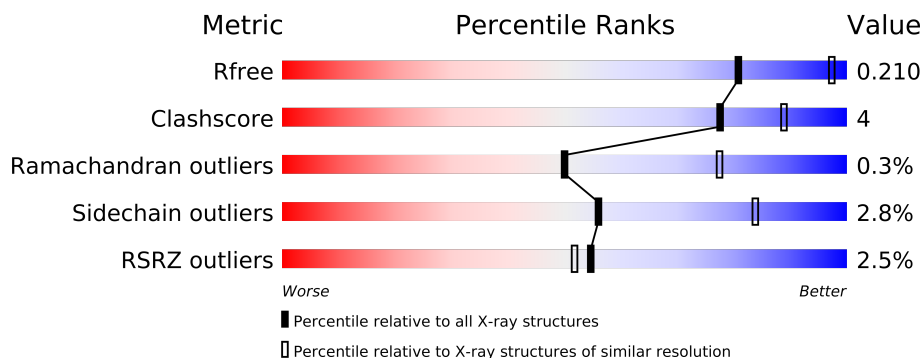
The following versions of software and data (see [references](#)) were used in the production of this report:

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	518	
1	B	518	
1	C	518	
1	D	518	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	GLU	A	519	-	X
3	GLU	C	2519	-	X
3	GLU	D	3519	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16327 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 Glutamate–cysteine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4009	2546	685	760	18			
1	B	503	Total	C	N	O	S	0	0	0
			3933	2508	669	738	18			
1	C	504	Total	C	N	O	S	0	0	0
			3925	2508	662	737	18			
1	D	499	Total	C	N	O	S	0	0	0
			3909	2490	666	735	18			

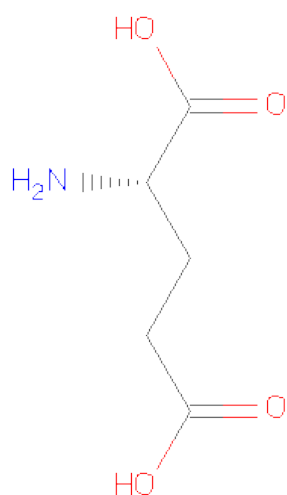
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	106	SER	CYS	ENGINEERED	UNP P0A6W9
A	164	SER	CYS	ENGINEERED	UNP P0A6W9
A	205	SER	CYS	ENGINEERED	UNP P0A6W9
A	223	SER	CYS	ENGINEERED	UNP P0A6W9
B	106	SER	CYS	ENGINEERED	UNP P0A6W9
B	164	SER	CYS	ENGINEERED	UNP P0A6W9
B	205	SER	CYS	ENGINEERED	UNP P0A6W9
B	223	SER	CYS	ENGINEERED	UNP P0A6W9
C	106	SER	CYS	ENGINEERED	UNP P0A6W9
C	164	SER	CYS	ENGINEERED	UNP P0A6W9
C	205	SER	CYS	ENGINEERED	UNP P0A6W9
C	223	SER	CYS	ENGINEERED	UNP P0A6W9
D	106	SER	CYS	ENGINEERED	UNP P0A6W9
D	164	SER	CYS	ENGINEERED	UNP P0A6W9
D	205	SER	CYS	ENGINEERED	UNP P0A6W9
D	223	SER	CYS	ENGINEERED	UNP P0A6W9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

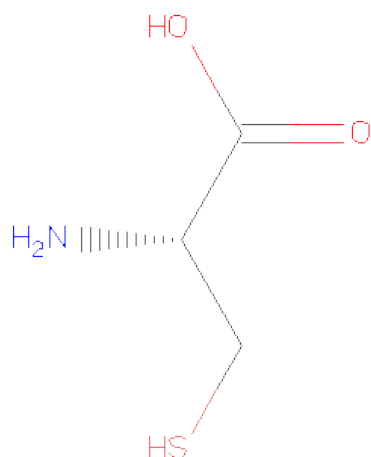
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Mg 3	0	0
2	A	4	Total 4	Mg 4	0	0
2	D	3	Total 3	Mg 3	0	0
2	C	3	Total 3	Mg 3	0	0

- Molecule 3 is GLUTAMIC ACID (three-letter code: GLU) (formula: $C_5H_9NO_4$).



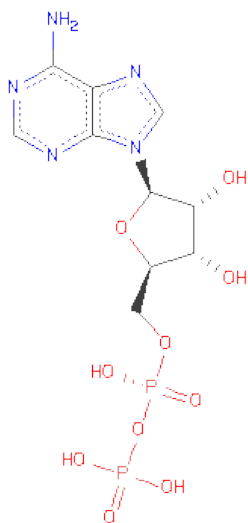
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 10	C 5	N 1	O 4	0	0
3	B	1	Total 10	C 5	N 1	O 4	0	0
3	C	1	Total 10	C 5	N 1	O 4	0	0
3	D	1	Total 10	C 5	N 1	O 4	0	0

- Molecule 4 is CYSTEINE (three-letter code: CYS) (formula: $C_3H_7NO_2S$).



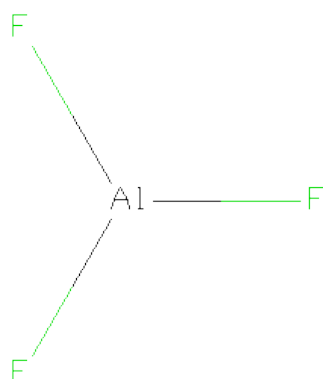
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
4	D	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Al	F	0	0
			4	1	3		
6	B	1	Total	Al	F	0	0
			4	1	3		
6	C	1	Total	Al	F	0	0
			4	1	3		
6	D	1	Total	Al	F	0	0
			4	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	174	Total	O	0	0
			174	174		
7	B	66	Total	O	0	0
			66	66		

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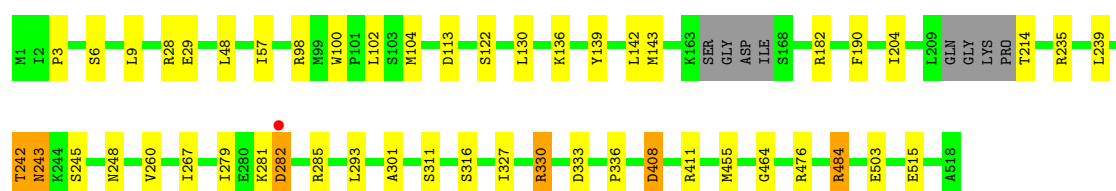
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	27	Total	O	0	0
			27	27		
7	D	79	Total	O	0	0
			79	79		

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.

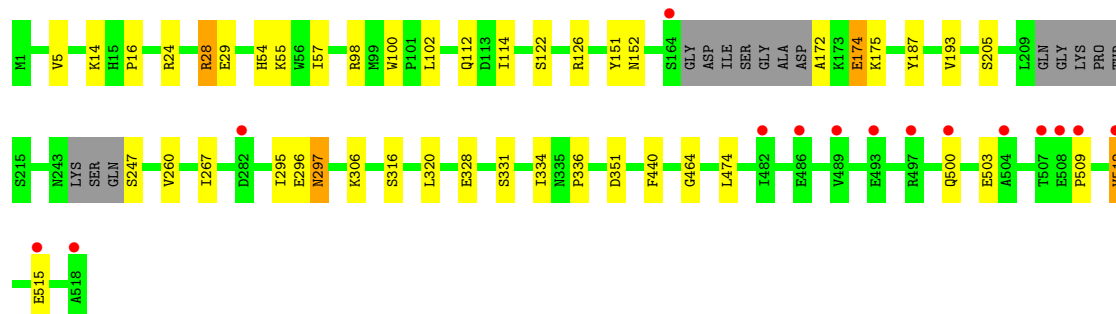
- Molecule 1: Glutamate–cysteine ligase

Chain A: 



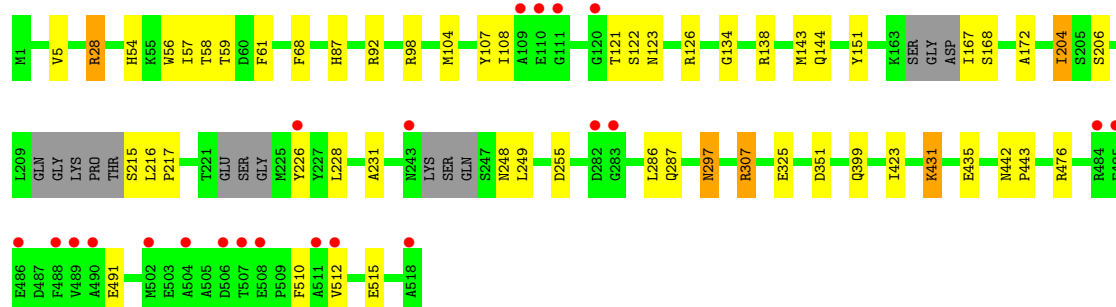
- Molecule 1: Glutamate–cysteine ligase

Chain B: 



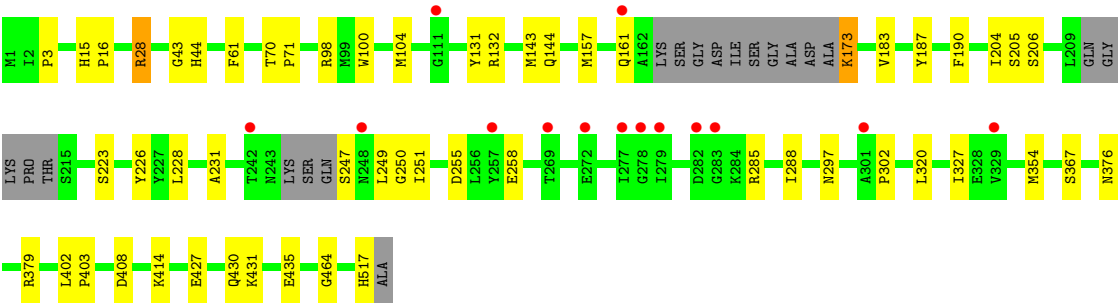
- Molecule 1: Glutamate–cysteine ligase

Chain C: 



- Molecule 1: Glutamate–cysteine ligase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	325.23Å 325.23Å 105.18Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.60 39.76 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.60) 100.0 (39.76-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.18 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.162 , 0.191 0.182 , 0.210	Depositor DCC
R_{free} test set	6408 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 22.8	EDS
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 127525 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16327	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: MG, ADP, AF3

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	0.83	0/4096	0.81	1/5547 (0.0%)
1	B	0.67	0/4019	0.73	0/5447
1	C	0.63	0/4010	0.68	0/5431
1	D	0.70	0/3993	0.74	2/5414 (0.0%)
All	All	0.71	0/16118	0.74	3/21839 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	132	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	A	113	ASP	CB-CG-OD1	-5.67	113.19	118.30
1	D	285	ARG	NE-CZ-NH1	-5.32	117.64	120.30

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	4009	0	3901	28	0
1	B	3933	0	3810	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3925	0	3793	31	0
1	D	3909	0	3776	27	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	10	0	5	1	0
3	B	10	0	5	1	0
3	C	10	0	5	1	0
3	D	10	0	5	0	0
4	A	7	0	4	0	0
4	B	7	0	4	0	0
4	C	7	0	4	1	0
4	D	7	0	4	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
5	C	27	0	12	0	0
5	D	27	0	12	0	0
6	A	4	0	0	0	0
6	B	4	0	0	0	0
6	C	4	0	0	0	0
6	D	4	0	0	0	0
7	A	174	0	0	1	0
7	B	66	0	0	0	0
7	C	27	0	0	0	0
7	D	79	0	0	0	0
All	All	16327	0	15364	116	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 4.

All (116) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:255:ASP:HB3	1:D:258:GLU:HB2	1.56	0.88
1:A:139:TYR:HB3	1:A:242:THR:HB	1.66	0.77
1:A:143:MET:HG3	1:A:242:THR:HG23	1.69	0.74
1:C:104:MET:HE2	1:C:204:ILE:HG22	1.71	0.71
1:D:250:GLY:HA2	1:D:367:SER:OG	1.93	0.69
1:C:54:HIS:HD2	1:C:56:TRP:H	1.40	0.69
1:C:104:MET:CE	1:C:204:ILE:HG22	2.23	0.69
1:D:173:LYS:HG2	1:D:173:LYS:O	1.93	0.67
1:A:29:GLU:OE2	3:A:519:GLU:HG3	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:427:GLU:CB	1:D:427:GLU:OE2	2.46	0.63
1:B:509:PRO:HG2	1:B:512:VAL:HG13	1.82	0.61
1:A:245:SER:HB3	1:A:248:ASN:HB2	1.81	0.61
1:B:152:ASN:OD1	1:B:328:GLU:HG3	2.01	0.60
1:D:187:TYR:HE2	1:D:302:PRO:HB2	1.67	0.59
1:B:28:ARG:C	1:B:28:ARG:HD3	2.23	0.59
1:B:5:VAL:HG12	1:B:5:VAL:O	2.03	0.59
1:C:286:LEU:O	1:C:287:GLN:HB3	2.03	0.58
1:B:187:TYR:OH	1:B:331:SER:OG	2.22	0.58
1:C:5:VAL:O	1:C:5:VAL:HG12	2.04	0.57
1:B:267:ILE:HD11	1:B:296:GLU:HG2	1.87	0.56
1:C:491:GLU:HA	1:C:491:GLU:OE1	2.06	0.56
1:B:14:LYS:C	1:B:16:PRO:HD3	2.27	0.54
1:C:58:THR:OG1	1:C:59:THR:N	2.40	0.53
1:D:131:TYR:HB2	1:D:288:ILE:HD11	1.90	0.53
1:A:100:TRP:CH2	1:A:464:GLY:HA3	2.44	0.53
1:C:107:TYR:O	1:C:108:ILE:HG12	2.09	0.52
1:B:267:ILE:HD13	1:B:295:ILE:HA	1.91	0.52
1:A:476:ARG:HD2	7:A:548:HOH:O	2.10	0.52
1:A:408:ASP:OD1	1:A:411:ARG:NH2	2.43	0.51
1:C:228:LEU:HB2	1:C:231:ALA:HB2	1.91	0.51
1:D:431:LYS:O	1:D:435:GLU:HG3	2.11	0.51
1:B:267:ILE:CD1	1:B:296:GLU:HG2	2.41	0.51
1:B:174:GLU:HG2	1:B:174:GLU:O	2.11	0.50
1:B:297:ASN:N	1:B:297:ASN:OD1	2.42	0.50
1:A:48:LEU:HD13	1:A:57:ILE:HG21	1.94	0.49
1:D:327:ILE:C	1:D:327:ILE:HD12	2.32	0.49
1:A:301:ALA:O	1:A:330:ARG:HD3	2.12	0.49
1:A:139:TYR:HB3	1:A:242:THR:CB	2.38	0.48
1:C:134:GLY:O	1:C:138:ARG:HG3	2.12	0.48
1:D:376:ASN:OD1	1:D:379:ARG:NH1	2.47	0.48
1:D:402:LEU:HB3	1:D:403:PRO:HD3	1.96	0.48
1:B:151:TYR:OH	1:B:351:ASP:OD1	2.32	0.48
1:C:151:TYR:OH	1:C:351:ASP:OD1	2.30	0.48
1:A:104:MET:HE2	1:A:204:ILE:HG13	1.95	0.47
1:C:68:PHE:CD2	1:C:87:HIS:CE1	3.03	0.47
1:D:414:LYS:HE3	1:D:430:GLN:HB3	1.96	0.47
1:C:107:TYR:C	1:C:108:ILE:HG12	2.34	0.47
1:B:122:SER:HB3	1:B:503:GLU:HG3	1.94	0.47
1:B:193:VAL:HG23	1:B:440:PHE:HZ	1.80	0.47
1:C:297:ASN:OD1	1:C:297:ASN:N	2.48	0.47
1:D:247:SER:C	1:D:249:LEU:H	2.19	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:104:MET:CE	1:D:204:ILE:HG13	2.45	0.46
1:A:235:ARG:HD3	1:A:333:ASP:OD1	2.15	0.46
1:B:260:VAL:HG11	1:B:320:LEU:HG	1.97	0.46
1:C:92:ARG:HD2	1:C:476:ARG:O	2.15	0.46
1:D:206:SER:HB3	1:D:226:TYR:HE1	1.79	0.46
1:B:172:ALA:O	1:B:175:LYS:N	2.50	0.45
1:D:327:ILE:O	1:D:327:ILE:HD12	2.15	0.45
1:B:334:ILE:O	1:B:336:PRO:HD3	2.16	0.45
1:D:61:PHE:CG	1:D:144:GLN:HB3	2.52	0.45
1:B:24:ARG:HA	1:B:152:ASN:O	2.17	0.45
1:A:243:ASN:OD1	1:A:243:ASN:N	2.43	0.45
1:A:122:SER:HB3	1:A:503:GLU:HG3	1.99	0.45
1:C:167:ILE:O	1:C:167:ILE:HG13	2.16	0.45
1:A:267:ILE:HD13	1:A:293:LEU:HB2	1.98	0.44
1:B:100:TRP:CH2	1:B:464:GLY:HA3	2.52	0.44
1:A:3:PRO:HD3	1:A:190:PHE:CZ	2.52	0.44
1:C:431:LYS:HE2	1:C:435:GLU:OE2	2.17	0.44
1:C:249:LEU:HD23	1:C:249:LEU:HA	1.76	0.44
1:A:104:MET:CE	1:A:204:ILE:HG13	2.48	0.44
1:B:112:GLN:O	1:B:114:ILE:HD12	2.17	0.44
1:D:28:ARG:C	1:D:28:ARG:HD3	2.38	0.44
1:D:320:LEU:HA	1:D:320:LEU:HD12	1.87	0.44
1:C:121:THR:O	1:C:126:ARG:NH2	2.51	0.44
1:D:15:HIS:N	1:D:16:PRO:HD3	2.33	0.44
1:B:267:ILE:O	1:B:267:ILE:CG2	2.67	0.43
1:C:307:ARG:CZ	1:C:325:GLU:HB2	2.48	0.43
1:D:100:TRP:CH2	1:D:464:GLY:HA3	2.54	0.43
1:C:104:MET:HE1	1:C:204:ILE:HG22	2.01	0.43
1:C:442:ASN:HA	1:C:443:PRO:HD2	1.90	0.43
1:A:484:ARG:HA	1:A:484:ARG:HD3	1.85	0.43
1:A:130:LEU:HD11	1:A:285:ARG:HG3	2.00	0.43
1:A:142:LEU:HA	1:A:142:LEU:HD12	1.83	0.43
1:D:402:LEU:C	1:D:402:LEU:HD23	2.38	0.42
1:B:267:ILE:HG22	1:B:267:ILE:O	2.18	0.42
1:A:327:ILE:HA	1:A:327:ILE:HD13	1.73	0.42
1:C:104:MET:HE1	1:C:204:ILE:CG2	2.49	0.42
1:D:43:GLY:O	1:D:44:HIS:C	2.58	0.42
3:C:2519:GLU:OE1	4:C:2520:CYS:HA	2.20	0.42
1:D:255:ASP:HB3	1:D:258:GLU:CB	2.38	0.42
1:D:183:VAL:CG1	1:D:354:MET:HE3	2.49	0.42
1:D:228:LEU:HB2	1:D:231:ALA:HB2	2.01	0.42
1:C:226:TYR:N	1:C:226:TYR:CD1	2.87	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:143:MET:HG2	1:C:143:MET:O	2.18	0.42
1:A:214:THR:HG21	1:A:239:LEU:HD21	2.02	0.42
1:C:123:ASN:OD1	1:C:510:PHE:HA	2.20	0.42
1:A:102:LEU:HD23	1:A:336:PRO:HB3	2.02	0.42
1:A:281:LYS:O	1:A:282:ASP:HB2	2.20	0.41
1:B:122:SER:O	1:B:126:ARG:HG3	2.20	0.41
1:A:260:VAL:HG13	1:A:316:SER:HB2	2.02	0.41
1:C:216:LEU:HA	1:C:217:PRO:HD3	1.81	0.41
1:C:512:VAL:O	1:C:515:GLU:HB3	2.21	0.41
1:D:70:THR:HA	1:D:71:PRO:HD3	1.83	0.41
1:C:28:ARG:C	1:C:28:ARG:HD3	2.41	0.41
1:B:512:VAL:O	1:B:515:GLU:HG2	2.21	0.41
1:B:296:GLU:OE2	1:B:316:SER:OG	2.37	0.40
1:A:267:ILE:HG22	1:A:267:ILE:O	2.19	0.40
1:C:61:PHE:CG	1:C:144:GLN:HB3	2.55	0.40
1:A:102:LEU:HD13	1:A:455:MET:CE	2.51	0.40
1:B:296:GLU:H	1:B:296:GLU:HG3	1.68	0.40
1:B:102:LEU:HD23	1:B:336:PRO:HB3	2.03	0.40
1:B:54:HIS:HB3	1:B:57:ILE:O	2.21	0.40
1:C:54:HIS:CD2	1:C:57:ILE:H	2.40	0.40
1:A:9:LEU:HA	1:A:9:LEU:HD23	1.92	0.40
1:D:3:PRO:HD3	1:D:190:PHE:CZ	2.57	0.40
1:B:29:GLU:OE2	3:B:1519:GLU:HB2	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	504/518 (97%)	488 (97%)	14 (3%)	2 (0%)	43	72
1	B	495/518 (96%)	481 (97%)	14 (3%)	0	100	100
1	C	494/518 (95%)	466 (94%)	25 (5%)	3 (1%)	33	63
1	D	491/518 (95%)	471 (96%)	19 (4%)	1 (0%)	56	82

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1984/2072 (96%)	1906 (96%)	72 (4%)	6 (0%)	50 77

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	248	ASN
1	A	515	GLU
1	C	122	SER
1	C	172	ALA
1	A	282	ASP
1	D	161	GLN

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	416/434 (96%)	404 (97%)	12 (3%)	55 83
1	B	401/434 (92%)	390 (97%)	11 (3%)	57 85
1	C	396/434 (91%)	384 (97%)	12 (3%)	53 82
1	D	400/434 (92%)	389 (97%)	11 (3%)	56 84
All	All	1613/1736 (93%)	1567 (97%)	46 (3%)	56 83

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	28	ARG
1	A	98	ARG
1	A	136	LYS
1	A	182	ARG
1	A	242	THR
1	A	243	ASN
1	A	279	ILE
1	A	311	SER
1	A	330	ARG

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Mol	Chain	Res	Type
1	A	408	ASP
1	A	484	ARG
1	B	28	ARG
1	B	55	LYS
1	B	98	ARG
1	B	174	GLU
1	B	205	SER
1	B	247	SER
1	B	297	ASN
1	B	306	LYS
1	B	474	LEU
1	B	500	GLN
1	B	512	VAL
1	C	28	ARG
1	C	98	ARG
1	C	168	SER
1	C	204	ILE
1	C	206	SER
1	C	215	SER
1	C	255	ASP
1	C	297	ASN
1	C	307	ARG
1	C	399	GLN
1	C	423	ILE
1	C	431	LYS
1	D	28	ARG
1	D	98	ARG
1	D	143	MET
1	D	157	MET
1	D	173	LYS
1	D	205	SER
1	D	223	SER
1	D	251	ILE
1	D	297	ASN
1	D	408	ASP
1	D	517	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	418	GLN
1	B	418	GLN

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Mol	Chain	Res	Type
1	C	54	HIS
1	C	418	GLN
1	D	404	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 29 ligands modelled in this entry, 13 are monoatomic - leaving 16 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	GLU	A	519	2,6	9,9,9	1.06	0	11,11,11	1.87	3 (27%)
4	CYS	A	520	6	6,6,6	1.08	0	7,7,7	1.36	1 (14%)
5	ADP	A	521	2,6	29,29,29	0.91	2 (6%)	45,45,45	2.33	14 (31%)
6	AF3	A	522	3,2,5,4,7	0,3,3	0.00	-	0,3,3	0.00	-
3	GLU	B	1519	2,6	9,9,9	0.92	0	11,11,11	1.27	2 (18%)
4	CYS	B	1520	-	6,6,6	0.74	0	7,7,7	1.68	3 (42%)
5	ADP	B	1521	2,6	29,29,29	1.10	2 (6%)	45,45,45	1.88	7 (15%)
6	AF3	B	1522	1,3,2,5	0,3,3	0.00	-	0,3,3	0.00	-
3	GLU	C	2519	2,6	9,9,9	0.85	0	11,11,11	1.17	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	CYS	C	2520	-	6,6,6	0.83	0	7,7,7	1.27	0
5	ADP	C	2521	2,6	29,29,29	1.08	3 (10%)	45,45,45	1.89	8 (17%)
6	AF3	C	2522	1,3,2,5	0,3,3	0.00	-	0,3,3	0.00	-
3	GLU	D	3519	2,6	9,9,9	0.87	0	11,11,11	1.38	2 (18%)
4	CYS	D	3520	6	6,6,6	1.05	0	7,7,7	1.66	3 (42%)
5	ADP	D	3521	2,6	29,29,29	1.21	3 (10%)	45,45,45	1.88	9 (20%)
6	AF3	D	3522	1,3,2,5,4,7	0,3,3	0.00	-	0,3,3	0.00	-

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	GLU	A	519	2,6	-	0/9/9/9	0/0/0/0
4	CYS	A	520	6	-	0/6/6/6	0/0/0/0
5	ADP	A	521	2,6	-	0/16/32/32	0/1/3/3
6	AF3	A	522	3,2,5,4,7	-	0/0/0/0	0/0/0/0
3	GLU	B	1519	2,6	-	0/9/9/9	0/0/0/0
4	CYS	B	1520	-	-	0/6/6/6	0/0/0/0
5	ADP	B	1521	2,6	-	0/16/32/32	0/1/3/3
6	AF3	B	1522	1,3,2,5	-	0/0/0/0	0/0/0/0
3	GLU	C	2519	2,6	-	0/9/9/9	0/0/0/0
4	CYS	C	2520	-	-	0/6/6/6	0/0/0/0
5	ADP	C	2521	2,6	-	0/16/32/32	0/1/3/3
6	AF3	C	2522	1,3,2,5	-	0/0/0/0	0/0/0/0
3	GLU	D	3519	2,6	-	0/9/9/9	0/0/0/0
4	CYS	D	3520	6	-	0/6/6/6	0/0/0/0
5	ADP	D	3521	2,6	-	0/16/32/32	0/1/3/3
6	AF3	D	3522	1,3,2,5,4,7	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	3521	ADP	C5-C4	3.10	1.47	1.40
5	B	1521	ADP	C4-N9	-2.87	1.33	1.37
5	B	1521	ADP	C5-C4	2.71	1.46	1.40
5	C	2521	ADP	C5-C4	2.54	1.46	1.40
5	D	3521	ADP	C4-N9	-2.54	1.34	1.37
5	C	2521	ADP	C4-N9	-2.52	1.34	1.37
5	D	3521	ADP	C2'-C1'	-2.28	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	521	ADP	C5-C4	2.22	1.45	1.40
5	A	521	ADP	C4-N9	-2.17	1.34	1.37
5	C	2521	ADP	C2'-C1'	-2.09	1.50	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	521	ADP	N3-C2-N1	-9.18	121.04	128.71
5	B	1521	ADP	N3-C2-N1	-7.61	122.35	128.71
5	C	2521	ADP	N3-C2-N1	-6.55	123.23	128.71
5	D	3521	ADP	N3-C2-N1	-5.87	123.80	128.71
5	C	2521	ADP	N3-C4-N9	5.13	134.69	125.43
5	B	1521	ADP	N3-C4-N9	5.12	134.68	125.43
5	A	521	ADP	C8-N9-C4	4.99	110.70	106.90
5	D	3521	ADP	N3-C4-N9	4.88	134.24	125.43
5	A	521	ADP	N3-C4-N9	4.57	133.69	125.43
3	A	519	GLU	C-CA-N	4.51	116.83	109.36
5	A	521	ADP	C4-C5-N7	-4.16	105.96	109.52
5	D	3521	ADP	C8-N9-C4	4.07	110.01	106.90
5	A	521	ADP	C1'-N9-C4	-3.94	119.82	126.64
5	C	2521	ADP	C4-C5-N7	-3.75	106.31	109.52
5	C	2521	ADP	C8-N9-C4	3.33	109.44	106.90
5	B	1521	ADP	C5-C4-N3	-3.05	119.06	125.70
5	C	2521	ADP	C5-C4-N3	-3.00	119.18	125.70
3	A	519	GLU	OXT-C-O	-2.93	117.44	124.07
5	D	3521	ADP	C4-C5-N7	-2.92	107.02	109.52
3	B	1519	GLU	C-CA-N	2.85	114.08	109.36
4	D	3520	CYS	OXT-C-O	-2.83	117.67	124.07
4	A	520	CYS	OXT-C-O	-2.75	117.85	124.07
4	B	1520	CYS	C-CA-N	2.75	113.92	109.36
3	D	3519	GLU	C-CA-N	2.75	113.91	109.36
5	B	1521	ADP	C4-C5-N7	-2.74	107.18	109.52
5	A	521	ADP	C2-N3-C4	2.72	121.75	114.01
5	A	521	ADP	O3'-C3'-C4'	-2.70	103.12	111.08
5	B	1521	ADP	PA-O3A-PB	-2.68	123.83	131.68
5	B	1521	ADP	C2-N3-C4	2.65	121.55	114.01
5	D	3521	ADP	C5-C4-N3	-2.62	119.99	125.70
5	D	3521	ADP	C1'-N9-C4	-2.60	122.14	126.64
5	A	521	ADP	PA-O3A-PB	-2.60	124.07	131.68
5	D	3521	ADP	O3B-PB-O1B	2.56	118.82	110.44
5	A	521	ADP	C5-C4-N3	-2.50	120.25	125.70
5	B	1521	ADP	O4'-C1'-N9	2.43	110.70	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2521	ADP	C2-N3-C4	2.40	120.85	114.01
5	C	2521	ADP	O3'-C3'-C4'	-2.39	104.03	111.08
5	A	521	ADP	C2-N1-C6	2.37	123.06	118.77
3	D	3519	GLU	OXT-C-O	-2.35	118.77	124.07
5	A	521	ADP	N7-C8-N9	-2.32	107.80	114.36
5	D	3521	ADP	O2A-PA-O3A	2.31	116.10	105.14
4	D	3520	CYS	OXT-C-CA	2.25	121.94	116.88
5	D	3521	ADP	C2-N3-C4	2.23	120.36	114.01
5	A	521	ADP	O3B-PB-O1B	2.22	117.69	110.44
4	B	1520	CYS	OXT-C-O	-2.21	119.07	124.07
3	B	1519	GLU	OXT-C-O	-2.19	119.12	124.07
3	A	519	GLU	O-C-CA	2.13	124.52	118.36
4	B	1520	CYS	OXT-C-CA	2.13	121.65	116.88
5	C	2521	ADP	O2'-C2'-C1'	-2.10	104.86	111.23
3	C	2519	GLU	OXT-C-O	-2.10	119.33	124.07
5	A	521	ADP	O3B-PB-O2B	2.08	115.70	107.61
5	A	521	ADP	O2A-PA-O3A	2.08	114.99	105.14
4	D	3520	CYS	C-CA-N	2.07	112.78	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	510/518 (98%)	-0.33	1 (0%) 93 94	18, 30, 53, 75	0
1	B	503/518 (97%)	-0.14	15 (2%) 48 45	26, 39, 61, 89	0
1	C	504/518 (97%)	-0.00	22 (4%) 33 29	30, 45, 69, 84	0
1	D	499/518 (96%)	-0.08	14 (2%) 50 48	24, 40, 66, 91	0
All	All	2016/2072 (97%)	-0.14	52 (2%) 54 50	18, 39, 64, 91	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	518	ALA	6.1
1	C	109	ALA	5.2
1	C	507	THR	4.4
1	C	111	GLY	3.7
1	B	164	SER	3.6
1	C	518	ALA	3.4
1	B	500	GLN	3.3
1	C	486	GLU	3.1
1	D	283	GLY	3.1
1	D	279	ILE	3.1
1	B	507	THR	3.0
1	D	272	GLU	2.9
1	C	489	VAL	2.9
1	B	512	VAL	2.8
1	D	257	TYR	2.8
1	C	226	TYR	2.8
1	C	504	ALA	2.8
1	C	508	GLU	2.8
1	D	161	GLN	2.7
1	C	110	GLU	2.7
1	C	120	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	248	ASN	2.6
1	C	283	GLY	2.6
1	C	506	ASP	2.6
1	D	269	THR	2.6
1	D	282	ASP	2.5
1	B	508	GLU	2.5
1	C	512	VAL	2.4
1	B	489	VAL	2.4
1	C	282	ASP	2.4
1	D	242	THR	2.4
1	B	482	ILE	2.4
1	C	511	ALA	2.3
1	B	486	GLU	2.3
1	A	282	ASP	2.3
1	B	493	GLU	2.3
1	C	488	PHE	2.3
1	B	504	ALA	2.3
1	C	243	ASN	2.2
1	C	484	ARG	2.2
1	B	282	ASP	2.2
1	C	502	MET	2.1
1	D	111	GLY	2.1
1	C	490	ALA	2.1
1	B	497	ARG	2.1
1	D	329	VAL	2.1
1	C	485	GLU	2.1
1	B	509	PRO	2.1
1	D	301	ALA	2.0
1	D	277	ILE	2.0
1	B	515	GLU	2.0
1	D	278	GLY	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
3	GLU	A	519	10/10	0.28	3.15	68,69,71,71	0
3	GLU	D	3519	10/10	0.36	2.66	46,48,49,49	0
3	GLU	C	2519	10/10	0.26	2.15	67,68,69,70	0
2	MG	C	2525	1/1	0.21	1.24	45,45,45,45	0
4	CYS	C	2520	7/7	0.18	1.04	53,55,55,55	0
6	AF3	B	1522	4/4	0.21	0.62	57,58,59,60	0
4	CYS	A	520	7/7	0.14	0.52	51,52,53,53	0
6	AF3	A	522	4/4	0.19	0.30	49,51,52,55	0
3	GLU	B	1519	10/10	0.19	0.17	50,52,54,54	0
4	CYS	B	1520	7/7	0.15	0.15	48,48,49,49	0
4	CYS	D	3520	7/7	0.18	0.09	50,52,54,54	0
5	ADP	B	1521	27/27	0.15	-0.03	33,36,37,38	0
6	AF3	C	2522	4/4	0.20	-0.12	59,60,60,62	0
2	MG	D	3523	1/1	0.23	-0.29	38,38,38,38	0
5	ADP	C	2521	27/27	0.15	-0.33	35,41,45,46	0
5	ADP	D	3521	27/27	0.15	-0.37	31,34,37,37	0
2	MG	C	2524	1/1	0.20	-0.41	47,47,47,47	0
5	ADP	A	521	27/27	0.15	-0.56	29,31,34,35	0
2	MG	B	1524	1/1	0.21	-0.57	36,36,36,36	0
2	MG	C	2523	1/1	0.15	-0.67	46,46,46,46	0
6	AF3	D	3522	4/4	0.23	-0.68	57,58,58,62	0
2	MG	A	525	1/1	0.14	-0.78	26,26,26,26	0
2	MG	A	524	1/1	0.20	-0.89	34,34,34,34	0
2	MG	D	3525	1/1	0.17	-1.28	37,37,37,37	0
2	MG	A	523	1/1	0.12	-1.44	40,40,40,40	0
2	MG	D	3524	1/1	0.21	-1.74	35,35,35,35	0
2	MG	B	1523	1/1	0.15	-1.99	45,45,45,45	0
2	MG	B	1525	1/1	0.12	-2.70	37,37,37,37	0
2	MG	A	526	1/1	0.08	-2.73	44,44,44,44	0

6.5 Other polymers ⓘ

There are no such residues in this entry.