



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:28 PM UTC

PDB ID : 2OA6 / pdb_00002oa6
Title : Aristolochene synthase from *Aspergillus terreus* complexed with pyrophosphate
Authors : Shishova, E.Y.; Di Costanzo, L.; Cane, D.E.; Christianson, D.W.
Deposited on : 2006-12-15
Resolution : 2.15 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

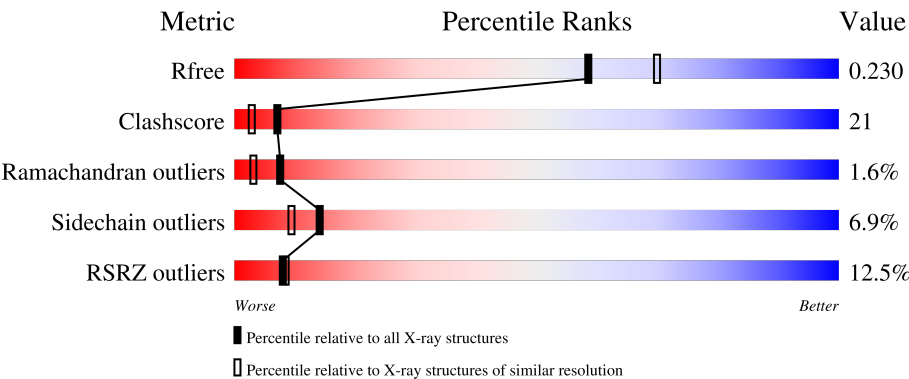
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	320	8% 66% 23% 8%
1	B	320	7% 64% 26% 8%
1	C	320	17% 51% 34% 5% 9%
1	D	320	15% 52% 38% 5%

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	BME	A	1273	-	-	-	X
2	BME	D	1271	-	-	X	-

2 Entry composition [i](#)

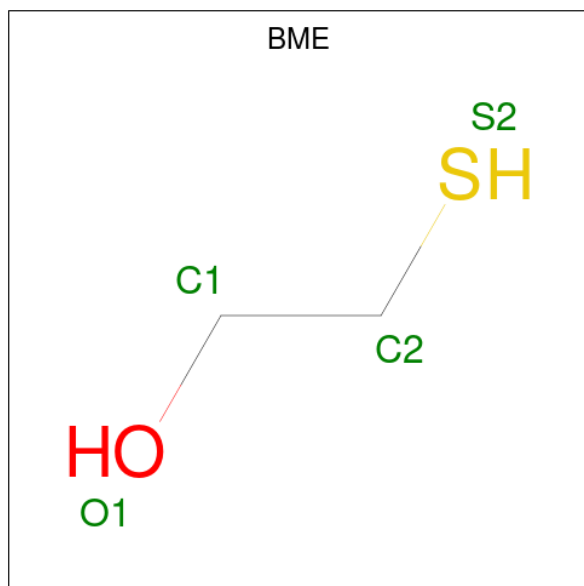
There are 6 unique types of molecules in this entry. The entry contains 9891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Aristolochene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	0	0
			2392	1529	403	445	15			
1	B	295	Total	C	N	O	S	0	0	0
			2393	1531	403	444	15			
1	C	292	Total	C	N	O	S	0	0	0
			2369	1517	398	439	15			
1	D	306	Total	C	N	O	S	0	0	0
			2467	1574	417	461	15			

- Molecule 2 is BETA-MERCAPTOETHANOL (CCD ID: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			4	2	1	1		
2	C	1	Total	C	O	S	0	0
			4	2	1	1		

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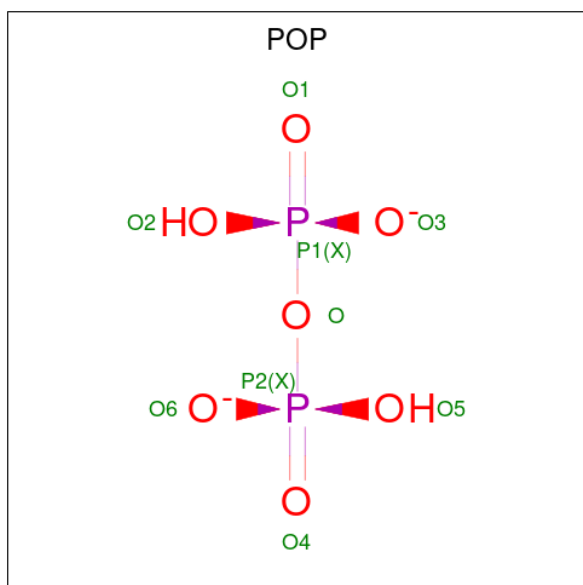
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

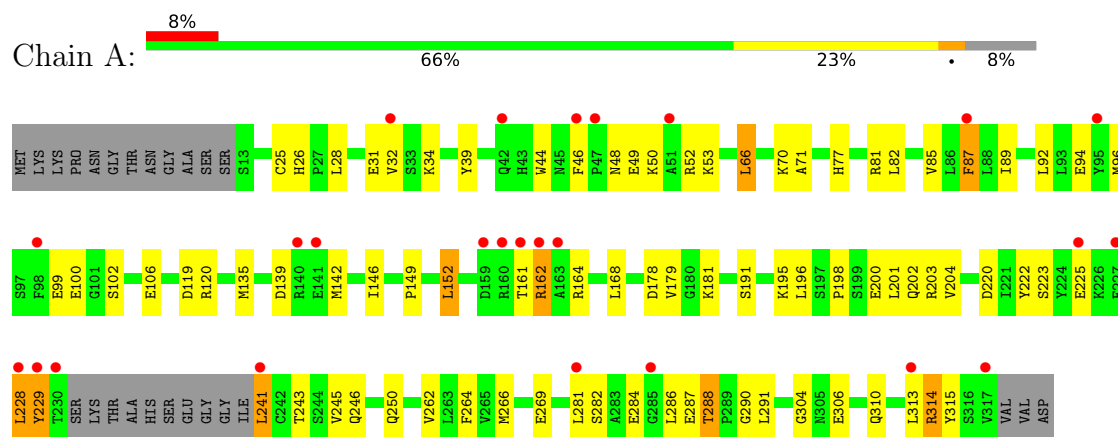
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	62	Total	O	0	0
			62	62		
6	B	65	Total	O	0	0
			65	65		
6	C	44	Total	O	0	0
			44	44		
6	D	65	Total	O	0	0
			65	65		

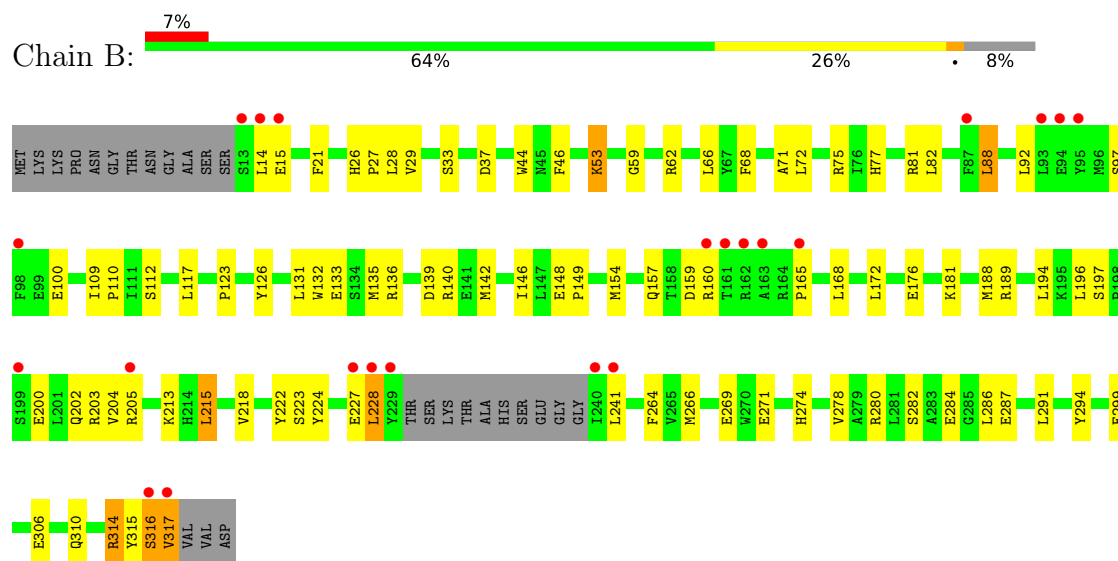
3 Residue-property plots [i](#)

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

• Molecule 1: Aristolochene synthase

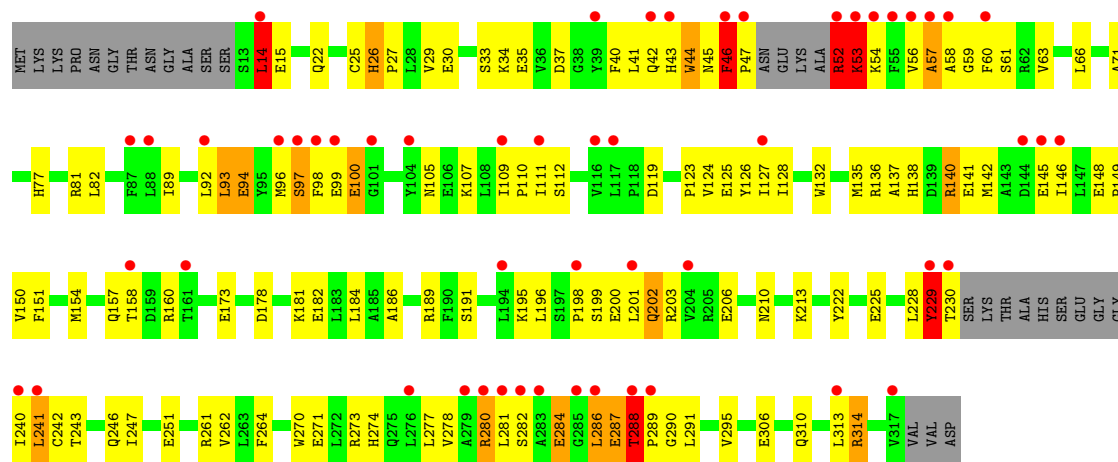


• Molecule 1: Aristolochene synthase

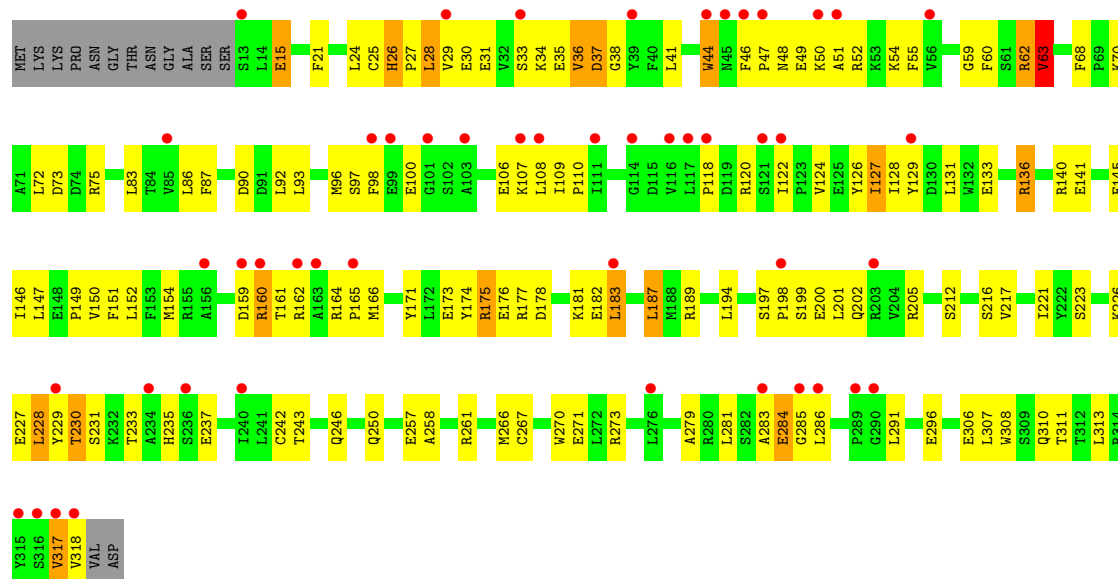


• Molecule 1: Aristolochene synthase





• Molecule 1: Aristolochene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.92Å 147.50Å 82.57Å 90.00° 96.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 50.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.15) 96.3 (50.00-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.273 0.237 , 0.230	Depositor DCC
R_{free} test set	3810 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.3	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9891	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

¹Theoretical 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: POP, GOL, MG, 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	0.50	0/2445	0.92	3/3309 (0.1%)
1	B	0.54	0/2446	0.93	3/3310 (0.1%)
1	C	0.53	1/2421 (0.0%)	0.97	8/3276 (0.2%)
1	D	0.50	0/2522	0.97	13/3414 (0.4%)
All	All	0.52	1/9834 (0.0%)	0.95	27/13309 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	ARG	N-CA	5.50	1.56	1.46

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	GLY	N-CA-C	-7.53	103.77	112.50
1	D	317	VAL	N-CA-C	7.17	117.92	107.75
1	C	100	GLU	N-CA-C	-7.04	103.68	111.36
1	C	46	PHE	C-N-CD	-6.82	97.04	125.00
1	A	26	HIS	CA-C-N	6.74	126.25	119.24
1	A	26	HIS	C-N-CA	6.74	126.25	119.24
1	D	36	VAL	N-CA-C	-6.48	101.20	109.30
1	D	147	LEU	N-CA-C	6.27	118.67	111.02
1	D	26	HIS	CA-C-N	6.04	126.47	119.47
1	D	26	HIS	C-N-CA	6.04	126.47	119.47
1	B	88	LEU	N-CA-C	-5.96	104.70	111.07
1	C	57	ALA	N-CA-C	-5.89	98.25	110.80
1	D	140	ARG	N-CA-C	5.81	117.28	111.07
1	D	284	GLU	N-CA-C	-5.76	101.76	110.28
1	C	26	HIS	CA-C-N	5.72	125.84	119.32
1	C	26	HIS	C-N-CA	5.72	125.84	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	258	ALA	N-CA-C	-5.55	105.31	111.36
1	C	313	LEU	N-CA-C	-5.54	106.02	112.89
1	C	44	TRP	N-CA-C	5.46	118.56	110.48
1	D	127	ILE	N-CA-C	-5.45	105.19	110.42
1	B	224	TYR	N-CA-C	5.34	117.54	111.02
1	D	63	VAL	CB-CA-C	-5.33	104.87	112.22
1	D	73	ASP	N-CA-C	5.27	118.50	111.75
1	C	119	ASP	N-CA-C	-5.27	100.51	108.67
1	B	29	VAL	N-CA-C	5.26	115.89	110.36
1	A	119	ASP	N-CA-C	-5.21	100.59	108.67
1	D	311	THR	N-CA-C	5.03	119.62	112.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2392	0	2365	78	0
1	B	2393	0	2369	78	0
1	C	2369	0	2345	119	0
1	D	2467	0	2439	136	0
2	A	4	0	6	1	0
2	C	4	0	6	1	0
2	D	8	0	12	7	0
3	D	3	0	0	0	0
4	D	9	0	0	0	0
5	D	6	0	8	1	0
6	A	62	0	0	2	0
6	B	65	0	0	1	0
6	C	44	0	0	3	0
6	D	65	0	0	1	0
All	All	9891	0	9550	402	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 21.

All (402) 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:C:47:PRO:HG2	1:C:52:ARG:NH1	1.69	1.08
1:A:288:THR:HG22	1:A:291:LEU:H	1.15	1.07
1:C:47:PRO:HG2	1:C:52:ARG:HH12	1.19	1.05
1:D:150:VAL:HG12	1:D:154:MET:HE2	1.38	1.05
1:A:77:HIS:O	1:A:81:ARG:HG3	1.62	0.98
1:B:77:HIS:HD2	1:B:81:ARG:HE	1.02	0.98
1:D:171:TYR:CZ	1:D:175:ARG:HG3	2.00	0.97
1:D:36:VAL:O	1:D:37:ASP:HB2	1.64	0.95
1:D:242:CYS:SG	2:D:1272:BME:S2	2.56	0.94
1:D:25:CYS:SG	2:D:1271:BME:S2	2.44	0.92
1:C:53:LYS:HA	1:C:53:LYS:HZ1	1.32	0.91
1:B:314:ARG:HH11	1:B:314:ARG:HB2	1.35	0.90
1:D:200:GLU:HB3	1:D:291:LEU:HD11	1.55	0.89
1:D:48:ASN:ND2	1:D:50:LYS:HB3	1.87	0.89
1:B:53:LYS:HE3	1:B:53:LYS:HA	1.53	0.89
1:C:200:GLU:OE2	1:C:288:THR:HG21	1.74	0.88
1:C:140:ARG:H	1:C:140:ARG:HD2	1.39	0.88
1:C:53:LYS:HA	1:C:53:LYS:NZ	1.89	0.87
1:D:150:VAL:HG22	1:D:183:LEU:HD13	1.57	0.86
1:A:200:GLU:OE1	1:A:288:THR:HG21	1.75	0.86
1:D:273:ARG:HG2	1:D:273:ARG:HH11	1.40	0.86
1:A:314:ARG:HH11	1:A:314:ARG:HB2	1.38	0.86
1:B:77:HIS:CD2	1:B:81:ARG:HE	1.93	0.85
1:C:314:ARG:HG2	1:C:314:ARG:HH11	1.41	0.85
1:B:316:SER:O	1:B:317:VAL:HG13	1.76	0.84
1:C:25:CYS:SG	2:C:1270:BME:S2	2.51	0.83
1:A:288:THR:CG2	1:A:291:LEU:H	1.92	0.82
1:C:306:GLU:O	1:C:310:GLN:HG3	1.80	0.82
1:D:197:SER:OG	1:D:200:GLU:HG3	1.80	0.81
1:D:162:ARG:HD3	1:D:174:TYR:OH	1.82	0.80
1:C:140:ARG:HD2	1:C:140:ARG:N	1.98	0.79
1:B:135:MET:HE1	1:B:146:ILE:HD11	1.65	0.78
1:D:223:SER:O	1:D:227:GLU:HG3	1.84	0.78
1:C:150:VAL:HG12	1:C:154:MET:HE2	1.65	0.77
1:B:26:HIS:HD2	1:B:28:LEU:H	1.32	0.77
1:D:97:SER:OG	1:D:100:GLU:HG3	1.85	0.77
1:D:54:LYS:HZ1	1:D:317:VAL:HG11	1.50	0.76
1:D:281:LEU:HD21	1:D:291:LEU:HD23	1.69	0.75
1:A:225:GLU:HB2	6:A:1280:HOH:O	1.86	0.74
1:B:135:MET:CE	1:B:146:ILE:HD11	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:ARG:HB3	1:D:160:ARG:HH11	1.53	0.74
1:A:246:GLN:O	1:A:250:GLN:HG2	1.87	0.73
1:C:241:LEU:HD12	1:C:246:GLN:NE2	2.03	0.73
1:C:280:ARG:O	1:C:284:GLU:HG2	1.89	0.73
1:D:152:LEU:HD21	1:D:177:ARG:CD	2.19	0.72
1:A:77:HIS:HD2	1:A:81:ARG:HD2	1.53	0.72
1:C:135:MET:HE1	1:C:146:ILE:HD11	1.71	0.72
1:D:151:PHE:HD1	1:D:154:MET:CE	2.02	0.72
1:B:77:HIS:HD2	1:B:81:ARG:NE	1.84	0.71
1:D:151:PHE:HD1	1:D:154:MET:HE3	1.56	0.71
1:C:288:THR:HG22	1:C:290:GLY:H	1.56	0.71
1:B:72:LEU:HD12	1:B:75:ARG:HD3	1.73	0.70
1:B:181:LYS:HG3	1:B:215:LEU:HD23	1.72	0.70
1:A:135:MET:HE1	1:A:146:ILE:HD11	1.73	0.70
1:B:194:LEU:HB3	1:B:196:LEU:HD11	1.74	0.70
1:B:223:SER:O	1:B:227:GLU:HG2	1.92	0.70
1:C:98:PHE:CD2	1:C:160:ARG:HG3	2.26	0.70
1:D:93:LEU:HB2	5:D:2647:GOL:H32	1.74	0.70
1:B:197:SER:OG	1:B:200:GLU:HG3	1.92	0.69
1:B:314:ARG:HB2	1:B:314:ARG:NH1	2.07	0.69
1:A:241:LEU:HD23	1:A:241:LEU:O	1.92	0.69
1:A:288:THR:HG22	1:A:291:LEU:N	1.99	0.69
1:C:274:HIS:O	1:C:278:VAL:HG23	1.93	0.69
1:C:52:ARG:HD2	1:C:52:ARG:O	1.93	0.69
1:C:96:MET:HB2	1:C:100:GLU:HB2	1.75	0.69
1:D:48:ASN:HD21	1:D:50:LYS:HB3	1.58	0.69
1:D:228:LEU:O	1:D:231:SER:HB3	1.93	0.68
1:C:146:ILE:C	1:C:149:PRO:HD2	2.19	0.67
1:D:149:PRO:HB3	1:D:182:GLU:HB3	1.76	0.67
1:C:123:PRO:O	1:C:127:ILE:HG22	1.94	0.67
1:C:288:THR:HG22	1:C:290:GLY:N	2.09	0.67
1:D:63:VAL:HG22	1:D:308:TRP:NE1	2.10	0.67
1:C:288:THR:HG23	1:C:289:PRO:HD2	1.77	0.67
1:A:250:GLN:HE21	1:B:165:PRO:HG3	1.61	0.66
1:B:135:MET:HE1	1:B:146:ILE:CD1	2.25	0.66
1:C:189:ARG:CD	1:C:196:LEU:HD23	2.26	0.66
1:D:284:GLU:HB2	1:D:286:LEU:HG	1.77	0.66
1:C:314:ARG:HG2	1:C:314:ARG:NH1	2.07	0.65
1:A:152:LEU:HD22	1:A:179:VAL:HG11	1.79	0.65
1:C:77:HIS:HD2	1:C:81:ARG:HE	1.45	0.64
1:B:282:SER:HB2	1:B:287:GLU:OE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:59:GLY:O	1:D:62:ARG:HG2	1.96	0.64
1:D:273:ARG:HG2	1:D:273:ARG:NH1	2.11	0.64
1:B:194:LEU:HB3	1:B:196:LEU:CD1	2.27	0.64
1:D:141:GLU:CD	1:D:141:GLU:H	2.04	0.64
1:C:107:LYS:O	1:C:110:PRO:HD2	1.98	0.63
1:C:30:GLU:OE2	1:C:34:LYS:HE3	1.98	0.63
1:C:229:TYR:HD2	1:C:229:TYR:C	2.06	0.63
1:D:226:LYS:O	1:D:230:THR:HG23	1.99	0.63
1:A:314:ARG:HB2	1:A:314:ARG:NH1	2.13	0.62
1:C:59:GLY:HA3	1:C:63:VAL:HG23	1.80	0.62
1:D:26:HIS:CE1	1:D:28:LEU:HG	2.34	0.62
1:C:154:MET:HA	1:C:157:GLN:OE1	2.00	0.62
1:D:29:VAL:HG21	2:D:1271:BME:H21	1.82	0.62
1:B:222:TYR:CZ	1:B:310:GLN:HG2	2.34	0.62
1:A:48:ASN:OD1	1:A:50:LYS:HB3	1.99	0.62
1:A:201:LEU:O	1:A:204:VAL:HG12	2.00	0.62
1:C:140:ARG:H	1:C:140:ARG:CD	2.03	0.62
1:D:200:GLU:HB3	1:D:291:LEU:CD1	2.29	0.62
1:C:46:PHE:CD1	1:C:53:LYS:HG2	2.35	0.62
1:C:154:MET:O	1:C:157:GLN:HG2	2.00	0.62
1:A:25:CYS:SG	2:A:1273:BME:S2	2.67	0.62
1:D:226:LYS:HD2	6:D:4357:HOH:O	2.00	0.62
1:D:54:LYS:NZ	1:D:317:VAL:HG11	2.14	0.61
1:B:160:ARG:HG3	1:B:160:ARG:HH11	1.66	0.61
1:B:227:GLU:HB3	1:B:241:LEU:HD11	1.83	0.61
1:D:152:LEU:HD21	1:D:177:ARG:CG	2.31	0.61
1:C:42:GLN:O	1:C:42:GLN:HG3	1.99	0.61
1:C:229:TYR:C	1:C:229:TYR:CD2	2.77	0.61
1:D:161:THR:HG23	1:D:164:ARG:NH1	2.15	0.61
1:A:146:ILE:C	1:A:149:PRO:HD2	2.25	0.61
1:D:98:PHE:CZ	1:D:237:GLU:HB2	2.36	0.61
1:B:181:LYS:HE2	1:B:215:LEU:HB3	1.83	0.61
1:D:107:LYS:HZ3	1:D:108:LEU:HD21	1.66	0.61
1:C:189:ARG:HD2	1:C:196:LEU:HD23	1.81	0.61
1:C:40:PHE:CZ	1:C:127:ILE:HD11	2.36	0.61
1:D:181:LYS:HG2	1:D:212:SER:HB2	1.83	0.61
1:B:109:ILE:HB	1:B:110:PRO:HD3	1.83	0.60
1:A:229:TYR:HD2	1:A:229:TYR:O	1.82	0.60
1:B:97:SER:OG	1:B:100:GLU:HG3	2.00	0.60
1:B:26:HIS:HE1	1:B:71:ALA:O	1.85	0.60
1:C:124:VAL:O	1:C:128:ILE:HG12	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:VAL:HG22	1:D:318:VAL:N	2.16	0.60
1:C:47:PRO:CG	1:C:52:ARG:HH12	2.06	0.60
1:C:247:ILE:O	1:C:251:GLU:HG3	2.02	0.60
1:A:178:ASP:OD2	1:A:181:LYS:HG2	2.02	0.59
1:C:123:PRO:HA	1:C:126:TYR:CE2	2.38	0.59
1:B:112:SER:O	1:B:136:ARG:NH2	2.35	0.59
1:D:107:LYS:NZ	1:D:108:LEU:HD21	2.17	0.59
1:B:53:LYS:HE3	1:B:53:LYS:CA	2.31	0.59
1:D:152:LEU:HD21	1:D:177:ARG:HD2	1.85	0.58
1:C:140:ARG:HG3	1:C:140:ARG:HH11	1.67	0.58
1:D:146:ILE:O	1:D:150:VAL:HG23	2.02	0.58
1:A:313:LEU:N	1:A:313:LEU:HD12	2.18	0.58
1:C:111:ILE:CD1	1:C:125:GLU:HG2	2.33	0.58
1:B:172:LEU:HB3	1:B:213:LYS:HD2	1.86	0.58
1:A:135:MET:CE	1:A:146:ILE:HD11	2.34	0.58
1:A:203:ARG:HD2	1:A:291:LEU:CD1	2.33	0.57
1:D:36:VAL:O	1:D:37:ASP:CB	2.47	0.57
1:C:282:SER:HA	1:C:287:GLU:HG3	1.87	0.57
1:D:98:PHE:CE2	1:D:237:GLU:HB2	2.39	0.57
1:A:164:ARG:NH1	1:C:173:GLU:HG3	2.19	0.57
1:B:82:LEU:HD13	1:B:82:LEU:C	2.30	0.56
1:B:314:ARG:HH11	1:B:314:ARG:CB	2.15	0.56
1:D:151:PHE:HA	1:D:154:MET:HE3	1.87	0.56
1:C:200:GLU:C	1:C:202:GLN:H	2.11	0.56
1:D:151:PHE:CD1	1:D:154:MET:CE	2.87	0.56
1:D:63:VAL:HG13	1:D:308:TRP:CG	2.41	0.56
1:D:171:TYR:CE1	1:D:175:ARG:HG3	2.41	0.56
1:D:29:VAL:HG21	2:D:1271:BME:C2	2.36	0.56
1:D:166:MET:HE3	1:D:171:TYR:HA	1.88	0.56
1:C:89:ILE:O	1:C:93:LEU:HG	2.06	0.55
1:D:124:VAL:O	1:D:128:ILE:HG12	2.06	0.55
1:D:62:ARG:HB2	2:D:1271:BME:H22	1.88	0.55
1:D:63:VAL:HG13	1:D:308:TRP:CD2	2.41	0.55
1:A:44:TRP:HB3	1:A:46:PHE:CE1	2.42	0.55
1:C:41:LEU:HD11	1:C:56:VAL:HG23	1.89	0.55
1:A:203:ARG:HD2	1:A:291:LEU:HD11	1.88	0.55
1:D:54:LYS:CE	1:D:317:VAL:HG11	2.37	0.55
1:B:189:ARG:HD3	1:B:294:TYR:CE1	2.42	0.55
1:A:96:MET:HE3	1:A:100:GLU:OE2	2.07	0.54
1:C:210:ASN:ND2	1:C:273:ARG:HD3	2.22	0.54
1:D:54:LYS:HZ1	1:D:317:VAL:CG1	2.17	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ALA:C	1:C:140:ARG:HH12	2.16	0.54
1:D:317:VAL:CG2	1:D:318:VAL:N	2.69	0.54
1:B:53:LYS:HA	1:B:53:LYS:CE	2.34	0.54
1:C:228:LEU:C	1:C:230:THR:H	2.15	0.54
1:A:66:LEU:HD22	1:A:304:GLY:HA2	1.89	0.54
1:B:204:VAL:HG11	1:B:291:LEU:HD22	1.91	0.54
1:C:111:ILE:HD13	1:C:125:GLU:HG2	1.88	0.54
1:C:138:HIS:HE1	6:C:1305:HOH:O	1.91	0.53
1:D:21:PHE:CE2	1:D:271:GLU:HG2	2.43	0.53
1:D:152:LEU:C	1:D:152:LEU:HD23	2.32	0.53
1:D:37:ASP:O	1:D:41:LEU:HG	2.09	0.53
1:D:96:MET:HB3	1:D:100:GLU:HB2	1.91	0.53
1:D:26:HIS:HE1	1:D:28:LEU:HG	1.70	0.53
1:A:49:GLU:OE2	1:A:53:LYS:HE3	2.07	0.53
1:D:189:ARG:HH12	1:D:201:LEU:CD2	2.22	0.53
1:D:202:GLN:NE2	1:D:205:ARG:NH1	2.57	0.53
1:A:250:GLN:HG3	1:B:165:PRO:HD3	1.91	0.52
1:D:162:ARG:O	2:D:1272:BME:H11	2.09	0.52
1:A:222:TYR:CZ	1:A:310:GLN:HG2	2.44	0.52
1:A:282:SER:O	1:A:284:GLU:O	2.28	0.52
1:D:133:GLU:HA	1:D:136:ARG:HH12	1.74	0.52
1:A:71:ALA:HB1	1:A:191:SER:HB3	1.91	0.52
1:B:21:PHE:CE2	1:B:271:GLU:HG2	2.44	0.52
1:C:44:TRP:HD1	1:C:46:PHE:CG	2.28	0.52
1:D:109:ILE:HB	1:D:110:PRO:HD3	1.92	0.52
1:A:77:HIS:CD2	1:A:81:ARG:HD2	2.41	0.52
1:C:142:MET:HG3	1:C:195:LYS:HE2	1.91	0.52
1:D:141:GLU:CD	1:D:141:GLU:N	2.68	0.52
1:B:88:LEU:O	1:B:92:LEU:HD13	2.10	0.51
1:D:273:ARG:HH11	1:D:273:ARG:CG	2.16	0.51
1:D:63:VAL:HG22	1:D:308:TRP:CE2	2.45	0.51
1:B:59:GLY:O	1:B:62:ARG:HB3	2.11	0.51
1:B:112:SER:HB3	1:B:132:TRP:CD1	2.45	0.51
1:B:133:GLU:OE2	1:B:136:ARG:NH1	2.44	0.51
1:B:316:SER:C	1:B:317:VAL:HG22	2.35	0.51
1:D:257:GLU:HG3	1:D:261:ARG:NH1	2.25	0.51
1:B:176:GLU:HG3	1:B:213:LYS:HD3	1.93	0.51
1:C:140:ARG:HG3	1:C:140:ARG:NH1	2.26	0.51
1:C:230:THR:HG21	1:C:240:ILE:HG21	1.92	0.51
1:D:35:GLU:CD	1:D:35:GLU:H	2.18	0.51
1:D:106:GLU:O	1:D:110:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:GLN:O	1:C:43:HIS:CD2	2.64	0.50
1:C:123:PRO:HB2	6:C:1286:HOH:O	2.10	0.50
1:D:48:ASN:HD22	1:D:50:LYS:HB3	1.75	0.50
1:C:222:TYR:CZ	1:C:310:GLN:HG2	2.47	0.50
1:A:152:LEU:CD2	1:A:179:VAL:HG11	2.41	0.50
1:C:44:TRP:HD1	1:C:46:PHE:CD2	2.29	0.50
1:C:112:SER:O	1:C:136:ARG:NH2	2.45	0.50
1:A:200:GLU:O	1:A:203:ARG:HG2	2.12	0.50
1:B:26:HIS:CD2	1:B:28:LEU:H	2.21	0.50
1:A:282:SER:C	1:A:284:GLU:H	2.20	0.49
1:B:202:GLN:OE1	1:B:205:ARG:CZ	2.60	0.49
1:C:45:ASN:ND2	1:C:123:PRO:HG2	2.28	0.49
1:C:92:LEU:O	1:C:94:GLU:N	2.45	0.49
1:D:31:GLU:O	1:D:35:GLU:OE1	2.30	0.49
1:D:70:LYS:HE2	1:D:296:GLU:OE2	2.13	0.49
1:D:171:TYR:OH	1:D:175:ARG:HD2	2.13	0.49
1:A:39:TYR:CD1	1:A:81:ARG:NH2	2.80	0.49
1:A:66:LEU:HD22	1:A:304:GLY:CA	2.42	0.49
1:A:71:ALA:CB	1:A:191:SER:HB3	2.43	0.49
1:D:160:ARG:HH11	1:D:160:ARG:CB	2.23	0.49
1:D:176:GLU:HA	1:D:212:SER:OG	2.13	0.49
1:D:284:GLU:OE2	1:D:286:LEU:HD11	2.13	0.49
1:A:49:GLU:HA	1:A:52:ARG:HD3	1.93	0.48
1:C:35:GLU:OE2	1:C:81:ARG:NH2	2.42	0.48
1:D:285:GLY:O	1:D:286:LEU:HD23	2.12	0.48
1:C:146:ILE:HA	1:C:149:PRO:HD2	1.93	0.48
1:C:52:ARG:O	1:C:53:LYS:HB2	2.13	0.48
1:C:314:ARG:NH1	1:C:314:ARG:CG	2.76	0.48
1:D:68:PHE:CE1	1:D:187:LEU:HD13	2.49	0.48
1:C:189:ARG:HD3	1:C:196:LEU:HD23	1.94	0.48
1:A:70:LYS:HB2	6:A:1300:HOH:O	2.13	0.48
1:C:59:GLY:O	1:C:61:SER:N	2.46	0.48
1:D:217:VAL:O	1:D:221:ILE:HG13	2.13	0.48
1:A:288:THR:HG23	1:A:290:GLY:N	2.28	0.48
1:B:68:PHE:CE2	1:B:188:MET:HB2	2.48	0.48
1:B:72:LEU:HD12	1:B:75:ARG:CD	2.43	0.47
1:B:316:SER:O	1:B:317:VAL:CG1	2.57	0.47
1:D:273:ARG:NH1	1:D:273:ARG:CG	2.74	0.47
1:B:203:ARG:HD2	1:B:286:LEU:HD13	1.96	0.47
1:B:135:MET:HE2	1:B:146:ILE:HD11	1.95	0.47
1:B:203:ARG:NE	1:B:286:LEU:HB3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:ILE:HB	1:C:110:PRO:HD3	1.97	0.47
1:C:281:LEU:HD21	1:C:291:LEU:HD13	1.97	0.47
1:D:175:ARG:NH2	1:D:178:ASP:OD2	2.42	0.47
1:C:29:VAL:HG13	1:C:30:GLU:N	2.30	0.47
1:D:54:LYS:NZ	1:D:317:VAL:HG21	2.29	0.47
1:A:282:SER:C	1:A:284:GLU:N	2.69	0.46
1:B:269:GLU:OE2	1:C:261:ARG:HD2	2.15	0.46
1:A:250:GLN:CG	1:B:165:PRO:HD3	2.44	0.46
1:C:46:PHE:CD2	1:C:46:PHE:N	2.84	0.46
1:D:267:CYS:HA	1:D:270:TRP:CE3	2.50	0.46
1:D:284:GLU:O	1:D:286:LEU:N	2.48	0.46
1:A:99:GLU:H	1:A:99:GLU:CD	2.24	0.46
1:A:142:MET:HE2	1:A:195:LYS:NZ	2.30	0.46
1:D:136:ARG:HH11	1:D:136:ARG:HB2	1.80	0.46
1:C:198:PRO:O	1:C:202:GLN:HB2	2.16	0.46
1:D:175:ARG:HD3	1:D:216:SER:HB3	1.98	0.46
1:D:54:LYS:HZ1	1:D:317:VAL:CB	2.29	0.46
1:B:306:GLU:O	1:B:310:GLN:HG3	2.15	0.45
1:C:141:GLU:O	1:C:145:GLU:HG2	2.17	0.45
1:C:278:VAL:HG22	1:C:295:VAL:HG11	1.97	0.45
1:B:160:ARG:HG3	1:B:160:ARG:NH1	2.31	0.45
1:D:33:SER:O	1:D:36:VAL:O	2.34	0.45
1:A:28:LEU:O	1:A:32:VAL:HG23	2.16	0.45
1:B:154:MET:O	1:B:157:GLN:HB2	2.16	0.45
1:C:98:PHE:HD2	1:C:158:THR:O	1.99	0.45
1:B:148:GLU:HB2	1:B:149:PRO:HD3	1.98	0.45
1:D:120:ARG:NH1	1:D:126:TYR:HB2	2.31	0.45
1:A:135:MET:HE1	1:A:146:ILE:CD1	2.43	0.45
1:D:152:LEU:C	1:D:152:LEU:CD2	2.89	0.45
1:A:281:LEU:HD13	1:A:286:LEU:HB2	1.97	0.45
1:C:14:LEU:C	1:C:14:LEU:HD23	2.42	0.45
1:D:235:HIS:CE1	1:D:237:GLU:HG2	2.51	0.45
1:D:160:ARG:H	1:D:160:ARG:HG2	1.35	0.45
1:D:306:GLU:O	1:D:310:GLN:HG3	2.17	0.45
1:A:306:GLU:O	1:A:310:GLN:HG3	2.17	0.45
1:C:71:ALA:HB1	1:C:191:SER:HB3	1.99	0.45
1:B:123:PRO:HA	1:B:126:TYR:CE2	2.52	0.44
1:B:139:ASP:OD1	1:B:142:MET:HG3	2.17	0.44
1:C:97:SER:OG	1:C:100:GLU:HG3	2.17	0.44
1:C:271:GLU:O	1:C:274:HIS:HB3	2.16	0.44
1:C:151:PHE:HD1	1:C:154:MET:HE3	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLU:HB3	1:C:277:LEU:HD13	1.99	0.44
1:D:31:GLU:O	1:D:34:LYS:HB2	2.17	0.44
1:C:93:LEU:HD11	1:C:105:ASN:HD21	1.80	0.44
1:D:133:GLU:HA	1:D:136:ARG:NH1	2.33	0.44
1:B:140:ARG:O	1:B:140:ARG:HG2	2.17	0.44
1:D:201:LEU:N	1:D:201:LEU:HD12	2.33	0.44
1:C:213:LYS:HE3	1:C:270:TRP:CE2	2.52	0.44
1:D:150:VAL:CG2	1:D:183:LEU:HD13	2.39	0.44
1:D:197:SER:C	1:D:199:SER:H	2.26	0.44
1:A:198:PRO:O	1:A:202:GLN:HG2	2.17	0.44
1:B:21:PHE:CZ	1:B:299:GLU:HG3	2.53	0.44
1:C:146:ILE:CA	1:C:149:PRO:HD2	2.47	0.44
1:C:287:GLU:O	1:C:288:THR:CB	2.66	0.44
1:D:60:PHE:O	1:D:63:VAL:HG23	2.18	0.44
1:A:31:GLU:H	1:A:31:GLU:CD	2.26	0.43
1:B:274:HIS:O	1:B:278:VAL:HG23	2.18	0.43
1:C:199:SER:O	1:C:203:ARG:HG3	2.16	0.43
1:A:142:MET:HE2	1:A:195:LYS:HG3	1.98	0.43
1:A:250:GLN:NE2	1:B:165:PRO:HG3	2.29	0.43
1:C:97:SER:C	1:C:99:GLU:H	2.26	0.43
1:C:229:TYR:CD2	1:C:229:TYR:O	2.71	0.43
1:D:46:PHE:CD2	1:D:52:ARG:NH1	2.86	0.43
1:D:60:PHE:HA	1:D:63:VAL:HG23	1.99	0.43
1:C:109:ILE:HG23	1:C:151:PHE:CE1	2.53	0.43
1:C:127:ILE:HG23	1:C:128:ILE:N	2.34	0.43
1:D:229:TYR:CZ	1:D:233:THR:HG21	2.53	0.43
1:B:280:ARG:O	1:B:284:GLU:HG3	2.19	0.43
1:A:85:VAL:O	1:A:89:ILE:HG13	2.18	0.43
1:A:161:THR:O	1:A:162:ARG:HB3	2.17	0.43
1:D:150:VAL:CG1	1:D:154:MET:HE2	2.29	0.43
1:B:218:VAL:HG11	1:B:306:GLU:HA	2.00	0.43
1:C:288:THR:CG2	1:C:290:GLY:H	2.29	0.43
1:A:220:ASP:HB3	1:A:245:VAL:HG23	2.00	0.43
1:B:181:LYS:HD2	1:B:181:LYS:N	2.33	0.43
1:C:33:SER:O	1:C:37:ASP:HB2	2.19	0.43
1:C:178:ASP:O	1:C:182:GLU:HG3	2.18	0.43
1:A:228:LEU:O	1:A:229:TYR:HB3	2.19	0.43
1:A:223:SER:HB3	1:A:315:TYR:CE1	2.54	0.43
1:A:284:GLU:HB3	1:A:286:LEU:HG	2.01	0.43
1:D:159:ASP:O	1:D:162:ARG:HG2	2.18	0.43
1:A:229:TYR:C	1:A:229:TYR:CD2	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:GLU:C	1:C:286:LEU:H	2.27	0.42
1:D:52:ARG:O	1:D:55:PHE:HB3	2.19	0.42
1:D:68:PHE:HE1	1:D:187:LEU:HD13	1.83	0.42
1:A:288:THR:HG23	1:A:290:GLY:H	1.83	0.42
1:B:316:SER:O	1:B:317:VAL:HG22	2.19	0.42
1:C:124:VAL:HA	1:C:127:ILE:CG2	2.50	0.42
1:D:118:PRO:HD3	1:D:129:TYR:CG	2.53	0.42
1:A:102:SER:O	1:A:106:GLU:HB2	2.18	0.42
1:A:139:ASP:OD2	1:A:142:MET:HE3	2.18	0.42
1:C:136:ARG:O	1:C:140:ARG:HG3	2.18	0.42
1:C:178:ASP:OD2	1:C:181:LYS:HG2	2.18	0.42
1:D:29:VAL:HG13	1:D:30:GLU:N	2.33	0.42
1:D:72:LEU:HD12	1:D:75:ARG:HD3	2.01	0.42
1:D:122:ILE:HG22	1:D:124:VAL:HG12	2.01	0.42
1:A:281:LEU:HD12	1:A:287:GLU:HA	2.00	0.42
1:B:44:TRP:HB3	1:B:46:PHE:CE1	2.54	0.42
1:C:46:PHE:HA	1:C:47:PRO:HD2	1.47	0.42
1:C:146:ILE:HG22	1:C:186:ALA:HB1	2.01	0.42
1:D:25:CYS:SG	2:D:1271:BME:C2	3.07	0.42
1:A:266:MET:O	1:A:269:GLU:HB2	2.19	0.42
1:C:132:TRP:O	1:C:136:ARG:HG3	2.18	0.42
1:C:200:GLU:HB3	1:C:291:LEU:HD21	2.02	0.42
1:D:26:HIS:HA	1:D:27:PRO:HD3	1.75	0.42
1:D:197:SER:HG	1:D:200:GLU:HG3	1.83	0.42
1:C:206:GLU:HB3	1:C:277:LEU:CD1	2.49	0.42
1:D:205:ARG:HH11	1:D:205:ARG:HG3	1.85	0.42
1:D:189:ARG:HH12	1:D:201:LEU:HD21	1.84	0.42
1:A:87:PHE:HD2	1:A:87:PHE:HA	1.69	0.42
1:C:14:LEU:C	1:C:14:LEU:CD2	2.92	0.42
1:A:250:GLN:HE21	1:B:165:PRO:CG	2.32	0.41
1:B:26:HIS:CD2	1:B:27:PRO:HD2	2.55	0.41
1:C:284:GLU:O	1:C:286:LEU:N	2.46	0.41
1:D:44:TRP:HD1	1:D:127:ILE:HD12	1.85	0.41
1:D:152:LEU:HD21	1:D:177:ARG:HG2	2.01	0.41
1:D:164:ARG:HB2	1:D:165:PRO:HD2	2.02	0.41
1:D:197:SER:O	1:D:199:SER:N	2.53	0.41
1:A:201:LEU:HA	1:A:204:VAL:HG12	2.02	0.41
1:D:47:PRO:HD2	1:D:51:ALA:CB	2.50	0.41
1:D:49:GLU:HA	1:D:52:ARG:HG2	2.02	0.41
1:A:284:GLU:C	1:A:286:LEU:H	2.27	0.41
1:C:281:LEU:O	1:C:284:GLU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLU:HA	1:B:136:ARG:NH1	2.36	0.41
1:D:15:GLU:OE1	1:D:15:GLU:HA	2.21	0.41
1:D:63:VAL:HG22	1:D:308:TRP:CD1	2.54	0.41
1:B:266:MET:HE2	1:C:262:VAL:HG11	2.02	0.41
1:B:266:MET:HE3	1:B:266:MET:HB2	1.90	0.41
1:C:124:VAL:C	1:C:127:ILE:HG22	2.46	0.41
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.85	0.41
1:C:97:SER:C	1:C:99:GLU:N	2.78	0.41
1:D:246:GLN:O	1:D:250:GLN:HG3	2.20	0.41
1:B:59:GLY:HA2	6:B:331:HOH:O	2.20	0.41
1:C:26:HIS:ND1	1:C:27:PRO:HD2	2.36	0.41
1:C:240:ILE:HG22	1:C:241:LEU:N	2.36	0.41
1:D:44:TRP:HD1	1:D:127:ILE:CD1	2.34	0.41
1:D:152:LEU:CD2	1:D:177:ARG:HB3	2.51	0.41
1:D:175:ARG:O	1:D:176:GLU:C	2.63	0.41
1:D:176:GLU:HG3	1:D:212:SER:OG	2.21	0.41
1:A:288:THR:HG22	1:A:291:LEU:HB2	2.03	0.41
1:A:313:LEU:HD12	1:A:313:LEU:H	1.82	0.41
1:B:146:ILE:C	1:B:149:PRO:HD2	2.46	0.41
1:B:223:SER:HB3	1:B:315:TYR:CZ	2.56	0.41
1:C:58:ALA:O	1:C:59:GLY:C	2.63	0.41
1:D:146:ILE:HG22	1:D:150:VAL:HG23	2.03	0.41
1:A:99:GLU:CD	1:A:99:GLU:N	2.79	0.40
1:B:203:ARG:HE	1:B:286:LEU:HB3	1.84	0.40
1:A:262:VAL:HG21	1:D:266:MET:HE2	2.03	0.40
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.84	0.40
1:C:225:GLU:HG2	6:C:1299:HOH:O	2.20	0.40
1:D:87:PHE:O	1:D:90:ASP:HB3	2.21	0.40
1:A:142:MET:HE2	1:A:195:LYS:HZ2	1.87	0.40
1:A:229:TYR:HD2	1:A:229:TYR:C	2.30	0.40
1:C:282:SER:CA	1:C:287:GLU:HG3	2.50	0.40
1:A:39:TYR:CG	1:A:81:ARG:NH2	2.90	0.40
1:B:33:SER:O	1:B:37:ASP:HB2	2.21	0.40
1:D:279:ALA:O	1:D:283:ALA:N	2.45	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	291/320 (91%)	280 (96%)	9 (3%)	2 (1%)	18	13
1	B	291/320 (91%)	284 (98%)	6 (2%)	1 (0%)	36	34
1	C	286/320 (89%)	261 (91%)	11 (4%)	14 (5%)	1	0
1	D	304/320 (95%)	289 (95%)	13 (4%)	2 (1%)	18	13
All	All	1172/1280 (92%)	1114 (95%)	39 (3%)	19 (2%)	7	3

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	54	LYS
1	C	57	ALA
1	C	93	LEU
1	C	288	THR
1	D	37	ASP
1	C	53	LYS
1	C	60	PHE
1	C	287	GLU
1	C	241	LEU
1	C	284	GLU
1	C	286	LEU
1	A	162	ARG
1	C	14	LEU
1	C	229	TYR
1	C	242	CYS
1	A	120	ARG
1	C	201	LEU
1	B	316	SER
1	D	198	PRO

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	260/279 (93%)	244 (94%)	16 (6%)	16	12
1	B	260/279 (93%)	247 (95%)	13 (5%)	22	18
1	C	258/279 (92%)	238 (92%)	20 (8%)	11	7
1	D	268/279 (96%)	245 (91%)	23 (9%)	10	5
All	All	1046/1116 (94%)	974 (93%)	72 (7%)	14	9

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	66	LEU
1	A	82	LEU
1	A	87	PHE
1	A	92	LEU
1	A	94	GLU
1	A	152	LEU
1	A	168	LEU
1	A	196	LEU
1	A	228	LEU
1	A	229	TYR
1	A	241	LEU
1	A	243	THR
1	A	264	PHE
1	A	288	THR
1	A	314	ARG
1	B	14	LEU
1	B	15	GLU
1	B	53	LYS
1	B	66	LEU
1	B	117	LEU
1	B	131	LEU
1	B	159	ASP
1	B	168	LEU

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Mol	Chain	Res	Type
1	B	215	LEU
1	B	228	LEU
1	B	264	PHE
1	B	314	ARG
1	B	317	VAL
1	C	14	LEU
1	C	15	GLU
1	C	22	GLN
1	C	46	PHE
1	C	52	ARG
1	C	53	LYS
1	C	66	LEU
1	C	82	LEU
1	C	94	GLU
1	C	97	SER
1	C	140	ARG
1	C	148	GLU
1	C	184	LEU
1	C	202	GLN
1	C	229	TYR
1	C	243	THR
1	C	264	PHE
1	C	280	ARG
1	C	288	THR
1	C	314	ARG
1	D	15	GLU
1	D	24	LEU
1	D	28	LEU
1	D	44	TRP
1	D	62	ARG
1	D	63	VAL
1	D	83	LEU
1	D	86	LEU
1	D	92	LEU
1	D	131	LEU
1	D	136	ARG
1	D	145	GLU
1	D	160	ARG
1	D	173	GLU
1	D	175	ARG
1	D	183	LEU
1	D	187	LEU

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Mol	Chain	Res	Type
1	D	194	LEU
1	D	228	LEU
1	D	230	THR
1	D	243	THR
1	D	307	LEU
1	D	313	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	219	ASN
1	A	250	GLN
1	A	301	GLN
1	A	305	ASN
1	B	26	HIS
1	B	42	GLN
1	B	77	HIS
1	B	210	ASN
1	B	219	ASN
1	C	22	GLN
1	C	45	ASN
1	C	77	HIS
1	C	138	HIS
1	C	210	ASN
1	C	219	ASN
1	C	246	GLN
1	C	250	GLN
1	D	22	GLN
1	D	42	GLN
1	D	202	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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	BME	C	1270	-	3,3,3	0.19	0	2,2,2	0.92	0
2	BME	D	1271	-	3,3,3	0.40	0	2,2,2	0.97	0
5	GOL	D	2647	3	5,5,5	0.65	0	5,5,5	0.42	0
2	BME	D	1272	-	3,3,3	0.64	0	2,2,2	0.67	0
4	POP	D	4293	3	6,8,8	1.12	0	12,13,13	0.92	1 (8%)
2	BME	A	1273	-	3,3,3	0.51	0	2,2,2	0.29	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	BME	C	1270	-	-	0/1/1/1	-
2	BME	D	1271	-	-	0/1/1/1	-
5	GOL	D	2647	3	-	0/4/4/4	-
2	BME	D	1272	-	-	0/1/1/1	-
4	POP	D	4293	3	-	0/6/6/6	-
2	BME	A	1273	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4293	POP	O5-P2-O	2.06	111.55	104.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1270	BME	1	0
2	D	1271	BME	5	0
5	D	2647	GOL	1	0
2	D	1272	BME	2	0
2	A	1273	BME	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/320 (92%)	0.57	25 (8%) 16 18	24, 38, 65, 79	0
1	B	295/320 (92%)	0.43	22 (7%) 20 23	24, 37, 63, 80	0
1	C	292/320 (91%)	1.09	53 (18%) 3 4	23, 46, 76, 90	0
1	D	306/320 (95%)	1.10	49 (16%) 5 5	23, 46, 69, 81	0
All	All	1188/1280 (92%)	0.80	149 (12%) 8 8	23, 41, 70, 90	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	47	PRO	7.5
1	C	286	LEU	6.7
1	C	46	PHE	5.9
1	D	46	PHE	5.6
1	A	317	VAL	5.6
1	D	114	GLY	5.4
1	D	318	VAL	5.3
1	C	98	PHE	5.2
1	C	52	ARG	5.2
1	A	98	PHE	5.1
1	B	229	TYR	4.9
1	A	229	TYR	4.7
1	C	240	ILE	4.5
1	C	229	TYR	4.3
1	C	241	LEU	4.2
1	C	60	PHE	4.2
1	B	317	VAL	4.2
1	A	230	THR	4.1
1	B	240	ILE	4.1
1	D	117	LEU	4.0
1	C	230	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	57	ALA	3.7
1	A	241	LEU	3.7
1	A	87	PHE	3.7
1	C	56	VAL	3.6
1	C	317	VAL	3.5
1	D	160	ARG	3.5
1	C	116	VAL	3.4
1	D	317	VAL	3.4
1	C	288	THR	3.4
1	D	234	ALA	3.4
1	A	160	ARG	3.3
1	B	161	THR	3.3
1	D	116	VAL	3.3
1	B	162	ARG	3.3
1	C	54	LYS	3.3
1	B	228	LEU	3.2
1	A	47	PRO	3.2
1	D	122	ILE	3.1
1	C	53	LYS	3.1
1	C	283	ALA	3.1
1	D	240	ILE	3.1
1	D	44	TRP	3.1
1	C	87	PHE	3.1
1	B	165	PRO	3.1
1	B	205	ARG	3.1
1	C	96	MET	3.1
1	D	315	TYR	3.0
1	A	227	GLU	3.0
1	D	159	ASP	3.0
1	D	162	ARG	2.9
1	C	55	PHE	2.9
1	B	316	SER	2.9
1	D	45	ASN	2.9
1	C	198	PRO	2.9
1	B	98	PHE	2.9
1	D	236	SER	2.9
1	D	283	ALA	2.9
1	C	281	LEU	2.8
1	C	289	PRO	2.8
1	B	160	ARG	2.8
1	D	101	GLY	2.8
1	A	161	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	87	PHE	2.8
1	C	161	THR	2.7
1	C	127	ILE	2.7
1	D	13	SER	2.7
1	D	99	GLU	2.7
1	A	163	ALA	2.7
1	B	241	LEU	2.7
1	D	198	PRO	2.7
1	B	163	ALA	2.7
1	D	156	ALA	2.7
1	C	92	LEU	2.7
1	D	286	LEU	2.6
1	C	97	SER	2.6
1	C	101	GLY	2.6
1	C	201	LEU	2.6
1	D	50	LYS	2.6
1	D	108	LEU	2.6
1	D	47	PRO	2.6
1	D	276	LEU	2.6
1	A	51	ALA	2.5
1	C	276	LEU	2.5
1	C	109	ILE	2.5
1	C	111	ILE	2.5
1	D	111	ILE	2.5
1	A	225	GLU	2.5
1	B	93	LEU	2.5
1	D	290	GLY	2.5
1	C	204	VAL	2.4
1	C	158	THR	2.4
1	D	316	SER	2.4
1	D	289	PRO	2.4
1	C	88	LEU	2.4
1	D	33	SER	2.4
1	C	58	ALA	2.4
1	D	183	LEU	2.4
1	C	99	GLU	2.4
1	A	46	PHE	2.4
1	D	107	LYS	2.4
1	D	163	ALA	2.3
1	A	159	ASP	2.3
1	A	162	ARG	2.3
1	C	282	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	95	TYR	2.3
1	D	229	TYR	2.3
1	D	203	ARG	2.3
1	C	279	ALA	2.3
1	D	51	ALA	2.3
1	B	14	LEU	2.3
1	C	144	ASP	2.3
1	D	165	PRO	2.3
1	C	117	LEU	2.3
1	A	95	TYR	2.3
1	D	121	SER	2.2
1	B	94	GLU	2.2
1	D	285	GLY	2.2
1	A	141	GLU	2.2
1	B	227	GLU	2.2
1	C	194	LEU	2.2
1	B	199	SER	2.2
1	D	118	PRO	2.2
1	A	285	GLY	2.2
1	C	145	GLU	2.2
1	D	85	VAL	2.1
1	A	42	GLN	2.1
1	C	43	HIS	2.1
1	D	56	VAL	2.1
1	A	140	ARG	2.1
1	C	313	LEU	2.1
1	D	129	TYR	2.1
1	D	98	PHE	2.1
1	A	32	VAL	2.1
1	D	29	VAL	2.1
1	D	103	ALA	2.1
1	C	14	LEU	2.1
1	B	15	GLU	2.1
1	C	146	ILE	2.1
1	A	228	LEU	2.0
1	A	281	LEU	2.0
1	A	313	LEU	2.0
1	C	42	GLN	2.0
1	C	280	ARG	2.0
1	C	39	TYR	2.0
1	C	104	TYR	2.0
1	C	285	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	13	SER	2.0
1	D	39	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BME	A	1273	4/4	0.65	0.51	54,55,55,55	4
2	BME	D	1271	4/4	0.86	0.20	50,50,50,52	0
2	BME	D	1272	4/4	0.88	0.17	53,57,57,57	0
2	BME	C	1270	4/4	0.90	0.15	47,48,51,53	0
5	GOL	D	2647	6/6	0.91	0.16	46,49,50,51	0
3	MG	D	703	1/1	0.93	0.07	38,38,38,38	0
3	MG	D	701	1/1	0.97	0.06	56,56,56,56	0
4	POP	D	4293	9/9	0.97	0.06	36,39,39,39	0
3	MG	D	702	1/1	0.97	0.06	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.