



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:25 am GMT

PDB ID : 1JYV
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH ONPG
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.75 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

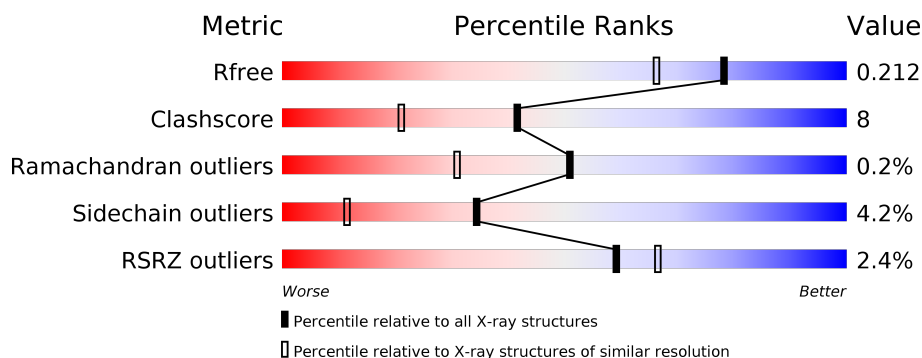
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>
1	B	1023	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>25%</div> <div>5%</div> <div>• •</div> </div> </div>
1	C	1023	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>23%</div> <div>• •</div> </div> </div>
1	D	1023	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>20%</div> <div>5%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	C	3104	-	-	-	X
4	145	D	2002	-	-	-	X
5	DMS	A	8405	-	-	-	X
5	DMS	A	8406	-	-	-	X
5	DMS	A	8407	-	-	-	X
5	DMS	A	8412	-	-	X	-
5	DMS	A	8416	-	-	-	X
5	DMS	A	8417	-	-	-	X
5	DMS	A	8420	-	-	-	X
5	DMS	A	8423	-	-	-	X
5	DMS	A	8501	-	-	-	X
5	DMS	A	8502	-	-	-	X
5	DMS	A	8504	-	-	-	X
5	DMS	B	8405	-	-	-	X
5	DMS	B	8407	-	-	-	X
5	DMS	B	8419	-	-	-	X
5	DMS	B	8420	-	-	-	X
5	DMS	B	8423	-	-	-	X
5	DMS	B	8425	-	-	-	X
5	DMS	B	8508	-	-	-	X
5	DMS	C	8403	-	-	-	X
5	DMS	C	8407	-	-	-	X
5	DMS	C	8415	-	X	-	-
5	DMS	C	8419	-	-	-	X
5	DMS	C	8420	-	-	-	X
5	DMS	C	8425	-	-	-	X
5	DMS	C	8503	-	-	-	X
5	DMS	C	8705	-	-	-	X
5	DMS	D	8404	-	-	-	X
5	DMS	D	8406	-	-	-	X
5	DMS	D	8407	-	-	-	X
5	DMS	D	8417	-	-	-	X
5	DMS	D	8419	-	-	-	X
5	DMS	D	8420	-	-	-	X
5	DMS	D	8425	-	-	-	X
5	DMS	D	8703	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37222 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

Continued on next page...

Continued from previous page...

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

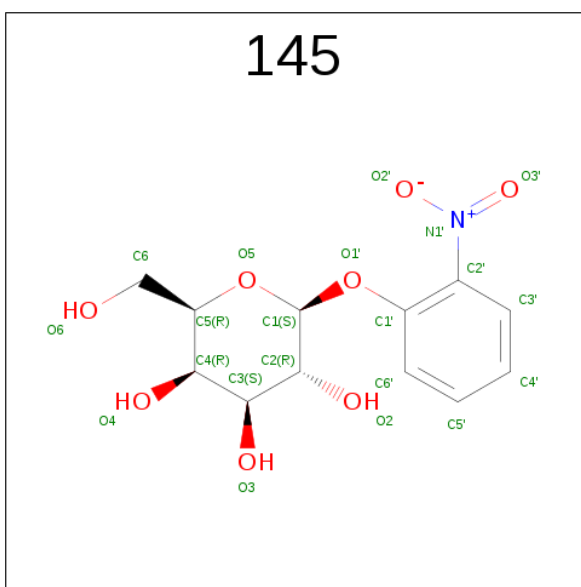
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

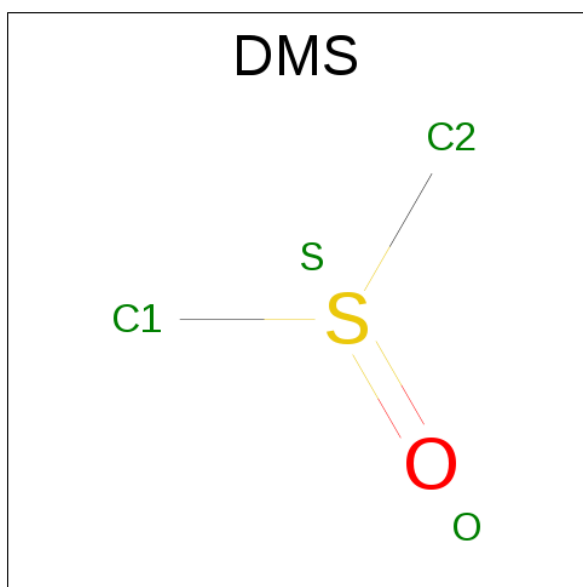
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Na 4 4	0	0
3	A	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0

- Molecule 4 is 1-O-[O-NITROPHENYL]-BETA-D-GALACTOPYRANOSE (three-letter code: 145) (formula: C₁₂H₁₅NO₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			21	12	1	8		
4	A	1	Total	C	N	O	0	0
			21	12	1	8		
4	B	1	Total	C	N	O	0	0
			21	12	1	8		
4	B	1	Total	C	N	O	0	0
			21	12	1	8		
4	C	1	Total	C	N	O	0	0
			21	12	1	8		
4	C	1	Total	C	N	O	0	0
			21	12	1	8		
4	D	1	Total	C	N	O	0	0
			21	12	1	8		
4	D	1	Total	C	N	O	0	0
			21	12	1	8		

- 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		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

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	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

Continued on next page...

Continued from previous page...

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	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

Continued on next page...

Continued from previous page...

[illegible]

Continued on next page...

Continued from previous page...

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	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

Continued on next page...

Continued from previous page...

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

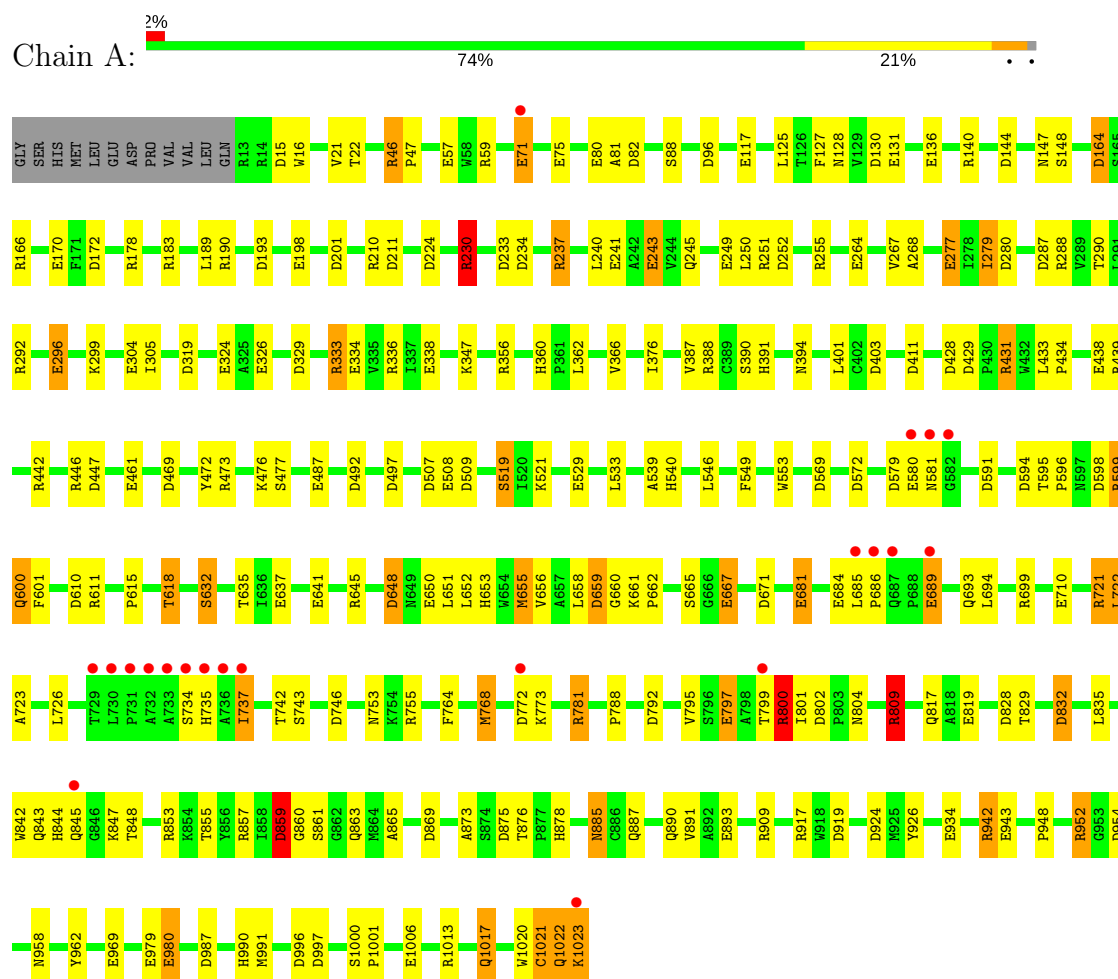
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1060	Total O 1060 1060	0	0
6	B	1013	Total O 1013 1013	0	0
6	C	987	Total O 987 987	0	0
6	D	1021	Total O 1021 1021	0	0

3 Residue-property plots [i](#)

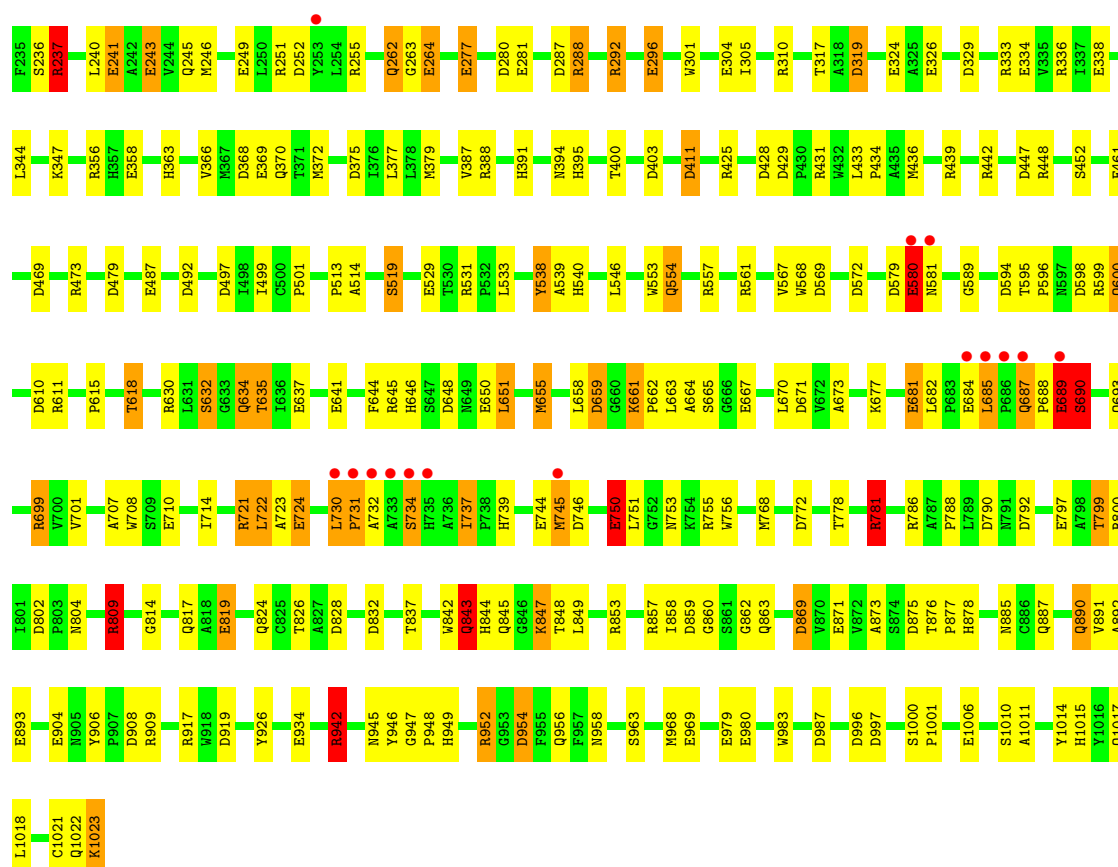
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Beta-Galactosidase

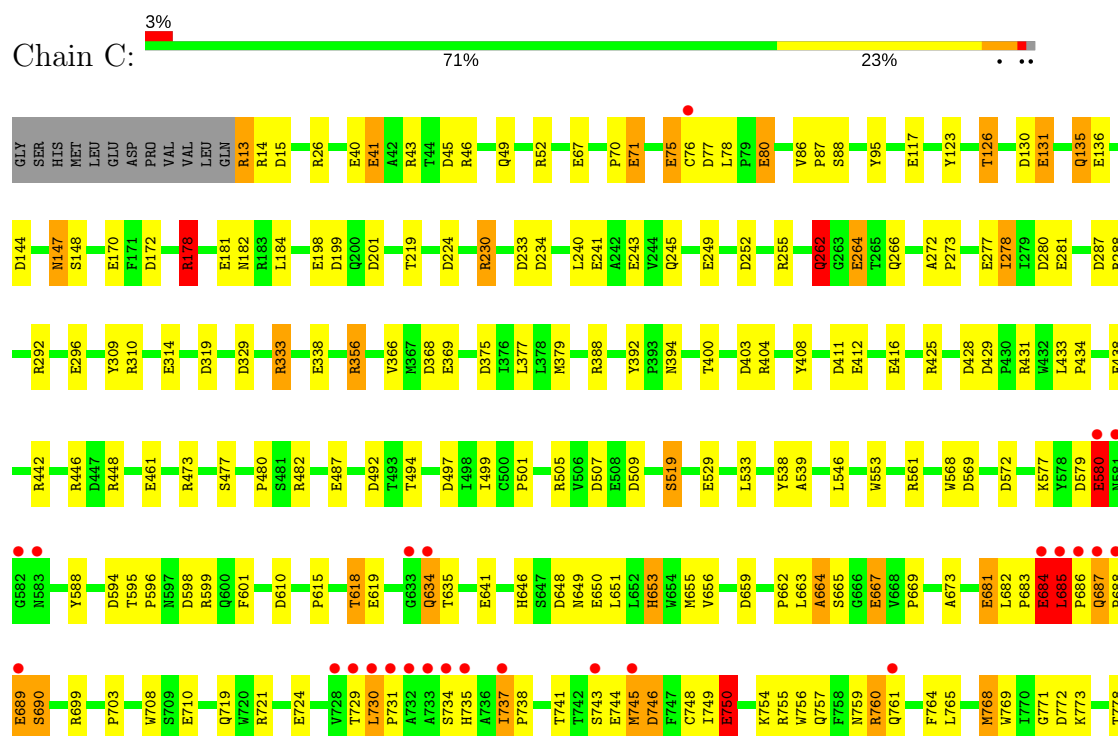


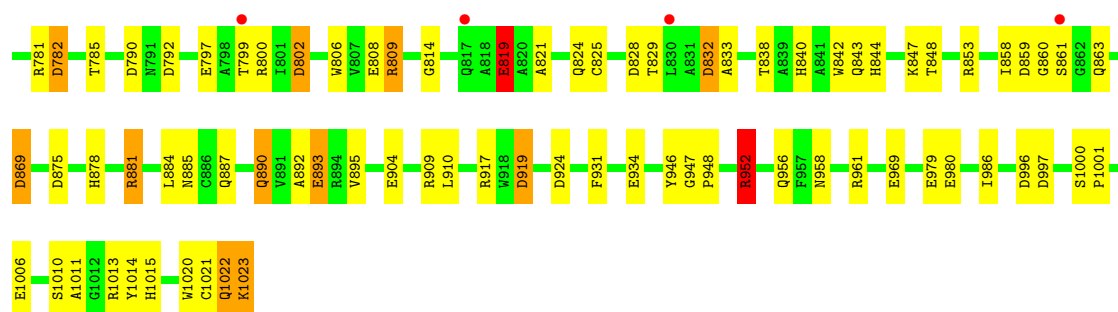
• Molecule 1: Beta-Galactosidase



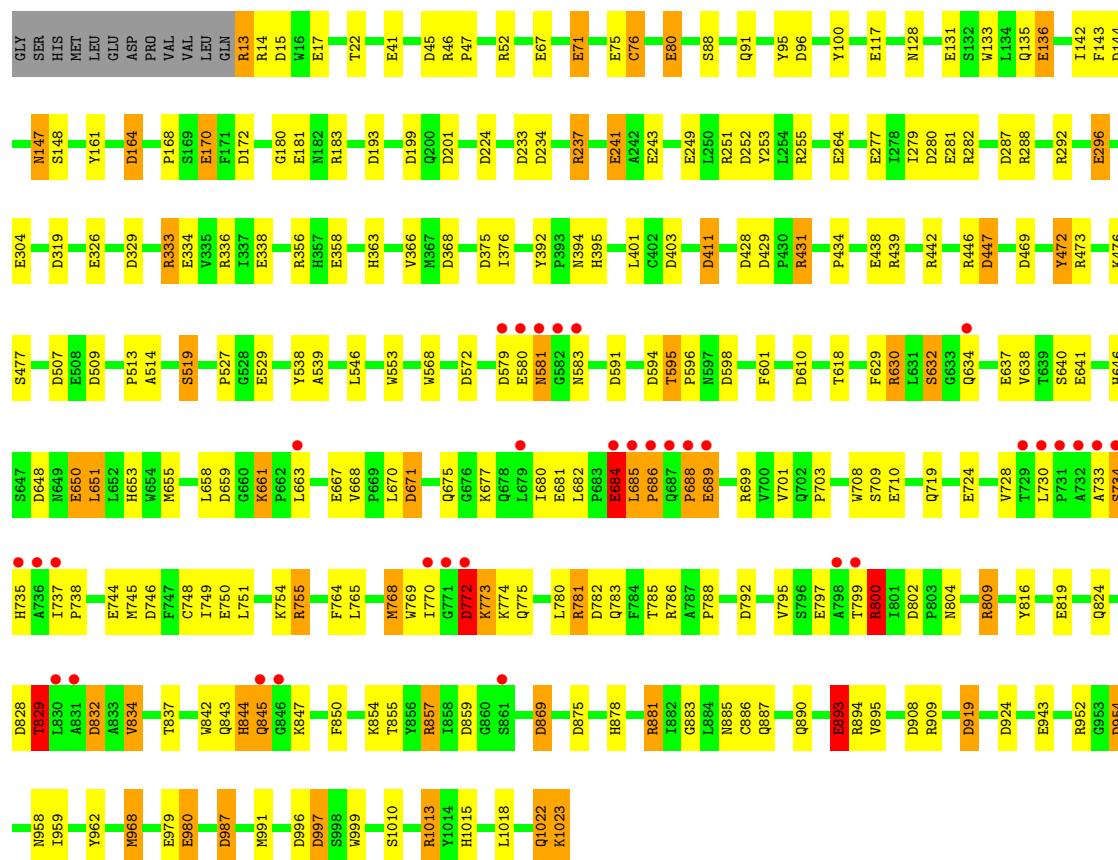
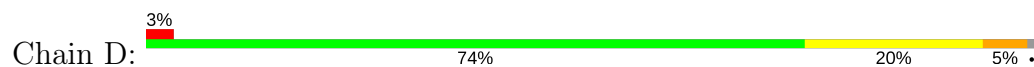


- Molecule 1: Beta-Galactosidase





• 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	149.49Å 167.46Å 200.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 1.75 29.85 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.90-1.75) 90.9 (29.85-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 1.75Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.180 , 0.240 0.162 , 0.212	Depositor DCC
R_{free} test set	6599 reflections (1.47%)	DCC
Wilson B-factor (Å ²)	15.1	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 89.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	37222	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 37.42 % 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 4.3036e-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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, DMS, 145

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	1.10	44/8383 (0.5%)	1.62	155/11437 (1.4%)
1	B	1.11	48/8383 (0.6%)	1.64	177/11437 (1.5%)
1	C	1.10	46/8383 (0.5%)	1.64	173/11437 (1.5%)
1	D	1.11	43/8383 (0.5%)	1.59	163/11437 (1.4%)
All	All	1.10	181/33532 (0.5%)	1.62	668/45748 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	2	0
1	D	1	0
All	All	3	0

All (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	684	GLU	CD-OE2	10.26	1.36	1.25
1	D	893	GLU	CD-OE2	9.38	1.35	1.25
1	D	71	GLU	CD-OE2	8.89	1.35	1.25
1	C	80	GLU	CD-OE2	8.45	1.34	1.25
1	C	1006	GLU	CD-OE2	8.41	1.34	1.25
1	D	170	GLU	CD-OE2	8.22	1.34	1.25
1	C	461	GLU	CD-OE2	8.17	1.34	1.25
1	A	487	GLU	CD-OE2	8.11	1.34	1.25
1	D	131	GLU	CD-OE2	8.06	1.34	1.25
1	C	980	GLU	CD-OE2	7.86	1.34	1.25
1	C	71	GLU	CD-OE2	7.76	1.34	1.25
1	D	980	GLU	CD-OE2	7.75	1.34	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	934	GLU	CD-OE2	7.74	1.34	1.25
1	A	684	GLU	CD-OE2	7.70	1.34	1.25
1	B	296	GLU	CD-OE2	7.57	1.33	1.25
1	C	296	GLU	CD-OE2	7.55	1.33	1.25
1	A	249	GLU	CD-OE2	7.54	1.33	1.25
1	A	681	GLU	CD-OE2	7.52	1.33	1.25
1	A	580	GLU	CD-OE2	7.51	1.33	1.25
1	D	80	GLU	CD-OE2	7.47	1.33	1.25
1	D	979	GLU	CD-OE2	7.44	1.33	1.25
1	C	619	GLU	CD-OE2	7.43	1.33	1.25
1	A	170	GLU	CD-OE2	7.40	1.33	1.25
1	B	71	GLU	CD-OE2	7.38	1.33	1.25
1	B	277	GLU	CD-OE2	7.38	1.33	1.25
1	A	529	GLU	CD-OE2	7.37	1.33	1.25
1	D	580	GLU	CD-OE2	7.30	1.33	1.25
1	A	80	GLU	CD-OE2	7.28	1.33	1.25
1	D	681	GLU	CD-OE2	7.27	1.33	1.25
1	B	684	GLU	CD-OE2	7.22	1.33	1.25
1	B	324	GLU	CD-OE2	7.19	1.33	1.25
1	D	684	GLU	CD-OE2	7.18	1.33	1.25
1	B	57	GLU	CD-OE2	7.16	1.33	1.25
1	A	296	GLU	CD-OE2	7.10	1.33	1.25
1	A	277	GLU	CD-OE2	7.09	1.33	1.25
1	B	980	GLU	CD-OE2	7.09	1.33	1.25
1	B	198	GLU	CD-OE2	7.00	1.33	1.25
1	C	744	GLU	CD-OE2	6.98	1.33	1.25
1	A	131	GLU	CD-OE2	6.98	1.33	1.25
1	C	641	GLU	CD-OE1	-6.96	1.18	1.25
1	B	744	GLU	CD-OE2	6.94	1.33	1.25
1	C	338	GLU	CD-OE2	6.94	1.33	1.25
1	A	980	GLU	CD-OE2	6.92	1.33	1.25
1	B	689	GLU	CD-OE2	6.91	1.33	1.25
1	B	117	GLU	CD-OE2	6.91	1.33	1.25
1	B	819	GLU	CD-OE2	6.91	1.33	1.25
1	B	358	GLU	CD-OE2	6.90	1.33	1.25
1	D	277	GLU	CD-OE2	6.88	1.33	1.25
1	B	264	GLU	CD-OE2	6.88	1.33	1.25
1	C	277	GLU	CD-OE2	6.87	1.33	1.25
1	C	710	GLU	CD-OE2	6.85	1.33	1.25
1	C	904	GLU	CD-OE1	-6.82	1.18	1.25
1	A	57	GLU	CD-OE2	6.81	1.33	1.25
1	C	689	GLU	CD-OE2	6.81	1.33	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	641	GLU	CD-OE1	-6.79	1.18	1.25
1	C	893	GLU	CD-OE2	6.78	1.33	1.25
1	D	136	GLU	CD-OE2	6.76	1.33	1.25
1	D	689	GLU	CD-OE2	6.71	1.33	1.25
1	A	338	GLU	CD-OE2	6.71	1.33	1.25
1	B	281	GLU	CD-OE2	6.71	1.33	1.25
1	B	710	GLU	CD-OE2	6.70	1.33	1.25
1	D	17	GLU	CD-OE2	6.69	1.33	1.25
1	D	338	GLU	CD-OE2	6.67	1.32	1.25
1	A	710	GLU	CD-OE2	6.66	1.32	1.25
1	B	249	GLU	CD-OE2	6.66	1.32	1.25
1	B	487	GLU	CD-OE2	6.65	1.32	1.25
1	A	117	GLU	CD-OE2	6.65	1.32	1.25
1	A	75	GLU	CD-OE2	6.63	1.32	1.25
1	B	1006	GLU	CD-OE2	6.63	1.32	1.25
1	C	580	GLU	CD-OE2	6.62	1.32	1.25
1	A	934	GLU	CD-OE2	6.62	1.32	1.25
1	D	334	GLU	CD-OE2	6.60	1.32	1.25
1	D	710	GLU	CD-OE2	6.59	1.32	1.25
1	C	487	GLU	CD-OE2	6.57	1.32	1.25
1	C	819	GLU	CD-OE2	6.52	1.32	1.25
1	B	241	GLU	CD-OE2	6.52	1.32	1.25
1	B	529	GLU	CD-OE2	6.48	1.32	1.25
1	A	71	GLU	CD-OE2	6.45	1.32	1.25
1	B	641	GLU	CD-OE1	-6.43	1.18	1.25
1	C	170	GLU	CD-OE2	6.42	1.32	1.25
1	C	667	GLU	CD-OE2	6.39	1.32	1.25
1	D	281	GLU	CD-OE2	6.39	1.32	1.25
1	C	750	GLU	CD-OE2	6.36	1.32	1.25
1	B	41	GLU	CD-OE2	6.34	1.32	1.25
1	B	904	GLU	CD-OE2	6.31	1.32	1.25
1	B	893	GLU	CD-OE2	6.26	1.32	1.25
1	B	461	GLU	CD-OE2	6.25	1.32	1.25
1	A	689	GLU	CD-OE2	6.25	1.32	1.25
1	B	170	GLU	CD-OE2	6.25	1.32	1.25
1	C	75	GLU	CD-OE2	6.21	1.32	1.25
1	B	75	GLU	CD-OE2	6.19	1.32	1.25
1	D	667	GLU	CD-OE2	6.15	1.32	1.25
1	B	326	GLU	CD-OE2	6.14	1.32	1.25
1	A	243	GLU	CD-OE2	6.12	1.32	1.25
1	C	117	GLU	CD-OE2	6.11	1.32	1.25
1	B	580	GLU	CD-OE2	6.10	1.32	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	667	GLU	CD-OE2	6.07	1.32	1.25
1	D	296	GLU	CD-OE2	6.05	1.32	1.25
1	D	650	GLU	CD-OE2	6.05	1.32	1.25
1	B	750	GLU	CD-OE2	6.01	1.32	1.25
1	B	131	GLU	CD-OE2	6.00	1.32	1.25
1	B	650	GLU	CD-OE2	6.00	1.32	1.25
1	B	681	GLU	CD-OE2	5.99	1.32	1.25
1	D	41	GLU	CD-OE2	5.97	1.32	1.25
1	D	724	GLU	CD-OE2	5.97	1.32	1.25
1	D	819	GLU	CD-OE2	5.93	1.32	1.25
1	B	969	GLU	CD-OE2	5.93	1.32	1.25
1	A	264	GLU	CD-OE2	5.92	1.32	1.25
1	A	943	GLU	CD-OE2	5.92	1.32	1.25
1	D	641	GLU	CD-OE1	-5.90	1.19	1.25
1	C	797	GLU	CD-OE2	5.89	1.32	1.25
1	C	681	GLU	CD-OE2	5.88	1.32	1.25
1	D	529	GLU	CD-OE2	5.86	1.32	1.25
1	B	724	GLU	CD-OE2	5.80	1.32	1.25
1	A	893	GLU	CD-OE2	5.78	1.32	1.25
1	A	136	GLU	CD-OE2	5.78	1.32	1.25
1	A	508	GLU	CD-OE2	5.77	1.31	1.25
1	D	438	GLU	CD-OE2	5.76	1.31	1.25
1	C	281	GLU	CD-OE2	5.76	1.31	1.25
1	C	969	GLU	CD-OE2	5.74	1.31	1.25
1	D	264	GLU	CD-OE2	5.74	1.31	1.25
1	A	1006	GLU	CD-OE2	5.73	1.31	1.25
1	C	249	GLU	CD-OE2	5.73	1.31	1.25
1	B	369	GLU	CD-OE2	5.71	1.31	1.25
1	D	637	GLU	CD-OE2	5.71	1.31	1.25
1	C	412	GLU	CD-OE2	5.70	1.31	1.25
1	A	797	GLU	CD-OE1	-5.69	1.19	1.25
1	C	198	GLU	CD-OE2	5.69	1.31	1.25
1	B	338	GLU	CD-OE2	5.67	1.31	1.25
1	C	131	GLU	CD-OE2	5.67	1.31	1.25
1	D	181	GLU	CD-OE2	5.67	1.31	1.25
1	B	304	GLU	CD-OE2	5.66	1.31	1.25
1	B	136	GLU	CD-OE2	5.66	1.31	1.25
1	D	249	GLU	CD-OE2	5.66	1.31	1.25
1	C	264	GLU	CD-OE2	5.63	1.31	1.25
1	A	324	GLU	CD-OE2	5.63	1.31	1.25
1	A	304	GLU	CD-OE2	5.60	1.31	1.25
1	D	744	GLU	CD-OE2	5.58	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	369	GLU	CD-OE2	5.58	1.31	1.25
1	D	641	GLU	CD-OE2	5.56	1.31	1.25
1	A	198	GLU	CD-OE2	5.55	1.31	1.25
1	D	117	GLU	CD-OE2	5.54	1.31	1.25
1	D	241	GLU	CD-OE2	5.53	1.31	1.25
1	C	181	GLU	CD-OE2	5.50	1.31	1.25
1	C	241	GLU	CD-OE2	5.45	1.31	1.25
1	B	243	GLU	CD-OE2	5.44	1.31	1.25
1	B	67	GLU	CD-OE2	5.44	1.31	1.25
1	A	650	GLU	CD-OE2	5.41	1.31	1.25
1	C	724	GLU	CD-OE2	5.38	1.31	1.25
1	D	75	GLU	CD-OE2	5.37	1.31	1.25
1	A	637	GLU	CD-OE2	5.37	1.31	1.25
1	C	136	GLU	CD-OE2	5.37	1.31	1.25
1	C	529	GLU	CD-OE2	5.36	1.31	1.25
1	D	750	GLU	CD-OE2	5.35	1.31	1.25
1	D	243	GLU	CD-OE2	5.35	1.31	1.25
1	C	650	GLU	CD-OE2	5.34	1.31	1.25
1	A	296	GLU	CD-OE1	-5.32	1.19	1.25
1	A	667	GLU	CD-OE2	5.32	1.31	1.25
1	C	979	GLU	CD-OE2	5.31	1.31	1.25
1	B	181	GLU	CD-OE2	5.26	1.31	1.25
1	A	461	GLU	CD-OE1	-5.25	1.19	1.25
1	B	934	GLU	CD-OE2	5.24	1.31	1.25
1	C	416	GLU	CD-OE2	5.24	1.31	1.25
1	A	979	GLU	CD-OE2	5.22	1.31	1.25
1	D	943	GLU	CD-OE2	5.20	1.31	1.25
1	A	943	GLU	CD-OE1	-5.19	1.20	1.25
1	A	969	GLU	CD-OE2	5.19	1.31	1.25
1	D	326	GLU	CD-OE2	5.17	1.31	1.25
1	D	358	GLU	CD-OE2	5.17	1.31	1.25
1	B	979	GLU	CD-OE2	5.16	1.31	1.25
1	B	334	GLU	CD-OE1	-5.15	1.20	1.25
1	A	326	GLU	CD-OE2	5.12	1.31	1.25
1	D	304	GLU	CD-OE2	5.12	1.31	1.25
1	B	80	GLU	CD-OE2	5.10	1.31	1.25
1	D	67	GLU	CD-OE2	5.09	1.31	1.25
1	C	67	GLU	CD-OE2	5.09	1.31	1.25
1	C	314	GLU	CD-OE2	5.05	1.31	1.25
1	A	334	GLU	CD-OE2	5.05	1.31	1.25
1	A	819	GLU	CD-OE2	5.04	1.31	1.25
1	A	461	GLU	CD-OE2	5.03	1.31	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	41	GLU	CD-OE2	5.02	1.31	1.25

All (668) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	809	ARG	NE-CZ-NH1	19.59	130.09	120.30
1	B	942	ARG	NE-CZ-NH1	17.39	128.99	120.30
1	B	687	GLN	C-N-CD	-15.95	85.52	120.60
1	C	699	ARG	NE-CZ-NH1	15.62	128.11	120.30
1	B	942	ARG	NE-CZ-NH2	-14.81	112.89	120.30
1	A	755	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	A	442	ARG	NE-CZ-NH2	-12.96	113.82	120.30
1	C	952	ARG	NE-CZ-NH1	12.86	126.73	120.30
1	A	755	ARG	NE-CZ-NH2	-12.21	114.19	120.30
1	C	442	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	A	917	ARG	NE-CZ-NH2	-11.96	114.32	120.30
1	B	336	ARG	NE-CZ-NH1	11.81	126.20	120.30
1	D	172	ASP	CB-CG-OD2	-11.77	107.71	118.30
1	A	230	ARG	NE-CZ-NH1	11.66	126.13	120.30
1	A	599	ARG	NE-CZ-NH1	-11.61	114.50	120.30
1	B	442	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	224	ASP	CB-CG-OD1	11.24	128.41	118.30
1	C	473	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	A	431	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	A	442	ARG	NE-CZ-NH1	10.91	125.76	120.30
1	D	996	ASP	CB-CG-OD2	-10.71	108.66	118.30
1	B	610	ASP	CB-CG-OD2	-10.67	108.70	118.30
1	C	43	ARG	NE-CZ-NH1	10.58	125.59	120.30
1	A	610	ASP	CB-CG-OD1	10.54	127.79	118.30
1	B	288	ARG	NE-CZ-NH2	-10.51	115.05	120.30
1	C	952	ARG	NE-CZ-NH2	-10.50	115.05	120.30
1	C	431	ARG	NE-CZ-NH2	-10.35	115.12	120.30
1	B	292	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	D	431	ARG	NE-CZ-NH2	-10.33	115.14	120.30
1	C	199	ASP	CB-CG-OD1	10.28	127.55	118.30
1	B	772	ASP	CB-CG-OD2	-10.27	109.06	118.30
1	C	333	ARG	NE-CZ-NH2	-10.21	115.19	120.30
1	B	469	ASP	CB-CG-OD1	10.21	127.49	118.30
1	C	909	ARG	NE-CZ-NH2	-10.20	115.20	120.30
1	C	699	ARG	NE-CZ-NH2	-10.14	115.23	120.30
1	D	144	ASP	CB-CG-OD1	10.13	127.42	118.30
1	A	336	ARG	NE-CZ-NH1	10.04	125.32	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	439	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	A	388	ARG	NE-CZ-NH2	-9.91	115.35	120.30
1	B	572	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	B	648	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	D	800	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	B	252	ASP	CB-CG-OD2	-9.71	109.56	118.30
1	B	809	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	C	429	ASP	CB-CG-OD2	-9.61	109.65	118.30
1	C	333	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	A	172	ASP	CB-CG-OD2	-9.58	109.68	118.30
1	C	178	ARG	NE-CZ-NH2	-9.53	115.53	120.30
1	C	539[A]	ALA	CB-CA-C	-9.53	95.81	110.10
1	C	539[B]	ALA	CB-CA-C	-9.53	95.81	110.10
1	A	469	ASP	CB-CG-OD2	-9.52	109.74	118.30
1	D	255	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	D	996	ASP	CB-CG-OD1	9.45	126.80	118.30
1	D	507	ASP	CB-CG-OD2	-9.38	109.86	118.30
1	D	786	ARG	NE-CZ-NH2	-9.29	115.65	120.30
1	A	251	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	B	919	ASP	CB-CG-OD2	-9.26	109.97	118.30
1	D	632	SER	N-CA-CB	9.26	124.39	110.50
1	A	952	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	C	233	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	C	233	ASP	CB-CG-OD1	9.19	126.57	118.30
1	B	388	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	D	786	ARG	NE-CZ-NH1	9.11	124.86	120.30
1	D	881	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	A	952	ARG	NE-CZ-NH2	-9.08	115.76	120.30
1	B	594	ASP	CB-CG-OD1	9.05	126.44	118.30
1	C	255	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	C	507	ASP	CB-CG-OD1	9.03	126.43	118.30
1	B	610	ASP	CB-CG-OD1	9.01	126.41	118.30
1	C	802	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	B	166	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	D	802	ASP	CB-CG-OD2	-8.95	110.24	118.30
1	C	909	ARG	NE-CZ-NH1	8.91	124.76	120.30
1	A	233	ASP	CB-CG-OD1	8.90	126.31	118.30
1	A	233	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	B	469	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	D	193	ASP	CB-CG-OD2	-8.86	110.33	118.30
1	D	234	ASP	CB-CG-OD2	-8.79	110.39	118.30
1	C	429	ASP	CB-CG-OD1	8.78	126.20	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	853	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	D	224	ASP	CB-CG-OD1	8.73	126.15	118.30
1	B	46	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	B	792	ASP	CB-CG-OD2	-8.71	110.47	118.30
1	D	368	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	D	610	ASP	CB-CG-OD1	8.70	126.13	118.30
1	B	772	ASP	CB-CG-OD1	8.66	126.10	118.30
1	D	659	ASP	CB-CG-OD2	-8.64	110.53	118.30
1	B	671	ASP	CB-CG-OD1	8.63	126.07	118.30
1	A	439	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	A	224	ASP	CB-CG-OD2	-8.62	110.55	118.30
1	B	45	ASP	CB-CG-OD1	8.62	126.05	118.30
1	B	425	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	C	802	ASP	CB-CG-OD1	8.61	126.05	118.30
1	B	539[A]	ALA	CB-CA-C	-8.60	97.20	110.10
1	B	539[B]	ALA	CB-CA-C	-8.60	97.20	110.10
1	C	26	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	A	287	ASP	CB-CG-OD1	8.59	126.03	118.30
1	B	671	ASP	CB-CG-OD2	-8.57	110.58	118.30
1	D	733	ALA	N-CA-CB	8.57	122.09	110.10
1	D	509	ASP	CB-CG-OD1	8.57	126.01	118.30
1	B	439	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	859	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	B	439	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	D	287	ASP	CB-CG-OD1	8.49	125.94	118.30
1	B	958	ASN	N-CA-CB	8.48	125.86	110.60
1	B	561	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	505	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	A	997	ASP	CB-CG-OD2	-8.45	110.70	118.30
1	D	539[A]	ALA	CB-CA-C	-8.44	97.44	110.10
1	D	539[B]	ALA	CB-CA-C	-8.44	97.44	110.10
1	C	792	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	C	224	ASP	CB-CG-OD1	8.39	125.85	118.30
1	D	859	ASP	CB-CG-OD2	-8.37	110.77	118.30
1	D	648	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	A	234	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	B	287	ASP	CB-CG-OD1	8.34	125.80	118.30
1	C	442	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	C	255	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	C	782	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	D	746	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	D	172	ASP	CB-CG-OD1	8.26	125.73	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	961	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	B	875	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	D	15	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	A	539[A]	ALA	CB-CA-C	-8.19	97.82	110.10
1	A	539[B]	ALA	CB-CA-C	-8.19	97.82	110.10
1	C	579	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	C	799	THR	CA-CB-CG2	-8.19	100.94	112.40
1	B	875	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	594	ASP	CB-CG-OD1	8.15	125.64	118.30
1	B	853	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	288	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	D	403	ASP	CB-CG-OD2	-8.12	111.00	118.30
1	A	954	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	D	287	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	46	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	B	869	ASP	CB-CG-OD1	8.06	125.56	118.30
1	B	233	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	A	802	ASP	CB-CG-OD1	8.04	125.53	118.30
1	B	594	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	D	144	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	A	802	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	469	ASP	CB-CG-OD1	7.99	125.49	118.30
1	C	403	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	A	201	ASP	CB-CG-OD2	-7.98	111.11	118.30
1	A	255	ARG	NE-CZ-NH2	-7.94	116.33	120.30
1	C	411	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	D	15	ASP	CB-CG-OD1	7.92	125.43	118.30
1	A	869	ASP	CB-CG-OD1	7.87	125.39	118.30
1	C	853	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	B	579	ASP	CB-CG-OD1	7.83	125.35	118.30
1	C	428	ASP	CB-CG-OD1	7.82	125.33	118.30
1	A	942	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	D	255	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	A	792	ASP	CB-CG-OD1	7.76	125.29	118.30
1	C	685	LEU	N-CA-CB	7.76	125.92	110.40
1	B	909	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	C	772	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	B	234	ASP	CB-CG-OD1	7.75	125.27	118.30
1	B	425	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	869	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	D	859	ASP	CB-CG-OD1	7.73	125.26	118.30
1	B	1018	LEU	CB-CA-C	-7.73	95.52	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	HIS	CA-CB-CG	-7.70	100.51	113.60
1	A	1021	CYS	CA-CB-SG	-7.68	100.17	114.00
1	B	942	ARG	CD-NE-CZ	7.67	134.34	123.60
1	B	429	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	C	832	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	D	507	ASP	CB-CG-OD1	7.64	125.18	118.30
1	D	336	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	952	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	D	333	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	329	ASP	CB-CG-OD2	-7.57	111.48	118.30
1	A	439	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	792	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	428	ASP	CB-CG-OD1	7.55	125.09	118.30
1	C	473	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	C	538	TYR	CB-CG-CD1	-7.53	116.48	121.00
1	A	721	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	D	164	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	C	509	ASP	CB-CG-OD1	7.52	125.07	118.30
1	C	184	LEU	CB-CA-C	-7.52	95.92	110.20
1	A	130	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	B	611	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	A	287	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	B	237	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	D	234	ASP	CB-CG-OD1	7.48	125.03	118.30
1	D	952	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	C	598	ASP	CB-CG-OD1	7.45	125.01	118.30
1	B	648	ASP	CB-CG-OD1	7.45	125.01	118.30
1	C	996	ASP	CB-CG-OD1	7.44	124.99	118.30
1	A	610	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	987	ASP	CB-CG-OD1	7.41	124.97	118.30
1	B	473	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	C	869	ASP	CB-CG-OD1	7.39	124.95	118.30
1	B	172	ASP	CB-CG-OD1	7.38	124.95	118.30
1	D	659	ASP	CB-CG-OD1	7.38	124.95	118.30
1	B	329	ASP	CB-CG-OD1	7.38	124.94	118.30
1	D	572	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	632	SER	N-CA-CB	7.33	121.49	110.50
1	C	792	ASP	CB-CG-OD1	7.32	124.89	118.30
1	C	958	ASN	N-CA-CB	7.31	123.75	110.60
1	D	591	ASP	CB-CG-OD1	7.31	124.88	118.30
1	D	403	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	598	ASP	CB-CG-OD2	-7.25	111.78	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	659	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	D	572	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	A	809	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	572	ASP	CB-CG-OD1	7.24	124.82	118.30
1	B	368	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	310	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	579	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	C	809	ARG	CD-NE-CZ	7.19	133.67	123.60
1	A	329	ASP	CB-CG-OD1	7.19	124.77	118.30
1	B	288	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	C	288	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	B	43	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	C	772	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	699	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	C	497	ASP	CB-CG-OD1	7.13	124.72	118.30
1	D	13	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	832	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	172	ASP	CB-CG-OD1	7.11	124.70	118.30
1	D	199	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	659	ASP	CB-CG-OD1	7.07	124.67	118.30
1	A	987	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	B	144	ASP	CB-CG-OD1	7.07	124.66	118.30
1	D	630	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	781	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	579	ASP	CB-CG-OD1	7.05	124.64	118.30
1	B	746	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	D	469	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	C	561	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	D	869	ASP	CB-CG-OD1	7.02	124.61	118.30
1	A	411	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	D	980	GLU	C-N-CA	-7.01	107.57	122.30
1	D	282	ARG	NE-CZ-NH2	-7.01	116.79	120.30
1	A	403	ASP	CB-CG-OD1	7.01	124.61	118.30
1	B	356	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	77	ASP	CB-CG-OD1	7.00	124.60	118.30
1	C	403	ASP	CB-CG-OD1	7.00	124.59	118.30
1	A	857	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	B	579	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	C	924	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	B	859	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	144	ASP	CB-CG-OD1	6.95	124.56	118.30
1	A	166	ARG	NE-CZ-NH2	-6.95	116.83	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	809	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	D	14	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	D	329	ASP	CB-CG-OD1	6.95	124.55	118.30
1	C	411	ASP	CB-CG-OD1	6.95	124.55	118.30
1	C	126	THR	CA-CB-CG2	-6.94	102.68	112.40
1	C	859	ASP	CB-CG-OD1	6.94	124.55	118.30
1	C	760	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	A	190	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	832	ASP	CB-CG-OD1	6.90	124.51	118.30
1	B	802	ASP	CB-CG-OD1	6.90	124.51	118.30
1	C	790	ASP	CB-CG-OD1	6.88	124.49	118.30
1	D	164	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	164	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	B	857	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	828	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	D	610	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	A	509	ASP	CB-CG-OD1	6.83	124.44	118.30
1	C	859	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	280	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	A	15	ASP	CB-CG-OD1	6.78	124.41	118.30
1	D	924	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	428	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	D	809	ARG	NE-CZ-NH2	6.76	123.68	120.30
1	C	13	ARG	N-CA-CB	6.76	122.77	110.60
1	B	997	ASP	CB-CG-OD1	6.75	124.38	118.30
1	D	734	SER	CA-C-N	-6.75	102.34	117.20
1	A	280	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	C	43	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	C	477	SER	N-CA-CB	-6.73	100.40	110.50
1	B	280	ASP	CB-CG-OD1	6.73	124.36	118.30
1	B	45	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	C	828	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	C	746	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	233	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	411	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	832	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	B	246	MET	CG-SD-CE	-6.70	89.47	100.20
1	C	919	ASP	CB-CG-OD1	6.70	124.33	118.30
1	D	446	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	447	ASP	CB-CG-OD1	6.69	124.32	118.30
1	C	234	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	B	13	ARG	NE-CZ-NH1	6.68	123.64	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	591	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	D	924	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	C	172	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	96	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	B	164	ASP	CB-CG-OD1	6.64	124.28	118.30
1	C	664	ALA	CB-CA-C	-6.63	100.15	110.10
1	C	15	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	509	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	375	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	772	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	429	ASP	CB-CG-OD1	6.58	124.22	118.30
1	D	193	ASP	CB-CG-OD1	6.57	124.22	118.30
1	D	987	ASP	CB-CG-OD1	6.57	124.22	118.30
1	C	199	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	D	854	LYS	CB-CA-C	-6.57	97.26	110.40
1	D	952	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	919	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	375	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	630	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	C	952	ARG	CD-NE-CZ	6.52	132.72	123.60
1	A	319	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	D	469	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	96	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	572	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	B	996	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	B	557	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	859	ASP	CB-CG-OD1	6.49	124.14	118.30
1	C	721	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	C	832	ASP	CB-CG-OD1	6.48	124.13	118.30
1	C	961	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	842	TRP	CG-CD2-CE3	-6.48	128.07	133.90
1	A	46	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	648	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	368	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	B	234	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	C	425	ARG	NE-CZ-NH2	6.45	123.52	120.30
1	D	958	ASN	N-CA-CB	6.45	122.20	110.60
1	D	594	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	D	832	ASP	CB-CG-OD1	6.44	124.09	118.30
1	B	292	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	45	ASP	CB-CG-OD1	6.43	124.09	118.30
1	B	734	SER	N-CA-CB	6.42	120.13	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	D	919	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	15	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	C	946	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	C	579	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	648	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	C	287	ASP	CB-CG-OD1	6.36	124.03	118.30
1	C	719	GLN	CB-CA-C	-6.36	97.67	110.40
1	B	411	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	B	859	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	594	ASP	CB-CG-OD1	6.32	123.99	118.30
1	D	832	ASP	N-CA-CB	-6.32	99.22	110.60
1	A	924	ASP	CB-CG-OD1	6.32	123.98	118.30
1	B	26	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	446	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	319	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	C	699	ARG	CD-NE-CZ	6.29	132.41	123.60
1	A	252	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	B	768	MET	CG-SD-CE	6.28	110.25	100.20
1	C	280	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	B	598	ASP	CB-CG-OD1	6.27	123.95	118.30
1	D	442	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	233	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	598	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	569	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	D	772	ASP	CB-CG-OD1	6.24	123.92	118.30
1	D	233	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	B	319	ASP	CB-CG-OD1	6.24	123.91	118.30
1	C	746	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	D	962	TYR	CB-CG-CD1	-6.23	117.26	121.00
1	D	224	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	659	ASP	CB-CG-OD1	6.22	123.90	118.30
1	C	890	GLN	N-CA-CB	-6.22	99.41	110.60
1	D	719	GLN	CB-CA-C	-6.21	97.97	110.40
1	B	786	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	996	ASP	CB-CG-OD1	6.21	123.89	118.30
1	C	553	TRP	CA-CB-CG	-6.19	101.94	113.70
1	D	100	TYR	CB-CG-CD1	-6.18	117.29	121.00
1	D	997	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	140	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	C	924	ASP	CB-CG-OD1	6.17	123.86	118.30
1	D	356	ARG	NE-CZ-NH1	6.17	123.38	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	659	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	D	782	ASP	CB-CG-OD1	6.15	123.84	118.30
1	D	252	ASP	CB-CG-OD1	6.15	123.83	118.30
1	C	505	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	211	ASP	CB-CG-OD1	6.15	123.83	118.30
1	C	404	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	140	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	336	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	255	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	329	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	C	790	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	A	572	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	356	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	509	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	B	690	SER	N-CA-CB	6.08	119.62	110.50
1	C	853	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	C	431	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	D	442	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	D	319	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	22	THR	CA-CB-CG2	-6.05	103.93	112.40
1	A	572	ASP	CB-CG-OD2	-6.04	112.87	118.30
1	A	648	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	C	507	ASP	CB-CG-OD2	-6.02	112.89	118.30
1	A	875	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	136	GLU	CB-CA-C	-6.01	98.38	110.40
1	C	147	ASN	N-CA-CB	-6.00	99.80	110.60
1	A	477	SER	N-CA-CB	6.00	119.50	110.50
1	A	721	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	52	ARG	CB-CA-C	-5.99	98.42	110.40
1	C	252	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	507	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	869	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	A	210	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	C	219	THR	CA-CB-CG2	-5.97	104.05	112.40
1	A	438	GLU	CG-CD-OE2	-5.96	106.38	118.30
1	D	802	ASP	CB-CG-OD1	5.96	123.66	118.30
1	A	569	ASP	CB-CG-OD1	5.95	123.66	118.30
1	D	598	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	741	THR	CA-CB-CG2	-5.95	104.08	112.40
1	C	610	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	C	234	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	333	ARG	NE-CZ-NH1	5.93	123.26	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	591	ASP	CB-CG-OD1	5.92	123.63	118.30
1	D	869	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	618	THR	CA-CB-CG2	-5.92	104.12	112.40
1	D	183	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	D	429	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	368	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	183	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	A	201	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	686	PRO	N-CA-CB	5.89	110.37	103.30
1	A	429	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	221	GLN	N-CA-CB	-5.89	100.00	110.60
1	B	224	ASP	CB-CG-OD1	5.88	123.60	118.30
1	C	917	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	C	875	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	388	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	519	SER	N-CA-CB	-5.88	101.68	110.50
1	C	446	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	919	ASP	CB-CG-OD1	5.87	123.59	118.30
1	B	252	ASP	CB-CG-OD1	5.86	123.57	118.30
1	D	829	THR	N-CA-CB	5.86	121.43	110.30
1	B	255	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	161	TYR	N-CA-CB	-5.86	100.06	110.60
1	D	280	ASP	CB-CG-OD1	5.85	123.56	118.30
1	D	828	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	B	996	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	211	ASP	CB-CG-OD1	5.84	123.56	118.30
1	B	157	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	230	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	799	THR	CA-CB-CG2	-5.83	104.24	112.40
1	A	251	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	164	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	B	172	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	509	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	D	428	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	448	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	B	15	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	681	GLU	CB-CG-CD	-5.79	98.56	114.20
1	B	388	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	B	832	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	408	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	C	842	TRP	CB-CA-C	-5.78	98.84	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	781	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	B	199	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	B	926	TYR	CB-CG-CD2	-5.76	117.55	121.00
1	C	76	CYS	CA-CB-SG	-5.76	103.64	114.00
1	D	579	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	D	890	GLN	N-CA-CB	-5.75	100.25	110.60
1	C	809	ARG	NH1-CZ-NH2	-5.75	113.08	119.40
1	A	772	ASP	CB-CA-C	5.75	121.90	110.40
1	C	201	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	B	557	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	255	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	492	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	D	45	ASP	CB-CG-OD1	5.73	123.45	118.30
1	A	82	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	540[A]	HIS	N-CA-CB	-5.72	100.30	110.60
1	A	540[B]	HIS	N-CA-CB	-5.72	100.30	110.60
1	A	553	TRP	CA-CB-CG	-5.72	102.83	113.70
1	B	699	ARG	CD-NE-CZ	5.72	131.61	123.60
1	B	954	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	403	ASP	CB-CG-OD2	-5.72	113.16	118.30
1	A	997	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	844	HIS	CA-CB-CG	-5.71	103.89	113.60
1	D	75	GLU	CG-CD-OE1	5.71	129.72	118.30
1	D	781	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	52	ARG	CB-CA-C	-5.70	98.99	110.40
1	C	997	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	164	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	768	MET	N-CA-CB	5.68	120.83	110.60
1	A	144	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	909	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	161	TYR	N-CA-CB	-5.67	100.39	110.60
1	C	172	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	768	MET	N-CA-CB	5.67	120.80	110.60
1	A	569	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	D	288	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	C	280	ASP	CB-CG-OD1	5.66	123.39	118.30
1	D	770	ILE	N-CA-C	-5.66	95.73	111.00
1	D	75	GLU	CG-CD-OE2	-5.64	107.01	118.30
1	D	834	VAL	CA-CB-CG1	-5.64	102.44	110.90
1	B	828	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	C	277	GLU	CA-CB-CG	-5.64	101.00	113.40
1	B	781	ARG	CD-NE-CZ	5.63	131.49	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	610	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	375	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	B	568	TRP	CA-CB-CG	-5.62	103.03	113.70
1	C	842	TRP	CA-CB-CG	-5.61	103.04	113.70
1	C	292	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	611	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	C	13	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	962	TYR	CB-CG-CD2	5.60	124.36	121.00
1	A	962	TYR	CB-CG-CD1	-5.59	117.64	121.00
1	C	840	HIS	CB-CA-C	-5.59	99.21	110.40
1	A	21	VAL	CA-CB-CG2	-5.59	102.51	110.90
1	D	147	ASN	N-CA-CB	-5.59	100.54	110.60
1	A	746	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	D	832	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	494	THR	CA-CB-CG2	-5.57	104.60	112.40
1	B	287	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	B	737	ILE	N-CA-CB	5.57	123.60	110.80
1	D	199	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	594	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	B	368	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	D	842	TRP	CH2-CZ2-CE2	-5.55	111.84	117.40
1	D	875	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	853	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	C	95	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	A	671	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	D	538	TYR	CB-CG-CD2	5.53	124.32	121.00
1	D	553	TRP	CA-CB-CG	-5.53	103.20	113.70
1	B	497	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	632	SER	N-CA-CB	5.52	118.77	110.50
1	A	828	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	479	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	519	SER	N-CA-CB	-5.51	102.24	110.50
1	C	782	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	193	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	279	ILE	CB-CG1-CD1	-5.49	98.53	113.90
1	A	336	ARG	CD-NE-CZ	5.49	131.29	123.60
1	B	790	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	519	SER	N-CA-CB	-5.49	102.27	110.50
1	B	553	TRP	CA-CB-CG	-5.49	103.28	113.70
1	B	531	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	C	492	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	B	193	ASP	CB-CG-OD1	5.47	123.22	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	279	ILE	CB-CG1-CD1	-5.46	98.60	113.90
1	D	253	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	D	595	THR	CA-CB-CG2	-5.46	104.76	112.40
1	D	76	CYS	N-CA-CB	5.45	120.41	110.60
1	B	76	CYS	CA-CB-SG	-5.44	104.21	114.00
1	B	954	ASP	CB-CG-OD1	5.44	123.19	118.30
1	C	438	GLU	CG-CD-OE2	-5.44	107.43	118.30
1	D	991	MET	CG-SD-CE	5.44	108.90	100.20
1	D	968	MET	N-CA-CB	-5.43	100.82	110.60
1	A	497	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	A	431	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	D	52	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	262	GLN	N-CA-C	-5.39	96.44	111.00
1	C	588	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	D	855	THR	N-CA-CB	5.38	120.53	110.30
1	C	659	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	519	SER	N-CA-CB	-5.38	102.44	110.50
1	A	618	THR	CA-CB-CG2	-5.36	104.90	112.40
1	A	356	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	635	THR	CA-CB-CG2	-5.36	104.90	112.40
1	C	123	TYR	CB-CA-C	-5.35	99.69	110.40
1	C	881	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	D	800	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	909	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	561	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	252	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	319	ASP	CB-CG-OD1	5.32	123.08	118.30
1	C	800	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	909	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	D	395	HIS	N-CA-CB	-5.31	101.04	110.60
1	B	569	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	319	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	746	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	546	LEU	N-CA-CB	5.29	120.99	110.40
1	C	869	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	C	230	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	B	436	MET	CG-SD-CE	5.29	108.66	100.20
1	B	987	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	95	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	B	428	ASP	CB-CG-OD1	5.28	123.06	118.30
1	B	400	THR	CA-CB-OG1	-5.27	97.93	109.00
1	A	193	ASP	CB-CG-OD1	5.26	123.04	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	949	HIS	CB-CA-C	-5.26	99.87	110.40
1	B	431	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	480	PRO	CA-N-CD	5.26	119.07	111.70
1	B	344	LEU	CA-CB-CG	-5.26	103.20	115.30
1	C	653	HIS	N-CA-CB	5.26	120.07	110.60
1	A	829	THR	CA-CB-CG2	-5.25	105.04	112.40
1	B	403	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	130	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	671	ASP	CB-CG-OD1	5.25	123.02	118.30
1	D	411	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	768	MET	N-CA-CB	5.24	120.03	110.60
1	B	746	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	310	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	954	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	442	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	A	746	ASP	CB-CA-C	-5.23	99.95	110.40
1	C	598	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	B	722	LEU	O-C-N	-5.22	114.35	122.70
1	D	95	TYR	CG-CD2-CE2	-5.22	117.13	121.30
1	C	329	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	917	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	D	477	SER	N-CA-CB	5.20	118.30	110.50
1	B	843	GLN	O-C-N	5.19	131.00	122.70
1	C	599	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	B	96	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	792	ASP	CB-CG-OD1	5.18	122.97	118.30
1	D	919	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	252	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	850	PHE	CB-CA-C	-5.18	100.05	110.40
1	D	14	ARG	N-CA-CB	-5.17	101.28	110.60
1	B	828	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	234	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	746	ASP	CB-CA-C	-5.17	100.07	110.40
1	B	59	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	472	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	C	448	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	D	447	ASP	CB-CG-OD1	5.16	122.94	118.30
1	D	52	ARG	CB-CA-C	-5.15	100.09	110.40
1	C	650	GLU	CG-CD-OE1	5.15	128.60	118.30
1	C	821	ALA	N-CA-CB	5.15	117.31	110.10
1	C	49	GLN	CB-CA-C	-5.15	100.10	110.40
1	B	170	GLU	CG-CD-OE2	-5.15	108.01	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	618	THR	CA-CB-CG2	-5.15	105.19	112.40
1	D	80	GLU	CB-CA-C	-5.15	100.11	110.40
1	A	96	ASP	N-CA-CB	5.14	119.85	110.60
1	B	540[A]	HIS	N-CA-CB	-5.14	101.36	110.60
1	B	540[B]	HIS	N-CA-CB	-5.14	101.36	110.60
1	D	782	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	549	PHE	CB-CG-CD1	-5.12	117.22	120.80
1	C	931	PHE	N-CA-C	-5.12	97.18	111.00
1	B	908	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	144	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	D	908	ASP	CB-CG-OD2	-5.11	113.71	118.30
1	D	842	TRP	CA-CB-CG	-5.10	104.00	113.70
1	C	594	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	527	PRO	N-CA-CB	5.09	109.41	103.30
1	D	251	ARG	CD-NE-CZ	5.09	130.73	123.60
1	B	842	TRP	CB-CG-CD2	-5.09	119.99	126.60
1	A	446	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	885	ASN	CB-CA-C	5.09	120.57	110.40
1	A	917	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	D	22	THR	CA-CB-CG2	-5.07	105.30	112.40
1	C	40	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	B	906	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	B	538	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	D	746	ASP	CB-CA-C	-5.06	100.28	110.40
1	A	492	ASP	CB-CG-OD1	5.06	122.85	118.30
1	D	699	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	648	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	492	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	707	ALA	CB-CA-C	-5.04	102.54	110.10
1	C	568	TRP	CA-CB-CG	-5.04	104.12	113.70
1	D	568	TRP	CA-CB-CG	-5.04	104.13	113.70
1	A	788	PRO	N-CA-CB	5.03	109.34	103.30
1	A	800	ARG	CA-CB-CG	5.02	124.45	113.40
1	A	958	ASN	N-CA-CB	5.02	119.63	110.60
1	C	130	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	C	482	ARG	CB-CA-C	-5.02	100.36	110.40
1	D	734	SER	O-C-N	5.02	130.73	122.70
1	D	997	ASP	CB-CG-OD1	5.02	122.82	118.30
1	D	857	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	C	400	THR	CA-CB-CG2	-5.01	105.39	112.40
1	A	249	GLU	OE1-CD-OE2	5.01	129.31	123.30
1	B	185	ALA	N-CA-CB	5.00	117.10	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	411	ASP	CB-CG-OD2	-5.00	113.80	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	13	ARG	CA
1	C	685	LEU	CA
1	D	733	ALA	CA

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	108	0
1	B	8128	0	7712	141	0
1	C	8128	0	7712	125	0
1	D	8128	0	7712	132	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	42	0	29	2	0
4	B	42	0	29	1	0
4	C	42	0	29	2	0
4	D	42	0	29	4	0
5	A	108	0	162	7	0
5	B	100	0	150	5	0
5	C	108	0	162	5	0
5	D	112	0	168	15	0
6	A	1060	0	0	16	3
6	B	1013	0	0	14	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	987	0	0	14	2
6	D	1021	0	0	15	0
All	All	37222	0	31606	518	3

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 8.

All (518) 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:B:8407:DMS:S	5:B:8407:DMS:C2	2.01	1.48
5:B:8502:DMS:S	5:B:8502:DMS:C1	2.01	1.46
5:D:8407:DMS:S	5:D:8407:DMS:C2	2.04	1.46
5:C:8415:DMS:C2	5:C:8415:DMS:S	2.04	1.45
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.37	1.21
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.41	1.16
1:B:942:ARG:HH21	1:B:954:ASP:HB2	1.07	1.10
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.37	1.07
1:C:634:GLN:H	1:C:634:GLN:NE2	1.57	1.02
1:D:651:LEU:HD21	1:D:653:HIS:CE1	2.00	0.96
1:D:581:ASN:HD22	1:D:583:ASN:ND2	1.63	0.95
1:D:581:ASN:HD22	1:D:583:ASN:HD22	1.05	0.94
1:A:473:ARG:NH1	1:A:476:LYS:HB2	1.85	0.91
1:C:634:GLN:H	1:C:634:GLN:HE21	1.02	0.91
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.07	0.89
1:A:655:MET:HE2	1:A:656:VAL:N	1.88	0.88
1:D:737:ILE:HD12	1:D:738:PRO:CD	2.03	0.88
1:A:1022:GLN:HG2	1:A:1023:LYS:N	1.91	0.86
1:D:658:LEU:O	1:D:661:LYS:HG3	1.75	0.85
1:B:942:ARG:HH21	1:B:954:ASP:CB	1.89	0.84
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.42	0.84
1:B:942:ARG:NH2	1:B:954:ASP:HB2	1.91	0.83
1:D:133:TRP:HE1	5:D:8703:DMS:H23	1.41	0.83
1:B:651:LEU:O	1:B:651:LEU:HD23	1.80	0.81
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.43	0.81
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.63	0.81
1:B:600:GLN:H	1:B:600:GLN:HE21	1.24	0.80
1:A:942:ARG:HB3	6:A:9413:HOH:O	1.78	0.80
1:A:600:GLN:H	1:A:600:GLN:HE21	1.30	0.80
1:D:651:LEU:CD2	1:D:701:VAL:HB	2.11	0.80
1:D:133:TRP:HE1	5:D:8703:DMS:C2	1.96	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:748:CYS:C	1:C:749:ILE:HD12	2.04	0.78
1:D:128:ASN:HB3	1:D:180:GLY:O	1.83	0.78
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.66	0.77
6:B:9369:HOH:O	5:C:8420:DMS:H21	1.82	0.77
1:A:809:ARG:HH11	1:A:809:ARG:HG2	1.49	0.77
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.14	0.77
1:C:745:MET:HG2	6:C:9532:HOH:O	1.84	0.77
1:C:634:GLN:N	1:C:634:GLN:NE2	2.34	0.76
1:C:615:PRO:O	1:C:618:THR:HG22	1.86	0.76
1:D:629:PHE:O	1:D:630:ARG:HD3	1.85	0.76
1:D:1013:ARG:HD3	6:D:9311:HOH:O	1.84	0.76
1:D:292:ARG:HH12	5:D:8412:DMS:C2	1.99	0.75
1:B:778:THR:HG23	1:B:887:GLN:HB3	1.69	0.74
1:C:131:GLU:HG3	1:C:135:GLN:NE2	2.02	0.74
1:D:800:ARG:HD2	6:D:9504:HOH:O	1.87	0.74
1:B:658:LEU:O	1:B:661:LYS:HG3	1.86	0.73
1:C:765:LEU:HD21	1:C:768:MET:CE	2.19	0.73
1:C:771:GLY:HA2	6:C:9614:HOH:O	1.88	0.73
1:C:843:GLN:HG2	1:C:848:THR:HA	1.71	0.73
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.71	0.72
1:D:737:ILE:HD12	1:D:738:PRO:HD2	1.69	0.72
1:D:237:ARG:NH1	6:D:9268:HOH:O	2.21	0.72
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.51	0.72
1:C:743:SER:O	1:C:760:ARG:NH1	2.22	0.72
1:B:890:GLN:HG3	1:B:891:VAL:N	2.05	0.72
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.70	0.72
1:B:237:ARG:HD2	1:B:296:GLU:OE1	1.89	0.72
1:B:615:PRO:O	1:B:618:THR:HG22	1.90	0.71
1:B:262:GLN:HE21	1:B:263:GLY:N	1.87	0.71
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.24	0.70
1:B:131:GLU:OE2	1:B:134:LEU:HB2	1.91	0.70
1:B:236:SER:C	1:B:237:ARG:HG2	2.10	0.70
1:B:693:GLN:NE2	1:B:723:ALA:O	2.23	0.70
1:C:41:GLU:HG2	1:C:46:ARG:NH2	2.05	0.70
1:D:749:ILE:N	1:D:749:ILE:HD12	2.06	0.70
1:C:737:ILE:HD12	1:C:832:ASP:C	2.12	0.70
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.73	0.69
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.04	0.69
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.75	0.69
1:D:292:ARG:HH12	5:D:8412:DMS:H22	1.56	0.69
1:D:581:ASN:ND2	1:D:583:ASN:HD22	1.87	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:HIS:HD2	6:C:8797:HOH:O	1.75	0.69
1:D:809:ARG:HG2	1:D:809:ARG:HH11	1.58	0.69
1:D:237:ARG:HG2	1:D:237:ARG:HH11	1.58	0.68
1:A:887:GLN:NE2	1:A:980:GLU:O	2.25	0.68
1:D:804:ASN:HD22	1:D:809:ARG:HH21	0.73	0.68
1:D:887:GLN:NE2	1:D:980:GLU:O	2.25	0.68
5:A:8503:DMS:H21	6:A:9019:HOH:O	1.94	0.68
1:B:243:GLU:OE2	1:B:245:GLN:NE2	2.26	0.68
1:B:681:GLU:HA	1:B:681:GLU:OE2	1.93	0.68
1:A:878:HIS:HD2	6:A:8675:HOH:O	1.77	0.68
1:C:750:GLU:HG2	6:C:9529:HOH:O	1.94	0.68
1:B:693:GLN:CD	1:B:721:ARG:HG2	2.14	0.67
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.27	0.67
1:A:387:VAL:HG22	6:A:9621:HOH:O	1.93	0.67
1:A:237:ARG:HB3	1:A:237:ARG:NH1	2.08	0.67
1:B:262:GLN:HE21	1:B:262:GLN:C	1.96	0.67
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.75	0.67
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.28	0.66
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.61	0.66
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.09	0.66
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.29	0.66
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.77	0.65
1:C:634:GLN:N	1:C:634:GLN:HE21	1.86	0.65
1:A:809:ARG:CG	1:A:809:ARG:HH11	2.08	0.65
1:B:634:GLN:HE21	1:B:685:LEU:HG	1.61	0.65
1:C:737:ILE:HG13	1:C:738:PRO:HD2	1.79	0.64
1:D:773:LYS:HD2	1:D:774:LYS:O	1.97	0.64
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.30	0.64
1:B:878:HIS:HD2	6:B:8694:HOH:O	1.79	0.64
1:B:634:GLN:HG2	1:B:682:LEU:O	1.98	0.64
1:B:251:ARG:NH1	5:B:8416:DMS:O	2.30	0.64
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.09	0.64
1:C:745:MET:HE3	1:C:745:MET:HA	1.78	0.64
1:A:431:ARG:HG3	6:A:9354:HOH:O	1.97	0.64
5:B:8420:DMS:H23	6:B:9580:HOH:O	1.98	0.63
1:C:131:GLU:HG3	1:C:135:GLN:HE21	1.61	0.63
1:A:615:PRO:O	1:A:618:THR:HG22	1.99	0.63
1:D:1022:GLN:O	1:D:1023:LYS:HB2	1.98	0.63
1:A:651:LEU:HD12	1:A:651:LEU:C	2.20	0.62
1:A:237:ARG:NH1	6:A:9130:HOH:O	2.28	0.62
1:D:651:LEU:HD21	1:D:653:HIS:HE1	1.59	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:C	1:C:651:LEU:HD12	2.20	0.62
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.65	0.62
1:D:893:GLU:HG2	1:D:894:ARG:HG2	1.82	0.62
1:B:635:THR:HG23	1:B:681:GLU:OE1	2.00	0.62
1:C:655:MET:HE2	1:C:665:SER:HB3	1.81	0.62
1:C:684:GLU:HG2	1:C:684:GLU:O	1.99	0.62
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.15	0.62
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.64	0.61
1:A:861:SER:OG	1:A:863:GLN:HG3	2.01	0.61
1:B:751:LEU:HD23	1:B:862:GLY:HA2	1.82	0.61
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.35	0.61
1:D:651:LEU:HD23	1:D:651:LEU:O	2.01	0.61
1:C:1023:LYS:HE3	1:C:1023:LYS:CA	2.31	0.61
1:C:646:HIS:HB3	6:C:9551:HOH:O	2.00	0.60
1:C:135:GLN:HG3	6:C:9667:HOH:O	2.01	0.60
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.36	0.60
1:D:781:ARG:NH1	6:D:9459:HOH:O	2.34	0.60
5:D:8703:DMS:H23	6:D:9650:HOH:O	2.02	0.60
1:D:748:CYS:C	1:D:749:ILE:HD12	2.20	0.60
1:C:737:ILE:HG13	1:C:738:PRO:CD	2.32	0.59
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.68	0.59
1:D:651:LEU:HD23	1:D:651:LEU:C	2.23	0.59
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.84	0.59
1:B:843:GLN:HB3	1:B:847:LYS:O	2.03	0.58
1:B:847:LYS:HG2	1:B:849:LEU:HD23	1.86	0.58
1:A:655:MET:HE2	1:A:656:VAL:H	1.66	0.58
1:B:655:MET:HE2	1:B:664:ALA:O	2.04	0.58
1:A:277:GLU:H	1:A:277:GLU:CD	2.07	0.58
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.03	0.58
5:C:8425:DMS:H21	6:C:9506:HOH:O	2.03	0.58
1:A:178:ARG:HD2	6:A:9459:HOH:O	2.04	0.58
1:C:88:SER:HA	1:C:366:VAL:HG21	1.85	0.57
1:C:768:MET:HE1	1:C:1020:TRP:CZ3	2.39	0.57
1:D:703:PRO:HG2	5:D:8425:DMS:H11	1.86	0.57
1:B:651:LEU:C	1:B:651:LEU:HD23	2.25	0.57
1:C:765:LEU:CD2	1:C:768:MET:HE2	2.35	0.57
1:D:133:TRP:NE1	5:D:8703:DMS:C2	2.66	0.57
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.39	0.57
1:A:595:THR:HA	1:A:596:PRO:C	2.25	0.57
1:B:595:THR:HA	1:B:596:PRO:C	2.25	0.57
1:A:865:ALA:HB1	1:A:1017:GLN:HE22	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:947:GLY:O	1:B:1023:LYS:HE3	2.05	0.56
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.35	0.56
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.87	0.56
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.40	0.56
1:D:878:HIS:HD2	6:D:8810:HOH:O	1.89	0.56
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.74	0.56
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.41	0.56
1:B:847:LYS:HG3	1:B:848:THR:N	2.20	0.56
1:D:773:LYS:HG3	1:D:775:GLN:HE21	1.71	0.56
1:D:581:ASN:ND2	1:D:583:ASN:ND2	2.46	0.55
1:C:750:GLU:OE2	1:C:755:ARG:HD2	2.06	0.55
1:D:754:LYS:HE2	1:D:1022:GLN:HG2	1.88	0.55
1:A:726:LEU:HD22	1:B:871:GLU:OE1	2.06	0.55
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.41	0.55
1:A:737:ILE:HD13	1:A:737:ILE:C	2.27	0.55
1:C:1023:LYS:HE3	1:C:1023:LYS:HA	1.88	0.55
1:D:843:GLN:HA	1:D:847:LYS:O	2.07	0.55
1:A:768:MET:HE3	1:A:1020:TRP:CZ2	2.43	0.54
1:A:952:ARG:NH2	1:A:1021:CYS:SG	2.78	0.54
1:C:356:ARG:HD2	1:C:379:MET:CE	2.36	0.54
1:D:135:GLN:C	1:D:136:GLU:HG2	2.26	0.54
1:A:890:GLN:OE1	1:A:948:PRO:HD3	2.08	0.54
1:A:268:ALA:HA	5:A:8602:DMS:H22	1.90	0.54
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.90	0.54
1:D:237:ARG:CB	1:D:237:ARG:HH11	2.21	0.54
1:B:618:THR:HG23	6:B:9572:HOH:O	2.06	0.54
1:B:178:ARG:HG3	1:B:178:ARG:O	2.06	0.54
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.89	0.54
1:D:473:ARG:HD3	6:D:8720:HOH:O	2.06	0.54
1:C:649:ASN:OD1	1:C:703:PRO:HD2	2.07	0.54
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.43	0.54
1:C:1020:TRP:HD1	1:C:1021:CYS:N	2.06	0.54
1:C:595:THR:HA	1:C:596:PRO:C	2.27	0.54
1:A:230:ARG:NH1	1:A:241:GLU:OE2	2.40	0.53
1:A:88:SER:HA	1:A:366:VAL:HG21	1.90	0.53
1:D:800:ARG:HG3	1:D:800:ARG:O	2.07	0.53
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.67	0.53
4:D:2002:145:O2'	4:D:2002:145:O1'	2.25	0.53
1:B:347:LYS:HG3	1:B:644:PHE:CE2	2.43	0.53
1:C:833:ALA:HB1	1:C:858:ILE:O	2.08	0.53
1:A:658:LEU:O	1:A:661:LYS:HG3	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.44	0.53
1:A:843:GLN:HA	1:A:847:LYS:O	2.08	0.53
1:A:290:THR:HB	5:A:8412:DMS:H22	1.90	0.53
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.90	0.53
5:B:8407:DMS:C1	5:B:8407:DMS:C2	2.86	0.53
1:C:1023:LYS:C	6:C:9668:HOH:O	2.47	0.53
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.91	0.53
1:B:788:PRO:HD2	1:B:968:MET:HB2	1.91	0.53
1:C:601:PHE:CD1	4:C:2002:145:H3'	2.44	0.53
1:C:682:LEU:HB3	1:C:683:PRO:CD	2.38	0.53
1:C:756:TRP:CD2	1:C:858:ILE:HD13	2.43	0.53
1:A:292:ARG:HH12	5:A:8412:DMS:C2	2.22	0.52
1:B:945:ASN:HB3	1:B:1023:LYS:HE2	1.91	0.52
4:B:2002:145:O1'	4:B:2002:145:O2'	2.26	0.52
4:C:2002:145:O1'	4:C:2002:145:O2'	2.27	0.52
1:D:618:THR:HG21	6:D:9049:HOH:O	2.08	0.52
1:C:651:LEU:HD13	1:C:667:GLU:HG2	1.92	0.52
1:C:952:ARG:NH2	1:C:1021:CYS:SG	2.82	0.52
1:D:1022:GLN:C	1:D:1022:GLN:HE21	2.13	0.52
1:C:759:ASN:OD1	1:C:761:GLN:N	2.41	0.52
1:B:751:LEU:HD23	1:B:862:GLY:CA	2.40	0.52
1:A:648:ASP:OD2	6:A:9498:HOH:O	2.19	0.51
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.46	0.51
1:B:804:ASN:HD22	1:B:809:ARG:NH2	2.09	0.51
1:D:595:THR:HA	1:D:596:PRO:C	2.29	0.51
1:D:618:THR:HG23	6:D:9065:HOH:O	2.10	0.51
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.91	0.51
1:B:128:ASN:HB2	1:B:181:GLU:OE2	2.10	0.51
1:B:78:LEU:HD23	6:B:9098:HOH:O	2.11	0.51
1:C:785:THR:O	1:C:881:ARG:HD2	2.09	0.51
5:C:8503:DMS:H12	6:C:9140:HOH:O	2.10	0.51
1:B:630:ARG:HH21	1:B:637:GLU:CD	2.13	0.51
1:D:237:ARG:NH1	1:D:237:ARG:HG2	2.22	0.51
1:D:675:GLN:HG3	6:D:9549:HOH:O	2.10	0.51
1:A:844:HIS:HD2	6:A:9428:HOH:O	1.92	0.51
1:B:745:MET:SD	1:B:745:MET:N	2.80	0.51
1:A:797:GLU:O	1:A:801:ILE:HD13	2.12	0.50
1:B:245:GLN:HG2	1:B:288:ARG:CG	2.39	0.50
1:B:88:SER:HA	1:B:366:VAL:HG21	1.92	0.50
1:B:580:GLU:CD	1:B:580:GLU:H	2.14	0.50
1:D:431:ARG:NE	6:D:9592:HOH:O	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LEU:CD1	1:A:653:HIS:CD2	2.94	0.50
1:B:689:GLU:O	1:B:690:SER:OG	2.26	0.50
1:D:292:ARG:HH12	5:D:8412:DMS:H23	1.72	0.50
1:A:376:ILE:HD12	1:A:401:LEU:HB3	1.94	0.50
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.80	0.50
1:D:88:SER:HA	1:D:366:VAL:HG21	1.93	0.50
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.26	0.50
1:A:843:GLN:HG2	1:A:848:THR:HA	1.93	0.50
1:A:835:LEU:HD11	1:A:855:THR:HB	1.94	0.50
1:D:653:HIS:ND1	1:D:701:VAL:CG2	2.75	0.50
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.12	0.50
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.26	0.50
1:D:135:GLN:O	1:D:136:GLU:HG2	2.12	0.50
1:C:745:MET:HE3	1:C:745:MET:CA	2.38	0.50
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.93	0.49
1:C:687:GLN:HG3	1:C:688:PRO:CD	2.26	0.49
1:D:241:GLU:HG3	1:D:292:ARG:HG2	1.94	0.49
1:C:861:SER:OG	1:C:863:GLN:HG3	2.12	0.49
5:D:8407:DMS:C2	5:D:8407:DMS:C1	2.87	0.49
1:C:126:THR:HA	1:C:182:ASN:O	2.12	0.49
1:C:266:GLN:O	5:C:8602:DMS:H22	2.11	0.49
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.94	0.49
1:D:668:VAL:HG11	1:D:680:ILE:HG12	1.95	0.49
1:A:237:ARG:HG2	1:A:296:GLU:OE1	2.13	0.49
1:C:745:MET:HE3	1:C:761:GLN:OE1	2.13	0.49
5:D:8416:DMS:H21	6:D:9390:HOH:O	2.12	0.49
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.75	0.49
1:A:292:ARG:NH1	5:A:8412:DMS:C2	2.76	0.49
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.95	0.49
1:D:601:PHE:CD1	4:D:2002:145:H3'	2.48	0.49
1:D:634:GLN:O	1:D:634:GLN:HG3	2.11	0.49
1:C:13:ARG:O	1:C:14:ARG:C	2.48	0.49
1:D:809:ARG:NH1	1:D:809:ARG:HG2	2.25	0.49
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.95	0.49
1:A:693:GLN:NE2	1:A:723:ALA:O	2.46	0.48
1:A:694:LEU:HB2	1:A:723:ALA:O	2.13	0.48
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.95	0.48
1:B:135:GLN:NE2	6:B:9398:HOH:O	2.28	0.48
1:C:782:ASP:HA	1:C:884:LEU:HD23	1.95	0.48
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.44	0.48
1:D:785:THR:HB	1:D:816:TYR:CE2	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:ARG:HG3	6:A:9370:HOH:O	2.14	0.48
1:C:580:GLU:HG3	1:C:580:GLU:H	1.27	0.48
5:A:8502:DMS:H12	6:A:9335:HOH:O	2.14	0.48
1:C:749:ILE:HD12	1:C:749:ILE:N	2.28	0.48
1:D:765:LEU:HD21	1:D:768:MET:SD	2.54	0.48
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.95	0.48
1:B:942:ARG:HD2	1:B:942:ARG:N	2.27	0.48
1:C:569:ASP:HB2	6:C:9491:HOH:O	2.13	0.48
1:D:363:HIS:HD2	6:D:9312:HOH:O	1.96	0.48
1:A:655:MET:HE2	1:A:655:MET:C	2.34	0.48
1:B:655:MET:HE2	1:B:655:MET:CA	2.44	0.48
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.95	0.48
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.49	0.48
1:A:859:ASP:OD1	1:A:861:SER:OG	2.23	0.48
1:D:795:VAL:HB	4:D:2002:145:C5'	2.43	0.48
1:D:737:ILE:HD13	1:D:832:ASP:HA	1.95	0.48
1:A:178:ARG:HG3	6:A:9459:HOH:O	2.14	0.48
1:C:689:GLU:O	1:C:690:SER:HB3	2.13	0.48
1:D:513:PRO:O	1:D:514:ALA:HB3	2.14	0.48
1:B:251:ARG:NH1	1:B:251:ARG:HB3	2.29	0.47
5:D:8703:DMS:C2	6:D:9650:HOH:O	2.60	0.47
1:A:721:ARG:NH2	6:A:9643:HOH:O	2.47	0.47
1:C:655:MET:CE	1:C:665:SER:HB3	2.44	0.47
1:C:682:LEU:CB	1:C:683:PRO:CD	2.90	0.47
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.44	0.47
1:B:722:LEU:O	1:B:723:ALA:C	2.52	0.47
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.43	0.47
1:C:634:GLN:CA	1:C:634:GLN:NE2	2.76	0.47
1:C:1000:SER:O	1:C:1001:PRO:C	2.53	0.47
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.96	0.47
1:A:521:LYS:HE2	6:A:9027:HOH:O	2.13	0.47
1:C:230:ARG:HG3	1:C:230:ARG:NH1	2.27	0.47
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.32	0.47
1:B:533:LEU:HD23	1:B:533:LEU:C	2.35	0.47
1:D:749:ILE:N	1:D:749:ILE:CD1	2.76	0.47
1:B:379:MET:HE1	1:B:387:VAL:HB	1.96	0.47
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.19	0.47
1:D:824:GLN:NE2	1:D:837:THR:HG22	2.30	0.47
1:A:795:VAL:HG11	4:A:2001:145:H4'	1.97	0.47
1:B:131:GLU:HA	1:B:131:GLU:OE2	2.15	0.47
1:D:797:GLU:HB2	1:D:800:ARG:HG3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:TRP:NE1	5:D:8703:DMS:H23	2.20	0.47
1:B:46:ARG:HB3	1:B:47:PRO:CD	2.44	0.47
1:B:693:GLN:OE1	1:B:721:ARG:HG2	2.15	0.47
1:B:75:GLU:OE1	1:B:75:GLU:HA	2.15	0.47
1:C:178:ARG:HD3	6:C:9559:HOH:O	2.14	0.47
1:D:376:ILE:CD1	1:D:401:LEU:HB3	2.45	0.47
1:A:128:ASN:HB2	6:A:9493:HOH:O	2.15	0.47
1:D:1022:GLN:HG3	1:D:1022:GLN:O	2.14	0.47
1:A:742:THR:HG22	1:A:743:SER:N	2.29	0.46
1:D:143:PHE:O	1:D:168:PRO:HA	2.15	0.46
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.97	0.46
1:D:651:LEU:HD23	1:D:701:VAL:HB	1.95	0.46
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.97	0.46
1:C:737:ILE:HG13	1:C:738:PRO:N	2.28	0.46
1:D:772:ASP:OD1	1:D:772:ASP:N	2.44	0.46
1:D:773:LYS:CG	1:D:775:GLN:NE2	2.79	0.46
1:A:809:ARG:NH1	1:A:809:ARG:HG2	2.24	0.46
1:A:734:SER:OG	1:A:860:GLY:HA3	2.15	0.46
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.45	0.46
1:D:703:PRO:HG2	5:D:8425:DMS:C1	2.45	0.46
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.97	0.46
1:B:699:ARG:HE	1:B:714:ILE:HD13	1.81	0.46
1:D:845:GLN:OE1	1:D:845:GLN:CA	2.64	0.46
1:A:473:ARG:HH12	1:A:476:LYS:HB2	1.73	0.46
1:D:832:ASP:OD1	1:D:832:ASP:N	2.44	0.46
1:A:147:ASN:HA	1:A:148:SER:HA	1.58	0.46
1:C:819:GLU:HG3	1:C:819:GLU:H	1.51	0.46
1:D:147:ASN:HA	1:D:148:SER:HA	1.68	0.46
1:D:634:GLN:NE2	1:D:682:LEU:O	2.49	0.46
1:C:737:ILE:CG1	1:C:738:PRO:HD2	2.43	0.46
1:C:890:GLN:HE21	1:C:892:ALA:HB2	1.80	0.46
1:B:845:GLN:OE1	1:B:845:GLN:HA	2.16	0.46
1:C:278:ILE:HD13	1:C:278:ILE:N	2.30	0.46
1:B:730:LEU:O	1:B:731:PRO:C	2.54	0.45
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.98	0.45
1:B:799:THR:HG23	6:B:9561:HOH:O	2.15	0.45
1:D:473:ARG:NH1	1:D:476:LYS:HB2	2.29	0.45
1:A:656:VAL:CG1	1:A:694:LEU:HD22	2.47	0.45
1:B:262:GLN:NE2	1:B:262:GLN:CA	2.80	0.45
1:B:734:SER:OG	1:B:860:GLY:HA3	2.16	0.45
1:C:806:TRP:CE2	1:C:809:ARG:NH2	2.85	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:ALA:O	1:A:876:THR:HG22	2.17	0.45
1:A:433:LEU:N	1:A:434:PRO:CD	2.80	0.45
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.99	0.45
1:C:243:GLU:OE2	1:C:245:GLN:NE2	2.49	0.45
1:A:753:ASN:OD1	1:A:753:ASN:N	2.50	0.45
1:C:41:GLU:HG2	1:C:46:ARG:HH21	1.78	0.45
1:D:844:HIS:N	1:D:847:LYS:O	2.49	0.45
1:B:46:ARG:HB3	1:B:47:PRO:HD2	1.99	0.45
1:B:655:MET:CE	1:B:665:SER:HB3	2.47	0.45
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.51	0.45
1:C:147:ASN:HA	1:C:148:SER:HA	1.55	0.45
1:D:133:TRP:NE1	5:D:8703:DMS:H22	2.32	0.45
1:B:890:GLN:OE1	1:B:948:PRO:HD3	2.17	0.44
1:B:91:GLN:HG2	1:B:98:PRO:HA	1.99	0.44
1:C:832:ASP:OD1	1:C:832:ASP:N	2.45	0.44
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.53	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.62	0.44
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.99	0.44
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.53	0.44
1:A:601:PHE:CD1	4:A:2002:145:H3'	2.52	0.44
1:B:183:ARG:HG2	6:B:8922:HOH:O	2.16	0.44
1:D:638:VAL:O	1:D:677:LYS:HA	2.18	0.44
1:D:737:ILE:HA	1:D:737:ILE:HD12	1.61	0.44
1:A:59:ARG:NH2	1:A:81:ALA:HB3	2.33	0.44
1:B:245:GLN:HG2	1:B:288:ARG:CD	2.48	0.44
1:B:817:GLN:NE2	1:B:817:GLN:HA	2.33	0.44
1:D:869:ASP:OD1	1:D:1015:HIS:ND1	2.50	0.44
1:B:554:GLN:HG3	6:B:9427:HOH:O	2.17	0.44
1:C:802:ASP:O	1:C:808:GLU:HG3	2.18	0.44
1:D:640:SER:O	1:D:675:GLN:HA	2.18	0.44
1:B:1000:SER:O	1:B:1001:PRO:C	2.54	0.44
1:B:599:ARG:HH11	1:B:600:GLN:NE2	2.16	0.44
1:B:778:THR:HG23	1:B:887:GLN:CB	2.44	0.44
1:B:781:ARG:HD3	6:B:9573:HOH:O	2.18	0.44
1:A:847:LYS:NZ	1:B:724:GLU:O	2.50	0.43
1:C:240:LEU:HD23	1:C:240:LEU:C	2.39	0.43
1:C:41:GLU:CG	1:C:46:ARG:NH2	2.79	0.43
1:C:669:PRO:HB3	6:C:9640:HOH:O	2.18	0.43
1:D:686:PRO:O	1:D:688:PRO:HD3	2.17	0.43
1:D:755:ARG:HG3	1:D:769:TRP:HB2	2.00	0.43
1:D:845:GLN:HA	1:D:845:GLN:OE1	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:GLN:HG3	1:A:891:VAL:N	2.33	0.43
1:B:128:ASN:HB2	6:B:9470:HOH:O	2.18	0.43
1:B:662:PRO:O	1:B:663:LEU:HD23	2.18	0.43
1:B:226:HIS:ND1	6:B:9139:HOH:O	2.36	0.43
1:C:734:SER:CB	1:C:860:GLY:HA3	2.48	0.43
1:C:947:GLY:HA3	1:C:948:PRO:HD2	1.79	0.43
1:B:241:GLU:CD	1:B:292:ARG:HE	2.22	0.43
1:B:630:ARG:NE	1:B:637:GLU:OE1	2.44	0.43
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.99	0.43
1:D:684:GLU:HG2	1:D:685:LEU:N	2.34	0.43
1:D:844:HIS:O	1:D:845:GLN:HB2	2.18	0.43
1:A:658:LEU:O	1:A:659:ASP:C	2.55	0.43
1:D:738:PRO:HB3	1:D:751:LEU:HB2	2.00	0.43
1:D:829:THR:HG23	1:D:834:VAL:HG22	1.99	0.43
1:A:1000:SER:O	1:A:1001:PRO:C	2.56	0.43
1:B:632:SER:N	1:B:635:THR:O	2.33	0.43
1:C:824:GLN:O	1:C:838:THR:HA	2.19	0.43
1:A:660:GLY:O	1:A:662:PRO:HD3	2.18	0.43
1:B:814:GLY:HA3	1:B:844:HIS:CG	2.54	0.43
1:C:847:LYS:HG3	1:C:848:THR:N	2.30	0.43
1:D:472:TYR:O	1:D:476:LYS:HG2	2.18	0.43
1:D:824:GLN:NE2	1:D:837:THR:CG2	2.82	0.43
1:B:1017:GLN:HB2	6:B:9518:HOH:O	2.18	0.43
1:B:538:TYR:O	1:B:567:VAL:HA	2.19	0.43
1:C:824:GLN:CG	1:C:825:CYS:N	2.81	0.43
1:A:694:LEU:HB3	1:A:722:LEU:HB2	2.01	0.42
1:A:832:ASP:OD1	1:A:832:ASP:N	2.52	0.42
1:B:658:LEU:O	1:B:659:ASP:C	2.55	0.42
1:B:730:LEU:H	1:B:730:LEU:HG	1.24	0.42
1:A:800:ARG:CG	6:A:9370:HOH:O	2.67	0.42
1:C:533:LEU:C	1:C:533:LEU:HD23	2.39	0.42
1:C:655:MET:SD	1:C:664:ALA:O	2.77	0.42
1:C:910:LEU:C	1:C:910:LEU:HD12	2.40	0.42
1:D:795:VAL:HG11	4:D:2001:145:H4'	2.01	0.42
1:A:473:ARG:HD2	1:A:473:ARG:HA	1.92	0.42
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.18	0.42
1:B:513:PRO:O	1:B:514:ALA:HB3	2.19	0.42
1:B:637:GLU:OE2	1:B:677:LYS:HE3	2.19	0.42
1:C:655:MET:SD	1:C:656:VAL:N	2.93	0.42
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.84	0.42
1:A:651:LEU:HD11	1:A:653:HIS:CD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:TRP:CH2	1:B:452:SER:HA	2.55	0.42
1:D:893:GLU:HG3	1:D:894:ARG:HD2	2.00	0.42
1:A:655:MET:HB2	1:A:655:MET:HE3	1.80	0.42
1:B:634:GLN:NE2	1:B:685:LEU:HG	2.32	0.42
1:B:826:THR:OG1	1:B:837:THR:HB	2.19	0.42
1:A:125:LEU:O	1:A:183:ARG:HA	2.20	0.42
1:A:305:ILE:HD11	1:A:645:ARG:HB3	2.01	0.42
1:C:1013:ARG:HD3	6:C:9297:HOH:O	2.18	0.42
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.83	0.42
1:D:431:ARG:NH2	6:D:9592:HOH:O	2.52	0.42
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.68	0.42
1:B:797:GLU:HB2	1:B:800:ARG:HG3	2.01	0.42
1:B:869:ASP:OD1	1:B:1015:HIS:ND1	2.53	0.42
1:C:1013:ARG:NH2	1:D:954:ASP:OD2	2.47	0.42
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.55	0.42
1:C:262:GLN:HB2	1:C:309:TYR:CE2	2.54	0.42
1:B:952:ARG:NH2	1:B:1021:CYS:SG	2.86	0.41
1:A:292:ARG:HH12	5:A:8412:DMS:H21	1.83	0.41
1:A:652:LEU:O	1:A:667:GLU:HA	2.20	0.41
1:B:127:PHE:CD2	1:B:127:PHE:N	2.88	0.41
1:C:655:MET:HE3	1:C:662:PRO:HB3	2.01	0.41
1:C:869:ASP:OD1	1:C:1015:HIS:ND1	2.34	0.41
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.37	0.41
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.55	0.41
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.01	0.41
1:C:577:LYS:HE3	1:C:577:LYS:HB3	1.87	0.41
1:D:737:ILE:HD12	1:D:738:PRO:HD3	1.98	0.41
1:D:745:MET:HE3	1:D:745:MET:HB2	1.79	0.41
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.20	0.41
1:A:472:TYR:O	1:A:476:LYS:HG2	2.20	0.41
1:B:372:MET:CE	1:B:395:HIS:HB3	2.50	0.41
1:D:893:GLU:HG2	1:D:894:ARG:CG	2.50	0.41
1:A:240:LEU:C	1:A:240:LEU:HD23	2.41	0.41
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.03	0.41
1:B:262:GLN:NE2	1:B:263:GLY:N	2.64	0.41
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.55	0.41
1:B:663:LEU:HD23	1:B:663:LEU:HA	1.56	0.41
1:B:756:TRP:CD2	1:B:858:ILE:HD13	2.55	0.41
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.54	0.41
1:C:646:HIS:CE1	1:C:673:ALA:CB	3.03	0.41
1:C:730:LEU:HA	1:C:731:PRO:HD3	1.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:783:GLN:HG2	1:D:881:ARG:HD2	2.02	0.41
1:A:299:LYS:HB3	1:A:299:LYS:HE3	1.83	0.41
1:B:240:LEU:HD23	1:B:240:LEU:C	2.41	0.41
1:C:814:GLY:HA3	1:C:844:HIS:CG	2.56	0.41
1:D:745:MET:O	1:D:745:MET:HG3	2.21	0.41
1:D:893:GLU:CG	1:D:894:ARG:CD	2.99	0.41
1:D:959:ILE:HD13	1:D:959:ILE:HG21	1.87	0.41
1:C:895:VAL:O	1:C:919:ASP:HA	2.20	0.41
1:D:764:PHE:CE1	1:D:781:ARG:NH1	2.89	0.41
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.56	0.41
1:A:390:SER:HA	1:A:391:HIS:HA	1.87	0.41
1:B:100:TYR:HB3	1:B:589:GLY:HA2	2.02	0.41
1:B:873:ALA:O	1:B:876:THR:HG22	2.19	0.41
1:B:372:MET:HE1	1:B:395:HIS:HB3	2.03	0.41
1:D:895:VAL:O	1:D:919:ASP:HA	2.21	0.41
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.56	0.40
1:C:844:HIS:HD2	6:C:9538:HOH:O	2.04	0.40
1:B:200:GLN:HG2	1:B:391:HIS:HB2	2.04	0.40
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.39	0.40
1:B:78:LEU:HA	1:B:79:PRO:HD3	1.89	0.40
1:B:942:ARG:HE	1:B:954:ASP:HA	1.86	0.40
1:D:797:GLU:HB2	1:D:800:ARG:CG	2.51	0.40
1:A:279:ILE:HD13	1:A:279:ILE:HG21	1.76	0.40
1:B:377:LEU:HD22	1:B:708:TRP:CA	2.51	0.40
1:B:753:ASN:ND2	6:B:9504:HOH:O	2.52	0.40
1:B:809:ARG:NH1	1:B:809:ARG:HG2	2.18	0.40
1:C:824:GLN:HG2	1:C:825:CYS:N	2.34	0.40
1:D:780:LEU:HA	1:D:886:CYS:HB3	2.03	0.40
1:A:127:PHE:N	1:A:127:PHE:CD2	2.88	0.40
1:A:533:LEU:C	1:A:533:LEU:HD23	2.42	0.40
1:C:757:GLN:OE1	1:C:769:TRP:HH2	2.04	0.40
1:A:655:MET:HE3	1:A:665:SER:HB3	2.03	0.40
1:A:842:TRP:C	1:A:843:GLN:HG3	2.41	0.40
1:A:990:HIS:HD2	1:A:991:MET:O	2.05	0.40
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.56	0.40
1:B:132:SER:O	1:B:135:GLN:HG2	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:9649:HOH:O	6:C:9528:HOH:O[3_544]	2.07	0.13
6:A:9494:HOH:O	6:B:9578:HOH:O[2_454]	2.10	0.10
6:A:9651:HOH:O	6:C:9654:HOH:O[2_554]	2.18	0.02

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%)	974 (96%)	35 (4%)	2 (0%)	51	31
1	B	1011/1023 (99%)	968 (96%)	39 (4%)	4 (0%)	38	18
1	C	1011/1023 (99%)	966 (96%)	44 (4%)	1 (0%)	55	35
1	D	1011/1023 (99%)	972 (96%)	37 (4%)	2 (0%)	51	31
All	All	4044/4092 (99%)	3880 (96%)	155 (4%)	9 (0%)	51	31

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	688	PRO
1	B	732	ALA
1	B	731	PRO
1	B	690	SER
1	A	164	ASP
1	D	688	PRO
1	A	722	LEU
1	C	690	SER
1	D	164	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	865/875 (99%)	836 (97%)	29 (3%)	42	17
1	B	865/875 (99%)	821 (95%)	44 (5%)	28	7
1	C	865/875 (99%)	829 (96%)	36 (4%)	34	11
1	D	865/875 (99%)	828 (96%)	37 (4%)	33	11
All	All	3460/3500 (99%)	3314 (96%)	146 (4%)	34	11

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	230	ARG
1	A	237	ARG
1	A	250	LEU
1	A	267	VAL
1	A	333	ARG
1	A	347	LYS
1	A	394	ASN
1	A	519	SER
1	A	546	LEU
1	A	581	ASN
1	A	600	GLN
1	A	632	SER
1	A	655	MET
1	A	689	GLU
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	799	THR
1	A	800	ARG
1	A	809	ARG
1	A	817	GLN
1	A	859	ASP
1	A	885	ASN
1	A	926	TYR
1	A	1013	ARG
1	A	1017	GLN
1	A	1022	GLN
1	A	1023	LYS
1	B	80	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	181	GLU
1	B	230	ARG
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	277	GLU
1	B	333	ARG
1	B	370	GLN
1	B	394	ASN
1	B	519	SER
1	B	554	GLN
1	B	580	GLU
1	B	581	ASN
1	B	600	GLN
1	B	634	GLN
1	B	635	THR
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	685	LEU
1	B	687	GLN
1	B	689	GLU
1	B	690	SER
1	B	721	ARG
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	750	GLU
1	B	755	ARG
1	B	781	ARG
1	B	809	ARG
1	B	819	GLU
1	B	824	GLN
1	B	843	GLN
1	B	847	LYS
1	B	877	PRO
1	B	885	ASN
1	B	890	GLN
1	B	917	ARG
1	B	942	ARG
1	B	956	GLN
1	B	1022	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1023	LYS
1	C	71	GLU
1	C	75	GLU
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG
1	C	262	GLN
1	C	264	GLU
1	C	278	ILE
1	C	333	ARG
1	C	392	TYR
1	C	394	ASN
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	634	GLN
1	C	663	LEU
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	729	THR
1	C	730	LEU
1	C	735	HIS
1	C	737	ILE
1	C	745	MET
1	C	750	GLU
1	C	773	LYS
1	C	819	GLU
1	C	829	THR
1	C	885	ASN
1	C	893	GLU
1	C	952	ARG
1	C	956	GLN
1	C	986	ILE
1	C	1022	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	76	CYS
1	D	80	GLU
1	D	237	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	333	ARG
1	D	392	TYR
1	D	394	ASN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	632	SER
1	D	651	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	684	GLU
1	D	685	LEU
1	D	689	GLU
1	D	728	VAL
1	D	730	LEU
1	D	734	SER
1	D	735	HIS
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	799	THR
1	D	800	ARG
1	D	829	THR
1	D	845	GLN
1	D	857	ARG
1	D	885	ASN
1	D	893	GLU
1	D	1013	ARG
1	D	1018	LEU
1	D	1022	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	135	GLN
1	A	262	GLN
1	A	600	GLN
1	A	614	HIS
1	A	624	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	702	GLN
1	A	761	GLN
1	A	824	GLN
1	A	844	HIS
1	A	878	HIS
1	A	1017	GLN
1	B	262	GLN
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	634	GLN
1	B	646	HIS
1	B	687	GLN
1	B	693	GLN
1	B	704	ASN
1	B	804	ASN
1	B	817	GLN
1	B	878	HIS
1	B	965	GLN
1	C	135	GLN
1	C	163	GLN
1	C	266	GLN
1	C	624	GLN
1	C	634	GLN
1	C	646	HIS
1	C	687	GLN
1	C	824	GLN
1	C	878	HIS
1	C	977	HIS
1	D	135	GLN
1	D	163	GLN
1	D	363	HIS
1	D	510	GLN
1	D	583	ASN
1	D	624	GLN
1	D	628	GLN
1	D	704	ASN
1	D	804	ASN
1	D	824	GLN
1	D	878	HIS
1	D	977	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1022	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 148 ligands modelled in this entry, 33 are monoatomic - leaving 115 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$
4	145	A	2001	3	20,22,22	0.96	0	26,31,31	1.46	3 (11%)
4	145	A	2002	-	20,22,22	0.85	0	26,31,31	1.32	3 (11%)
5	DMS	A	8401	-	3,3,3	0.65	0	3,3,3	0.83	0
5	DMS	A	8402	-	3,3,3	1.49	0	3,3,3	0.28	0
5	DMS	A	8403	-	3,3,3	1.44	1 (33%)	3,3,3	0.36	0
5	DMS	A	8404	-	3,3,3	1.06	0	3,3,3	0.70	0
5	DMS	A	8405	-	3,3,3	0.85	0	3,3,3	0.29	0
5	DMS	A	8406	-	3,3,3	0.34	0	3,3,3	1.06	0
5	DMS	A	8407	-	3,3,3	2.52	2 (66%)	3,3,3	0.23	0
5	DMS	A	8408	-	3,3,3	0.64	0	3,3,3	1.66	1 (33%)
5	DMS	A	8409	-	3,3,3	2.03	1 (33%)	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8410	-	3,3,3	1.09	0	3,3,3	0.34	0
5	DMS	A	8411	-	3,3,3	0.75	0	3,3,3	0.39	0
5	DMS	A	8412	-	3,3,3	0.62	0	3,3,3	0.35	0
5	DMS	A	8413	-	3,3,3	2.04	2 (66%)	3,3,3	0.34	0
5	DMS	A	8414	-	3,3,3	1.22	0	3,3,3	0.13	0
5	DMS	A	8415	-	3,3,3	1.08	0	3,3,3	0.70	0
5	DMS	A	8416	-	3,3,3	0.54	0	3,3,3	0.39	0
5	DMS	A	8417	-	3,3,3	2.06	1 (33%)	3,3,3	1.04	0
5	DMS	A	8419	-	3,3,3	0.76	0	3,3,3	0.33	0
5	DMS	A	8420	-	3,3,3	1.07	0	3,3,3	0.36	0
5	DMS	A	8421	-	3,3,3	0.19	0	3,3,3	0.36	0
5	DMS	A	8423	-	3,3,3	1.24	0	3,3,3	0.86	0
5	DMS	A	8425	3	3,3,3	1.96	1 (33%)	3,3,3	0.64	0
5	DMS	A	8501	-	3,3,3	1.16	0	3,3,3	0.32	0
5	DMS	A	8502	-	3,3,3	1.27	0	3,3,3	1.29	1 (33%)
5	DMS	A	8503	-	3,3,3	0.33	0	3,3,3	0.20	0
5	DMS	A	8504	-	3,3,3	0.63	0	3,3,3	0.30	0
5	DMS	A	8602	-	3,3,3	0.83	0	3,3,3	0.55	0
4	145	B	2001	3	20,22,22	1.11	2 (10%)	26,31,31	0.97	0
4	145	B	2002	-	20,22,22	0.88	0	26,31,31	1.23	2 (7%)
5	DMS	B	8401	-	3,3,3	0.58	0	3,3,3	0.28	0
5	DMS	B	8402	-	3,3,3	0.58	0	3,3,3	0.08	0
5	DMS	B	8403	-	3,3,3	1.19	0	3,3,3	0.45	0
5	DMS	B	8404	-	3,3,3	1.27	0	3,3,3	1.37	1 (33%)
5	DMS	B	8405	-	3,3,3	1.41	0	3,3,3	0.54	0
5	DMS	B	8407	-	3,3,3	2.11	1 (33%)	3,3,3	0.24	0
5	DMS	B	8408	-	3,3,3	1.43	1 (33%)	3,3,3	0.33	0
5	DMS	B	8409	-	3,3,3	2.20	1 (33%)	3,3,3	0.57	0
5	DMS	B	8410	-	3,3,3	0.72	0	3,3,3	0.31	0
5	DMS	B	8411	-	3,3,3	1.21	1 (33%)	3,3,3	0.42	0
5	DMS	B	8412	-	3,3,3	1.88	1 (33%)	3,3,3	0.18	0
5	DMS	B	8413	-	3,3,3	1.65	1 (33%)	3,3,3	0.13	0
5	DMS	B	8414	-	3,3,3	1.09	0	3,3,3	0.45	0
5	DMS	B	8415	-	3,3,3	1.99	1 (33%)	3,3,3	1.39	1 (33%)
5	DMS	B	8416	-	3,3,3	0.53	0	3,3,3	0.52	0
5	DMS	B	8417	-	3,3,3	0.92	0	3,3,3	0.21	0
5	DMS	B	8419	-	3,3,3	0.61	0	3,3,3	0.41	0
5	DMS	B	8420	-	3,3,3	1.50	1 (33%)	3,3,3	0.44	0
5	DMS	B	8421	-	3,3,3	0.69	0	3,3,3	0.99	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8423	-	3,3,3	0.97	0	3,3,3	0.10	0
5	DMS	B	8425	3	3,3,3	1.84	1 (33%)	3,3,3	0.59	0
5	DMS	B	8502	-	3,3,3	2.30	1 (33%)	3,3,3	0.44	0
5	DMS	B	8504	-	3,3,3	1.04	0	3,3,3	0.83	0
5	DMS	B	8508	-	3,3,3	2.13	1 (33%)	3,3,3	0.36	0
5	DMS	B	8601	-	3,3,3	2.07	1 (33%)	3,3,3	1.02	0
4	145	C	2001	3	20,22,22	0.73	0	26,31,31	1.21	5 (19%)
4	145	C	2002	-	20,22,22	0.83	1 (5%)	26,31,31	1.09	1 (3%)
5	DMS	C	8401	-	3,3,3	0.85	0	3,3,3	0.51	0
5	DMS	C	8402	-	3,3,3	1.02	0	3,3,3	0.81	0
5	DMS	C	8403	-	3,3,3	1.24	0	3,3,3	0.44	0
5	DMS	C	8404	-	3,3,3	1.18	0	3,3,3	1.14	0
5	DMS	C	8405	-	3,3,3	1.47	1 (33%)	3,3,3	0.55	0
5	DMS	C	8407	-	3,3,3	2.20	2 (66%)	3,3,3	0.54	0
5	DMS	C	8408	-	3,3,3	1.35	0	3,3,3	0.53	0
5	DMS	C	8409	-	3,3,3	2.07	1 (33%)	3,3,3	0.82	0
5	DMS	C	8410	-	3,3,3	1.25	0	3,3,3	0.21	0
5	DMS	C	8411	-	3,3,3	1.04	0	3,3,3	0.42	0
5	DMS	C	8412	-	3,3,3	0.84	0	3,3,3	0.32	0
5	DMS	C	8413	-	3,3,3	1.32	0	3,3,3	0.18	0
5	DMS	C	8414	-	3,3,3	1.05	0	3,3,3	0.81	0
5	DMS	C	8415	-	3,3,3	2.65	2 (66%)	3,3,3	1.72	1 (33%)
5	DMS	C	8416	-	3,3,3	0.75	0	3,3,3	0.10	0
5	DMS	C	8417	-	3,3,3	1.02	0	3,3,3	0.83	0
5	DMS	C	8419	-	3,3,3	1.03	0	3,3,3	0.46	0
5	DMS	C	8420	-	3,3,3	1.88	1 (33%)	3,3,3	0.22	0
5	DMS	C	8421	-	3,3,3	0.62	0	3,3,3	0.67	0
5	DMS	C	8423	-	3,3,3	0.63	0	3,3,3	0.34	0
5	DMS	C	8425	3	3,3,3	1.78	1 (33%)	3,3,3	0.38	0
5	DMS	C	8501	-	3,3,3	1.42	1 (33%)	3,3,3	1.00	0
5	DMS	C	8503	-	3,3,3	1.05	0	3,3,3	0.21	0
5	DMS	C	8504	-	3,3,3	0.81	0	3,3,3	0.29	0
5	DMS	C	8601	-	3,3,3	0.74	0	3,3,3	1.04	0
5	DMS	C	8602	-	3,3,3	1.08	0	3,3,3	0.27	0
5	DMS	C	8705	-	3,3,3	1.10	0	3,3,3	0.21	0
4	145	D	2001	3	20,22,22	1.12	2 (10%)	26,31,31	1.39	4 (15%)
4	145	D	2002	-	20,22,22	0.51	0	26,31,31	0.95	1 (3%)
5	DMS	D	8401	-	3,3,3	0.95	0	3,3,3	0.82	0
5	DMS	D	8402	-	3,3,3	1.58	1 (33%)	3,3,3	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8403	-	3,3,3	0.58	0	3,3,3	0.70	0
5	DMS	D	8404	-	3,3,3	1.08	0	3,3,3	0.47	0
5	DMS	D	8405	-	3,3,3	0.73	0	3,3,3	0.80	0
5	DMS	D	8406	-	3,3,3	1.14	0	3,3,3	0.68	0
5	DMS	D	8407	-	3,3,3	2.81	2 (66%)	3,3,3	0.31	0
5	DMS	D	8408	-	3,3,3	0.80	0	3,3,3	0.22	0
5	DMS	D	8409	-	3,3,3	2.20	1 (33%)	3,3,3	0.61	0
5	DMS	D	8410	-	3,3,3	1.49	0	3,3,3	0.45	0
5	DMS	D	8411	-	3,3,3	1.03	0	3,3,3	0.27	0
5	DMS	D	8412	-	3,3,3	0.92	0	3,3,3	0.50	0
5	DMS	D	8413	-	3,3,3	1.93	1 (33%)	3,3,3	0.66	0
5	DMS	D	8414	-	3,3,3	0.65	0	3,3,3	0.33	0
5	DMS	D	8415	-	3,3,3	2.47	1 (33%)	3,3,3	0.46	0
5	DMS	D	8416	-	3,3,3	1.32	1 (33%)	3,3,3	0.50	0
5	DMS	D	8417	-	3,3,3	1.36	0	3,3,3	1.13	0
5	DMS	D	8419	-	3,3,3	0.40	0	3,3,3	0.18	0
5	DMS	D	8420	-	3,3,3	1.29	1 (33%)	3,3,3	0.38	0
5	DMS	D	8421	-	3,3,3	0.55	0	3,3,3	0.36	0
5	DMS	D	8423	-	3,3,3	1.30	0	3,3,3	0.29	0
5	DMS	D	8425	3	3,3,3	0.37	0	3,3,3	0.65	0
5	DMS	D	8501	-	3,3,3	0.34	0	3,3,3	0.72	0
5	DMS	D	8503	-	3,3,3	0.72	0	3,3,3	0.33	0
5	DMS	D	8508	-	3,3,3	1.77	1 (33%)	3,3,3	0.46	0
5	DMS	D	8701	-	3,3,3	1.84	0	3,3,3	0.45	0
5	DMS	D	8703	-	3,3,3	2.30	2 (66%)	3,3,3	0.24	0
5	DMS	D	8705	-	3,3,3	1.66	0	3,3,3	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	145	A	2001	3	-	0/8/30/30	0/2/2/2
4	145	A	2002	-	-	0/8/30/30	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	8415	-	-	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	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	8425	3	-	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	8602	-	-	0/0/0/0	0/0/0/0
4	145	B	2001	3	-	0/8/30/30	0/2/2/2
4	145	B	2002	-	-	0/8/30/30	0/2/2/2
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	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8425	3	-	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	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
4	145	C	2001	3	-	0/8/30/30	0/2/2/2
4	145	C	2002	-	-	0/8/30/30	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	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	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	8425	3	-	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	8601	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8705	-	-	0/0/0/0	0/0/0/0
4	145	D	2001	3	-	0/8/30/30	0/2/2/2
4	145	D	2002	-	-	0/8/30/30	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8407	-	-	0/0/0/0	0/0/0/0
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	8415	-	-	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	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	8425	3	-	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	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	8705	-	-	0/0/0/0	0/0/0/0

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8417	DMS	C1-S	-3.51	1.49	1.75
5	D	8420	DMS	C2-S	-2.18	1.59	1.75
5	D	8416	DMS	C2-S	-2.09	1.60	1.75
5	B	8411	DMS	C1-S	2.08	1.91	1.75
5	A	8413	DMS	C2-S	2.08	1.91	1.75
5	B	8408	DMS	C1-S	2.15	1.92	1.75
5	D	8703	DMS	C1-S	2.16	1.92	1.75
5	C	8501	DMS	O-S	2.18	1.65	1.50
5	D	8402	DMS	C2-S	2.18	1.92	1.75
5	C	8405	DMS	C1-S	2.19	1.92	1.75
5	A	8403	DMS	C2-S	2.23	1.92	1.75
4	D	2001	145	O3'-N1'	2.28	1.26	1.22
5	B	8420	DMS	C2-S	2.31	1.93	1.75
4	C	2002	145	O3'-N1'	2.35	1.27	1.22
5	B	8413	DMS	O-S	2.35	1.66	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2001	145	O3'-N1'	2.37	1.27	1.22
4	B	2001	145	O3-C3	2.38	1.48	1.43
5	D	8413	DMS	O-S	2.42	1.66	1.50
5	C	8407	DMS	O-S	2.45	1.66	1.50
5	A	8413	DMS	C1-S	2.48	1.94	1.75
5	C	8415	DMS	C1-S	2.50	1.94	1.75
4	D	2001	145	O3-C3	2.54	1.48	1.43
5	B	8601	DMS	C2-S	2.61	1.95	1.75
5	C	8425	DMS	O-S	2.68	1.68	1.50
5	B	8412	DMS	C1-S	2.77	1.96	1.75
5	D	8508	DMS	O-S	2.78	1.69	1.50
5	D	8703	DMS	O-S	2.81	1.69	1.50
5	A	8425	DMS	O-S	2.85	1.69	1.50
5	B	8425	DMS	O-S	2.90	1.69	1.50
5	B	8508	DMS	C1-S	2.92	1.97	1.75
5	B	8415	DMS	C2-S	2.92	1.97	1.75
5	C	8407	DMS	C2-S	2.92	1.97	1.75
5	D	8407	DMS	O-S	2.96	1.70	1.50
5	A	8407	DMS	C2-S	2.96	1.98	1.75
5	A	8407	DMS	O-S	3.13	1.71	1.50
5	C	8420	DMS	O-S	3.18	1.71	1.50
5	C	8409	DMS	O-S	3.18	1.71	1.50
5	A	8409	DMS	O-S	3.23	1.72	1.50
5	B	8502	DMS	C1-S	3.44	2.01	1.75
5	B	8407	DMS	C2-S	3.45	2.01	1.75
5	B	8409	DMS	O-S	3.54	1.74	1.50
5	D	8415	DMS	O-S	3.58	1.74	1.50
5	D	8409	DMS	O-S	3.61	1.74	1.50
5	D	8407	DMS	C2-S	3.78	2.04	1.75
5	C	8415	DMS	C2-S	3.84	2.04	1.75

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2002	145	C1-C2-C3	-3.00	104.41	109.98
4	D	2002	145	O1'-C1'-C2'	-2.94	113.88	117.13
4	A	2001	145	O3-C3-C2	-2.68	104.52	110.36
4	C	2002	145	C6-C5-C4	-2.60	106.92	113.00
4	A	2001	145	O1'-C1-C2	-2.59	103.28	107.11
4	A	2002	145	O5-C1-C2	-2.46	105.55	110.30
4	B	2002	145	C1-C2-C3	-2.30	105.71	109.98
4	D	2001	145	C5'-C4'-C3'	-2.14	117.27	120.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2001	145	C1-O5-C5	-2.11	109.75	113.72
4	C	2001	145	O5-C1-O1'	-2.08	103.14	108.39
4	C	2001	145	O1'-C1-C2	-2.07	104.05	107.11
4	D	2001	145	O4-C4-C5	2.00	114.32	109.28
4	A	2002	145	C4'-C5'-C6'	2.02	122.99	120.21
4	C	2001	145	O4-C4-C5	2.09	114.55	109.28
4	C	2001	145	O6-C6-C5	2.21	118.79	111.34
5	A	8502	DMS	C2-S-C1	2.24	110.05	98.44
4	D	2001	145	C1'-O1'-C1	2.27	122.27	118.23
5	B	8404	DMS	C2-S-C1	2.36	110.71	98.44
5	B	8415	DMS	C2-S-C1	2.38	110.80	98.44
4	B	2002	145	O5-C5-C4	2.58	114.42	109.66
5	A	8408	DMS	C2-S-C1	2.86	113.29	98.44
5	C	8415	DMS	C2-S-C1	2.93	113.64	98.44
4	D	2001	145	O1'-C1'-C2'	2.99	120.44	117.13
4	A	2001	145	O1'-C1'-C2'	4.67	122.30	117.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

24 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	145	1	0
4	A	2002	145	1	0
5	A	8412	DMS	4	0
5	A	8502	DMS	1	0
5	A	8503	DMS	1	0
5	A	8602	DMS	1	0
4	B	2002	145	1	0
5	B	8407	DMS	2	0
5	B	8416	DMS	1	0
5	B	8420	DMS	1	0
5	B	8502	DMS	1	0
4	C	2002	145	2	0
5	C	8415	DMS	1	0
5	C	8420	DMS	1	0
5	C	8425	DMS	1	0
5	C	8503	DMS	1	0
5	C	8602	DMS	1	0
4	D	2001	145	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	2002	145	3	0
5	D	8407	DMS	2	0
5	D	8412	DMS	3	0
5	D	8416	DMS	1	0
5	D	8425	DMS	2	0
5	D	8703	DMS	7	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.30	21 (2%) 64 71	11, 18, 46, 100	0
1	B	1011/1023 (98%)	-0.24	16 (1%) 72 80	11, 19, 48, 99	0
1	C	1011/1023 (98%)	-0.19	29 (2%) 52 59	11, 20, 51, 100	0
1	D	1011/1023 (98%)	-0.23	33 (3%) 47 54	11, 19, 50, 100	0
All	All	4044/4092 (98%)	-0.24	99 (2%) 59 66	11, 19, 49, 100	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	11.0
1	C	732	ALA	10.2
1	C	730	LEU	9.3
1	D	732	ALA	9.1
1	B	731	PRO	8.9
1	D	735	HIS	8.8
1	D	730	LEU	7.7
1	C	731	PRO	7.5
1	B	689	GLU	7.2
1	C	735	HIS	6.1
1	B	685	LEU	6.0
1	D	686	PRO	5.9
1	A	733	ALA	5.3
1	B	732	ALA	5.3
1	A	732	ALA	5.2
1	B	730	LEU	5.2
1	D	734	SER	5.1
1	A	731	PRO	5.0
1	A	730	LEU	4.9
1	B	733	ALA	4.8
1	B	686	PRO	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	581	ASN	4.8
1	A	686	PRO	4.7
1	D	687	GLN	4.7
1	C	733	ALA	4.5
1	D	731	PRO	4.5
1	D	733	ALA	4.5
1	C	689	GLU	4.4
1	C	745	MET	4.3
1	D	689	GLU	4.1
1	D	580	GLU	4.1
1	C	687	GLN	4.0
1	A	689	GLU	4.0
1	D	685	LEU	3.9
1	B	687	GLN	3.9
1	A	736	ALA	3.9
1	B	684	GLU	3.9
1	B	735	HIS	3.8
1	C	830	LEU	3.8
1	D	845	GLN	3.8
1	C	685	LEU	3.8
1	A	734	SER	3.8
1	A	580	GLU	3.7
1	D	663	LEU	3.7
1	D	736	ALA	3.6
1	C	686	PRO	3.4
1	D	688	PRO	3.4
1	A	687	GLN	3.3
1	D	684	GLU	3.3
1	D	831	ALA	3.2
1	A	582	GLY	3.1
1	A	737	ILE	3.1
1	C	634	GLN	3.0
1	C	734	SER	2.9
1	D	799	THR	2.9
1	A	772	ASP	2.9
1	A	685	LEU	2.8
1	C	580	GLU	2.8
1	D	798	ALA	2.8
1	D	634	GLN	2.8
1	A	799	THR	2.7
1	D	737	ILE	2.7
1	D	679	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	582	GLY	2.6
1	D	771	GLY	2.6
1	D	582	GLY	2.6
1	C	633	GLY	2.6
1	C	76	CYS	2.6
1	A	845	GLN	2.6
1	B	79	PRO	2.5
1	A	729	THR	2.5
1	C	743	SER	2.5
1	B	745	MET	2.5
1	A	71	GLU	2.5
1	B	734	SER	2.4
1	A	581	ASN	2.4
1	D	770	ILE	2.4
1	D	830	LEU	2.4
1	C	684	GLU	2.4
1	C	581	ASN	2.4
1	B	253	TYR	2.4
1	D	846	GLY	2.3
1	C	729	THR	2.3
1	C	799	THR	2.3
1	C	728	VAL	2.3
1	D	772	ASP	2.3
1	B	580	GLU	2.3
1	D	583	ASN	2.2
1	D	861	SER	2.2
1	A	1023	LYS	2.2
1	D	729	THR	2.2
1	D	579	ASP	2.2
1	C	688	PRO	2.1
1	C	761	GLN	2.1
1	B	581	ASN	2.1
1	C	737	ILE	2.1
1	C	817	GLN	2.0
1	C	861	SER	2.0
1	C	583	ASN	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	DMS	B	8407	4/4	0.91	0.14	9.39	27,39,40,47	0
5	DMS	D	8703	4/4	0.91	0.15	7.58	32,38,49,53	0
5	DMS	A	8406	4/4	0.94	0.18	6.32	16,52,70,78	0
5	DMS	A	8423	4/4	0.93	0.19	5.74	36,59,67,100	0
5	DMS	D	8420	4/4	0.92	0.13	5.60	27,51,77,94	0
5	DMS	A	8504	4/4	0.96	0.10	5.46	21,36,41,87	0
5	DMS	A	8502	4/4	0.95	0.12	5.14	29,30,54,72	0
5	DMS	C	8503	4/4	0.79	0.22	5.11	46,82,100,100	0
5	DMS	A	8416	4/4	0.96	0.23	4.84	24,53,80,100	0
5	DMS	B	8419	4/4	0.93	0.17	4.84	33,56,58,66	0
5	DMS	D	8407	4/4	0.91	0.12	4.67	26,50,53,55	0
5	DMS	A	8417	4/4	0.94	0.20	4.39	25,30,33,100	0
5	DMS	D	8404	4/4	0.95	0.11	4.38	21,31,44,100	0
5	DMS	B	8420	4/4	0.94	0.11	4.35	39,42,46,52	0
5	DMS	A	8407	4/4	0.92	0.13	4.31	25,38,39,47	0
5	DMS	B	8508	4/4	0.95	0.13	3.95	29,49,50,57	0
5	DMS	D	8417	4/4	0.88	0.18	3.77	26,41,80,100	0
5	DMS	C	8420	4/4	0.96	0.10	3.69	40,41,57,100	0
5	DMS	A	8420	4/4	0.96	0.10	3.64	37,44,52,62	0
5	DMS	B	8423	4/4	0.94	0.12	3.63	37,56,72,72	0
5	DMS	C	8403	4/4	0.99	0.12	3.50	23,24,25,27	0
5	DMS	D	8425	4/4	0.94	0.19	3.21	22,24,28,56	4
5	DMS	D	8419	4/4	0.97	0.10	3.16	34,36,55,72	0
5	DMS	B	8425	4/4	0.94	0.13	2.50	29,35,36,43	0
5	DMS	C	8425	4/4	0.94	0.14	2.44	42,44,49,71	0
5	DMS	C	8419	4/4	0.91	0.12	2.33	35,37,40,57	0
5	DMS	D	8406	4/4	0.97	0.11	2.12	26,27,31,35	0
5	DMS	C	8705	4/4	0.80	0.18	2.10	35,45,50,100	0
5	DMS	A	8501	4/4	0.93	0.12	2.08	20,28,34,38	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	B	8405	4/4	0.99	0.09	2.08	23,28,29,31	0
5	DMS	A	8405	4/4	0.99	0.09	2.05	20,24,25,27	0
4	145	D	2002	21/21	0.92	0.14	2.05	23,35,50,55	0
5	DMS	C	8407	4/4	0.95	0.12	2.05	30,39,40,50	0
3	NA	C	3104	1/1	0.97	0.13	2.01	30,30,30,30	0
5	DMS	D	8423	4/4	0.95	0.10	1.94	31,39,55,58	0
5	DMS	D	8705	4/4	0.93	0.15	1.81	26,36,43,45	0
3	NA	D	3104	1/1	0.84	0.11	1.77	36,36,36,36	0
4	145	A	2001	21/21	0.95	0.10	1.68	14,17,45,95	0
5	DMS	A	8419	4/4	0.97	0.11	1.64	36,44,49,52	0
4	145	B	2002	21/21	0.92	0.13	1.61	23,31,41,50	0
5	DMS	A	8401	4/4	0.99	0.08	1.60	12,14,16,18	0
5	DMS	C	8405	4/4	0.98	0.08	1.58	27,31,31,32	0
5	DMS	D	8508	4/4	0.95	0.10	1.49	34,39,44,51	0
4	145	C	2002	21/21	0.89	0.12	1.49	24,34,43,47	0
5	DMS	D	8501	4/4	0.94	0.09	1.45	25,31,36,46	0
5	DMS	D	8403	4/4	0.99	0.08	1.45	18,25,25,27	0
5	DMS	B	8408	4/4	0.97	0.10	1.44	31,36,40,100	0
5	DMS	D	8402	4/4	0.98	0.09	1.42	18,23,24,26	0
4	145	A	2002	21/21	0.90	0.13	1.35	20,30,41,43	0
5	DMS	C	8602	4/4	0.95	0.12	1.31	43,49,52,100	0
5	DMS	A	8412	4/4	0.99	0.12	1.29	34,34,37,60	0
5	DMS	D	8408	4/4	0.98	0.08	1.24	17,31,35,38	0
5	DMS	C	8423	4/4	0.93	0.11	1.24	38,42,44,58	0
4	145	D	2001	21/21	0.96	0.08	1.19	12,19,47,57	0
5	DMS	B	8417	4/4	0.88	0.13	1.06	30,33,36,69	0
5	DMS	A	8404	4/4	0.97	0.08	1.05	22,27,36,40	0
5	DMS	B	8404	4/4	0.97	0.06	0.99	20,21,36,39	0
3	NA	A	3104	1/1	0.98	0.09	0.97	25,25,25,25	0
5	DMS	C	8417	4/4	0.95	0.12	0.86	23,35,47,52	0
5	DMS	C	8411	4/4	0.98	0.12	0.85	24,28,30,35	0
5	DMS	B	8401	4/4	0.99	0.08	0.85	15,17,17,20	0
5	DMS	C	8404	4/4	0.98	0.06	0.85	21,24,28,31	0
5	DMS	B	8502	4/4	0.96	0.09	0.83	30,31,44,100	0
5	DMS	A	8403	4/4	0.99	0.08	0.81	21,24,27,27	0
5	DMS	C	8412	4/4	0.99	0.09	0.67	26,33,44,100	0
5	DMS	C	8501	4/4	0.96	0.09	0.66	18,28,36,48	0
5	DMS	D	8405	4/4	0.99	0.08	0.65	24,25,25,30	0
5	DMS	C	8401	4/4	1.00	0.07	0.38	15,17,21,23	0
5	DMS	C	8408	4/4	0.98	0.09	0.37	25,41,48,100	0
4	145	B	2001	21/21	0.96	0.09	0.33	11,15,38,47	0
5	DMS	C	8402	4/4	0.99	0.06	0.32	18,22,23,28	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	B	8412	4/4	0.99	0.09	0.30	27,33,35,37	0
3	NA	B	3104	1/1	0.97	0.09	0.28	32,32,32,32	0
5	DMS	D	8701	4/4	0.99	0.08	0.25	15,16,20,38	0
4	145	C	2001	21/21	0.96	0.08	0.18	13,17,38,55	0
2	MG	D	3105	1/1	0.98	0.10	0.14	31,31,31,31	0
5	DMS	D	8412	4/4	0.99	0.08	0.04	26,28,31,100	0
5	DMS	A	8425	4/4	0.96	0.09	0.03	28,32,41,42	0
5	DMS	B	8504	4/4	0.93	0.10	-0.04	35,35,69,100	0
5	DMS	B	8403	4/4	0.99	0.07	-0.28	16,21,26,26	0
2	MG	B	3105	1/1	0.99	0.08	-0.33	27,27,27,27	0
5	DMS	B	8402	4/4	0.98	0.06	-0.35	16,21,22,23	0
5	DMS	A	8408	4/4	0.98	0.07	-0.39	22,35,39,47	0
5	DMS	A	8411	4/4	0.99	0.07	-0.63	23,24,28,31	0
5	DMS	A	8402	4/4	0.99	0.07	-0.73	16,17,22,28	0
2	MG	B	3002	1/1	0.99	0.05	-1.04	17,17,17,17	0
3	NA	A	3103	1/1	0.99	0.07	-1.05	25,25,25,25	0
3	NA	C	3102	1/1	0.99	0.04	-1.07	17,17,17,17	0
5	DMS	B	8411	4/4	0.99	0.06	-1.13	26,27,31,100	0
5	DMS	D	8401	4/4	1.00	0.05	-1.16	15,16,18,19	0
3	NA	D	3102	1/1	1.00	0.05	-1.22	15,15,15,15	0
2	MG	D	3002	1/1	0.99	0.05	-1.37	17,17,17,17	0
3	NA	A	3102	1/1	0.99	0.05	-1.39	15,15,15,15	0
2	MG	C	3002	1/1	0.99	0.05	-1.44	15,15,15,15	0
5	DMS	D	8411	4/4	0.99	0.04	-1.57	23,25,28,59	0
3	NA	C	3103	1/1	0.97	0.05	-1.91	26,26,26,26	0
2	MG	A	3001	1/1	0.99	0.04	-1.97	17,17,17,17	0
3	NA	D	3103	1/1	0.97	0.06	-2.00	26,26,26,26	0
3	NA	B	3103	1/1	0.99	0.04	-2.11	25,25,25,25	0
2	MG	C	3001	1/1	0.99	0.05	-2.12	15,15,15,15	0
2	MG	A	3002	1/1	0.99	0.04	-2.24	17,17,17,17	0
3	NA	B	3102	1/1	0.99	0.04	-2.27	16,16,16,16	0
3	NA	A	3101	1/1	0.99	0.06	-2.36	17,17,17,17	0
2	MG	B	3001	1/1	0.99	0.04	-2.73	15,15,15,15	0
2	MG	D	3001	1/1	0.99	0.04	-2.92	15,15,15,15	0
3	NA	B	3101	1/1	0.98	0.06	-4.24	16,16,16,16	0
3	NA	C	3101	1/1	1.00	0.03	-5.32	15,15,15,15	0
3	NA	D	3101	1/1	0.99	0.04	-9.45	16,16,16,16	0
2	MG	B	3003	1/1	0.85	0.26	-	48,48,48,48	0
5	DMS	C	8413	4/4	0.96	0.14	-	32,33,45,45	0
5	DMS	C	8421	4/4	0.98	0.09	-	37,49,62,63	0
2	MG	A	3005	1/1	0.95	0.06	-	31,31,31,31	0
5	DMS	C	8410	4/4	0.97	0.13	-	24,34,37,39	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	A	8415	4/4	0.94	0.15	-	24,63,100,100	0
5	DMS	A	8410	4/4	0.97	0.12	-	28,36,39,52	0
5	DMS	A	8413	4/4	0.95	0.14	-	33,35,42,51	0
5	DMS	D	8413	4/4	0.97	0.12	-	31,33,40,55	0
5	DMS	B	8601	4/4	0.97	0.10	-	33,35,37,42	0
5	DMS	D	8415	4/4	0.96	0.11	-	25,49,64,100	0
5	DMS	D	8421	4/4	0.97	0.13	-	32,54,78,100	0
5	DMS	A	8602	4/4	0.93	0.19	-	54,58,100,100	0
5	DMS	D	8410	4/4	0.99	0.11	-	25,34,43,53	0
5	DMS	C	8504	4/4	0.96	0.08	-	47,50,51,69	0
2	MG	A	3003	1/1	0.84	0.19	-	61,61,61,61	0
2	MG	D	3005	1/1	0.96	0.08	-	27,27,27,27	0
5	DMS	B	8415	4/4	0.89	0.12	-	30,34,37,73	0
5	DMS	A	8503	4/4	0.93	0.17	-	31,100,100,100	0
5	DMS	C	8416	4/4	0.94	0.23	-	64,66,100,100	0
5	DMS	C	8415	4/4	0.91	0.14	-	26,32,41,61	0
5	DMS	B	8421	4/4	0.96	0.10	-	32,43,53,100	0
5	DMS	D	8414	4/4	0.98	0.15	-	26,44,58,100	0
5	DMS	A	8414	4/4	0.94	0.14	-	27,38,66,100	0
5	DMS	C	8601	4/4	0.97	0.10	-	37,38,41,43	0
5	DMS	A	8421	4/4	0.91	0.16	-	51,60,61,74	0
5	DMS	D	8409	4/4	0.98	0.12	-	29,37,43,100	0
5	DMS	B	8409	4/4	0.97	0.11	-	25,34,44,45	0
5	DMS	B	8414	4/4	0.95	0.14	-	22,49,74,100	0
5	DMS	C	8414	4/4	0.98	0.10	-	26,35,50,100	0
5	DMS	C	8409	4/4	0.94	0.13	-	29,40,45,47	0
5	DMS	D	8416	4/4	0.95	0.25	-	34,35,54,77	0
2	MG	C	3006	1/1	0.95	0.14	-	41,41,41,41	0
5	DMS	B	8410	4/4	0.95	0.12	-	29,42,60,100	0
5	DMS	A	8409	4/4	0.97	0.12	-	30,41,46,100	0
5	DMS	D	8503	4/4	0.93	0.18	-	31,76,100,100	0
2	MG	A	3105	1/1	0.98	0.12	-	31,31,31,31	0
5	DMS	B	8413	4/4	0.95	0.15	-	47,48,50,100	0
2	MG	C	3105	1/1	0.97	0.10	-	26,26,26,26	0
5	DMS	B	8416	4/4	0.90	0.19	-	46,55,71,100	0

6.5 Other polymers

There are no such residues in this entry.