



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 03:07 PM EST

PDB ID : 2OA6  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

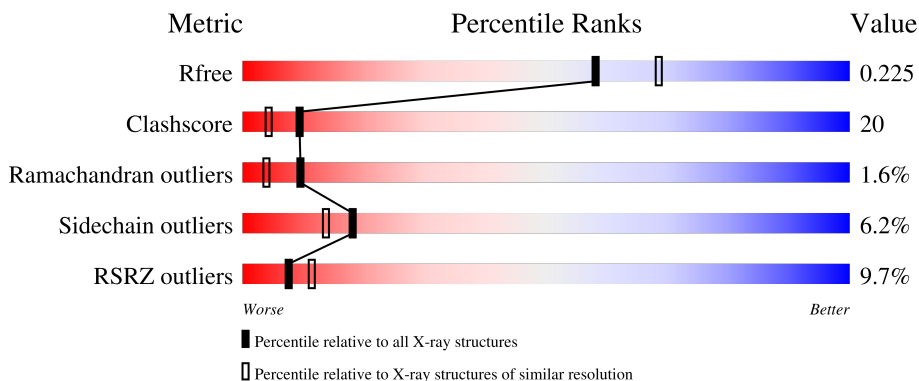
# 1 Overall quality at a glance i

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))
$R_{free}$	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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  $\geq 3$ , 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	 6% 68% 21% 8%
1	B	320	 5% 64% 26% 8%
1	C	320	 11% 53% 33% 9%
1	D	320	 14% 55% 38% 8%

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](#)

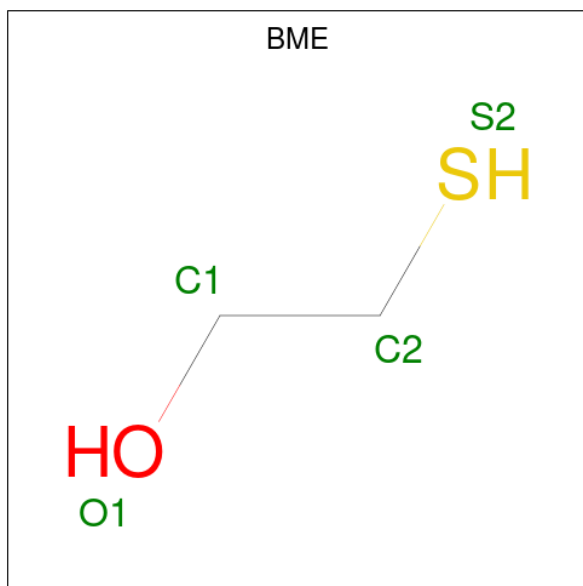
There are 6 unique types of molecules in this entry. The entry contains 9891 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

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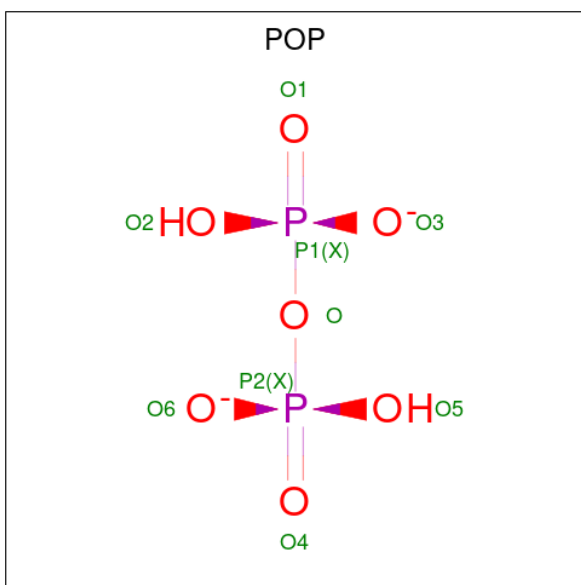
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	O	S	0	0
			4	2	1	1		
2	D	1	Total	C	O	S	0	0
			4	2	1	1		

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

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

- Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H<sub>2</sub>O<sub>7</sub>P<sub>2</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

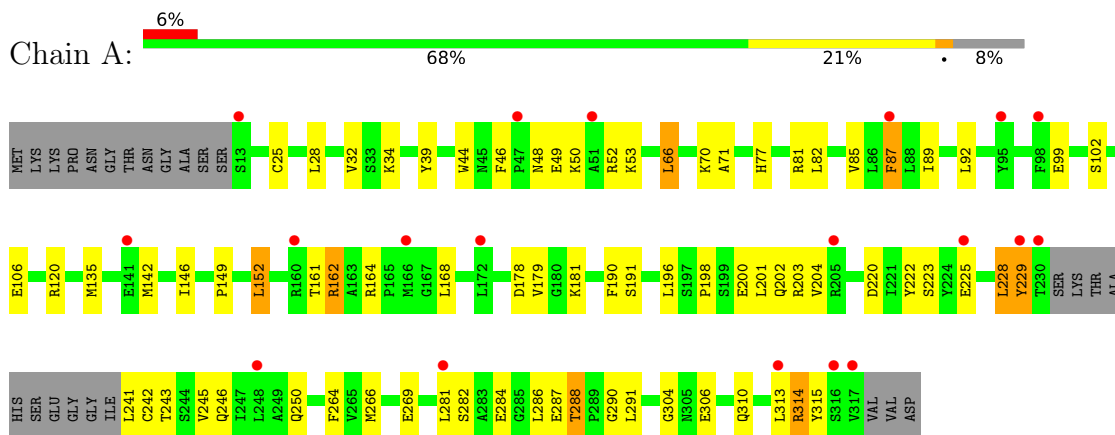
- Molecule 6 is water.

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

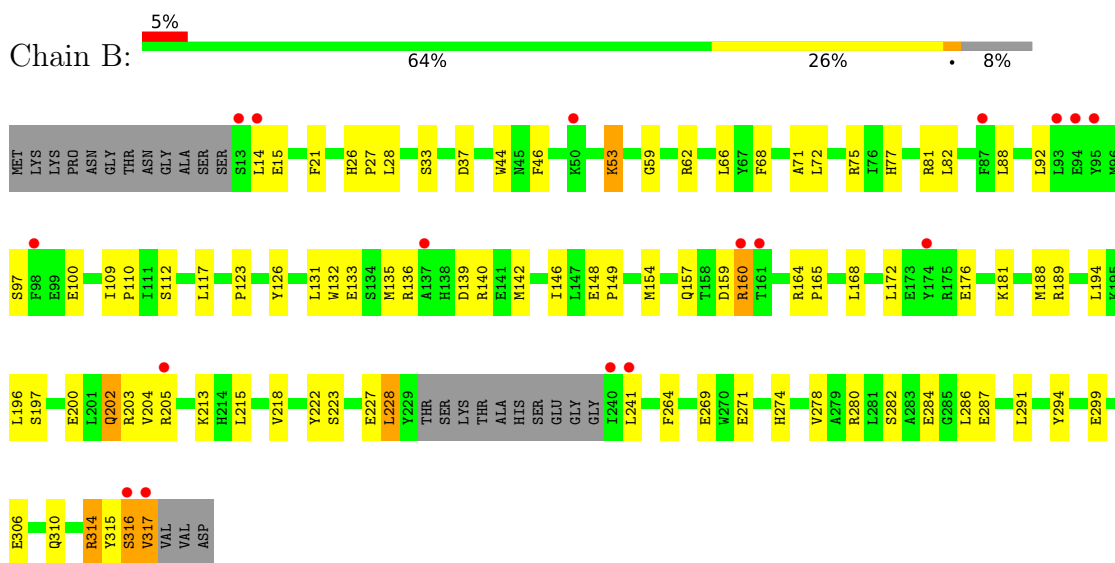
### 3 Residue-property plots [i](#)

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

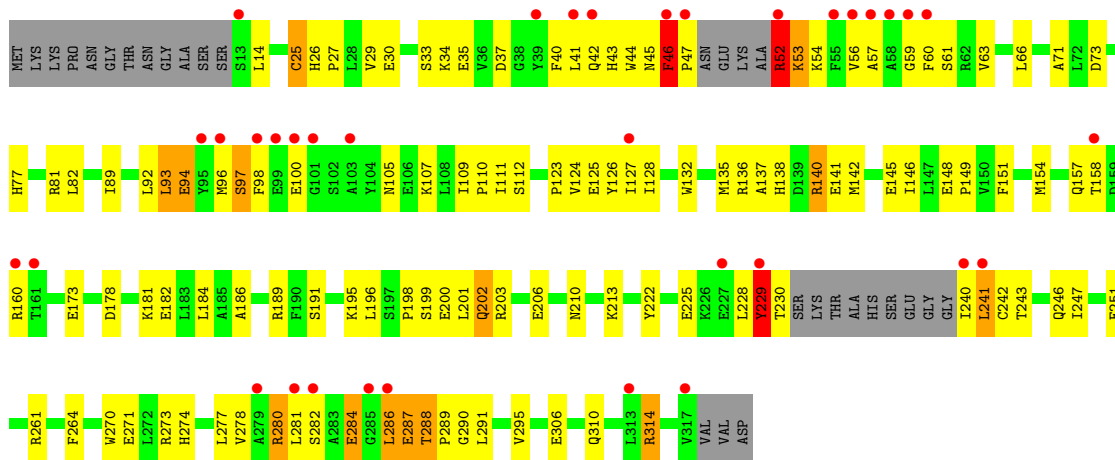


- Molecule 1: Aristolochene synthase

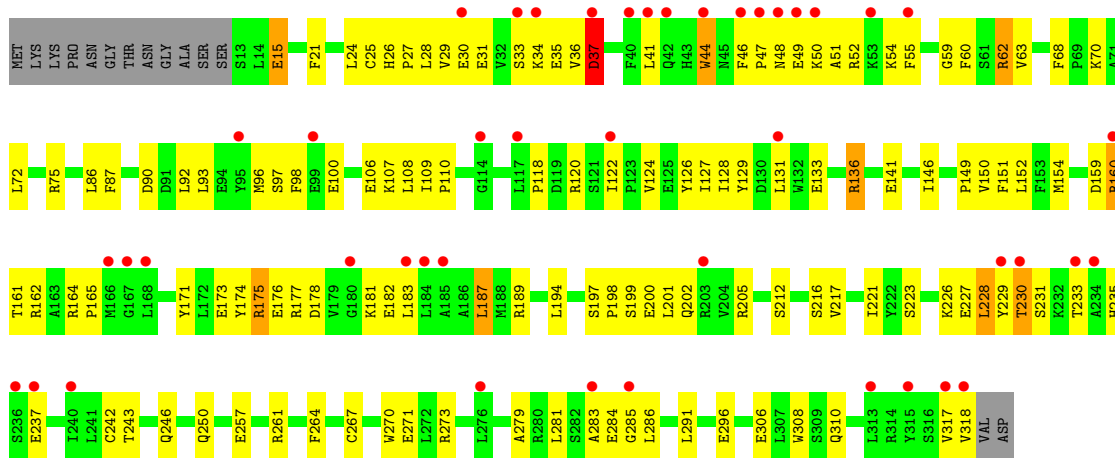


- Molecule 1: Aristolochene synthase





• Molecule 1: Aristolochene synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.92Å 147.50Å 82.57Å 90.00° 96.71° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 46.78 – 2.15	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.15) 96.3 (46.78-2.15)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.16Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.229 , 0.273 0.225 , 0.225	Depositor DCC
$R_{free}$ test set	3810 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtrriage
Anisotropy	0.089	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, POP, 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	0.44	0/2445	0.61	0/3309
1	B	0.45	0/2446	0.61	0/3310
1	C	0.45	1/2421 (0.0%)	0.68	1/3276 (0.0%)
1	D	0.44	0/2522	0.61	0/3414
All	All	0.44	1/9834 (0.0%)	0.63	1/13309 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	ARG	N-CA	5.18	1.56	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	46	PHE	C-N-CD	-10.71	97.04	120.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	68	0
1	B	2393	0	2369	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2369	0	2345	110	0
1	D	2467	0	2439	133	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	3	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	379	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 20.

All (379) 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: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:25:CYS:SG	2:D:1271:BME:S2	2.44	0.96
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: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:NZ	1:C:53:LYS:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:LYS:HA	1:C:53:LYS:HZ1	1.46	0.79
1:C:140:ARG:HD2	1:C:140:ARG:N	1.98	0.79
1:D:54:LYS:HZ1	1:D:317:VAL:HG11	1.45	0.79
1:D:223:SER:O	1:D:227:GLU:HG3	1.84	0.78
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: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
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: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: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: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:B:135:MET:HE1	1:B:146:ILE:HD11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:151:PHE:HD1	1:D:154:MET:HE3	1.61	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
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:151:PHE:CD1	1:D:154:MET:HE3	2.32	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:146:ILE:C	1:C:149:PRO:HD2	2.19	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: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:D:161:THR:HG23	1:D:164:ARG:NH1	2.15	0.61
1:D:98:PHE:CZ	1:D:237:GLU:HB2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:135:MET:HE1	1:B:146:ILE:CD1	2.31	0.60
1:C:124:VAL:O	1:C:128:ILE:HG12	2.02	0.60
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:D:141:GLU:CD	1:D:141:GLU:H	2.04	0.59
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:A:25:CYS:SG	2:A:1273:BME:S2	2.67	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:B:135:MET:HE2	1:B:146:ILE:HD11	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:C:229:TYR:HD2	1:C:229:TYR:C	2.06	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:D:150:VAL:HG12	1:D:154:MET:CE	2.34	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:314:ARG:HH11	1:B:314:ARG:CB	2.15	0.56
1:C:229:TYR:C	1:C:229:TYR:CD2	2.77	0.56
1:A:146:ILE:C	1:A:149:PRO:HD2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:VAL:HG21	2:D:1271:BME:C2	2.36	0.56
1:D:151:PHE:CD1	1:D:154:MET:CE	2.87	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:C:210:ASN:ND2	1:C:273:ARG:HD3	2.22	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: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: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:C:135:MET:HE3	1:C:146:ILE:HD11	1.89	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:54:LYS:HZ1	1:D:317:VAL:CG1	2.19	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:A:135:MET:HE1	1:A:146:ILE:HD11	1.90	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:82:LEU:HD13	1:B:82:LEU:C	2.30	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:C:200:GLU:C	1:C:202:GLN:H	2.11	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:106:GLU:O	1:D:110:PRO:HD3	2.11	0.51
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:C:228:LEU:C	1:C:230:THR:H	2.15	0.50
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:137:ALA:C	1:C:140:ARG:HH12	2.16	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:152:LEU:C	1:D:152:LEU:HD23	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:203:ARG:NE	1:B:286:LEU:HB3	2.30	0.47
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:D:141:GLU:CD	1:D:141:GLU:N	2.68	0.47
1:D:150:VAL:HG12	1:D:154:MET:HE1	1.96	0.47
1:B:269:GLU:OE2	1:C:261:ARG:HD2	2.15	0.46
1:A:142:MET:HE2	6:A:1279:HOH:O	2.14	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:B:316:SER:C	1:B:317:VAL:HG22	2.35	0.46
1:A:282:SER:C	1:A:284:GLU:N	2.69	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:35:GLU:CD	1:D:35:GLU:H	2.18	0.46
1:D:175:ARG:HD3	1:D:216:SER:HB3	1.98	0.46
1:D:150:VAL:HG12	1:D:154:MET:HE2	1.97	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:A:282:SER:C	1:A:284:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:281:LEU:HD13	1:A:286:LEU:HB2	1.97	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: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: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:135:MET:CE	1:C:146:ILE:HD11	2.48	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: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:250:GLN:NE2	1:B:165:PRO:HG3	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:D:109:ILE:HG12	1:D:154:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:H	1:A:99:GLU:CD	2.24	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:C:281:LEU:O	1:C:284:GLU:HB2	2.21	0.41
1:B:133:GLU:HA	1:B:136:ARG:NH1	2.36	0.41
1:D:15:GLU:HA	1:D:15:GLU:OE1	2.21	0.41
1:D:63:VAL:HG22	1:D:308:TRP:CD1	2.54	0.41
1:A:135:MET:HE3	1:A:190:PHE:CE2	2.55	0.41
1:C:41:LEU:HD23	1:C:41:LEU:HA	1.85	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: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:223:SER:HB3	1:B:315:TYR:CZ	2.56	0.41
1:D:146:ILE:HG22	1:D:150:VAL:HG23	2.03	0.41
1:B:203:ARG:HE	1:B:286:LEU:HB3	1.84	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:D:152:LEU:C	1:D:152:LEU:CD2	2.89	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 [\(i\)](#)

### 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	291/320 (91%)	280 (96%)	9 (3%)	2 (1%)	22	15
1	B	291/320 (91%)	284 (98%)	6 (2%)	1 (0%)	41	37
1	C	286/320 (89%)	261 (91%)	11 (4%)	14 (5%)	2	0
1	D	304/320 (95%)	289 (95%)	13 (4%)	2 (1%)	22	15
All	All	1172/1280 (92%)	1114 (95%)	39 (3%)	19 (2%)	9	4

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 [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	260/279 (93%)	245 (94%)	15 (6%)	20	15
1	B	260/279 (93%)	245 (94%)	15 (6%)	20	15
1	C	258/279 (92%)	241 (93%)	17 (7%)	16	11
1	D	268/279 (96%)	250 (93%)	18 (7%)	16	11
All	All	1046/1116 (94%)	981 (94%)	65 (6%)	18	14

All (65) 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	152	LEU
1	A	168	LEU
1	A	196	LEU
1	A	228	LEU
1	A	229	TYR
1	A	242	CYS
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	160	ARG
1	B	164	ARG
1	B	168	LEU
1	B	202	GLN
1	B	228	LEU
1	B	264	PHE
1	B	314	ARG
1	B	317	VAL
1	C	25	CYS
1	C	46	PHE
1	C	52	ARG

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Mol	Chain	Res	Type
1	C	66	LEU
1	C	73	ASP
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	314	ARG
1	D	15	GLU
1	D	24	LEU
1	D	37	ASP
1	D	44	TRP
1	D	62	ARG
1	D	86	LEU
1	D	92	LEU
1	D	131	LEU
1	D	136	ARG
1	D	160	ARG
1	D	173	GLU
1	D	175	ARG
1	D	187	LEU
1	D	194	LEU
1	D	228	LEU
1	D	230	THR
1	D	243	THR
1	D	264	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) 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

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Mol	Chain	Res	Type
1	B	42	GLN
1	B	77	HIS
1	B	219	ASN
1	B	305	ASN
1	C	45	ASN
1	C	138	HIS
1	C	210	ASN
1	C	246	GLN
1	C	275	GLN
1	D	22	GLN
1	D	42	GLN
1	D	202	GLN
1	D	275	GLN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

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	D	1272	-	3,3,3	0.77	0	1,2,2	0.65	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	POP	D	4293	3	6,8,8	1.07	0	13,13,13	1.81	2 (15%)
2	BME	C	1270	-	3,3,3	0.25	0	1,2,2	1.10	0
5	GOL	D	2647	3	5,5,5	0.63	0	5,5,5	0.38	0
2	BME	D	1271	-	3,3,3	0.41	0	1,2,2	1.32	0
2	BME	A	1273	-	3,3,3	0.50	0	1,2,2	0.34	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	D	1272	-	-	0/1/1/1	-
4	POP	D	4293	3	-	0/6/6/6	-
2	BME	C	1270	-	-	0/1/1/1	-
5	GOL	D	2647	3	-	0/4/4/4	-
2	BME	D	1271	-	-	0/1/1/1	-
2	BME	A	1273	-	-	0/1/1/1	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	4293	POP	P2-O-P1	-5.69	113.29	132.83
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	D	1272	BME	2	0
2	C	1270	BME	1	0
5	D	2647	GOL	1	0
2	D	1271	BME	5	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	295/320 (92%)	0.59	19 (6%) 19 26	24, 38, 65, 79	0
1	B	295/320 (92%)	0.49	17 (5%) 23 31	24, 37, 63, 80	0
1	C	292/320 (91%)	0.94	35 (11%) 4 6	23, 46, 76, 90	0
1	D	306/320 (95%)	1.07	44 (14%) 2 3	23, 46, 69, 81	0
All	All	1188/1280 (92%)	0.77	115 (9%) 7 11	23, 41, 70, 90	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	98	PHE	7.9
1	C	46	PHE	7.7
1	C	47	PRO	7.2
1	D	46	PHE	6.8
1	D	317	VAL	6.4
1	D	234	ALA	6.2
1	B	13	SER	5.6
1	C	286	LEU	5.6
1	D	50	LYS	5.6
1	C	13	SER	5.3
1	A	230	THR	5.1
1	D	318	VAL	5.0
1	D	236	SER	4.9
1	C	229	TYR	4.8
1	D	47	PRO	4.8
1	C	56	VAL	4.8
1	C	240	ILE	4.5
1	B	240	ILE	4.5
1	A	317	VAL	4.4
1	C	317	VAL	4.4
1	B	160	ARG	4.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	13	SER	4.1
1	C	52	ARG	4.1
1	D	48	ASN	4.0
1	D	283	ALA	3.9
1	B	317	VAL	3.9
1	A	160	ARG	3.8
1	C	285	GLY	3.7
1	A	229	TYR	3.7
1	C	313	LEU	3.5
1	D	313	LEU	3.5
1	B	316	SER	3.4
1	B	161	THR	3.4
1	A	98	PHE	3.4
1	D	203	ARG	3.3
1	A	47	PRO	3.3
1	D	114	GLY	3.3
1	D	233	THR	3.3
1	D	285	GLY	3.2
1	D	183	LEU	3.1
1	D	276	LEU	3.1
1	A	316	SER	3.0
1	D	122	ILE	3.0
1	D	95	TYR	3.0
1	D	229	TYR	3.0
1	C	160	ARG	3.0
1	C	99	GLU	3.0
1	B	241	LEU	2.9
1	D	41	LEU	2.9
1	B	94	GLU	2.9
1	C	227	GLU	2.8
1	D	166	MET	2.8
1	A	51	ALA	2.8
1	C	279	ALA	2.8
1	D	168	LEU	2.8
1	B	137	ALA	2.8
1	D	37	ASP	2.8
1	D	30	GLU	2.7
1	A	248	LEU	2.7
1	C	96	MET	2.7
1	B	95	TYR	2.7
1	C	59	GLY	2.7
1	C	60	PHE	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	205	ARG	2.6
1	A	205	ARG	2.6
1	B	50	LYS	2.6
1	C	241	LEU	2.6
1	C	58	ALA	2.5
1	D	315	TYR	2.5
1	D	42	GLN	2.5
1	C	127	ILE	2.5
1	D	240	ILE	2.5
1	B	93	LEU	2.5
1	B	98	PHE	2.5
1	C	55	PHE	2.5
1	B	14	LEU	2.5
1	D	237	GLU	2.5
1	C	101	GLY	2.5
1	A	225	GLU	2.5
1	D	40	PHE	2.5
1	A	141	GLU	2.4
1	D	117	LEU	2.4
1	D	184	LEU	2.4
1	C	158	THR	2.4
1	D	55	PHE	2.4
1	C	39	TYR	2.3
1	D	167	GLY	2.3
1	D	160	ARG	2.3
1	D	34	LYS	2.3
1	C	42	GLN	2.3
1	A	172	LEU	2.3
1	D	131	LEU	2.3
1	C	161	THR	2.3
1	D	230	THR	2.3
1	D	49	GLU	2.3
1	C	57	ALA	2.2
1	D	180	GLY	2.2
1	C	281	LEU	2.2
1	C	100	GLU	2.2
1	A	95	TYR	2.2
1	C	95	TYR	2.2
1	D	185	ALA	2.2
1	A	166	MET	2.2
1	A	87	PHE	2.2
1	C	41	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	99	GLU	2.1
1	B	87	PHE	2.1
1	D	33	SER	2.1
1	A	281	LEU	2.1
1	B	174	TYR	2.1
1	A	313	LEU	2.1
1	D	53	LYS	2.1
1	C	103	ALA	2.0
1	C	282	SER	2.0
1	D	44	TRP	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	BME	A	1273	4/4	0.53	0.49	54,55,55,55	4
3	MG	D	703	1/1	0.86	0.08	38,38,38,38	0
2	BME	D	1271	4/4	0.87	0.26	50,50,50,52	0
2	BME	D	1272	4/4	0.90	0.16	53,57,57,57	0
2	BME	C	1270	4/4	0.91	0.17	47,48,51,53	0
3	MG	D	701	1/1	0.93	0.04	56,56,56,56	0
3	MG	D	702	1/1	0.94	0.05	51,51,51,51	0
5	GOL	D	2647	6/6	0.94	0.21	46,49,50,51	0
4	POP	D	4293	9/9	0.97	0.11	36,39,39,39	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.