



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:01 AM GMT

PDB ID : 3HWW
Title : Crystal structure of menaquinone synthesis protein MenD from E. coli in complex with oxoglutarate
Authors : Priyadarshi, A.; Hwang, K.Y.
Deposited on : 2009-06-19
Resolution : 1.95 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>

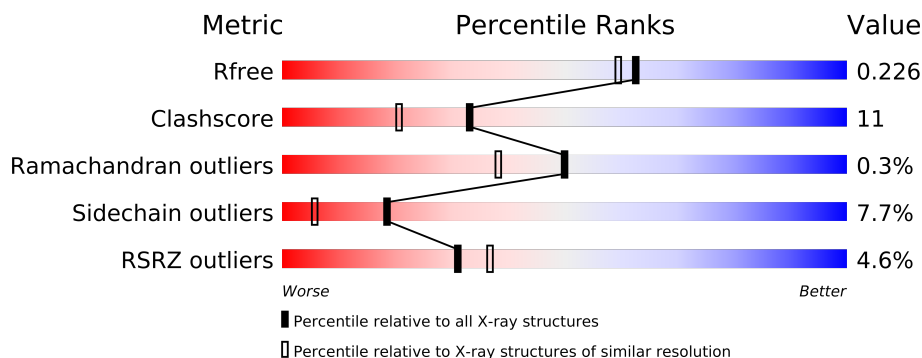
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.95 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	1321 (1.96-1.96)
Clashscore	79885	1488 (1.96-1.96)
Ramachandran outliers	78287	1475 (1.96-1.96)
Sidechain outliers	78261	1475 (1.96-1.96)
RSRZ outliers	66119	1321 (1.96-1.96)

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	556	
1	D	556	

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

Mol	Type	Chain	Res	Geometry	Electron density
4	NA	A	559	-	X
4	NA	A	564	-	X
4	NA	A	566	-	X
4	NA	A	567	-	X
4	NA	A	571	-	X
4	NA	A	575	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	NA	A	578	-	X
4	NA	D	559	-	X
4	NA	D	561	-	X
4	NA	D	573	-	X
4	NA	D	579	-	X
5	CL	A	563	-	X
6	GOL	A	577	-	X
6	GOL	A	579	-	X
6	GOL	A	580	-	X
6	GOL	D	569	-	X

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 8750 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.

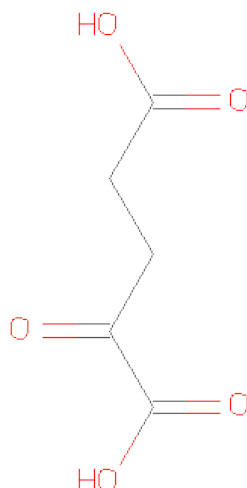
- Molecule 1 is a protein called 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylatesynthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			4190	2657	756	762	15			
1	D	532	Total	C	N	O	S	0	0	0
			4132	2616	749	754	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	36	LEU	PRO	ENGINEERED	UNP P17109
D	36	LEU	PRO	ENGINEERED	UNP P17109

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total	Na	0	0
			18	18		
4	D	19	Total	Na	0	0
			19	19		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 7 is water.

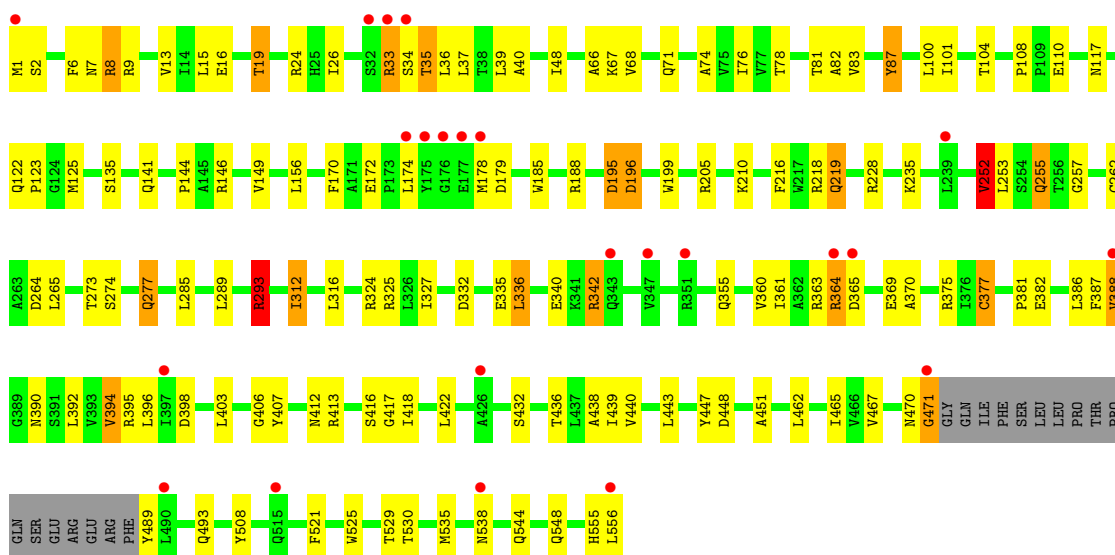
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	176	Total	O	0	0
			176	176		
7	D	155	Total	O	0	0
			155	155		

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.

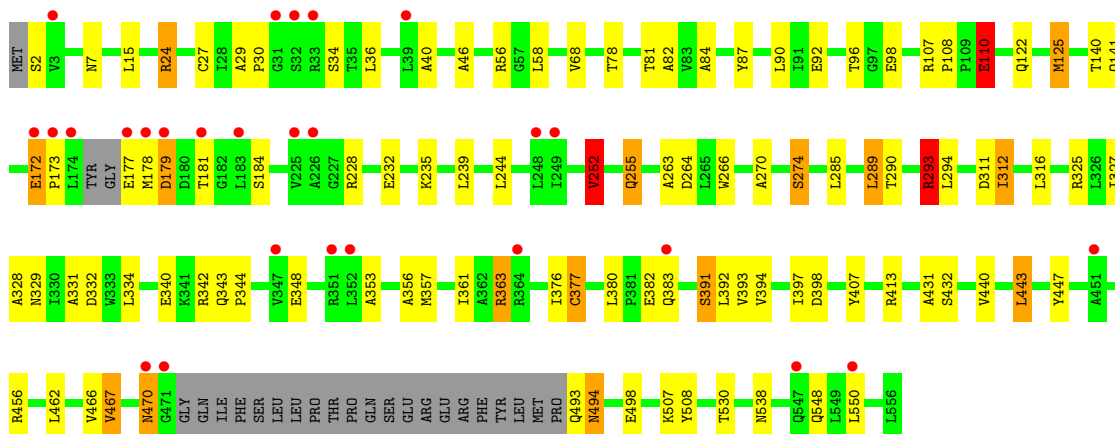
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylatesynthase

Chain A: 



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylatesynthase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.91Å 117.91Å 175.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.32 – 1.95 34.31 – 1.95	Depositor EDS
% Data completeness (in resolution range)	94.2 (34.32-1.95) 94.2 (34.31-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.209 , 0.255 0.212 , 0.226	Depositor DCC
R_{free} test set	4290 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	3 of 85134 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8750	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: GOL, MG, AKG, NA, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	5/4292 (0.1%)	0.99	10/5854 (0.2%)
1	D	1.00	4/4230 (0.1%)	0.97	11/5767 (0.2%)
All	All	1.03	9/8522 (0.1%)	0.98	21/11621 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	467	VAL	C-O	21.21	1.63	1.23
1	A	467	VAL	C-O	20.04	1.61	1.23
1	A	471	GLY	C-O	-17.31	0.95	1.23
1	A	377	CYS	CB-SG	-9.02	1.67	1.82
1	D	466	VAL	C-N	-7.35	1.17	1.34
1	A	489	TYR	CD1-CE1	-5.49	1.31	1.39
1	A	196	ASP	CB-CG	-5.41	1.40	1.51
1	D	92	GLU	CG-CD	5.39	1.60	1.51
1	D	377	CYS	CB-SG	-5.18	1.73	1.81

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	D	228	ARG	NE-CZ-NH2	-9.75	115.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	196	ASP	N-CA-CB	-9.18	94.07	110.60
1	D	125	MET	CG-SD-CE	-8.56	86.51	100.20
1	D	252	VAL	CB-CA-C	-7.52	97.11	111.40
1	A	285	LEU	CA-CB-CG	7.36	132.24	115.30
1	A	228	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	D	293	ARG	NE-CZ-NH1	6.59	123.60	120.30
1	D	311	ASP	N-CA-CB	6.58	122.45	110.60
1	A	252	VAL	CB-CA-C	-6.26	99.50	111.40
1	D	90	LEU	CB-CG-CD1	-6.21	100.44	111.00
1	A	146	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	324	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	D	107	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	A	196	ASP	CB-CG-OD1	-5.65	113.21	118.30
1	A	146	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	56	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	D	110	GLU	CA-CB-CG	5.18	124.80	113.40
1	A	293	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	244	LEU	CA-CB-CG	5.13	127.10	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	195	ASP	Peptide

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	4190	0	4162	107	0
1	D	4132	0	4100	78	0
2	A	10	0	4	1	0
2	D	10	0	4	2	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	18	0	0	0	0
4	D	19	0	0	0	0
5	A	1	0	0	1	0
5	D	1	0	0	0	0
6	A	18	0	24	15	0
6	D	18	0	24	0	0
7	A	176	0	0	5	0
7	D	155	0	0	7	0
All	All	8750	0	8318	184	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 11.

All (184) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:467:VAL:C	1:D:467:VAL:O	1.63	1.35
1:D:377:CYS:HB2	7:D:680:HOH:O	1.44	1.18
1:D:172:GLU:HG3	1:D:173:PRO:HA	1.15	1.08
1:D:172:GLU:HG3	1:D:173:PRO:CA	1.88	1.03
1:A:364:ARG:HG3	1:A:364:ARG:HH21	1.23	1.00
1:A:342:ARG:HH11	1:A:342:ARG:HG3	1.27	1.00
1:A:293:ARG:HH11	1:A:293:ARG:HG2	1.28	0.95
1:D:312:ILE:HD11	1:D:316:LEU:HD21	1.54	0.89
1:D:172:GLU:CG	1:D:173:PRO:HA	2.04	0.87
1:A:216:PHE:O	1:A:219:GLN:HG3	1.76	0.85
1:A:7:ASN:HB3	1:A:36:LEU:HD13	1.58	0.84
1:D:7:ASN:HB3	1:D:36:LEU:HD13	1.60	0.83
1:A:188:ARG:HD3	6:A:579:GOL:H31	1.61	0.82
1:D:329:ASN:HD22	1:D:332:ASP:H	1.29	0.80
1:A:185:TRP:CD1	6:A:579:GOL:H32	2.17	0.79
1:A:144:PRO:CA	6:A:579:GOL:H12	2.13	0.79
1:A:470:ASN:N	1:A:471:GLY:HA2	1.98	0.78
1:A:16:GLU:O	1:A:19:THR:HB	1.82	0.78
1:A:342:ARG:HG3	1:A:342:ARG:NH1	1.96	0.77
1:D:252:VAL:HG22	1:D:398:ASP:HB2	1.66	0.76
1:D:293:ARG:HG2	1:D:293:ARG:HH11	1.51	0.76
1:D:363:ARG:HH11	1:D:363:ARG:CB	1.98	0.75
1:D:470:ASN:N	1:D:470:ASN:HD22	1.83	0.74
1:A:144:PRO:HA	6:A:579:GOL:H12	1.69	0.74
1:A:364:ARG:CG	1:A:364:ARG:HH21	1.98	0.72
1:A:219:GLN:HB3	1:A:342:ARG:NH2	2.05	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:144:PRO:HA	6:A:579:GOL:C1	2.22	0.69
1:D:290:THR:OG1	1:D:413:ARG:NH1	2.24	0.69
1:D:122:GLN:O	1:D:125:MET:HB2	1.93	0.69
1:A:342:ARG:HH11	1:A:342:ARG:CG	2.03	0.69
1:A:33:ARG:HG3	1:A:78:THR:OG1	1.92	0.68
1:D:470:ASN:H	1:D:470:ASN:HD22	1.42	0.68
1:A:342:ARG:NH1	1:A:342:ARG:CG	2.57	0.68
1:A:293:ARG:NH1	1:A:293:ARG:HG2	2.01	0.67
1:A:252:VAL:HG13	1:A:398:ASP:HA	1.76	0.66
1:D:329:ASN:ND2	1:D:332:ASP:H	1.93	0.66
1:D:293:ARG:NH1	1:D:293:ARG:HG2	2.08	0.66
1:D:377:CYS:SG	7:D:680:HOH:O	2.53	0.65
1:D:377:CYS:CB	7:D:680:HOH:O	2.20	0.65
1:D:264:ASP:O	1:D:293:ARG:HG3	1.98	0.64
1:D:2:SER:OG	1:D:177:GLU:HG3	1.97	0.64
1:D:327:ILE:N	1:D:327:ILE:HD12	2.12	0.64
1:D:7:ASN:HB3	1:D:36:LEU:CD1	2.26	0.64
1:A:144:PRO:HB3	6:A:579:GOL:H12	1.80	0.63
1:A:33:ARG:HD3	1:A:33:ARG:O	1.98	0.63
1:A:7:ASN:HB3	1:A:36:LEU:CD1	2.29	0.63
1:A:293:ARG:HH11	1:A:293:ARG:CG	2.07	0.63
1:A:26:ILE:HG13	1:A:74:ALA:HB3	1.81	0.62
1:D:312:ILE:HG12	1:D:316:LEU:HD11	1.82	0.62
1:A:364:ARG:HG3	1:A:364:ARG:NH2	2.03	0.62
1:A:144:PRO:CB	6:A:579:GOL:H12	2.30	0.61
1:D:363:ARG:NH2	1:D:548:GLN:OE1	2.34	0.60
1:A:1:MET:HG3	7:A:707:HOH:O	2.01	0.60
1:D:377:CYS:HA	1:D:380:LEU:HG	1.84	0.60
1:A:332:ASP:O	1:A:335:GLU:HB2	2.01	0.59
1:D:329:ASN:HD21	1:D:331:ALA:HB3	1.69	0.58
1:D:108:PRO:HB2	1:D:110:GLU:OE1	2.04	0.57
1:D:363:ARG:HH11	1:D:363:ARG:HB3	1.68	0.57
1:A:15:LEU:HD12	1:A:40:ALA:HB3	1.87	0.57
1:D:293:ARG:CG	1:D:293:ARG:HH11	2.18	0.57
1:D:252:VAL:CG2	1:D:398:ASP:HB2	2.35	0.57
1:A:465:ILE:HD11	1:A:521:PHE:HZ	1.70	0.56
1:A:8:ARG:CG	1:A:8:ARG:HH21	2.19	0.56
1:A:9:ARG:HD3	7:A:607:HOH:O	2.08	0.54
1:D:493:GLN:HG2	1:D:494:ASN:H	1.73	0.54
1:A:108:PRO:HB2	1:A:110:GLU:OE1	2.07	0.54
1:D:391:SER:OG	2:D:557:AKG:H32	2.08	0.54
1:D:24:ARG:NE	1:D:46:ALA:O	2.38	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:108:PRO:HD3	1:A:170:PHE:O	2.07	0.53
1:D:27:CYS:HB3	1:D:58:LEU:HD11	1.89	0.53
1:A:264:ASP:O	1:A:293:ARG:HG3	2.08	0.53
1:D:470:ASN:ND2	1:D:470:ASN:N	2.55	0.53
1:A:188:ARG:HH11	6:A:579:GOL:H31	1.74	0.53
1:D:15:LEU:CD1	1:D:40:ALA:HB3	2.38	0.53
1:A:386:LEU:HD11	1:A:439:ILE:HD12	1.91	0.52
1:A:417:GLY:HA2	6:A:577:GOL:H31	1.91	0.52
1:D:493:GLN:CG	1:D:494:ASN:H	2.24	0.51
1:A:364:ARG:NH1	7:A:694:HOH:O	2.44	0.51
1:A:355:GLN:HB3	1:A:556:LEU:HD21	1.91	0.51
1:D:470:ASN:ND2	1:D:470:ASN:H	2.06	0.50
1:A:312:ILE:HG12	1:A:316:LEU:HD11	1.93	0.50
1:A:274:SER:HA	1:A:277:GLN:NE2	2.26	0.50
1:A:67:LYS:NZ	7:A:588:HOH:O	2.42	0.50
1:A:544:GLN:HG3	1:A:548:GLN:NE2	2.27	0.50
1:D:462:LEU:O	1:D:530:THR:HA	2.12	0.50
1:A:68:VAL:HG11	1:A:432:SER:HB3	1.93	0.50
1:D:2:SER:N	7:D:696:HOH:O	2.44	0.50
1:A:312:ILE:HD11	1:A:316:LEU:HD21	1.93	0.50
1:A:462:LEU:O	1:A:530:THR:HA	2.12	0.50
1:A:117:ASN:ND2	7:A:627:HOH:O	2.22	0.49
1:D:27:CYS:HB3	1:D:58:LEU:CD1	2.43	0.49
6:A:577:GOL:H2	7:D:679:HOH:O	2.11	0.49
1:A:219:GLN:HB3	1:A:342:ARG:CZ	2.41	0.49
1:D:353:ALA:O	1:D:356:ALA:HB3	2.12	0.49
1:A:264:ASP:O	1:A:293:ARG:CG	2.61	0.49
1:D:172:GLU:HG3	1:D:173:PRO:N	2.28	0.49
1:A:253:LEU:HD11	1:A:413:ARG:HG3	1.95	0.48
1:A:443:LEU:N	2:A:557:AKG:O2	2.43	0.48
1:A:8:ARG:HH21	1:A:8:ARG:CB	2.26	0.48
1:A:195:ASP:OD1	1:A:196:ASP:HB3	2.13	0.48
1:D:470:ASN:OD1	1:D:494:ASN:HA	2.13	0.48
1:A:24:ARG:HG3	1:A:48:ILE:HD12	1.95	0.48
1:A:188:ARG:CD	6:A:579:GOL:H31	2.38	0.48
1:D:252:VAL:HG22	1:D:398:ASP:CB	2.41	0.48
1:D:363:ARG:HB2	1:D:363:ARG:HH11	1.75	0.48
1:A:26:ILE:HD11	1:A:76:ILE:HD11	1.95	0.47
1:A:361:ILE:C	1:A:363:ARG:H	2.18	0.47
1:A:101:ILE:N	1:A:101:ILE:HD13	2.29	0.47
1:D:494:ASN:HB3	7:D:710:HOH:O	2.14	0.47
1:A:235:LYS:HE3	1:A:406:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:68:VAL:HG11	1:D:432:SER:HB3	1.98	0.46
1:A:15:LEU:HD12	1:A:40:ALA:CB	2.45	0.46
1:A:8:ARG:HH21	1:A:8:ARG:HG2	1.80	0.46
1:A:418:ILE:N	6:A:577:GOL:H32	2.31	0.46
1:D:68:VAL:HB	1:D:431:ALA:CB	2.46	0.46
1:A:81:THR:O	1:A:82:ALA:C	2.54	0.46
1:A:255:GLN:HG2	1:A:407:TYR:O	2.16	0.46
1:A:66:ALA:HB1	5:A:563:CL:CL	2.53	0.46
1:A:218:ARG:NH1	1:A:340:GLU:HG3	2.31	0.46
1:A:387:PHE:O	1:A:438:ALA:HA	2.15	0.46
1:A:422:LEU:HB2	1:A:451:ALA:HB3	1.98	0.45
1:A:122:GLN:HA	1:A:125:MET:HG3	1.97	0.45
1:D:255:GLN:HG2	1:D:407:TYR:O	2.17	0.45
1:D:263:ALA:HA	1:D:266:TRP:CE2	2.52	0.45
1:A:370:ALA:HA	1:A:396:LEU:HD13	1.99	0.45
1:D:232:GLU:HG2	7:D:601:HOH:O	2.17	0.45
1:A:493:GLN:HB3	1:D:456:ARG:NH2	2.32	0.45
1:D:289:LEU:HG	1:D:294:LEU:HD21	1.99	0.44
1:A:2:SER:HB3	1:A:179:ASP:OD2	2.17	0.44
1:A:100:LEU:C	1:A:101:ILE:HD13	2.37	0.44
1:A:262:CYS:HB3	1:A:265:LEU:HD12	2.00	0.44
1:A:87:TYR:HB3	1:D:84:ALA:HB1	1.99	0.44
1:A:6:PHE:CE1	1:A:141:GLN:HG2	2.53	0.44
1:D:270:ALA:O	1:D:274:SER:HB2	2.17	0.44
1:D:81:THR:O	1:D:82:ALA:C	2.55	0.44
1:A:34:SER:HB3	1:A:78:THR:HA	1.99	0.43
1:D:443:LEU:HB2	2:D:557:AKG:O2	2.18	0.43
1:A:13:VAL:CG1	1:A:149:VAL:HG12	2.49	0.43
1:A:390:ASN:OD1	1:A:413:ARG:HD3	2.18	0.43
1:D:34:SER:HB3	1:D:78:THR:HA	2.00	0.43
1:D:29:ALA:HA	1:D:30:PRO:HD2	1.82	0.43
1:A:257:GLY:HA2	1:A:403:LEU:O	2.19	0.43
1:D:285:LEU:N	1:D:285:LEU:HD22	2.34	0.43
1:D:327:ILE:O	1:D:328:ALA:HB2	2.19	0.43
1:D:493:GLN:CG	1:D:494:ASN:N	2.82	0.43
1:D:255:GLN:HE21	1:D:255:GLN:HB2	1.60	0.43
1:D:343:GLN:HA	1:D:344:PRO:HD3	1.93	0.43
1:A:327:ILE:HD12	1:A:327:ILE:N	2.34	0.43
1:A:395:ARG:HG3	1:A:395:ARG:HH11	1.84	0.42
1:A:274:SER:HA	1:A:277:GLN:HE21	1.85	0.42
1:A:418:ILE:HG23	6:A:577:GOL:H32	2.00	0.42
1:D:179:ASP:HB3	1:D:181:THR:H	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:36:LEU:HD11	1:A:174:LEU:HD22	2.02	0.42
1:A:436:THR:HB	1:A:462:LEU:HD12	2.02	0.42
1:A:149:VAL:CG2	1:A:199:TRP:HB3	2.50	0.42
1:D:393:VAL:O	1:D:397:ILE:HG13	2.20	0.42
1:A:395:ARG:NH1	1:A:395:ARG:HG3	2.35	0.42
1:A:381:PRO:HD3	1:A:525:TRP:CZ2	2.55	0.42
1:A:149:VAL:CG2	1:A:199:TRP:CB	2.98	0.41
1:A:465:ILE:HD11	1:A:521:PHE:CZ	2.53	0.41
1:A:369:GLU:HG2	1:A:396:LEU:CD1	2.50	0.41
1:A:144:PRO:HA	6:A:579:GOL:H11	1.99	0.41
1:D:68:VAL:HB	1:D:431:ALA:HB3	2.02	0.41
1:A:422:LEU:HG	1:A:448:ASP:HB3	2.01	0.41
1:A:361:ILE:O	1:A:364:ARG:HG2	2.20	0.41
1:A:210:LYS:HG3	1:A:336:LEU:HG	2.02	0.41
1:A:34:SER:O	1:A:37:LEU:N	2.52	0.41
1:A:388:VAL:HG13	1:A:394:VAL:HG21	2.01	0.41
1:D:15:LEU:HD12	1:D:40:ALA:HB3	2.03	0.41
1:A:508:TYR:H	6:A:580:GOL:H11	1.86	0.41
1:D:334:LEU:HA	1:D:334:LEU:HD23	1.92	0.41
1:D:96:THR:OG1	1:D:98:GLU:OE1	2.29	0.41
1:D:376:ILE:HD12	1:D:376:ILE:HA	1.87	0.40
1:A:122:GLN:N	1:A:123:PRO:CD	2.85	0.40
1:A:83:VAL:HG13	1:A:104:THR:HG21	2.02	0.40
1:A:35:THR:HG23	1:A:39:LEU:CD1	2.51	0.40
1:D:498:GLU:HB2	1:D:508:TYR:CE2	2.57	0.40
1:A:360:VAL:O	1:A:363:ARG:HB2	2.21	0.40
1:D:327:ILE:N	1:D:327:ILE:CD1	2.81	0.40
1:A:412:ASN:O	1:A:416:SER:HA	2.21	0.40
1:D:235:LYS:HB2	1:D:235:LYS:HE3	1.86	0.40
1:D:29:ALA:HB2	1:D:58:LEU:HD22	2.03	0.40
1:A:277:GLN:HB2	1:A:277:GLN:HE21	1.47	0.40
1:D:382:GLU:O	1:D:383:GLN: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	535/556 (96%)	512 (96%)	22 (4%)	1 (0%)	56	46
1	D	526/556 (95%)	503 (96%)	21 (4%)	2 (0%)	43	30
All	All	1061/1112 (95%)	1015 (96%)	43 (4%)	3 (0%)	50	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	THR
1	D	178	MET
1	D	179	ASP

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	436/452 (96%)	401 (92%)	35 (8%)	17	5
1	D	430/452 (95%)	398 (93%)	32 (7%)	20	6
All	All	866/904 (96%)	799 (92%)	67 (8%)	18	6

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	19	THR
1	A	33	ARG
1	A	71	GLN
1	A	87	TYR
1	A	135	SER
1	A	156	LEU
1	A	172	GLU
1	A	178	MET
1	A	205	ARG
1	A	219	GLN
1	A	252	VAL

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Mol	Chain	Res	Type
1	A	255	GLN
1	A	273	THR
1	A	277	GLN
1	A	289	LEU
1	A	293	ARG
1	A	312	ILE
1	A	325	ARG
1	A	336	LEU
1	A	342	ARG
1	A	364	ARG
1	A	365	ASP
1	A	375	ARG
1	A	377	CYS
1	A	382	GLU
1	A	388	VAL
1	A	392	LEU
1	A	394	VAL
1	A	440	VAL
1	A	447	TYR
1	A	529	THR
1	A	535	MET
1	A	538	ASN
1	A	555	HIS
1	D	24	ARG
1	D	87	TYR
1	D	110	GLU
1	D	140	THR
1	D	141	GLN
1	D	172	GLU
1	D	184	SER
1	D	239	LEU
1	D	252	VAL
1	D	255	GLN
1	D	274	SER
1	D	289	LEU
1	D	293	ARG
1	D	312	ILE
1	D	325	ARG
1	D	340	GLU
1	D	342	ARG
1	D	348	GLU
1	D	357	MET

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Mol	Chain	Res	Type
1	D	361	ILE
1	D	363	ARG
1	D	391	SER
1	D	392	LEU
1	D	394	VAL
1	D	440	VAL
1	D	443	LEU
1	D	447	TYR
1	D	470	ASN
1	D	494	ASN
1	D	507	LYS
1	D	538	ASN
1	D	550	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	GLN
1	A	277	GLN
1	A	284	GLN
1	A	296	GLN
1	A	493	GLN
1	D	141	GLN
1	D	296	GLN
1	D	329	ASN
1	D	470	ASN
1	D	538	ASN
1	D	547	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 49 ligands modelled in this entry, 41 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$
2	AKG	A	557	3	9,9,9	4.36	3 (33%)	11,11,11	5.97	4 (36%)
6	GOL	A	577	-	5,5,5	0.41	0	5,5,5	0.89	0
6	GOL	A	579	4	5,5,5	0.55	0	5,5,5	1.81	2 (40%)
6	GOL	A	580	-	5,5,5	0.49	0	5,5,5	0.60	0
2	AKG	D	557	3	9,9,9	0.97	0	11,11,11	1.67	3 (27%)
6	GOL	D	569	-	5,5,5	0.41	0	5,5,5	0.36	0
6	GOL	D	571	-	5,5,5	0.36	0	5,5,5	0.64	0
6	GOL	D	581	-	5,5,5	0.42	0	5,5,5	0.09	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	AKG	A	557	3	-	0/9/9/9	0/0/0/0
6	GOL	A	577	-	-	0/4/4/4	0/0/0/0
6	GOL	A	579	4	-	0/4/4/4	0/0/0/0
6	GOL	A	580	-	-	0/4/4/4	0/0/0/0
2	AKG	D	557	3	-	0/9/9/9	0/0/0/0
6	GOL	D	569	-	-	0/4/4/4	0/0/0/0
6	GOL	D	571	-	-	0/4/4/4	0/0/0/0
6	GOL	D	581	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	557	AKG	C3-C2	-11.36	1.36	1.51
2	A	557	AKG	C2-C1	-5.16	1.39	1.54
2	A	557	AKG	O5-C2	3.43	1.31	1.23

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	557	AKG	O5-C2-C3	-16.71	85.11	120.77
2	A	557	AKG	O5-C2-C1	6.01	135.07	118.80
2	A	557	AKG	C3-C2-C1	5.97	138.83	118.34
2	A	557	AKG	C3-C4-C5	-5.48	103.35	113.53
2	D	557	AKG	O2-C1-C2	3.05	121.09	114.37
6	A	579	GOL	O3-C3-C2	2.70	122.87	109.71
2	D	557	AKG	O5-C2-C3	-2.66	115.08	120.77
2	D	557	AKG	O2-C1-O1	-2.29	118.19	123.62
6	A	579	GOL	O1-C1-C2	2.07	119.80	109.71

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	539/556 (96%)	0.14	23 (4%)	34 39	21, 34, 57, 82	11 (2%)
1	D	532/556 (95%)	0.19	27 (5%)	27 33	22, 36, 58, 79	10 (1%)
All	All	1071/1112 (96%)	0.16	50 (4%)	31 36	21, 35, 57, 82	21 (1%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	TYR	8.1
1	A	174	LEU	5.6
1	D	174	LEU	5.4
1	A	177	GLU	5.1
1	A	178	MET	4.8
1	D	32	SER	4.6
1	D	471	GLY	4.5
1	A	176	GLY	4.2
1	D	178	MET	4.0
1	A	1	MET	3.9
1	A	34	SER	3.6
1	D	351	ARG	3.5
1	D	33	ARG	3.4
1	A	365	ASP	3.3
1	D	470	ASN	3.3
1	A	351	ARG	3.2
1	D	31	GLY	3.2
1	D	177	GLU	3.2
1	A	32	SER	3.1
1	A	33	ARG	3.0
1	D	173	PRO	2.9
1	A	556	LEU	2.8
1	D	225	VAL	2.8
1	A	515	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	249	ILE	2.6
1	A	490	LEU	2.6
1	D	248	LEU	2.5
1	A	471	GLY	2.5
1	D	39	LEU	2.5
1	D	352	LEU	2.4
1	D	172	GLU	2.3
1	D	3	VAL	2.3
1	D	347	VAL	2.3
1	A	239	LEU	2.3
1	D	179	ASP	2.3
1	D	364	ARG	2.2
1	D	226	ALA	2.1
1	A	388	VAL	2.1
1	D	550	LEU	2.1
1	D	181	THR	2.1
1	A	347	VAL	2.1
1	D	383	GLN	2.1
1	A	343	GLN	2.1
1	A	397	ILE	2.0
1	A	538	ASN	2.0
1	D	547	GLN	2.0
1	D	451	ALA	2.0
1	A	364	ARG	2.0
1	D	183	LEU	2.0
1	A	426	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NA	A	571	1/1	0.36	19.35	45,45,45,45	0
4	NA	A	566	1/1	0.11	8.35	49,49,49,49	0
6	GOL	A	580	6/6	0.45	8.22	64,69,69,70	0
4	NA	D	573	1/1	0.20	5.71	49,49,49,49	0
4	NA	A	575	1/1	0.15	4.87	35,35,35,35	0
6	GOL	D	569	6/6	0.14	4.70	72,75,75,75	0
4	NA	A	578	1/1	0.26	4.26	69,69,69,69	0
4	NA	A	559	1/1	0.13	3.91	40,40,40,40	0
4	NA	A	567	1/1	0.29	3.55	51,51,51,51	0
6	GOL	A	577	6/6	0.21	3.30	57,57,58,59	0
4	NA	D	561	1/1	0.19	2.97	47,47,47,47	0
4	NA	D	579	1/1	0.14	2.59	72,72,72,72	0
4	NA	D	559	1/1	0.17	2.42	37,37,37,37	0
6	GOL	A	579	6/6	0.20	2.41	46,50,53,53	0
5	CL	A	563	1/1	0.15	2.39	62,62,62,62	0
4	NA	A	564	1/1	0.15	2.19	43,43,43,43	0
2	AKG	A	557	10/10	0.18	1.25	70,72,73,75	0
4	NA	D	563	1/1	0.12	1.15	44,44,44,44	0
4	NA	A	570	1/1	0.17	1.07	44,44,44,44	0
4	NA	D	567	1/1	0.10	0.95	41,41,41,41	0
4	NA	D	560	1/1	0.11	0.88	50,50,50,50	0
4	NA	A	573	1/1	0.14	0.49	40,40,40,40	0
4	NA	A	565	1/1	0.10	0.32	40,40,40,40	0
4	NA	A	576	1/1	0.14	0.26	34,34,34,34	0
4	NA	D	566	1/1	0.10	0.25	24,24,24,24	0
4	NA	A	569	1/1	0.14	0.24	64,64,64,64	0
4	NA	D	576	1/1	0.19	0.18	52,52,52,52	0
6	GOL	D	571	6/6	0.13	0.05	59,64,65,66	0
2	AKG	D	557	10/10	0.12	0.01	61,68,69,69	0
4	NA	A	560	1/1	0.10	-0.11	67,67,67,67	0
4	NA	D	574	1/1	0.12	-0.13	47,47,47,47	0
5	CL	D	568	1/1	0.07	-0.30	58,58,58,58	0
4	NA	D	565	1/1	0.07	-0.42	37,37,37,37	0
6	GOL	D	581	6/6	0.13	-0.53	78,80,82,82	0
4	NA	D	562	1/1	0.10	-0.54	40,40,40,40	0
4	NA	D	570	1/1	0.09	-0.64	32,32,32,32	0
4	NA	D	577	1/1	0.14	-0.66	49,49,49,49	0
4	NA	D	564	1/1	0.08	-0.76	45,45,45,45	0
3	MG	D	558	1/1	0.10	-0.87	41,41,41,41	0
4	NA	A	568	1/1	0.08	-0.87	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NA	D	572	1/1	0.10	-0.90	48,48,48,48	0
3	MG	A	558	1/1	0.05	-1.13	45,45,45,45	0
4	NA	D	575	1/1	0.07	-1.18	37,37,37,37	0
4	NA	D	580	1/1	0.10	-1.34	43,43,43,43	0
4	NA	A	572	1/1	0.10	-1.52	34,34,34,34	0
4	NA	D	578	1/1	0.09	-1.83	49,49,49,49	0
4	NA	A	574	1/1	0.06	-1.90	47,47,47,47	0
4	NA	A	561	1/1	0.06	-2.36	38,38,38,38	0
4	NA	A	562	1/1	0.05	-2.86	32,32,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.