



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

PDB ID : 1JZ8
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH ALLOLACTOSE
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

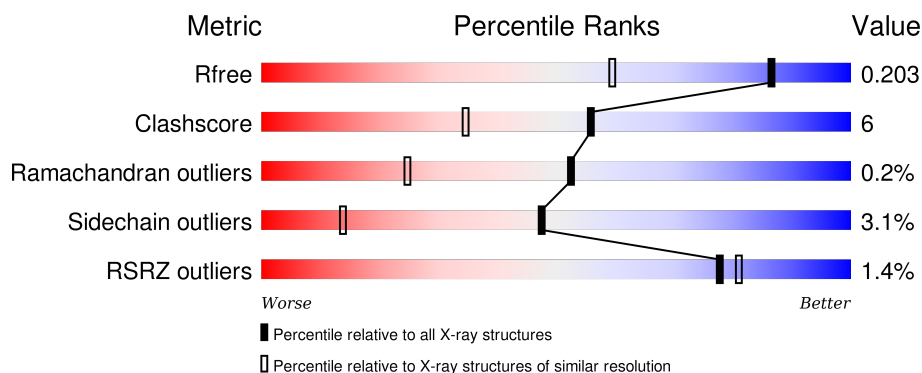
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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	1023	<div> <div>2%</div> <div>76%</div> <div>19%</div> <div>..</div> </div>
1	B	1023	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	C	1023	<div> <div>2%</div> <div>76%</div> <div>19%</div> <div>..</div> </div>
1	D	1023	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LAK	A	2001	-	-	-	X
2	LAK	B	2001[A]	X	-	-	X
2	LAK	B	2002[B]	X	-	-	X
2	LAK	C	2001	-	-	-	X
2	LAK	D	2001	-	-	-	X
5	DMS	A	8403	-	-	-	X
5	DMS	A	8404	-	-	-	X
5	DMS	A	8406	-	-	-	X
5	DMS	A	8407	-	-	-	X
5	DMS	A	8408	-	-	-	X
5	DMS	A	8413	-	X	-	-
5	DMS	A	8417	-	-	-	X
5	DMS	A	8418	-	-	-	X
5	DMS	A	8419	-	-	-	X
5	DMS	A	8420	-	-	-	X
5	DMS	A	8423	-	-	-	X
5	DMS	A	8425	-	X	-	-
5	DMS	A	8501	-	-	-	X
5	DMS	A	8502	-	X	-	-
5	DMS	A	8504	-	-	-	X
5	DMS	A	8506	-	-	-	X
5	DMS	B	8404	-	-	-	X
5	DMS	B	8405	-	-	-	X
5	DMS	B	8407	-	-	-	X
5	DMS	B	8408	-	-	-	X
5	DMS	B	8415	-	-	X	-
5	DMS	B	8417	-	-	-	X
5	DMS	B	8418	-	-	X	-
5	DMS	B	8419	-	-	-	X
5	DMS	B	8420	-	-	-	X
5	DMS	B	8423	-	-	-	X
5	DMS	B	8425	-	-	-	X
5	DMS	B	8501	-	-	X	X
5	DMS	B	8504	-	-	-	X
5	DMS	B	8506	-	-	-	X
5	DMS	B	8508	-	-	-	X
5	DMS	C	8404	-	-	-	X
5	DMS	C	8405	-	-	-	X
5	DMS	C	8406	-	-	-	X
5	DMS	C	8407	-	-	-	X
5	DMS	C	8408	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	C	8417	-	-	-	X
5	DMS	C	8418	-	-	X	X
5	DMS	C	8419	-	-	-	X
5	DMS	C	8420	-	-	-	X
5	DMS	C	8423	-	-	-	X
5	DMS	C	8425	-	-	-	X
5	DMS	C	8501	-	-	-	X
5	DMS	C	8506	-	-	-	X
5	DMS	C	8508	-	-	-	X
5	DMS	D	8403	-	-	-	X
5	DMS	D	8404	-	-	-	X
5	DMS	D	8406	-	-	-	X
5	DMS	D	8407	-	-	-	X
5	DMS	D	8417	-	-	-	X
5	DMS	D	8418	-	-	-	X
5	DMS	D	8419	-	-	-	X
5	DMS	D	8420	-	-	-	X
5	DMS	D	8423	-	-	-	X
5	DMS	D	8425	-	-	-	X
5	DMS	D	8501	-	-	-	X
5	DMS	D	8506	-	-	-	X
5	DMS	D	8508	-	-	-	X
5	DMS	D	8701	-	-	-	X
5	DMS	D	8703	-	-	-	X
5	DMS	D	8705	-	-	X	X
6	TAR	B	2003[C]	X	-	X	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 37685 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 Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	B	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	C	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	D	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

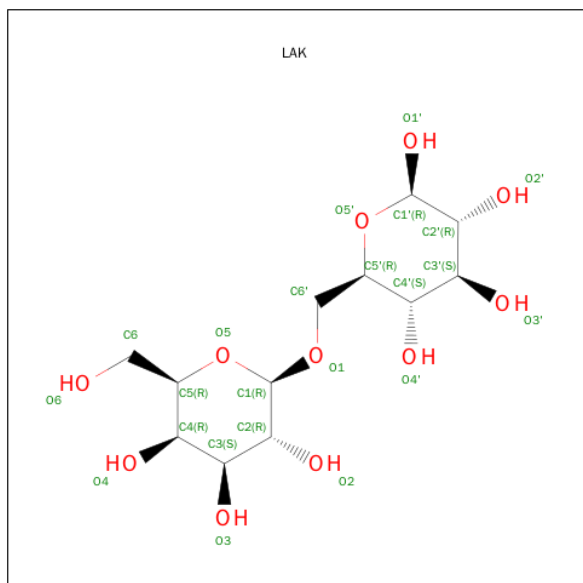
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	CLONING ARTIFACT	? P00722
A	2	SER	MET	CLONING ARTIFACT	? P00722
A	3	HIS	ILE	CLONING ARTIFACT	? P00722
A	4	MET	THR	CLONING ARTIFACT	? P00722
A	5	LEU	ASP	CLONING ARTIFACT	? P00722
A	6	GLU	SER	CLONING ARTIFACT	? P00722
A	7	ASP	LEU	CLONING ARTIFACT	? P00722
A	8	PRO	ALA	CLONING ARTIFACT	? P00722
A	537	GLN	GLU	ENGINEERED	? P00722
B	1	GLY	THR	CLONING ARTIFACT	? P00722
B	2	SER	MET	CLONING ARTIFACT	? P00722
B	3	HIS	ILE	CLONING ARTIFACT	? P00722
B	4	MET	THR	CLONING ARTIFACT	? P00722
B	5	LEU	ASP	CLONING ARTIFACT	? P00722
B	6	GLU	SER	CLONING ARTIFACT	? P00722
B	7	ASP	LEU	CLONING ARTIFACT	? P00722
B	8	PRO	ALA	CLONING ARTIFACT	? P00722
B	537	GLN	GLU	ENGINEERED	? P00722
C	1	GLY	THR	CLONING ARTIFACT	? P00722
C	2	SER	MET	CLONING ARTIFACT	? P00722
C	3	HIS	ILE	CLONING ARTIFACT	? P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	THR	CLONING ARTIFACT	? P00722
C	5	LEU	ASP	CLONING ARTIFACT	? P00722
C	6	GLU	SER	CLONING ARTIFACT	? P00722
C	7	ASP	LEU	CLONING ARTIFACT	? P00722
C	8	PRO	ALA	CLONING ARTIFACT	? P00722
C	537	GLN	GLU	ENGINEERED	? P00722
D	1	GLY	THR	CLONING ARTIFACT	? P00722
D	2	SER	MET	CLONING ARTIFACT	? P00722
D	3	HIS	ILE	CLONING ARTIFACT	? P00722
D	4	MET	THR	CLONING ARTIFACT	? P00722
D	5	LEU	ASP	CLONING ARTIFACT	? P00722
D	6	GLU	SER	CLONING ARTIFACT	? P00722
D	7	ASP	LEU	CLONING ARTIFACT	? P00722
D	8	PRO	ALA	CLONING ARTIFACT	? P00722
D	537	GLN	GLU	ENGINEERED	? P00722

- Molecule 2 is SUGAR (BETA-D-GALACTOPYRANOSYL-1-6-BETA-D-GLUCOPYRANOSE) (three-letter code: LAK) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	1
			23	12	11		
2	B	1	Total	C	O	0	1
			9	4	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

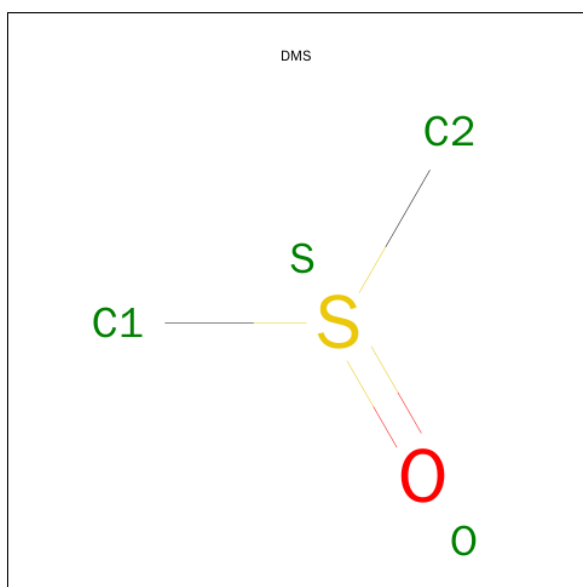
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	A	4	Total	Mg	0	0
			4	4		
3	D	4	Total	Mg	0	0
			4	4		
3	C	5	Total	Mg	0	0
			5	5		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Na	0	0
			4	4		
4	A	4	Total	Na	0	0
			4	4		
4	D	4	Total	Na	0	0
			4	4		
4	C	4	Total	Na	0	0
			4	4		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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

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

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

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

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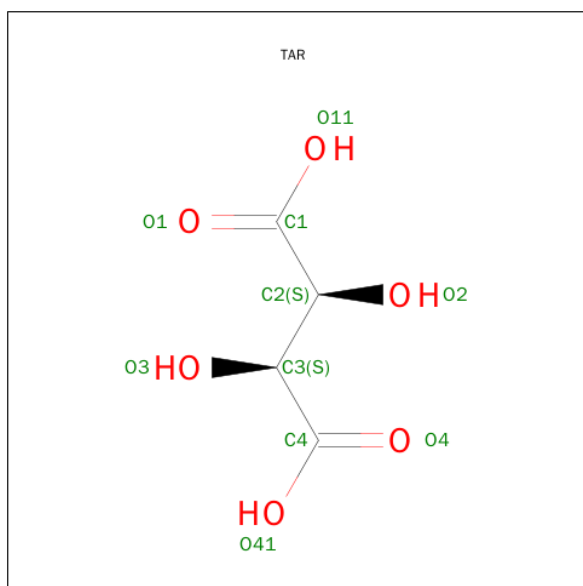
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2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

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

- Molecule 6 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	1
			9	4	5		

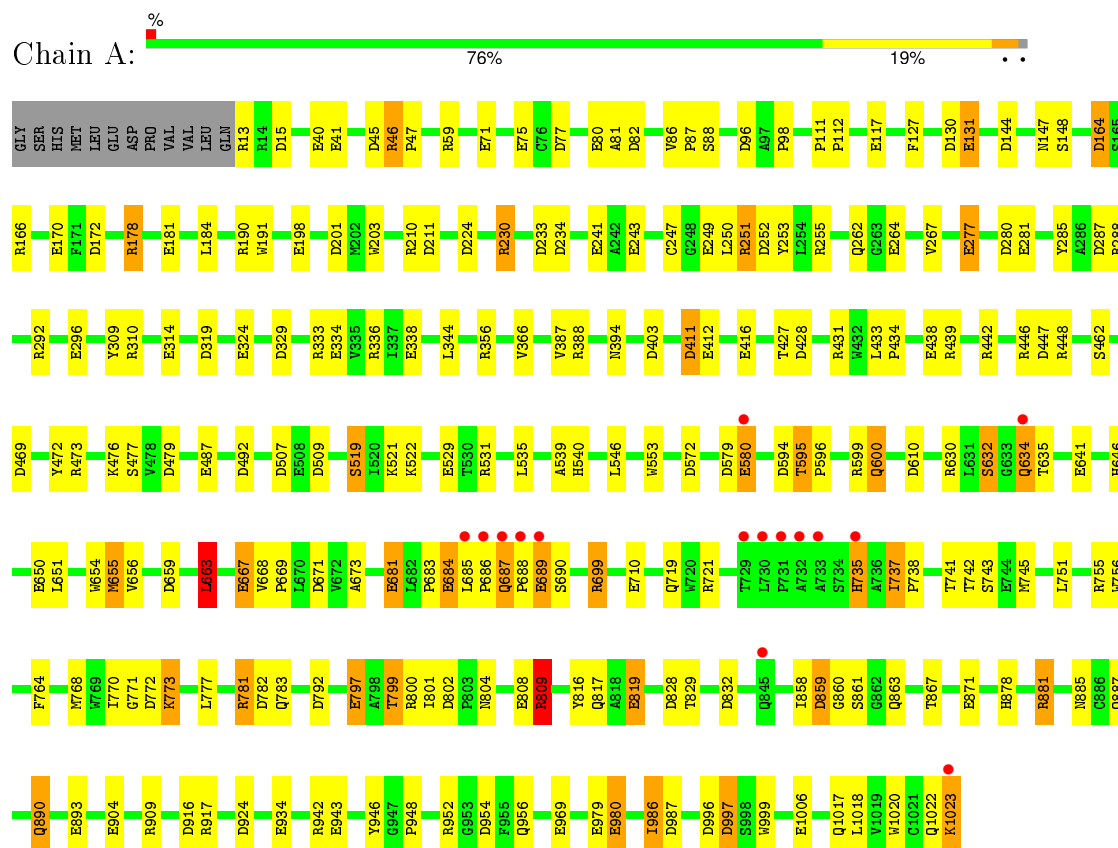
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1144	Total 1144	O 1144	0	0
7	B	1148	Total 1148	O 1148	0	0
7	C	1126	Total 1126	O 1126	0	0
7	D	1105	Total 1105	O 1105	0	0

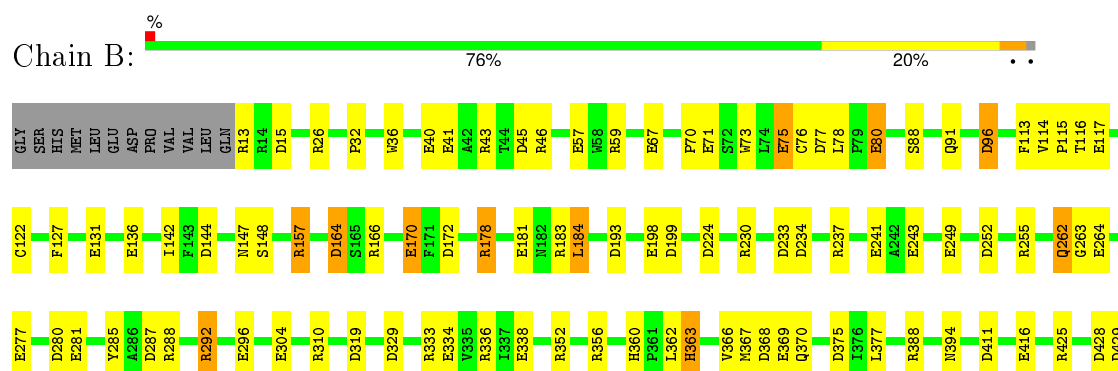
3 Residue-property plots

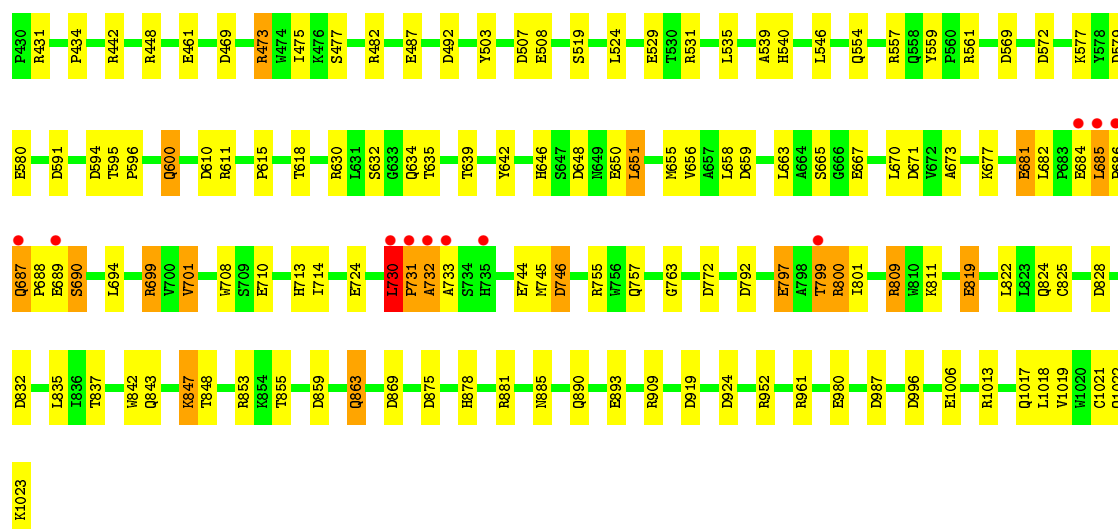
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Beta-Galactosidase

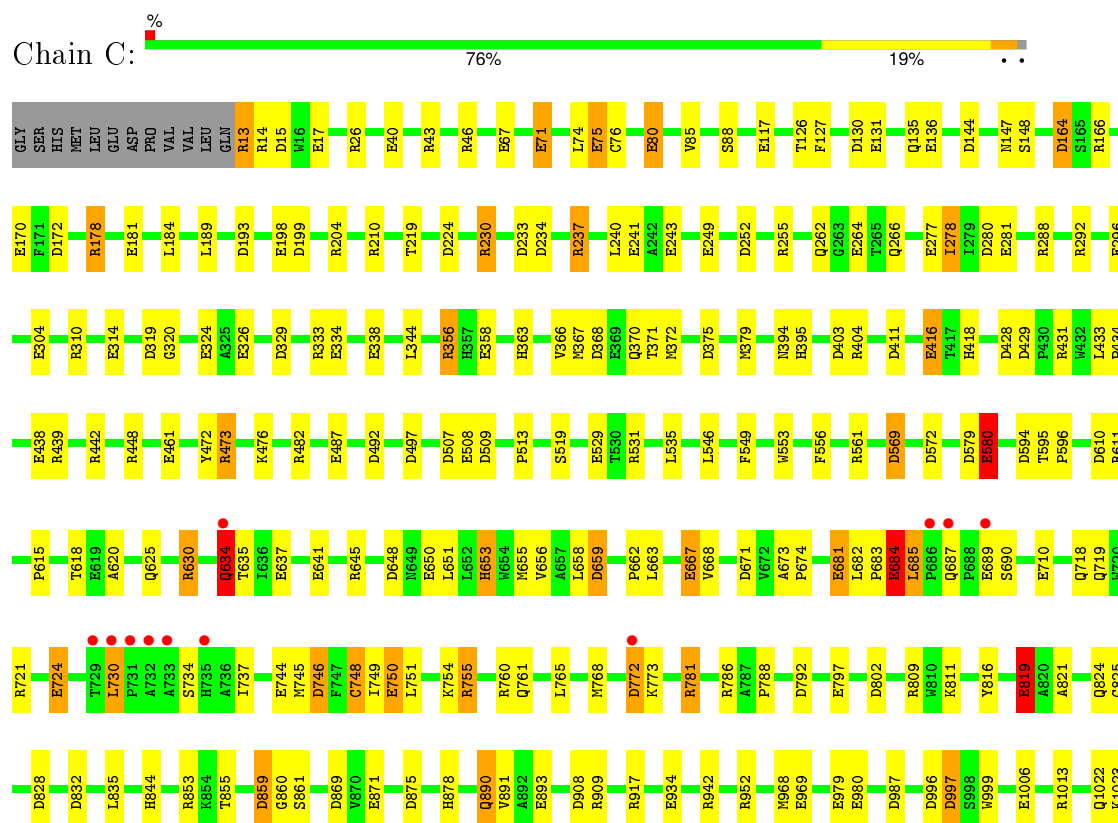


• Molecule 1: Beta-Galactosidase

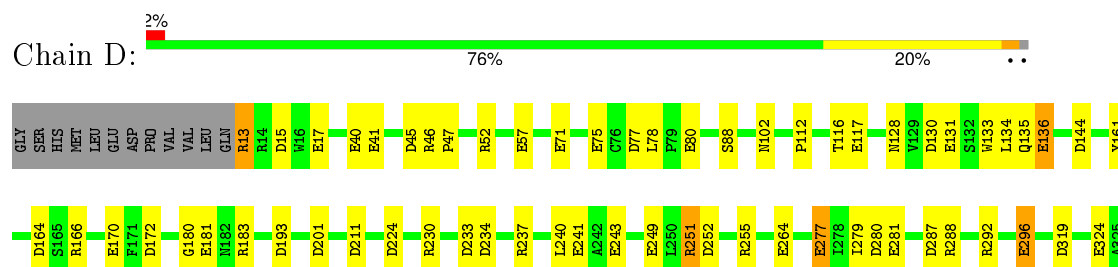


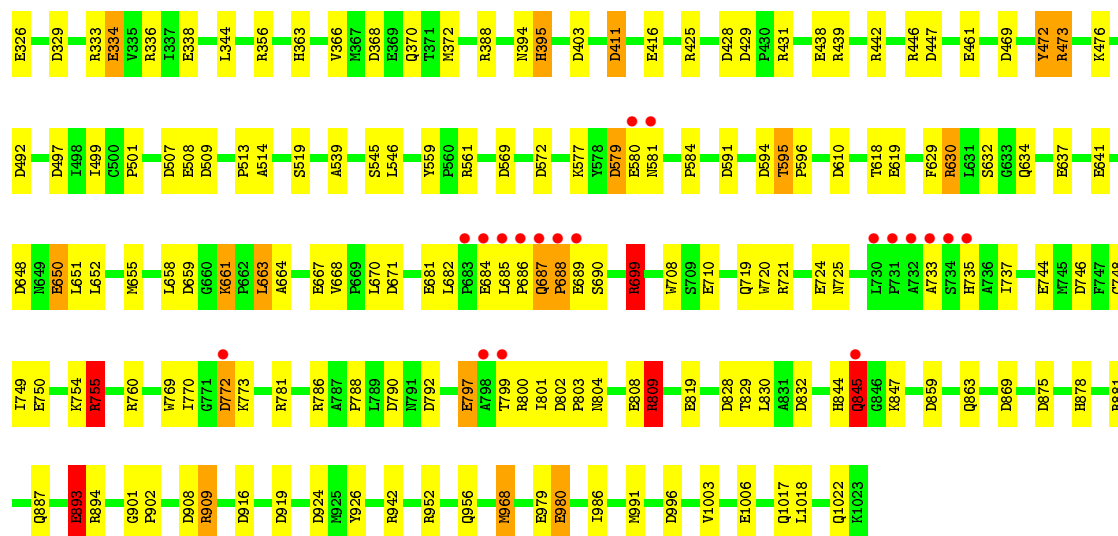


• Molecule 1: Beta-Galactosidase



• Molecule 1: Beta-Galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.39Å 168.71Å 200.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	18.00 – 1.50 18.00 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (18.00-1.50) 97.8 (18.00-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 1.51Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.165 , 0.208 0.162 , 0.203	Depositor DCC
R_{free} test set	11385 reflections (1.49%)	DCC
Wilson B-factor (Å ²)	10.8	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 82.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 777574 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	37685	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.54 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.7464e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, DMS, TAR, LAK

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.19	52/8383 (0.6%)	1.53	143/11437 (1.3%)
1	B	1.21	46/8383 (0.5%)	1.51	154/11437 (1.3%)
1	C	1.21	52/8383 (0.6%)	1.54	152/11437 (1.3%)
1	D	1.21	51/8383 (0.6%)	1.50	146/11437 (1.3%)
All	All	1.20	201/33532 (0.6%)	1.52	595/45748 (1.3%)

All (201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	893	GLU	CD-OE2	11.37	1.38	1.25
1	D	71	GLU	CD-OE2	10.62	1.37	1.25
1	A	296	GLU	CD-OE2	10.38	1.37	1.25
1	C	684	GLU	CD-OE2	9.95	1.36	1.25
1	C	80	GLU	CD-OE2	9.65	1.36	1.25
1	B	1006	GLU	CD-OE2	9.58	1.36	1.25
1	A	1006	GLU	CD-OE2	9.26	1.35	1.25
1	D	650	GLU	CD-OE2	9.24	1.35	1.25
1	D	243	GLU	CD-OE2	9.19	1.35	1.25
1	D	80	GLU	CD-OE2	9.16	1.35	1.25
1	C	934	GLU	CD-OE2	9.13	1.35	1.25
1	B	296	GLU	CD-OE2	8.82	1.35	1.25
1	C	71	GLU	CD-OE2	8.66	1.35	1.25
1	B	650	GLU	CD-OE2	8.54	1.35	1.25
1	D	75	GLU	CD-OE2	8.50	1.34	1.25
1	D	580	GLU	CD-OE2	8.49	1.34	1.25
1	D	980	GLU	CD-OE2	8.27	1.34	1.25
1	B	487	GLU	CD-OE2	8.17	1.34	1.25
1	A	580	GLU	CD-OE2	8.08	1.34	1.25
1	B	819	GLU	CD-OE2	8.06	1.34	1.25
1	B	684	GLU	CD-OE2	7.94	1.34	1.25
1	A	808	GLU	CD-OE2	7.87	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	GLU	CD-OE2	7.81	1.34	1.25
1	C	281	GLU	CD-OE2	7.79	1.34	1.25
1	A	689	GLU	CD-OE2	7.76	1.34	1.25
1	B	181	GLU	CD-OE2	7.74	1.34	1.25
1	B	80	GLU	CD-OE2	7.72	1.34	1.25
1	B	170	GLU	CD-OE2	7.68	1.34	1.25
1	C	529	GLU	CD-OE2	7.67	1.34	1.25
1	C	170	GLU	CD-OE2	7.64	1.34	1.25
1	C	641	GLU	CD-OE1	-7.58	1.17	1.25
1	C	819	GLU	CD-OE2	7.56	1.33	1.25
1	D	170	GLU	CD-OE2	7.54	1.33	1.25
1	A	243	GLU	CD-OE2	7.49	1.33	1.25
1	B	529	GLU	CD-OE2	7.49	1.33	1.25
1	B	744	GLU	CD-OE2	7.48	1.33	1.25
1	C	681	GLU	CD-OE2	7.44	1.33	1.25
1	A	979	GLU	CD-OE2	7.43	1.33	1.25
1	C	630	ARG	NE-CZ	7.42	1.42	1.33
1	C	442	ARG	CZ-NH1	7.38	1.42	1.33
1	A	487	GLU	CD-OE2	7.38	1.33	1.25
1	D	637	GLU	CD-OE2	7.36	1.33	1.25
1	B	198	GLU	CD-OE2	7.35	1.33	1.25
1	A	80	GLU	CD-OE2	7.32	1.33	1.25
1	A	969	GLU	CD-OE2	7.30	1.33	1.25
1	D	334	GLU	CD-OE2	7.28	1.33	1.25
1	B	136	GLU	CD-OE2	7.28	1.33	1.25
1	D	797	GLU	CD-OE2	7.24	1.33	1.25
1	A	684	GLU	CD-OE2	7.22	1.33	1.25
1	A	710	GLU	CD-OE2	7.20	1.33	1.25
1	D	17	GLU	CD-OE2	7.19	1.33	1.25
1	B	580	GLU	CD-OE2	7.18	1.33	1.25
1	D	641	GLU	CD-OE1	-7.17	1.17	1.25
1	C	580	GLU	CD-OE2	7.15	1.33	1.25
1	D	684	GLU	CD-OE2	7.13	1.33	1.25
1	D	281	GLU	CD-OE2	7.12	1.33	1.25
1	C	334	GLU	CD-OE2	7.11	1.33	1.25
1	B	710	GLU	CD-OE2	7.10	1.33	1.25
1	B	71	GLU	CD-OE2	7.07	1.33	1.25
1	C	797	GLU	CD-OE2	7.06	1.33	1.25
1	D	136	GLU	CD-OE2	7.04	1.33	1.25
1	B	243	GLU	CD-OE2	7.02	1.33	1.25
1	A	681	GLU	CD-OE2	6.98	1.33	1.25
1	B	40	GLU	CD-OE2	6.95	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	326	GLU	CD-OE2	6.94	1.33	1.25
1	A	893	GLU	CD-OE2	6.91	1.33	1.25
1	D	681	GLU	CD-OE2	6.89	1.33	1.25
1	D	277	GLU	CD-OE2	6.88	1.33	1.25
1	A	170	GLU	CD-OE2	6.81	1.33	1.25
1	B	980	GLU	CD-OE2	6.76	1.33	1.25
1	B	334	GLU	CD-OE1	-6.74	1.18	1.25
1	D	689	GLU	CD-OE2	6.72	1.33	1.25
1	B	689	GLU	CD-OE2	6.72	1.33	1.25
1	A	334	GLU	CD-OE2	6.69	1.33	1.25
1	C	461	GLU	CD-OE2	6.68	1.32	1.25
1	A	277	GLU	CD-OE2	6.67	1.32	1.25
1	C	264	GLU	CD-OE2	6.67	1.32	1.25
1	C	75	GLU	CD-OE2	6.67	1.32	1.25
1	A	412	GLU	CD-OE2	6.66	1.32	1.25
1	A	249	GLU	CD-OE2	6.59	1.32	1.25
1	C	241	GLU	CD-OE2	6.59	1.32	1.25
1	C	1006	GLU	CD-OE2	6.57	1.32	1.25
1	C	277	GLU	CD-OE2	6.57	1.32	1.25
1	D	241	GLU	CD-OE2	6.56	1.32	1.25
1	C	198	GLU	CD-OE2	6.51	1.32	1.25
1	C	744	GLU	CD-OE2	6.50	1.32	1.25
1	B	249	GLU	CD-OE2	6.49	1.32	1.25
1	D	750	GLU	CD-OE2	6.48	1.32	1.25
1	D	117	GLU	CD-OE2	6.47	1.32	1.25
1	A	442	ARG	CZ-NH1	6.47	1.41	1.33
1	D	710	GLU	CD-OE2	6.46	1.32	1.25
1	C	117	GLU	CD-OE2	6.44	1.32	1.25
1	C	136	GLU	CD-OE2	6.40	1.32	1.25
1	A	980	GLU	CD-OE2	6.39	1.32	1.25
1	A	131	GLU	CD-OE2	6.37	1.32	1.25
1	A	338	GLU	CD-OE2	6.37	1.32	1.25
1	C	416	GLU	CD-OE2	6.36	1.32	1.25
1	C	750	GLU	CD-OE2	6.35	1.32	1.25
1	C	487	GLU	CD-OE2	6.32	1.32	1.25
1	D	667	GLU	CD-OE2	6.31	1.32	1.25
1	B	667	GLU	CD-OE2	6.31	1.32	1.25
1	B	369	GLU	CD-OE2	6.30	1.32	1.25
1	C	243	GLU	CD-OE2	6.29	1.32	1.25
1	D	724	GLU	CD-OE2	6.29	1.32	1.25
1	A	117	GLU	CD-OE2	6.28	1.32	1.25
1	A	324	GLU	CD-OE1	-6.22	1.18	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	744	GLU	CD-OE2	6.21	1.32	1.25
1	C	689	GLU	CD-OE2	6.21	1.32	1.25
1	A	241	GLU	CD-OE2	6.19	1.32	1.25
1	C	710	GLU	CD-OE2	6.17	1.32	1.25
1	B	67	GLU	CD-OE1	-6.17	1.18	1.25
1	C	338	GLU	CD-OE2	6.17	1.32	1.25
1	D	181	GLU	CD-OE2	6.16	1.32	1.25
1	B	281	GLU	CD-OE2	6.13	1.32	1.25
1	D	699	ARG	CZ-NH2	6.12	1.41	1.33
1	A	438	GLU	CD-OE2	6.11	1.32	1.25
1	B	797	GLU	CD-OE2	6.11	1.32	1.25
1	C	724	GLU	CD-OE2	6.04	1.32	1.25
1	C	296	GLU	CD-OE2	6.04	1.32	1.25
1	D	461	GLU	CD-OE2	6.02	1.32	1.25
1	A	264	GLU	CD-OE2	6.00	1.32	1.25
1	A	416	GLU	CD-OE2	5.99	1.32	1.25
1	B	304	GLU	CD-OE2	5.99	1.32	1.25
1	C	181	GLU	CD-OE2	5.95	1.32	1.25
1	B	241	GLU	CD-OE2	5.95	1.32	1.25
1	D	264	GLU	CD-OE2	5.93	1.32	1.25
1	C	969	GLU	CD-OE2	5.92	1.32	1.25
1	D	41	GLU	CD-OE2	5.92	1.32	1.25
1	C	893	GLU	CD-OE2	5.92	1.32	1.25
1	D	979	GLU	CD-OE2	5.91	1.32	1.25
1	B	310	ARG	CZ-NH1	5.91	1.40	1.33
1	D	296	GLU	CD-OE2	5.85	1.32	1.25
1	B	75	GLU	CD-OE2	5.85	1.32	1.25
1	D	324	GLU	CD-OE1	-5.85	1.19	1.25
1	A	71	GLU	CD-OE2	5.83	1.32	1.25
1	A	314	GLU	CD-OE1	-5.80	1.19	1.25
1	D	819	GLU	CD-OE2	5.78	1.32	1.25
1	B	893	GLU	CD-OE2	5.77	1.32	1.25
1	C	314	GLU	CD-OE1	-5.76	1.19	1.25
1	B	131	GLU	CD-OE2	5.75	1.31	1.25
1	C	324	GLU	CD-OE2	5.73	1.31	1.25
1	B	338	GLU	CD-OE2	5.72	1.31	1.25
1	C	67	GLU	CD-OE2	5.71	1.31	1.25
1	C	508	GLU	CD-OE2	5.71	1.31	1.25
1	D	619	GLU	CD-OE2	5.70	1.31	1.25
1	D	249	GLU	CD-OE2	5.69	1.31	1.25
1	A	797	GLU	CD-OE2	5.69	1.31	1.25
1	C	40	GLU	CD-OE2	5.68	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	57	GLU	CD-OE2	5.66	1.31	1.25
1	D	338	GLU	CD-OE2	5.65	1.31	1.25
1	B	842	TRP	CD2-CE3	-5.63	1.31	1.40
1	D	131	GLU	CD-OE2	5.63	1.31	1.25
1	C	358	GLU	CD-OE2	5.61	1.31	1.25
1	A	943	GLU	CD-OE2	5.55	1.31	1.25
1	C	17	GLU	CD-OE2	5.54	1.31	1.25
1	A	650	GLU	CD-OE2	5.54	1.31	1.25
1	D	508	GLU	CD-OE2	5.53	1.31	1.25
1	C	667	GLU	CD-OE2	5.53	1.31	1.25
1	C	980	GLU	CD-OE2	5.51	1.31	1.25
1	B	41	GLU	CD-OE2	5.50	1.31	1.25
1	A	191	TRP	NE1-CE2	5.48	1.44	1.37
1	B	117	GLU	CD-OE2	5.46	1.31	1.25
1	B	508	GLU	CD-OE2	5.45	1.31	1.25
1	A	641	GLU	CD-OE1	-5.45	1.19	1.25
1	A	40	GLU	CD-OE2	5.45	1.31	1.25
1	C	304	GLU	CD-OE2	5.44	1.31	1.25
1	D	442	ARG	CZ-NH1	5.43	1.40	1.33
1	A	281	GLU	CD-OE2	5.40	1.31	1.25
1	D	442	ARG	CZ-NH2	5.40	1.40	1.33
1	A	667	GLU	CD-OE2	5.39	1.31	1.25
1	D	40	GLU	CD-OE2	5.38	1.31	1.25
1	D	57	GLU	CD-OE1	-5.37	1.19	1.25
1	B	724	GLU	CD-OE2	5.36	1.31	1.25
1	A	529	GLU	CD-OE2	5.35	1.31	1.25
1	D	438	GLU	CD-OE2	5.34	1.31	1.25
1	C	650	GLU	CD-OE2	5.31	1.31	1.25
1	A	181	GLU	CD-OE2	5.30	1.31	1.25
1	C	131	GLU	CD-OE2	5.30	1.31	1.25
1	B	264	GLU	CD-OE2	5.25	1.31	1.25
1	A	800	ARG	CZ-NH1	5.25	1.39	1.33
1	B	277	GLU	CD-OE2	5.24	1.31	1.25
1	C	979	GLU	CD-OE2	5.22	1.31	1.25
1	C	326	GLU	CD-OE2	5.22	1.31	1.25
1	D	808	GLU	CD-OE1	-5.21	1.20	1.25
1	D	425	ARG	NE-CZ	5.20	1.39	1.33
1	A	198	GLU	CD-OE2	5.19	1.31	1.25
1	A	310	ARG	CZ-NH2	5.17	1.39	1.33
1	A	871	GLU	CD-OE2	5.17	1.31	1.25
1	C	249	GLU	CD-OE2	5.15	1.31	1.25
1	B	681	GLU	CD-OE2	5.14	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	416	GLU	CD-OE2	5.14	1.31	1.25
1	A	904	GLU	CD-OE2	5.14	1.31	1.25
1	B	32	PRO	N-CD	5.12	1.55	1.47
1	B	461	GLU	CD-OE1	-5.12	1.20	1.25
1	A	772	ASP	CG-OD2	5.10	1.37	1.25
1	A	934	GLU	CD-OE2	5.08	1.31	1.25
1	A	819	GLU	CD-OE2	5.08	1.31	1.25
1	D	1006	GLU	CD-OE2	5.06	1.31	1.25
1	A	41	GLU	CD-OE2	5.04	1.31	1.25
1	D	442	ARG	NE-CZ	5.04	1.39	1.33
1	A	909	ARG	NE-CZ	5.00	1.39	1.33

All (595) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	ARG	NE-CZ-NH1	26.47	133.53	120.30
1	C	442	ARG	NE-CZ-NH2	-17.31	111.64	120.30
1	A	431	ARG	NE-CZ-NH2	-17.25	111.67	120.30
1	D	473	ARG	NE-CZ-NH1	13.79	127.19	120.30
1	A	442	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	C	473	ARG	NE-CZ-NH1	12.77	126.68	120.30
1	C	630	ARG	CD-NE-CZ	12.39	140.95	123.60
1	A	431	ARG	NE-CZ-NH1	12.32	126.46	120.30
1	A	442	ARG	NE-CZ-NH1	12.08	126.34	120.30
1	A	909	ARG	NE-CZ-NH1	11.95	126.28	120.30
1	D	172	ASP	CB-CG-OD2	-11.85	107.64	118.30
1	C	721	ARG	NE-CZ-NH1	11.81	126.20	120.30
1	A	356	ARG	NE-CZ-NH2	-11.72	114.44	120.30
1	C	442	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	A	251	ARG	NE-CZ-NH1	11.51	126.05	120.30
1	B	336	ARG	NE-CZ-NH1	11.35	125.98	120.30
1	D	630	ARG	NE-CZ-NH1	11.17	125.88	120.30
1	A	755	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	D	431	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	A	917	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	D	439	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	B	368	ASP	CB-CG-OD1	10.23	127.51	118.30
1	A	224	ASP	CB-CG-OD1	10.12	127.40	118.30
1	D	183	ARG	NE-CZ-NH1	-10.11	115.24	120.30
1	A	172	ASP	CB-CG-OD2	-10.06	109.25	118.30
1	B	853	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	755	ARG	NE-CZ-NH2	-10.03	115.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	B	832	ASP	CB-CG-OD1	9.86	127.17	118.30
1	A	233	ASP	CB-CG-OD1	9.79	127.11	118.30
1	D	579	ASP	CB-CG-OD2	-9.65	109.61	118.30
1	D	648	ASP	CB-CG-OD2	-9.57	109.69	118.30
1	B	388	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	A	234	ASP	CB-CG-OD2	-9.50	109.75	118.30
1	B	671	ASP	CB-CG-OD2	-9.44	109.80	118.30
1	D	952	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	B	755	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	B	832	ASP	CB-CG-OD2	-9.39	109.84	118.30
1	C	579	ASP	CB-CG-OD2	-9.38	109.86	118.30
1	A	288	ARG	NE-CZ-NH2	-9.35	115.63	120.30
1	D	781	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	B	288	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	B	252	ASP	CB-CG-OD2	-9.25	109.98	118.30
1	C	43	ARG	NE-CZ-NH1	9.24	124.92	120.30
1	C	224	ASP	CB-CG-OD1	9.20	126.58	118.30
1	A	233	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	B	630	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	D	15	ASP	CB-CG-OD2	-9.17	110.05	118.30
1	A	428	ASP	CB-CG-OD1	9.16	126.55	118.30
1	B	319	ASP	CB-CG-OD2	-9.16	110.06	118.30
1	B	772	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	A	610	ASP	CB-CG-OD1	9.07	126.47	118.30
1	C	531	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	509	ASP	CB-CG-OD1	9.07	126.46	118.30
1	D	172	ASP	CB-CG-OD1	8.98	126.38	118.30
1	B	648	ASP	CB-CG-OD2	-8.93	110.26	118.30
1	B	319	ASP	CB-CG-OD1	8.91	126.32	118.30
1	C	233	ASP	CB-CG-OD1	8.88	126.30	118.30
1	D	996	ASP	CB-CG-OD2	-8.84	110.34	118.30
1	D	755	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	234	ASP	CB-CG-OD1	8.83	126.24	118.30
1	A	428	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	B	800	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	C	561	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	439	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	D	996	ASP	CB-CG-OD1	8.65	126.08	118.30
1	A	659	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	D	442	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	A	255	ARG	NE-CZ-NH2	-8.57	116.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	909	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	D	439	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	B	579	ASP	CB-CG-OD1	8.46	125.91	118.30
1	A	46	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	D	909	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	A	356	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	C	853	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	B	557	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	356	ARG	NE-CZ-NH2	-8.31	116.14	120.30
1	B	469	ASP	CB-CG-OD1	8.29	125.76	118.30
1	D	869	ASP	CB-CG-OD1	8.29	125.76	118.30
1	C	288	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	659	ASP	CB-CG-OD1	8.27	125.74	118.30
1	A	924	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	B	531	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	C	792	ASP	CB-CG-OD1	8.23	125.71	118.30
1	C	255	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	D	859	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	A	816	TYR	CB-CG-CD2	-8.18	116.09	121.00
1	B	233	ASP	CB-CG-OD1	8.18	125.67	118.30
1	C	233	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	D	234	ASP	CB-CG-OD1	8.14	125.63	118.30
1	C	431	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	987	ASP	CB-CG-OD1	8.13	125.61	118.30
1	D	561	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	A	144	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	809	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	A	599	ARG	NE-CZ-NH1	-8.03	116.29	120.30
1	A	954	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	C	448	ARG	NE-CZ-NH2	-8.01	116.30	120.30
1	B	368	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	B	610	ASP	CB-CG-OD1	7.98	125.48	118.30
1	D	13	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	336	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	D	429	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	D	561	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	B	288	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	A	594	ASP	CB-CG-OD1	7.88	125.39	118.30
1	C	772	ASP	CB-CG-OD2	-7.87	111.21	118.30
1	C	648	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	D	630	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	172	ASP	CB-CG-OD1	7.85	125.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	786	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	B	800	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	C	802	ASP	CB-CG-OD1	7.84	125.36	118.30
1	B	77	ASP	CB-CG-OD1	7.84	125.35	118.30
1	A	632	SER	N-CA-CB	7.83	122.24	110.50
1	B	287	ASP	CB-CG-OD1	7.81	125.33	118.30
1	C	832	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	B	875	ASP	CB-CG-OD1	7.79	125.31	118.30
1	C	996	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	557	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	D	429	ASP	CB-CG-OD1	7.75	125.28	118.30
1	A	909	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	772	ASP	CB-CG-OD1	7.72	125.25	118.30
1	D	255	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	B	166	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	C	85	VAL	CA-CB-CG2	-7.71	99.33	110.90
1	B	178	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	C	204	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	C	809	ARG	NE-CZ-NH2	7.68	124.14	120.30
1	A	946	TYR	CB-CG-CD2	-7.67	116.40	121.00
1	C	199	ASP	CB-CG-OD1	7.66	125.19	118.30
1	D	507	ASP	CB-CG-OD2	-7.65	111.41	118.30
1	C	909	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	C	26	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	C	869	ASP	CB-CG-OD1	7.62	125.16	118.30
1	B	469	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	319	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	A	255	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	C	144	ASP	CB-CG-OD1	7.60	125.14	118.30
1	D	288	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	234	ASP	CB-CG-OD1	7.58	125.12	118.30
1	A	509	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	B	234	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	B	329	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	B	648	ASP	CB-CG-OD1	7.55	125.09	118.30
1	B	594	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	A	687	GLN	C-N-CD	-7.53	104.03	120.60
1	B	482	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	B	26	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	C	630	ARG	NH1-CZ-NH2	-7.48	111.17	119.40
1	D	52	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	166	ARG	NE-CZ-NH2	-7.45	116.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	671	ASP	CB-CG-OD1	7.44	124.99	118.30
1	B	96	ASP	CB-CG-OD2	-7.43	111.62	118.30
1	B	442	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	A	13	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	D	446	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	C	917	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	C	659	ASP	CB-CG-OD1	7.37	124.94	118.30
1	C	832	ASP	CB-CG-OD1	7.36	124.93	118.30
1	D	45	ASP	CB-CG-OD1	7.35	124.92	118.30
1	D	255	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	D	166	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	B	428	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	859	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	B	519	SER	N-CA-CB	-7.30	99.55	110.50
1	C	772	ASP	CB-CG-OD1	7.29	124.86	118.30
1	D	786	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	D	579	ASP	CB-CG-OD1	7.29	124.86	118.30
1	D	403	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	C	610	ASP	CB-CG-OD1	7.27	124.84	118.30
1	B	178	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	C	875	ASP	CB-CG-OD1	7.25	124.82	118.30
1	C	509	ASP	CB-CG-OD1	7.25	124.82	118.30
1	D	924	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	D	356	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	96	ASP	CB-CG-OD1	7.24	124.81	118.30
1	B	594	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	853	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	C	492	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	D	659	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	B	919	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	C	908	ASP	CB-CG-OD1	7.15	124.74	118.30
1	B	492	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	D	828	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	B	473	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	C	828	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	D	13	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	329	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	579	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	D	733	ALA	N-CA-CB	7.10	120.05	110.10
1	C	473	ARG	NH1-CZ-NH2	-7.09	111.61	119.40
1	B	233	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	D	800	ARG	NE-CZ-NH1	7.07	123.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	952	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	579	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	B	46	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	193	ASP	CB-CG-OD1	7.02	124.62	118.30
1	C	46	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	D	224	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	996	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	D	403	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	172	ASP	CB-CG-OD1	6.99	124.59	118.30
1	B	809	ARG	CG-CD-NE	6.97	126.45	111.80
1	A	507	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	B	909	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	C	172	ASP	CB-CG-OD1	6.92	124.53	118.30
1	D	469	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	482	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	82	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	224	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	B	699	ARG	NE-CZ-NH2	6.90	123.75	120.30
1	C	594	ASP	CB-CG-OD1	6.90	124.51	118.30
1	D	425	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	C	561	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	C	136	GLU	CB-CA-C	-6.86	96.69	110.40
1	C	255	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	D	648	ASP	CB-CG-OD1	6.85	124.46	118.30
1	B	388	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	746	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	C	909	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	329	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	924	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	411	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	319	ASP	CB-CG-OD1	6.80	124.42	118.30
1	D	832	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	610	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	572	ASP	CB-CG-OD1	6.78	124.40	118.30
1	D	594	ASP	CB-CG-OD1	6.78	124.40	118.30
1	B	280	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	A	832	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	569	ASP	CB-CG-OD1	6.73	124.36	118.30
1	B	569	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	C	319	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	D	130	ASP	CB-CG-OD1	6.72	124.34	118.30
1	A	828	ASP	CB-CG-OD1	6.71	124.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	755	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	B	919	ASP	CB-CG-OD1	6.70	124.33	118.30
1	D	632	SER	N-CA-CB	6.70	120.55	110.50
1	D	859	ASP	CB-CG-OD1	6.70	124.33	118.30
1	C	579	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	802	ASP	CB-CG-OD1	6.68	124.31	118.30
1	D	287	ASP	CB-CG-OD1	6.68	124.31	118.30
1	D	442	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	B	310	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	746	ASP	CB-CG-OD1	6.67	124.30	118.30
1	D	356	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	368	ASP	CB-CG-OD1	6.66	124.29	118.30
1	A	411	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	A	446	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	741	THR	CA-CB-CG2	-6.65	103.09	112.40
1	B	559	TYR	CB-CG-CD2	-6.65	117.01	121.00
1	C	76	CYS	N-CA-CB	-6.65	98.63	110.60
1	C	280	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	D	875	ASP	CB-CG-OD1	6.64	124.28	118.30
1	B	610	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	B	539[A]	ALA	CB-CA-C	-6.63	100.15	110.10
1	B	539[B]	ALA	CB-CA-C	-6.63	100.15	110.10
1	B	144	ASP	CB-CG-OD1	6.63	124.27	118.30
1	C	74	LEU	CB-CG-CD1	-6.62	99.74	111.00
1	A	802	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	781	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	507	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	255	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	C	166	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	572	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	D	446	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	255	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	D	809	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	C	659	ASP	CB-CG-OD2	-6.57	112.38	118.30
1	D	234	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	B	659	ASP	CB-CG-OD1	6.57	124.21	118.30
1	C	234	ASP	CB-CG-OD1	6.57	124.21	118.30
1	C	828	ASP	CB-CG-OD1	6.56	124.21	118.30
1	B	77	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	B	367	MET	CG-SD-CE	6.55	110.69	100.20
1	A	699	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	D	919	ASP	CB-CG-OD2	-6.53	112.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	569	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	D	329	ASP	CB-CG-OD2	-6.50	112.44	118.30
1	D	746	ASP	CB-CG-OD1	6.50	124.16	118.30
1	C	952	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	821	ALA	N-CA-CB	6.49	119.19	110.10
1	C	507	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	411	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	875	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	285	TYR	CZ-CE2-CD2	-6.48	113.97	119.80
1	A	211	ASP	CB-CG-OD1	6.45	124.11	118.30
1	C	310	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	952	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	952	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	287	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	285	TYR	CB-CG-CD1	-6.41	117.16	121.00
1	C	859	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	D	193	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	D	428	ASP	CB-CG-OD1	6.39	124.05	118.30
1	D	233	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	B	280	ASP	CB-CG-OD1	6.38	124.04	118.30
1	A	800	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	997	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	D	802	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	828	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	B	183	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	539[A]	ALA	CB-CA-C	-6.34	100.59	110.10
1	A	539[B]	ALA	CB-CA-C	-6.34	100.59	110.10
1	A	792	ASP	CB-CG-OD1	6.34	124.00	118.30
1	A	519	SER	N-CA-CB	-6.33	101.00	110.50
1	A	881	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	572	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	403	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	996	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	579	ASP	CB-CG-OD1	6.32	123.99	118.30
1	D	77	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	D	80	GLU	OE1-CD-OE2	6.31	130.88	123.30
1	C	869	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	809	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	B	113	PHE	CB-CG-CD1	-6.28	116.40	120.80
1	D	1018	LEU	CB-CA-C	-6.28	98.28	110.20
1	B	96	ASP	CB-CG-OD1	6.25	123.93	118.30
1	D	368	ASP	CB-CG-OD2	-6.25	112.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	952	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	C	338	GLU	CG-CD-OE2	-6.24	105.82	118.30
1	C	368	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	C	356	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	130	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	428	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	329	ASP	CB-CG-OD1	6.23	123.90	118.30
1	D	772	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	144	ASP	CB-CG-OD1	6.22	123.90	118.30
1	D	980	GLU	C-N-CA	-6.21	109.25	122.30
1	D	252	ASP	CB-CG-OD1	6.20	123.88	118.30
1	D	509	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	B	287	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	B	172	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	B	292	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	859	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	816	TYR	CB-CG-CD1	6.15	124.69	121.00
1	D	924	ASP	CB-CG-OD1	6.15	123.83	118.30
1	C	43	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	561	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	497	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	591	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	287	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	425	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	C	890	GLN	N-CA-CB	-6.10	99.61	110.60
1	A	130	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	429	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	164	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	771	GLY	N-CA-C	-6.09	97.87	113.10
1	C	755	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	479	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	210	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	926	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	B	431	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	492	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	199	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	230	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	828	ASP	CB-CG-OD1	6.05	123.75	118.30
1	C	630	ARG	CA-CB-CG	6.05	126.72	113.40
1	A	859	ASP	CB-CG-OD1	6.04	123.74	118.30
1	C	280	ASP	CB-CG-OD1	6.03	123.73	118.30
1	D	388	ARG	NE-CZ-NH2	-6.03	117.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	987	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	B	1018	LEU	CB-CA-C	-6.02	98.76	110.20
1	A	403	ASP	CB-CG-OD1	6.01	123.71	118.30
1	D	719	GLN	CB-CA-C	-6.01	98.37	110.40
1	C	630	ARG	CG-CD-NE	6.01	124.41	111.80
1	C	204	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	792	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	748	CYS	CA-CB-SG	-5.99	103.22	114.00
1	B	157	ARG	NE-CZ-NH2	5.97	123.29	120.30
1	D	201	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	B	448	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	828	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	B	792	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	C	13	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	C	509	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	C	781	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	D	287	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	77	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	C	671	ASP	CB-CG-OD1	5.93	123.63	118.30
1	C	252	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	252	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	D	431	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	D	919	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	280	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	252	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	859	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	329	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	987	ASP	CB-CG-OD1	5.88	123.60	118.30
1	C	439	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	869	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	890	GLN	N-CA-CB	-5.87	100.03	110.60
1	D	252	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	C	492	ASP	CB-CG-OD1	5.84	123.56	118.30
1	C	375	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	954	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	648	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	251	ARG	CG-CD-NE	-5.82	99.59	111.80
1	C	553	TRP	CA-CB-CG	-5.79	102.69	113.70
1	C	792	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	952	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	45	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	591	ASP	CB-CG-OD1	5.78	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	507	ASP	CB-CG-OD1	5.76	123.49	118.30
1	B	1013	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	611	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	D	572	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	319	ASP	CB-CG-OD1	5.76	123.49	118.30
1	C	210	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	A	190	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	183	ARG	CD-NE-CZ	-5.75	115.55	123.60
1	B	701	VAL	CA-CB-CG2	-5.75	102.28	110.90
1	A	15	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	C	230	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	509	ASP	CB-CG-OD1	5.73	123.46	118.30
1	A	388	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	572	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	280	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	C	572	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	721	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	442	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	569	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	997	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	199	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	D	610	ASP	CB-CG-OD1	5.68	123.42	118.30
1	C	252	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	288	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	279	ILE	CA-CB-CG2	5.67	122.25	110.90
1	B	411	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	D	411	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	D	942	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	193	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	329	ASP	CB-CG-OD1	5.66	123.39	118.30
1	D	77	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	611	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	D	559	TYR	CB-CG-CD1	5.64	124.38	121.00
1	D	211	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	917	ARG	NE-CZ-NH1	-5.63	117.48	120.30
1	B	116	THR	CA-CB-CG2	-5.62	104.53	112.40
1	B	755	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	247	CYS	CA-CB-SG	-5.61	103.91	114.00
1	B	961	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	980	GLU	C-N-CA	-5.61	110.53	122.30
1	C	126	THR	CA-CB-CG2	-5.60	104.56	112.40
1	C	987	ASP	CB-CG-OD1	5.56	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	472	TYR	CB-CG-CD1	5.56	124.33	121.00
1	C	234	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	267	VAL	CG1-CB-CG2	-5.55	102.03	110.90
1	B	352	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	733	ALA	N-CA-CB	5.54	117.86	110.10
1	A	719	GLN	CB-CA-C	-5.53	99.33	110.40
1	D	416	GLU	CG-CD-OE1	5.53	129.36	118.30
1	A	663	LEU	CB-CA-C	-5.53	99.69	110.20
1	D	324	GLU	N-CA-CB	5.52	120.54	110.60
1	B	632	SER	N-CA-CB	5.51	118.77	110.50
1	C	671	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	59	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	D	569	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	C	634	GLN	N-CA-CB	-5.49	100.72	110.60
1	C	219	THR	CA-CB-CG2	-5.49	104.72	112.40
1	D	926	TYR	CB-CG-CD1	5.48	124.29	121.00
1	A	832	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	809	ARG	CG-CD-NE	5.47	123.29	111.80
1	B	224	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	429	ASP	CB-CG-OD1	5.46	123.22	118.30
1	D	497	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	201	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	760	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	292	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	829	THR	CA-CB-CG2	-5.43	104.79	112.40
1	C	237	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	201	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	15	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	559	TYR	CB-CG-CD1	5.41	124.25	121.00
1	D	908	ASP	CB-CG-OD2	-5.39	113.44	118.30
1	D	746	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	C	507	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	164	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	755	ARG	CA-CB-CG	5.38	125.23	113.40
1	C	594	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	D	792	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	178	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	477	SER	N-CA-CB	5.36	118.53	110.50
1	C	519	SER	N-CA-CB	-5.35	102.47	110.50
1	B	184	LEU	CB-CA-C	-5.35	100.03	110.20
1	B	730	LEU	CB-CA-C	5.35	120.36	110.20
1	D	161	TYR	CZ-CE2-CD2	-5.34	114.99	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	917	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	D	781	ARG	CD-NE-CZ	5.34	131.08	123.60
1	A	46	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	746	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	233	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	595	THR	CA-CB-CG2	-5.34	104.92	112.40
1	A	832	ASP	N-CA-CB	-5.33	101.00	110.60
1	B	431	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	503	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	D	473	ARG	CD-NE-CZ	5.32	131.05	123.60
1	A	469	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	924	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	942	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	594	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	D	472	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	D	671	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	280	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	C	375	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	D	116	THR	CA-CB-CG2	-5.28	105.02	112.40
1	D	473	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	43	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	319	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	D	721	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	C	610	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	D	790	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	C	531	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	80	GLU	CG-CD-OE2	-5.25	107.80	118.30
1	D	319	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	439	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	D	869	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	411	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	786	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	522	LYS	CD-CE-NZ	-5.21	99.71	111.70
1	B	611	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	A	540[A]	HIS	N-CA-CB	-5.20	101.24	110.60
1	A	540[B]	HIS	N-CA-CB	-5.20	101.24	110.60
1	A	996	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	893	GLU	CA-CB-CG	5.20	124.84	113.40
1	B	843	GLN	O-C-N	5.19	131.01	122.70
1	B	164	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	429	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	863	GLN	CA-CB-CG	-5.19	101.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	524	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	D	395	HIS	N-CA-CB	-5.19	101.26	110.60
1	D	803	PRO	N-CA-CB	5.18	109.52	103.30
1	B	659	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	B	15	ASP	CB-CG-OD2	-5.17	113.64	118.30
1	A	782	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	A	916	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	76	CYS	CA-CB-SG	-5.17	104.69	114.00
1	A	800	ARG	N-CA-CB	-5.17	101.30	110.60
1	C	719	GLN	CB-CA-C	-5.16	100.08	110.40
1	A	671	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	B	492	ASP	CB-CG-OD1	5.15	122.93	118.30
1	B	881	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	B	296	GLU	OE1-CD-OE2	5.15	129.47	123.30
1	B	363	HIS	CA-CB-CG	-5.15	104.85	113.60
1	A	942	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	917	ARG	CD-NE-CZ	-5.14	116.41	123.60
1	D	881	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	802	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	C	371	THR	CA-CB-CG2	-5.12	105.23	112.40
1	C	1013	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	492	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	645	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	859	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	375	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	482	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	404	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	178	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	875	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	469	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	B	642	TYR	CB-CG-CD2	5.09	124.05	121.00
1	A	531	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	842	TRP	CG-CD2-CE3	-5.08	129.33	133.90
1	B	540[A]	HIS	N-CA-CB	-5.08	101.47	110.60
1	B	540[B]	HIS	N-CA-CB	-5.08	101.47	110.60
1	D	559	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	1018	LEU	CB-CA-C	-5.07	100.56	110.20
1	C	997	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	336	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	15	ASP	CB-CG-OD1	5.07	122.86	118.30
1	D	916	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	553	TRP	CA-CB-CG	-5.06	104.08	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	292	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	875	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	D	786	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	403	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	D	968	MET	CG-SD-CE	5.05	108.28	100.20
1	A	448	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	C	193	ASP	CB-CG-OD1	5.04	122.84	118.30
1	C	871	GLU	CB-CA-C	-5.04	100.33	110.40
1	D	52	ARG	CB-CA-C	-5.04	100.33	110.40
1	C	556	PHE	CB-CG-CD1	5.04	124.33	120.80
1	B	164	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	673	ALA	N-CA-CB	-5.03	103.06	110.10
1	A	309	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	A	782	ASP	CB-CG-OD1	5.03	122.82	118.30
1	A	164	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	630	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	721	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	D	800	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	D	671	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	D	845	GLN	C-N-CA	-5.01	111.78	122.30
1	D	721	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	C	438	GLU	CG-CD-OE2	-5.00	108.30	118.30

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	8128	0	7712	98	0
1	B	8128	0	7712	96	0
1	C	8128	0	7712	98	0
1	D	8128	0	7712	80	0
2	A	23	0	21	0	0
2	B	32	0	16	3	0
2	C	23	0	21	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	23	0	21	1	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	120	0	180	12	0
5	B	128	0	192	22	0
5	C	128	0	192	14	0
5	D	132	0	195	20	0
6	B	9	0	6	9	0
7	A	1144	0	0	11	0
7	B	1148	0	0	13	0
7	C	1126	0	0	14	0
7	D	1105	0	0	12	0
All	All	37685	0	31692	404	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 6.

All (404) 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)
5:A:8403:DMS:S	5:A:8403:DMS:C2	2.02	1.47
5:D:8423:DMS:C1	5:D:8423:DMS:S	2.01	1.47
5:C:8415:DMS:C2	5:C:8415:DMS:S	2.01	1.46
5:B:8407:DMS:S	5:B:8407:DMS:C2	2.05	1.45
5:B:8601:DMS:C2	5:B:8601:DMS:S	2.04	1.44
5:D:8429:DMS:C2	5:D:8429:DMS:S	2.05	1.43
5:D:8704:DMS:C1	5:D:8704:DMS:S	2.05	1.43
5:B:8415:DMS:C2	5:B:8415:DMS:S	2.06	1.42
5:B:8508:DMS:C1	5:B:8508:DMS:S	2.11	1.37
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.47	1.13
1:A:634:GLN:H	1:A:634:GLN:NE2	1.44	1.12
1:B:655:MET:HE2	1:B:665:SER:HB3	1.38	1.05
1:D:809:ARG:HG2	1:D:809:ARG:HH11	1.27	0.98
1:B:685:LEU:HD23	1:B:686:PRO:HD2	1.45	0.95
1:B:600:GLN:H	1:B:600:GLN:HE21	1.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.66	0.93
1:A:809:ARG:HH11	1:A:809:ARG:HG2	1.33	0.93
1:B:730:LEU:HD12	1:B:730:LEU:H	1.34	0.91
1:D:804:ASN:HD22	1:D:809:ARG:HH21	1.17	0.90
1:A:685:LEU:HD23	1:A:686:PRO:HD2	1.56	0.88
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.04	0.88
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.56	0.87
1:B:655:MET:CE	1:B:665:SER:HB3	2.06	0.85
1:A:634:GLN:H	1:A:634:GLN:HE21	1.23	0.85
1:C:745:MET:HA	1:C:761:GLN:HE22	1.44	0.83
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.22	0.81
1:A:292:ARG:HH12	5:A:8412:DMS:C2	1.93	0.81
1:B:685:LEU:CD2	1:B:686:PRO:HD2	2.10	0.80
1:A:600:GLN:H	1:A:600:GLN:HE21	1.30	0.79
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.62	0.79
1:D:658:LEU:O	1:D:661:LYS:HG3	1.83	0.79
1:A:1023:LYS:CB	1:A:1023:LYS:HZ2	1.94	0.78
1:A:735:HIS:ND1	1:A:735:HIS:N	2.31	0.78
1:B:262:GLN:HE21	1:B:263:GLY:N	1.82	0.78
1:A:292:ARG:HH12	5:A:8412:DMS:H23	1.48	0.77
1:A:685:LEU:CD2	1:A:686:PRO:HD2	2.15	0.76
1:A:737:ILE:HD11	7:A:9656:HOH:O	1.85	0.76
1:B:687:GLN:HG3	1:B:688:PRO:HD2	1.68	0.75
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.17	0.75
1:C:745:MET:HG2	7:C:9490:HOH:O	1.87	0.74
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.18	0.73
1:C:580:GLU:HG2	7:C:9648:HOH:O	1.88	0.73
1:A:634:GLN:N	1:A:634:GLN:NE2	2.29	0.73
1:A:1022:GLN:CG	1:A:1023:LYS:HZ1	2.02	0.73
1:C:367:MET:HA	1:C:367:MET:HE3	1.71	0.73
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.02	0.73
1:A:1022:GLN:HG2	1:A:1023:LYS:HE3	1.72	0.72
1:D:663:LEU:HD21	1:D:686:PRO:HG2	1.72	0.72
1:D:292:ARG:HH12	5:D:8412:DMS:H22	1.54	0.71
1:B:651:LEU:O	1:B:651:LEU:HD23	1.90	0.71
1:B:1017:GLN:HB2	7:B:9693:HOH:O	1.89	0.71
1:B:685:LEU:HD23	1:B:686:PRO:CD	2.20	0.71
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.06	0.71
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.71	0.70
1:B:1022:GLN:HG2	1:B:1023:LYS:N	2.05	0.70
1:D:685:LEU:HB3	1:D:686:PRO:CD	2.20	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.26	0.69
1:C:788:PRO:HD3	1:C:968:MET:CE	2.22	0.69
1:D:797:GLU:O	1:D:801:ILE:HD13	1.93	0.69
1:A:797:GLU:O	1:A:801:ILE:HD13	1.93	0.68
1:C:630:ARG:HD3	1:C:637:GLU:OE1	1.93	0.67
1:C:230:ARG:NH1	5:C:8418:DMS:H11	2.10	0.67
5:A:8420:DMS:H21	7:D:9535:HOH:O	1.95	0.66
1:C:278:ILE:HD13	1:C:278:ILE:N	2.11	0.66
1:B:230:ARG:HH21	5:B:8418:DMS:H11	1.60	0.66
1:A:861:SER:OG	1:A:863:GLN:HG3	1.95	0.66
1:D:809:ARG:NH1	1:D:809:ARG:HG2	2.04	0.65
1:C:356:ARG:HD2	1:C:379:MET:CE	2.26	0.65
1:B:473:ARG:NH1	1:B:477:SER:HB2	2.11	0.65
1:A:770:ILE:O	1:A:773:LYS:HD3	1.97	0.65
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.29	0.65
1:D:134:LEU:HA	5:D:8705:DMS:H22	1.77	0.65
1:A:277:GLU:H	1:A:277:GLU:CD	1.96	0.65
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.30	0.64
1:B:878:HIS:HD2	7:B:8805:HOH:O	1.79	0.64
1:A:685:LEU:HD23	1:A:686:PRO:CD	2.26	0.64
1:B:863:GLN:HG2	1:B:1019:VAL:HG11	1.79	0.64
1:C:230:ARG:NH1	7:C:8967:HOH:O	2.30	0.64
1:B:262:GLN:HE21	1:B:262:GLN:C	2.01	0.64
1:D:687:GLN:OE1	1:D:687:GLN:N	2.31	0.63
1:B:890:GLN:HB2	7:B:9801:HOH:O	1.98	0.63
1:B:1022:GLN:HG2	1:B:1023:LYS:O	1.99	0.63
1:C:816:TYR:CE1	1:C:968:MET:HE1	2.34	0.63
1:A:878:HIS:HD2	7:A:8676:HOH:O	1.81	0.63
5:D:8703:DMS:H23	7:D:9708:HOH:O	1.98	0.62
1:B:745:MET:HE2	1:B:745:MET:HA	1.79	0.62
1:D:135:GLN:C	1:D:136:GLU:HG2	2.19	0.62
5:B:8423:DMS:H13	7:B:9818:HOH:O	1.99	0.62
1:D:663:LEU:CD2	1:D:686:PRO:HG2	2.29	0.62
1:A:1022:GLN:HG2	1:A:1023:LYS:CE	2.30	0.62
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.82	0.62
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.35	0.61
1:B:600:GLN:N	1:B:600:GLN:HE21	1.94	0.61
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.83	0.61
5:D:8429:DMS:C2	5:D:8429:DMS:C1	2.78	0.61
1:D:749:ILE:N	1:D:749:ILE:HD12	2.15	0.60
1:C:878:HIS:HD2	7:C:8701:HOH:O	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:618:THR:HG21	7:D:9060:HOH:O	2.00	0.60
1:A:1022:GLN:CD	1:A:1023:LYS:HZ1	2.05	0.60
1:C:595:THR:HG22	5:C:8413:DMS:S	2.41	0.60
1:B:157:ARG:HD3	7:B:9582:HOH:O	2.02	0.59
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.83	0.59
1:B:687:GLN:HG3	1:B:688:PRO:CD	2.30	0.59
1:C:178:ARG:HD2	7:C:9579:HOH:O	2.01	0.59
1:A:773:LYS:HD3	1:A:773:LYS:H	1.67	0.59
1:B:655:MET:HE2	1:B:665:SER:CB	2.22	0.59
1:B:730:LEU:H	1:B:730:LEU:CD1	1.95	0.59
1:D:579:ASP:OD1	1:D:581:ASN:HB2	2.01	0.59
1:A:887:GLN:NE2	1:A:980:GLU:O	2.34	0.59
1:D:878:HIS:HD2	7:D:8818:HOH:O	1.85	0.59
1:D:363:HIS:HD2	7:D:9332:HOH:O	1.84	0.58
1:B:699:ARG:HH21	5:B:8415:DMS:C1	2.17	0.58
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.86	0.58
1:B:615:PRO:O	1:B:618:THR:HG22	2.03	0.58
1:B:797:GLU:O	1:B:801:ILE:HD13	2.04	0.58
1:A:1023:LYS:HB2	1:A:1023:LYS:HZ2	1.69	0.58
1:C:237:ARG:HB3	1:C:237:ARG:NH1	2.19	0.58
1:C:367:MET:HB3	1:C:372:MET:CE	2.34	0.57
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.86	0.57
1:D:664:ALA:HB3	1:D:685:LEU:CD2	2.34	0.57
1:C:473:ARG:NH2	7:C:8614:HOH:O	2.37	0.57
1:C:651:LEU:C	1:C:651:LEU:HD12	2.24	0.57
1:C:749:ILE:HD12	1:C:749:ILE:N	2.20	0.57
1:C:788:PRO:HD3	1:C:968:MET:HE3	1.88	0.56
1:D:748:CYS:C	1:D:749:ILE:HD12	2.25	0.56
1:A:595:THR:HA	1:A:596:PRO:C	2.25	0.56
1:C:367:MET:HE1	7:C:9665:HOH:O	2.05	0.56
1:A:387:VAL:HG22	7:A:9694:HOH:O	2.06	0.56
1:B:658:LEU:HB2	1:B:663:LEU:HD11	1.87	0.56
1:A:651:LEU:HD12	1:A:651:LEU:C	2.25	0.56
1:C:811:LYS:HD2	5:C:8424:DMS:C1	2.36	0.56
1:B:800:ARG:HD3	7:B:9817:HOH:O	2.06	0.56
1:A:292:ARG:HH12	5:A:8412:DMS:H22	1.72	0.55
1:C:367:MET:HB3	1:C:372:MET:HE2	1.86	0.55
1:D:473:ARG:NE	7:D:9481:HOH:O	2.31	0.55
1:C:367:MET:HE3	1:C:367:MET:CA	2.35	0.55
1:D:618:THR:HG23	7:D:9077:HOH:O	2.05	0.55
1:A:809:ARG:CG	1:A:809:ARG:HH11	2.12	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LYS:HE2	7:A:9035:HOH:O	2.07	0.55
1:A:646:HIS:ND1	7:A:9463:HOH:O	2.28	0.54
1:B:36:TRP:HZ2	5:B:8501:DMS:C1	2.21	0.54
1:D:663:LEU:CD2	1:D:686:PRO:HD2	2.37	0.54
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.89	0.54
1:C:356:ARG:HD2	1:C:379:MET:HE3	1.88	0.54
1:A:654:TRP:CZ2	1:A:683:PRO:HG2	2.43	0.54
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.90	0.54
1:B:363:HIS:HD2	7:B:9311:HOH:O	1.90	0.54
1:B:230:ARG:HH21	5:B:8418:DMS:C1	2.20	0.54
1:A:88:SER:HA	1:A:366:VAL:HG21	1.90	0.54
1:B:639:THR:OG1	1:B:677:LYS:HD3	2.08	0.54
1:B:699:ARG:NH1	7:B:9823:HOH:O	2.41	0.53
1:B:797:GLU:HG2	1:B:799:THR:HG23	1.89	0.53
1:A:655:MET:HE2	1:A:656:VAL:N	2.23	0.53
5:D:8428:DMS:H22	7:D:9768:HOH:O	2.08	0.53
1:A:688:PRO:C	1:A:690:SER:H	2.11	0.53
1:D:595:THR:HA	1:D:596:PRO:C	2.29	0.52
5:C:8406:DMS:H13	7:C:9718:HOH:O	2.09	0.52
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.90	0.52
1:C:230:ARG:CZ	5:C:8418:DMS:H12	2.40	0.52
1:C:724:GLU:O	1:D:847:LYS:NZ	2.42	0.51
1:A:764:PHE:CE2	1:A:781:ARG:NH1	2.78	0.51
1:B:45:ASP:O	5:B:8501:DMS:H11	2.10	0.51
7:B:9512:HOH:O	5:C:8420:DMS:H21	2.10	0.51
1:C:240:LEU:HD23	1:C:240:LEU:C	2.31	0.51
5:A:8428:DMS:H11	7:A:8812:HOH:O	2.10	0.51
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.46	0.51
1:A:251:ARG:HA	5:A:8416:DMS:S	2.51	0.51
1:B:651:LEU:C	1:B:651:LEU:HD23	2.31	0.51
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.94	0.50
1:B:634:GLN:HG2	1:B:682:LEU:O	2.12	0.50
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.46	0.50
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.95	0.50
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.12	0.50
1:B:713:HIS:ND1	7:B:9513:HOH:O	2.35	0.50
1:D:634:GLN:OE1	1:D:682:LEU:O	2.29	0.50
1:A:688:PRO:O	1:A:690:SER:N	2.45	0.49
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.94	0.49
5:B:8407:DMS:C1	5:B:8407:DMS:C2	2.89	0.49
1:B:699:ARG:NH2	5:B:8415:DMS:C1	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:600:GLN:H	1:B:600:GLN:NE2	1.97	0.49
1:D:664:ALA:CB	1:D:685:LEU:HD23	2.42	0.49
1:A:668:VAL:HG12	1:A:669:PRO:O	2.12	0.49
1:A:699:ARG:NH2	7:A:9479:HOH:O	2.46	0.49
1:A:738:PRO:HD3	1:A:751:LEU:HD13	1.95	0.49
1:A:773:LYS:N	1:A:773:LYS:HD3	2.27	0.49
1:C:844:HIS:HD2	7:C:9496:HOH:O	1.95	0.49
1:C:835:LEU:HD11	1:C:855:THR:HB	1.93	0.49
1:C:824:GLN:HG3	1:C:825:CYS:N	2.28	0.49
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.48	0.49
1:C:634:GLN:OE1	1:C:635:THR:OG1	2.29	0.49
1:D:133:TRP:O	5:D:8705:DMS:H22	2.13	0.49
1:B:36:TRP:HZ2	5:B:8501:DMS:H12	1.78	0.49
1:A:685:LEU:O	1:A:687:GLN:NE2	2.46	0.49
1:C:824:GLN:CG	1:C:825:CYS:N	2.74	0.48
1:C:595:THR:HA	1:C:596:PRO:C	2.33	0.48
1:D:663:LEU:HD23	1:D:686:PRO:HD2	1.95	0.48
1:C:651:LEU:O	1:C:651:LEU:HD12	2.12	0.48
1:C:730:LEU:H	1:C:730:LEU:HD12	1.78	0.48
1:A:230:ARG:NH1	5:A:8418:DMS:C1	2.76	0.48
1:A:738:PRO:HD3	1:A:860:GLY:HA2	1.94	0.48
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.48	0.48
1:A:251:ARG:HH11	5:A:8416:DMS:H22	1.78	0.48
1:C:230:ARG:NH1	5:C:8418:DMS:C1	2.75	0.48
1:C:147:ASN:HA	1:C:148:SER:HA	1.64	0.48
1:A:867:THR:HB	7:A:9360:HOH:O	2.13	0.48
1:A:147:ASN:HA	1:A:148:SER:HA	1.60	0.48
1:C:615:PRO:O	1:C:618:THR:HG22	2.13	0.47
1:B:655:MET:SD	1:B:656:VAL:N	2.88	0.47
1:C:816:TYR:CE1	1:C:968:MET:CE	2.98	0.47
1:A:742:THR:HG22	1:A:743:SER:N	2.28	0.47
1:D:686:PRO:O	1:D:687:GLN:HG3	2.14	0.47
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.96	0.47
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.98	0.47
1:A:178:ARG:HD2	7:A:9492:HOH:O	2.13	0.47
1:C:655:MET:CE	1:C:662:PRO:HB3	2.44	0.47
5:B:8428:DMS:H12	7:B:9754:HOH:O	2.14	0.47
1:D:134:LEU:O	5:D:8705:DMS:H21	2.15	0.47
1:C:730:LEU:CD1	1:C:730:LEU:H	2.04	0.47
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.13	0.47
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:THR:OG1	1:B:681:GLU:OE2	2.28	0.47
1:D:230:ARG:HH21	5:D:8418:DMS:H11	1.80	0.47
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.97	0.47
1:B:687:GLN:CG	1:B:688:PRO:HD2	2.42	0.47
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.50	0.47
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.95	0.47
1:D:88:SER:HA	1:D:366:VAL:HG21	1.97	0.47
1:C:655:MET:SD	1:C:656:VAL:N	2.88	0.46
1:D:134:LEU:CA	5:D:8705:DMS:H22	2.45	0.46
1:B:36:TRP:CZ2	5:B:8501:DMS:H13	2.51	0.46
1:D:251:ARG:NH2	7:D:9800:HOH:O	2.47	0.46
1:B:685:LEU:CG	1:B:686:PRO:HD2	2.45	0.46
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.50	0.46
1:C:88:SER:HA	1:C:366:VAL:HG21	1.96	0.46
1:B:230:ARG:NH2	5:B:8418:DMS:C1	2.78	0.46
1:D:651:LEU:HD12	1:D:668:VAL:O	2.14	0.46
1:D:133:TRP:HE1	5:D:8703:DMS:H23	1.79	0.46
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.41	0.46
1:A:634:GLN:H	1:A:634:GLN:CD	2.07	0.46
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.96	0.46
1:D:128:ASN:HB3	1:D:180:GLY:O	2.15	0.46
1:A:230:ARG:NH1	5:A:8418:DMS:H12	2.31	0.46
1:C:653:HIS:CE1	1:C:667:GLU:CG	3.00	0.45
1:C:320:GLY:HA2	5:C:8406:DMS:O	2.16	0.45
1:C:781:ARG:NH1	7:C:9379:HOH:O	2.49	0.45
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.79	0.45
1:B:824:GLN:OE1	1:B:837:THR:HG22	2.16	0.45
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.98	0.45
1:A:1022:GLN:CD	1:A:1023:LYS:NZ	2.70	0.45
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.80	0.45
1:B:811:LYS:HD2	5:B:8424:DMS:C1	2.45	0.45
1:D:663:LEU:HD23	1:D:686:PRO:CD	2.46	0.45
1:B:36:TRP:CZ2	5:B:8501:DMS:C1	3.00	0.45
1:C:658:LEU:O	1:C:659:ASP:C	2.53	0.45
1:A:1022:GLN:NE2	1:A:1023:LYS:HE2	2.32	0.45
1:C:595:THR:O	1:C:595:THR:HG23	2.15	0.45
1:B:595:THR:HA	1:B:596:PRO:C	2.37	0.45
1:B:147:ASN:HA	1:B:148:SER:HA	1.66	0.45
1:A:819:GLU:HG3	7:A:9703:HOH:O	2.17	0.45
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.99	0.45
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:997:ASP:HB2	1:A:999:TRP:CZ2	2.52	0.44
1:D:725:ASN:HB2	7:D:9591:HOH:O	2.17	0.44
1:D:887:GLN:OE1	1:D:980:GLU:O	2.36	0.44
1:D:991:MET:HE2	1:D:1003:VAL:HG21	1.99	0.44
1:B:178:ARG:HG3	1:B:178:ARG:O	2.18	0.44
1:B:847:LYS:HG3	1:B:848:THR:N	2.32	0.44
1:C:625:GLN:NE2	7:C:8830:HOH:O	2.45	0.44
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.34	0.44
1:C:667:GLU:C	1:C:668:VAL:HG23	2.37	0.44
1:C:655:MET:HE3	1:C:662:PRO:HB3	1.99	0.44
1:B:262:GLN:NE2	1:B:262:GLN:CA	2.80	0.44
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.47	0.44
1:B:809:ARG:NH2	7:B:9728:HOH:O	2.51	0.44
1:D:829:THR:O	1:D:830:LEU:HD23	2.17	0.44
1:A:600:GLN:N	1:A:600:GLN:HE21	2.07	0.44
1:C:237:ARG:CB	1:C:237:ARG:HH11	2.31	0.44
1:B:824:GLN:HG2	1:B:825:CYS:N	2.33	0.44
1:A:687:GLN:HG3	7:A:9470:HOH:O	2.18	0.44
1:A:251:ARG:HG3	1:A:253:TYR:CZ	2.52	0.44
1:C:751:LEU:HD21	1:C:860:GLY:O	2.19	0.43
1:C:765:LEU:HD21	1:C:768:MET:CE	2.48	0.43
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.52	0.43
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.48	0.43
1:C:890:GLN:HG3	1:C:891:VAL:N	2.33	0.43
1:A:59:ARG:HG2	5:A:8502:DMS:H11	2.00	0.43
1:B:731:PRO:O	1:B:732:ALA:HB2	2.17	0.43
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.54	0.43
1:C:230:ARG:HG3	5:C:8418:DMS:C1	2.49	0.43
1:C:718:GLN:HG2	5:C:8503:DMS:C1	2.48	0.43
1:D:128:ASN:HB2	7:D:9726:HOH:O	2.19	0.43
1:A:756:TRP:CD2	1:A:858:ILE:HD13	2.53	0.43
1:A:663:LEU:HA	1:A:663:LEU:HD22	1.71	0.43
1:B:663:LEU:HD12	1:B:694:LEU:CD2	2.49	0.43
1:C:266:GLN:O	5:C:8602:DMS:H22	2.19	0.43
1:D:629:PHE:O	1:D:630:ARG:HD3	2.18	0.43
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.00	0.43
1:D:770:ILE:HA	1:D:770:ILE:HD13	1.67	0.43
1:A:654:TRP:HZ2	1:A:683:PRO:HG2	1.83	0.43
1:B:699:ARG:NH2	5:B:8415:DMS:H11	2.34	0.43
1:C:968:MET:HE2	1:C:968:MET:HB2	1.59	0.43
1:A:251:ARG:HH11	5:A:8416:DMS:C2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:754:LYS:HG2	1:D:770:ILE:CD1	2.48	0.43
1:D:664:ALA:HB3	1:D:685:LEU:HD23	2.00	0.43
1:D:708:TRP:CZ2	5:D:8403:DMS:H12	2.54	0.43
1:D:720:TRP:NE1	5:D:8503:DMS:O	2.48	0.43
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.01	0.43
1:B:88:SER:HA	1:B:366:VAL:HG21	2.01	0.43
1:C:748:CYS:C	1:C:749:ILE:HD12	2.39	0.42
1:D:78:LEU:HA	1:D:78:LEU:HD23	1.89	0.42
1:D:682:LEU:HD23	1:D:682:LEU:HA	1.76	0.42
1:B:577:LYS:HB3	1:B:577:LYS:HE3	1.87	0.42
1:B:70:PRO:HG2	1:B:78:LEU:HD21	2.01	0.42
1:A:890:GLN:OE1	1:A:948:PRO:HD3	2.19	0.42
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.19	0.42
1:B:262:GLN:NE2	1:B:262:GLN:HA	2.34	0.42
1:C:997:ASP:HB2	1:C:999:TRP:CE2	2.54	0.42
1:D:577:LYS:O	1:D:584:PRO:HA	2.19	0.42
1:A:59:ARG:NH2	1:A:81:ALA:HB3	2.35	0.42
5:D:8423:DMS:C1	5:D:8423:DMS:C2	2.96	0.42
1:C:230:ARG:CZ	5:C:8418:DMS:C1	2.97	0.42
1:A:859:ASP:OD1	1:A:861:SER:OG	2.27	0.42
1:B:1022:GLN:HG2	1:B:1023:LYS:H	1.83	0.42
1:C:655:MET:SD	1:C:656:VAL:O	2.77	0.42
1:A:472:TYR:O	1:A:476:LYS:HG2	2.20	0.42
1:C:472:TYR:OH	1:C:476:LYS:HE2	2.19	0.42
1:C:684:GLU:HG2	1:C:685:LEU:N	2.34	0.42
1:C:651:LEU:HD13	1:C:653:HIS:ND1	2.35	0.42
1:B:230:ARG:NH2	5:B:8418:DMS:H12	2.34	0.42
1:A:688:PRO:O	1:A:689:GLU:HB2	2.18	0.42
1:A:745:MET:HE2	1:A:745:MET:HB3	1.80	0.42
1:D:650:GLU:HB3	1:D:670:LEU:HD12	2.02	0.42
1:A:1022:GLN:CG	1:A:1023:LYS:NZ	2.80	0.42
1:C:127:PHE:HE1	1:C:184:LEU:HG	1.85	0.42
1:D:893:GLU:HG2	1:D:894:ARG:HG2	2.02	0.42
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.54	0.42
1:A:986:ILE:HG21	1:A:986:ILE:HD12	1.83	0.42
1:D:699:ARG:HB3	1:D:699:ARG:HE	1.51	0.42
1:A:684:GLU:HG2	1:A:685:LEU:N	2.35	0.41
1:B:651:LEU:HD22	1:B:701:VAL:O	2.20	0.41
1:C:367:MET:CE	1:C:367:MET:HA	2.47	0.41
1:B:763:GLY:HA3	1:B:822:LEU:HD13	2.01	0.41
1:A:668:VAL:HG13	1:A:669:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.55	0.41
1:A:111:PRO:HA	1:A:112:PRO:HA	1.85	0.41
1:D:46:ARG:HB3	1:D:47:PRO:HD2	2.02	0.41
1:B:292:ARG:NH1	5:B:8412:DMS:H22	2.36	0.41
1:A:1022:GLN:NE2	1:A:1023:LYS:CE	2.84	0.41
1:C:653:HIS:ND1	1:C:667:GLU:CG	2.78	0.41
1:B:114:VAL:HB	1:B:115:PRO:HD2	2.01	0.41
1:B:730:LEU:HD12	1:B:730:LEU:N	2.17	0.41
1:D:134:LEU:HA	5:D:8705:DMS:C2	2.50	0.41
1:D:788:PRO:HD2	1:D:968:MET:HG3	2.03	0.41
1:B:699:ARG:HE	1:B:714:ILE:HD13	1.85	0.41
1:A:634:GLN:N	1:A:634:GLN:HE21	2.03	0.41
1:D:545:SER:O	1:D:909:ARG:HD3	2.21	0.41
1:C:749:ILE:O	1:C:755:ARG:HA	2.21	0.41
1:D:102:ASN:HB3	5:D:8506:DMS:H11	2.02	0.41
1:D:844:HIS:O	1:D:845:GLN:HB2	2.20	0.41
1:D:663:LEU:CD2	1:D:686:PRO:CG	2.98	0.41
1:C:788:PRO:HD3	1:C:968:MET:HE2	2.01	0.41
1:D:230:ARG:NH2	5:D:8418:DMS:C1	2.84	0.41
1:C:363:HIS:HD2	7:C:9215:HOH:O	2.03	0.41
1:B:475:ILE:HG21	1:B:475:ILE:HD13	1.86	0.41
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.37	0.41
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.56	0.41
1:D:240:LEU:HD23	1:D:240:LEU:C	2.42	0.41
1:D:513:PRO:O	1:D:514:ALA:HB3	2.21	0.41
2:D:2001:LAK:C4	7:D:9024:HOH:O	2.68	0.41
1:B:13:ARG:NH1	7:C:8622:HOH:O	2.54	0.41
1:C:13:ARG:O	1:C:14:ARG:C	2.59	0.41
1:C:859:ASP:OD1	1:C:861:SER:OG	2.27	0.41
1:A:737:ILE:HD12	1:A:738:PRO:O	2.21	0.40
1:C:278:ILE:HD12	1:C:278:ILE:HA	1.82	0.40
1:B:663:LEU:CD1	1:B:694:LEU:HD21	2.51	0.40
5:B:8501:DMS:H22	7:B:9183:HOH:O	2.21	0.40
1:B:127:PHE:N	1:B:127:PHE:CD1	2.90	0.40
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.50	0.40
1:C:746:ASP:HA	1:C:760:ARG:HG3	2.03	0.40
1:D:688:PRO:C	1:D:690:SER:H	2.23	0.40
1:C:811:LYS:HD2	5:C:8424:DMS:S	2.62	0.40
1:B:646:HIS:ND1	1:B:673:ALA:HA	2.37	0.40
1:B:360:HIS:HE1	1:B:362:LEU:HD12	1.85	0.40
1:B:835:LEU:HD11	1:B:855:THR:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:687:GLN:HA	1:D:688:PRO:HD3	1.48	0.40
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.91	0.40
1:C:819:GLU:H	1:C:819:GLU:HG2	1.25	0.40
1:C:569:ASP:HB2	7:C:9439:HOH:O	2.22	0.40
1:B:745:MET:HE2	1:B:745:MET:CA	2.48	0.40
1:C:416:GLU:OE2	1:C:418:HIS:HB2	2.21	0.40
1:D:472:TYR:O	1:D:476:LYS:HG2	2.21	0.40
1:A:427:THR:HG21	1:A:462:SER:HB3	2.02	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	1011/1023 (99%)	977 (97%)	33 (3%)	1 (0%)	56	26
1	B	1011/1023 (99%)	976 (96%)	31 (3%)	4 (0%)	39	14
1	C	1011/1023 (99%)	979 (97%)	31 (3%)	1 (0%)	56	26
1	D	1011/1023 (99%)	978 (97%)	29 (3%)	4 (0%)	39	14
All	All	4044/4092 (99%)	3910 (97%)	124 (3%)	10 (0%)	52	25

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	731	PRO
1	B	732	ALA
1	B	690	SER
1	D	688	PRO
1	D	539[A]	ALA
1	D	539[B]	ALA
1	C	164	ASP

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Mol	Chain	Res	Type
1	D	164	ASP
1	A	164	ASP
1	B	164	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	865/875 (99%)	836 (97%)	29 (3%)	44	11
1	B	865/875 (99%)	844 (98%)	21 (2%)	57	22
1	C	865/875 (99%)	835 (96%)	30 (4%)	43	11
1	D	865/875 (99%)	837 (97%)	28 (3%)	46	13
All	All	3460/3500 (99%)	3352 (97%)	108 (3%)	47	14

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	GLU
1	A	250	LEU
1	A	262	GLN
1	A	333	ARG
1	A	344	LEU
1	A	394	ASN
1	A	473	ARG
1	A	519	SER
1	A	535	LEU
1	A	546	LEU
1	A	580	GLU
1	A	595	THR
1	A	600	GLN
1	A	632	SER
1	A	634	GLN
1	A	655	MET
1	A	663	LEU
1	A	667	GLU

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Mol	Chain	Res	Type
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	799	THR
1	A	809	ARG
1	A	817	GLN
1	A	885	ASN
1	A	956	GLN
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	76	CYS
1	B	80	GLU
1	B	237	ARG
1	B	262	GLN
1	B	333	ARG
1	B	370	GLN
1	B	394	ASN
1	B	535	LEU
1	B	546	LEU
1	B	554	GLN
1	B	600	GLN
1	B	651	LEU
1	B	685	LEU
1	B	687	GLN
1	B	690	SER
1	B	730	LEU
1	B	799	THR
1	B	819	GLU
1	B	847	LYS
1	B	863	GLN
1	B	885	ASN
1	C	71	GLU
1	C	75	GLU
1	C	80	GLU
1	C	135	GLN
1	C	189	LEU
1	C	262	GLN
1	C	278	ILE
1	C	333	ARG
1	C	344	LEU
1	C	370	GLN

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Mol	Chain	Res	Type
1	C	394	ASN
1	C	513	PRO
1	C	535	LEU
1	C	546	LEU
1	C	580	GLU
1	C	634	GLN
1	C	653	HIS
1	C	663	LEU
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	690	SER
1	C	730	LEU
1	C	737	ILE
1	C	750	GLU
1	C	772	ASP
1	C	773	LYS
1	C	819	GLU
1	C	1023	LYS
1	D	13	ARG
1	D	112	PRO
1	D	277	GLU
1	D	333	ARG
1	D	344	LEU
1	D	370	GLN
1	D	394	ASN
1	D	519	SER
1	D	546	LEU
1	D	652	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	687	GLN
1	D	699	ARG
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	799	THR
1	D	809	ARG

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Mol	Chain	Res	Type
1	D	845	GLN
1	D	893	GLU
1	D	956	GLN
1	D	986	ILE
1	D	1017	GLN
1	D	1022	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	GLN
1	A	600	GLN
1	A	624	GLN
1	A	634	GLN
1	A	675	GLN
1	A	817	GLN
1	A	824	GLN
1	A	844	HIS
1	A	878	HIS
1	A	977	HIS
1	A	1017	GLN
1	A	1022	GLN
1	B	262	GLN
1	B	363	HIS
1	B	510	GLN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	675	GLN
1	B	687	GLN
1	B	878	HIS
1	C	49	GLN
1	C	266	GLN
1	C	363	HIS
1	C	624	GLN
1	C	761	GLN
1	C	844	HIS
1	C	878	HIS
1	C	977	HIS
1	D	294	ASN
1	D	363	HIS

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Mol	Chain	Res	Type
1	D	624	GLN
1	D	628	GLN
1	D	804	ASN
1	D	878	HIS
1	D	887	GLN
1	D	977	HIS

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 ⓘ

Of 165 ligands modelled in this entry, 32 are monoatomic - leaving 133 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	LAK	A	2001	4	24,24,24	1.24	3 (12%)	35,35,35	1.23	3 (8%)
5	DMS	A	8401	-	3,3,3	0.79	0	3,3,3	0.42	0
5	DMS	A	8402	-	3,3,3	1.73	1 (33%)	3,3,3	0.28	0
5	DMS	A	8403	-	3,3,3	2.26	1 (33%)	3,3,3	0.54	0
5	DMS	A	8404	-	3,3,3	1.28	0	3,3,3	0.22	0
5	DMS	A	8405	-	3,3,3	1.30	1 (33%)	3,3,3	0.71	0
5	DMS	A	8406	-	3,3,3	0.92	0	3,3,3	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8407	-	3,3,3	2.38	1 (33%)	3,3,3	1.22	1 (33%)
5	DMS	A	8408	-	3,3,3	0.26	0	3,3,3	0.73	0
5	DMS	A	8409	-	3,3,3	2.70	1 (33%)	3,3,3	0.88	0
5	DMS	A	8410	-	3,3,3	1.12	0	3,3,3	0.67	0
5	DMS	A	8411	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	A	8412	-	3,3,3	0.80	0	3,3,3	0.38	0
5	DMS	A	8413	-	3,3,3	2.52	3 (100%)	3,3,3	0.67	0
5	DMS	A	8414	-	3,3,3	1.82	1 (33%)	3,3,3	0.20	0
5	DMS	A	8416	-	3,3,3	2.32	1 (33%)	3,3,3	0.41	0
5	DMS	A	8417	-	3,3,3	1.47	1 (33%)	3,3,3	0.61	0
5	DMS	A	8418	-	3,3,3	0.99	0	3,3,3	0.36	0
5	DMS	A	8419	-	3,3,3	0.93	0	3,3,3	0.56	0
5	DMS	A	8420	-	3,3,3	1.24	0	3,3,3	0.84	0
5	DMS	A	8421	-	3,3,3	1.17	0	3,3,3	0.87	0
5	DMS	A	8423	-	3,3,3	2.00	2 (66%)	3,3,3	0.44	0
5	DMS	A	8424	-	3,3,3	1.23	0	3,3,3	0.35	0
5	DMS	A	8425	4	3,3,3	2.53	3 (100%)	3,3,3	1.05	0
5	DMS	A	8428	-	3,3,3	1.24	1 (33%)	3,3,3	0.38	0
5	DMS	A	8501	-	3,3,3	1.40	0	3,3,3	0.57	0
5	DMS	A	8502	-	3,3,3	2.22	2 (66%)	3,3,3	1.51	1 (33%)
5	DMS	A	8503	-	3,3,3	1.06	0	3,3,3	1.19	1 (33%)
5	DMS	A	8504	-	3,3,3	1.32	1 (33%)	3,3,3	0.34	0
5	DMS	A	8506	-	3,3,3	2.32	2 (66%)	3,3,3	0.41	0
5	DMS	A	8602	-	3,3,3	1.11	0	3,3,3	0.43	0
2	LAK	B	2001[A]	-	24,24,24	1.24	2 (8%)	35,35,35	1.44	7 (20%)
2	LAK	B	2002[B]	-	5,8,24	1.42	1 (20%)	4,10,35	1.68	1 (25%)
6	TAR	B	2003[C]	-	5,8,9	1.45	1 (20%)	4,10,12	1.57	1 (25%)
5	DMS	B	8401	-	3,3,3	0.88	0	3,3,3	0.37	0
5	DMS	B	8402	-	3,3,3	1.89	2 (66%)	3,3,3	0.52	0
5	DMS	B	8403	-	3,3,3	1.57	0	3,3,3	0.40	0
5	DMS	B	8404	-	3,3,3	1.27	0	3,3,3	0.22	0
5	DMS	B	8405	-	3,3,3	1.45	0	3,3,3	0.54	0
5	DMS	B	8407	-	3,3,3	2.87	2 (66%)	3,3,3	0.25	0
5	DMS	B	8408	-	3,3,3	0.88	0	3,3,3	0.14	0
5	DMS	B	8409	-	3,3,3	2.29	1 (33%)	3,3,3	0.41	0
5	DMS	B	8410	-	3,3,3	1.68	1 (33%)	3,3,3	0.25	0
5	DMS	B	8411	-	3,3,3	1.08	0	3,3,3	0.41	0
5	DMS	B	8412	-	3,3,3	0.80	0	3,3,3	0.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8413	-	3,3,3	2.94	2 (66%)	3,3,3	0.56	0
5	DMS	B	8414	-	3,3,3	0.55	0	3,3,3	1.02	0
5	DMS	B	8415	-	3,3,3	2.72	1 (33%)	3,3,3	1.00	0
5	DMS	B	8416	-	3,3,3	1.14	0	3,3,3	0.34	0
5	DMS	B	8417	-	3,3,3	1.29	0	3,3,3	0.36	0
5	DMS	B	8418	-	3,3,3	0.72	0	3,3,3	0.53	0
5	DMS	B	8419	-	3,3,3	1.29	0	3,3,3	0.25	0
5	DMS	B	8420	-	3,3,3	1.69	1 (33%)	3,3,3	0.47	0
5	DMS	B	8421	-	3,3,3	0.32	0	3,3,3	0.30	0
5	DMS	B	8423	-	3,3,3	0.72	0	3,3,3	0.63	0
5	DMS	B	8424	-	3,3,3	0.98	0	3,3,3	0.13	0
5	DMS	B	8425	4	3,3,3	2.33	2 (66%)	3,3,3	0.29	0
5	DMS	B	8428	-	3,3,3	1.55	1 (33%)	3,3,3	0.32	0
5	DMS	B	8429	-	3,3,3	2.50	2 (66%)	3,3,3	0.76	0
5	DMS	B	8501	-	3,3,3	1.00	0	3,3,3	0.27	0
5	DMS	B	8502	-	3,3,3	1.18	0	3,3,3	2.03	1 (33%)
5	DMS	B	8504	-	3,3,3	0.43	0	3,3,3	0.31	0
5	DMS	B	8506	-	3,3,3	1.62	1 (33%)	3,3,3	0.45	0
5	DMS	B	8508	-	3,3,3	3.18	2 (66%)	3,3,3	0.70	0
5	DMS	B	8601	-	3,3,3	2.23	1 (33%)	3,3,3	0.91	0
5	DMS	B	8706	-	3,3,3	1.72	1 (33%)	3,3,3	0.41	0
2	LAK	C	2001	4	24,24,24	1.31	3 (12%)	35,35,35	1.37	5 (14%)
5	DMS	C	8401	-	3,3,3	1.08	0	3,3,3	0.36	0
5	DMS	C	8402	-	3,3,3	1.88	1 (33%)	3,3,3	0.43	0
5	DMS	C	8403	-	3,3,3	1.22	0	3,3,3	0.48	0
5	DMS	C	8404	-	3,3,3	0.91	0	3,3,3	0.76	0
5	DMS	C	8405	-	3,3,3	1.76	1 (33%)	3,3,3	0.60	0
5	DMS	C	8406	-	3,3,3	0.77	0	3,3,3	0.19	0
5	DMS	C	8407	-	3,3,3	1.71	1 (33%)	3,3,3	0.44	0
5	DMS	C	8408	-	3,3,3	0.89	0	3,3,3	0.71	0
5	DMS	C	8409	-	3,3,3	2.35	1 (33%)	3,3,3	0.70	0
5	DMS	C	8410	-	3,3,3	1.19	0	3,3,3	0.23	0
5	DMS	C	8411	-	3,3,3	1.01	0	3,3,3	0.37	0
5	DMS	C	8412	-	3,3,3	1.66	1 (33%)	3,3,3	0.45	0
5	DMS	C	8413	-	3,3,3	2.09	1 (33%)	3,3,3	0.53	0
5	DMS	C	8414	-	3,3,3	1.26	0	3,3,3	0.93	0
5	DMS	C	8415	-	3,3,3	2.56	2 (66%)	3,3,3	0.92	0
5	DMS	C	8416	-	3,3,3	2.11	2 (66%)	3,3,3	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8417	-	3,3,3	0.79	0	3,3,3	0.98	0
5	DMS	C	8418	-	3,3,3	1.98	1 (33%)	3,3,3	1.43	1 (33%)
5	DMS	C	8419	-	3,3,3	0.87	0	3,3,3	0.21	0
5	DMS	C	8420	-	3,3,3	2.44	1 (33%)	3,3,3	0.90	0
5	DMS	C	8421	-	3,3,3	1.18	0	3,3,3	1.16	0
5	DMS	C	8423	-	3,3,3	1.07	0	3,3,3	0.38	0
5	DMS	C	8424	-	3,3,3	1.13	0	3,3,3	0.59	0
5	DMS	C	8425	4	3,3,3	1.61	1 (33%)	3,3,3	0.34	0
5	DMS	C	8429	-	3,3,3	1.38	1 (33%)	3,3,3	0.32	0
5	DMS	C	8501	-	3,3,3	1.08	0	3,3,3	1.17	0
5	DMS	C	8503	-	3,3,3	0.94	0	3,3,3	0.78	0
5	DMS	C	8504	-	3,3,3	1.18	0	3,3,3	0.29	0
5	DMS	C	8506	-	3,3,3	1.09	0	3,3,3	0.55	0
5	DMS	C	8508	-	3,3,3	2.53	1 (33%)	3,3,3	0.52	0
5	DMS	C	8601	-	3,3,3	1.11	0	3,3,3	1.03	0
5	DMS	C	8602	-	3,3,3	1.30	1 (33%)	3,3,3	0.18	0
2	LAK	D	2001	4	24,24,24	1.34	4 (16%)	35,35,35	1.17	3 (8%)
5	DMS	D	8401	-	3,3,3	1.22	0	3,3,3	0.41	0
5	DMS	D	8402	-	3,3,3	1.24	0	3,3,3	0.29	0
5	DMS	D	8403	-	3,3,3	1.33	0	3,3,3	0.45	0
5	DMS	D	8404	-	3,3,3	1.38	1 (33%)	3,3,3	0.16	0
5	DMS	D	8405	-	3,3,3	0.93	0	3,3,3	0.50	0
5	DMS	D	8406	-	3,3,3	1.07	0	3,3,3	0.57	0
5	DMS	D	8407	-	3,3,3	2.83	2 (66%)	3,3,3	0.33	0
5	DMS	D	8408	-	3,3,3	1.46	0	3,3,3	0.11	0
5	DMS	D	8409	-	3,3,3	2.44	1 (33%)	3,3,3	1.02	0
5	DMS	D	8410	-	3,3,3	1.15	0	3,3,3	0.16	0
5	DMS	D	8411	-	3,3,3	0.73	0	3,3,3	0.10	0
5	DMS	D	8412	-	3,3,3	0.80	0	3,3,3	0.59	0
5	DMS	D	8413	-	3,3,3	1.74	1 (33%)	3,3,3	0.49	0
5	DMS	D	8414	-	3,3,3	0.42	0	3,3,3	0.28	0
5	DMS	D	8416	-	3,3,3	0.75	0	3,3,3	0.28	0
5	DMS	D	8417	-	3,3,3	1.51	1 (33%)	3,3,3	0.68	0
5	DMS	D	8418	-	3,3,3	1.38	0	3,3,3	0.92	0
5	DMS	D	8419	-	3,3,3	0.44	0	3,3,3	0.14	0
5	DMS	D	8420	-	3,3,3	2.37	1 (33%)	3,3,3	0.30	0
5	DMS	D	8421	-	3,3,3	0.88	0	3,3,3	0.35	0
5	DMS	D	8423	-	3,3,3	2.44	2 (66%)	3,3,3	0.38	0
5	DMS	D	8424	-	3,3,3	1.29	0	3,3,3	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8425	4	3,3,3	1.37	1 (33%)	3,3,3	1.16	1 (33%)
5	DMS	D	8428	-	3,3,3	1.15	0	3,3,3	0.40	0
5	DMS	D	8429	-	3,3,3	2.34	1 (33%)	3,3,3	0.37	0
5	DMS	D	8501	-	3,3,3	0.95	0	3,3,3	0.09	0
5	DMS	D	8503	-	3,3,3	0.84	0	3,3,3	0.60	0
5	DMS	D	8506	-	3,3,3	1.54	1 (33%)	3,3,3	0.46	0
5	DMS	D	8508	-	3,3,3	1.74	1 (33%)	3,3,3	0.80	0
5	DMS	D	8701	-	3,3,3	2.39	2 (66%)	3,3,3	0.69	0
5	DMS	D	8703	-	3,3,3	1.35	0	3,3,3	0.14	0
5	DMS	D	8704	-	3,3,3	2.23	1 (33%)	3,3,3	0.57	0
5	DMS	D	8705	-	3,3,3	2.94	1 (33%)	3,3,3	1.64	1 (33%)

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	LAK	A	2001	4	-	0/7/47/47	0/2/2/2
5	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8418	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8424	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	A	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	A	8428	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8503	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8602	-	-	0/0/0/0	0/0/0/0
2	LAK	B	2001[A]	-	1/1/10/10	0/7/47/47	0/2/2/2
2	LAK	B	2002[B]	-	1/1/3/10	0/6/10/47	0/0/0/2
6	TAR	B	2003[C]	-	1/1/3/4	0/6/10/12	0/0/0/0
5	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8418	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8424	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	B	8428	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8429	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8601	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	B	8706	-	-	0/0/0/0	0/0/0/0
2	LAK	C	2001	4	-	0/7/47/47	0/2/2/2
5	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8418	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8424	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	C	8429	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8503	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
2	LAK	D	2001	4	-	0/7/47/47	0/2/2/2
5	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8407	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8418	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8424	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	D	8428	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8429	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8503	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8704	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8705	-	-	0/0/0/0	0/0/0/0

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	8705	DMS	C1-S	-5.01	1.37	1.75
5	D	8420	DMS	C2-S	-3.89	1.45	1.75
5	A	8416	DMS	O-S	-3.68	1.24	1.50
5	C	8418	DMS	C1-S	-2.38	1.57	1.75
5	A	8414	DMS	O-S	-2.30	1.34	1.50
5	A	8504	DMS	C1-S	-2.27	1.58	1.75
2	D	2001	LAK	O2-C2	2.02	1.47	1.43
5	A	8405	DMS	O-S	2.03	1.64	1.50
5	A	8428	DMS	C2-S	2.03	1.91	1.75
5	C	8602	DMS	O-S	2.06	1.64	1.50
2	A	2001	LAK	O2-C2	2.06	1.47	1.43
5	A	8417	DMS	O-S	2.09	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8402	DMS	O-S	2.11	1.64	1.50
5	C	8412	DMS	O-S	2.11	1.64	1.50
5	A	8506	DMS	C2-S	2.16	1.92	1.75
5	B	8425	DMS	C2-S	2.16	1.92	1.75
5	D	8423	DMS	C2-S	2.16	1.92	1.75
5	D	8425	DMS	C2-S	2.16	1.92	1.75
5	A	8423	DMS	C2-S	2.18	1.92	1.75
5	A	8425	DMS	C2-S	2.23	1.92	1.75
2	D	2001	LAK	O3-C3	2.23	1.48	1.43
5	B	8402	DMS	C2-S	2.24	1.93	1.75
5	A	8402	DMS	C2-S	2.25	1.93	1.75
5	C	8415	DMS	C1-S	2.27	1.93	1.75
2	B	2001[A]	LAK	C4-C5	2.27	1.57	1.53
2	C	2001	LAK	O2-C2	2.27	1.48	1.43
5	C	8405	DMS	O-S	2.28	1.65	1.50
5	D	8701	DMS	C1-S	2.29	1.93	1.75
5	A	8413	DMS	C1-S	2.29	1.93	1.75
5	A	8423	DMS	O-S	2.31	1.66	1.50
5	C	8425	DMS	O-S	2.34	1.66	1.50
5	D	8404	DMS	C2-S	2.34	1.93	1.75
5	C	8407	DMS	O-S	2.37	1.66	1.50
5	C	8416	DMS	O-S	2.37	1.66	1.50
5	C	8429	DMS	O-S	2.39	1.66	1.50
5	A	8413	DMS	O-S	2.43	1.66	1.50
5	B	8428	DMS	C1-S	2.43	1.94	1.75
5	A	8425	DMS	C1-S	2.44	1.94	1.75
2	A	2001	LAK	C4-C5	2.47	1.58	1.53
5	B	8506	DMS	C2-S	2.48	1.94	1.75
5	D	8417	DMS	C2-S	2.50	1.95	1.75
5	D	8508	DMS	O-S	2.52	1.67	1.50
5	D	8407	DMS	C2-S	2.52	1.95	1.75
5	A	8502	DMS	C1-S	2.53	1.95	1.75
5	B	8410	DMS	C1-S	2.55	1.95	1.75
5	B	8413	DMS	C2-S	2.60	1.95	1.75
5	D	8413	DMS	O-S	2.63	1.68	1.50
5	B	8420	DMS	C2-S	2.64	1.96	1.75
2	D	2001	LAK	C1'-C2'	2.66	1.58	1.52
5	D	8506	DMS	O-S	2.66	1.68	1.50
6	B	2003[C]	TAR	O2-C2	2.67	1.48	1.42
5	C	8402	DMS	C2-S	2.68	1.96	1.75
5	B	8508	DMS	O-S	2.69	1.68	1.50
5	C	8416	DMS	C2-S	2.71	1.96	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2001	LAK	O2'-C2'	2.73	1.49	1.43
5	B	8706	DMS	O-S	2.76	1.69	1.50
5	C	8413	DMS	O-S	2.80	1.69	1.50
5	A	8413	DMS	C2-S	2.82	1.97	1.75
5	A	8506	DMS	C1-S	2.83	1.97	1.75
5	D	8701	DMS	O-S	2.84	1.69	1.50
5	A	8502	DMS	C2-S	2.85	1.97	1.75
5	B	8429	DMS	C2-S	2.86	1.97	1.75
5	A	8425	DMS	O-S	2.87	1.69	1.50
2	B	2002[B]	LAK	C3'-C2'	2.91	1.56	1.53
2	C	2001	LAK	O4-C4	3.00	1.50	1.43
5	B	8407	DMS	O-S	3.13	1.71	1.50
5	B	8429	DMS	O-S	3.15	1.71	1.50
2	A	2001	LAK	O4-C4	3.22	1.50	1.43
2	D	2001	LAK	O4-C4	3.32	1.50	1.43
5	D	8423	DMS	C1-S	3.38	2.01	1.75
5	C	8415	DMS	C2-S	3.39	2.01	1.75
5	B	8425	DMS	O-S	3.39	1.73	1.50
2	B	2001[A]	LAK	O4-C4	3.42	1.51	1.43
5	B	8409	DMS	O-S	3.43	1.73	1.50
5	A	8403	DMS	C2-S	3.44	2.02	1.75
5	A	8407	DMS	O-S	3.67	1.75	1.50
5	B	8601	DMS	C2-S	3.70	2.04	1.75
5	D	8429	DMS	C2-S	3.79	2.05	1.75
5	D	8704	DMS	C1-S	3.83	2.05	1.75
5	D	8409	DMS	O-S	3.86	1.76	1.50
5	B	8407	DMS	C2-S	3.87	2.05	1.75
5	D	8407	DMS	O-S	3.87	1.76	1.50
5	C	8409	DMS	O-S	3.95	1.77	1.50
5	B	8415	DMS	C2-S	3.99	2.06	1.75
5	C	8420	DMS	O-S	4.01	1.77	1.50
5	B	8413	DMS	O-S	4.19	1.79	1.50
5	C	8508	DMS	O-S	4.33	1.80	1.50
5	A	8409	DMS	O-S	4.42	1.80	1.50
5	B	8508	DMS	C1-S	4.58	2.11	1.75

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001[A]	LAK	O2-C2-C1	-3.55	102.24	110.02
2	D	2001	LAK	O2-C2-C1	-3.27	102.85	110.02
2	C	2001	LAK	O2-C2-C1	-3.13	103.16	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	LAK	O3-C3-C2	-2.87	103.88	110.34
5	D	8705	DMS	C2-S-C1	-2.83	83.86	98.46
2	B	2001[A]	LAK	C1'-O5'-C5'	-2.77	108.34	113.47
2	B	2001[A]	LAK	O3-C3-C2	-2.71	104.24	110.34
2	C	2001	LAK	C1'-C2'-C3'	-2.54	106.66	110.43
5	C	8418	DMS	C2-S-C1	-2.47	85.69	98.46
2	A	2001	LAK	O2-C2-C1	-2.36	104.85	110.02
2	C	2001	LAK	C6'-O1-C1	-2.26	109.07	113.82
2	A	2001	LAK	C1'-O5'-C5'	-2.19	109.43	113.47
2	C	2001	LAK	C2'-C3'-C4'	-2.08	106.91	110.79
2	B	2001[A]	LAK	O2-C2-C3	-2.05	105.72	110.34
5	A	8503	DMS	C2-S-C1	-2.05	87.90	98.46
5	D	8425	DMS	C2-S-C1	2.01	108.83	98.46
2	D	2001	LAK	O1-C1-C2	2.02	110.59	108.04
2	C	2001	LAK	O1-C1-C2	2.10	110.69	108.04
5	A	8407	DMS	C2-S-C1	2.11	109.37	98.46
2	D	2001	LAK	C1'-C2'-C3'	2.52	114.17	110.43
6	B	2003[C]	TAR	C4-C3-C2	2.54	116.17	111.94
2	B	2001[A]	LAK	C2'-C3'-C4'	2.56	115.57	110.79
5	A	8502	DMS	C2-S-C1	2.61	111.93	98.46
2	B	2001[A]	LAK	C1'-C2'-C3'	2.61	114.32	110.43
2	B	2002[B]	LAK	C4'-C3'-C2'	2.98	116.90	111.94
2	B	2001[A]	LAK	O1-C1-C2	3.29	112.19	108.04
5	B	8502	DMS	C2-S-C1	3.51	116.60	98.46

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	2003[C]	TAR	C3
2	B	2001[A]	LAK	C2'
2	B	2002[B]	LAK	C2'

There are no torsion outliers.

There are no ring outliers.

39 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8403	DMS	1	0
5	A	8412	DMS	3	0
5	A	8416	DMS	3	0
5	A	8418	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8420	DMS	1	0
5	A	8428	DMS	1	0
5	A	8502	DMS	1	0
2	B	2002[B]	LAK	3	0
6	B	2003[C]	TAR	9	0
5	B	8407	DMS	2	0
5	B	8412	DMS	1	0
5	B	8415	DMS	4	0
5	B	8418	DMS	4	0
5	B	8423	DMS	1	0
5	B	8424	DMS	1	0
5	B	8428	DMS	1	0
5	B	8501	DMS	6	0
5	B	8508	DMS	1	0
5	B	8601	DMS	1	0
5	C	8406	DMS	2	0
5	C	8413	DMS	1	0
5	C	8415	DMS	1	0
5	C	8418	DMS	5	0
5	C	8420	DMS	1	0
5	C	8424	DMS	2	0
5	C	8503	DMS	1	0
5	C	8602	DMS	1	0
2	D	2001	LAK	1	0
5	D	8403	DMS	1	0
5	D	8412	DMS	2	0
5	D	8418	DMS	2	0
5	D	8423	DMS	2	0
5	D	8428	DMS	1	0
5	D	8429	DMS	2	0
5	D	8503	DMS	1	0
5	D	8506	DMS	1	0
5	D	8703	DMS	2	0
5	D	8704	DMS	1	0
5	D	8705	DMS	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.71	15 (1%) 76 79	7, 12, 42, 100	0
1	B	1011/1023 (98%)	-0.73	11 (1%) 82 85	6, 12, 39, 100	0
1	C	1011/1023 (98%)	-0.69	11 (1%) 82 85	6, 13, 43, 100	0
1	D	1011/1023 (98%)	-0.66	19 (1%) 70 73	6, 13, 44, 98	0
All	All	4044/4092 (98%)	-0.70	56 (1%) 78 81	6, 13, 43, 100	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	10.1
1	A	735	HIS	8.8
1	C	732	ALA	8.1
1	D	732	ALA	7.7
1	C	730	LEU	7.5
1	D	686	PRO	7.1
1	D	730	LEU	6.9
1	D	735	HIS	6.8
1	B	689	GLU	6.5
1	A	687	GLN	6.3
1	B	730	LEU	6.2
1	D	689	GLU	6.2
1	C	731	PRO	5.7
1	B	732	ALA	5.6
1	B	731	PRO	5.6
1	C	689	GLU	5.3
1	A	730	LEU	5.2
1	C	686	PRO	5.1
1	D	731	PRO	5.1
1	B	687	GLN	4.8
1	D	687	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	687	GLN	4.5
1	A	731	PRO	4.5
1	C	735	HIS	4.4
1	C	733	ALA	4.3
1	A	685	LEU	4.3
1	D	684	GLU	4.1
1	B	686	PRO	4.1
1	A	732	ALA	4.0
1	A	1023	LYS	3.7
1	B	733	ALA	3.7
1	D	685	LEU	3.7
1	B	684	GLU	3.7
1	D	580	GLU	3.7
1	A	689	GLU	3.6
1	D	581	ASN	3.4
1	D	688	PRO	3.1
1	D	733	ALA	3.1
1	B	735	HIS	3.1
1	D	683	PRO	3.1
1	A	733	ALA	3.1
1	A	580	GLU	3.0
1	C	729	THR	3.0
1	A	634	GLN	2.9
1	A	688	PRO	2.7
1	C	772	ASP	2.6
1	B	685	LEU	2.6
1	D	772	ASP	2.3
1	C	634	GLN	2.3
1	D	734	SER	2.2
1	D	799	THR	2.1
1	B	799	THR	2.1
1	A	729	THR	2.1
1	D	798	ALA	2.1
1	D	845	GLN	2.0
1	A	845	GLN	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
6	TAR	B	2003[C]	9/10	0.71	0.31	147.44	13,38,100,100	9
2	LAK	B	2002[B]	9/23	0.79	0.36	106.44	6,56,100,100	9
5	DMS	B	8506	4/4	0.98	0.10	21.59	26,26,29,100	0
2	LAK	D	2001	23/23	0.94	0.12	18.49	13,21,100,100	0
5	DMS	B	8420	4/4	0.89	0.15	17.82	36,40,43,53	0
2	LAK	C	2001	23/23	0.96	0.12	14.37	10,17,100,100	0
5	DMS	B	8423	4/4	0.95	0.09	11.95	26,28,45,50	0
5	DMS	D	8423	4/4	0.90	0.14	11.64	30,37,42,50	0
2	LAK	B	2001[A]	23/23	0.94	0.12	11.29	11,18,100,100	9
5	DMS	C	8419	4/4	0.93	0.13	10.62	30,32,43,52	0
5	DMS	D	8420	4/4	0.94	0.13	10.26	18,67,81,83	0
5	DMS	A	8406	4/4	0.93	0.15	10.19	24,45,69,72	0
5	DMS	C	8501	4/4	0.93	0.12	10.16	18,26,37,46	0
5	DMS	D	8404	4/4	0.93	0.10	9.75	18,19,41,53	0
2	LAK	A	2001	23/23	0.96	0.10	9.25	12,21,100,100	0
5	DMS	A	8420	4/4	0.96	0.12	8.54	24,30,31,47	0
5	DMS	A	8417	4/4	0.94	0.13	8.37	24,26,73,100	0
5	DMS	B	8419	4/4	0.92	0.12	7.79	32,48,65,100	0
5	DMS	C	8506	4/4	0.98	0.08	7.56	26,26,31,74	0
5	DMS	D	8703	4/4	0.85	0.16	7.48	25,51,52,58	0
5	DMS	C	8417	4/4	0.91	0.10	7.28	26,27,50,61	0
5	DMS	A	8506	4/4	0.98	0.09	7.07	27,28,46,63	0
5	DMS	B	8508	4/4	0.89	0.10	6.92	19,40,41,55	0
5	DMS	C	8508	4/4	0.83	0.11	6.82	30,35,35,81	0
5	DMS	A	8504	4/4	0.97	0.10	6.67	20,32,35,94	0
5	DMS	D	8417	4/4	0.88	0.14	6.61	26,27,85,92	0
5	DMS	D	8406	4/4	0.97	0.09	6.51	18,18,21,39	0
5	DMS	C	8420	4/4	0.96	0.09	6.21	25,32,35,40	0
5	DMS	D	8506	4/4	0.98	0.09	6.03	19,32,44,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	A	8419	4/4	0.91	0.11	5.62	33,38,46,47	0
5	DMS	B	8404	4/4	0.97	0.07	5.62	18,21,28,28	0
5	DMS	A	8407	4/4	0.97	0.09	5.16	18,25,28,31	0
5	DMS	B	8407	4/4	0.97	0.11	4.96	25,29,30,30	0
5	DMS	D	8407	4/4	0.96	0.10	4.95	22,29,31,63	0
5	DMS	A	8501	4/4	0.94	0.11	4.75	16,27,35,36	0
5	DMS	C	8404	4/4	0.97	0.07	4.74	15,16,21,26	0
5	DMS	D	8418	4/4	0.90	0.14	4.62	25,70,78,100	0
5	DMS	B	8408	4/4	0.98	0.10	4.53	22,25,31,38	0
5	DMS	D	8403	4/4	0.96	0.08	4.19	16,23,25,26	0
5	DMS	B	8417	4/4	0.92	0.11	4.05	27,29,70,100	0
5	DMS	D	8419	4/4	0.94	0.10	4.03	27,39,41,43	0
5	DMS	A	8418	4/4	0.88	0.16	3.99	34,39,76,100	0
5	DMS	C	8406	4/4	0.93	0.18	3.70	42,44,99,100	0
5	DMS	C	8423	4/4	0.94	0.09	3.63	28,31,48,48	0
5	DMS	C	8418	4/4	0.93	0.15	3.62	20,27,56,100	0
5	DMS	A	8404	4/4	0.97	0.07	3.60	17,23,23,27	0
5	DMS	D	8508	4/4	0.94	0.09	3.52	31,36,41,53	0
5	DMS	D	8501	4/4	0.88	0.10	3.33	23,29,37,52	0
5	DMS	A	8423	4/4	0.95	0.10	3.14	28,42,51,73	0
5	DMS	B	8501	4/4	0.91	0.13	3.06	27,44,56,64	0
5	DMS	D	8701	4/4	0.98	0.07	2.99	13,14,17,31	0
5	DMS	D	8705	4/4	0.95	0.12	2.66	8,44,50,78	0
5	DMS	A	8408	4/4	0.96	0.08	2.64	15,29,31,48	0
5	DMS	C	8425	4/4	0.99	0.10	2.61	26,28,29,42	0
5	DMS	C	8407	4/4	0.98	0.08	2.44	23,24,30,34	0
5	DMS	A	8403	4/4	0.98	0.06	2.42	19,19,21,24	0
5	DMS	C	8405	4/4	0.98	0.09	2.37	21,23,23,24	0
5	DMS	C	8408	4/4	0.97	0.07	2.33	15,28,29,37	0
5	DMS	D	8425	4/4	0.83	0.18	2.28	35,42,59,100	0
5	DMS	B	8425	4/4	0.97	0.09	2.24	17,26,26,32	0
5	DMS	B	8504	4/4	0.95	0.09	2.11	20,35,38,43	0
5	DMS	B	8405	4/4	0.99	0.09	2.11	22,24,28,34	0
5	DMS	C	8602	4/4	0.95	0.11	1.97	43,47,57,68	0
5	DMS	D	8405	4/4	0.99	0.08	1.87	20,20,23,36	0
5	DMS	C	8412	4/4	0.97	0.08	1.86	25,26,29,72	0
5	DMS	A	8412	4/4	0.96	0.11	1.83	29,38,100,100	0
5	DMS	D	8412	4/4	0.99	0.09	1.70	24,26,27,35	0
5	DMS	B	8411	4/4	0.99	0.06	1.29	17,20,20,100	0
5	DMS	A	8502	4/4	0.92	0.12	1.27	18,23,49,54	0
5	DMS	D	8408	4/4	0.98	0.07	1.21	17,27,27,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NA	D	3104	1/1	0.93	0.09	1.21	27,27,27,27	0
5	DMS	B	8502	4/4	0.96	0.07	1.20	16,22,30,36	0
4	NA	D	3103	1/1	0.96	0.08	1.19	24,24,24,24	0
5	DMS	B	8706	4/4	0.94	0.12	1.10	37,41,42,42	0
5	DMS	C	8402	4/4	0.98	0.06	1.05	12,22,23,26	0
5	DMS	B	8402	4/4	0.99	0.06	0.90	14,14,18,23	0
5	DMS	B	8412	4/4	0.98	0.08	0.81	23,28,28,30	0
5	DMS	A	8405	4/4	0.99	0.06	0.81	18,22,22,31	0
5	DMS	B	8403	4/4	0.99	0.05	0.71	15,15,22,23	0
5	DMS	B	8401	4/4	0.99	0.05	0.56	12,16,16,19	0
5	DMS	A	8402	4/4	0.98	0.06	0.54	11,18,20,27	0
5	DMS	B	8418	4/4	0.91	0.09	0.53	26,30,63,96	0
4	NA	B	3104	1/1	0.97	0.08	0.48	24,24,24,24	0
5	DMS	C	8403	4/4	0.99	0.05	0.35	17,19,21,21	0
5	DMS	A	8425	4/4	0.97	0.08	0.29	23,26,30,32	0
5	DMS	C	8411	4/4	0.99	0.06	0.25	15,20,25,25	0
4	NA	B	3102	1/1	1.00	0.04	0.21	9,9,9,9	0
4	NA	C	3104	1/1	0.98	0.08	0.10	22,22,22,22	0
5	DMS	A	8401	4/4	0.99	0.04	-0.07	10,11,13,13	0
4	NA	A	3104	1/1	0.97	0.06	-0.11	20,20,20,20	0
5	DMS	C	8401	4/4	0.99	0.04	-0.15	11,12,16,17	0
5	DMS	D	8402	4/4	0.99	0.04	-0.52	12,15,17,18	0
5	DMS	A	8411	4/4	0.99	0.05	-0.52	16,21,21,48	0
5	DMS	D	8411	4/4	0.99	0.05	-0.55	17,17,22,40	0
5	DMS	D	8401	4/4	0.99	0.04	-0.80	11,12,15,16	0
4	NA	D	3102	1/1	1.00	0.04	-0.85	9,9,9,9	0
4	NA	B	3103	1/1	0.99	0.04	-0.97	18,18,18,18	0
4	NA	C	3103	1/1	0.99	0.04	-1.04	18,18,18,18	0
4	NA	A	3103	1/1	0.98	0.04	-1.33	20,20,20,20	0
3	MG	C	3001	1/1	1.00	0.03	-1.46	8,8,8,8	0
4	NA	C	3102	1/1	1.00	0.03	-1.54	10,10,10,10	0
3	MG	D	3002	1/1	0.99	0.03	-1.98	12,12,12,12	0
4	NA	A	3101	1/1	1.00	0.03	-2.27	10,10,10,10	0
3	MG	B	3002	1/1	0.99	0.03	-2.53	11,11,11,11	0
4	NA	A	3102	1/1	1.00	0.02	-2.68	9,9,9,9	0
3	MG	A	3001	1/1	1.00	0.03	-2.70	9,9,9,9	0
3	MG	D	3001	1/1	1.00	0.02	-3.03	8,8,8,8	0
3	MG	A	3002	1/1	0.99	0.03	-3.13	11,11,11,11	0
4	NA	B	3101	1/1	1.00	0.02	-3.14	10,10,10,10	0
3	MG	B	3001	1/1	1.00	0.02	-3.48	8,8,8,8	0
4	NA	C	3101	1/1	1.00	0.02	-4.40	9,9,9,9	0
4	NA	D	3101	1/1	1.00	0.02	-5.12	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	C	3002	1/1	1.00	0.01	-6.29	10,10,10,10	0
5	DMS	B	8428	4/4	0.85	0.13	-	34,38,57,61	0
5	DMS	B	8416	4/4	0.94	0.10	-	33,46,47,50	0
5	DMS	C	8504	4/4	0.92	0.14	-	31,37,46,100	0
5	DMS	D	8428	4/4	0.91	0.19	-	39,47,61,65	0
5	DMS	A	8416	4/4	0.95	0.16	-	16,31,40,100	0
5	DMS	B	8601	4/4	0.98	0.08	-	27,34,36,44	0
5	DMS	D	8413	4/4	0.99	0.10	-	25,26,26,41	0
5	DMS	B	8421	4/4	0.93	0.13	-	31,49,52,100	0
3	MG	A	3105	1/1	0.89	0.16	-	45,45,45,45	0
5	DMS	A	8414	4/4	0.95	0.13	-	23,24,55,100	0
5	DMS	C	8414	4/4	0.98	0.08	-	17,37,46,48	0
5	DMS	A	8428	4/4	0.91	0.21	-	53,66,100,100	0
5	DMS	C	8413	4/4	0.98	0.12	-	24,25,27,30	0
5	DMS	D	8414	4/4	0.96	0.11	-	21,35,76,100	0
5	DMS	B	8413	4/4	0.97	0.10	-	28,28,29,34	0
5	DMS	C	8503	4/4	0.85	0.17	-	23,50,50,52	0
5	DMS	B	8414	4/4	0.96	0.11	-	22,38,40,100	0
5	DMS	A	8413	4/4	0.96	0.12	-	24,28,29,34	0
5	DMS	D	8409	4/4	0.97	0.09	-	27,33,36,42	0
5	DMS	D	8410	4/4	0.98	0.06	-	14,27,27,39	0
5	DMS	C	8424	4/4	0.92	0.17	-	41,60,100,100	0
5	DMS	D	8416	4/4	0.93	0.14	-	25,32,44,100	0
3	MG	B	3105	1/1	0.99	0.11	-	35,35,35,35	0
5	DMS	B	8429	4/4	0.95	0.12	-	29,40,45,51	0
3	MG	A	3005	1/1	0.97	0.09	-	25,25,25,25	0
3	MG	C	3004	1/1	0.97	0.17	-	36,36,36,36	0
5	DMS	D	8704	4/4	0.82	0.21	-	31,32,100,100	0
5	DMS	C	8421	4/4	0.97	0.11	-	30,37,41,49	0
5	DMS	A	8424	4/4	0.93	0.15	-	34,35,70,100	0
5	DMS	D	8421	4/4	0.96	0.12	-	32,46,51,66	0
5	DMS	D	8424	4/4	0.83	0.20	-	47,57,87,100	0
5	DMS	D	8429	4/4	0.87	0.19	-	26,51,82,100	0
5	DMS	C	8416	4/4	0.96	0.17	-	32,43,43,44	0
5	DMS	B	8410	4/4	0.98	0.06	-	19,27,33,35	0
5	DMS	D	8503	4/4	0.90	0.17	-	23,38,49,100	0
5	DMS	C	8415	4/4	0.95	0.10	-	19,25,31,38	0
5	DMS	C	8601	4/4	0.96	0.12	-	39,40,55,57	0
5	DMS	A	8410	4/4	0.98	0.07	-	17,27,32,34	0
3	MG	C	3006	1/1	0.95	0.14	-	24,24,24,24	0
5	DMS	A	8503	4/4	0.96	0.12	-	28,42,100,100	0
5	DMS	B	8424	4/4	0.80	0.19	-	50,74,76,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	A	8421	4/4	0.88	0.18	-	34,46,61,63	0
3	MG	D	3005	1/1	0.99	0.10	-	21,21,21,21	0
5	DMS	C	8409	4/4	0.97	0.11	-	23,32,33,35	0
5	DMS	C	8410	4/4	0.99	0.05	-	17,27,28,30	0
5	DMS	B	8409	4/4	0.98	0.08	-	23,26,28,30	0
5	DMS	C	8429	4/4	0.95	0.11	-	41,42,51,100	0
3	MG	D	3105	1/1	0.97	0.10	-	36,36,36,36	0
5	DMS	A	8409	4/4	0.95	0.12	-	27,28,41,51	0
5	DMS	B	8415	4/4	0.96	0.11	-	19,28,30,38	0
3	MG	C	3105	1/1	0.93	0.11	-	35,35,35,35	0
5	DMS	A	8602	4/4	0.97	0.17	-	35,52,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.