



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2018 – 09:56 AM EDT

PDB ID : 5XVV
Title : Crystal Structure of Forward Inhibited *Aspergillus niger* Glutamate Dehydrogenase With Both Apo- and Alpha Ketoglutarate Bound Subunits
Authors : Prakash, P.; Puneekar, N.S.; Bhaumik, P.
Deposited on : 2017-06-28
Resolution : 2.25 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

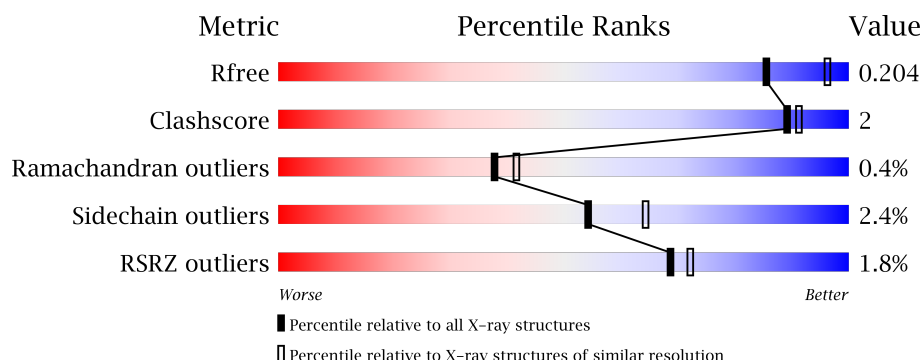
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.



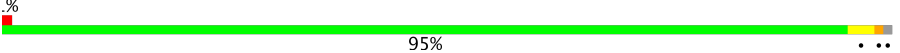
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (2.26-2.26)

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	460	<div> <div>0.2%</div> <div>92% 7%</div> </div>
1	B	460	<div> <div>3%</div> <div>94% 5%</div> </div>
1	C	460	<div> <div>4%</div> <div>92% 7%</div> </div>
1	D	460	<div> <div>0.2%</div> <div>94% . .</div> </div>
1	E	460	<div> <div>0.2%</div> <div>93% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	460	

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	GOL	A	501	-	-	-	X
2	GOL	A	502	-	-	-	X
2	GOL	A	507	-	-	-	X
2	GOL	B	501	-	-	-	X
2	GOL	B	502	-	-	-	X
2	GOL	B	503	-	-	-	X
2	GOL	B	504	-	-	-	X
2	GOL	C	502	-	-	-	X
2	GOL	E	501	-	-	-	X
2	GOL	E	503	-	-	-	X
2	GOL	E	504	-	-	-	X
2	GOL	F	501	-	-	-	X
2	GOL	F	503	-	-	-	X
3	AKG	A	508	-	-	-	X
3	AKG	B	506	-	-	-	X
3	AKG	C	504	-	-	-	X
4	BME	A	509	-	-	-	X
4	BME	B	507	-	-	-	X
4	BME	C	505	-	-	-	X
4	BME	D	501	-	-	-	X
4	BME	E	505	-	-	X	X
4	BME	F	504	-	-	-	X

2 Entry composition [i](#)

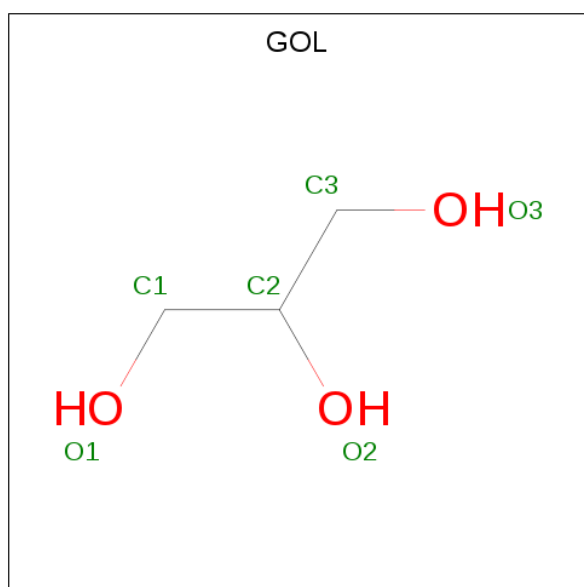
There are 5 unique types of molecules in this entry. The entry contains 22611 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase.

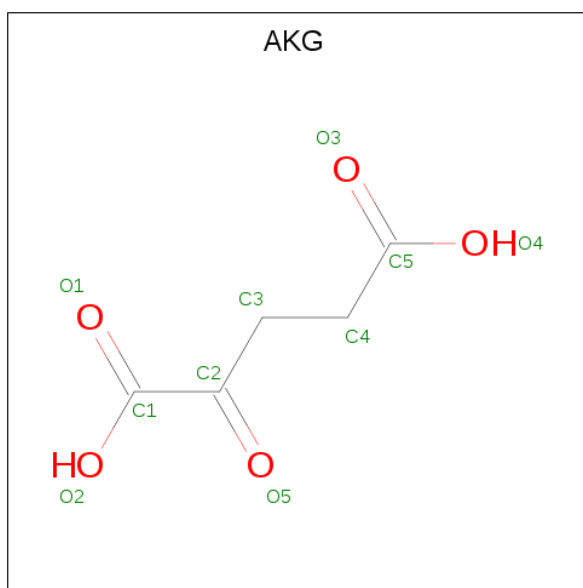
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	6	0
			3491	2205	606	667	13			
1	B	459	Total	C	N	O	S	0	3	0
			3496	2201	612	670	13			
1	C	459	Total	C	N	O	S	0	3	0
			3484	2195	607	669	13			
1	D	458	Total	C	N	O	S	0	4	0
			3483	2197	606	666	14			
1	E	458	Total	C	N	O	S	0	2	0
			3476	2191	606	666	13			
1	F	457	Total	C	N	O	S	0	4	0
			3479	2193	606	667	13			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



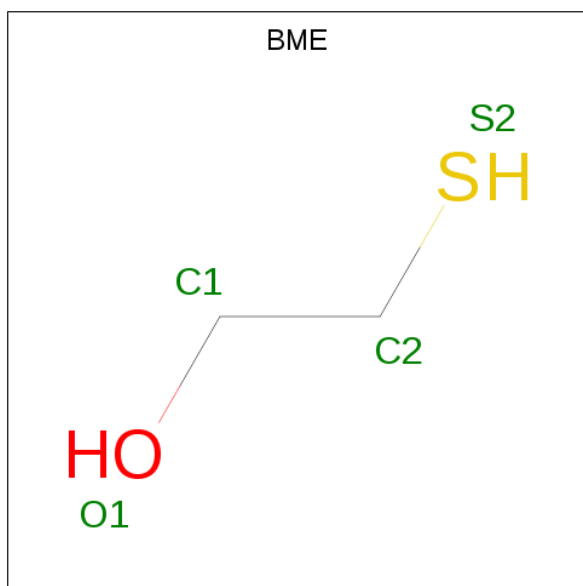
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



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

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	D	1	Total C O S 4 2 1 1	0	0
4	E	1	Total C O S 4 2 1 1	0	0
4	F	1	Total C O S 4 2 1 1	0	0

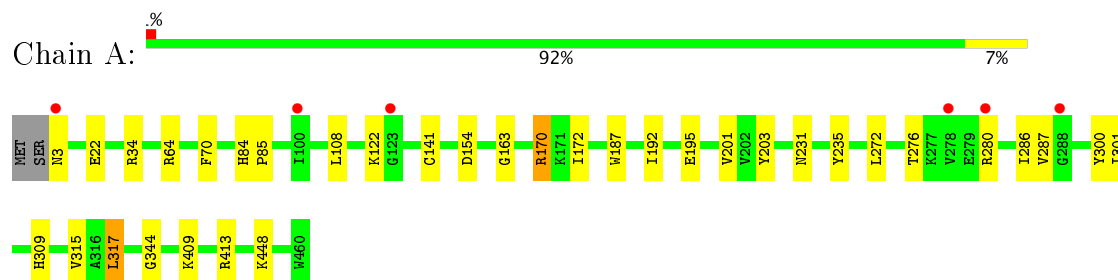
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	279	Total O 279 279	0	0
5	B	246	Total O 246 246	0	0
5	C	221	Total O 221 221	0	0
5	D	252	Total O 252 252	0	0
5	E	252	Total O 252 252	0	0
5	F	266	Total O 266 266	0	0

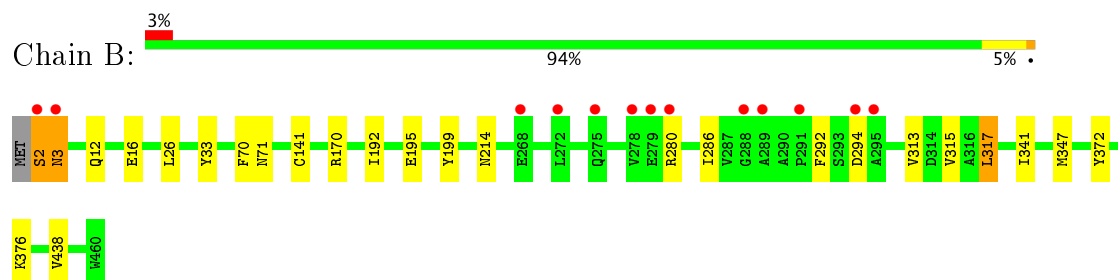
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

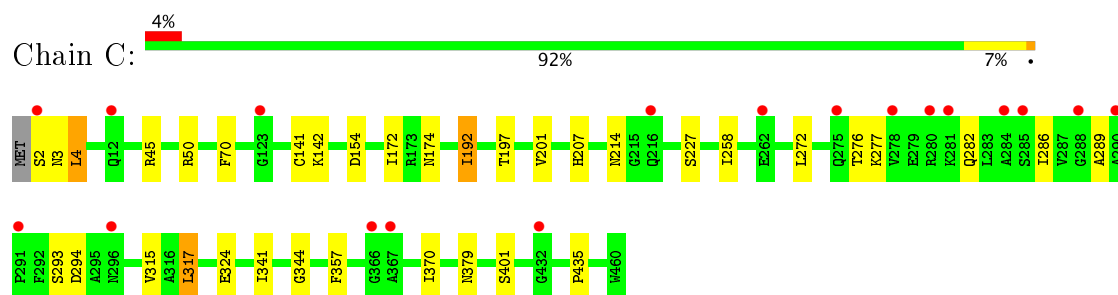
- Molecule 1: Glutamate dehydrogenase



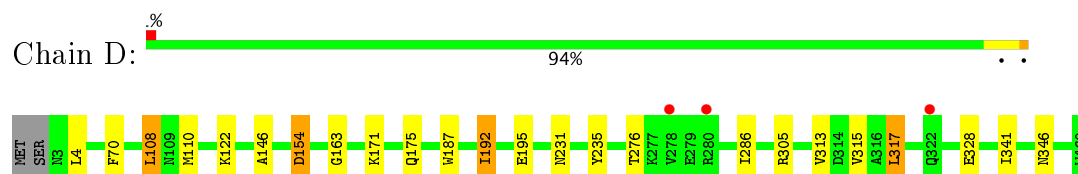
- Molecule 1: Glutamate dehydrogenase



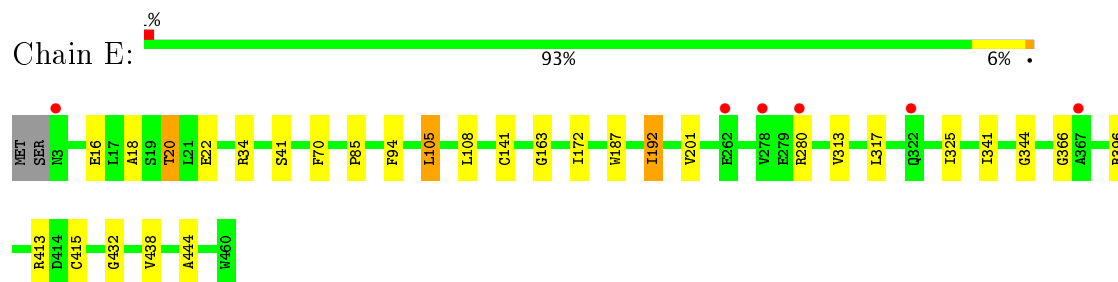
- Molecule 1: Glutamate dehydrogenase



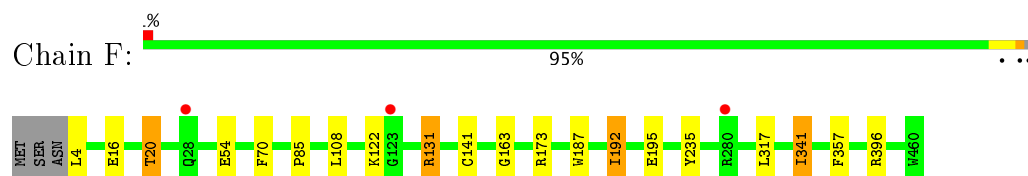
- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.26 Å 92.15 Å 111.06 Å 103.40° 93.95° 120.36°	Depositor
Resolution (Å)	33.00 – 2.25 32.63 – 2.25	Depositor EDS
% Data completeness (in resolution range)	95.5 (33.00-2.25) 84.8 (32.63-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.24 Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.158 , 0.199 0.167 , 0.204	Depositor DCC
R_{free} test set	6786 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	22611	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: GOL, AKG, BME

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	0.56	0/3580	0.73	3/4841 (0.1%)
1	B	0.56	0/3570	0.75	2/4825 (0.0%)
1	C	0.56	0/3564	0.72	3/4818 (0.1%)
1	D	0.56	0/3566	0.72	2/4821 (0.0%)
1	E	0.55	0/3553	0.70	0/4803
1	F	0.56	0/3559	0.72	2/4811 (0.0%)
All	All	0.56	0/21392	0.72	12/28919 (0.0%)

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	B	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	B	170	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	C	45	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	C	45	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	A	170	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	413	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	D	305	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	108	LEU	CA-CB-CG	5.42	127.78	115.30
1	C	50	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	F	131	ARG	NE-CZ-NH1	5.34	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	396	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	280	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	SER	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	3491	0	3437	21	0
1	B	3496	0	3422	14	0
1	C	3484	0	3414	24	0
1	D	3483	0	3420	9	0
1	E	3476	0	3407	18	0
1	F	3479	0	3411	9	0
2	A	42	0	56	3	0
2	B	30	0	40	0	0
2	C	18	0	24	0	0
2	E	24	0	32	0	0
2	F	18	0	24	0	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
3	C	10	0	4	0	0
4	A	4	0	5	0	0
4	B	4	0	5	1	0
4	C	4	0	5	3	0
4	D	4	0	5	0	0
4	E	4	0	6	6	0
4	F	4	0	6	2	0
5	A	279	0	0	1	0
5	B	246	0	0	8	0
5	C	221	0	0	9	0
5	D	252	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	252	0	0	1	0
5	F	266	0	0	1	0
All	All	22611	0	20731	92	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 2.

All (92) 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:E:141[A]:CYS:SG	4:E:505:BME:S2	2.51	1.03
1:D:110:MET:SD	5:D:714:HOH:O	2.20	0.99
1:B:199:TYR:CE1	5:B:712:HOH:O	2.16	0.98
1:A:141[A]:CYS:SG	1:A:172[A]:ILE:HD13	2.02	0.98
1:A:141[A]:CYS:SG	1:A:172[A]:ILE:CD1	2.55	0.95
1:F:141[A]:CYS:SG	4:F:504:BME:S2	2.64	0.89
1:E:172:ILE:HG22	4:E:505:BME:H22	1.61	0.83
1:E:105:LEU:HD12	1:E:415:CYS:SG	2.26	0.75
1:C:172:ILE:HG22	4:E:505:BME:H11	1.74	0.70
1:E:141[B]:CYS:SG	4:E:505:BME:S2	2.67	0.69
1:A:448:LYS:NZ	2:A:503:GOL:O2	2.27	0.67
1:E:172:ILE:CG2	4:E:505:BME:H22	2.24	0.67
1:A:231[A]:ASN:ND2	5:A:601:HOH:O	2.28	0.66
1:A:141[A]:CYS:SG	1:A:172[A]:ILE:HD11	2.39	0.62
1:C:3:ASN:ND2	5:C:602:HOH:O	2.28	0.61
1:B:372:TYR:O	5:B:601:HOH:O	2.16	0.60
1:C:172:ILE:CG2	4:E:505:BME:H11	2.33	0.58
1:C:379:ASN:CG	5:C:601:HOH:O	2.42	0.58
1:A:276:THR:HG21	1:A:286:ILE:HG21	1.85	0.58
1:A:3:ASN:ND2	1:E:85:PRO:O	2.37	0.57
1:E:413:ARG:NH1	5:E:603:HOH:O	2.38	0.56
1:B:2:SER:HA	1:F:85:PRO:O	2.05	0.55
1:A:301:ILE:HD13	1:A:309:HIS:CG	2.42	0.54
1:C:379:ASN:HA	5:C:650:HOH:O	2.07	0.54
1:B:2:SER:N	5:B:603:HOH:O	2.41	0.54
1:C:344:GLY:O	5:C:601:HOH:O	2.18	0.54
1:C:379:ASN:CB	5:C:601:HOH:O	2.56	0.53
1:E:105:LEU:CD1	1:E:415:CYS:SG	2.96	0.52
1:A:272:LEU:O	1:A:276:THR:HG23	2.09	0.51
1:E:192:ILE:O	1:E:192:ILE:HG22	2.11	0.51
1:E:163:GLY:HA2	1:E:187:TRP:CH2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:276:THR:HG21	1:D:286:ILE:HG21	1.93	0.51
1:B:199:TYR:CZ	5:B:712:HOH:O	2.48	0.50
1:C:341:ILE:CD1	1:C:370:ILE:HD11	2.42	0.50
1:A:172[B]:ILE:HG22	4:F:504:BME:H11	1.95	0.49
1:F:16:GLU:O	1:F:20:THR:HG23	2.12	0.49
1:B:141[B]:CYS:SG	4:B:507:BME:S2	2.97	0.49
1:F:54:GLU:O	1:F:131:ARG:HD2	2.12	0.49
1:D:315:VAL:HG12	1:D:317:LEU:HD13	1.95	0.48
1:F:173:ARG:HD2	5:F:717:HOH:O	2.12	0.48
1:B:438:VAL:N	5:B:601:HOH:O	2.46	0.48
1:D:171:LYS:NZ	5:D:604:HOH:O	2.45	0.48
1:B:286:ILE:HD12	1:B:292:PHE:CE2	2.50	0.47
1:B:2:SER:OG	1:B:3:ASN:N	2.47	0.47
1:C:272:LEU:O	1:C:276:THR:HG23	2.14	0.47
1:F:192:ILE:HG22	1:F:192:ILE:O	2.15	0.47
1:E:201:VAL:HG21	1:E:344:GLY:HA2	1.96	0.47
1:D:175:GLN:HB2	5:D:601:HOH:O	2.13	0.47
1:E:16:GLU:O	1:E:20:THR:HG23	2.15	0.46
1:D:146:ALA:O	1:E:396:ARG:NH1	2.48	0.46
1:C:227:SER:OG	1:C:324:GLU:OE2	2.32	0.46
1:D:195:GLU:HG3	1:D:235:TYR:CD1	2.51	0.46
1:B:33:TYR:CE1	5:B:705:HOH:O	2.67	0.46
1:A:201[A]:VAL:HG11	1:A:344:GLY:HA2	1.98	0.45
1:A:287:VAL:HG21	1:A:300:TYR:HB2	1.98	0.45
1:A:3:ASN:OD1	1:A:3:ASN:C	2.54	0.45
1:C:141[B]:CYS:HG	4:C:505:BME:C2	2.30	0.45
1:C:207:HIS:HE1	5:C:625:HOH:O	1.99	0.45
1:F:195:GLU:HG3	1:F:235:TYR:CD1	2.50	0.45
1:D:163:GLY:HA2	1:D:187:TRP:CH2	2.52	0.45
2:A:501:GOL:H32	1:C:174:ASN:OD1	2.17	0.44
1:E:105:LEU:CD2	1:E:444:ALA:HB3	2.47	0.44
1:A:22:GLU:OE2	1:A:34:ARG:NH1	2.51	0.44
1:C:258:ILE:HD12	5:C:655:HOH:O	2.17	0.44
1:C:197:THR:O	1:C:201:VAL:HG23	2.18	0.44
1:E:22:GLU:OE2	1:E:34:ARG:NH1	2.37	0.43
1:E:366:GLY:N	1:E:432:GLY:O	2.50	0.43
1:F:163:GLY:HA2	1:F:187:TRP:CH2	2.53	0.43
1:A:195:GLU:HG3	1:A:235:TYR:CD1	2.54	0.43
1:A:64:ARG:NH1	2:A:506:GOL:O2	2.50	0.43
1:B:315:VAL:HG12	1:B:317:LEU:HD13	2.00	0.42
1:C:276:THR:HG21	1:C:286:ILE:HG21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:VAL:HG12	1:A:317:LEU:HD13	2.02	0.42
1:C:315:VAL:HG12	1:C:317:LEU:HD13	2.02	0.42
1:E:18:ALA:O	1:E:22:GLU:HG2	2.20	0.42
1:A:163:GLY:HA2	1:A:187:TRP:CH2	2.55	0.41
1:B:195:GLU:CG	5:B:712:HOH:O	2.67	0.41
1:A:203:TYR:CZ	1:A:409:LYS:HE3	2.55	0.41
1:D:192:ILE:O	1:D:192:ILE:HG22	2.20	0.41
1:C:192:ILE:HG22	1:C:192:ILE:O	2.21	0.41
1:C:435:PRO:HG3	5:C:646:HOH:O	2.20	0.41
1:A:84:HIS:CG	1:A:85:PRO:HD2	2.55	0.41
1:C:379:ASN:ND2	5:C:601:HOH:O	2.53	0.41
1:E:325:ILE:CD1	1:E:341:ILE:HD11	2.51	0.41
1:F:341:ILE:HD13	1:F:357:PHE:CZ	2.56	0.41
1:C:341:ILE:HD12	1:C:357:PHE:CE1	2.55	0.41
1:A:22:GLU:CD	1:A:34:ARG:HH12	2.24	0.41
1:C:141[B]:CYS:SG	4:C:505:BME:S2	3.08	0.41
1:B:12:GLN:O	1:B:16:GLU:HG3	2.21	0.40
1:C:142:LYS:CG	4:C:505:BME:H12	2.51	0.40
1:B:71:ASN:ND2	5:B:609:HOH:O	2.53	0.40
1:C:2:SER:HB3	1:C:4:LEU:HD13	2.04	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	462/460 (100%)	450 (97%)	10 (2%)	2 (0%)	38	42
1	B	460/460 (100%)	449 (98%)	9 (2%)	2 (0%)	38	42
1	C	460/460 (100%)	443 (96%)	13 (3%)	4 (1%)	20	17
1	D	460/460 (100%)	449 (98%)	9 (2%)	2 (0%)	38	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	458/460 (100%)	444 (97%)	13 (3%)	1 (0%)	51	60
1	F	459/460 (100%)	447 (97%)	11 (2%)	1 (0%)	51	60
All	All	2759/2760 (100%)	2682 (97%)	65 (2%)	12 (0%)	38	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ILE
1	B	294	ASP
1	C	192	ILE
1	B	192	ILE
1	C	294	ASP
1	D	192	ILE
1	F	192	ILE
1	C	154	ASP
1	C	289	ALA
1	D	154	ASP
1	E	192	ILE
1	A	154	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	361/357 (101%)	356 (99%)	5 (1%)	71	81
1	B	359/357 (101%)	349 (97%)	10 (3%)	49	58
1	C	359/357 (101%)	351 (98%)	8 (2%)	57	67
1	D	359/357 (101%)	348 (97%)	11 (3%)	45	55
1	E	357/357 (100%)	347 (97%)	10 (3%)	49	58
1	F	358/357 (100%)	351 (98%)	7 (2%)	60	70
All	All	2153/2142 (100%)	2102 (98%)	51 (2%)	54	64

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	PHE
1	A	108	LEU
1	A	122	LYS
1	A	170	ARG
1	A	317	LEU
1	B	3	ASN
1	B	26	LEU
1	B	70	PHE
1	B	214	ASN
1	B	280	ARG
1	B	313	VAL
1	B	317	LEU
1	B	341	ILE
1	B	347	MET
1	B	376	LYS
1	C	4	LEU
1	C	70	PHE
1	C	214	ASN
1	C	277	LYS
1	C	282	GLN
1	C	293	SER
1	C	317	LEU
1	C	401	SER
1	D	4	LEU
1	D	70	PHE
1	D	108	LEU
1	D	122	LYS
1	D	154	ASP
1	D	231	ASN
1	D	313	VAL
1	D	317	LEU
1	D	328	GLU
1	D	341	ILE
1	D	346	ASN
1	E	20	THR
1	E	41	SER
1	E	70	PHE
1	E	94	PHE
1	E	105	LEU
1	E	108	LEU
1	E	280	ARG
1	E	313	VAL
1	E	317	LEU

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Mol	Chain	Res	Type
1	E	438	VAL
1	F	4	LEU
1	F	20	THR
1	F	70	PHE
1	F	108	LEU
1	F	122	LYS
1	F	317	LEU
1	F	341	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	207	HIS
1	A	214	ASN
1	B	214	ASN
1	B	260	ASN
1	B	442	ASN
1	C	207	HIS
1	C	211	HIS
1	C	379	ASN
1	D	12	GLN
1	E	48	GLN
1	E	331	GLN
1	F	254	GLN
1	F	331	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

31 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	A	501	-	5,5,5	0.19	0	5,5,5	0.72	0
2	GOL	A	502	-	5,5,5	0.44	0	5,5,5	1.32	0
2	GOL	A	503	-	5,5,5	0.43	0	5,5,5	0.44	0
2	GOL	A	504	-	5,5,5	0.42	0	5,5,5	0.55	0
2	GOL	A	505	-	5,5,5	0.27	0	5,5,5	0.36	0
2	GOL	A	506	-	5,5,5	0.67	0	5,5,5	1.08	0
2	GOL	A	507	-	5,5,5	0.19	0	5,5,5	0.36	0
3	AKG	A	508	-	3,9,9	1.11	0	4,11,11	1.47	0
4	BME	A	509	1	3,3,3	0.89	0	2,2,2	0.72	0
2	GOL	B	501	-	5,5,5	0.31	0	5,5,5	0.43	0
2	GOL	B	502	-	5,5,5	0.73	0	5,5,5	1.11	0
2	GOL	B	503	-	5,5,5	0.32	0	5,5,5	0.33	0
2	GOL	B	504	-	5,5,5	0.21	0	5,5,5	0.91	0
2	GOL	B	505	-	5,5,5	0.12	0	5,5,5	0.61	0
3	AKG	B	506	-	3,9,9	0.23	0	4,11,11	1.78	1 (25%)
4	BME	B	507	1	3,3,3	0.44	0	2,2,2	0.24	0
2	GOL	C	501	-	5,5,5	0.28	0	5,5,5	0.39	0
2	GOL	C	502	-	5,5,5	0.19	0	5,5,5	0.33	0
2	GOL	C	503	-	5,5,5	0.48	0	5,5,5	0.53	0
3	AKG	C	504	-	3,9,9	0.61	0	4,11,11	2.29	1 (25%)
4	BME	C	505	1	3,3,3	0.28	0	2,2,2	0.66	0
4	BME	D	501	1	3,3,3	0.37	0	2,2,2	0.41	0
2	GOL	E	501	-	5,5,5	0.49	0	5,5,5	0.98	0
2	GOL	E	502	-	5,5,5	0.39	0	5,5,5	0.23	0
2	GOL	E	503	-	5,5,5	0.58	0	5,5,5	1.12	0
2	GOL	E	504	-	5,5,5	0.31	0	5,5,5	0.48	0
4	BME	E	505	-	3,3,3	0.90	0	2,2,2	1.17	0
2	GOL	F	501	-	5,5,5	0.46	0	5,5,5	0.77	0
2	GOL	F	502	-	5,5,5	0.23	0	5,5,5	0.24	0
2	GOL	F	503	-	5,5,5	0.32	0	5,5,5	0.42	0
4	BME	F	504	-	3,3,3	0.33	0	2,2,2	1.32	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	GOL	A	501	-	-	0/4/4/4	0/0/0/0
2	GOL	A	502	-	-	0/4/4/4	0/0/0/0
2	GOL	A	503	-	-	0/4/4/4	0/0/0/0
2	GOL	A	504	-	-	0/4/4/4	0/0/0/0
2	GOL	A	505	-	-	0/4/4/4	0/0/0/0
2	GOL	A	506	-	-	0/4/4/4	0/0/0/0
2	GOL	A	507	-	-	0/4/4/4	0/0/0/0
3	AKG	A	508	-	-	0/3/9/9	0/0/0/0
4	BME	A	509	1	-	0/1/1/1	0/0/0/0
2	GOL	B	501	-	-	0/4/4/4	0/0/0/0
2	GOL	B	502	-	-	0/4/4/4	0/0/0/0
2	GOL	B	503	-	-	0/4/4/4	0/0/0/0
2	GOL	B	504	-	-	0/4/4/4	0/0/0/0
2	GOL	B	505	-	-	0/4/4/4	0/0/0/0
3	AKG	B	506	-	-	0/3/9/9	0/0/0/0
4	BME	B	507	1	-	0/1/1/1	0/0/0/0
2	GOL	C	501	-	-	0/4/4/4	0/0/0/0
2	GOL	C	502	-	-	0/4/4/4	0/0/0/0
2	GOL	C	503	-	-	0/4/4/4	0/0/0/0
3	AKG	C	504	-	-	0/3/9/9	0/0/0/0
4	BME	C	505	1	-	0/1/1/1	0/0/0/0
4	BME	D	501	1	-	0/1/1/1	0/0/0/0
2	GOL	E	501	-	-	0/4/4/4	0/0/0/0
2	GOL	E	502	-	-	0/4/4/4	0/0/0/0
2	GOL	E	503	-	-	0/4/4/4	0/0/0/0
2	GOL	E	504	-	-	0/4/4/4	0/0/0/0
4	BME	E	505	-	-	0/1/1/1	0/0/0/0
2	GOL	F	501	-	-	0/4/4/4	0/0/0/0
2	GOL	F	502	-	-	0/4/4/4	0/0/0/0
2	GOL	F	503	-	-	0/4/4/4	0/0/0/0
4	BME	F	504	-	-	0/1/1/1	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	504	AKG	C4-C3-C2	-4.35	102.99	113.04
3	B	506	AKG	C3-C4-C5	-2.99	107.55	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	GOL	1	0
2	A	503	GOL	1	0
2	A	506	GOL	1	0
4	B	507	BME	1	0
4	C	505	BME	3	0
4	E	505	BME	6	0
4	F	504	BME	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	458/460 (99%)	-0.46	6 (1%) 77 80	14, 20, 41, 69	0
1	B	459/460 (99%)	-0.33	13 (2%) 53 57	15, 24, 50, 78	0
1	C	459/460 (99%)	-0.28	18 (3%) 40 44	15, 24, 57, 81	0
1	D	458/460 (99%)	-0.49	3 (0%) 87 88	16, 23, 40, 71	0
1	E	458/460 (99%)	-0.46	6 (1%) 77 80	15, 23, 41, 65	0
1	F	457/460 (99%)	-0.46	3 (0%) 87 88	16, 21, 37, 63	0
All	All	2749/2760 (99%)	-0.41	49 (1%) 69 72	14, 23, 44, 81	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	ARG	4.7
1	B	2	SER	4.1
1	B	280	ARG	4.0
1	C	367	ALA	3.9
1	E	280	ARG	3.8
1	B	278	VAL	3.3
1	C	2	SER	3.0
1	A	288	GLY	2.8
1	E	278	VAL	2.8
1	E	367	ALA	2.8
1	C	291	PRO	2.7
1	B	288	GLY	2.7
1	D	278	VAL	2.7
1	E	3	ASN	2.7
1	C	288	GLY	2.7
1	B	291	PRO	2.6
1	F	28	GLN	2.6
1	C	281	LYS	2.6
1	A	280	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	285	SER	2.5
1	C	278	VAL	2.5
1	B	294	ASP	2.5
1	B	272	LEU	2.4
1	C	290	ALA	2.4
1	B	3	ASN	2.4
1	C	296	ASN	2.4
1	B	289	ALA	2.4
1	E	322	GLN	2.3
1	B	295	ALA	2.3
1	C	216	GLN	2.3
1	B	275	GLN	2.2
1	D	280	ARG	2.2
1	D	322	GLN	2.2
1	A	278[A]	VAL	2.2
1	C	262	GLU	2.2
1	B	268	GLU	2.2
1	C	12	GLN	2.2
1	F	123	GLY	2.2
1	C	275	GLN	2.1
1	F	280	ARG	2.1
1	C	284	ALA	2.1
1	B	279	GLU	2.1
1	A	3	ASN	2.1
1	A	100	ILE	2.1
1	E	262	GLU	2.1
1	A	123	GLY	2.1
1	C	432	GLY	2.0
1	C	123	GLY	2.0
1	C	366	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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	E	503	6/6	0.88	0.18	11.80	30,31,32,35	0
2	GOL	B	502	6/6	0.78	0.16	11.65	34,37,38,38	0
4	BME	E	505	4/4	0.78	0.33	11.49	53,53,57,63	0
4	BME	C	505	4/4	0.83	0.29	9.64	52,55,56,56	0
2	GOL	F	501	6/6	0.81	0.21	8.12	39,48,49,54	0
4	BME	F	504	4/4	0.79	0.24	7.99	57,62,65,70	0
4	BME	B	507	4/4	0.90	0.21	7.85	55,56,57,57	0
3	AKG	B	506	10/10	0.68	0.33	7.40	44,56,70,79	1
2	GOL	F	503	6/6	0.80	0.23	6.83	54,58,60,60	0
4	BME	A	509	4/4	0.68	0.26	6.48	53,54,54,57	0
2	GOL	B	503	6/6	0.90	0.24	5.99	59,64,67,72	0
2	GOL	B	504	6/6	0.85	0.17	5.71	36,39,40,42	0
2	GOL	A	502	6/6	0.89	0.21	5.08	33,37,39,42	0
4	BME	D	501	4/4	0.82	0.19	4.96	64,67,68,69	0
2	GOL	B	501	6/6	0.93	0.13	3.95	27,32,36,37	0
2	GOL	E	501	6/6	0.92	0.18	3.75	39,42,44,49	0
2	GOL	A	507	6/6	0.78	0.27	3.14	77,80,82,84	0
2	GOL	C	502	6/6	0.88	0.22	3.12	50,54,56,61	0
2	GOL	A	501	6/6	0.90	0.18	2.96	35,38,41,46	0
2	GOL	E	504	6/6	0.89	0.15	2.53	36,38,39,40	0
3	AKG	A	508	10/10	0.86	0.27	2.49	33,38,50,58	0
3	AKG	C	504	10/10	0.90	0.17	2.47	34,42,51,57	0
2	GOL	A	504	6/6	0.85	0.16	1.97	50,52,54,55	0
2	GOL	B	505	6/6	0.88	0.16	1.95	46,48,49,55	0
2	GOL	E	502	6/6	0.83	0.18	1.59	46,52,53,55	0
2	GOL	C	501	6/6	0.94	0.11	0.73	28,30,32,35	0
2	GOL	A	503	6/6	0.88	0.14	0.43	26,30,34,35	0
2	GOL	A	505	6/6	0.94	0.13	0.14	43,45,47,49	0
2	GOL	A	506	6/6	0.96	0.10	-0.54	39,41,45,46	0
2	GOL	F	502	6/6	0.89	0.33	-	56,57,58,59	0
2	GOL	C	503	6/6	0.78	0.25	-	46,51,53,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.