



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:17 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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

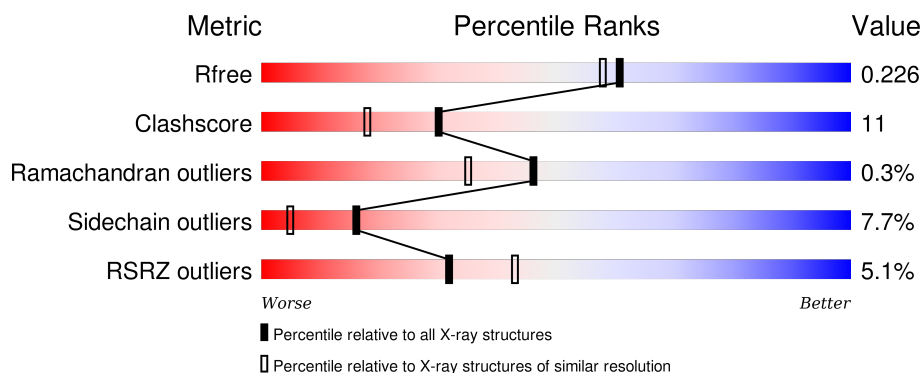
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (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. 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	556	<div> <div>4%</div> <div>71%</div> <div>22%</div> <div>• •</div> </div>
1	D	556	<div> <div>6%</div> <div>77%</div> <div>16%</div> <div>• • •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AKG	A	557	-	-	-	X
4	NA	A	571	-	-	-	X
4	NA	D	561	-	-	-	X
4	NA	D	567	-	-	-	X
5	CL	A	563	-	-	-	X
6	GOL	A	577	-	-	X	-
6	GOL	A	579	-	-	X	X

2 Entry composition [i](#)

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

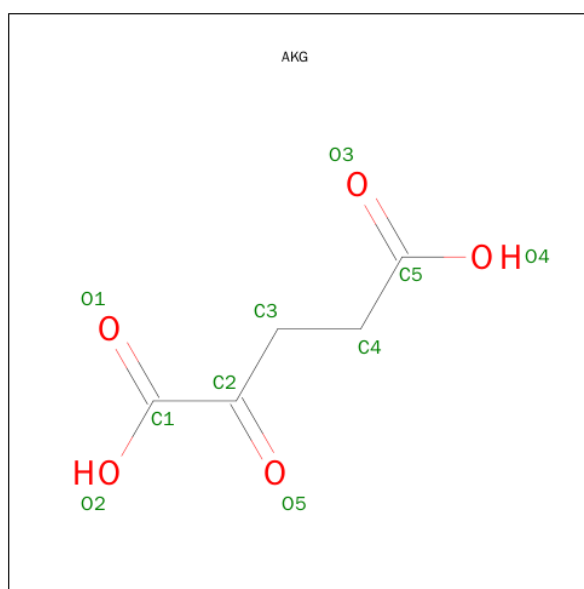
- Molecule 1 is a protein called 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

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		

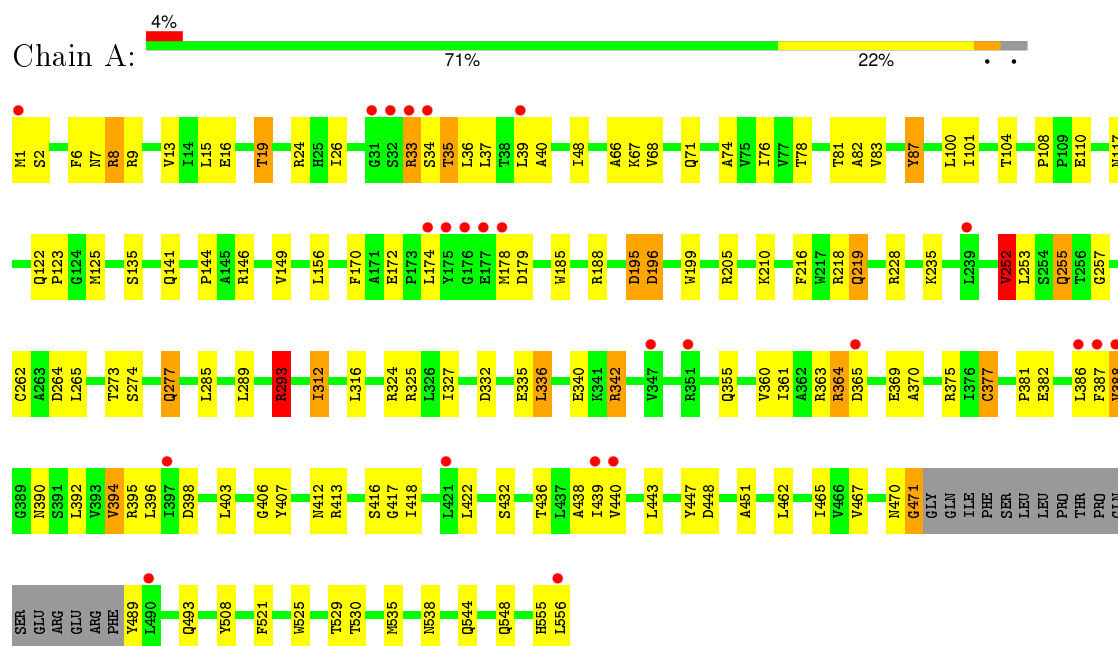
- Molecule 7 is water.

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

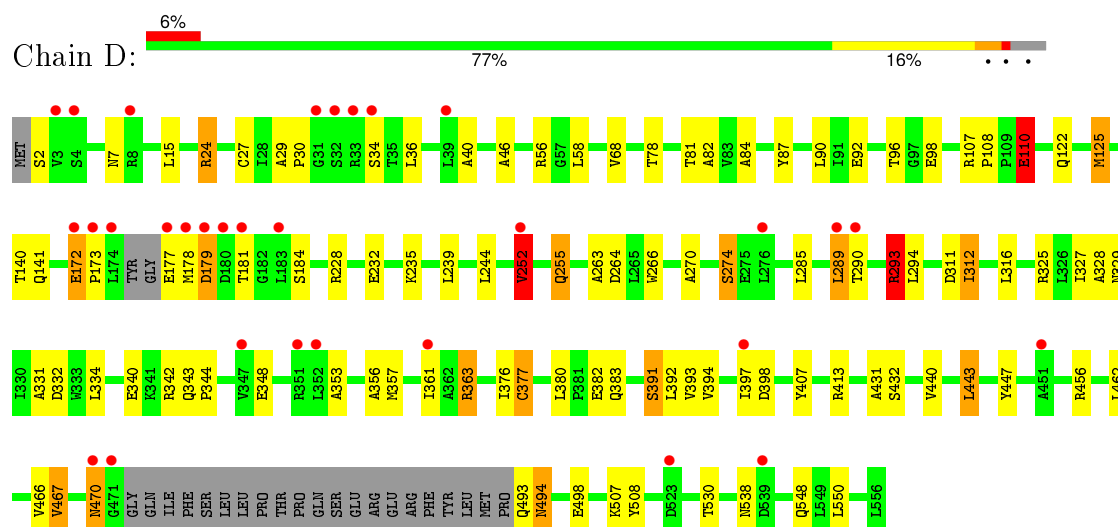
3 Residue-property plots [i](#)

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-carboxylate synthase



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



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 0.210 , 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 , 41.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 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	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
3	D	1	0	0	0	0
4	A	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 11.

All (184) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:ARG:NE	1:D:46:ALA:O	2.38	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 [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	535/556 (96%)	512 (96%)	22 (4%)	1 (0%)	52	43
1	D	526/556 (95%)	503 (96%)	21 (4%)	2 (0%)	39	27
All	All	1061/1112 (95%)	1015 (96%)	43 (4%)	3 (0%)	46	35

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 [i](#)

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%)	15	4
1	D	430/452 (95%)	398 (93%)	32 (7%)	17	5
All	All	866/904 (96%)	799 (92%)	67 (8%)	16	5

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	3,9,9	6.02	2 (66%)	4,11,11	10.31	3 (75%)
6	GOL	A	577	-	5,5,5	0.44	0	5,5,5	0.86	0
6	GOL	A	579	4	5,5,5	0.60	0	5,5,5	1.73	1 (20%)
6	GOL	A	580	-	5,5,5	0.53	0	5,5,5	0.60	0
2	AKG	D	557	3	3,9,9	0.56	0	4,11,11	1.84	1 (25%)
6	GOL	D	569	-	5,5,5	0.44	0	5,5,5	0.32	0
6	GOL	D	571	-	5,5,5	0.38	0	5,5,5	0.61	0
6	GOL	D	581	-	5,5,5	0.44	0	5,5,5	0.11	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	-	0/3/9/9	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	-	0/3/9/9	0/0/0/0
6	GOL	D	569	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	557	AKG	C3-C2	-9.09	1.36	1.51
2	A	557	AKG	O5-C2	5.09	1.31	1.22

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	557	AKG	O5-C2-C3	-18.60	85.11	120.28
2	A	557	AKG	C3-C4-C5	-5.13	103.35	112.75
2	D	557	AKG	O5-C2-C3	-2.75	115.08	120.28
6	A	579	GOL	O3-C3-C2	2.62	122.87	110.18
2	A	557	AKG	C3-C2-C1	7.22	138.83	121.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	557	AKG	1	0
6	A	577	GOL	4	0
6	A	579	GOL	10	0
6	A	580	GOL	1	0
2	D	557	AKG	2	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	539/556 (96%)	0.14	24 (4%)	37 48	21, 34, 57, 82	11 (2%)
1	D	532/556 (95%)	0.18	31 (5%)	26 37	22, 36, 58, 79	10 (1%)
All	All	1071/1112 (96%)	0.16	55 (5%)	32 43	21, 35, 57, 82	21 (1%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	175	TYR	6.5
1	D	32	SER	5.6
1	A	174	LEU	5.3
1	A	177	GLU	4.8
1	D	174	LEU	4.7
1	D	173	PRO	4.5
1	A	34	SER	4.3
1	D	31	GLY	4.3
1	D	178	MET	4.1
1	A	351	ARG	4.0
1	A	556	LEU	4.0
1	A	176	GLY	3.9
1	A	178	MET	3.9
1	D	39	LEU	3.7
1	A	365	ASP	3.7
1	D	3	VAL	3.6
1	D	33	ARG	3.6
1	D	172	GLU	3.4
1	A	388	VAL	3.3
1	D	177	GLU	3.2
1	D	181	THR	3.2
1	D	4	SER	3.1
1	D	471	GLY	2.9
1	A	39	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	351	ARG	2.9
1	A	347	VAL	2.9
1	A	1	MET	2.8
1	D	347	VAL	2.8
1	D	470	ASN	2.7
1	A	32	SER	2.6
1	D	289	LEU	2.5
1	D	523	ASP	2.5
1	D	451	ALA	2.5
1	A	33	ARG	2.5
1	D	361	ILE	2.4
1	D	180	ASP	2.4
1	D	352	LEU	2.4
1	D	183	LEU	2.4
1	A	387	PHE	2.4
1	A	439	ILE	2.4
1	D	179	ASP	2.4
1	D	276	LEU	2.3
1	A	490	LEU	2.3
1	A	397	ILE	2.3
1	A	239	LEU	2.2
1	D	290	THR	2.2
1	D	397	ILE	2.2
1	D	539	ASP	2.2
1	A	421	LEU	2.1
1	D	252	VAL	2.1
1	D	8	ARG	2.1
1	A	31	GLY	2.1
1	A	386	LEU	2.0
1	A	440	VAL	2.0
1	D	34	SER	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 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NA	A	571	1/1	0.97	0.23	15.85	45,45,45,45	0
6	GOL	A	579	6/6	0.81	0.26	5.61	46,50,53,53	0
5	CL	A	563	1/1	0.93	0.17	5.16	62,62,62,62	0
4	NA	D	561	1/1	0.94	0.17	2.89	47,47,47,47	0
4	NA	D	567	1/1	0.98	0.14	2.63	41,41,41,41	0
2	AKG	A	557	10/10	0.83	0.21	2.44	70,72,73,75	0
4	NA	D	566	1/1	0.99	0.14	1.57	24,24,24,24	0
4	NA	A	575	1/1	0.98	0.12	1.52	35,35,35,35	0
6	GOL	A	577	6/6	0.84	0.14	1.29	57,57,58,59	0
4	NA	A	570	1/1	0.96	0.18	1.28	44,44,44,44	0
4	NA	D	565	1/1	0.99	0.08	0.83	37,37,37,37	0
4	NA	A	576	1/1	0.98	0.19	0.67	34,34,34,34	0
5	CL	D	568	1/1	0.99	0.10	0.46	58,58,58,58	0
4	NA	D	572	1/1	0.95	0.12	0.38	48,48,48,48	0
4	NA	A	559	1/1	0.97	0.08	0.21	40,40,40,40	0
2	AKG	D	557	10/10	0.86	0.13	0.13	61,68,69,69	0
4	NA	D	560	1/1	0.96	0.09	-0.06	50,50,50,50	0
4	NA	A	568	1/1	0.99	0.09	-0.16	33,33,33,33	0
4	NA	D	559	1/1	0.99	0.08	-0.33	37,37,37,37	0
4	NA	D	570	1/1	1.00	0.09	-0.54	32,32,32,32	0
4	NA	D	577	1/1	0.97	0.11	-0.62	49,49,49,49	0
4	NA	A	565	1/1	0.97	0.08	-0.72	40,40,40,40	0
4	NA	A	573	1/1	0.98	0.08	-0.75	40,40,40,40	0
4	NA	D	578	1/1	0.94	0.12	-0.77	49,49,49,49	0
4	NA	A	564	1/1	0.98	0.07	-0.85	43,43,43,43	0
4	NA	D	580	1/1	0.97	0.13	-0.86	43,43,43,43	0
3	MG	A	558	1/1	0.95	0.10	-0.96	45,45,45,45	0
4	NA	D	562	1/1	0.98	0.06	-0.98	40,40,40,40	0
4	NA	D	575	1/1	0.99	0.06	-1.74	37,37,37,37	0
4	NA	A	572	1/1	0.99	0.05	-1.76	34,34,34,34	0
4	NA	D	563	1/1	0.99	0.07	-1.81	44,44,44,44	0
4	NA	D	576	1/1	0.94	0.10	-1.93	52,52,52,52	0
4	NA	A	561	1/1	0.99	0.07	-1.95	38,38,38,38	0
4	NA	A	562	1/1	0.98	0.06	-2.19	32,32,32,32	0
4	NA	A	574	1/1	0.96	0.07	-2.57	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	D	558	1/1	0.96	0.10	-	41,41,41,41	0
6	GOL	D	571	6/6	0.90	0.10	-	59,64,65,66	0
4	NA	A	578	1/1	0.87	0.24	-	69,69,69,69	0
4	NA	A	560	1/1	0.70	0.13	-	67,67,67,67	0
4	NA	A	566	1/1	0.95	0.14	-	49,49,49,49	0
4	NA	D	574	1/1	0.92	0.09	-	47,47,47,47	0
4	NA	D	573	1/1	0.93	0.15	-	49,49,49,49	0
6	GOL	A	580	6/6	0.80	0.39	-	64,69,69,70	0
4	NA	D	579	1/1	0.83	0.38	-	72,72,72,72	0
4	NA	A	567	1/1	0.93	0.19	-	51,51,51,51	0
6	GOL	D	569	6/6	0.68	0.15	-	72,75,75,75	0
4	NA	A	569	1/1	0.92	0.13	-	64,64,64,64	0
6	GOL	D	581	6/6	0.81	0.11	-	78,80,82,82	0
4	NA	D	564	1/1	0.95	0.09	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.