



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:16 AM GMT

PDB ID : 3DYO
Title : E. coli (lacZ) beta-galactosidase (H418N) in complex with IPTG
Authors : Juers, D.H.; Huber, R.E.; Matthews, B.W.
Deposited on : 2008-07-28
Resolution : 1.80 Å(reported)

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

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

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

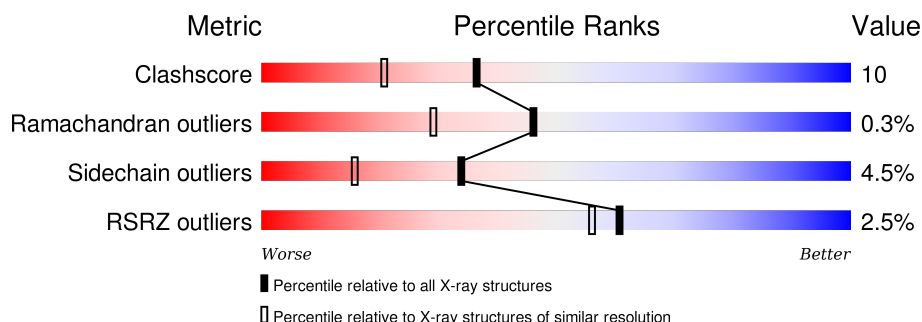
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	
1	B	1023	
1	C	1023	
1	D	1023	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	3012	-	-	-	X
4	IPT	A	2003	-	-	-	X
4	IPT	B	2003	-	-	-	X
4	IPT	B	2004	-	-	-	X
4	IPT	C	2003	-	-	-	X
4	IPT	D	2003	-	-	-	X
5	DMS	A	8403	-	-	-	X
5	DMS	A	8416	-	-	-	X
5	DMS	A	8417	-	-	-	X
5	DMS	A	8419	-	-	-	X
5	DMS	A	8420	-	-	-	X
5	DMS	A	8423	-	-	-	X
5	DMS	B	8401	-	-	-	X
5	DMS	B	8403	-	-	-	X
5	DMS	B	8405	-	-	-	X
5	DMS	B	8407	-	-	-	X
5	DMS	B	8417	-	-	-	X
5	DMS	B	8420	-	-	-	X
5	DMS	B	8423	-	-	-	X
5	DMS	B	8425	-	-	-	X
5	DMS	B	8506	-	-	X	X
5	DMS	C	8403	-	-	-	X
5	DMS	C	8404	-	-	-	X
5	DMS	C	8411	-	-	X	-
5	DMS	C	8420	-	-	-	X
5	DMS	C	8425	-	-	-	X
5	DMS	C	8501	-	-	-	X
5	DMS	D	8403	-	-	-	X
5	DMS	D	8405	-	-	-	X
5	DMS	D	8417	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36820 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	0	0
			8123	5136	1439	1510	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP P00722
A	2	SER	-	EXPRESSION TAG	UNP P00722
A	3	HIS	-	EXPRESSION TAG	UNP P00722
A	4	MET	-	EXPRESSION TAG	UNP P00722
A	5	LEU	-	EXPRESSION TAG	UNP P00722
A	6	GLU	-	EXPRESSION TAG	UNP P00722
A	7	ASP	-	EXPRESSION TAG	UNP P00722
A	8	PRO	-	EXPRESSION TAG	UNP P00722
A	418	ASN	HIS	ENGINEERED	UNP P00722
B	1	GLY	-	EXPRESSION TAG	UNP P00722
B	2	SER	-	EXPRESSION TAG	UNP P00722
B	3	HIS	-	EXPRESSION TAG	UNP P00722
B	4	MET	-	EXPRESSION TAG	UNP P00722
B	5	LEU	-	EXPRESSION TAG	UNP P00722
B	6	GLU	-	EXPRESSION TAG	UNP P00722
B	7	ASP	-	EXPRESSION TAG	UNP P00722
B	8	PRO	-	EXPRESSION TAG	UNP P00722
B	418	ASN	HIS	ENGINEERED	UNP P00722
C	1	GLY	-	EXPRESSION TAG	UNP P00722
C	2	SER	-	EXPRESSION TAG	UNP P00722
C	3	HIS	-	EXPRESSION TAG	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	EXPRESSION TAG	UNP P00722
C	5	LEU	-	EXPRESSION TAG	UNP P00722
C	6	GLU	-	EXPRESSION TAG	UNP P00722
C	7	ASP	-	EXPRESSION TAG	UNP P00722
C	8	PRO	-	EXPRESSION TAG	UNP P00722
C	418	ASN	HIS	ENGINEERED	UNP P00722
D	1	GLY	-	EXPRESSION TAG	UNP P00722
D	2	SER	-	EXPRESSION TAG	UNP P00722
D	3	HIS	-	EXPRESSION TAG	UNP P00722
D	4	MET	-	EXPRESSION TAG	UNP P00722
D	5	LEU	-	EXPRESSION TAG	UNP P00722
D	6	GLU	-	EXPRESSION TAG	UNP P00722
D	7	ASP	-	EXPRESSION TAG	UNP P00722
D	8	PRO	-	EXPRESSION TAG	UNP P00722
D	418	ASN	HIS	ENGINEERED	UNP P00722

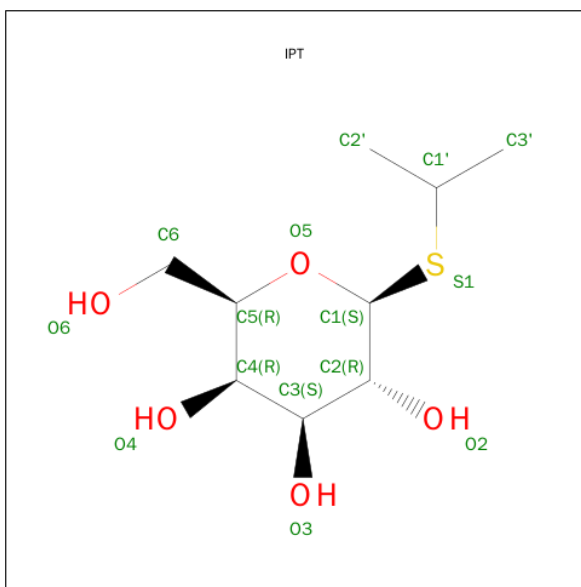
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 4 is ISOPROPYL-1-BETA-D-THIOGALACTOSIDE (three-letter code: IPT) (formula: C₉H₁₈O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			15	9	5	1		
4	A	1	Total	C	O	S	0	0
			15	9	5	1		
4	A	1	Total	C	O	S	0	0
			15	9	5	1		
4	B	1	Total	C	O	S	0	0
			15	9	5	1		
4	B	1	Total	C	O	S	0	0
			15	9	5	1		
4	B	1	Total	C	O	S	0	0
			15	9	5	1		
4	C	1	Total	C	O	S	0	0
			15	9	5	1		
4	C	1	Total	C	O	S	0	0
			15	9	5	1		
4	C	1	Total	C	O	S	0	0
			15	9	5	1		
4	D	1	Total	C	O	S	0	0
			15	9	5	1		
4	D	1	Total	C	O	S	0	0
			15	9	5	1		
4	D	1	Total	C	O	S	0	0
			15	9	5	1		

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



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

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

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

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

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

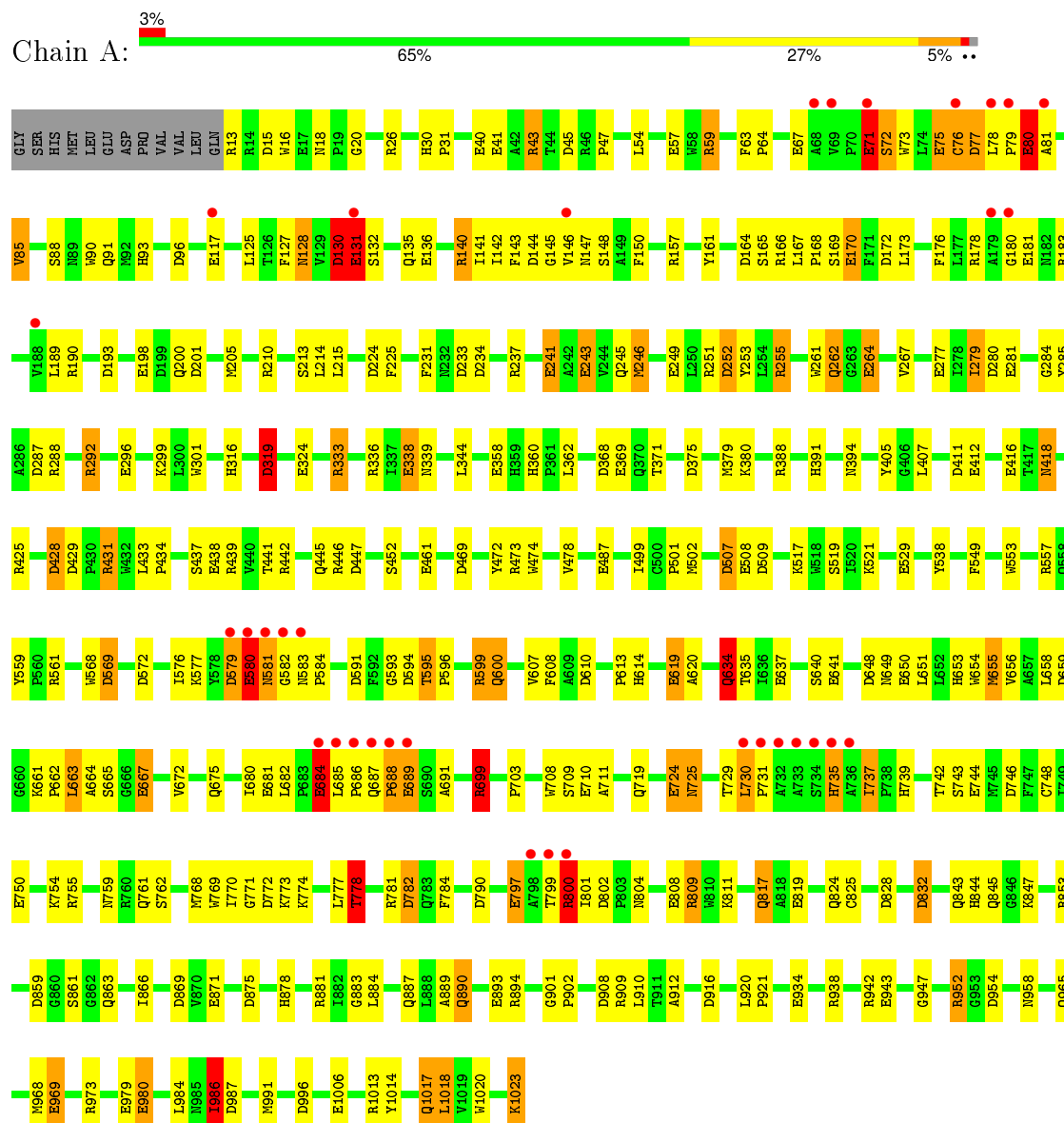
- Molecule 6 is water.

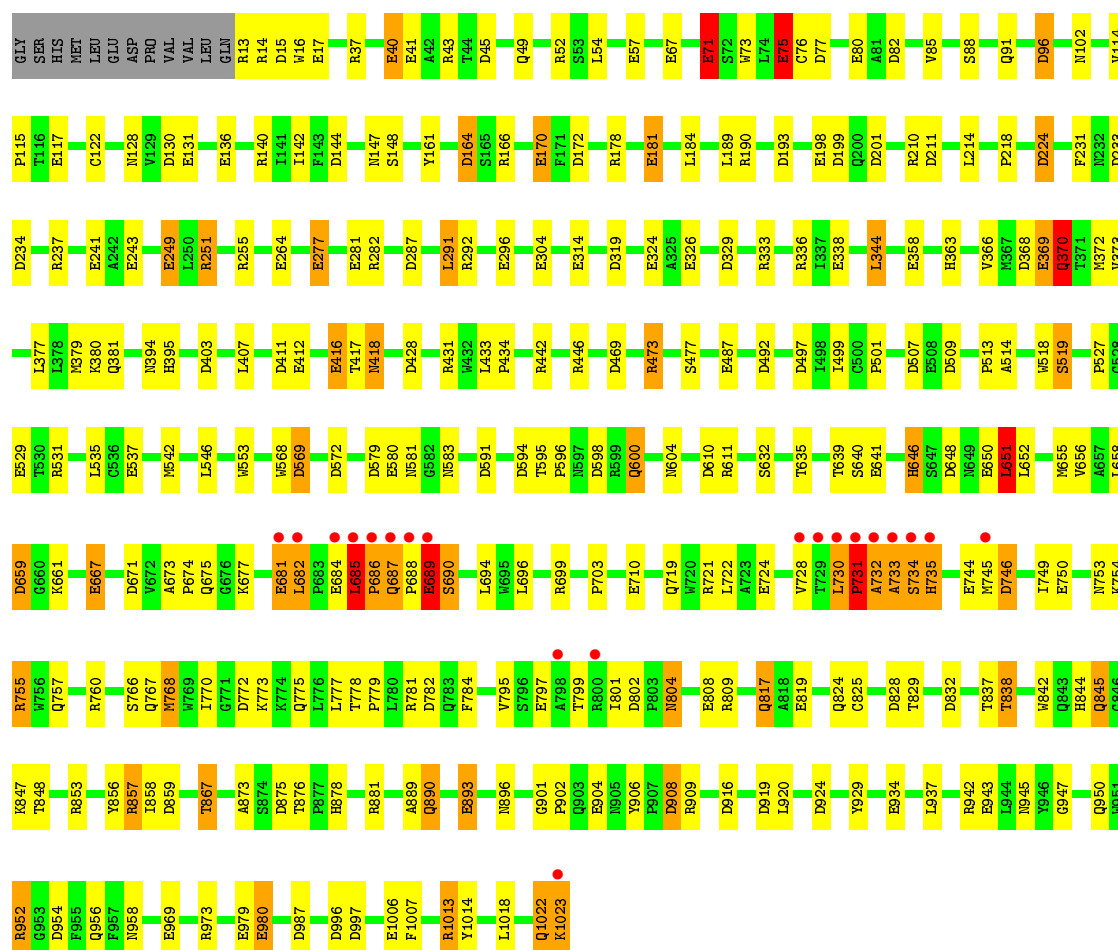
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	862	Total 862	O 862	0	0
6	B	995	Total 995	O 995	0	0
6	C	974	Total 974	O 974	0	0
6	D	897	Total 897	O 897	0	0

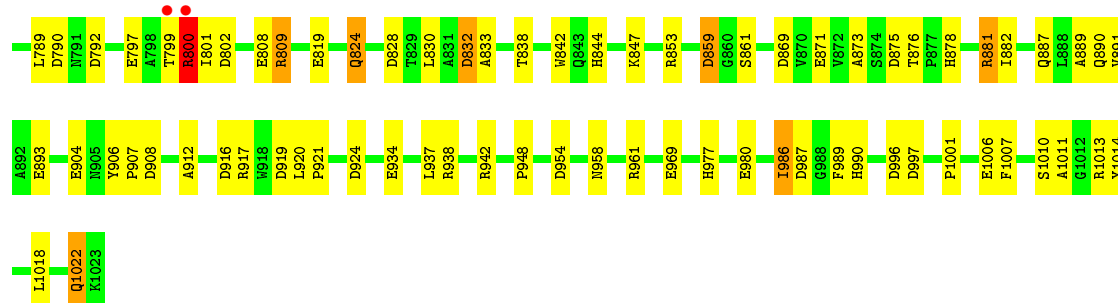
3 Residue-property plots

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

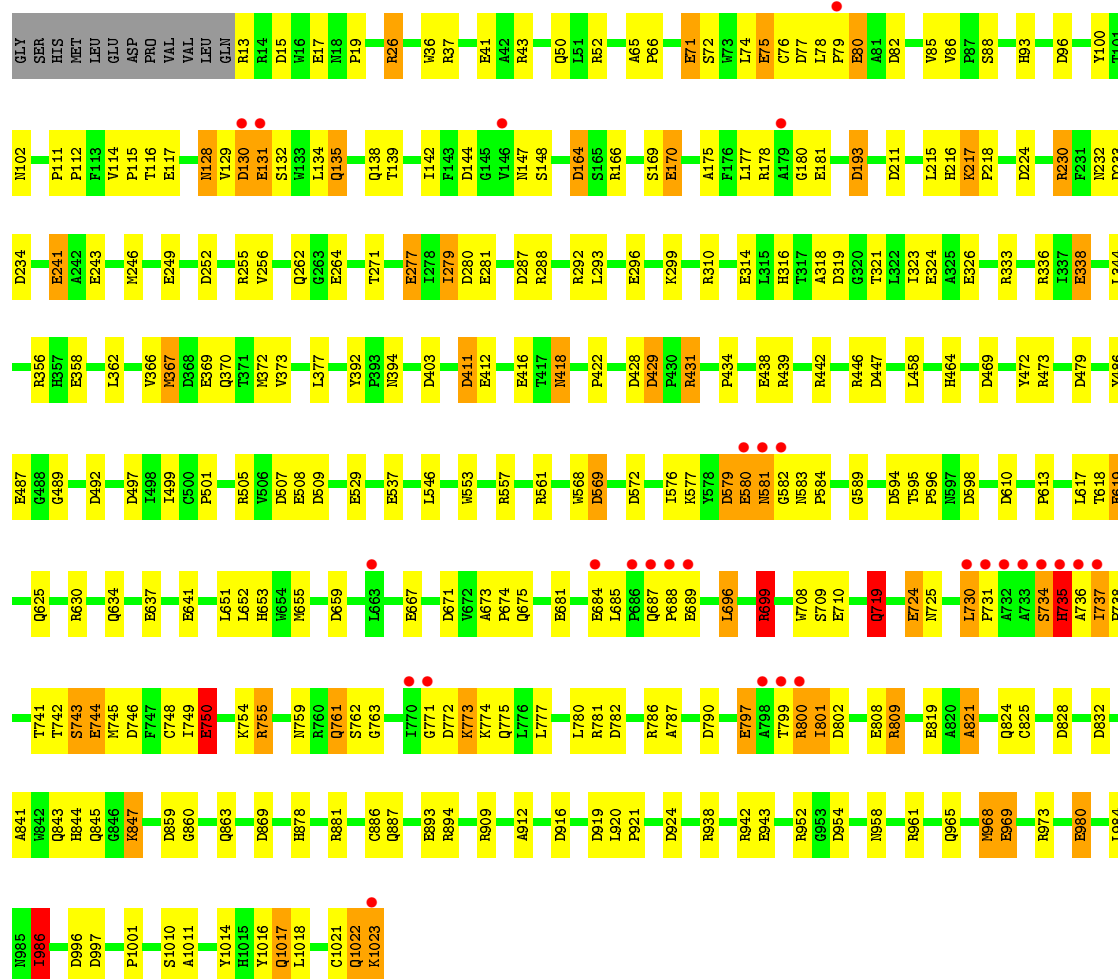
• Molecule 1: Beta-galactosidase







• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.01Å 162.52Å 204.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.95 – 1.80	Depositor EDS
% Data completeness (in resolution range)	1.5 (30.00-1.80) 97.7 (29.95-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.80Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.173 , 0.241 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 90.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 452647 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36820	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 40.80 % 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 2.5942e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1.09	52/8364 (0.6%)	1.66	169/11411 (1.5%)
1	B	1.11	52/8364 (0.6%)	1.62	174/11411 (1.5%)
1	C	1.11	46/8364 (0.5%)	1.63	164/11411 (1.4%)
1	D	1.06	45/8364 (0.5%)	1.62	154/11411 (1.3%)
All	All	1.09	195/33456 (0.6%)	1.63	661/45644 (1.4%)

All (195) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	619	GLU	CD-OE2	9.61	1.36	1.25
1	B	641	GLU	CD-OE1	-8.74	1.16	1.25
1	B	241	GLU	CD-OE2	8.39	1.34	1.25
1	A	241	GLU	CD-OE2	8.30	1.34	1.25
1	B	650	GLU	CD-OE2	8.26	1.34	1.25
1	D	241	GLU	CD-OE2	8.20	1.34	1.25
1	B	537	GLU	CD-OE2	7.92	1.34	1.25
1	B	412	GLU	CD-OE2	7.92	1.34	1.25
1	C	277	GLU	CD-OE2	7.89	1.34	1.25
1	D	750	GLU	CD-OE2	7.88	1.34	1.25
1	A	117	GLU	CD-OE2	7.85	1.34	1.25
1	C	689	GLU	CD-OE2	7.82	1.34	1.25
1	C	181	GLU	CD-OE2	7.80	1.34	1.25
1	D	689	GLU	CD-OE2	7.74	1.34	1.25
1	C	684	GLU	CD-OE2	7.74	1.34	1.25
1	C	41	GLU	CD-OE2	7.72	1.34	1.25
1	A	750	GLU	CD-OE2	7.69	1.34	1.25
1	B	71	GLU	CD-OE2	7.65	1.34	1.25
1	D	580	GLU	CD-OE2	7.62	1.34	1.25
1	D	71	GLU	CD-OE2	7.59	1.33	1.25
1	B	277	GLU	CD-OE2	7.56	1.33	1.25
1	A	198	GLU	CD-OE2	7.49	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	819	GLU	CD-OE2	7.49	1.33	1.25
1	B	117	GLU	CD-OE2	7.46	1.33	1.25
1	D	487	GLU	CD-OE2	7.46	1.33	1.25
1	C	893	GLU	CD-OE2	7.39	1.33	1.25
1	D	296	GLU	CD-OE2	7.37	1.33	1.25
1	A	131	GLU	CD-OE2	7.28	1.33	1.25
1	A	980	GLU	CD-OE2	7.27	1.33	1.25
1	A	619	GLU	CD-OE2	7.22	1.33	1.25
1	A	71	GLU	CD-OE2	7.19	1.33	1.25
1	B	710	GLU	CD-OE2	7.13	1.33	1.25
1	B	41	GLU	CD-OE2	7.12	1.33	1.25
1	D	710	GLU	CD-OE2	7.10	1.33	1.25
1	C	136	GLU	CD-OE2	7.05	1.33	1.25
1	A	67	GLU	CD-OE2	7.02	1.33	1.25
1	A	710	GLU	CD-OE2	6.99	1.33	1.25
1	A	684	GLU	CD-OE2	6.98	1.33	1.25
1	C	750	GLU	CD-OE2	6.98	1.33	1.25
1	C	744	GLU	CD-OE2	6.97	1.33	1.25
1	A	580	GLU	CD-OE2	6.95	1.33	1.25
1	A	667	GLU	CD-OE2	6.92	1.33	1.25
1	C	131	GLU	CD-OE2	6.90	1.33	1.25
1	B	934	GLU	CD-OE2	6.88	1.33	1.25
1	A	181	GLU	CD-OE2	6.88	1.33	1.25
1	B	170	GLU	CD-OE2	6.87	1.33	1.25
1	D	980	GLU	CD-OE2	6.86	1.33	1.25
1	B	744	GLU	CD-OE2	6.85	1.33	1.25
1	D	529	GLU	CD-OE2	6.80	1.33	1.25
1	D	819	GLU	CD-OE2	6.79	1.33	1.25
1	D	412	GLU	CD-OE2	6.79	1.33	1.25
1	D	537	GLU	CD-OE2	6.76	1.33	1.25
1	C	487	GLU	CD-OE2	6.76	1.33	1.25
1	A	529	GLU	CD-OE2	6.75	1.33	1.25
1	C	667	GLU	CD-OE2	6.75	1.33	1.25
1	B	979	GLU	CD-OE2	6.73	1.33	1.25
1	C	969	GLU	CD-OE2	6.72	1.33	1.25
1	B	304	GLU	CD-OE2	6.71	1.33	1.25
1	C	580	GLU	CD-OE2	6.71	1.33	1.25
1	D	75	GLU	CD-OE2	6.71	1.33	1.25
1	C	71	GLU	CD-OE2	6.64	1.32	1.25
1	C	338	GLU	CD-OE2	6.64	1.32	1.25
1	A	412	GLU	CD-OE2	6.63	1.32	1.25
1	B	819	GLU	CD-OE2	6.62	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	304	GLU	CD-OE2	6.61	1.32	1.25
1	A	277	GLU	CD-OE2	6.59	1.32	1.25
1	A	744	GLU	CD-OE2	6.59	1.32	1.25
1	A	136	GLU	CD-OE2	6.58	1.32	1.25
1	D	264	GLU	CD-OE2	6.57	1.32	1.25
1	B	893	GLU	CD-OE2	6.57	1.32	1.25
1	D	281	GLU	CD-OE2	6.52	1.32	1.25
1	D	181	GLU	CD-OE2	6.51	1.32	1.25
1	C	249	GLU	CD-OE2	6.51	1.32	1.25
1	A	41	GLU	CD-OE2	6.47	1.32	1.25
1	C	710	GLU	CD-OE2	6.47	1.32	1.25
1	C	75	GLU	CD-OE2	6.46	1.32	1.25
1	D	41	GLU	CD-OE2	6.46	1.32	1.25
1	B	326	GLU	CD-OE2	6.45	1.32	1.25
1	C	724	GLU	CD-OE2	6.42	1.32	1.25
1	A	243	GLU	CD-OE2	6.41	1.32	1.25
1	A	689	GLU	CD-OE2	6.37	1.32	1.25
1	D	684	GLU	CD-OE2	6.36	1.32	1.25
1	B	131	GLU	CD-OE2	6.36	1.32	1.25
1	B	338	GLU	CD-OE2	6.35	1.32	1.25
1	C	650	GLU	CD-OE2	6.34	1.32	1.25
1	A	264	GLU	CD-OE2	6.32	1.32	1.25
1	B	689	GLU	CD-OE2	6.30	1.32	1.25
1	C	637	GLU	CD-OE2	6.30	1.32	1.25
1	C	641	GLU	CD-OE1	-6.30	1.18	1.25
1	A	979	GLU	CD-OE2	6.28	1.32	1.25
1	D	667	GLU	CD-OE2	6.28	1.32	1.25
1	C	980	GLU	CD-OE2	6.25	1.32	1.25
1	B	684	GLU	CD-OE2	6.22	1.32	1.25
1	B	724	GLU	CD-OE2	6.21	1.32	1.25
1	B	136	GLU	CD-OE2	6.21	1.32	1.25
1	A	724	GLU	CD-OE2	6.20	1.32	1.25
1	D	277	GLU	CD-OE2	6.20	1.32	1.25
1	A	819	GLU	CD-OE2	6.18	1.32	1.25
1	A	487	GLU	CD-OE2	6.17	1.32	1.25
1	A	934	GLU	CD-OE2	6.15	1.32	1.25
1	B	797	GLU	CD-OE2	6.14	1.32	1.25
1	B	57	GLU	CD-OE2	6.12	1.32	1.25
1	D	131	GLU	CD-OE2	6.11	1.32	1.25
1	A	641	GLU	CD-OE1	-6.11	1.19	1.25
1	A	797	GLU	CD-OE2	6.10	1.32	1.25
1	C	681	GLU	CD-OE2	6.09	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	969	GLU	CD-OE2	6.08	1.32	1.25
1	C	904	GLU	CD-OE2	6.05	1.32	1.25
1	D	338	GLU	CD-OE2	6.02	1.32	1.25
1	A	508	GLU	CD-OE1	-6.01	1.19	1.25
1	A	80	GLU	CD-OE2	6.00	1.32	1.25
1	D	619	GLU	CD-OE2	6.00	1.32	1.25
1	A	943	GLU	CD-OE2	5.99	1.32	1.25
1	B	980	GLU	CD-OE2	5.99	1.32	1.25
1	D	249	GLU	CD-OE2	5.98	1.32	1.25
1	A	1006	GLU	CD-OE2	5.97	1.32	1.25
1	B	667	GLU	CD-OE2	5.93	1.32	1.25
1	A	170	GLU	CD-OE2	5.92	1.32	1.25
1	C	40	GLU	CD-OE2	5.90	1.32	1.25
1	D	969	GLU	CD-OE2	5.90	1.32	1.25
1	D	744	GLU	CD-OE2	5.88	1.32	1.25
1	C	264	GLU	CD-OE2	5.87	1.32	1.25
1	A	338	GLU	CD-OE2	5.86	1.32	1.25
1	A	438	GLU	CD-OE2	5.85	1.32	1.25
1	A	281	GLU	CD-OE2	5.84	1.32	1.25
1	D	808	GLU	CD-OE2	5.84	1.32	1.25
1	C	358	GLU	CD-OE2	5.81	1.32	1.25
1	C	808	GLU	CD-OE2	5.81	1.32	1.25
1	A	637	GLU	CD-OE2	5.80	1.32	1.25
1	D	797	GLU	CD-OE2	5.79	1.32	1.25
1	C	243	GLU	CD-OE1	-5.76	1.19	1.25
1	A	461	GLU	CD-OE2	5.76	1.31	1.25
1	B	487	GLU	CD-OE2	5.73	1.31	1.25
1	C	117	GLU	CD-OE2	5.73	1.31	1.25
1	B	969	GLU	CD-OE2	5.72	1.31	1.25
1	C	797	GLU	CD-OE2	5.69	1.31	1.25
1	A	358	GLU	CD-OE2	5.68	1.31	1.25
1	B	943	GLU	CD-OE2	5.67	1.31	1.25
1	C	296	GLU	CD-OE2	5.66	1.31	1.25
1	C	412	GLU	CD-OE2	5.64	1.31	1.25
1	A	40	GLU	CD-OE2	5.62	1.31	1.25
1	B	296	GLU	CD-OE2	5.59	1.31	1.25
1	D	17	GLU	CD-OE2	5.59	1.31	1.25
1	B	249	GLU	CD-OE2	5.58	1.31	1.25
1	D	369	GLU	CD-OE2	5.56	1.31	1.25
1	D	508	GLU	CD-OE2	5.56	1.31	1.25
1	C	326	GLU	CD-OE2	5.56	1.31	1.25
1	A	75	GLU	CD-OE2	5.54	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	871	GLU	CD-OE2	5.54	1.31	1.25
1	A	893	GLU	CD-OE2	5.54	1.31	1.25
1	D	641	GLU	CD-OE2	5.54	1.31	1.25
1	C	241	GLU	CD-OE2	5.53	1.31	1.25
1	B	943	GLU	CD-OE1	-5.51	1.19	1.25
1	B	580	GLU	CD-OE2	5.46	1.31	1.25
1	C	369	GLU	CD-OE1	-5.46	1.19	1.25
1	B	529	GLU	CD-OE2	5.45	1.31	1.25
1	C	934	GLU	CD-OE2	5.44	1.31	1.25
1	B	750	GLU	CD-OE2	5.41	1.31	1.25
1	B	75	GLU	CD-OE2	5.39	1.31	1.25
1	D	438	GLU	CD-OE2	5.38	1.31	1.25
1	B	904	GLU	CD-OE2	5.38	1.31	1.25
1	B	1006	GLU	CD-OE2	5.37	1.31	1.25
1	C	871	GLU	CD-OE1	-5.37	1.19	1.25
1	C	170	GLU	CD-OE2	5.36	1.31	1.25
1	B	17	GLU	CD-OE2	5.36	1.31	1.25
1	B	181	GLU	CD-OE2	5.35	1.31	1.25
1	B	264	GLU	CD-OE2	5.35	1.31	1.25
1	B	314	GLU	CD-OE2	5.34	1.31	1.25
1	B	40	GLU	CD-OE2	5.34	1.31	1.25
1	A	369	GLU	CD-OE2	5.32	1.31	1.25
1	A	57	GLU	CD-OE2	5.31	1.31	1.25
1	B	243	GLU	CD-OE2	5.31	1.31	1.25
1	B	281	GLU	CD-OE2	5.30	1.31	1.25
1	A	249	GLU	CD-OE2	5.29	1.31	1.25
1	A	324	GLU	CD-OE2	5.29	1.31	1.25
1	C	1006	GLU	CD-OE2	5.28	1.31	1.25
1	D	314	GLU	CD-OE2	5.27	1.31	1.25
1	C	904	GLU	CD-OE1	-5.26	1.19	1.25
1	D	681	GLU	CD-OE2	5.24	1.31	1.25
1	D	358	GLU	CD-OE2	5.20	1.31	1.25
1	B	198	GLU	CD-OE2	5.19	1.31	1.25
1	D	326	GLU	CD-OE2	5.19	1.31	1.25
1	A	296	GLU	CD-OE2	5.18	1.31	1.25
1	B	369	GLU	CD-OE2	5.16	1.31	1.25
1	D	170	GLU	CD-OE2	5.15	1.31	1.25
1	B	358	GLU	CD-OE2	5.13	1.31	1.25
1	D	943	GLU	CD-OE2	5.13	1.31	1.25
1	D	893	GLU	CD-OE2	5.12	1.31	1.25
1	D	117	GLU	CD-OE2	5.11	1.31	1.25
1	D	324	GLU	CD-OE2	5.08	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	243	GLU	CD-OE2	5.07	1.31	1.25
1	A	681	GLU	CD-OE2	5.07	1.31	1.25
1	B	80	GLU	CD-OE2	5.05	1.31	1.25
1	B	67	GLU	CD-OE2	5.01	1.31	1.25
1	D	724	GLU	CD-OE2	5.00	1.31	1.25

All (661) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	809	ARG	NE-CZ-NH1	20.37	130.49	120.30
1	A	251	ARG	NE-CZ-NH1	16.10	128.35	120.30
1	D	809	ARG	NE-CZ-NH1	14.65	127.62	120.30
1	A	251	ARG	NE-CZ-NH2	-14.48	113.06	120.30
1	D	699	ARG	NE-CZ-NH1	13.84	127.22	120.30
1	A	336	ARG	NE-CZ-NH1	13.28	126.94	120.30
1	B	442	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	A	446	ARG	NE-CZ-NH1	13.13	126.86	120.30
1	B	442	ARG	NE-CZ-NH2	-13.00	113.80	120.30
1	C	130	ASP	CB-CG-OD1	12.89	129.90	118.30
1	A	319	ASP	CB-CG-OD2	-12.87	106.72	118.30
1	A	45	ASP	CB-CG-OD1	12.51	129.56	118.30
1	C	43	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	A	319	ASP	CB-CG-OD1	12.38	129.44	118.30
1	A	853	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	A	699	ARG	NE-CZ-NH1	12.07	126.34	120.30
1	A	952	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	B	685	LEU	C-N-CD	-11.78	94.69	120.60
1	A	431	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	D	280	ASP	CB-CG-OD2	-11.50	107.95	118.30
1	B	237	ARG	NE-CZ-NH2	-11.37	114.61	120.30
1	A	446	ARG	NE-CZ-NH2	-11.29	114.65	120.30
1	B	336	ARG	NE-CZ-NH1	11.17	125.89	120.30
1	A	43	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	A	942	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	D	610	ASP	CB-CG-OD1	11.04	128.24	118.30
1	B	648	ASP	CB-CG-OD2	-11.02	108.39	118.30
1	D	671	ASP	CB-CG-OD1	10.98	128.19	118.30
1	D	942	ARG	NE-CZ-NH1	10.87	125.74	120.30
1	D	193	ASP	CB-CG-OD2	-10.81	108.57	118.30
1	B	237	ARG	NE-CZ-NH1	10.69	125.64	120.30
1	D	507	ASP	CB-CG-OD2	-10.68	108.69	118.30
1	C	997	ASP	CB-CG-OD2	-10.67	108.70	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ASP	CB-CG-OD1	10.54	127.78	118.30
1	D	255	ARG	NE-CZ-NH1	10.43	125.52	120.30
1	C	178	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	C	942	ARG	NE-CZ-NH1	10.17	125.39	120.30
1	C	439	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	C	230	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	C	255	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	C	234	ASP	CB-CG-OD2	-9.96	109.33	118.30
1	B	172	ASP	CB-CG-OD2	-9.90	109.39	118.30
1	D	809	ARG	NE-CZ-NH2	-9.89	115.35	120.30
1	B	492	ASP	CB-CG-OD2	-9.82	109.46	118.30
1	B	924	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	D	288	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	C	336	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	C	442	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	A	429	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	C	144	ASP	CB-CG-OD1	9.52	126.87	118.30
1	A	333	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	C	428	ASP	CB-CG-OD1	9.46	126.81	118.30
1	B	919	ASP	CB-CG-OD2	-9.44	109.80	118.30
1	B	319	ASP	CB-CG-OD2	-9.43	109.82	118.30
1	D	336	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	C	630	ARG	NE-CZ-NH1	9.37	124.98	120.30
1	A	287	ASP	CB-CG-OD2	-9.36	109.88	118.30
1	A	659	ASP	CB-CG-OD2	-9.35	109.88	118.30
1	D	952	ARG	NE-CZ-NH1	9.35	124.98	120.30
1	B	648	ASP	CB-CG-OD1	9.29	126.66	118.30
1	B	473	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	A	287	ASP	CB-CG-OD1	9.26	126.64	118.30
1	C	431	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	D	782	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	A	469	ASP	CB-CG-OD1	9.14	126.53	118.30
1	C	507	ASP	CB-CG-OD2	-9.13	110.08	118.30
1	B	45	ASP	CB-CG-OD1	9.12	126.51	118.30
1	B	233	ASP	CB-CG-OD2	-9.13	110.09	118.30
1	D	997	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	B	1013	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	853	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	B	987	ASP	CB-CG-OD1	8.97	126.37	118.30
1	C	492	ASP	CB-CG-OD2	-8.97	110.22	118.30
1	A	952	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	A	255	ARG	NE-CZ-NH2	-8.96	115.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	699	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	D	507	ASP	CB-CG-OD1	8.89	126.31	118.30
1	D	572	ASP	CB-CG-OD1	8.89	126.30	118.30
1	D	790	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	D	671	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	A	755	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	C	531	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	C	671	ASP	CB-CG-OD1	8.78	126.20	118.30
1	D	961	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	D	429	ASP	CB-CG-OD2	-8.76	110.42	118.30
1	D	43	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	D	255	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	D	13	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	375	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	B	916	ASP	CB-CG-OD2	-8.69	110.48	118.30
1	C	230	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	D	610	ASP	CB-CG-OD2	-8.66	110.51	118.30
1	A	45	ASP	CB-CG-OD2	-8.64	110.52	118.30
1	D	832	ASP	CB-CG-OD2	-8.64	110.53	118.30
1	B	973	ARG	NE-CZ-NH2	8.61	124.61	120.30
1	C	507	ASP	CB-CG-OD1	8.61	126.05	118.30
1	C	439	ARG	NE-CZ-NH2	-8.59	116.01	120.30
1	C	224	ASP	CB-CG-OD1	8.57	126.01	118.30
1	D	318	ALA	N-CA-CB	-8.53	98.16	110.10
1	C	802	ASP	CB-CG-OD1	8.50	125.95	118.30
1	D	193	ASP	CB-CG-OD1	8.48	125.93	118.30
1	D	572	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	C	802	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	B	579	ASP	CB-CG-OD1	8.44	125.89	118.30
1	C	782	ASP	CB-CG-OD2	-8.40	110.73	118.30
1	D	859	ASP	CB-CG-OD1	8.36	125.82	118.30
1	A	557	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	D	446	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	B	579	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	C	388	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	233	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	B	172	ASP	CB-CG-OD1	8.29	125.76	118.30
1	B	671	ASP	CB-CG-OD1	8.28	125.75	118.30
1	B	507	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	B	1013	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	954	ASP	CB-CG-OD1	8.28	125.75	118.30
1	A	172	ASP	CB-CG-OD2	-8.24	110.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	648	ASP	CB-CG-OD2	-8.24	110.89	118.30
1	C	919	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	D	252	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	B	919	ASP	CB-CG-OD1	8.19	125.67	118.30
1	C	875	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	43	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	735	HIS	CA-CB-CG	-8.12	99.80	113.60
1	C	790	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	D	954	ASP	CB-CG-OD1	8.10	125.59	118.30
1	A	252	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	B	201	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	B	671	ASP	CB-CG-OD2	-8.05	111.05	118.30
1	C	43	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	D	469	ASP	CB-CG-OD1	8.04	125.54	118.30
1	A	288	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	B	996	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	A	13	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	507	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	C	996	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	246	MET	CG-SD-CE	-7.99	87.41	100.20
1	D	782	ASP	CB-CG-OD1	7.95	125.45	118.30
1	C	809	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	96	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	D	952	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	D	234	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	D	924	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	A	507	ASP	CB-CG-OD1	7.87	125.38	118.30
1	A	832	ASP	CB-CG-OD2	-7.86	111.23	118.30
1	C	1022	GLN	CG-CD-OE1	7.85	137.30	121.60
1	A	610	ASP	CB-CG-OD1	7.85	125.36	118.30
1	D	211	ASP	CB-CG-OD2	-7.84	111.25	118.30
1	C	234	ASP	CB-CG-OD1	7.82	125.33	118.30
1	D	356	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	809	ARG	NE-CZ-NH2	7.76	124.18	120.30
1	C	247	CYS	CA-CB-SG	-7.73	100.09	114.00
1	B	954	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	A	77	ASP	CB-CG-OD2	-7.72	111.36	118.30
1	D	411	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	267	VAL	CG1-CB-CG2	-7.70	98.59	110.90
1	D	82	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	428	ASP	CB-CG-OD1	7.69	125.22	118.30
1	C	997	ASP	CB-CG-OD1	7.68	125.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	C	428	ASP	CB-CG-OD2	-7.66	111.40	118.30
1	C	772	ASP	CB-CG-OD1	7.66	125.19	118.30
1	B	77	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	B	210	ARG	N-CA-CB	7.62	124.32	110.60
1	D	557	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	A	954	ASP	CB-CG-OD2	-7.57	111.48	118.30
1	C	531	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	D	52	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	211	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	C	916	ASP	CB-CG-OD1	7.54	125.09	118.30
1	D	411	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	C	442	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	B	319	ASP	CB-CG-OD1	7.47	125.03	118.30
1	C	1022	GLN	N-CA-CB	7.47	124.04	110.60
1	D	469	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	C	634	GLN	N-CA-CB	7.44	123.99	110.60
1	C	446	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	B	531	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	C	130	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	D	429	ASP	CB-CG-OD1	7.37	124.93	118.30
1	C	211	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	C	875	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	B	531	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	507	ASP	CB-CG-OD1	7.32	124.88	118.30
1	A	916	ASP	CB-CG-OD1	7.31	124.88	118.30
1	C	329	ASP	CB-CG-OD1	7.30	124.87	118.30
1	C	760	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	B	193	ASP	CB-CG-OD1	7.30	124.87	118.30
1	C	958	ASN	N-CA-CB	7.30	123.74	110.60
1	B	996	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	431	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	659	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	D	881	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	B	14	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	C	447	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	B	755	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	B	144	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	C	178	ARG	CD-NE-CZ	7.21	133.70	123.60
1	A	15	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	D	288	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	96	ASP	CB-CG-OD2	-7.19	111.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	234	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	233	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	782	ASP	CB-CG-OD1	7.17	124.75	118.30
1	D	579	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	A	782	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	A	800	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	D	958	ASN	N-CA-CB	7.09	123.36	110.60
1	A	140	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	C	288	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	D	252	ASP	CB-CG-OD1	7.08	124.67	118.30
1	C	144	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	B	942	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	C	671	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	D	919	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	869	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	1018	LEU	CB-CA-C	-7.03	96.85	110.20
1	D	954	ASP	CB-CG-OD2	-7.03	111.98	118.30
1	D	439	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	D	924	ASP	CB-CG-OD1	7.02	124.61	118.30
1	B	908	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	D	973	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	D	997	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	908	ASP	CB-CG-OD1	6.99	124.59	118.30
1	D	832	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	77	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	569	ASP	CB-CG-OD1	6.98	124.58	118.30
1	B	832	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	D	442	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	C	288	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	B	76	CYS	N-CA-CB	-6.97	98.05	110.60
1	A	802	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	875	ASP	CB-CG-OD1	6.96	124.56	118.30
1	B	997	ASP	N-CA-CB	6.95	123.11	110.60
1	D	719	GLN	N-CA-CB	6.95	123.11	110.60
1	A	251	ARG	CD-NE-CZ	6.95	133.32	123.60
1	A	828	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	B	287	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	B	916	ASP	CB-CG-OD1	6.93	124.54	118.30
1	C	172	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	C	735	HIS	CA-CB-CG	-6.91	101.86	113.60
1	C	721	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	D	280	ASP	CB-CG-OD1	6.89	124.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	755	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	D	919	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	B	853	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	569	ASP	CB-CG-OD1	6.87	124.49	118.30
1	B	193	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	869	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	C	594	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	610	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	C	987	ASP	CB-CG-OD1	6.83	124.45	118.30
1	C	809	ARG	CD-NE-CZ	6.83	133.16	123.60
1	D	164	ASP	CB-CG-OD1	6.83	124.45	118.30
1	D	497	ASP	CB-CG-OD1	6.83	124.45	118.30
1	D	557	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	699	ARG	CB-CA-C	-6.82	96.77	110.40
1	C	287	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	832	ASP	CB-CG-OD1	6.78	124.41	118.30
1	C	919	ASP	CB-CG-OD1	6.78	124.40	118.30
1	D	492	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	B	857	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	C	193	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	C	287	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	C	954	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	C	166	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	610	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	C	772	ASP	CB-CG-OD2	-6.71	112.27	118.30
1	A	809	ARG	NE-CZ-NH1	-6.70	116.95	120.30
1	B	45	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	B	772	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	B	43	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	857	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	C	648	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	828	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	579	ASP	CB-CG-OD1	6.67	124.31	118.30
1	A	648	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	D	324	GLU	N-CA-CB	6.67	122.60	110.60
1	D	1018	LEU	CB-CA-C	-6.67	97.53	110.20
1	C	233	ASP	CB-CG-OD1	6.66	124.29	118.30
1	C	411	ASP	CB-CG-OD1	6.64	124.28	118.30
1	C	1022	GLN	OE1-CD-NE2	-6.63	106.65	121.90
1	C	403	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	B	52	ARG	CB-CA-C	-6.62	97.16	110.40
1	D	287	ASP	CB-CG-OD2	-6.61	112.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	A	439	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	C	411	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	411	ASP	CB-CG-OD2	-6.59	112.36	118.30
1	A	667	GLU	CB-CG-CD	-6.58	96.44	114.20
1	C	479	ASP	CB-CG-OD1	6.58	124.22	118.30
1	D	279	ILE	CA-CB-CG2	6.57	124.05	110.90
1	A	746	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	B	954	ASP	CB-CG-OD1	6.57	124.21	118.30
1	B	734	SER	N-CA-C	6.57	128.73	111.00
1	A	859	ASP	CB-CG-OD1	6.56	124.20	118.30
1	C	659	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	164	ASP	CB-CG-OD1	6.54	124.19	118.30
1	B	598	ASP	CB-CG-OD1	6.52	124.17	118.30
1	D	82	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	429	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	961	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	572	ASP	CB-CG-OD1	6.50	124.16	118.30
1	C	193	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	952	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	699	ARG	CD-NE-CZ	6.50	132.69	123.60
1	C	46	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	C	368	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	184	LEU	CB-CA-C	-6.49	97.87	110.20
1	A	442	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	1014	TYR	CB-CG-CD1	6.48	124.89	121.00
1	C	610	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	C	996	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	368	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	610	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	790	ASP	CB-CG-OD1	6.47	124.12	118.30
1	D	15	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	1018	LEU	CB-CA-C	-6.45	97.94	110.20
1	C	77	ASP	CB-CG-OD1	6.45	124.11	118.30
1	D	594	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	C	859	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	B	52	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	908	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	1018	LEU	CB-CA-C	-6.44	97.97	110.20
1	D	735	HIS	N-CA-CB	-6.44	99.01	110.60
1	A	224	ASP	CB-CG-OD1	6.43	124.09	118.30
1	C	735	HIS	CB-CA-C	6.43	123.26	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	916	ASP	CB-CG-OD1	6.41	124.07	118.30
1	D	828	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	D	828	ASP	CB-CG-OD1	6.38	124.05	118.30
1	B	282	ARG	NE-CZ-NH2	6.37	123.48	120.30
1	B	287	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	428	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	96	ASP	CB-CG-OD1	6.35	124.02	118.30
1	B	734	SER	CA-C-N	-6.35	103.24	117.20
1	A	285	TYR	CB-CG-CD2	-6.34	117.20	121.00
1	D	594	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	659	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	287	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	996	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	D	428	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	D	96	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	A	15	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	201	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	371	THR	CA-CB-CG2	-6.28	103.61	112.40
1	A	782	ASP	CB-CG-OD1	6.28	123.95	118.30
1	D	746	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	C	792	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	809	ARG	CD-NE-CZ	-6.23	114.88	123.60
1	B	721	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	591	ASP	CB-CG-OD1	6.22	123.90	118.30
1	C	924	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	594	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	579	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	859	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	D	772	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	233	ASP	CB-CG-OD1	6.20	123.88	118.30
1	C	15	ASP	CB-CG-OD1	6.17	123.86	118.30
1	C	828	ASP	CB-CG-OD1	6.17	123.85	118.30
1	C	1013	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	D	367	MET	CG-SD-CE	6.16	110.06	100.20
1	C	303	ALA	N-CA-CB	6.15	118.71	110.10
1	B	591	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	C	403	ASP	CB-CG-OD1	6.14	123.82	118.30
1	D	13	ARG	NE-CZ-NH2	-6.13	117.24	120.30
1	B	772	ASP	CB-CG-OD1	6.12	123.81	118.30
1	A	130	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	A	172	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	446	ARG	NE-CZ-NH2	-6.11	117.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	881	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	948	PRO	CB-CA-C	-6.11	96.73	112.00
1	D	234	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	201	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	D	781	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	856	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	C	546	LEU	N-CA-CB	6.09	122.58	110.40
1	C	572	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	634	GLN	N-CA-CB	6.08	121.55	110.60
1	B	1014	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	B	233	ASP	CB-CG-OD1	6.07	123.77	118.30
1	D	431	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	A	59	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	D	211	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	634	GLN	CB-CA-C	6.07	122.53	110.40
1	B	782	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	A	667	GLU	CB-CA-C	-6.04	98.31	110.40
1	B	733	ALA	C-N-CA	-6.04	106.59	121.70
1	C	572	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	D	909	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	B	735	HIS	CB-CA-C	6.03	122.45	110.40
1	D	473	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	C	961	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	431	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	157	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	C	734	SER	N-CA-CB	5.99	119.49	110.50
1	C	781	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	781	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	D	986	ILE	CG1-CB-CG2	-5.99	98.22	111.40
1	D	938	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	924	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	954	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	719	GLN	CB-CA-C	-5.96	98.47	110.40
1	A	991	MET	CG-SD-CE	5.96	109.74	100.20
1	D	473	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	D	802	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	A	748	CYS	CA-CB-SG	-5.96	103.27	114.00
1	C	368	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	561	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	A	561	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	388	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	875	ASP	CB-CG-OD2	-5.93	112.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	920	LEU	CB-CA-C	-5.93	98.94	110.20
1	C	924	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	659	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	52	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	D	569	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	894	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	B	598	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	C	469	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	790	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	255	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	538	TYR	CB-CG-CD2	5.88	124.53	121.00
1	A	553	TRP	CA-CB-CG	-5.88	102.53	113.70
1	A	472	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	B	82	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	832	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	659	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	916	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	D	144	ASP	CB-CG-OD1	5.85	123.56	118.30
1	D	553	TRP	CA-CB-CG	-5.85	102.59	113.70
1	D	1010	SER	N-CA-CB	-5.84	101.74	110.50
1	A	292	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	C	184	LEU	CB-CG-CD2	-5.82	101.10	111.00
1	C	211	ASP	CB-CG-OD1	5.82	123.54	118.30
1	C	1022	GLN	CB-CA-C	-5.81	98.77	110.40
1	D	869	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	405	TYR	CB-CG-CD2	-5.79	117.53	121.00
1	B	140	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	859	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	569	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	842	TRP	CA-CB-CG	-5.78	102.72	113.70
1	D	164	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	D	479	ASP	CB-CG-OD1	5.77	123.50	118.30
1	D	598	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	B	324	GLU	CG-CD-OE1	5.76	129.81	118.30
1	A	778	THR	N-CA-CB	5.75	121.23	110.30
1	B	130	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	B	336	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	B	889	ALA	C-N-CA	-5.73	107.36	121.70
1	B	952	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	280	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	90	TRP	CB-CA-C	5.71	121.82	110.40
1	C	746	ASP	CB-CA-C	-5.71	98.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	909	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	234	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	599	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	917	ARG	CD-NE-CZ	-5.68	115.65	123.60
1	B	15	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	473	ARG	CD-NE-CZ	5.66	131.52	123.60
1	C	809	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
1	B	650	GLU	CB-CA-C	-5.65	99.10	110.40
1	A	509	ASP	CB-CG-OD1	5.65	123.38	118.30
1	D	569	ASP	CB-CG-OD1	5.65	123.38	118.30
1	D	772	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	237	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	166	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	C	869	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	144	ASP	CB-CG-OD1	5.62	123.36	118.30
1	C	116	THR	CA-CB-CG2	-5.61	104.55	112.40
1	B	234	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	699	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	375	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	746	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	659	ASP	CB-CG-OD2	-5.59	113.26	118.30
1	B	909	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	650	GLU	CB-CA-C	-5.59	99.21	110.40
1	C	889	ALA	N-CA-CB	-5.59	102.27	110.10
1	C	832	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	632	SER	N-CA-CB	5.59	118.88	110.50
1	C	183	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	958	ASN	N-CA-CB	5.59	120.66	110.60
1	B	161	TYR	N-CA-CB	-5.58	100.55	110.60
1	D	26	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	403	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	368	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	96	ASP	CB-CG-OD1	5.56	123.31	118.30
1	D	15	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	D	497	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	D	699	ARG	CD-NE-CZ	5.54	131.36	123.60
1	C	252	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	731	PRO	CA-N-CD	-5.54	103.75	111.50
1	D	310	ARG	NE-CZ-NH1	-5.53	117.53	120.30
1	B	224	ASP	CB-CG-OD1	5.53	123.28	118.30
1	D	175	ALA	CB-CA-C	-5.53	101.81	110.10
1	A	938	ARG	N-CA-CB	5.52	120.53	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	472	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	A	319	ASP	N-CA-CB	5.52	120.53	110.60
1	B	838	THR	CA-CB-CG2	-5.51	104.68	112.40
1	A	469	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	C	611	ARG	N-CA-CB	5.51	120.52	110.60
1	C	632	SER	N-CA-CB	5.51	118.76	110.50
1	A	130	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	439	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	15	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	755	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	442	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	251	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	D	561	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	85	VAL	CA-CB-CG2	-5.49	102.66	110.90
1	D	144	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	A	431	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	77	ASP	CB-CG-OD1	5.48	123.24	118.30
1	B	164	ASP	CB-CG-OD1	5.47	123.23	118.30
1	B	469	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	B	828	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	80	GLU	CG-CD-OE2	-5.47	107.36	118.30
1	A	894	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	B	802	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	929	TYR	CB-CG-CD1	5.46	124.28	121.00
1	B	417	THR	CA-CB-CG2	-5.46	104.76	112.40
1	C	789	LEU	CB-CA-C	-5.46	99.83	110.20
1	D	916	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	252	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	557	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	329	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	B	650	GLU	CG-CD-OE1	5.45	129.20	118.30
1	B	553	TRP	CA-CB-CG	-5.45	103.34	113.70
1	D	996	ASP	CB-CG-OD1	5.45	123.21	118.30
1	C	800	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	D	509	ASP	CB-CG-OD1	5.43	123.18	118.30
1	B	973	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	C	482	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	255	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	469	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	889	ALA	O-C-N	-5.41	114.05	122.70
1	A	599	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	C	881	ARG	NE-CZ-NH1	5.41	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	201	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	486	TYR	CB-CG-CD2	-5.39	117.76	121.00
1	B	178	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	403	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	B	731	PRO	N-CD-CG	5.38	111.27	103.20
1	C	710	GLU	CB-CA-C	-5.38	99.64	110.40
1	D	746	ASP	CB-CA-C	-5.38	99.64	110.40
1	D	821	ALA	N-CA-CB	5.38	117.63	110.10
1	A	559	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	D	832	ASP	N-CA-CB	-5.37	100.94	110.60
1	A	538	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	D	909	ARG	N-CA-CB	5.36	120.25	110.60
1	B	368	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	553	TRP	CA-CB-CG	-5.36	103.52	113.70
1	B	875	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	B	859	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	572	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	1013	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	509	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	428	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	218	PRO	N-CA-CB	5.33	109.69	103.30
1	B	329	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	942	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
1	B	446	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	968	MET	CA-CB-CG	5.29	122.30	113.30
1	D	659	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	755	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	C	579	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	986	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	D	403	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	B	497	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	594	ASP	CB-CG-OD1	5.27	123.05	118.30
1	B	611	ARG	N-CA-CB	5.27	120.09	110.60
1	B	651	LEU	CB-CG-CD2	5.27	119.96	111.00
1	D	699	ARG	N-CA-CB	5.27	120.09	110.60
1	D	997	ASP	N-CA-CB	5.27	120.08	110.60
1	D	233	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	916	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	685	LEU	N-CA-CB	5.26	120.92	110.40
1	B	997	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	D	786	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	996	ASP	CB-CG-OD1	5.25	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	ARG	N-CA-CB	5.24	120.03	110.60
1	A	280	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	B	594	ASP	CB-CG-OD1	5.23	123.01	118.30
1	D	224	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	591	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	768	MET	N-CA-CB	5.22	120.00	110.60
1	C	680	ILE	CA-CB-CG1	-5.22	101.08	111.00
1	B	166	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	234	ASP	CB-CG-OD1	5.21	122.99	118.30
1	B	492	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	14	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	B	997	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	43	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	D	800	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	52	ARG	N-CA-CB	-5.21	101.23	110.60
1	C	379	MET	CA-CB-CG	-5.20	104.47	113.30
1	C	447	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	237	ARG	CB-CA-C	-5.18	100.04	110.40
1	B	199	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	336	ARG	CD-NE-CZ	5.18	130.85	123.60
1	C	157	ARG	CD-NE-CZ	5.18	130.85	123.60
1	D	178	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	968	MET	N-CA-CB	-5.17	101.29	110.60
1	B	370	GLN	CA-CB-CG	-5.17	102.03	113.40
1	C	625	GLN	CG-CD-OE1	-5.17	111.26	121.60
1	D	439	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	190	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	D	744	GLU	CG-CD-OE2	-5.15	108.00	118.30
1	C	262	GLN	C-N-CA	-5.15	111.49	122.30
1	B	958	ASN	N-CA-CB	5.14	119.86	110.60
1	A	735	HIS	N-CA-CB	-5.14	101.34	110.60
1	C	509	ASP	CB-CG-OD1	5.14	122.93	118.30
1	D	894	ARG	CB-CA-C	-5.14	100.13	110.40
1	A	13	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	381	GLN	CA-CB-CG	-5.13	102.11	113.40
1	A	193	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	719	GLN	CA-CB-CG	5.13	124.68	113.40
1	B	344	LEU	CA-CB-CG	-5.13	103.51	115.30
1	C	799	THR	CA-CB-CG2	-5.12	105.22	112.40
1	B	82	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	B	929	TYR	CB-CG-CD2	-5.12	117.93	121.00
1	B	85	VAL	CB-CA-C	-5.12	101.68	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	446	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	869	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	379	MET	CG-SD-CE	-5.12	92.02	100.20
1	C	719	GLN	CB-CA-C	-5.11	100.17	110.40
1	D	230	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	D	233	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	319	ASP	CA-CB-CG	5.11	124.64	113.40
1	B	416	GLU	CG-CD-OE2	-5.11	108.08	118.30
1	B	781	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	52	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	650	GLU	CG-CD-OE2	-5.09	108.12	118.30
1	B	572	ASP	CB-CG-OD1	5.08	122.88	118.30
1	D	961	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	431	ARG	CA-CB-CG	-5.08	102.22	113.40
1	D	859	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	C	52	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	161	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	C	842	TRP	CA-CB-CG	-5.08	104.06	113.70
1	C	446	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	D	96	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	973	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	A	190	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	610	ASP	CB-CG-OD1	5.05	122.85	118.30
1	C	853	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	D	505	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	B	37	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	804	ASN	N-CA-CB	-5.04	101.52	110.60
1	A	1014	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	D	116	THR	CA-CB-CG2	-5.04	105.35	112.40
1	C	792	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	B	845	GLN	C-N-CA	-5.03	111.73	122.30
1	A	324	GLU	N-CA-CB	5.03	119.65	110.60
1	B	719	GLN	CB-CA-C	-5.03	100.34	110.40
1	A	1023	LYS	N-CA-CB	5.03	119.65	110.60
1	C	184	LEU	CB-CA-C	-5.02	100.65	110.20
1	D	696	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	C	598	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	164	ASP	CB-CG-OD2	-5.01	113.80	118.30
1	C	938	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	A	648	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8123	0	7715	202	0
1	B	8123	0	7715	136	0
1	C	8123	0	7715	121	0
1	D	8123	0	7715	149	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
4	A	45	0	53	0	0
4	B	45	0	53	3	0
4	C	45	0	53	1	0
4	D	45	0	53	1	0
5	A	96	0	144	13	0
5	B	104	0	156	18	0
5	C	96	0	144	14	0
5	D	92	0	138	6	0
6	A	862	0	0	19	0
6	B	995	0	0	20	0
6	C	974	0	0	12	0
6	D	897	0	0	12	0
All	All	36820	0	31654	615	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (615) 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:D:8403:DMS:C2	5:D:8403:DMS:S	2.08	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:GLN:HE21	1:A:1018:LEU:N	1.46	1.11
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.16	1.08
1:D:750:GLU:HG3	1:D:755:ARG:HG3	1.37	1.06
1:A:730:LEU:HD22	1:A:731:PRO:HD2	1.36	1.05
1:B:369:GLU:HG2	1:B:370:GLN:HE22	1.16	1.05
1:D:316:HIS:HA	1:D:323:ILE:HD12	1.44	0.99
1:A:685:LEU:HD23	1:A:686:PRO:HD2	1.45	0.99
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.43	0.99
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.30	0.95
1:A:600:GLN:H	1:A:600:GLN:HE21	0.95	0.94
1:C:643:LEU:HD23	1:C:675:GLN:NE2	1.87	0.90
1:B:600:GLN:H	1:B:600:GLN:HE21	1.14	0.89
1:A:1017:GLN:HE21	1:A:1018:LEU:H	1.09	0.89
1:D:735:HIS:N	1:D:735:HIS:ND1	2.16	0.89
1:C:737:ILE:CD1	1:C:738:PRO:HD2	2.03	0.89
1:B:804:ASN:HD22	1:B:809:ARG:NH2	1.71	0.88
1:B:804:ASN:ND2	1:B:809:ARG:HH21	1.74	0.86
1:B:369:GLU:HG2	1:B:370:GLN:NE2	1.90	0.86
1:B:795:VAL:HG12	5:B:8506:DMS:H22	1.59	0.84
1:A:241:GLU:HG2	1:A:292:ARG:HG2	1.57	0.84
5:A:8420:DMS:H21	6:D:4743:HOH:O	1.78	0.84
1:C:277:GLU:HG2	6:C:4832:HOH:O	1.78	0.82
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.14	0.82
1:D:777:LEU:HD13	1:D:980:GLU:HG3	1.60	0.82
1:D:730:LEU:HG	1:D:731:PRO:HD2	1.61	0.82
1:A:1017:GLN:NE2	1:A:1018:LEU:N	2.27	0.82
1:B:777:LEU:CD1	1:B:980:GLU:HG2	2.10	0.82
1:C:251:ARG:HH11	1:C:251:ARG:HB3	1.44	0.81
1:A:231:PHE:O	5:A:8417:DMS:H22	1.80	0.81
1:D:750:GLU:CG	1:D:755:ARG:HG3	2.09	0.81
5:C:8502:DMS:H23	6:C:4944:HOH:O	1.81	0.81
1:A:579:ASP:OD2	1:A:583:ASN:HB2	1.81	0.81
1:D:730:LEU:CD2	1:D:731:PRO:HD2	2.10	0.81
1:B:730:LEU:O	1:B:730:LEU:HD13	1.81	0.80
1:D:750:GLU:HG3	1:D:755:ARG:CG	2.10	0.80
1:B:251:ARG:HD2	5:B:8416:DMS:O	1.82	0.80
1:A:655:MET:HG3	1:A:656:VAL:N	1.96	0.80
1:C:653:HIS:ND1	1:C:667:GLU:HG2	1.97	0.80
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.17	0.79
1:A:890:GLN:OE1	1:A:947:GLY:HA3	1.82	0.79
1:D:730:LEU:CG	1:D:731:PRO:HD2	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:GLU:O	1:A:135:GLN:HG2	1.83	0.78
1:C:630:ARG:HH11	1:C:630:ARG:HB3	1.49	0.78
1:B:1023:LYS:HA	6:B:4995:HOH:O	1.83	0.78
1:A:730:LEU:CD2	1:A:731:PRO:HD2	2.14	0.78
1:D:797:GLU:O	1:D:801:ILE:HD13	1.84	0.78
1:B:777:LEU:HD11	1:B:980:GLU:HG2	1.64	0.77
1:B:251:ARG:HA	5:B:8416:DMS:O	1.83	0.77
1:D:262:GLN:HE22	1:D:299:LYS:HD2	1.48	0.77
5:A:8410:DMS:H21	6:A:4506:HOH:O	1.84	0.77
1:D:759:ASN:OD1	1:D:761:GLN:HG3	1.83	0.77
1:A:279:ILE:HD11	1:D:422:PRO:HG3	1.66	0.77
1:D:730:LEU:HD23	1:D:731:PRO:HD2	1.65	0.77
1:C:251:ARG:NH1	1:C:251:ARG:HB3	2.00	0.76
1:D:1022:GLN:HG3	1:D:1023:LYS:HG3	1.67	0.76
1:B:844:HIS:CE1	1:B:845:GLN:HG3	2.21	0.76
1:C:685:LEU:HD23	1:C:686:PRO:HD2	1.65	0.76
1:C:685:LEU:HD23	1:C:686:PRO:CD	2.17	0.75
1:D:750:GLU:HG2	1:D:754:LYS:O	1.87	0.75
1:B:292:ARG:HH12	5:B:8412:DMS:C2	1.99	0.75
1:A:431:ARG:HG3	6:A:4683:HOH:O	1.86	0.75
1:A:769:TRP:NE1	1:A:774:LYS:HD3	2.01	0.75
1:A:634:GLN:HB2	1:A:682:LEU:HB2	1.69	0.74
1:B:809:ARG:NH1	1:B:809:ARG:HG2	2.00	0.74
1:A:600:GLN:NE2	1:A:600:GLN:H	1.79	0.74
1:D:130:ASP:OD1	1:D:132:SER:N	2.20	0.74
1:C:251:ARG:HA	5:C:8416:DMS:O	1.87	0.73
1:A:581:ASN:HD22	1:A:583:ASN:HD22	1.36	0.73
1:A:600:GLN:N	1:A:600:GLN:HE21	1.80	0.73
1:A:279:ILE:HD11	1:D:422:PRO:CG	2.19	0.72
1:A:797:GLU:O	1:A:801:ILE:HD13	1.89	0.72
1:D:128:ASN:HB3	1:D:180:GLY:O	1.90	0.72
1:A:655:MET:HE3	1:A:664:ALA:O	1.89	0.72
1:A:292:ARG:HH12	5:A:8412:DMS:H22	1.53	0.72
1:D:651:LEU:CD2	1:D:653:HIS:HE1	2.04	0.71
1:A:684:GLU:O	1:A:686:PRO:HD3	1.90	0.71
1:A:965:GLN:O	1:A:969:GLU:HG3	1.89	0.71
1:B:757:GLN:NE2	1:B:766:SER:OG	2.23	0.71
1:C:576:ILE:HD12	5:C:8411:DMS:H12	1.72	0.71
1:C:576:ILE:N	1:C:576:ILE:HD13	2.05	0.71
1:D:618:THR:HG23	6:D:4358:HOH:O	1.89	0.71
1:B:370:GLN:N	1:B:370:GLN:HE21	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLN:HG2	1:A:682:LEU:O	1.91	0.70
1:B:804:ASN:ND2	1:B:809:ARG:NH2	2.35	0.70
1:D:749:ILE:N	1:D:749:ILE:HD12	2.06	0.69
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.74	0.69
5:A:8412:DMS:H23	6:A:4624:HOH:O	1.92	0.69
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.27	0.69
1:B:370:GLN:N	1:B:370:GLN:NE2	2.40	0.69
1:D:316:HIS:HA	1:D:323:ILE:CD1	2.20	0.69
1:B:249:GLU:CG	1:B:251:ARG:HD3	2.23	0.69
1:A:800:ARG:CZ	1:A:800:ARG:HB2	2.22	0.69
1:C:737:ILE:HD13	1:C:832:ASP:HA	1.75	0.69
1:B:847:LYS:HG3	1:B:848:THR:N	2.08	0.68
1:A:808:GLU:OE1	1:A:811:LYS:NZ	2.25	0.68
1:A:656:VAL:HG21	1:A:685:LEU:CD1	2.23	0.68
1:A:130:ASP:OD1	1:A:132:SER:N	2.26	0.67
1:D:1016:TYR:C	1:D:1017:GLN:HG3	2.14	0.67
1:A:768:MET:HE3	1:A:1020:TRP:CZ2	2.29	0.67
1:A:686:PRO:O	1:A:687:GLN:NE2	2.28	0.67
1:B:102:ASN:HB3	5:B:8506:DMS:H11	1.75	0.67
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.30	0.66
1:C:685:LEU:CD2	1:C:686:PRO:HD2	2.24	0.66
1:D:78:LEU:HB3	1:D:80:GLU:OE2	1.96	0.66
1:D:755:ARG:NH1	1:D:771:GLY:O	2.28	0.66
1:A:608:PHE:CE1	1:A:614:HIS:HD2	2.14	0.66
1:A:863:GLN:HE22	1:A:952:ARG:HH22	1.44	0.66
1:D:887:GLN:NE2	1:D:980:GLU:O	2.28	0.66
1:A:730:LEU:HD22	1:A:731:PRO:CD	2.21	0.66
1:D:984:LEU:HD21	1:D:986:ILE:HG13	1.78	0.66
1:D:777:LEU:CD1	1:D:980:GLU:HG3	2.26	0.65
1:B:249:GLU:HG2	1:B:251:ARG:HD3	1.76	0.65
5:B:8504:DMS:H12	6:B:4832:HOH:O	1.95	0.65
1:D:262:GLN:NE2	1:D:299:LYS:HD2	2.10	0.65
1:A:135:GLN:HG3	6:A:4816:HOH:O	1.96	0.65
1:C:770:ILE:HD12	1:C:775:GLN:CD	2.17	0.65
1:D:131:GLU:OE1	1:D:134:LEU:HB2	1.97	0.65
1:D:580:GLU:OE1	1:D:580:GLU:HA	1.97	0.65
1:A:1017:GLN:NE2	1:A:1018:LEU:H	1.90	0.65
1:A:130:ASP:C	1:A:130:ASP:OD1	2.36	0.64
1:A:770:ILE:O	1:A:773:LYS:HE2	1.96	0.64
1:C:251:ARG:CB	1:C:251:ARG:HH11	2.09	0.64
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.12	0.64
1:B:75:GLU:OE1	1:B:75:GLU:HA	1.98	0.64
1:A:72:SER:OG	6:A:4467:HOH:O	2.15	0.64
1:A:319:ASP:CB	6:A:4830:HOH:O	2.47	0.63
1:A:778:THR:HG21	6:A:4708:HOH:O	1.99	0.63
1:A:579:ASP:O	1:A:582:GLY:N	2.29	0.63
1:C:576:ILE:HD12	5:C:8411:DMS:C1	2.29	0.63
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.81	0.63
1:A:474:TRP:O	1:A:478:VAL:HG22	1.99	0.63
1:C:696:LEU:HB2	1:C:722:LEU:HD11	1.81	0.62
1:A:655:MET:HE2	1:A:662:PRO:HA	1.80	0.62
1:B:687:GLN:HB3	1:B:688:PRO:HD2	1.80	0.62
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.34	0.62
1:A:737:ILE:O	1:A:737:ILE:HD13	1.99	0.62
1:C:576:ILE:CD1	5:C:8411:DMS:H12	2.29	0.62
1:A:319:ASP:HB2	6:A:4830:HOH:O	1.99	0.62
1:D:416:GLU:OE2	1:D:418:ASN:HB2	2.00	0.62
1:A:759:ASN:OD1	1:A:762:SER:N	2.32	0.62
1:C:643:LEU:HD23	1:C:675:GLN:HE22	1.61	0.62
1:B:54:LEU:HD11	1:B:214:LEU:HG	1.82	0.61
1:C:890:GLN:HG3	1:C:891:VAL:N	2.14	0.61
1:A:73:TRP:HA	1:A:76:CYS:O	1.99	0.61
1:A:292:ARG:HH12	5:A:8412:DMS:C2	2.12	0.61
1:D:618:THR:HG21	6:D:4343:HOH:O	2.00	0.61
1:A:581:ASN:HD22	1:A:583:ASN:ND2	1.97	0.61
1:A:441:THR:O	1:A:445:GLN:HG3	2.00	0.61
1:B:950:GLN:OE1	1:B:952:ARG:HD3	2.00	0.61
1:C:43:ARG:NH1	1:C:264:GLU:OE1	2.28	0.61
1:A:130:ASP:OD1	1:A:131:GLU:N	2.34	0.61
1:B:656:VAL:CG1	1:B:694:LEU:HD22	2.31	0.60
1:D:878:HIS:HD2	6:D:4105:HOH:O	1.83	0.60
1:C:292:ARG:HH12	5:C:8412:DMS:C2	2.13	0.60
1:A:685:LEU:HD23	1:A:686:PRO:CD	2.28	0.60
5:C:8421:DMS:H22	6:C:4539:HOH:O	2.02	0.60
1:A:771:GLY:O	1:A:773:LYS:HD3	2.01	0.60
1:B:675:GLN:HG3	6:B:4808:HOH:O	2.00	0.60
1:A:887:GLN:NE2	1:A:980:GLU:O	2.34	0.60
1:D:241:GLU:HG2	1:D:292:ARG:HG2	1.83	0.60
1:D:800:ARG:NH1	1:D:800:ARG:HB2	2.16	0.60
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.84	0.60
1:B:639:THR:OG1	1:B:677:LYS:HE3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.83	0.60
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.84	0.60
1:D:277:GLU:H	1:D:277:GLU:CD	2.03	0.59
1:A:778:THR:HG23	1:A:887:GLN:HB3	1.84	0.59
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.84	0.59
1:B:369:GLU:CG	1:B:370:GLN:HE22	2.04	0.59
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.68	0.59
1:A:656:VAL:HG21	1:A:685:LEU:HD13	1.84	0.59
1:A:651:LEU:CD2	1:A:703:PRO:HG3	2.27	0.59
1:C:750:GLU:HG3	6:C:4736:HOH:O	2.02	0.59
1:B:844:HIS:ND1	1:B:845:GLN:HG3	2.17	0.59
1:D:71:GLU:CD	1:D:71:GLU:H	2.07	0.59
1:C:844:HIS:HD2	6:C:4824:HOH:O	1.86	0.58
1:C:554:GLN:HG3	6:C:4934:HOH:O	2.01	0.58
1:A:54:LEU:HD11	1:A:214:LEU:HD13	1.86	0.58
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.85	0.58
1:B:277:GLU:HG2	6:B:4822:HOH:O	2.02	0.58
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.04	0.57
1:A:777:LEU:HG	1:A:889:ALA:HA	1.86	0.57
1:A:984:LEU:HD21	1:A:986:ILE:HG13	1.86	0.57
1:B:890:GLN:OE1	1:B:947:GLY:HA3	2.04	0.57
1:D:36:TRP:O	1:D:37:ARG:HD3	2.04	0.57
1:A:878:HIS:HD2	6:A:4073:HOH:O	1.86	0.57
1:C:878:HIS:HD2	6:C:4098:HOH:O	1.87	0.57
1:B:363:HIS:HD2	6:B:4596:HOH:O	1.87	0.57
5:D:8503:DMS:O	6:D:4264:HOH:O	2.15	0.57
1:A:742:THR:HG22	1:A:743:SER:N	2.19	0.57
1:B:689:GLU:O	1:B:690:SER:HB2	2.04	0.57
1:D:773:LYS:HD2	1:D:774:LYS:O	2.05	0.57
1:B:128:ASN:HB2	6:B:4847:HOH:O	2.05	0.57
1:A:685:LEU:O	1:A:687:GLN:OE1	2.23	0.57
1:A:769:TRP:HE1	1:A:774:LYS:HD3	1.70	0.57
1:B:635:THR:HG23	1:B:681:GLU:OE2	2.04	0.56
1:B:646:HIS:ND1	6:B:4823:HOH:O	2.33	0.56
1:A:656:VAL:HG21	1:A:685:LEU:HD11	1.86	0.56
1:B:370:GLN:HB2	6:B:4525:HOH:O	2.05	0.56
1:A:595:THR:HA	1:A:596:PRO:C	2.25	0.56
1:C:662:PRO:O	1:C:663:LEU:HD23	2.06	0.56
1:B:795:VAL:HG12	5:B:8506:DMS:C2	2.32	0.56
1:D:131:GLU:HG3	1:D:135:GLN:OE1	2.05	0.55
1:B:1023:LYS:HD3	1:B:1023:LYS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:LEU:C	1:B:730:LEU:HD13	2.24	0.55
1:D:844:HIS:CE1	1:D:845:GLN:HG2	2.42	0.55
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.89	0.55
1:A:252:ASP:HB2	5:A:8416:DMS:O	2.07	0.55
1:A:655:MET:HB3	1:A:699:ARG:HH22	1.72	0.55
1:B:754:LYS:HE2	1:B:1022:GLN:HG2	1.88	0.55
1:D:131:GLU:OE2	1:D:135:GLN:HG2	2.07	0.55
1:B:890:GLN:O	1:B:890:GLN:HG3	2.02	0.55
1:C:363:HIS:HD2	6:C:4598:HOH:O	1.90	0.55
1:C:367:MET:HE2	1:C:372:MET:HG2	1.89	0.55
1:A:146:VAL:HG11	1:A:150:PHE:CD2	2.41	0.54
1:C:378:LEU:HG	6:C:4568:HOH:O	2.08	0.54
1:D:777:LEU:HD13	1:D:980:GLU:CG	2.36	0.54
1:D:730:LEU:HD23	1:D:731:PRO:CD	2.35	0.54
1:D:625:GLN:NE2	6:D:4231:HOH:O	2.41	0.54
1:C:131:GLU:OE2	1:C:135:GLN:HG3	2.07	0.54
1:B:473:ARG:NH1	6:B:4701:HOH:O	2.24	0.54
1:A:664:ALA:HB3	1:A:685:LEU:HD21	1.88	0.54
1:B:878:HIS:HD2	6:B:4098:HOH:O	1.89	0.54
1:C:251:ARG:HD2	5:C:8416:DMS:O	2.08	0.54
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.23	0.54
1:A:130:ASP:OD2	1:A:132:SER:OG	2.22	0.54
1:D:734:SER:OG	1:D:860:GLY:HA3	2.08	0.54
1:D:1022:GLN:HE21	1:D:1023:LYS:CG	2.21	0.54
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.90	0.53
1:C:630:ARG:NH1	1:C:630:ARG:HB3	2.21	0.53
1:D:675:GLN:HG3	6:D:4777:HOH:O	2.07	0.53
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.43	0.53
1:C:88:SER:HA	1:C:366:VAL:HG21	1.89	0.53
1:D:130:ASP:OD1	1:D:130:ASP:C	2.46	0.53
1:A:866:ILE:O	1:A:1017:GLN:NE2	2.42	0.52
1:D:651:LEU:HD21	1:D:653:HIS:HE1	1.74	0.52
1:B:687:GLN:HA	1:B:687:GLN:NE2	2.23	0.52
1:C:646:HIS:HB3	6:C:4836:HOH:O	2.08	0.52
1:B:595:THR:HA	1:B:596:PRO:C	2.29	0.52
1:C:292:ARG:HH12	5:C:8412:DMS:H23	1.74	0.52
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.91	0.52
1:D:367:MET:HE2	1:D:372:MET:HG2	1.91	0.52
1:B:231:PHE:O	5:B:8417:DMS:H22	2.10	0.52
1:B:581:ASN:HB2	6:B:4827:HOH:O	2.10	0.52
1:D:1022:GLN:HG3	1:D:1023:LYS:CG	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:GLU:HA	1:D:134:LEU:HD12	1.90	0.52
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.92	0.52
1:B:655:MET:HG2	6:B:4962:HOH:O	2.09	0.52
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.92	0.52
1:B:16:TRP:CG	1:B:189:LEU:HD13	2.45	0.52
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.92	0.52
1:A:128:ASN:HB2	1:A:180:GLY:C	2.31	0.52
1:A:79:PRO:HD2	1:A:80:GLU:HG3	1.92	0.52
1:A:502:MET:O	1:A:517:LYS:HE3	2.10	0.52
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.35	0.51
1:A:608:PHE:CE1	1:A:614:HIS:CD2	2.96	0.51
1:D:1022:GLN:NE2	1:D:1023:LYS:CG	2.73	0.51
1:A:577:LYS:O	1:A:584:PRO:HA	2.10	0.51
1:D:725:ASN:HB2	6:D:4779:HOH:O	2.10	0.51
1:D:824:GLN:HG2	1:D:825:CYS:N	2.26	0.51
1:C:640:SER:O	1:C:675:GLN:HA	2.10	0.51
1:A:769:TRP:CE2	1:A:774:LYS:HD3	2.45	0.51
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.93	0.51
1:C:319:ASP:OD1	1:C:319:ASP:C	2.49	0.51
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.91	0.51
1:C:859:ASP:OD1	1:C:861:SER:OG	2.25	0.51
1:B:292:ARG:NH1	5:B:8412:DMS:C2	2.73	0.51
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.26	0.51
1:D:579:ASP:O	1:D:582:GLY:N	2.43	0.51
1:C:595:THR:HA	1:C:596:PRO:C	2.32	0.51
1:C:651:LEU:HD11	1:C:667:GLU:HG2	1.92	0.50
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.41	0.50
1:D:338:GLU:HG2	6:D:4707:HOH:O	2.10	0.50
1:C:131:GLU:OE1	1:C:131:GLU:O	2.29	0.50
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.92	0.50
1:B:817:GLN:HG2	6:B:4364:HOH:O	2.11	0.50
1:C:809:ARG:NH2	1:C:1001:PRO:CG	2.74	0.50
1:A:131:GLU:HG2	1:A:135:GLN:NE2	2.26	0.50
1:C:772:ASP:OD1	1:C:772:ASP:N	2.40	0.50
1:B:685:LEU:O	1:B:686:PRO:O	2.29	0.50
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.93	0.50
1:D:595:THR:HA	1:D:596:PRO:C	2.32	0.50
1:C:431:ARG:HD2	6:C:4776:HOH:O	2.12	0.50
1:B:370:GLN:CA	1:B:370:GLN:NE2	2.74	0.50
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.46	0.50
1:A:93:HIS:CD2	5:A:8414:DMS:H11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:SER:HA	1:B:366:VAL:HG21	1.94	0.50
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.12	0.50
1:A:16:TRP:CD2	1:A:189:LEU:CD1	2.94	0.50
1:C:730:LEU:O	1:C:731:PRO:O	2.30	0.50
1:A:863:GLN:HE22	1:A:952:ARG:NH2	2.10	0.49
1:B:1013:ARG:NH1	6:B:4014:HOH:O	2.28	0.49
1:A:579:ASP:CG	1:A:583:ASN:HB2	2.31	0.49
1:B:583:ASN:ND2	6:B:4827:HOH:O	2.27	0.49
1:A:26:ARG:NH1	1:A:169:SER:OG	2.37	0.49
1:D:1022:GLN:HE21	1:D:1023:LYS:HG2	1.78	0.49
1:D:1022:GLN:CG	1:D:1023:LYS:HG3	2.40	0.49
1:C:685:LEU:HD23	1:C:686:PRO:HD3	1.91	0.49
1:B:777:LEU:HD13	1:B:980:GLU:HG2	1.91	0.49
1:B:730:LEU:CD1	1:B:730:LEU:N	2.76	0.49
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.94	0.49
1:A:77:ASP:HB2	6:A:4314:HOH:O	2.12	0.49
1:B:292:ARG:HH12	5:B:8412:DMS:H22	1.77	0.49
1:A:691:ALA:HA	1:A:725:ASN:HB2	1.93	0.49
1:A:653:HIS:HD2	1:A:667:GLU:HG2	1.77	0.49
1:A:658:LEU:O	1:A:661:LYS:HE2	2.12	0.49
1:A:338:GLU:HG2	6:A:4661:HOH:O	2.12	0.49
1:B:600:GLN:N	1:B:600:GLN:HE21	1.97	0.49
1:A:428:ASP:O	5:A:8420:DMS:H23	2.13	0.49
1:B:753:ASN:OD1	1:B:753:ASN:N	2.42	0.49
1:C:251:ARG:NH1	5:C:8416:DMS:O	2.46	0.49
1:C:682:LEU:CB	1:C:683:PRO:HD2	2.42	0.49
1:B:696:LEU:HB2	1:B:722:LEU:HD11	1.94	0.49
1:C:653:HIS:CE1	1:C:667:GLU:CG	2.91	0.48
1:D:37:ARG:NH2	1:D:218:PRO:HD3	2.27	0.48
1:C:147:ASN:HA	1:C:148:SER:HA	1.67	0.48
1:D:730:LEU:HG	1:D:731:PRO:CD	2.39	0.48
1:A:319:ASP:HB3	6:A:4830:HOH:O	2.10	0.48
1:D:800:ARG:NH1	1:D:800:ARG:CB	2.75	0.48
1:A:85:VAL:O	1:A:88:SER:HB3	2.12	0.48
1:D:130:ASP:OD1	1:D:132:SER:OG	2.25	0.48
1:A:255:ARG:HB2	1:A:316:HIS:CE1	2.48	0.48
1:A:264:GLU:HG3	6:A:4747:HOH:O	2.12	0.48
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.48	0.48
1:C:830:LEU:N	1:C:833:ALA:O	2.34	0.48
1:B:1022:GLN:HG3	1:B:1022:GLN:O	2.12	0.48
1:B:251:ARG:HA	5:B:8416:DMS:S	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:VAL:HG23	1:B:728:VAL:O	2.14	0.48
1:D:734:SER:HA	1:D:735:HIS:CE1	2.49	0.48
1:A:78:LEU:HB2	1:A:81:ALA:HB2	1.95	0.48
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.95	0.48
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.94	0.48
1:A:173:LEU:O	1:A:176:PHE:N	2.42	0.48
1:D:965:GLN:O	1:D:969:GLU:HG3	2.14	0.48
1:D:79:PRO:HG2	1:D:80:GLU:OE2	2.14	0.47
1:D:821:ALA:N	1:D:841:ALA:O	2.43	0.47
1:A:844:HIS:ND1	1:A:845:GLN:HG2	2.30	0.47
1:D:373:VAL:O	1:D:377:LEU:HG	2.14	0.47
1:A:380:LYS:O	5:A:8403:DMS:H13	2.14	0.47
1:D:26:ARG:HD2	1:D:169:SER:HA	1.95	0.47
1:A:580:GLU:OE2	1:A:580:GLU:HA	2.13	0.47
1:A:416:GLU:OE2	1:A:418:ASN:HB2	2.15	0.47
1:B:102:ASN:HD22	5:B:8506:DMS:C1	2.28	0.47
1:D:37:ARG:HG2	1:D:50:GLN:NE2	2.29	0.47
1:C:687:GLN:CG	1:C:688:PRO:HD2	2.44	0.47
1:D:742:THR:CG2	1:D:743:SER:N	2.78	0.47
1:A:824:GLN:HG2	1:A:825:CYS:N	2.28	0.47
1:D:734:SER:HA	1:D:735:HIS:ND1	2.29	0.47
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.49	0.47
1:C:689:GLU:O	1:C:690:SER:HB3	2.15	0.47
1:C:576:ILE:CD1	5:C:8411:DMS:C1	2.92	0.47
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.96	0.47
1:D:762:SER:OG	1:D:763:GLY:N	2.46	0.47
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.97	0.47
1:B:732:ALA:O	1:B:734:SER:HB3	2.15	0.47
1:B:71:GLU:OE1	1:B:71:GLU:N	2.48	0.47
1:A:664:ALA:CB	1:A:685:LEU:HD21	2.45	0.46
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.96	0.46
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.97	0.46
1:B:380:LYS:O	5:B:8403:DMS:H13	2.16	0.46
1:D:986:ILE:HD12	1:D:986:ILE:HG21	1.44	0.46
1:A:16:TRP:CG	1:A:189:LEU:CD1	2.98	0.46
1:A:687:GLN:HA	1:A:688:PRO:HD3	1.78	0.46
1:A:1017:GLN:C	1:A:1017:GLN:HE21	2.12	0.46
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.97	0.46
1:D:429:ASP:OD1	1:D:431:ARG:HG3	2.15	0.46
1:A:167:LEU:HB3	1:A:168:PRO:HD2	1.98	0.46
1:A:607:VAL:HG12	1:A:613:PRO:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:LEU:HD12	1:B:682:LEU:HA	1.59	0.46
1:A:521:LYS:HE3	6:A:4416:HOH:O	2.16	0.46
1:D:76:CYS:O	1:D:77:ASP:C	2.53	0.46
1:D:230:ARG:NH2	4:D:2003:IPT:O6	2.42	0.46
1:D:843:GLN:HA	1:D:847:LYS:O	2.16	0.46
1:D:749:ILE:N	1:D:749:ILE:CD1	2.78	0.46
1:A:145:GLY:N	1:A:210:ARG:HB2	2.31	0.46
1:A:599:ARG:HB2	1:A:600:GLN:HE21	1.82	0.45
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.50	0.45
1:B:658:LEU:O	1:B:661:LYS:HE3	2.16	0.45
1:D:748:CYS:C	1:D:749:ILE:HD12	2.36	0.45
1:D:292:ARG:C	1:D:293:LEU:HD12	2.37	0.45
1:C:13:ARG:O	1:C:14:ARG:C	2.53	0.45
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.98	0.45
4:C:2004:IPT:H1	4:C:2004:IPT:H3'3	1.55	0.45
1:B:369:GLU:CG	1:B:370:GLN:NE2	2.73	0.45
1:A:737:ILE:HD13	1:A:737:ILE:C	2.37	0.45
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.97	0.45
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.34	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.64	0.45
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.63	0.45
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.98	0.45
1:C:251:ARG:HD2	1:C:251:ARG:HA	1.76	0.45
1:D:984:LEU:CD2	1:D:986:ILE:HG13	2.46	0.45
1:B:595:THR:HG22	5:B:8413:DMS:S	2.56	0.45
1:C:1022:GLN:N	1:C:1022:GLN:NE2	2.65	0.45
1:A:832:ASP:N	1:A:832:ASP:OD1	2.48	0.45
1:C:651:LEU:HD11	1:C:653:HIS:HE1	1.76	0.45
1:C:131:GLU:HG3	1:C:135:GLN:NE2	2.31	0.45
1:B:906:TYR:CZ	1:B:937:LEU:HB2	2.52	0.45
1:C:608:PHE:CZ	1:C:614:HIS:CD2	3.05	0.45
1:B:867:THR:HG23	6:B:4435:HOH:O	2.17	0.45
1:A:59:ARG:NH2	1:A:81:ALA:O	2.50	0.45
1:D:809:ARG:NH2	1:D:1001:PRO:CG	2.80	0.45
1:A:754:LYS:NZ	6:A:4752:HOH:O	2.28	0.45
1:C:630:ARG:CB	1:C:630:ARG:NH1	2.79	0.45
1:B:687:GLN:HA	1:B:688:PRO:HD3	1.82	0.45
1:A:742:THR:CG2	1:A:743:SER:N	2.80	0.45
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.52	0.45
1:B:896:ASN:HB3	1:B:945:ASN:HB2	1.98	0.45
1:D:651:LEU:HD23	1:D:653:HIS:HE1	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:640:SER:O	1:B:675:GLN:HA	2.17	0.45
1:B:542:MET:HA	1:B:604:ASN:HA	1.98	0.45
1:A:739:HIS:CD2	6:A:4777:HOH:O	2.69	0.45
1:D:696:LEU:O	1:D:719:GLN:HB3	2.17	0.45
1:A:581:ASN:ND2	1:A:583:ASN:HD22	2.11	0.44
1:A:80:GLU:H	1:A:80:GLU:HG3	1.36	0.44
1:C:457:SER:HA	1:C:485:GLN:O	2.17	0.44
1:A:769:TRP:HA	1:A:773:LYS:O	2.17	0.44
1:D:800:ARG:CB	1:D:800:ARG:HH11	2.31	0.44
1:A:299:LYS:HE2	1:A:299:LYS:HA	1.98	0.44
1:B:291:LEU:HD22	1:B:291:LEU:N	2.32	0.44
1:C:906:TYR:CZ	1:C:937:LEU:HB2	2.52	0.44
1:C:737:ILE:HD12	1:C:738:PRO:CD	2.11	0.44
1:A:724:GLU:O	1:B:847:LYS:NZ	2.50	0.44
1:D:232:ASN:C	5:D:8417:DMS:H21	2.38	0.44
1:B:730:LEU:O	1:B:731:PRO:O	2.36	0.44
1:A:768:MET:CE	1:A:1020:TRP:CH2	3.00	0.44
1:C:768:MET:CE	1:C:776:LEU:HD11	2.47	0.44
1:D:241:GLU:HG3	6:D:4835:HOH:O	2.16	0.44
1:C:524:LEU:HD11	1:C:562:LEU:HG	1.99	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.62	0.44
1:B:513:PRO:O	1:B:514:ALA:HB3	2.17	0.44
1:D:139:THR:OG1	1:D:216:HIS:HD2	2.00	0.44
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.44
1:C:54:LEU:HD11	1:C:214:LEU:HD13	1.98	0.44
1:D:619:GLU:HA	1:D:912:ALA:HB2	1.99	0.44
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.64	0.44
1:D:458:LEU:HD11	1:D:472:TYR:HB2	2.00	0.44
1:B:873:ALA:O	1:B:876:THR:HG22	2.17	0.44
1:D:215:LEU:HD21	1:D:217:LYS:HD3	2.00	0.44
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.99	0.44
1:A:817:GLN:HB3	1:A:817:GLN:HE21	1.47	0.44
4:B:2001:IPT:C3'	5:B:8506:DMS:C2	2.96	0.44
1:A:634:GLN:CB	1:A:682:LEU:HB2	2.42	0.44
1:A:739:HIS:HD2	6:A:4777:HOH:O	2.00	0.44
1:A:654:TRP:CZ3	1:A:665:SER:HA	2.53	0.44
1:D:630:ARG:NE	1:D:637:GLU:OE1	2.50	0.44
1:B:754:LYS:CE	1:B:1022:GLN:HG2	2.48	0.43
1:D:111:PRO:HA	1:D:112:PRO:HA	1.64	0.43
1:B:651:LEU:HD13	1:B:703:PRO:HG3	2.00	0.43
1:D:737:ILE:HG13	1:D:738:PRO:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASN:ND2	5:B:8506:DMS:H13	2.33	0.43
1:D:1022:GLN:NE2	1:D:1023:LYS:HG3	2.32	0.43
1:B:416:GLU:OE2	1:B:418:ASN:HB2	2.19	0.43
1:D:577:LYS:O	1:D:584:PRO:HA	2.17	0.43
1:B:373:VAL:O	1:B:377:LEU:HG	2.18	0.43
1:C:824:GLN:O	1:C:838:THR:HA	2.18	0.43
1:D:651:LEU:CD2	1:D:653:HIS:CE1	2.93	0.43
1:C:873:ALA:O	1:C:876:THR:HG22	2.18	0.43
1:B:801:ILE:HD12	1:B:808:GLU:CD	2.39	0.43
1:C:375:ASP:O	1:C:379:MET:HG3	2.19	0.43
1:D:780:LEU:HA	1:D:886:CYS:HB3	2.00	0.43
1:A:91:GLN:OE1	1:A:205:MET:HB3	2.18	0.43
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.54	0.43
1:C:847:LYS:NZ	1:D:724:GLU:O	2.52	0.43
1:D:88:SER:HA	1:D:366:VAL:HG21	2.01	0.43
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.53	0.43
1:C:128:ASN:HA	1:C:180:GLY:O	2.19	0.43
5:D:8406:DMS:H22	6:D:4678:HOH:O	2.17	0.43
1:A:141:ILE:HA	1:A:213:SER:O	2.19	0.43
1:B:730:LEU:HD12	1:B:730:LEU:H	1.84	0.43
1:A:608:PHE:CD1	1:A:614:HIS:HD2	2.37	0.43
1:C:579:ASP:HB2	1:C:580:GLU:OE2	2.18	0.43
1:D:613:PRO:HB3	1:D:617:LEU:HD23	2.01	0.43
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.53	0.43
1:C:577:LYS:HE3	1:C:577:LYS:HB3	1.61	0.43
1:A:147:ASN:HA	1:A:165:SER:OG	2.19	0.43
1:A:599:ARG:HD2	1:A:600:GLN:NE2	2.34	0.43
1:B:102:ASN:ND2	5:B:8506:DMS:C1	2.82	0.43
1:B:809:ARG:CG	1:B:809:ARG:NH1	2.73	0.42
1:D:742:THR:HG22	1:D:743:SER:N	2.34	0.42
1:A:655:MET:HE2	1:A:663:LEU:H	1.84	0.42
1:A:777:LEU:HD23	1:A:777:LEU:HA	1.83	0.42
1:A:143:PHE:O	1:A:168:PRO:HA	2.20	0.42
1:C:430:PRO:HD3	5:C:8420:DMS:H23	2.01	0.42
1:D:74:LEU:HA	1:D:74:LEU:HD23	1.68	0.42
1:D:93:HIS:CD2	5:D:8414:DMS:C2	3.02	0.42
1:C:533:LEU:C	1:C:533:LEU:HD23	2.40	0.42
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.55	0.42
1:A:901:GLY:HA3	1:A:902:PRO:HA	1.73	0.42
1:A:771:GLY:O	1:A:772:ASP:HB2	2.20	0.42
1:B:13:ARG:NH2	1:C:13:ARG:HB2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ASN:O	1:B:527:PRO:HB3	2.20	0.42
1:A:640:SER:O	1:A:675:GLN:HA	2.20	0.42
1:A:379:MET:CE	1:A:407:LEU:HD13	2.50	0.42
1:A:47:PRO:HA	5:A:8501:DMS:O	2.19	0.42
1:C:390:SER:HA	1:C:391:HIS:HA	1.90	0.42
1:B:224:ASP:OD2	6:B:4836:HOH:O	2.22	0.42
1:C:733:ALA:O	1:C:735:HIS:CE1	2.73	0.42
1:B:730:LEU:HD22	1:B:730:LEU:C	2.40	0.42
1:A:984:LEU:HD11	1:A:986:ILE:HG12	2.01	0.42
1:B:181:GLU:CB	6:B:4882:HOH:O	2.67	0.42
1:A:843:GLN:HB3	1:A:847:LYS:O	2.19	0.42
1:D:100:TYR:HB3	1:D:589:GLY:HA2	2.02	0.42
5:C:8408:DMS:H12	6:C:4685:HOH:O	2.20	0.42
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.55	0.42
1:C:986:ILE:HG21	1:C:986:ILE:HD12	1.69	0.42
1:A:784:PHE:HA	1:A:881:ARG:O	2.20	0.42
1:C:739:HIS:HE1	1:C:741:THR:OG1	2.03	0.42
1:D:777:LEU:HA	1:D:777:LEU:HD23	1.90	0.42
1:A:131:GLU:HB3	1:A:135:GLN:NE2	2.35	0.42
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.49	0.42
1:C:131:GLU:OE2	1:C:135:GLN:NE2	2.49	0.42
1:D:584:PRO:HD2	6:D:4693:HOH:O	2.19	0.42
1:D:166:ARG:HG3	1:D:392:TYR:HB2	2.01	0.42
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.54	0.42
1:B:901:GLY:HA3	1:B:902:PRO:HA	1.77	0.42
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.55	0.42
1:B:749:ILE:HD13	1:B:858:ILE:HD12	2.00	0.42
1:D:256:VAL:O	1:D:271:THR:HA	2.20	0.42
1:A:655:MET:HE2	1:A:662:PRO:CA	2.48	0.42
1:B:784:PHE:HA	1:B:881:ARG:O	2.20	0.42
1:B:770:ILE:HD12	1:B:775:GLN:CD	2.41	0.42
1:D:316:HIS:HB2	1:D:321:THR:O	2.19	0.41
1:D:79:PRO:CD	1:D:80:GLU:OE2	2.68	0.41
1:A:952:ARG:HG3	1:A:952:ARG:HH11	1.84	0.41
1:C:673:ALA:O	1:C:674:PRO:C	2.56	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.74	0.41
1:A:301:TRP:CH2	1:A:452:SER:HA	2.55	0.41
1:D:699:ARG:HH12	5:D:8415:DMS:C1	2.33	0.41
1:C:615:PRO:O	1:C:618:THR:HG22	2.19	0.41
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.94	0.41
1:D:800:ARG:HB2	1:D:800:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:LEU:CD2	1:A:986:ILE:HG13	2.49	0.41
1:B:824:GLN:O	1:B:838:THR:HA	2.19	0.41
5:A:8415:DMS:C1	6:A:4769:HOH:O	2.68	0.41
1:A:655:MET:CE	1:A:662:PRO:HB3	2.51	0.41
1:B:804:ASN:HD21	1:B:809:ARG:HH21	1.64	0.41
1:A:599:ARG:HB2	1:A:600:GLN:NE2	2.35	0.41
1:A:319:ASP:OD2	6:A:4764:HOH:O	2.22	0.41
1:A:593:GLY:O	1:A:595:THR:HG22	2.20	0.41
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.55	0.41
1:D:85:VAL:HG12	1:D:86:VAL:N	2.35	0.41
1:C:977:HIS:O	1:C:977:HIS:CD2	2.73	0.41
1:C:765:LEU:HD21	1:C:768:MET:CE	2.50	0.41
1:D:787:ALA:HA	1:D:968:MET:HE2	2.02	0.41
1:D:576:ILE:HA	1:D:576:ILE:HD13	1.77	0.41
1:A:253:TYR:CD1	1:A:253:TYR:C	2.94	0.41
1:D:799:THR:HG23	1:D:799:THR:O	2.18	0.41
1:A:132:SER:HA	1:A:135:GLN:CG	2.50	0.41
1:A:861:SER:OG	1:A:863:GLN:HG3	2.21	0.41
1:A:71:GLU:O	1:A:72:SER:C	2.58	0.41
1:D:138:GLN:O	1:D:216:HIS:HA	2.21	0.41
1:D:464:HIS:HB2	1:D:489:GLY:HA3	2.02	0.41
1:A:804:ASN:O	1:A:809:ARG:HD2	2.20	0.41
1:A:125:LEU:O	1:A:183:ARG:HA	2.21	0.41
1:A:127:PHE:N	1:A:127:PHE:CD2	2.88	0.41
1:A:844:HIS:CE1	1:A:845:GLN:HG2	2.54	0.41
1:B:291:LEU:CD2	1:B:291:LEU:N	2.83	0.41
1:D:581:ASN:HD22	1:D:583:ASN:ND2	2.18	0.41
1:C:989:PHE:N	1:C:989:PHE:CD1	2.89	0.41
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.38	0.41
1:D:262:GLN:NE2	1:D:299:LYS:CD	2.82	0.41
1:A:986:ILE:HG23	1:A:986:ILE:HD13	1.63	0.41
1:B:817:GLN:HG2	1:B:817:GLN:H	1.52	0.41
1:C:977:HIS:CG	1:C:977:HIS:O	2.74	0.41
1:C:784:PHE:HA	1:C:881:ARG:O	2.20	0.41
1:C:907:PRO:HG2	1:C:990:HIS:O	2.21	0.41
1:A:140:ARG:HG2	1:A:215:LEU:HB3	2.01	0.41
1:C:800:ARG:CZ	1:C:801:ILE:O	2.69	0.41
1:A:200:GLN:HG2	1:A:391:HIS:HB2	2.01	0.41
1:C:246:MET:HB3	1:C:274:PHE:CZ	2.55	0.41
1:D:362:LEU:HA	1:D:362:LEU:HD23	1.84	0.41
1:D:734:SER:C	1:D:736:ALA:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:ARG:CB	1:A:800:ARG:CZ	2.97	0.41
1:B:277:GLU:H	1:B:277:GLU:HG2	1.53	0.41
1:A:262:GLN:HA	1:A:262:GLN:OE1	2.21	0.41
1:D:246:MET:SD	1:D:246:MET:C	3.00	0.41
1:A:703:PRO:O	1:A:711:ALA:HB1	2.20	0.41
1:D:78:LEU:HA	1:D:79:PRO:HD2	1.81	0.41
1:C:768:MET:HE2	1:C:776:LEU:HD11	2.03	0.41
1:D:737:ILE:HD12	1:D:738:PRO:HD2	2.03	0.41
6:B:4763:HOH:O	5:C:8420:DMS:H21	2.21	0.41
1:B:652:LEU:O	1:B:667:GLU:HA	2.21	0.41
1:C:24:LEU:HB2	1:C:161:TYR:HB3	2.01	0.41
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.56	0.41
1:A:782:ASP:HA	1:A:884:LEU:HD23	2.02	0.41
1:A:883:GLY:HA3	1:A:987:ASP:HA	2.03	0.41
1:B:844:HIS:CE1	1:B:845:GLN:CG	3.00	0.41
1:A:142:ILE:HG23	1:A:170:GLU:HG2	2.01	0.41
1:A:18:ASN:C	1:A:20:GLY:H	2.24	0.41
1:A:576:ILE:CD1	5:A:8411:DMS:S	3.09	0.41
1:A:30:HIS:HB2	1:A:31:PRO:HD2	2.04	0.40
1:A:507:ASP:O	4:B:2004:IPT:H2	2.21	0.40
1:A:635:THR:HA	1:A:680:ILE:O	2.21	0.40
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.57	0.40
1:B:746:ASP:HA	1:B:760:ARG:HG3	2.03	0.40
4:B:2001:IPT:H3'2	5:B:8506:DMS:H13	2.03	0.40
1:C:882:ILE:CD1	1:C:1014:TYR:CD1	3.04	0.40
1:A:608:PHE:CD1	1:A:614:HIS:CD2	3.09	0.40
1:D:102:ASN:C	1:D:102:ASN:OD1	2.60	0.40
1:A:131:GLU:HB3	1:A:135:GLN:HE21	1.86	0.40
1:B:1023:LYS:N	1:B:1023:LYS:CD	2.84	0.40
1:C:663:LEU:HA	1:C:663:LEU:HD22	1.87	0.40
1:B:778:THR:HG23	1:B:779:PRO:HD2	2.02	0.40
1:B:518:TRP:O	1:B:519:SER:C	2.60	0.40
1:B:825:CYS:HA	1:B:837:THR:O	2.21	0.40
1:A:279:ILE:HD13	1:A:284:GLY:HA2	2.03	0.40
1:D:78:LEU:O	1:D:79:PRO:C	2.59	0.40
1:B:655:MET:HB3	6:B:4962:HOH:O	2.21	0.40
1:A:225:PHE:HA	1:A:243:GLU:O	2.21	0.40
1:B:767:GLN:HG3	1:B:768:MET:N	2.37	0.40
1:D:19:PRO:HA	1:D:193:ASP:OD1	2.22	0.40
1:B:687:GLN:CD	1:B:687:GLN:N	2.75	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	959 (95%)	49 (5%)	1 (0%)	56	38
1	B	1009/1023 (99%)	967 (96%)	35 (4%)	7 (1%)	26	11
1	C	1009/1023 (99%)	973 (96%)	34 (3%)	2 (0%)	52	35
1	D	1009/1023 (99%)	976 (97%)	30 (3%)	3 (0%)	46	29
All	All	4036/4092 (99%)	3875 (96%)	148 (4%)	13 (0%)	46	29

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	686	PRO
1	B	731	PRO
1	B	735	HIS
1	C	731	PRO
1	D	688	PRO
1	B	732	ALA
1	B	733	ALA
1	A	688	PRO
1	C	164	ASP
1	D	735	HIS
1	B	690	SER
1	D	164	ASP
1	B	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	864/875 (99%)	818 (95%)	46 (5%)	28	11
1	B	864/875 (99%)	827 (96%)	37 (4%)	35	17
1	C	864/875 (99%)	832 (96%)	32 (4%)	41	23
1	D	864/875 (99%)	822 (95%)	42 (5%)	31	13
All	All	3456/3500 (99%)	3299 (96%)	157 (4%)	34	16

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	72	SER
1	A	75	GLU
1	A	76	CYS
1	A	80	GLU
1	A	128	ASN
1	A	130	ASP
1	A	131	GLU
1	A	178	ARG
1	A	246	MET
1	A	262	GLN
1	A	279	ILE
1	A	319	ASP
1	A	333	ARG
1	A	344	LEU
1	A	394	ASN
1	A	418	ASN
1	A	437	SER
1	A	473	ARG
1	A	519	SER
1	A	580	GLU
1	A	581	ASN
1	A	595	THR
1	A	600	GLN
1	A	634	GLN
1	A	655	MET
1	A	663	LEU
1	A	672	VAL
1	A	684	GLU
1	A	689	GLU
1	A	699	ARG
1	A	725	ASN
1	A	729	THR

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Mol	Chain	Res	Type
1	A	730	LEU
1	A	735	HIS
1	A	737	ILE
1	A	761	GLN
1	A	778	THR
1	A	799	THR
1	A	800	ARG
1	A	817	GLN
1	A	890	GLN
1	A	910	LEU
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	40	GLU
1	B	49	GLN
1	B	71	GLU
1	B	75	GLU
1	B	291	LEU
1	B	333	ARG
1	B	344	LEU
1	B	370	GLN
1	B	394	ASN
1	B	418	ASN
1	B	477	SER
1	B	519	SER
1	B	535	LEU
1	B	546	LEU
1	B	600	GLN
1	B	646	HIS
1	B	651	LEU
1	B	681	GLU
1	B	682	LEU
1	B	685	LEU
1	B	687	GLN
1	B	689	GLU
1	B	730	LEU
1	B	745	MET
1	B	755	ARG
1	B	768	MET
1	B	773	LYS
1	B	799	THR
1	B	817	GLN

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Mol	Chain	Res	Type
1	B	829	THR
1	B	857	ARG
1	B	867	THR
1	B	890	GLN
1	B	893	GLU
1	B	956	GLN
1	B	1022	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	80	GLU
1	C	131	GLU
1	C	214	LEU
1	C	241	GLU
1	C	251	ARG
1	C	262	GLN
1	C	264	GLU
1	C	277	GLU
1	C	333	ARG
1	C	344	LEU
1	C	370	GLN
1	C	394	ASN
1	C	418	ASN
1	C	519	SER
1	C	535	LEU
1	C	576	ILE
1	C	634	GLN
1	C	651	LEU
1	C	653	HIS
1	C	663	LEU
1	C	681	GLU
1	C	684	GLU
1	C	687	GLN
1	C	728	VAL
1	C	730	LEU
1	C	737	ILE
1	C	772	ASP
1	C	773	LYS
1	C	800	ARG
1	C	824	GLN
1	C	986	ILE
1	D	72	SER
1	D	75	GLU

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Mol	Chain	Res	Type
1	D	80	GLU
1	D	128	ASN
1	D	129	VAL
1	D	130	ASP
1	D	135	GLN
1	D	177	LEU
1	D	217	LYS
1	D	279	ILE
1	D	319	ASP
1	D	333	ARG
1	D	344	LEU
1	D	370	GLN
1	D	394	ASN
1	D	418	ASN
1	D	546	LEU
1	D	581	ASN
1	D	634	GLN
1	D	652	LEU
1	D	655	MET
1	D	685	LEU
1	D	687	GLN
1	D	699	ARG
1	D	719	GLN
1	D	730	LEU
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	741	THR
1	D	743	SER
1	D	744	GLU
1	D	745	MET
1	D	750	GLU
1	D	761	GLN
1	D	773	LYS
1	D	801	ILE
1	D	847	LYS
1	D	986	ILE
1	D	1017	GLN
1	D	1022	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	583	ASN
1	A	600	GLN
1	A	653	HIS
1	A	675	GLN
1	A	687	GLN
1	A	702	GLN
1	A	739	HIS
1	A	804	ASN
1	A	817	GLN
1	A	863	GLN
1	A	878	HIS
1	A	977	HIS
1	A	1017	GLN
1	B	102	ASN
1	B	363	HIS
1	B	370	GLN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	687	GLN
1	B	702	GLN
1	B	757	GLN
1	B	804	ASN
1	B	817	GLN
1	B	878	HIS
1	B	1022	GLN
1	C	363	HIS
1	C	370	GLN
1	C	394	ASN
1	C	554	GLN
1	C	675	GLN
1	C	702	GLN
1	C	735	HIS
1	C	739	HIS
1	C	878	HIS
1	D	216	HIS
1	D	262	GLN
1	D	266	GLN
1	D	581	ASN
1	D	628	GLN
1	D	653	HIS
1	D	824	GLN

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Mol	Chain	Res	Type
1	D	878	HIS
1	D	903	GLN
1	D	977	HIS
1	D	1017	GLN
1	D	1022	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 141 ligands modelled in this entry, 32 are monoatomic - leaving 109 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	IPT	A	2001	3	15,15,15	0.73	0	19,21,21	1.17	1 (5%)
4	IPT	A	2002	-	15,15,15	1.02	1 (6%)	19,21,21	1.29	2 (10%)
4	IPT	A	2003	-	15,15,15	0.63	0	19,21,21	2.05	3 (15%)
5	DMS	A	8401	-	3,3,3	0.59	0	3,3,3	0.20	0
5	DMS	A	8402	-	3,3,3	1.66	1 (33%)	3,3,3	0.27	0
5	DMS	A	8403	-	3,3,3	1.72	1 (33%)	3,3,3	1.18	1 (33%)
5	DMS	A	8404	-	3,3,3	0.63	0	3,3,3	0.56	0
5	DMS	A	8405	-	3,3,3	0.64	0	3,3,3	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8406	-	3,3,3	0.53	0	3,3,3	0.38	0
5	DMS	A	8407	-	3,3,3	1.23	0	3,3,3	0.25	0
5	DMS	A	8408	-	3,3,3	0.51	0	3,3,3	0.18	0
5	DMS	A	8409	-	3,3,3	2.38	1 (33%)	3,3,3	0.27	0
5	DMS	A	8410	-	3,3,3	0.74	0	3,3,3	0.13	0
5	DMS	A	8411	-	3,3,3	0.76	0	3,3,3	0.20	0
5	DMS	A	8412	-	3,3,3	0.43	0	3,3,3	0.27	0
5	DMS	A	8413	-	3,3,3	2.17	1 (33%)	3,3,3	0.31	0
5	DMS	A	8414	-	3,3,3	0.91	0	3,3,3	0.52	0
5	DMS	A	8415	-	3,3,3	1.38	0	3,3,3	0.57	0
5	DMS	A	8416	-	3,3,3	0.89	0	3,3,3	0.24	0
5	DMS	A	8417	-	3,3,3	1.03	0	3,3,3	0.34	0
5	DMS	A	8419	-	3,3,3	0.60	0	3,3,3	0.34	0
5	DMS	A	8420	-	3,3,3	0.91	0	3,3,3	0.23	0
5	DMS	A	8421	-	3,3,3	0.85	0	3,3,3	0.21	0
5	DMS	A	8423	-	3,3,3	1.62	1 (33%)	3,3,3	0.16	0
5	DMS	A	8501	-	3,3,3	0.87	0	3,3,3	0.31	0
5	DMS	A	8502	-	3,3,3	2.00	1 (33%)	3,3,3	0.63	0
5	DMS	A	8504	-	3,3,3	0.63	0	3,3,3	0.13	0
4	IPT	B	2001	3	15,15,15	0.71	0	19,21,21	0.89	1 (5%)
4	IPT	B	2003	-	15,15,15	0.79	0	19,21,21	1.27	2 (10%)
4	IPT	B	2004	-	15,15,15	0.69	0	19,21,21	1.60	3 (15%)
5	DMS	B	8401	-	3,3,3	0.82	0	3,3,3	1.28	1 (33%)
5	DMS	B	8402	-	3,3,3	0.82	0	3,3,3	0.33	0
5	DMS	B	8403	-	3,3,3	1.40	1 (33%)	3,3,3	0.76	0
5	DMS	B	8404	-	3,3,3	1.26	1 (33%)	3,3,3	1.27	1 (33%)
5	DMS	B	8405	-	3,3,3	1.43	1 (33%)	3,3,3	0.50	0
5	DMS	B	8406	-	3,3,3	0.80	0	3,3,3	0.18	0
5	DMS	B	8407	-	3,3,3	1.82	1 (33%)	3,3,3	0.46	0
5	DMS	B	8408	-	3,3,3	1.31	0	3,3,3	0.38	0
5	DMS	B	8409	-	3,3,3	2.34	1 (33%)	3,3,3	0.47	0
5	DMS	B	8410	-	3,3,3	1.67	1 (33%)	3,3,3	0.55	0
5	DMS	B	8411	-	3,3,3	0.94	0	3,3,3	0.62	0
5	DMS	B	8412	-	3,3,3	0.87	0	3,3,3	0.54	0
5	DMS	B	8413	-	3,3,3	1.18	0	3,3,3	0.59	0
5	DMS	B	8414	-	3,3,3	1.32	1 (33%)	3,3,3	1.06	0
5	DMS	B	8415	-	3,3,3	1.65	1 (33%)	3,3,3	0.47	0
5	DMS	B	8416	-	3,3,3	0.66	0	3,3,3	0.73	0
5	DMS	B	8417	-	3,3,3	1.50	1 (33%)	3,3,3	1.80	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8420	-	3,3,3	2.43	2 (66%)	3,3,3	0.55	0
5	DMS	B	8421	-	3,3,3	0.55	0	3,3,3	0.49	0
5	DMS	B	8423	-	3,3,3	1.73	1 (33%)	3,3,3	0.52	0
5	DMS	B	8425	3	3,3,3	1.08	0	3,3,3	0.20	0
5	DMS	B	8427	-	3,3,3	0.76	0	3,3,3	0.21	0
5	DMS	B	8501	-	3,3,3	1.47	1 (33%)	3,3,3	0.37	0
5	DMS	B	8502	-	3,3,3	1.29	1 (33%)	3,3,3	1.08	0
5	DMS	B	8504	-	3,3,3	0.41	0	3,3,3	0.19	0
5	DMS	B	8506	-	3,3,3	1.59	1 (33%)	3,3,3	0.41	0
4	IPT	C	2001	3	15,15,15	0.64	0	19,21,21	1.14	1 (5%)
4	IPT	C	2003	-	15,15,15	0.70	0	19,21,21	1.43	3 (15%)
4	IPT	C	2004	-	15,15,15	0.42	0	19,21,21	1.54	3 (15%)
5	DMS	C	8401	-	3,3,3	1.21	0	3,3,3	0.68	0
5	DMS	C	8402	-	3,3,3	1.56	1 (33%)	3,3,3	0.51	0
5	DMS	C	8403	-	3,3,3	1.66	1 (33%)	3,3,3	0.44	0
5	DMS	C	8404	-	3,3,3	1.45	1 (33%)	3,3,3	1.11	0
5	DMS	C	8405	-	3,3,3	0.83	0	3,3,3	0.18	0
5	DMS	C	8407	-	3,3,3	1.57	1 (33%)	3,3,3	0.52	0
5	DMS	C	8408	-	3,3,3	0.49	0	3,3,3	1.22	1 (33%)
5	DMS	C	8409	-	3,3,3	1.10	0	3,3,3	0.25	0
5	DMS	C	8410	-	3,3,3	1.77	1 (33%)	3,3,3	0.54	0
5	DMS	C	8411	-	3,3,3	2.16	2 (66%)	3,3,3	0.21	0
5	DMS	C	8412	-	3,3,3	1.14	0	3,3,3	0.41	0
5	DMS	C	8413	-	3,3,3	1.74	1 (33%)	3,3,3	0.15	0
5	DMS	C	8414	-	3,3,3	0.94	0	3,3,3	0.98	0
5	DMS	C	8415	-	3,3,3	1.88	1 (33%)	3,3,3	0.20	0
5	DMS	C	8416	-	3,3,3	0.74	0	3,3,3	0.15	0
5	DMS	C	8420	-	3,3,3	1.03	0	3,3,3	0.18	0
5	DMS	C	8421	-	3,3,3	0.39	0	3,3,3	0.31	0
5	DMS	C	8423	-	3,3,3	1.47	0	3,3,3	0.45	0
5	DMS	C	8425	3	3,3,3	1.63	1 (33%)	3,3,3	0.16	0
5	DMS	C	8427	-	3,3,3	0.10	0	3,3,3	0.46	0
5	DMS	C	8501	-	3,3,3	1.27	1 (33%)	3,3,3	0.95	0
5	DMS	C	8502	-	3,3,3	0.62	0	3,3,3	1.25	1 (33%)
5	DMS	C	8503	-	3,3,3	1.03	0	3,3,3	0.24	0
5	DMS	C	8504	-	3,3,3	0.66	0	3,3,3	0.25	0
4	IPT	D	2001	3	15,15,15	0.46	0	19,21,21	1.34	2 (10%)
4	IPT	D	2002	-	15,15,15	0.92	1 (6%)	19,21,21	1.12	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IPT	D	2003	-	15,15,15	0.57	0	19,21,21	1.58	5 (26%)
5	DMS	D	8401	-	3,3,3	2.21	2 (66%)	3,3,3	0.94	0
5	DMS	D	8402	-	3,3,3	1.91	1 (33%)	3,3,3	0.29	0
5	DMS	D	8403	-	3,3,3	2.49	1 (33%)	3,3,3	0.41	0
5	DMS	D	8404	-	3,3,3	1.24	0	3,3,3	0.19	0
5	DMS	D	8405	-	3,3,3	0.96	0	3,3,3	0.36	0
5	DMS	D	8406	-	3,3,3	0.98	0	3,3,3	0.74	0
5	DMS	D	8407	-	3,3,3	1.45	1 (33%)	3,3,3	0.40	0
5	DMS	D	8408	-	3,3,3	1.00	0	3,3,3	0.50	0
5	DMS	D	8409	-	3,3,3	2.28	1 (33%)	3,3,3	0.88	0
5	DMS	D	8410	-	3,3,3	1.28	0	3,3,3	0.43	0
5	DMS	D	8411	-	3,3,3	1.40	1 (33%)	3,3,3	0.63	0
5	DMS	D	8412	-	3,3,3	1.43	1 (33%)	3,3,3	0.52	0
5	DMS	D	8413	-	3,3,3	1.20	0	3,3,3	0.07	0
5	DMS	D	8414	-	3,3,3	0.80	0	3,3,3	0.37	0
5	DMS	D	8415	-	3,3,3	1.78	0	3,3,3	0.32	0
5	DMS	D	8416	-	3,3,3	1.14	0	3,3,3	0.10	0
5	DMS	D	8417	-	3,3,3	1.21	0	3,3,3	0.85	0
5	DMS	D	8419	-	3,3,3	0.56	0	3,3,3	0.24	0
5	DMS	D	8421	-	3,3,3	1.16	0	3,3,3	0.34	0
5	DMS	D	8423	-	3,3,3	0.63	0	3,3,3	0.18	0
5	DMS	D	8501	-	3,3,3	0.15	0	3,3,3	0.55	0
5	DMS	D	8503	-	3,3,3	0.81	0	3,3,3	0.17	0
5	DMS	D	8705	-	3,3,3	0.74	0	3,3,3	0.50	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	IPT	A	2001	3	-	0/6/26/26	0/1/1/1
4	IPT	A	2002	-	-	0/6/26/26	0/1/1/1
4	IPT	A	2003	-	-	0/6/26/26	0/1/1/1
5	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8407	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
4	IPT	B	2001	3	-	0/6/26/26	0/1/1/1
4	IPT	B	2003	-	-	0/6/26/26	0/1/1/1
4	IPT	B	2004	-	-	0/6/26/26	0/1/1/1
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	8406	-	-	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	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8425	3	-	0/0/0/0	0/0/0/0
5	DMS	B	8427	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	B	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8506	-	-	0/0/0/0	0/0/0/0
4	IPT	C	2001	3	-	0/6/26/26	0/1/1/1
4	IPT	C	2003	-	-	0/6/26/26	0/1/1/1
4	IPT	C	2004	-	-	0/6/26/26	0/1/1/1
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	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	8427	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8502	-	-	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
4	IPT	D	2001	3	-	0/6/26/26	0/1/1/1
4	IPT	D	2002	-	-	0/6/26/26	0/1/1/1
4	IPT	D	2003	-	-	0/6/26/26	0/1/1/1
5	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8408	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8423	-	-	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	8705	-	-	0/0/0/0	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8414	DMS	O-S	-2.06	1.35	1.50
5	B	8502	DMS	C1-S	2.01	1.91	1.75
5	D	8411	DMS	C1-S	2.02	1.91	1.75
5	B	8417	DMS	C2-S	2.03	1.91	1.75
5	B	8415	DMS	C1-S	2.04	1.91	1.75
5	D	8401	DMS	O-S	2.05	1.64	1.50
5	C	8411	DMS	C1-S	2.08	1.91	1.75
5	B	8404	DMS	C2-S	2.14	1.92	1.75
5	C	8402	DMS	O-S	2.16	1.65	1.50
5	B	8501	DMS	O-S	2.17	1.65	1.50
5	D	8412	DMS	O-S	2.18	1.65	1.50
5	C	8407	DMS	C2-S	2.19	1.92	1.75
5	C	8501	DMS	C2-S	2.19	1.92	1.75
5	B	8403	DMS	C2-S	2.22	1.92	1.75
5	D	8407	DMS	O-S	2.22	1.65	1.50
5	B	8410	DMS	C1-S	2.30	1.93	1.75
5	C	8415	DMS	O-S	2.34	1.66	1.50
5	B	8407	DMS	C2-S	2.37	1.94	1.75
5	C	8404	DMS	C2-S	2.39	1.94	1.75
5	B	8405	DMS	O-S	2.41	1.66	1.50
5	B	8423	DMS	O-S	2.44	1.66	1.50
4	A	2002	IPT	O5-C1	2.49	1.46	1.42
5	A	8402	DMS	O-S	2.50	1.67	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8410	DMS	C1-S	2.53	1.95	1.75
4	D	2002	IPT	O4-C4	2.54	1.49	1.43
5	A	8423	DMS	C1-S	2.58	1.95	1.75
5	B	8506	DMS	O-S	2.59	1.68	1.50
5	C	8413	DMS	O-S	2.67	1.68	1.50
5	C	8403	DMS	C2-S	2.69	1.96	1.75
5	D	8402	DMS	C2-S	2.74	1.96	1.75
5	B	8420	DMS	C2-S	2.75	1.96	1.75
5	C	8425	DMS	O-S	2.77	1.69	1.50
5	A	8403	DMS	C2-S	2.88	1.98	1.75
5	C	8411	DMS	C2-S	2.91	1.98	1.75
5	B	8420	DMS	C1-S	2.92	1.98	1.75
5	A	8502	DMS	O-S	2.94	1.70	1.50
5	D	8401	DMS	C1-S	3.06	1.99	1.75
5	D	8409	DMS	O-S	3.49	1.74	1.50
5	A	8413	DMS	O-S	3.53	1.74	1.50
5	A	8409	DMS	O-S	3.53	1.74	1.50
5	B	8409	DMS	O-S	3.73	1.75	1.50
5	D	8403	DMS	C2-S	4.22	2.08	1.75

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	IPT	C3-C4-C5	-6.25	99.31	110.20
4	D	2003	IPT	C3-C4-C5	-3.93	103.34	110.20
4	C	2003	IPT	C1-O5-C5	-3.20	106.64	112.74
4	A	2001	IPT	O5-C1-S1	-3.19	101.92	110.01
4	C	2003	IPT	O5-C1-S1	-3.18	101.95	110.01
4	A	2003	IPT	O2-C2-C3	-3.00	103.58	110.34
4	C	2003	IPT	O6-C6-C5	-2.97	101.52	111.33
4	A	2002	IPT	C1-C2-C3	-2.77	104.55	110.69
4	C	2004	IPT	C1-O5-C5	-2.74	107.51	112.74
4	B	2003	IPT	O5-C1-S1	-2.59	103.45	110.01
4	D	2001	IPT	O2-C2-C3	-2.44	104.84	110.34
4	D	2003	IPT	O6-C6-C5	-2.44	103.27	111.33
4	D	2003	IPT	O2-C2-C3	-2.30	105.15	110.34
4	B	2003	IPT	C1-O5-C5	-2.28	108.38	112.74
4	D	2003	IPT	O5-C1-S1	-2.27	104.27	110.01
4	B	2004	IPT	O3-C3-C2	-2.04	105.75	110.34
4	B	2001	IPT	C1-O5-C5	-2.02	108.88	112.74
4	A	2002	IPT	C1-O5-C5	-2.01	108.90	112.74
5	A	8403	DMS	C2-S-C1	2.04	109.00	98.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	8408	DMS	C2-S-C1	2.05	109.05	98.46
4	C	2004	IPT	O5-C1-C2	2.07	113.00	110.19
4	C	2001	IPT	C6-C5-C4	2.11	118.21	113.02
5	B	8404	DMS	C2-S-C1	2.11	109.35	98.46
5	C	8502	DMS	C2-S-C1	2.15	109.58	98.46
5	B	8401	DMS	C2-S-C1	2.16	109.64	98.46
4	D	2002	IPT	O4-C4-C3	2.22	115.33	110.34
4	D	2003	IPT	O3-C3-C4	2.37	115.68	110.34
4	A	2003	IPT	O3-C3-C4	2.94	116.95	110.34
4	B	2004	IPT	O5-C5-C4	3.02	115.34	109.68
5	B	8417	DMS	C2-S-C1	3.08	114.39	98.46
4	D	2001	IPT	C6-C5-C4	3.23	120.99	113.02
4	B	2004	IPT	C4-C3-C2	4.13	118.50	110.79
4	C	2004	IPT	C4-C3-C2	4.30	118.82	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

34 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8403	DMS	1	0
5	A	8410	DMS	1	0
5	A	8411	DMS	1	0
5	A	8412	DMS	3	0
5	A	8414	DMS	1	0
5	A	8415	DMS	1	0
5	A	8416	DMS	1	0
5	A	8417	DMS	1	0
5	A	8420	DMS	2	0
5	A	8501	DMS	1	0
4	B	2001	IPT	2	0
4	B	2004	IPT	1	0
5	B	8403	DMS	1	0
5	B	8412	DMS	3	0
5	B	8413	DMS	1	0
5	B	8416	DMS	3	0
5	B	8417	DMS	1	0
5	B	8504	DMS	1	0
5	B	8506	DMS	8	0
4	C	2004	IPT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8408	DMS	1	0
5	C	8411	DMS	4	0
5	C	8412	DMS	2	0
5	C	8416	DMS	3	0
5	C	8420	DMS	2	0
5	C	8421	DMS	1	0
5	C	8502	DMS	1	0
4	D	2003	IPT	1	0
5	D	8403	DMS	1	0
5	D	8406	DMS	1	0
5	D	8414	DMS	1	0
5	D	8415	DMS	1	0
5	D	8417	DMS	1	0
5	D	8503	DMS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.14	34 (3%)	49	43	11, 22, 52, 99	0
1	B	1011/1023 (98%)	-0.27	20 (1%)	68	64	10, 19, 49, 100	0
1	C	1011/1023 (98%)	-0.33	21 (2%)	67	62	11, 18, 46, 99	0
1	D	1011/1023 (98%)	-0.18	28 (2%)	56	51	13, 23, 51, 99	0
All	All	4044/4092 (98%)	-0.23	103 (2%)	61	56	10, 20, 50, 100	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	8.7
1	D	730	LEU	8.6
1	B	732	ALA	7.9
1	B	686	PRO	6.8
1	C	735	HIS	6.8
1	D	735	HIS	6.6
1	B	730	LEU	6.4
1	B	731	PRO	6.3
1	A	686	PRO	6.2
1	A	732	ALA	6.0
1	B	733	ALA	5.8
1	C	731	PRO	5.6
1	C	733	ALA	5.6
1	B	685	LEU	5.2
1	C	730	LEU	5.2
1	B	734	SER	5.2
1	C	687	GLN	5.2
1	B	687	GLN	5.1
1	D	734	SER	5.1
1	D	733	ALA	5.1
1	A	733	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	685	LEU	5.0
1	C	686	PRO	4.9
1	D	686	PRO	4.8
1	D	687	GLN	4.8
1	B	735	HIS	4.6
1	D	581	ASN	4.4
1	C	689	GLU	4.3
1	A	730	LEU	4.2
1	B	689	GLU	4.2
1	A	687	GLN	4.1
1	C	685	LEU	4.1
1	C	684	GLU	4.1
1	A	580	GLU	4.0
1	C	688	PRO	3.9
1	D	732	ALA	3.9
1	A	799	THR	3.8
1	B	688	PRO	3.8
1	D	684	GLU	3.8
1	D	79	PRO	3.7
1	C	800	ARG	3.7
1	D	582	GLY	3.6
1	D	580	GLU	3.5
1	D	689	GLU	3.4
1	A	71	GLU	3.3
1	A	689	GLU	3.2
1	D	800	ARG	3.2
1	C	732	ALA	3.1
1	A	800	ARG	3.1
1	D	799	THR	3.1
1	A	78	LEU	3.1
1	B	728	VAL	3.0
1	A	581	ASN	3.0
1	B	798	ALA	3.0
1	C	729	THR	2.9
1	A	684	GLU	2.9
1	A	734	SER	2.9
1	A	688	PRO	2.9
1	A	76	CYS	2.9
1	A	146	VAL	2.9
1	A	582	GLY	2.9
1	A	131	GLU	2.8
1	B	684	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	688	PRO	2.7
1	A	117	GLU	2.7
1	D	736	ALA	2.7
1	C	799	THR	2.6
1	A	188	VAL	2.6
1	D	131	GLU	2.6
1	B	729	THR	2.6
1	C	582	GLY	2.5
1	D	1023	LYS	2.5
1	A	179	ALA	2.5
1	A	79	PRO	2.5
1	A	731	PRO	2.5
1	D	731	PRO	2.5
1	A	69	VAL	2.4
1	C	580	GLU	2.4
1	D	179	ALA	2.4
1	A	579	ASP	2.4
1	D	130	ASP	2.4
1	B	800	ARG	2.4
1	B	1023	LYS	2.4
1	B	745	MET	2.4
1	D	771	GLY	2.3
1	D	770	ILE	2.3
1	C	581	ASN	2.3
1	D	737	ILE	2.3
1	A	180	GLY	2.2
1	C	319	ASP	2.2
1	A	81	ALA	2.2
1	D	663	LEU	2.2
1	A	736	ALA	2.2
1	A	68	ALA	2.1
1	D	146	VAL	2.1
1	A	798	ALA	2.1
1	B	681	GLU	2.1
1	C	745	MET	2.1
1	C	690	SER	2.1
1	B	682	LEU	2.0
1	C	728	VAL	2.0
1	D	798	ALA	2.0
1	A	583	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	A	8423	4/4	0.80	0.31	14.74	58,63,65,100	0
5	DMS	A	8420	4/4	0.92	0.16	13.39	45,55,55,65	0
5	DMS	B	8420	4/4	0.88	0.23	13.17	56,57,69,82	0
4	IPT	B	2004	15/15	0.90	0.20	9.93	31,45,99,100	0
5	DMS	C	8420	4/4	0.95	0.15	9.04	47,52,67,79	0
4	IPT	D	2003	15/15	0.90	0.20	9.02	28,36,55,63	0
5	DMS	A	8416	4/4	0.93	0.23	8.18	43,44,100,100	0
5	DMS	C	8403	4/4	0.95	0.16	7.28	23,33,36,100	0
5	DMS	B	8417	4/4	0.91	0.24	6.80	28,29,73,100	0
5	DMS	B	8423	4/4	0.90	0.14	5.34	35,58,73,80	0
5	DMS	D	8417	4/4	0.93	0.19	5.30	30,35,64,98	0
2	MG	A	3012	1/1	0.97	0.16	5.29	40,40,40,40	0
5	DMS	C	8404	4/4	0.96	0.10	4.85	20,23,40,53	0
5	DMS	A	8403	4/4	0.96	0.14	4.56	24,26,36,100	0
5	DMS	A	8417	4/4	0.91	0.18	4.49	30,36,38,100	0
5	DMS	C	8425	4/4	0.94	0.17	4.15	34,36,52,57	0
4	IPT	C	2003	15/15	0.93	0.18	4.04	18,28,47,67	0
5	DMS	B	8425	4/4	0.95	0.17	3.81	41,42,43,50	0
5	DMS	D	8403	4/4	0.96	0.12	3.45	28,33,42,42	0
5	DMS	B	8403	4/4	0.96	0.14	3.42	26,33,38,100	0
4	IPT	B	2003	15/15	0.92	0.17	3.37	23,30,38,42	0
4	IPT	A	2003	15/15	0.92	0.16	3.21	26,35,77,100	0
5	DMS	B	8407	4/4	0.96	0.10	3.02	25,39,43,50	0
5	DMS	B	8506	4/4	0.96	0.17	2.95	44,50,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	A	8419	4/4	0.91	0.15	2.88	38,62,71,100	0
5	DMS	B	8405	4/4	0.98	0.10	2.77	28,32,33,38	0
5	DMS	D	8405	4/4	0.98	0.11	2.62	33,33,39,39	0
5	DMS	B	8401	4/4	0.99	0.10	2.37	16,22,22,24	0
5	DMS	C	8501	4/4	0.93	0.11	2.00	25,48,53,60	0
5	DMS	D	8423	4/4	0.90	0.12	1.75	49,50,66,96	0
5	DMS	D	8407	4/4	0.96	0.10	1.75	25,34,40,44	0
3	NA	C	3104	1/1	0.98	0.14	1.75	26,26,26,26	0
5	DMS	C	8405	4/4	0.98	0.09	1.74	28,29,32,33	0
5	DMS	C	8408	4/4	0.97	0.11	1.70	31,35,41,100	0
5	DMS	D	8406	4/4	0.94	0.14	1.59	36,57,85,100	0
5	DMS	D	8501	4/4	0.94	0.13	1.51	31,37,48,74	0
4	IPT	A	2001	15/15	0.96	0.09	1.39	17,25,58,60	0
5	DMS	C	8502	4/4	0.97	0.08	1.36	28,29,41,44	0
5	DMS	D	8705	4/4	0.95	0.18	1.27	38,47,100,100	0
5	DMS	D	8401	4/4	0.98	0.09	1.25	14,22,23,26	0
5	DMS	A	8501	4/4	0.95	0.14	1.20	36,53,54,57	0
5	DMS	D	8419	4/4	0.97	0.12	1.16	55,62,64,72	0
3	NA	B	3104	1/1	0.98	0.14	1.16	29,29,29,29	0
5	DMS	A	8407	4/4	0.97	0.11	1.09	32,34,40,47	0
5	DMS	C	8423	4/4	0.96	0.10	1.09	27,40,47,77	0
5	DMS	A	8502	4/4	0.94	0.15	1.09	36,41,54,100	0
2	MG	D	3002	1/1	0.98	0.11	1.01	27,27,27,27	0
5	DMS	A	8412	4/4	0.97	0.15	0.99	36,51,51,65	0
5	DMS	B	8412	4/4	0.97	0.12	0.86	34,35,39,57	0
5	DMS	B	8408	4/4	0.97	0.09	0.81	39,42,42,56	0
4	IPT	D	2002	15/15	0.96	0.09	0.70	13,22,31,32	0
5	DMS	D	8402	4/4	0.97	0.08	0.66	12,25,29,42	0
4	IPT	D	2001	15/15	0.96	0.09	0.56	20,30,34,52	0
4	IPT	A	2002	15/15	0.96	0.09	0.54	15,22,30,34	0
3	NA	C	3101	1/1	0.99	0.10	0.52	15,15,15,15	0
5	DMS	B	8406	4/4	0.98	0.08	0.50	35,36,44,100	0
5	DMS	C	8401	4/4	0.99	0.08	0.47	15,15,21,22	0
5	DMS	B	8404	4/4	0.97	0.08	0.42	19,20,32,38	0
5	DMS	D	8404	4/4	0.98	0.08	0.30	18,30,34,35	0
5	DMS	C	8407	4/4	0.98	0.08	0.29	28,28,36,43	0
5	DMS	C	8412	4/4	0.98	0.10	0.27	31,35,37,54	0
5	DMS	B	8402	4/4	0.98	0.08	0.27	19,20,32,36	0
4	IPT	B	2001	15/15	0.96	0.09	0.27	16,20,28,33	0
5	DMS	A	8410	4/4	0.96	0.11	0.20	40,45,58,61	0
5	DMS	A	8408	4/4	0.96	0.11	0.16	31,37,48,82	0
5	DMS	C	8402	4/4	0.96	0.08	0.03	20,21,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	C	8410	4/4	0.96	0.10	-0.01	17,33,39,100	0
5	DMS	A	8405	4/4	0.98	0.09	-0.02	33,34,34,35	0
5	DMS	C	8504	4/4	0.95	0.09	-0.03	37,66,69,100	0
4	IPT	C	2001	15/15	0.97	0.09	-0.07	14,19,31,37	0
5	DMS	D	8408	4/4	0.98	0.11	-0.08	26,34,43,47	0
5	DMS	A	8504	4/4	0.96	0.12	-0.18	58,65,69,89	0
5	DMS	D	8412	4/4	0.97	0.10	-0.27	30,39,46,62	0
5	DMS	B	8410	4/4	0.98	0.10	-0.42	22,35,44,48	0
5	DMS	A	8411	4/4	0.98	0.09	-0.45	28,29,36,43	0
5	DMS	B	8411	4/4	0.99	0.07	-0.46	23,27,36,47	0
5	DMS	A	8401	4/4	0.99	0.07	-0.52	15,24,25,26	0
3	NA	A	3103	1/1	0.97	0.09	-0.60	33,33,33,33	0
5	DMS	D	8411	4/4	0.98	0.09	-0.71	27,35,38,100	0
5	DMS	B	8502	4/4	0.97	0.07	-0.82	19,29,62,68	0
5	DMS	C	8411	4/4	0.99	0.07	-0.89	21,23,23,27	0
5	DMS	A	8404	4/4	0.97	0.07	-0.93	24,33,36,44	0
5	DMS	B	8501	4/4	0.98	0.07	-0.97	21,24,32,32	0
3	NA	D	3103	1/1	0.97	0.08	-1.15	31,31,31,31	0
2	MG	B	3002	1/1	0.99	0.06	-1.28	19,19,19,19	0
3	NA	C	3103	1/1	0.99	0.07	-1.29	30,30,30,30	0
3	NA	B	3103	1/1	0.96	0.07	-1.41	31,31,31,31	0
3	NA	C	3102	1/1	0.99	0.06	-1.47	16,16,16,16	0
3	NA	B	3102	1/1	0.99	0.05	-1.52	15,15,15,15	0
2	MG	C	3002	1/1	0.99	0.05	-1.63	18,18,18,18	0
3	NA	A	3102	1/1	0.99	0.06	-1.79	15,15,15,15	0
2	MG	B	3011	1/1	0.95	0.09	-1.82	41,41,41,41	0
5	DMS	A	8406	4/4	0.98	0.07	-1.87	28,51,52,61	0
2	MG	B	3001	1/1	0.99	0.05	-1.93	16,16,16,16	0
2	MG	D	3001	1/1	0.99	0.06	-2.01	18,18,18,18	0
3	NA	D	3101	1/1	0.99	0.06	-2.07	19,19,19,19	0
2	MG	C	3001	1/1	1.00	0.06	-2.16	15,15,15,15	0
5	DMS	A	8402	4/4	0.99	0.06	-2.16	18,25,26,31	0
2	MG	A	3002	1/1	0.98	0.07	-2.40	23,23,23,23	0
3	NA	D	3102	1/1	0.99	0.05	-2.55	17,17,17,17	0
2	MG	A	3001	1/1	0.99	0.05	-2.65	17,17,17,17	0
3	NA	A	3101	1/1	0.99	0.05	-4.52	21,21,21,21	0
3	NA	B	3101	1/1	0.99	0.06	-4.55	17,17,17,17	0
5	DMS	D	8503	4/4	0.93	0.11	-	25,47,53,100	0
5	DMS	D	8413	4/4	0.93	0.19	-	39,40,52,56	0
5	DMS	A	8421	4/4	0.89	0.17	-	28,62,80,100	0
5	DMS	C	8503	4/4	0.94	0.10	-	38,47,52,55	0
5	DMS	D	8416	4/4	0.90	0.20	-	36,61,87,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	B	8414	4/4	0.97	0.11	-	24,42,50,100	0
5	DMS	B	8409	4/4	0.96	0.10	-	24,34,36,41	0
3	NA	C	3105	1/1	0.79	0.13	-	48,48,48,48	0
5	DMS	B	8416	4/4	0.88	0.29	-	21,75,100,100	0
3	NA	A	3105	1/1	0.96	0.05	-	46,46,46,46	0
5	DMS	B	8421	4/4	0.98	0.13	-	36,47,100,100	0
5	DMS	C	8427	4/4	0.95	0.14	-	38,49,72,73	0
4	IPT	C	2004	15/15	0.88	0.25	-	29,55,100,100	0
2	MG	A	3003	1/1	0.87	0.15	-	52,52,52,52	0
5	DMS	D	8415	4/4	0.97	0.07	-	26,30,37,48	0
5	DMS	B	8504	4/4	0.97	0.14	-	53,54,60,65	0
5	DMS	C	8414	4/4	0.95	0.12	-	23,41,47,52	0
5	DMS	A	8414	4/4	0.95	0.15	-	38,40,91,100	0
5	DMS	B	8415	4/4	0.93	0.12	-	28,32,48,100	0
5	DMS	C	8409	4/4	0.97	0.09	-	33,38,43,51	0
2	MG	D	3003	1/1	0.95	0.09	-	48,48,48,48	0
5	DMS	B	8413	4/4	0.95	0.15	-	32,42,44,69	0
5	DMS	C	8421	4/4	0.92	0.14	-	38,46,62,68	0
5	DMS	D	8414	4/4	0.97	0.17	-	30,61,100,100	0
5	DMS	C	8413	4/4	0.96	0.14	-	28,48,50,100	0
3	NA	D	3105	1/1	0.94	0.09	-	64,64,64,64	0
5	DMS	C	8416	4/4	0.91	0.28	-	22,78,100,100	0
5	DMS	B	8427	4/4	0.95	0.18	-	41,68,100,100	0
5	DMS	A	8409	4/4	0.94	0.12	-	38,39,50,66	0
5	DMS	D	8409	4/4	0.95	0.10	-	28,31,34,46	0
5	DMS	D	8421	4/4	0.86	0.17	-	47,55,65,100	0
5	DMS	D	8410	4/4	0.96	0.11	-	32,41,45,71	0
2	MG	B	3007	1/1	0.99	0.16	-	26,26,26,26	0
5	DMS	A	8413	4/4	0.93	0.16	-	44,46,52,52	0
3	NA	B	3105	1/1	0.91	0.11	-	48,48,48,48	0
5	DMS	C	8415	4/4	0.96	0.10	-	21,26,37,46	0
5	DMS	A	8415	4/4	0.95	0.10	-	27,31,48,49	0
2	MG	C	3003	1/1	0.96	0.09	-	15,15,15,15	1

6.5 Other polymers ⓘ

There are no such residues in this entry.