



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:28 AM UTC

PDB ID : 1JYV / pdb_00001jyv
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH ONPG
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

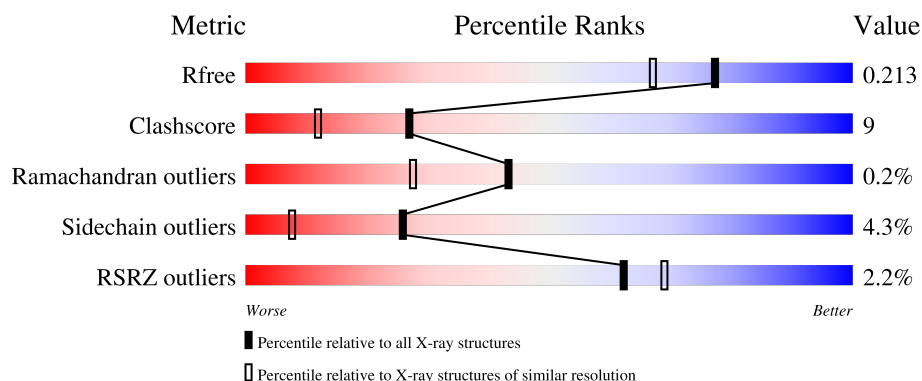
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	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
5	DMS	A	8412	-	-	X	-
5	DMS	C	8415	-	X	-	-
5	DMS	D	8703	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37222 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-Galactosidase.

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

There are 36 discrepancies between the modelled and reference sequences:

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

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

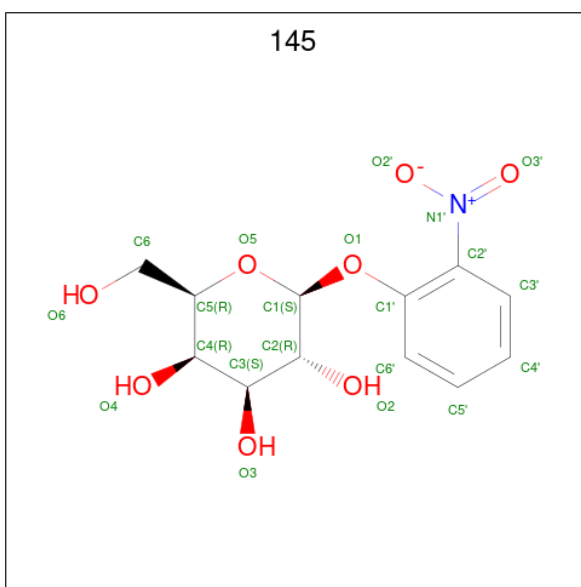
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is 2-nitrophenyl beta-D-galactopyranoside (CCD ID: 145) (formula: C₁₂H₁₅NO₈).



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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

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

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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	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0

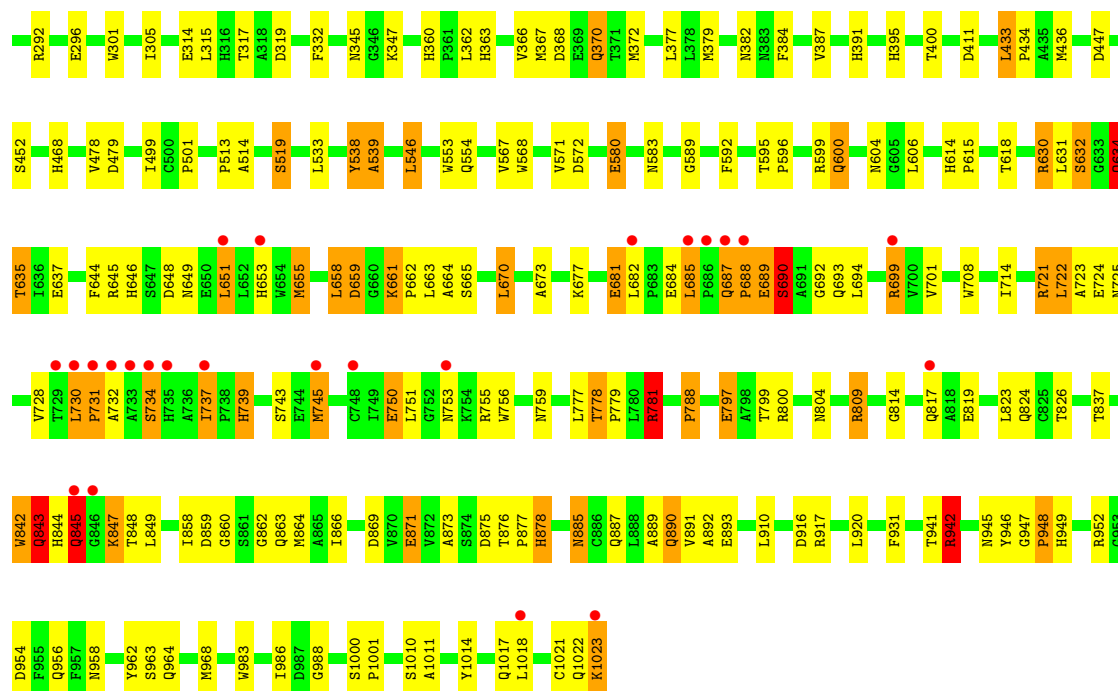
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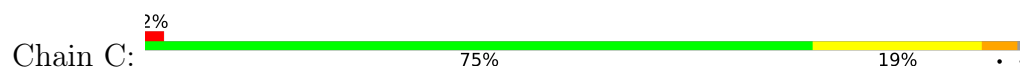
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4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

- Molecule 6 is water.

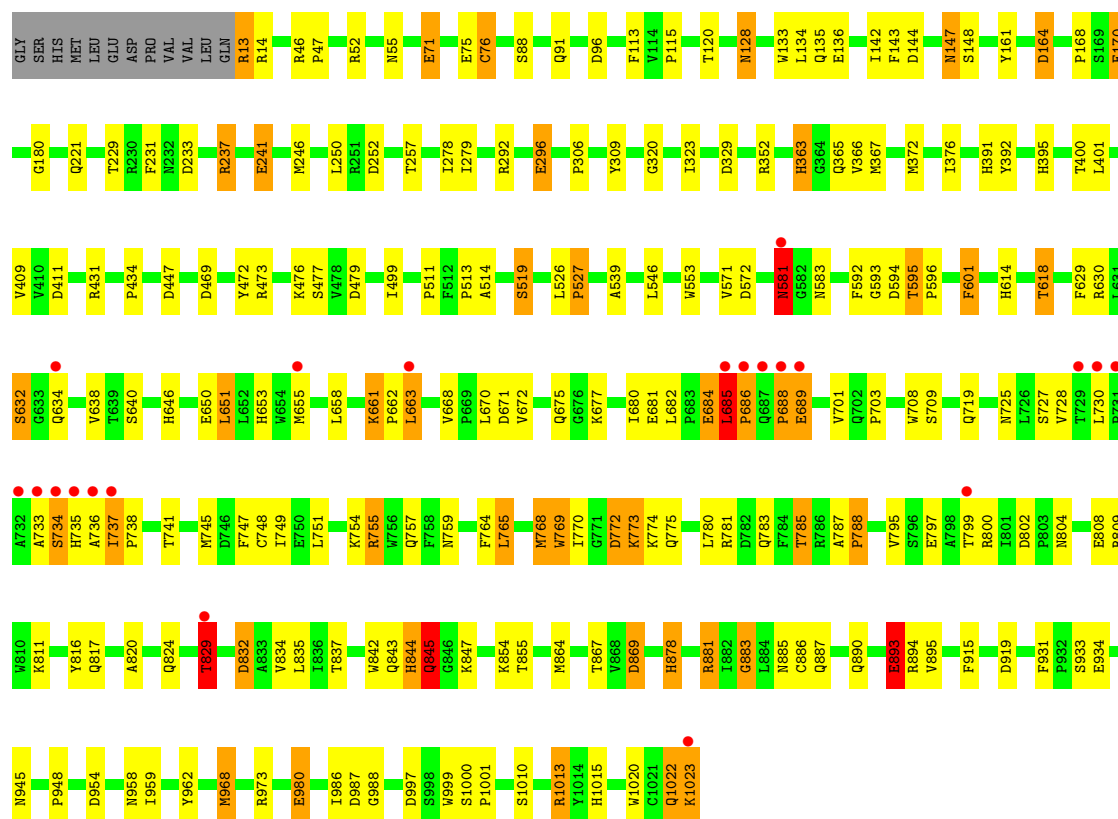
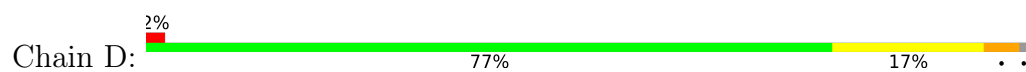
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1060	Total O 1060 1060	0	0
6	B	1013	Total O 1013 1013	0	0
6	C	987	Total O 987 987	0	0
6	D	1021	Total O 1021 1021	0	0



• Molecule 1: Beta-Galactosidase



• Molecule 1: Beta-Galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.49Å 167.46Å 200.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 1.75 29.90 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.90-1.75) 90.9 (29.90-1.75)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.68 (at 1.75Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.180 , 0.240 0.162 , 0.213	Depositor DCC
R_{free} test set	7151 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	15.1	Xtrriage
Anisotropy	0.408	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 87.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	37222	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3036e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.30	5/8383 (0.1%)	1.76	108/11437 (0.9%)
1	B	1.30	3/8383 (0.0%)	1.77	117/11437 (1.0%)
1	C	1.28	8/8383 (0.1%)	1.80	131/11437 (1.1%)
1	D	1.29	12/8383 (0.1%)	1.77	127/11437 (1.1%)
All	All	1.29	28/33532 (0.1%)	1.77	483/45748 (1.1%)

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

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

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	479	ASP	C-N	-8.36	1.25	1.34
1	C	111	PRO	CA-C	-7.24	1.47	1.51
1	D	883	GLY	C-O	6.73	1.30	1.23
1	D	734	SER	N-CA	-6.47	1.38	1.46
1	B	86	VAL	CA-C	6.21	1.57	1.52
1	C	479	ASP	C-N	-6.17	1.27	1.34
1	C	684	GLU	CD-OE2	6.10	1.36	1.25
1	D	170	GLU	C-O	5.85	1.31	1.24
1	B	468	HIS	CE1-NE2	5.80	1.38	1.32
1	D	391	HIS	CG-ND1	5.64	1.44	1.38
1	A	297	ASN	CA-C	-5.64	1.50	1.53
1	D	893	GLU	CD-OE2	5.59	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297	ASN	CA-C	-5.58	1.50	1.53
1	C	208	ILE	CA-C	-5.56	1.48	1.53
1	A	844	HIS	N-CA	-5.54	1.39	1.46
1	D	842	TRP	CA-C	-5.53	1.46	1.52
1	D	120	THR	C-N	5.46	1.36	1.33
1	D	479	ASP	C-N	-5.40	1.28	1.34
1	D	71	GLU	CD-OE2	5.30	1.35	1.25
1	C	499	ILE	N-CA	5.23	1.52	1.46
1	A	646	HIS	CG-CD2	5.18	1.41	1.35
1	A	126	THR	CA-C	-5.12	1.46	1.52
1	D	13	ARG	C-N	-5.09	1.27	1.33
1	D	511	PRO	CA-C	-5.05	1.48	1.53
1	C	80	GLU	CD-OE2	5.05	1.34	1.25
1	B	988	GLY	CA-C	5.04	1.57	1.52
1	C	1006	GLU	CD-OE2	5.03	1.34	1.25
1	D	881	ARG	NE-CZ	5.02	1.38	1.33

All (483) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	HIS	CA-CB-CG	-13.29	100.51	113.80
1	C	685	LEU	N-CA-CB	12.40	125.92	110.17
1	D	844	HIS	CA-CB-CG	-9.91	103.89	113.80
1	B	687	GLN	C-N-CD	-9.63	85.52	125.00
1	C	725	ASN	CA-CB-CG	-9.62	102.98	112.60
1	D	980	GLU	CA-C-N	-9.56	107.57	121.44
1	D	980	GLU	C-N-CA	-9.56	107.57	121.44
1	D	733	ALA	N-CA-C	9.21	122.21	110.24
1	D	632	SER	N-CA-CB	8.91	124.39	110.84
1	D	736	ALA	N-CA-C	8.91	123.55	109.65
1	B	737	ILE	N-CA-CB	8.85	123.60	111.21
1	C	747	PHE	CA-CB-CG	8.62	122.42	113.80
1	D	614	HIS	N-CA-C	-8.62	100.22	110.13
1	C	809	ARG	NE-CZ-NH1	8.60	130.09	121.50
1	D	869	ASP	CA-CB-CG	-8.57	104.03	112.60
1	D	727	SER	CA-C-N	-8.57	110.81	122.72
1	D	727	SER	C-N-CA	-8.57	110.81	122.72
1	C	274	PHE	CA-CB-CG	-8.54	105.26	113.80
1	D	323	ILE	N-CA-C	-8.37	103.67	111.45
1	C	363	HIS	CA-CB-CG	-8.36	105.44	113.80
1	B	681	GLU	CB-CG-CD	-8.26	98.56	112.60
1	B	725	ASN	CA-CB-CG	-8.26	104.34	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	770	ILE	N-CA-C	-8.23	95.73	107.75
1	D	363	HIS	CA-CB-CG	-8.20	105.60	113.80
1	C	184	LEU	CB-CA-C	-8.04	95.92	109.50
1	B	823	LEU	N-CA-C	-7.94	104.11	113.88
1	C	954	ASP	CA-CB-CG	-7.89	104.70	112.60
1	A	583	ASN	CA-CB-CG	-7.86	104.74	112.60
1	B	400	THR	CA-CB-OG1	-7.78	97.93	109.60
1	A	14	ARG	N-CA-CB	-7.78	101.64	110.35
1	B	958	ASN	N-CA-CB	7.71	125.86	111.53
1	C	598	ASP	CA-CB-CG	-7.71	104.89	112.60
1	A	82	ASP	CA-CB-CG	-7.67	104.93	112.60
1	D	733	ALA	N-CA-CB	7.61	122.09	109.92
1	B	942	ARG	NE-CZ-NH1	7.49	128.99	121.50
1	C	739	HIS	CA-CB-CG	-7.44	106.36	113.80
1	D	306	PRO	N-CA-CB	7.41	107.44	102.25
1	C	583	ASN	CA-CB-CG	-7.39	105.21	112.60
1	B	360	HIS	CA-CB-CG	-7.36	106.44	113.80
1	B	885	ASN	CA-CB-CG	7.36	119.96	112.60
1	B	221	GLN	N-CA-CB	-7.31	100.00	111.56
1	C	113	PHE	CA-CB-CG	-7.30	106.50	113.80
1	B	653	HIS	CA-CB-CG	7.30	121.10	113.80
1	A	279	ILE	CB-CG1-CD1	-7.27	98.53	113.80
1	D	832	ASP	N-CA-CB	-7.26	99.22	111.20
1	B	113	PHE	CA-CB-CG	-7.25	106.55	113.80
1	D	279	ILE	CB-CG1-CD1	-7.24	98.60	113.80
1	C	13	ARG	N-CA-CB	7.21	122.77	110.50
1	B	519	SER	N-CA-C	-7.18	99.81	110.23
1	C	890	GLN	N-CA-CB	-7.16	99.41	110.29
1	A	954	ASP	CA-CB-CG	-7.15	105.45	112.60
1	C	512	PHE	CA-C-O	7.11	128.72	120.69
1	B	942	ARG	CD-NE-CZ	7.10	134.34	124.40
1	A	519	SER	N-CA-C	-7.09	100.24	110.24
1	A	772	ASP	CB-CA-C	7.07	121.90	110.09
1	D	128	ASN	OD1-CG-ND2	7.05	129.65	122.60
1	D	893	GLU	CB-CG-CD	7.05	124.59	112.60
1	C	685	LEU	CB-CA-C	7.04	118.18	110.08
1	B	942	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	A	599	ARG	NE-CZ-NH1	-7.00	114.50	121.50
1	C	684	GLU	CB-CG-CD	6.99	124.49	112.60
1	D	278	ILE	CA-C-N	-6.98	113.95	121.84
1	D	278	ILE	C-N-CA	-6.98	113.95	121.84
1	C	667	GLU	CB-CG-CD	-6.97	100.75	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	147	ASN	N-CA-CB	-6.96	99.80	110.65
1	C	680	ILE	CA-C-N	-6.96	113.52	122.77
1	C	680	ILE	C-N-CA	-6.96	113.52	122.77
1	A	844	HIS	CA-CB-CG	-6.94	106.86	113.80
1	C	958	ASN	N-CA-CB	6.93	123.75	111.69
1	D	829	THR	N-CA-CB	6.92	121.43	110.57
1	D	527	PRO	N-CA-CB	6.91	109.41	103.19
1	D	890	GLN	N-CA-CB	-6.89	100.25	110.17
1	B	734	SER	N-CA-CB	6.87	120.13	109.48
1	C	209	PHE	CA-CB-CG	-6.85	106.95	113.80
1	B	433	LEU	CA-C-O	6.84	124.98	118.34
1	D	400	THR	CA-CB-OG1	-6.84	99.33	109.60
1	B	85	VAL	CA-C-N	6.84	129.28	123.33
1	B	85	VAL	C-N-CA	6.84	129.28	123.33
1	C	947	GLY	CA-C-N	6.83	126.97	119.87
1	C	947	GLY	C-N-CA	6.83	126.97	119.87
1	C	539[A]	ALA	CB-CA-C	6.82	123.99	110.42
1	C	539[B]	ALA	CB-CA-C	6.82	123.99	110.42
1	A	632	SER	N-CA-CB	6.79	121.49	110.90
1	B	777	LEU	N-CA-C	-6.79	105.12	113.41
1	A	788	PRO	N-CA-CB	6.78	109.34	103.31
1	D	988	GLY	N-CA-C	-6.76	103.72	113.86
1	C	931	PHE	CA-CB-CG	-6.76	107.04	113.80
1	C	737	ILE	N-CA-CB	6.75	120.66	111.21
1	D	128	ASN	CA-CB-CG	-6.73	105.87	112.60
1	D	931	PHE	CA-CB-CG	-6.73	107.07	113.80
1	B	211	ASP	N-CA-C	6.69	118.93	110.24
1	A	235	PHE	CA-CB-CG	-6.67	107.13	113.80
1	B	110	ASN	N-CA-CB	-6.67	103.17	110.71
1	B	725	ASN	OD1-CG-ND2	6.67	129.27	122.60
1	C	790	ASP	CA-CB-CG	-6.67	105.93	112.60
1	C	13	ARG	CA-C-N	-6.66	113.08	122.34
1	C	13	ARG	C-N-CA	-6.66	113.08	122.34
1	D	686	PRO	N-CA-CB	6.66	110.37	103.38
1	C	634	GLN	CA-C-O	6.65	129.19	121.34
1	B	539[A]	ALA	CB-CA-C	-6.64	97.20	110.42
1	B	539[B]	ALA	CB-CA-C	-6.64	97.20	110.42
1	C	736	ALA	N-CA-C	6.63	118.84	108.96
1	C	809	ARG	CD-NE-CZ	6.62	133.67	124.40
1	B	1018	LEU	CB-CA-C	-6.61	95.52	110.07
1	C	669	PRO	CB-CA-C	-6.61	102.77	111.23
1	C	699	ARG	NE-CZ-NH1	6.61	128.11	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ASN	OD1-CG-ND2	6.61	129.21	122.60
1	C	648	ASP	CA-CB-CG	-6.61	105.99	112.60
1	A	996	ASP	N-CA-C	-6.58	104.14	111.71
1	C	477	SER	N-CA-CB	-6.58	100.40	110.20
1	C	738	PRO	CA-C-N	-6.57	113.93	123.00
1	C	738	PRO	C-N-CA	-6.57	113.93	123.00
1	B	209	PHE	N-CA-C	6.56	121.44	113.17
1	C	277	GLU	CA-CB-CG	-6.55	101.00	114.10
1	A	570	TRP	N-CA-C	6.53	118.28	111.03
1	D	539[A]	ALA	CB-CA-C	-6.52	97.44	110.42
1	D	539[B]	ALA	CB-CA-C	-6.52	97.44	110.42
1	D	765	LEU	N-CA-C	-6.52	100.25	109.96
1	C	581	ASN	CA-CB-CG	-6.50	106.10	112.60
1	B	233	ASP	CA-C-N	-6.50	112.28	122.49
1	B	233	ASP	C-N-CA	-6.50	112.28	122.49
1	A	659	ASP	CA-CB-CG	-6.50	106.11	112.60
1	D	759	ASN	CA-CB-CG	-6.47	106.13	112.60
1	D	689	GLU	CA-C-N	6.41	130.47	121.24
1	D	689	GLU	C-N-CA	6.41	130.47	121.24
1	A	614	HIS	N-CA-C	-6.40	101.78	110.36
1	C	592	PHE	CA-CB-CG	-6.40	107.40	113.80
1	C	611	ARG	CB-CA-C	6.40	116.16	109.83
1	D	571	VAL	N-CA-C	6.40	117.99	108.46
1	A	264	GLU	CA-C-O	6.39	127.16	119.43
1	C	931	PHE	N-CA-C	-6.39	97.18	108.69
1	B	382	ASN	CA-CB-CG	-6.39	106.21	112.60
1	D	147	ASN	N-CA-CB	-6.38	100.54	110.55
1	C	497	ASP	CA-CB-CG	-6.35	106.25	112.60
1	C	614	HIS	N-CA-CB	6.35	117.11	109.74
1	B	71	GLU	CB-CG-CD	6.35	123.39	112.60
1	C	682	LEU	CA-C-N	6.34	126.31	120.03
1	C	682	LEU	C-N-CA	6.34	126.31	120.03
1	A	539[A]	ALA	CB-CA-C	-6.33	97.82	110.42
1	A	539[B]	ALA	CB-CA-C	-6.33	97.82	110.42
1	A	477	SER	N-CA-CB	6.33	119.50	110.13
1	B	120	THR	CA-C-N	-6.32	116.67	122.29
1	B	120	THR	C-N-CA	-6.32	116.67	122.29
1	C	111	PRO	O-C-N	6.31	124.21	121.31
1	C	249	GLU	N-CA-C	6.31	119.00	108.96
1	C	842	TRP	CB-CA-C	-6.29	98.84	109.72
1	C	601	PHE	CA-CB-CG	-6.27	107.53	113.80
1	C	319	ASP	CA-C-N	-6.24	113.57	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	ASP	C-N-CA	-6.24	113.57	122.00
1	A	778	THR	CA-CB-OG1	-6.24	100.24	109.60
1	A	832	ASP	N-CA-CB	-6.24	102.50	111.54
1	B	916	ASP	CA-CB-CG	-6.21	106.39	112.60
1	B	546	LEU	N-CA-CB	6.21	120.99	110.49
1	C	570	TRP	N-CA-C	6.21	117.92	111.03
1	C	320	GLY	CA-C-N	-6.21	114.16	122.72
1	C	320	GLY	C-N-CA	-6.21	114.16	122.72
1	B	722	LEU	O-C-N	-6.20	114.35	122.59
1	C	684	GLU	CB-CA-C	-6.20	101.44	110.06
1	A	1021	CYS	CA-CB-SG	-6.19	100.17	114.40
1	B	845	GLN	O-C-N	6.18	130.30	122.57
1	A	770	ILE	N-CA-CB	6.18	119.62	112.15
1	B	634	GLN	N-CA-C	-6.17	105.33	112.92
1	D	820	ALA	N-CA-C	6.17	118.85	108.23
1	D	785	THR	CA-CB-OG1	-6.17	100.35	109.60
1	D	161	TYR	N-CA-CB	-6.16	100.06	111.52
1	A	264	GLU	CA-C-N	-6.16	114.22	122.72
1	A	264	GLU	C-N-CA	-6.16	114.22	122.72
1	B	93	HIS	CA-CB-CG	-6.16	107.64	113.80
1	D	469	ASP	CA-CB-CG	-6.14	106.45	112.60
1	C	553	TRP	CA-CB-CG	-6.13	101.94	113.60
1	C	653	HIS	CA-CB-CG	6.13	119.93	113.80
1	D	878	HIS	CA-CB-CG	-6.11	107.69	113.80
1	B	875	ASP	CA-CB-CG	-6.11	106.49	112.60
1	D	968	MET	N-CA-CB	-6.11	100.82	110.28
1	B	52	ARG	CB-CA-C	-6.09	98.42	109.38
1	B	986	ILE	CB-CG1-CD1	-6.07	101.05	113.80
1	C	39	SER	N-CA-C	6.07	117.89	111.28
1	A	784	PHE	CA-CB-CG	-6.06	107.74	113.80
1	B	843	GLN	O-C-N	6.04	131.00	123.15
1	D	958	ASN	N-CA-CB	6.04	122.20	111.69
1	D	113	PHE	CA-CB-CG	-6.04	107.76	113.80
1	A	477	SER	CB-CA-C	-6.04	100.65	110.79
1	B	893	GLU	N-CA-C	6.04	117.94	111.36
1	C	735	HIS	CA-CB-CG	6.04	119.84	113.80
1	C	641	GLU	N-CA-CB	6.01	119.33	110.56
1	A	63	PHE	CA-CB-CG	-6.00	107.80	113.80
1	A	601	PHE	CA-CB-CG	-5.99	107.81	113.80
1	B	468	HIS	ND1-CG-CD2	5.99	112.09	106.10
1	A	659	ASP	CB-CA-C	-5.99	103.39	111.89
1	B	161	TYR	N-CA-CB	-5.99	100.39	111.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	442	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	A	193	ASP	CA-CB-CG	-5.97	106.63	112.60
1	B	878	HIS	CA-CB-CG	-5.97	107.83	113.80
1	D	329	ASP	CA-CB-CG	-5.96	106.64	112.60
1	A	499	ILE	N-CA-C	-5.95	100.98	108.84
1	D	14	ARG	N-CA-C	-5.95	100.66	109.11
1	B	370	GLN	CB-CG-CD	5.95	122.72	112.60
1	B	384	PHE	CA-CB-CG	-5.95	107.85	113.80
1	C	952	ARG	CD-NE-CZ	5.94	132.72	124.40
1	A	433	LEU	CA-C-O	5.94	124.10	118.34
1	A	790	ASP	CA-CB-CG	-5.94	106.66	112.60
1	D	395	HIS	N-CA-CB	-5.93	101.04	109.75
1	D	477	SER	CB-CA-C	-5.92	100.84	110.79
1	D	734	SER	O-C-N	5.92	130.73	123.21
1	C	653	HIS	N-CA-CB	5.91	120.07	110.43
1	A	832	ASP	CA-CB-CG	-5.91	106.69	112.60
1	C	719	GLN	CB-CA-C	-5.91	97.67	109.79
1	B	648	ASP	N-CA-C	5.91	119.55	112.93
1	B	692	GLY	O-C-N	5.90	128.67	123.06
1	B	759	ASN	CA-CB-CG	-5.90	106.70	112.60
1	C	482	ARG	CB-CA-C	-5.89	100.36	109.20
1	B	931	PHE	CA-CB-CG	-5.89	107.91	113.80
1	D	75	GLU	N-CA-CB	5.89	119.06	110.47
1	A	556	PHE	CA-CB-CG	5.87	119.67	113.80
1	D	787	ALA	N-CA-C	-5.87	98.82	109.44
1	D	734	SER	CA-C-O	5.86	126.93	120.71
1	C	771	GLY	CA-C-N	-5.85	112.89	122.54
1	C	771	GLY	C-N-CA	-5.85	112.89	122.54
1	A	274	PHE	CA-CB-CG	-5.84	107.96	113.80
1	B	842	TRP	CE2-CD2-CE3	5.84	124.64	118.80
1	D	309	TYR	N-CA-C	-5.84	100.88	109.81
1	D	511	PRO	N-CA-CB	5.83	106.33	102.25
1	B	842	TRP	CG-CD2-CE3	-5.83	128.07	133.90
1	B	788	PRO	N-CA-C	5.82	120.00	111.03
1	D	854	LYS	CB-CA-C	-5.82	97.26	110.07
1	A	705	ALA	CA-C-O	-5.81	115.13	121.87
1	A	928	PRO	CB-CA-C	-5.79	105.31	112.89
1	B	181	GLU	CB-CG-CD	5.78	122.43	112.60
1	A	730	LEU	CB-CA-C	5.78	117.75	109.26
1	B	869	ASP	CA-CB-CG	-5.75	106.85	112.60
1	C	664	ALA	CB-CA-C	-5.75	100.15	110.03
1	A	115	PRO	CB-CA-C	-5.74	103.88	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	649	ASN	N-CA-C	-5.73	100.95	109.83
1	C	699	ARG	CD-NE-CZ	5.72	132.41	124.40
1	C	297	ASN	CB-CA-C	-5.72	105.33	110.71
1	C	1019	VAL	N-CA-CB	5.71	118.66	111.46
1	A	14	ARG	N-CA-C	-5.71	101.66	109.71
1	D	685	LEU	N-CA-C	5.71	117.81	110.39
1	B	949	HIS	CB-CA-C	-5.70	99.87	109.50
1	D	618	THR	CA-CB-OG1	-5.70	101.06	109.60
1	A	948	PRO	CB-CA-C	-5.69	102.86	110.88
1	D	733	ALA	CA-C-N	-5.69	114.68	122.93
1	D	733	ALA	C-N-CA	-5.69	114.68	122.93
1	D	864	MET	CA-C-N	-5.69	114.17	122.19
1	D	864	MET	C-N-CA	-5.69	114.17	122.19
1	D	115	PRO	N-CA-CB	5.68	108.30	103.35
1	A	540[A]	HIS	CA-CB-CG	-5.67	108.12	113.80
1	A	540[B]	HIS	CA-CB-CG	-5.67	108.12	113.80
1	A	553	TRP	CA-CB-CG	-5.67	102.83	113.60
1	C	52	ARG	CB-CA-C	-5.67	98.99	109.37
1	A	746	ASP	CA-CB-CG	-5.67	106.93	112.60
1	D	595	THR	CB-CA-C	5.67	117.67	109.45
1	C	614	HIS	N-CA-C	-5.65	102.79	110.36
1	B	964	GLN	CA-C-O	5.63	126.52	120.55
1	A	869	ASP	CA-CB-CG	-5.63	106.97	112.60
1	D	144	ASP	CA-CB-CG	-5.63	106.97	112.60
1	C	799	THR	CA-CB-CG2	-5.62	100.94	110.50
1	D	14	ARG	N-CA-CB	-5.62	101.28	110.11
1	C	110	ASN	CA-C-O	5.62	127.85	120.16
1	B	658	LEU	CA-C-N	-5.60	114.41	122.36
1	B	658	LEU	C-N-CA	-5.60	114.41	122.36
1	C	262	GLN	N-CA-C	-5.60	96.44	107.69
1	C	704	ASN	CA-CB-CG	-5.60	107.00	112.60
1	D	519	SER	N-CA-C	-5.59	102.36	110.24
1	A	772	ASP	N-CA-CB	-5.58	102.23	110.49
1	A	721	ARG	CB-CA-C	-5.57	101.15	110.29
1	A	755	ARG	NE-CZ-NH2	-5.56	114.19	119.20
1	B	568	TRP	CA-CB-CG	-5.56	103.03	113.60
1	C	730	LEU	CA-C-N	5.56	125.74	119.90
1	C	730	LEU	C-N-CA	5.56	125.74	119.90
1	B	63	PHE	CA-CB-CG	-5.56	108.24	113.80
1	D	164	ASP	CA-CB-CG	-5.56	107.04	112.60
1	C	599	ARG	N-CA-C	5.56	116.76	108.31
1	C	842	TRP	CA-CB-CG	-5.56	103.04	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASN	CA-CB-CG	-5.55	107.05	112.60
1	D	844	HIS	CA-C-N	-5.55	114.37	122.19
1	D	844	HIS	C-N-CA	-5.55	114.37	122.19
1	A	416	GLU	CA-CB-CG	-5.55	103.01	114.10
1	B	571	VAL	N-CA-C	5.54	116.72	108.46
1	B	871	GLU	CB-CG-CD	-5.53	103.19	112.60
1	C	519	SER	N-CA-C	-5.53	102.44	110.24
1	D	320	GLY	CA-C-N	-5.53	114.39	122.19
1	D	320	GLY	C-N-CA	-5.53	114.39	122.19
1	D	948	PRO	CB-CA-C	-5.53	102.68	111.04
1	D	352	ARG	CA-C-N	-5.53	116.72	122.69
1	D	352	ARG	C-N-CA	-5.53	116.72	122.69
1	D	725	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	A	113	PHE	CA-CB-CG	-5.52	108.28	113.80
1	D	477	SER	N-CA-CB	5.52	118.30	110.13
1	D	662	PRO	N-CA-CB	5.51	108.10	103.25
1	A	360	HIS	CA-CB-CG	-5.51	108.29	113.80
1	B	345	ASN	CA-CB-CG	-5.51	107.09	112.60
1	D	802	ASP	CA-CB-CG	-5.51	107.09	112.60
1	D	572	ASP	CB-CA-C	-5.50	101.32	109.90
1	A	181	GLU	N-CA-C	5.49	118.19	109.96
1	B	631	LEU	CA-C-N	-5.49	114.48	122.44
1	B	631	LEU	C-N-CA	-5.49	114.48	122.44
1	C	442	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	B	920	LEU	O-C-N	5.48	125.22	121.71
1	D	553	TRP	CA-CB-CG	-5.47	103.20	113.60
1	B	479	ASP	CA-CB-CG	-5.47	107.13	112.60
1	D	719	GLN	CB-CA-C	-5.46	97.97	109.38
1	A	773	LYS	N-CA-C	5.46	117.64	108.96
1	C	431	ARG	CA-CB-CG	-5.46	103.19	114.10
1	C	832	ASP	N-CA-CB	-5.46	102.21	111.27
1	B	436	MET	CA-C-N	-5.45	112.97	120.28
1	B	436	MET	C-N-CA	-5.45	112.97	120.28
1	B	89	ASN	N-CA-C	-5.45	100.30	109.07
1	C	171	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	96	ASP	N-CA-CB	5.45	119.85	111.46
1	B	332	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	917	ARG	CD-NE-CZ	-5.44	116.78	124.40
1	C	674	PRO	N-CA-CB	5.44	108.17	103.27
1	B	592	PHE	CA-CB-CG	-5.43	108.36	113.80
1	B	553	TRP	CA-CB-CG	-5.43	103.28	113.60
1	C	844	HIS	CA-CB-CG	-5.43	108.37	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	THR	N-CA-C	-5.43	105.52	111.82
1	C	597	ASN	CA-CB-CG	-5.43	107.17	112.60
1	B	614	HIS	N-CA-C	-5.42	102.26	110.39
1	A	917	ARG	NE-CZ-NH2	-5.42	114.32	119.20
1	B	797	GLU	CA-CB-CG	-5.42	103.27	114.10
1	D	581	ASN	CA-CB-CG	5.42	118.02	112.60
1	A	243	GLU	CA-C-N	-5.41	115.43	122.94
1	A	243	GLU	C-N-CA	-5.41	115.43	122.94
1	A	799	THR	N-CA-CB	-5.41	101.33	110.41
1	D	499	ILE	N-CA-C	-5.41	101.70	108.84
1	A	755	ARG	NE-CZ-NH1	5.40	126.90	121.50
1	B	690	SER	N-CA-CB	5.40	119.62	110.49
1	C	768	MET	N-CA-CB	5.40	120.80	111.13
1	B	166	ARG	N-CA-C	5.40	119.84	112.88
1	C	784	PHE	CA-CB-CG	-5.39	108.41	113.80
1	D	747	PHE	CA-CB-CG	5.39	119.19	113.80
1	A	277	GLU	CB-CG-CD	5.39	121.76	112.60
1	A	345	ASN	CA-CB-CG	-5.39	107.21	112.60
1	D	592	PHE	CA-CB-CG	-5.38	108.42	113.80
1	D	835	LEU	CA-C-N	-5.36	116.55	123.19
1	D	835	LEU	C-N-CA	-5.36	116.55	123.19
1	B	859	ASP	CA-CB-CG	-5.35	107.25	112.60
1	D	945	ASN	CA-CB-CG	-5.35	107.25	112.60
1	C	370	GLN	CB-CG-CD	5.35	121.69	112.60
1	B	688	PRO	N-CA-CB	5.34	108.86	103.25
1	A	896	ASN	OD1-CG-ND2	5.33	127.93	122.60
1	A	100	TYR	CA-CB-CG	-5.33	104.31	113.90
1	C	850	PHE	CA-CB-CG	5.32	119.12	113.80
1	D	231	PHE	CA-CB-CG	-5.32	108.48	113.80
1	A	771	GLY	CA-C-N	-5.32	113.76	122.54
1	A	771	GLY	C-N-CA	-5.32	113.76	122.54
1	C	136	GLU	CB-CA-C	-5.31	98.38	110.07
1	A	845	GLN	CA-C-N	-5.31	115.11	122.86
1	A	845	GLN	C-N-CA	-5.31	115.11	122.86
1	C	782	ASP	CA-CB-CG	-5.31	107.29	112.60
1	D	409	VAL	N-CA-C	5.30	116.12	108.48
1	D	241	GLU	CB-CG-CD	-5.30	103.59	112.60
1	A	602	CYS	CA-C-N	-5.30	115.30	123.14
1	A	602	CYS	C-N-CA	-5.30	115.30	123.14
1	D	593	GLY	CA-C-O	5.30	124.90	119.02
1	B	314	GLU	CB-CA-C	-5.30	100.56	109.72
1	B	630	ARG	CA-C-N	-5.30	115.00	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	630	ARG	C-N-CA	-5.30	115.00	122.94
1	D	365	GLN	N-CA-CB	-5.29	102.81	110.70
1	C	433	LEU	CA-C-O	5.29	123.92	118.73
1	A	672	VAL	CB-CA-C	-5.29	102.74	110.62
1	C	123	TYR	CB-CA-C	-5.29	99.69	109.37
1	A	866	ILE	CB-CA-C	-5.28	102.82	110.63
1	D	76	CYS	O-C-N	5.28	129.39	123.27
1	D	229	THR	CA-C-O	-5.27	114.65	120.24
1	A	722	LEU	O-C-N	-5.27	115.58	122.59
1	B	728	VAL	CA-C-O	5.27	124.76	119.97
1	C	746	ASP	N-CA-C	5.27	116.81	108.96
1	C	846	GLY	CA-C-N	-5.27	115.29	122.93
1	C	846	GLY	C-N-CA	-5.27	115.29	122.93
1	D	134	LEU	N-CA-C	-5.27	105.59	112.23
1	D	855	THR	N-CA-CB	5.26	120.53	111.00
1	D	221	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	B	583	ASN	CA-CB-CG	-5.26	107.34	112.60
1	C	917	ARG	CD-NE-CZ	-5.25	117.05	124.40
1	D	257	THR	CA-C-N	-5.25	116.26	123.14
1	D	257	THR	C-N-CA	-5.25	116.26	123.14
1	C	479	ASP	CA-C-O	5.25	126.93	121.00
1	D	769	TRP	CA-C-O	5.24	126.68	120.66
1	B	75	GLU	CA-C-N	-5.24	112.69	121.75
1	B	75	GLU	C-N-CA	-5.24	112.69	121.75
1	D	915	PHE	CA-CB-CG	-5.24	108.56	113.80
1	A	736	ALA	N-CA-C	5.23	116.39	108.07
1	B	889	ALA	CA-C-O	5.23	125.99	119.97
1	D	817	GLN	CB-CG-CD	-5.23	103.71	112.60
1	B	986	ILE	CB-CA-C	5.23	118.20	110.77
1	C	952	ARG	NE-CZ-NH1	5.23	126.73	121.50
1	A	438	GLU	CG-CD-OE2	-5.23	106.38	118.40
1	B	739	HIS	CA-CB-CG	-5.23	108.57	113.80
1	C	510	GLN	CA-C-O	5.23	127.33	120.74
1	D	842	TRP	CA-C-O	-5.22	114.74	120.43
1	B	948	PRO	CB-CA-C	-5.22	104.16	110.00
1	B	694	LEU	CB-CA-C	-5.21	101.26	109.80
1	D	279	ILE	CA-CB-CG2	5.20	119.34	110.50
1	C	469	ASP	CA-CB-CG	-5.20	107.40	112.60
1	C	339	ASN	CA-CB-CG	-5.20	107.40	112.60
1	B	246	MET	CG-SD-CE	-5.19	89.47	100.90
1	B	368	ASP	CA-CB-CG	-5.19	107.41	112.60
1	B	257	THR	CA-C-N	-5.19	116.34	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	257	THR	C-N-CA	-5.19	116.34	123.14
1	B	572	ASP	CB-CA-C	-5.18	101.35	109.70
1	A	771	GLY	CA-C-O	5.18	127.16	120.89
1	A	234	ASP	CA-CB-CG	-5.17	107.43	112.60
1	A	800	ARG	CA-CB-CG	5.17	124.45	114.10
1	C	320	GLY	O-C-N	-5.17	116.75	122.55
1	B	659	ASP	CA-CB-CG	-5.16	107.44	112.60
1	A	746	ASP	N-CA-C	5.16	116.91	109.07
1	A	942	ARG	CA-CB-CG	-5.16	103.79	114.10
1	A	221	GLN	N-CA-CB	-5.15	103.42	111.56
1	C	746	ASP	N-CA-CB	-5.15	103.42	111.56
1	A	210	ARG	N-CA-CB	5.15	118.65	110.87
1	C	368	ASP	CA-CB-CG	-5.15	107.45	112.60
1	B	699	ARG	CD-NE-CZ	5.15	131.61	124.40
1	C	844	HIS	ND1-CG-CD2	5.14	111.24	106.10
1	A	14	ARG	CA-CB-CG	-5.13	103.83	114.10
1	C	348	PRO	N-CA-CB	5.13	107.40	103.30
1	C	835	LEU	N-CA-C	5.13	116.99	108.02
1	C	692	GLY	O-C-N	5.12	127.93	123.06
1	C	710	GLU	N-CA-CB	-5.12	102.66	110.45
1	D	392	TYR	N-CA-C	-5.12	103.52	108.13
1	B	538	TYR	O-C-N	5.12	128.90	123.42
1	C	499	ILE	CA-C-N	-5.12	117.16	122.89
1	C	499	ILE	C-N-CA	-5.12	117.16	122.89
1	A	522	LYS	CA-C-O	5.11	125.84	120.42
1	D	867	THR	CA-C-O	-5.11	114.84	120.36
1	B	315	LEU	N-CA-C	-5.10	100.92	109.24
1	C	989	PHE	CA-CB-CG	-5.10	108.70	113.80
1	B	670	LEU	CA-C-N	-5.10	114.00	122.92
1	B	670	LEU	C-N-CA	-5.10	114.00	122.92
1	C	96	ASP	N-CA-CB	5.10	119.31	111.46
1	D	788	PRO	N-CA-CB	5.10	107.85	103.31
1	A	747	PHE	N-CA-CB	5.10	118.55	110.55
1	D	663	LEU	N-CA-C	-5.10	106.40	113.18
1	D	601	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	97	ALA	N-CA-C	5.09	116.48	110.07
1	D	13	ARG	CA-C-N	-5.09	115.97	122.79
1	D	13	ARG	C-N-CA	-5.09	115.97	122.79
1	B	779	PRO	CB-CA-C	-5.08	104.56	111.12
1	C	739	HIS	ND1-CG-CD2	5.08	111.18	106.10
1	A	319	ASP	CA-CB-CG	-5.08	107.52	112.60
1	A	30	HIS	CA-CB-CG	-5.08	108.72	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ASN	N-CA-CB	-5.08	102.73	110.65
1	D	757	GLN	CA-CB-CG	-5.08	103.95	114.10
1	D	845	GLN	CA-C-N	-5.08	114.13	122.20
1	D	845	GLN	C-N-CA	-5.08	114.13	122.20
1	D	52	ARG	CB-CA-C	-5.07	100.09	109.37
1	D	395	HIS	ND1-CE1-NE2	5.07	113.47	108.40
1	D	76	CYS	N-CA-C	5.07	117.08	109.23
1	A	75	GLU	CA-C-N	-5.06	112.99	121.75
1	A	75	GLU	C-N-CA	-5.06	112.99	121.75
1	B	781	ARG	CD-NE-CZ	5.06	131.49	124.40
1	A	365	GLN	CA-CB-CG	-5.06	103.99	114.10
1	A	675	GLN	CA-CB-CG	-5.06	103.98	114.10
1	A	890	GLN	N-CA-CB	-5.06	102.60	110.29
1	D	681	GLU	N-CA-CB	5.06	118.67	110.17
1	A	872	VAL	CB-CA-C	-5.05	103.16	110.63
1	D	842	TRP	CA-CB-CG	-5.05	104.00	113.60
1	B	877	PRO	N-CA-CB	5.05	107.80	103.31
1	C	480	PRO	CA-N-CD	5.05	119.07	112.00
1	A	226	HIS	CB-CA-C	-5.05	100.56	109.70
1	A	770	ILE	N-CA-C	-5.05	98.70	106.72
1	B	632	SER	N-CA-CB	5.05	118.77	110.90
1	A	363	HIS	CA-CB-CG	-5.04	108.76	113.80
1	C	661	LYS	CA-C-O	5.04	122.57	119.29
1	D	75	GLU	CA-C-N	-5.04	113.97	122.29
1	D	75	GLU	C-N-CA	-5.04	113.97	122.29
1	D	519	SER	N-CA-CB	-5.04	101.68	109.69
1	C	859	ASP	CA-C-N	5.03	126.47	120.13
1	C	859	ASP	C-N-CA	5.03	126.47	120.13
1	C	210	ARG	N-CA-CB	5.03	118.60	111.05
1	B	237	ARG	CA-CB-CG	-5.03	104.04	114.10
1	D	734	SER	CB-CA-C	5.02	118.42	109.38
1	C	395	HIS	ND1-CG-CD2	5.02	111.12	106.10
1	C	345	ASN	CA-CB-CG	-5.02	107.58	112.60
1	A	725	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	A	735	HIS	CB-CA-C	5.01	117.39	111.22
1	A	702	GLN	CA-C-O	5.01	123.57	119.36
1	C	447	ASP	N-CA-C	5.01	120.01	113.30
1	B	519	SER	N-CA-CB	-5.01	102.27	109.83
1	B	606	LEU	N-CA-C	-5.01	106.68	112.89
1	D	296	GLU	CB-CG-CD	-5.01	104.09	112.60
1	D	768	MET	N-CA-CB	5.00	120.83	111.53

All (3) chirality outliers are listed below:

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

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8128	0	7712	124	0
1	B	8128	0	7712	163	0
1	C	8128	0	7712	133	0
1	D	8128	0	7712	147	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	42	0	27	2	0
4	B	42	0	27	1	0
4	C	42	0	27	2	0
4	D	42	0	27	4	0
5	A	108	0	162	15	0
5	B	100	0	150	18	0
5	C	108	0	162	14	0
5	D	112	0	168	24	0
6	A	1060	0	0	20	3
6	B	1013	0	0	18	1
6	C	987	0	0	21	2
6	D	1021	0	0	18	0
All	All	37222	0	31598	595	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (595) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:8407:DMS:C2	5:B:8407:DMS:S	2.01	1.48
5:B:8502:DMS:C1	5:B:8502:DMS:S	2.01	1.46
5:D:8407:DMS:C2	5:D:8407:DMS:S	2.04	1.46
5:C:8415:DMS:S	5:C:8415:DMS:C2	2.04	1.45
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.37	1.21
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.41	1.16
1:B:942:ARG:HH21	1:B:954:ASP:HB2	1.07	1.10
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.37	1.07
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.35	1.05
1:D:133:TRP:HE1	5:D:8703:DMS:H23	1.21	1.04
1:C:634:GLN:H	1:C:634:GLN:NE2	1.57	1.02
1:D:292:ARG:HH12	5:D:8412:DMS:H23	1.25	0.99
1:D:133:TRP:NE1	5:D:8703:DMS:H23	1.77	0.98
1:D:651:LEU:HD21	1:D:653:HIS:CE1	2.00	0.96
1:D:581:ASN:HD22	1:D:583:ASN:ND2	1.63	0.95
1:D:581:ASN:HD22	1:D:583:ASN:HD22	1.05	0.94
1:A:473:ARG:NH1	1:A:476:LYS:HB2	1.85	0.91
1:C:634:GLN:H	1:C:634:GLN:HE21	1.02	0.91
1:C:765:LEU:CD2	1:C:768:MET:HE2	2.01	0.91
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.07	0.89
1:D:737:ILE:HD12	1:D:738:PRO:CD	2.03	0.88
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.55	0.87
1:A:1022:GLN:HG2	1:A:1023:LYS:N	1.91	0.86
1:D:658:LEU:O	1:D:661:LYS:HG3	1.75	0.85
1:B:942:ARG:HH21	1:B:954:ASP:CB	1.89	0.84
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.42	0.84
1:B:942:ARG:NH2	1:B:954:ASP:HB2	1.91	0.83
5:D:8703:DMS:H21	6:D:9650:HOH:O	1.77	0.83
5:C:8417:DMS:H22	6:C:9329:HOH:O	1.78	0.83
1:C:748:CYS:C	1:C:749:ILE:HD12	2.04	0.82
1:B:651:LEU:O	1:B:651:LEU:HD23	1.80	0.81
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.43	0.81
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.63	0.81
1:B:600:GLN:H	1:B:600:GLN:HE21	1.24	0.80
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.17	0.80
1:A:942:ARG:HB3	6:A:9413:HOH:O	1.78	0.80
1:A:600:GLN:H	1:A:600:GLN:HE21	1.30	0.80
1:D:651:LEU:CD2	1:D:701:VAL:HB	2.11	0.80
1:D:133:TRP:HE1	5:D:8703:DMS:C2	1.96	0.79
1:A:655:MET:HE2	1:A:656:VAL:N	1.97	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:VAL:O	5:A:8602:DMS:H23	1.83	0.78
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.17	0.78
1:D:128:ASN:HB3	1:D:180:GLY:O	1.83	0.78
6:B:9369:HOH:O	5:C:8420:DMS:H22	1.82	0.77
1:A:809:ARG:HG2	1:A:809:ARG:HH11	1.49	0.77
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.14	0.77
1:C:745:MET:HG2	6:C:9532:HOH:O	1.84	0.77
1:C:655:MET:HE2	1:C:665:SER:HB3	1.67	0.76
1:C:634:GLN:NE2	1:C:634:GLN:N	2.34	0.76
1:C:615:PRO:O	1:C:618:THR:HG22	1.86	0.76
1:D:629:PHE:O	1:D:630:ARG:HD3	1.85	0.76
1:D:1013:ARG:HD3	6:D:9311:HOH:O	1.84	0.76
1:B:236:SER:C	1:B:237:ARG:HG2	2.10	0.75
1:C:737:ILE:HD12	1:C:832:ASP:C	2.12	0.74
5:C:8419:DMS:H13	6:C:9057:HOH:O	1.85	0.74
1:B:778:THR:HG23	1:B:887:GLN:HB3	1.69	0.74
1:C:131:GLU:HG3	1:C:135:GLN:NE2	2.02	0.74
1:D:800:ARG:HD2	6:D:9504:HOH:O	1.87	0.74
1:A:231:PHE:O	5:A:8417:DMS:H23	1.88	0.74
1:B:658:LEU:O	1:B:661:LYS:HG3	1.86	0.73
1:C:771:GLY:HA2	6:C:9614:HOH:O	1.88	0.73
1:C:843:GLN:HG2	1:C:848:THR:HA	1.71	0.73
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.71	0.72
1:D:737:ILE:HD12	1:D:738:PRO:HD2	1.69	0.72
1:D:237:ARG:NH1	6:D:9268:HOH:O	2.21	0.72
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.51	0.72
1:C:743:SER:O	1:C:760:ARG:NH1	2.22	0.72
1:B:693:GLN:CD	1:B:721:ARG:HG2	2.14	0.72
1:B:890:GLN:HG3	1:B:891:VAL:N	2.05	0.72
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.70	0.72
1:B:237:ARG:HD2	1:B:296:GLU:OE1	1.89	0.72
1:D:703:PRO:HG2	5:D:8425:DMS:H12	1.71	0.72
1:B:262:GLN:HE21	1:B:262:GLN:C	1.96	0.72
1:D:292:ARG:HH12	5:D:8412:DMS:C2	1.99	0.72
1:B:615:PRO:O	1:B:618:THR:HG22	1.90	0.71
1:B:262:GLN:HE21	1:B:263:GLY:N	1.87	0.71
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.24	0.70
1:B:131:GLU:OE2	1:B:134:LEU:HB2	1.91	0.70
1:B:693:GLN:NE2	1:B:723:ALA:O	2.23	0.70
1:C:41:GLU:HG2	1:C:46:ARG:NH2	2.05	0.70
1:D:749:ILE:HD12	1:D:749:ILE:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ASP:HA	5:D:8417:DMS:H13	1.74	0.70
1:D:367:MET:HB3	1:D:372:MET:HE2	1.73	0.70
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.73	0.69
1:B:699:ARG:NH2	5:B:8415:DMS:H11	2.07	0.69
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.04	0.69
1:D:581:ASN:ND2	1:D:583:ASN:HD22	1.87	0.69
1:C:878:HIS:HD2	6:C:8797:HOH:O	1.75	0.69
1:D:809:ARG:HH11	1:D:809:ARG:HG2	1.58	0.69
5:A:8415:DMS:H11	6:A:9519:HOH:O	1.93	0.69
1:D:237:ARG:HH11	1:D:237:ARG:HG2	1.58	0.68
1:C:765:LEU:HD21	1:C:768:MET:CE	2.19	0.68
1:A:887:GLN:NE2	1:A:980:GLU:O	2.25	0.68
1:D:804:ASN:HD22	1:D:809:ARG:HH21	0.73	0.68
1:D:887:GLN:NE2	1:D:980:GLU:O	2.25	0.68
5:A:8503:DMS:H22	6:A:9019:HOH:O	1.94	0.68
1:B:243:GLU:OE2	1:B:245:GLN:NE2	2.26	0.68
1:B:655:MET:HE2	1:B:664:ALA:O	1.94	0.68
5:B:8410:DMS:H22	6:B:8879:HOH:O	1.93	0.68
1:A:878:HIS:HD2	6:A:8675:HOH:O	1.77	0.68
1:C:750:GLU:HG2	6:C:9529:HOH:O	1.94	0.68
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.27	0.67
1:A:387:VAL:HG22	6:A:9621:HOH:O	1.93	0.67
1:A:237:ARG:HB3	1:A:237:ARG:NH1	2.08	0.67
1:A:651:LEU:C	1:A:651:LEU:HD12	2.20	0.67
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.75	0.67
1:C:367:MET:HB3	1:C:372:MET:HE2	1.77	0.67
1:C:651:LEU:HD12	1:C:651:LEU:C	2.20	0.67
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.28	0.66
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.61	0.66
1:D:973:ARG:O	5:D:8423:DMS:H12	1.95	0.66
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.09	0.66
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.29	0.66
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.77	0.65
1:A:973:ARG:O	5:A:8423:DMS:H12	1.96	0.65
1:C:634:GLN:HE21	1:C:634:GLN:N	1.86	0.65
1:A:809:ARG:HH11	1:A:809:ARG:CG	2.08	0.65
1:B:634:GLN:HE21	1:B:685:LEU:HG	1.61	0.65
1:C:737:ILE:HG13	1:C:738:PRO:HD2	1.79	0.64
1:D:748:CYS:C	1:D:749:ILE:HD12	2.20	0.64
1:D:773:LYS:HD2	1:D:774:LYS:O	1.97	0.64
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:878:HIS:HD2	6:B:8694:HOH:O	1.79	0.64
1:B:251:ARG:NH1	5:B:8416:DMS:O	2.30	0.64
1:B:634:GLN:HG2	1:B:682:LEU:O	1.98	0.64
1:B:681:GLU:HA	1:B:681:GLU:OE2	1.93	0.64
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.09	0.64
5:D:8410:DMS:H12	6:D:9660:HOH:O	1.97	0.64
1:A:292:ARG:HH12	5:A:8412:DMS:H22	1.60	0.64
1:A:431:ARG:HG3	6:A:9354:HOH:O	1.97	0.64
1:C:131:GLU:HG3	1:C:135:GLN:HE21	1.61	0.63
1:A:615:PRO:O	1:A:618:THR:HG22	1.99	0.63
1:D:651:LEU:C	1:D:651:LEU:HD23	2.23	0.63
1:D:1022:GLN:O	1:D:1023:LYS:HB2	1.98	0.63
1:A:277:GLU:H	1:A:277:GLU:CD	2.07	0.63
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.33	0.63
1:A:237:ARG:NH1	6:A:9130:HOH:O	2.28	0.62
1:D:651:LEU:HD21	1:D:653:HIS:HE1	1.59	0.62
1:B:651:LEU:HD23	1:B:651:LEU:C	2.25	0.62
5:C:8503:DMS:H13	6:C:9140:HOH:O	1.99	0.62
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.65	0.62
1:D:893:GLU:HG2	1:D:894:ARG:HG2	1.82	0.62
1:B:635:THR:HG23	1:B:681:GLU:OE1	2.00	0.62
1:B:595:THR:HA	1:B:596:PRO:C	2.25	0.62
1:C:684:GLU:HG2	1:C:684:GLU:O	1.99	0.62
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.15	0.62
1:C:745:MET:HE3	1:C:745:MET:HA	1.81	0.61
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.64	0.61
1:A:32:PRO:HB2	5:A:8404:DMS:H13	1.82	0.61
1:A:861:SER:OG	1:A:863:GLN:HG3	2.01	0.61
1:B:751:LEU:HD23	1:B:862:GLY:HA2	1.82	0.61
1:C:92:MET:HE2	1:C:92:MET:HA	1.83	0.61
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.35	0.61
1:D:651:LEU:HD23	1:D:651:LEU:O	2.01	0.61
1:B:699:ARG:HH21	5:B:8415:DMS:H11	1.65	0.61
1:C:1023:LYS:HE3	1:C:1023:LYS:CA	2.31	0.61
1:C:646:HIS:HB3	6:C:9551:HOH:O	2.00	0.60
1:A:595:THR:HA	1:A:596:PRO:C	2.25	0.60
1:C:135:GLN:HG3	6:C:9667:HOH:O	2.01	0.60
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.36	0.60
1:D:781:ARG:NH1	6:D:9459:HOH:O	2.34	0.60
1:C:266:GLN:HE21	5:C:8602:DMS:H23	1.66	0.60
1:D:135:GLN:C	1:D:136:GLU:HG2	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:C	1:A:737:ILE:HD13	2.27	0.59
1:C:737:ILE:HG13	1:C:738:PRO:CD	2.32	0.59
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.68	0.59
1:D:252:ASP:OD1	5:D:8416:DMS:H23	2.03	0.59
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.84	0.59
5:B:8420:DMS:H21	6:B:9083:HOH:O	2.03	0.59
1:B:843:GLN:HB3	1:B:847:LYS:O	2.03	0.58
1:B:847:LYS:HG2	1:B:849:LEU:HD23	1.86	0.58
1:C:595:THR:HA	1:C:596:PRO:C	2.27	0.58
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.38	0.58
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.03	0.58
5:C:8425:DMS:H22	6:C:9506:HOH:O	2.03	0.58
1:A:178:ARG:HD2	6:A:9459:HOH:O	2.04	0.58
1:C:88:SER:HA	1:C:366:VAL:HG21	1.85	0.57
1:C:1023:LYS:C	6:C:9668:HOH:O	2.47	0.57
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.39	0.57
5:C:8410:DMS:H11	6:C:9067:HOH:O	2.04	0.57
1:B:251:ARG:HD2	5:B:8416:DMS:H23	1.87	0.56
1:D:595:THR:HA	1:D:596:PRO:C	2.29	0.56
1:D:1022:GLN:HE21	1:D:1022:GLN:C	2.13	0.56
1:A:859:ASP:OD1	1:A:861:SER:OG	2.23	0.56
1:B:379:MET:HE1	1:B:387:VAL:HB	1.85	0.56
1:A:865:ALA:HB1	1:A:1017:GLN:HE22	1.70	0.56
1:B:947:GLY:O	1:B:1023:LYS:HE3	2.05	0.56
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.35	0.56
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.87	0.56
1:A:290:THR:O	5:A:8412:DMS:H23	2.06	0.56
1:D:878:HIS:HD2	6:D:8810:HOH:O	1.89	0.56
1:B:372:MET:HE2	6:B:8811:HOH:O	2.05	0.56
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.74	0.56
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.41	0.56
1:B:630:ARG:HH21	1:B:637:GLU:CD	2.13	0.56
1:B:847:LYS:HG3	1:B:848:THR:N	2.20	0.56
1:D:773:LYS:HG3	1:D:775:GLN:HE21	1.71	0.56
1:D:581:ASN:ND2	1:D:583:ASN:ND2	2.46	0.55
1:C:750:GLU:OE2	1:C:755:ARG:HD2	2.06	0.55
1:D:754:LYS:HE2	1:D:1022:GLN:HG2	1.88	0.55
1:A:726:LEU:HD22	1:B:871:GLU:OE1	2.06	0.55
1:B:580:GLU:CD	1:B:580:GLU:H	2.14	0.55
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.41	0.55
1:C:1023:LYS:HE3	1:C:1023:LYS:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:843:GLN:HA	1:D:847:LYS:O	2.07	0.55
1:A:952:ARG:NH2	1:A:1021:CYS:SG	2.78	0.54
1:A:890:GLN:OE1	1:A:948:PRO:HD3	2.08	0.54
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.21	0.54
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.90	0.54
1:B:133:TRP:NE1	5:B:8504:DMS:H12	2.22	0.54
1:B:618:THR:HG23	6:B:9572:HOH:O	2.06	0.54
1:B:178:ARG:HG3	1:B:178:ARG:O	2.06	0.54
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.89	0.54
1:D:473:ARG:HD3	6:D:8720:HOH:O	2.06	0.54
1:C:649:ASN:OD1	1:C:703:PRO:HD2	2.07	0.54
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.43	0.54
1:C:1020:TRP:HD1	1:C:1021:CYS:N	2.06	0.54
1:A:230:ARG:NH1	1:A:241:GLU:OE2	2.40	0.53
1:A:88:SER:HA	1:A:366:VAL:HG21	1.90	0.53
1:D:800:ARG:HG3	1:D:800:ARG:O	2.07	0.53
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.67	0.53
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.90	0.53
1:B:962:TYR:OH	5:B:8508:DMS:H23	2.07	0.53
4:D:2002:145:O1	4:D:2002:145:O2'	2.25	0.53
1:B:347:LYS:HG3	1:B:644:PHE:CE2	2.43	0.53
1:C:833:ALA:HB1	1:C:858:ILE:O	2.08	0.53
1:A:658:LEU:O	1:A:661:LYS:HG3	2.07	0.53
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.44	0.53
1:A:843:GLN:HA	1:A:847:LYS:O	2.08	0.53
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.90	0.53
5:B:8407:DMS:C2	5:B:8407:DMS:C1	2.86	0.53
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.91	0.53
1:B:788:PRO:HD2	1:B:968:MET:HB2	1.91	0.53
1:C:601:PHE:CD1	4:C:2002:145:H3'	2.44	0.53
1:C:682:LEU:HB3	1:C:683:PRO:CD	2.38	0.53
1:C:756:TRP:CD2	1:C:858:ILE:HD13	2.43	0.53
1:A:292:ARG:HH12	5:A:8412:DMS:C2	2.22	0.52
1:B:945:ASN:HB3	1:B:1023:LYS:HE2	1.91	0.52
4:B:2002:145:O2'	4:B:2002:145:O1	2.26	0.52
4:C:2002:145:O2'	4:C:2002:145:O1	2.27	0.52
1:D:618:THR:HG21	6:D:9049:HOH:O	2.08	0.52
1:C:651:LEU:HD13	1:C:667:GLU:HG2	1.92	0.52
1:C:952:ARG:NH2	1:C:1021:CYS:SG	2.82	0.52
5:D:8419:DMS:H13	6:D:9068:HOH:O	2.09	0.52
1:C:1000:SER:O	1:C:1001:PRO:C	2.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ARG:HH11	5:A:8416:DMS:H23	1.75	0.52
1:C:759:ASN:OD1	1:C:761:GLN:N	2.41	0.52
1:B:533:LEU:HD23	1:B:533:LEU:C	2.35	0.52
1:B:751:LEU:HD23	1:B:862:GLY:CA	2.40	0.52
1:A:648:ASP:OD2	6:A:9498:HOH:O	2.19	0.51
1:C:768:MET:HE1	1:C:1020:TRP:CE3	2.45	0.51
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.46	0.51
1:B:804:ASN:HD22	1:B:809:ARG:NH2	2.09	0.51
1:D:618:THR:HG23	6:D:9065:HOH:O	2.10	0.51
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.91	0.51
1:B:78:LEU:HD23	6:B:9098:HOH:O	2.11	0.51
1:B:128:ASN:HB2	1:B:181:GLU:OE2	2.10	0.51
1:C:785:THR:O	1:C:881:ARG:HD2	2.09	0.51
1:B:231:PHE:O	5:B:8417:DMS:H23	2.10	0.51
1:D:237:ARG:NH1	1:D:237:ARG:HG2	2.22	0.51
1:D:675:GLN:HG3	6:D:9549:HOH:O	2.10	0.51
1:A:844:HIS:HD2	6:A:9428:HOH:O	1.92	0.51
1:B:745:MET:SD	1:B:745:MET:N	2.80	0.51
1:A:797:GLU:O	1:A:801:ILE:HD13	2.12	0.50
1:B:245:GLN:HG2	1:B:288:ARG:CG	2.39	0.50
1:B:88:SER:HA	1:B:366:VAL:HG21	1.92	0.50
1:D:431:ARG:NE	6:D:9592:HOH:O	2.43	0.50
1:A:651:LEU:CD1	1:A:653:HIS:CD2	2.94	0.50
1:B:730:LEU:O	1:B:731:PRO:C	2.54	0.50
1:A:376:ILE:HD12	1:A:401:LEU:HB3	1.94	0.50
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.80	0.50
1:D:88:SER:HA	1:D:366:VAL:HG21	1.93	0.50
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.26	0.50
1:A:835:LEU:HD11	1:A:855:THR:HB	1.94	0.50
1:A:843:GLN:HG2	1:A:848:THR:HA	1.93	0.50
1:D:653:HIS:ND1	1:D:701:VAL:CG2	2.75	0.50
5:D:8503:DMS:H22	6:D:9153:HOH:O	2.11	0.50
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.12	0.50
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.26	0.50
1:D:135:GLN:O	1:D:136:GLU:HG2	2.12	0.50
1:A:508:GLU:OE2	5:A:8407:DMS:H11	2.12	0.50
1:C:703:PRO:HG2	5:C:8425:DMS:H12	1.93	0.50
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.93	0.49
1:C:687:GLN:HG3	1:C:688:PRO:CD	2.26	0.49
1:D:241:GLU:HG3	1:D:292:ARG:HG2	1.94	0.49
1:C:861:SER:OG	1:C:863:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:8407:DMS:C2	5:D:8407:DMS:C1	2.87	0.49
1:C:126:THR:HA	1:C:182:ASN:O	2.12	0.49
1:C:266:GLN:HB3	5:C:8602:DMS:H23	1.93	0.49
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.94	0.49
1:D:668:VAL:HG11	1:D:680:ILE:HG12	1.95	0.49
1:A:237:ARG:HG2	1:A:296:GLU:OE1	2.13	0.49
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.75	0.49
1:C:745:MET:HE3	1:C:761:GLN:OE1	2.13	0.49
1:C:768:MET:HE1	1:C:1020:TRP:CZ3	2.48	0.49
1:A:292:ARG:NH1	5:A:8412:DMS:C2	2.76	0.49
1:C:13:ARG:O	1:C:14:ARG:C	2.48	0.49
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.95	0.49
1:D:601:PHE:CD1	4:D:2002:145:H3'	2.48	0.49
1:D:634:GLN:O	1:D:634:GLN:HG3	2.11	0.49
1:B:743:SER:HB2	1:B:745:MET:HE1	1.95	0.49
1:D:809:ARG:HG2	1:D:809:ARG:NH1	2.25	0.49
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.95	0.49
1:A:693:GLN:NE2	1:A:723:ALA:O	2.46	0.48
1:A:694:LEU:HB2	1:A:723:ALA:O	2.13	0.48
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.95	0.48
1:D:808:GLU:OE1	1:D:811:LYS:NZ	2.43	0.48
1:B:135:GLN:NE2	6:B:9398:HOH:O	2.28	0.48
1:C:782:ASP:HA	1:C:884:LEU:HD23	1.95	0.48
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.44	0.48
1:D:785:THR:HB	1:D:816:TYR:CE2	2.47	0.48
1:A:800:ARG:HG3	6:A:9370:HOH:O	2.14	0.48
1:C:580:GLU:H	1:C:580:GLU:HG3	1.27	0.48
1:B:722:LEU:O	1:B:723:ALA:C	2.52	0.48
1:C:749:ILE:HD12	1:C:749:ILE:N	2.28	0.48
1:D:765:LEU:HD21	1:D:768:MET:SD	2.54	0.48
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.95	0.48
1:B:942:ARG:N	1:B:942:ARG:HD2	2.27	0.48
1:C:569:ASP:HB2	6:C:9491:HOH:O	2.13	0.48
1:D:363:HIS:HD2	6:D:9312:HOH:O	1.96	0.48
1:D:768:MET:HE1	1:D:1020:TRP:CE2	2.49	0.48
1:B:241:GLU:CD	1:B:292:ARG:HE	2.22	0.48
1:C:367:MET:HA	1:C:367:MET:HE2	1.95	0.48
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.95	0.48
1:A:658:LEU:O	1:A:659:ASP:C	2.55	0.48
1:D:292:ARG:NH1	5:D:8412:DMS:H23	2.09	0.48
1:C:240:LEU:C	1:C:240:LEU:HD23	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:737:ILE:HD13	1:D:832:ASP:HA	1.95	0.48
1:D:795:VAL:HB	4:D:2002:145:C5'	2.43	0.48
1:A:178:ARG:HG3	6:A:9459:HOH:O	2.14	0.48
1:A:577:LYS:NZ	6:A:9606:HOH:O	2.38	0.48
1:A:1000:SER:O	1:A:1001:PRO:C	2.56	0.48
1:C:689:GLU:O	1:C:690:SER:HB3	2.13	0.48
1:D:513:PRO:O	1:D:514:ALA:HB3	2.14	0.48
1:B:251:ARG:NH1	1:B:251:ARG:HB3	2.29	0.47
1:A:721:ARG:NH2	6:A:9643:HOH:O	2.47	0.47
1:C:682:LEU:CB	1:C:683:PRO:CD	2.90	0.47
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.44	0.47
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.43	0.47
1:B:658:LEU:O	1:B:659:ASP:C	2.55	0.47
1:C:634:GLN:NE2	1:C:634:GLN:CA	2.76	0.47
1:B:842:TRP:C	1:B:843:GLN:HG3	2.37	0.47
1:C:533:LEU:C	1:C:533:LEU:HD23	2.39	0.47
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.96	0.47
1:A:521:LYS:HE2	6:A:9027:HOH:O	2.13	0.47
1:C:230:ARG:HG3	1:C:230:ARG:NH1	2.27	0.47
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.32	0.47
1:B:1000:SER:O	1:B:1001:PRO:C	2.54	0.47
5:B:8508:DMS:H13	6:B:8731:HOH:O	2.15	0.47
1:D:749:ILE:N	1:D:749:ILE:CD1	2.76	0.47
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.19	0.47
1:D:824:GLN:NE2	1:D:837:THR:HG22	2.30	0.47
1:A:795:VAL:HG11	4:A:2001:145:H4'	1.97	0.47
1:B:131:GLU:OE2	1:B:131:GLU:HA	2.15	0.47
1:D:797:GLU:HB2	1:D:800:ARG:HG3	1.97	0.47
1:B:46:ARG:HB3	1:B:47:PRO:CD	2.44	0.47
1:C:178:ARG:HD3	6:C:9559:HOH:O	2.14	0.47
1:D:376:ILE:CD1	1:D:401:LEU:HB3	2.45	0.47
1:A:128:ASN:HB2	6:A:9493:HOH:O	2.15	0.47
1:D:1022:GLN:O	1:D:1022:GLN:HG3	2.14	0.47
1:A:742:THR:HG22	1:A:743:SER:N	2.29	0.46
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.97	0.46
1:D:143:PHE:O	1:D:168:PRO:HA	2.15	0.46
1:D:651:LEU:HD23	1:D:701:VAL:HB	1.95	0.46
1:C:745:MET:HE3	1:C:745:MET:CA	2.42	0.46
1:C:910:LEU:C	1:C:910:LEU:HD12	2.40	0.46
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.97	0.46
1:C:737:ILE:HG13	1:C:738:PRO:N	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ASN:O	5:D:8408:DMS:H21	2.16	0.46
1:D:772:ASP:OD1	1:D:772:ASP:N	2.44	0.46
1:D:773:LYS:CG	1:D:775:GLN:NE2	2.79	0.46
1:A:734:SER:OG	1:A:860:GLY:HA3	2.15	0.46
1:A:809:ARG:HG2	1:A:809:ARG:NH1	2.24	0.46
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.45	0.46
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.15	0.46
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.97	0.46
5:A:8410:DMS:H22	6:A:8862:HOH:O	2.15	0.46
1:B:699:ARG:HE	1:B:714:ILE:HD13	1.81	0.46
1:D:845:GLN:CA	1:D:845:GLN:OE1	2.64	0.46
1:A:240:LEU:C	1:A:240:LEU:HD23	2.41	0.46
1:A:473:ARG:HH12	1:A:476:LYS:HB2	1.73	0.46
5:A:8423:DMS:H11	6:A:9145:HOH:O	2.15	0.46
1:A:147:ASN:HA	1:A:148:SER:HA	1.58	0.46
1:C:356:ARG:HD2	1:C:379:MET:CE	2.36	0.46
1:C:819:GLU:H	1:C:819:GLU:HG3	1.51	0.46
1:D:147:ASN:HA	1:D:148:SER:HA	1.68	0.46
1:D:634:GLN:NE2	1:D:682:LEU:O	2.49	0.46
1:C:737:ILE:CG1	1:C:738:PRO:HD2	2.43	0.46
1:C:890:GLN:HE21	1:C:892:ALA:HB2	1.80	0.46
1:B:845:GLN:OE1	1:B:845:GLN:HA	2.16	0.46
1:C:278:ILE:HD13	1:C:278:ILE:N	2.30	0.46
5:C:8410:DMS:H22	6:C:8986:HOH:O	2.16	0.46
1:B:240:LEU:C	1:B:240:LEU:HD23	2.41	0.45
5:D:8410:DMS:H22	6:D:8996:HOH:O	2.15	0.45
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.98	0.45
1:B:799:THR:HG23	6:B:9561:HOH:O	2.15	0.45
1:D:473:ARG:NH1	1:D:476:LYS:HB2	2.29	0.45
1:A:656:VAL:CG1	1:A:694:LEU:HD22	2.47	0.45
1:B:262:GLN:CA	1:B:262:GLN:NE2	2.80	0.45
1:B:734:SER:OG	1:B:860:GLY:HA3	2.16	0.45
1:C:806:TRP:CE2	1:C:809:ARG:NH2	2.85	0.45
1:A:873:ALA:O	1:A:876:THR:HG22	2.17	0.45
1:B:910:LEU:C	1:B:910:LEU:HD12	2.42	0.45
5:C:8705:DMS:H21	6:C:9414:HOH:O	2.16	0.45
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.99	0.45
1:A:433:LEU:N	1:A:434:PRO:CD	2.80	0.45
6:A:9017:HOH:O	5:D:8420:DMS:H12	2.15	0.45
1:B:693:GLN:OE1	1:B:721:ARG:HG2	2.15	0.45
1:C:243:GLU:OE2	1:C:245:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:MET:HE3	1:A:655:MET:HB2	1.56	0.45
1:A:753:ASN:OD1	1:A:753:ASN:N	2.50	0.45
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.51	0.45
1:A:842:TRP:C	1:A:843:GLN:HG3	2.41	0.45
1:C:41:GLU:HG2	1:C:46:ARG:HH21	1.78	0.45
1:D:844:HIS:N	1:D:847:LYS:O	2.49	0.45
1:B:46:ARG:HB3	1:B:47:PRO:HD2	1.99	0.45
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.51	0.45
1:B:655:MET:CE	1:B:665:SER:HB3	2.47	0.45
1:C:147:ASN:HA	1:C:148:SER:HA	1.55	0.45
1:D:832:ASP:OD1	1:D:832:ASP:N	2.44	0.45
1:A:655:MET:HE2	1:A:656:VAL:H	1.78	0.44
1:B:91:GLN:HG2	1:B:98:PRO:HA	1.99	0.44
1:B:890:GLN:OE1	1:B:948:PRO:HD3	2.17	0.44
1:C:832:ASP:OD1	1:C:832:ASP:N	2.45	0.44
1:A:50:GLN:N	1:A:50:GLN:CD	2.75	0.44
1:A:533:LEU:C	1:A:533:LEU:HD23	2.42	0.44
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.53	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.62	0.44
1:B:233:ASP:HA	5:B:8417:DMS:H13	2.00	0.44
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.99	0.44
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.53	0.44
1:C:92:MET:HE2	1:C:92:MET:CA	2.46	0.44
1:A:601:PHE:CD1	4:A:2002:145:H3'	2.52	0.44
1:D:1000:SER:O	1:D:1001:PRO:C	2.60	0.44
1:B:183:ARG:HG2	6:B:8922:HOH:O	2.16	0.44
1:B:252:ASP:OD2	5:B:8416:DMS:H12	2.18	0.44
1:D:638:VAL:O	1:D:677:LYS:HA	2.18	0.44
1:D:737:ILE:HD12	1:D:737:ILE:HA	1.61	0.44
1:A:59:ARG:NH2	1:A:81:ALA:HB3	2.33	0.44
1:B:245:GLN:HG2	1:B:288:ARG:CD	2.48	0.44
1:D:869:ASP:OD1	1:D:1015:HIS:ND1	2.50	0.44
1:B:554:GLN:HG3	6:B:9427:HOH:O	2.17	0.44
1:B:662:PRO:C	1:B:663:LEU:HD23	2.43	0.44
1:C:802:ASP:O	1:C:808:GLU:HG3	2.18	0.44
1:C:658:LEU:O	1:C:659:ASP:C	2.59	0.44
1:D:640:SER:O	1:D:675:GLN:HA	2.18	0.44
1:B:599:ARG:HH11	1:B:600:GLN:NE2	2.16	0.44
1:B:778:THR:HG23	1:B:887:GLN:CB	2.44	0.44
1:B:781:ARG:HD3	6:B:9573:HOH:O	2.18	0.44
5:B:8409:DMS:H23	6:B:8953:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:847:LYS:NZ	1:B:724:GLU:O	2.50	0.43
1:B:941:THR:C	1:B:942:ARG:HD2	2.43	0.43
1:C:41:GLU:CG	1:C:46:ARG:NH2	2.79	0.43
1:C:669:PRO:HB3	6:C:9640:HOH:O	2.18	0.43
1:D:686:PRO:O	1:D:688:PRO:HD3	2.17	0.43
1:D:755:ARG:HG3	1:D:769:TRP:HB2	2.00	0.43
1:D:845:GLN:OE1	1:D:845:GLN:HA	2.18	0.43
1:A:890:GLN:HG3	1:A:891:VAL:N	2.33	0.43
1:B:128:ASN:HB2	6:B:9470:HOH:O	2.18	0.43
1:B:662:PRO:O	1:B:663:LEU:HD23	2.18	0.43
1:B:226:HIS:ND1	6:B:9139:HOH:O	2.36	0.43
1:C:734:SER:CB	1:C:860:GLY:HA3	2.48	0.43
1:C:947:GLY:HA3	1:C:948:PRO:HD2	1.79	0.43
1:B:630:ARG:NE	1:B:637:GLU:OE1	2.44	0.43
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.99	0.43
1:D:684:GLU:HG2	1:D:685:LEU:N	2.34	0.43
1:D:844:HIS:O	1:D:845:GLN:HB2	2.18	0.43
1:D:738:PRO:HB3	1:D:751:LEU:HB2	2.00	0.43
1:D:829:THR:HG23	1:D:834:VAL:HG22	1.99	0.43
1:A:536:CYS:C	1:A:537:GLN:HG3	2.44	0.43
1:A:844:HIS:O	1:A:845:GLN:C	2.61	0.43
1:B:632:SER:N	1:B:635:THR:O	2.33	0.43
1:B:817:GLN:NE2	1:B:817:GLN:HA	2.33	0.43
1:C:824:GLN:O	1:C:838:THR:HA	2.19	0.43
1:A:660:GLY:O	1:A:662:PRO:HD3	2.18	0.43
1:B:814:GLY:HA3	1:B:844:HIS:CG	2.54	0.43
1:C:847:LYS:HG3	1:C:848:THR:N	2.30	0.43
1:D:472:TYR:O	1:D:476:LYS:HG2	2.18	0.43
1:D:824:GLN:NE2	1:D:837:THR:CG2	2.82	0.43
1:A:708:TRP:CZ2	5:A:8403:DMS:H13	2.53	0.43
1:B:538:TYR:O	1:B:567:VAL:HA	2.19	0.43
1:B:538:TYR:C	1:B:539[B]:ALA:O	2.61	0.43
1:B:689:GLU:O	1:B:690:SER:OG	2.26	0.43
1:B:962:TYR:OH	5:B:8423:DMS:H21	2.19	0.43
1:B:1017:GLN:HB2	6:B:9518:HOH:O	2.18	0.43
1:C:824:GLN:CG	1:C:825:CYS:N	2.81	0.43
1:A:694:LEU:HB3	1:A:722:LEU:HB2	2.01	0.42
1:A:832:ASP:OD1	1:A:832:ASP:N	2.52	0.42
1:B:730:LEU:H	1:B:730:LEU:HG	1.24	0.42
1:A:745:MET:HE1	1:A:761:GLN:HB2	2.01	0.42
1:A:800:ARG:CG	6:A:9370:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:MET:SD	1:C:664:ALA:O	2.77	0.42
1:D:795:VAL:HG11	4:D:2001:145:H4'	2.01	0.42
1:A:473:ARG:HA	1:A:473:ARG:HD2	1.92	0.42
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.18	0.42
1:B:637:GLU:OE2	1:B:677:LYS:HE3	2.19	0.42
1:C:655:MET:SD	1:C:656:VAL:N	2.93	0.42
1:A:518:TRP:O	1:A:519:SER:C	2.62	0.42
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.84	0.42
1:A:651:LEU:HD11	1:A:653:HIS:CD2	2.54	0.42
1:B:301:TRP:CH2	1:B:452:SER:HA	2.55	0.42
1:D:893:GLU:HG3	1:D:894:ARG:HD2	2.00	0.42
1:A:460:ASN:O	1:A:461:GLU:C	2.62	0.42
1:B:634:GLN:NE2	1:B:685:LEU:HG	2.32	0.42
1:B:826:THR:OG1	1:B:837:THR:HB	2.19	0.42
1:D:962:TYR:OH	5:D:8508:DMS:H11	2.20	0.42
1:A:125:LEU:O	1:A:183:ARG:HA	2.20	0.42
1:A:305:ILE:HD11	1:A:645:ARG:HB3	2.01	0.42
1:C:1013:ARG:HD3	6:C:9297:HOH:O	2.18	0.42
1:B:92:MET:HE2	1:B:92:MET:HA	2.00	0.42
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.83	0.42
5:C:8419:DMS:H21	6:C:9478:HOH:O	2.20	0.42
1:D:431:ARG:NH2	6:D:9592:HOH:O	2.52	0.42
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.68	0.42
1:B:797:GLU:HB2	1:B:800:ARG:HG3	2.01	0.42
1:C:1013:ARG:NH2	1:D:954:ASP:OD2	2.47	0.42
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.55	0.42
1:C:262:GLN:HB2	1:C:309:TYR:CE2	2.54	0.42
1:B:952:ARG:NH2	1:B:1021:CYS:SG	2.86	0.41
1:D:754:LYS:C	1:D:755:ARG:HG2	2.45	0.41
1:A:253:TYR:CD1	1:A:253:TYR:C	2.97	0.41
1:A:652:LEU:O	1:A:667:GLU:HA	2.20	0.41
1:B:127:PHE:CD2	1:B:127:PHE:N	2.88	0.41
1:B:131:GLU:O	1:B:132:SER:C	2.61	0.41
1:C:869:ASP:OD1	1:C:1015:HIS:ND1	2.34	0.41
1:D:246:MET:SD	1:D:246:MET:C	3.03	0.41
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.37	0.41
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.55	0.41
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.01	0.41
1:C:577:LYS:HB3	1:C:577:LYS:HE3	1.87	0.41
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.20	0.41
1:D:737:ILE:HD12	1:D:738:PRO:HD3	1.98	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:TYR:O	1:A:476:LYS:HG2	2.20	0.41
1:B:655:MET:HE3	1:B:665:SER:HB3	2.02	0.41
1:D:893:GLU:HG2	1:D:894:ARG:CG	2.50	0.41
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.03	0.41
1:B:262:GLN:NE2	1:B:263:GLY:N	2.64	0.41
1:C:254:LEU:C	1:C:255:ARG:HG2	2.45	0.41
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.55	0.41
1:D:933:SER:O	1:D:934:GLU:C	2.63	0.41
1:B:372:MET:CE	1:B:395:HIS:HB3	2.50	0.41
1:B:663:LEU:HD23	1:B:663:LEU:HA	1.56	0.41
1:B:756:TRP:CD2	1:B:858:ILE:HD13	2.55	0.41
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.54	0.41
1:C:646:HIS:CE1	1:C:673:ALA:CB	3.03	0.41
1:C:730:LEU:HA	1:C:731:PRO:HD3	1.60	0.41
1:D:703:PRO:HG2	5:D:8425:DMS:C1	2.45	0.41
1:D:783:GLN:HG2	1:D:881:ARG:HD2	2.02	0.41
5:D:8416:DMS:H22	6:D:9390:HOH:O	2.21	0.41
1:A:299:LYS:HE3	1:A:299:LYS:HB3	1.83	0.41
1:D:250:LEU:O	5:D:8416:DMS:H13	2.20	0.41
1:B:513:PRO:O	1:B:514:ALA:HB3	2.19	0.41
1:B:655:MET:HE3	1:B:655:MET:HB2	1.61	0.41
1:C:685:LEU:O	1:C:686:PRO:C	2.63	0.41
1:C:814:GLY:HA3	1:C:844:HIS:CG	2.56	0.41
1:D:893:GLU:CG	1:D:894:ARG:CD	2.99	0.41
1:D:959:ILE:HD13	1:D:959:ILE:HG21	1.87	0.41
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.56	0.41
1:A:390:SER:HA	1:A:391:HIS:HA	1.87	0.41
1:B:100:TYR:HB3	1:B:589:GLY:HA2	2.02	0.41
1:B:864:MET:HE3	1:B:866:ILE:HD11	2.03	0.41
1:B:873:ALA:O	1:B:876:THR:HG22	2.19	0.41
1:C:538:TYR:C	1:C:539[B]:ALA:O	2.63	0.41
1:C:895:VAL:O	1:C:919:ASP:HA	2.20	0.41
1:D:745:MET:O	1:D:745:MET:HG3	2.21	0.41
1:D:764:PHE:CE1	1:D:781:ARG:NH1	2.89	0.41
1:B:580:GLU:CD	1:B:580:GLU:N	2.78	0.41
1:D:703:PRO:CG	5:D:8425:DMS:H12	2.48	0.41
1:D:844:HIS:O	1:D:845:GLN:C	2.64	0.41
1:D:895:VAL:O	1:D:919:ASP:HA	2.21	0.41
1:A:802:ASP:OD1	1:A:802:ASP:C	2.63	0.40
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.56	0.40
1:B:367:MET:HB3	1:B:372:MET:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:844:HIS:HD2	6:C:9538:HOH:O	2.04	0.40
5:C:8423:DMS:H11	6:C:9595:HOH:O	2.21	0.40
1:D:526:LEU:O	1:D:527:PRO:C	2.64	0.40
1:B:78:LEU:HA	1:B:79:PRO:HD3	1.89	0.40
1:B:200:GLN:HG2	1:B:391:HIS:HB2	2.04	0.40
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.39	0.40
1:B:942:ARG:HE	1:B:954:ASP:HA	1.86	0.40
1:D:797:GLU:HB2	1:D:800:ARG:CG	2.51	0.40
1:A:279:ILE:HG21	1:A:279:ILE:HD13	1.76	0.40
1:A:651:LEU:C	1:A:651:LEU:CD1	2.93	0.40
1:B:377:LEU:HD22	1:B:708:TRP:CA	2.51	0.40
1:B:753:ASN:ND2	6:B:9504:HOH:O	2.52	0.40
1:B:809:ARG:HG2	1:B:809:ARG:NH1	2.18	0.40
1:D:629:PHE:C	1:D:630:ARG:HD3	2.45	0.40
1:D:780:LEU:HA	1:D:886:CYS:HB3	2.03	0.40
1:A:127:PHE:CD2	1:A:127:PHE:N	2.88	0.40
1:A:655:MET:HE3	1:A:665:SER:HB3	2.02	0.40
1:C:757:GLN:OE1	1:C:769:TRP:HH2	2.04	0.40
1:A:990:HIS:HD2	1:A:991:MET:O	2.05	0.40
1:B:132:SER:O	1:B:135:GLN:HG2	2.21	0.40
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.56	0.40
1:C:662:PRO:C	1:C:663:LEU:HD23	2.46	0.40

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

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1011/1023 (99%)	974 (96%)	35 (4%)	2 (0%)	43	27
1	B	1011/1023 (99%)	968 (96%)	39 (4%)	4 (0%)	30	15
1	C	1011/1023 (99%)	966 (96%)	44 (4%)	1 (0%)	48	32
1	D	1011/1023 (99%)	972 (96%)	37 (4%)	2 (0%)	43	27
All	All	4044/4092 (99%)	3880 (96%)	155 (4%)	9 (0%)	43	27

All (9) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	865/875 (99%)	831 (96%)	34 (4%)	28	9
1	B	865/875 (99%)	819 (95%)	46 (5%)	20	5
1	C	865/875 (99%)	830 (96%)	35 (4%)	28	9
1	D	865/875 (99%)	830 (96%)	35 (4%)	28	9
All	All	3460/3500 (99%)	3310 (96%)	150 (4%)	26	8

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	230	ARG
1	A	237	ARG
1	A	250	LEU
1	A	267	VAL
1	A	277	GLU
1	A	344	LEU
1	A	347	LYS
1	A	431	ARG
1	A	478	VAL
1	A	519	SER
1	A	546	LEU
1	A	581	ASN
1	A	600	GLN
1	A	632	SER
1	A	655	MET
1	A	684	GLU
1	A	689	GLU
1	A	735	HIS
1	A	737	ILE
1	A	741	THR
1	A	773	LYS
1	A	799	THR
1	A	800	ARG
1	A	809	ARG
1	A	817	GLN
1	A	859	ASP
1	A	885	ASN
1	A	890	GLN
1	A	986	ILE
1	A	1013	ARG
1	A	1017	GLN
1	A	1022	GLN
1	A	1023	LYS
1	B	75	GLU
1	B	80	GLU
1	B	181	GLU
1	B	230	ARG
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	277	GLU
1	B	362	LEU

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Mol	Chain	Res	Type
1	B	370	GLN
1	B	478	VAL
1	B	519	SER
1	B	546	LEU
1	B	580	GLU
1	B	600	GLN
1	B	604	ASN
1	B	634	GLN
1	B	635	THR
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	684	GLU
1	B	685	LEU
1	B	687	GLN
1	B	689	GLU
1	B	690	SER
1	B	721	ARG
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	750	GLU
1	B	755	ARG
1	B	778	THR
1	B	781	ARG
1	B	809	ARG
1	B	819	GLU
1	B	824	GLN
1	B	843	GLN
1	B	845	GLN
1	B	847	LYS
1	B	885	ASN
1	B	890	GLN
1	B	942	ARG
1	B	956	GLN
1	B	1022	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	75	GLU
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG

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Mol	Chain	Res	Type
1	C	251	ARG
1	C	262	GLN
1	C	264	GLU
1	C	278	ILE
1	C	333	ARG
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	634	GLN
1	C	651	LEU
1	C	663	LEU
1	C	681	GLU
1	C	685	LEU
1	C	687	GLN
1	C	689	GLU
1	C	729	THR
1	C	730	LEU
1	C	735	HIS
1	C	737	ILE
1	C	745	MET
1	C	750	GLU
1	C	773	LYS
1	C	819	GLU
1	C	829	THR
1	C	893	GLU
1	C	956	GLN
1	C	986	ILE
1	C	1013	ARG
1	C	1022	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	76	CYS
1	D	237	ARG
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	594	ASP
1	D	632	SER
1	D	651	LEU
1	D	655	MET
1	D	661	LYS

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Mol	Chain	Res	Type
1	D	663	LEU
1	D	672	VAL
1	D	684	GLU
1	D	685	LEU
1	D	689	GLU
1	D	728	VAL
1	D	730	LEU
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	741	THR
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	799	THR
1	D	829	THR
1	D	845	GLN
1	D	885	ASN
1	D	893	GLU
1	D	986	ILE
1	D	1013	ARG
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	135	GLN
1	A	445	GLN
1	A	485	GLN
1	A	600	GLN
1	A	614	HIS
1	A	624	GLN
1	A	628	GLN
1	A	704	ASN
1	A	824	GLN
1	A	844	HIS
1	A	878	HIS
1	A	885	ASN
1	A	903	GLN
1	A	977	HIS

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Mol	Chain	Res	Type
1	A	1017	GLN
1	B	50	GLN
1	B	163	GLN
1	B	262	GLN
1	B	363	HIS
1	B	394	ASN
1	B	485	GLN
1	B	554	GLN
1	B	600	GLN
1	B	624	GLN
1	B	646	HIS
1	B	653	HIS
1	B	675	GLN
1	B	687	GLN
1	B	693	GLN
1	B	704	ASN
1	B	804	ASN
1	B	817	GLN
1	B	844	HIS
1	B	878	HIS
1	C	128	ASN
1	C	135	GLN
1	C	163	GLN
1	C	266	GLN
1	C	363	HIS
1	C	485	GLN
1	C	624	GLN
1	C	634	GLN
1	C	646	HIS
1	C	687	GLN
1	C	704	ASN
1	C	739	HIS
1	C	824	GLN
1	C	878	HIS
1	C	945	ASN
1	C	950	GLN
1	C	977	HIS
1	C	1017	GLN
1	D	135	GLN
1	D	163	GLN
1	D	262	GLN
1	D	297	ASN

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Mol	Chain	Res	Type
1	D	363	HIS
1	D	485	GLN
1	D	583	ASN
1	D	628	GLN
1	D	634	GLN
1	D	757	GLN
1	D	775	GLN
1	D	804	ASN
1	D	824	GLN
1	D	843	GLN
1	D	844	HIS
1	D	878	HIS
1	D	977	HIS
1	D	1022	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 148 ligands modelled in this entry, 33 are monoatomic - leaving 115 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8414	-	3,3,3	1.27	0	3,3,3	0.13	0
5	DMS	B	8403	-	3,3,3	1.23	0	3,3,3	0.46	0
5	DMS	A	8405	-	3,3,3	0.86	0	3,3,3	0.30	0
5	DMS	A	8406	-	3,3,3	0.36	0	3,3,3	1.08	0
5	DMS	B	8414	-	3,3,3	1.16	0	3,3,3	0.45	0
4	145	A	2002	-	22,22,22	0.94	1 (4%)	28,31,31	1.26	3 (10%)
5	DMS	B	8404	-	3,3,3	1.31	0	3,3,3	1.39	1 (33%)
5	DMS	B	8508	-	3,3,3	2.22	1 (33%)	3,3,3	0.37	0
5	DMS	D	8425	3	3,3,3	0.37	0	3,3,3	0.66	0
5	DMS	D	8417	-	3,3,3	1.40	0	3,3,3	1.14	0
5	DMS	B	8417	-	3,3,3	0.98	0	3,3,3	0.21	0
5	DMS	C	8416	-	3,3,3	0.77	0	3,3,3	0.10	0
5	DMS	A	8412	-	3,3,3	0.63	0	3,3,3	0.36	0
5	DMS	C	8705	-	3,3,3	1.14	0	3,3,3	0.21	0
5	DMS	B	8425	3	3,3,3	1.89	1 (33%)	3,3,3	0.60	0
5	DMS	C	8420	-	3,3,3	1.93	1 (33%)	3,3,3	0.22	0
5	DMS	C	8408	-	3,3,3	1.39	0	3,3,3	0.56	0
4	145	C	2002	-	22,22,22	0.92	1 (4%)	28,31,31	1.13	2 (7%)
5	DMS	A	8423	-	3,3,3	1.28	0	3,3,3	0.87	0
5	DMS	A	8503	-	3,3,3	0.33	0	3,3,3	0.20	0
5	DMS	C	8402	-	3,3,3	1.06	0	3,3,3	0.82	0
5	DMS	C	8602	-	3,3,3	1.11	0	3,3,3	0.28	0
5	DMS	B	8420	-	3,3,3	1.56	1 (33%)	3,3,3	0.45	0
5	DMS	D	8401	-	3,3,3	0.97	0	3,3,3	0.84	0
5	DMS	D	8412	-	3,3,3	0.95	0	3,3,3	0.50	0
5	DMS	B	8409	-	3,3,3	2.27	1 (33%)	3,3,3	0.58	0
5	DMS	C	8403	-	3,3,3	1.27	0	3,3,3	0.47	0
5	DMS	D	8410	-	3,3,3	1.53	1 (33%)	3,3,3	0.46	0
5	DMS	C	8407	-	3,3,3	2.29	2 (66%)	3,3,3	0.55	0
5	DMS	C	8504	-	3,3,3	0.86	0	3,3,3	0.29	0
5	DMS	C	8414	-	3,3,3	1.10	0	3,3,3	0.83	0
5	DMS	A	8403	-	3,3,3	1.49	1 (33%)	3,3,3	0.38	0
5	DMS	D	8416	-	3,3,3	1.39	1 (33%)	3,3,3	0.50	0
5	DMS	D	8423	-	3,3,3	1.34	0	3,3,3	0.30	0
5	DMS	B	8402	-	3,3,3	0.59	0	3,3,3	0.08	0
5	DMS	D	8701	-	3,3,3	1.90	1 (33%)	3,3,3	0.47	0
5	DMS	C	8601	-	3,3,3	0.76	0	3,3,3	1.06	0
5	DMS	C	8413	-	3,3,3	1.35	0	3,3,3	0.18	0
5	DMS	D	8705	-	3,3,3	1.73	0	3,3,3	0.82	0
5	DMS	B	8405	-	3,3,3	1.45	0	3,3,3	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8411	-	3,3,3	1.26	1 (33%)	3,3,3	0.42	0
4	145	D	2002	-	22,22,22	0.72	1 (4%)	28,31,31	1.28	3 (10%)
5	DMS	C	8419	-	3,3,3	1.07	0	3,3,3	0.47	0
5	DMS	C	8421	-	3,3,3	0.63	0	3,3,3	0.67	0
5	DMS	D	8404	-	3,3,3	1.12	0	3,3,3	0.47	0
5	DMS	B	8416	-	3,3,3	0.55	0	3,3,3	0.53	0
5	DMS	B	8408	-	3,3,3	1.48	1 (33%)	3,3,3	0.34	0
4	145	B	2002	-	22,22,22	0.96	1 (4%)	28,31,31	1.38	4 (14%)
5	DMS	C	8425	3	3,3,3	1.83	1 (33%)	3,3,3	0.39	0
5	DMS	C	8415	-	3,3,3	2.77	2 (66%)	3,3,3	1.75	1 (33%)
5	DMS	A	8602	-	3,3,3	0.86	0	3,3,3	0.55	0
5	DMS	A	8402	-	3,3,3	1.54	0	3,3,3	0.29	0
5	DMS	C	8410	-	3,3,3	1.29	0	3,3,3	0.21	0
5	DMS	B	8407	-	3,3,3	2.20	1 (33%)	3,3,3	0.25	0
5	DMS	A	8407	-	3,3,3	2.61	2 (66%)	3,3,3	0.23	0
5	DMS	A	8409	-	3,3,3	2.09	1 (33%)	3,3,3	0.59	0
5	DMS	D	8501	-	3,3,3	0.33	0	3,3,3	0.74	0
5	DMS	D	8408	-	3,3,3	0.84	0	3,3,3	0.23	0
5	DMS	A	8410	-	3,3,3	1.13	0	3,3,3	0.35	0
5	DMS	A	8416	-	3,3,3	0.56	0	3,3,3	0.40	0
5	DMS	B	8415	-	3,3,3	2.07	1 (33%)	3,3,3	1.41	1 (33%)
4	145	B	2001	3	22,22,22	1.19	3 (13%)	28,31,31	0.91	0
5	DMS	A	8425	3	3,3,3	2.02	1 (33%)	3,3,3	0.65	0
5	DMS	A	8501	-	3,3,3	1.19	0	3,3,3	0.33	0
5	DMS	D	8403	-	3,3,3	0.59	0	3,3,3	0.72	0
5	DMS	D	8415	-	3,3,3	2.55	2 (66%)	3,3,3	0.47	0
5	DMS	D	8703	-	3,3,3	2.39	2 (66%)	3,3,3	0.24	0
5	DMS	A	8502	-	3,3,3	1.32	1 (33%)	3,3,3	1.31	1 (33%)
5	DMS	D	8407	-	3,3,3	2.92	2 (66%)	3,3,3	0.32	0
5	DMS	D	8409	-	3,3,3	2.27	1 (33%)	3,3,3	0.62	0
5	DMS	C	8405	-	3,3,3	1.52	1 (33%)	3,3,3	0.57	0
5	DMS	A	8419	-	3,3,3	0.82	0	3,3,3	0.33	0
5	DMS	C	8411	-	3,3,3	1.07	0	3,3,3	0.42	0
5	DMS	B	8410	-	3,3,3	0.73	0	3,3,3	0.32	0
5	DMS	B	8504	-	3,3,3	1.09	0	3,3,3	0.85	0
5	DMS	A	8408	-	3,3,3	0.68	0	3,3,3	1.68	1 (33%)
4	145	D	2001	3	22,22,22	1.22	3 (13%)	28,31,31	1.34	5 (17%)
5	DMS	C	8409	-	3,3,3	2.13	1 (33%)	3,3,3	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8417	-	3,3,3	1.08	0	3,3,3	0.84	0
5	DMS	B	8502	-	3,3,3	2.39	2 (66%)	3,3,3	0.45	0
5	DMS	C	8503	-	3,3,3	1.08	0	3,3,3	0.22	0
5	DMS	A	8415	-	3,3,3	1.12	0	3,3,3	0.71	0
5	DMS	A	8411	-	3,3,3	0.77	0	3,3,3	0.40	0
5	DMS	B	8601	-	3,3,3	2.16	1 (33%)	3,3,3	1.03	0
5	DMS	A	8417	-	3,3,3	2.18	1 (33%)	3,3,3	1.05	0
5	DMS	D	8420	-	3,3,3	1.37	1 (33%)	3,3,3	0.38	0
5	DMS	D	8508	-	3,3,3	1.83	1 (33%)	3,3,3	0.48	0
5	DMS	B	8421	-	3,3,3	0.71	0	3,3,3	1.00	0
5	DMS	D	8414	-	3,3,3	0.70	0	3,3,3	0.34	0
5	DMS	C	8404	-	3,3,3	1.22	1 (33%)	3,3,3	1.16	0
5	DMS	D	8411	-	3,3,3	1.06	0	3,3,3	0.27	0
5	DMS	B	8419	-	3,3,3	0.64	0	3,3,3	0.41	0
5	DMS	D	8402	-	3,3,3	1.63	1 (33%)	3,3,3	0.39	0
5	DMS	C	8412	-	3,3,3	0.86	0	3,3,3	0.33	0
5	DMS	A	8401	-	3,3,3	0.66	0	3,3,3	0.85	0
5	DMS	B	8413	-	3,3,3	1.70	1 (33%)	3,3,3	0.14	0
5	DMS	C	8401	-	3,3,3	0.88	0	3,3,3	0.51	0
5	DMS	B	8423	-	3,3,3	0.99	0	3,3,3	0.11	0
5	DMS	C	8423	-	3,3,3	0.67	0	3,3,3	0.35	0
5	DMS	D	8405	-	3,3,3	0.74	0	3,3,3	0.82	0
4	145	A	2001	3	22,22,22	1.06	3 (13%)	28,31,31	1.46	4 (14%)
4	145	C	2001	3	22,22,22	0.90	1 (4%)	28,31,31	1.19	5 (17%)
5	DMS	A	8421	-	3,3,3	0.19	0	3,3,3	0.36	0
5	DMS	B	8412	-	3,3,3	1.96	1 (33%)	3,3,3	0.19	0
5	DMS	C	8501	-	3,3,3	1.47	1 (33%)	3,3,3	1.02	0
5	DMS	A	8420	-	3,3,3	1.11	0	3,3,3	0.37	0
5	DMS	A	8404	-	3,3,3	1.10	0	3,3,3	0.70	0
5	DMS	D	8421	-	3,3,3	0.56	0	3,3,3	0.37	0
5	DMS	B	8401	-	3,3,3	0.59	0	3,3,3	0.29	0
5	DMS	D	8413	-	3,3,3	1.99	1 (33%)	3,3,3	0.67	0
5	DMS	A	8504	-	3,3,3	0.68	0	3,3,3	0.30	0
5	DMS	D	8503	-	3,3,3	0.75	0	3,3,3	0.33	0
5	DMS	A	8413	-	3,3,3	2.12	2 (66%)	3,3,3	0.34	0
5	DMS	D	8406	-	3,3,3	1.18	0	3,3,3	0.71	0
5	DMS	D	8419	-	3,3,3	0.42	0	3,3,3	0.17	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
 '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	145	A	2001	3	-	1/8/30/30	0/2/2/2
4	145	C	2001	3	-	1/8/30/30	0/2/2/2
4	145	B	2002	-	-	1/8/30/30	0/2/2/2
4	145	D	2002	-	-	0/8/30/30	0/2/2/2
4	145	D	2001	3	-	1/8/30/30	0/2/2/2
4	145	C	2002	-	-	0/8/30/30	0/2/2/2
4	145	A	2002	-	-	0/8/30/30	0/2/2/2
4	145	B	2001	3	-	1/8/30/30	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8415	DMS	C2-S	4.02	2.04	1.76
5	D	8407	DMS	C2-S	3.96	2.04	1.76
5	D	8409	DMS	O-S	3.71	1.74	1.50
5	A	8417	DMS	C1-S	-3.71	1.49	1.76
5	D	8415	DMS	O-S	3.68	1.74	1.50
5	B	8409	DMS	O-S	3.64	1.74	1.50
5	B	8407	DMS	C2-S	3.61	2.01	1.76
5	B	8502	DMS	C1-S	3.59	2.01	1.76
5	A	8409	DMS	O-S	3.32	1.72	1.50
5	C	8409	DMS	O-S	3.27	1.71	1.50
5	C	8420	DMS	O-S	3.27	1.71	1.50
5	A	8407	DMS	O-S	3.22	1.71	1.50
5	A	8407	DMS	C2-S	3.10	1.98	1.76
5	C	8407	DMS	C2-S	3.05	1.97	1.76
5	B	8415	DMS	C2-S	3.05	1.97	1.76
5	B	8508	DMS	C1-S	3.05	1.97	1.76
5	D	8407	DMS	O-S	3.04	1.70	1.50
5	B	8425	DMS	O-S	2.97	1.69	1.50
5	A	8425	DMS	O-S	2.93	1.69	1.50
5	B	8412	DMS	C1-S	2.90	1.96	1.76
5	D	8703	DMS	O-S	2.88	1.69	1.50
5	D	8508	DMS	O-S	2.86	1.69	1.50
5	C	8425	DMS	O-S	2.75	1.68	1.50
5	B	8601	DMS	C2-S	2.72	1.95	1.76
5	C	8415	DMS	C1-S	2.61	1.94	1.76
5	A	8413	DMS	C1-S	2.59	1.94	1.76
5	C	8407	DMS	O-S	2.52	1.66	1.50
5	D	8413	DMS	O-S	2.48	1.66	1.50
4	B	2001	145	O3'-N1'	2.45	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2002	145	O3'-N1'	2.43	1.27	1.22
4	B	2001	145	O2'-N1'	-2.42	1.19	1.35
5	B	8413	DMS	O-S	2.42	1.66	1.50
5	B	8420	DMS	C2-S	2.41	1.93	1.76
4	D	2002	145	O2'-N1'	-2.37	1.19	1.35
4	D	2001	145	O3-C3	2.37	1.48	1.43
4	D	2001	145	O3'-N1'	2.35	1.26	1.22
5	A	8403	DMS	C2-S	2.32	1.92	1.76
5	D	8420	DMS	C2-S	-2.31	1.59	1.76
5	C	8405	DMS	C1-S	2.28	1.92	1.76
5	D	8402	DMS	C2-S	2.28	1.92	1.76
4	A	2001	145	O2'-N1'	-2.27	1.20	1.35
5	D	8703	DMS	C1-S	2.25	1.92	1.76
4	D	2001	145	O2'-N1'	-2.25	1.20	1.35
5	B	8408	DMS	C1-S	2.24	1.92	1.76
5	C	8501	DMS	O-S	2.23	1.65	1.50
5	D	8416	DMS	C2-S	-2.22	1.60	1.76
4	B	2001	145	O3-C3	2.21	1.48	1.43
4	C	2001	145	O2'-N1'	-2.17	1.20	1.35
5	A	8413	DMS	C2-S	2.16	1.91	1.76
5	B	8411	DMS	C1-S	2.16	1.91	1.76
4	A	2002	145	O2'-N1'	-2.13	1.21	1.35
4	B	2002	145	O2'-N1'	-2.07	1.21	1.35
5	A	8502	DMS	C1-S	2.05	1.90	1.76
5	B	8502	DMS	O-S	2.05	1.63	1.50
5	D	8415	DMS	C1-S	2.03	1.90	1.76
5	D	8410	DMS	O-S	2.03	1.63	1.50
4	A	2001	145	O3'-N1'	2.02	1.26	1.22
4	A	2001	145	C4'-C3'	-2.02	1.35	1.38
5	C	8404	DMS	C2-S	2.01	1.90	1.76
5	D	8701	DMS	O-S	2.00	1.63	1.50

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2002	145	C3'-C2'-N1'	4.36	121.13	116.47
4	A	2001	145	O1-C1'-C2'	4.14	122.30	117.31
4	B	2002	145	C3'-C2'-N1'	3.82	120.56	116.47
4	A	2001	145	C3'-C2'-N1'	-3.00	113.27	116.47
5	C	8415	DMS	C2-S-C1	2.97	113.64	98.42
5	A	8408	DMS	C2-S-C1	2.90	113.29	98.42
4	D	2002	145	O1-C1'-C2'	-2.84	113.88	117.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2002	145	C1-C2-C3	-2.66	104.41	110.01
4	A	2001	145	O1-C1-C2	-2.66	103.28	107.16
4	B	2002	145	O5-C5-C4	2.62	114.42	109.70
4	D	2001	145	O1-C1'-C2'	2.60	120.44	117.31
4	C	2002	145	C6-C5-C4	-2.49	106.92	113.02
4	A	2001	145	O3-C3-C2	-2.48	104.52	110.38
5	B	8415	DMS	C2-S-C1	2.42	110.80	98.42
4	D	2001	145	C5'-C4'-C3'	-2.41	117.27	120.24
5	B	8404	DMS	C2-S-C1	2.40	110.71	98.42
4	A	2002	145	O5-C1-C2	-2.34	105.55	110.37
4	C	2002	145	C3'-C2'-N1'	2.28	118.91	116.47
5	A	8502	DMS	C2-S-C1	2.27	110.05	98.42
4	D	2001	145	C1'-O1-C1	2.26	122.27	118.15
4	A	2002	145	C4'-C5'-C6'	2.23	122.99	120.24
4	C	2001	145	O6-C6-C5	2.19	118.79	111.33
4	B	2002	145	C4'-C5'-C6'	2.16	122.91	120.24
4	C	2001	145	O1-C1-C2	-2.13	104.05	107.16
4	D	2002	145	O3'-N1'-C2'	2.13	122.67	119.03
4	C	2001	145	O4-C4-C5	2.12	114.55	109.32
4	D	2001	145	C4'-C3'-C2'	2.12	122.08	118.60
4	C	2001	145	O5-C1-O1	-2.06	103.14	108.42
4	B	2002	145	C1-C2-C3	-2.04	105.71	110.01
4	C	2001	145	C1-O5-C5	-2.03	109.75	113.72
4	D	2001	145	O4-C4-C5	2.03	114.32	109.32

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2001	145	O5-C5-C6-O6
4	D	2001	145	O5-C5-C6-O6
4	B	2001	145	O5-C5-C6-O6
4	A	2001	145	O5-C5-C6-O6
4	B	2002	145	C4-C5-C6-O6

There are no ring outliers.

51 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	145	1	0
5	B	8508	DMS	2	0

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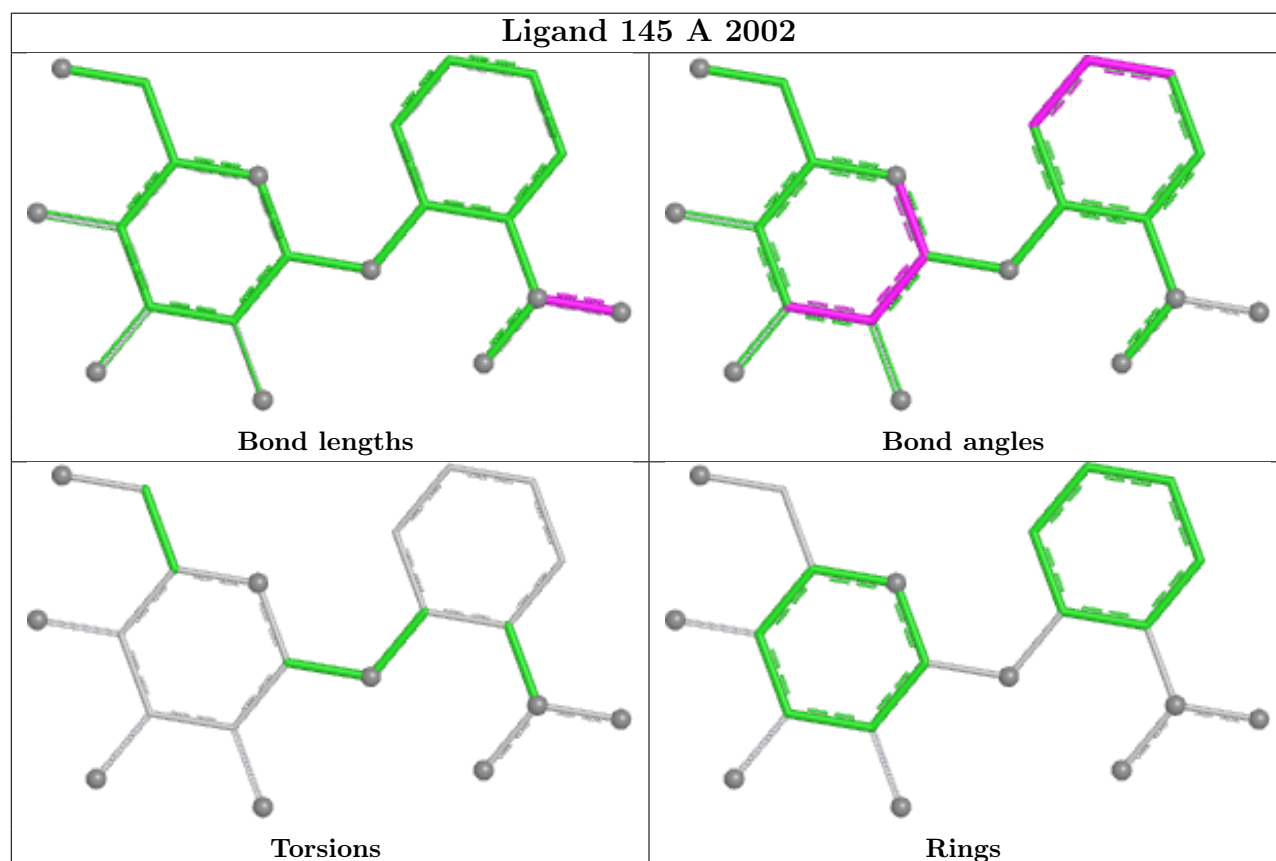
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8425	DMS	3	0
5	D	8417	DMS	1	0
5	B	8417	DMS	2	0
5	A	8412	DMS	4	0
5	C	8705	DMS	1	0
5	C	8420	DMS	1	0
4	C	2002	145	2	0
5	A	8423	DMS	2	0
5	A	8503	DMS	1	0
5	C	8602	DMS	2	0
5	B	8420	DMS	1	0
5	D	8412	DMS	3	0
5	B	8409	DMS	1	0
5	D	8410	DMS	2	0
5	A	8403	DMS	1	0
5	D	8416	DMS	3	0
5	D	8423	DMS	1	0
4	D	2002	145	3	0
5	C	8419	DMS	2	0
5	B	8416	DMS	3	0
4	B	2002	145	1	0
5	C	8425	DMS	2	0
5	C	8415	DMS	1	0
5	A	8602	DMS	1	0
5	C	8410	DMS	2	0
5	B	8407	DMS	2	0
5	A	8407	DMS	1	0
5	D	8408	DMS	1	0
5	A	8410	DMS	1	0
5	A	8416	DMS	1	0
5	B	8415	DMS	2	0
5	D	8703	DMS	4	0
5	D	8407	DMS	2	0
5	B	8410	DMS	1	0
5	B	8504	DMS	2	0
4	D	2001	145	1	0
5	C	8417	DMS	1	0
5	B	8502	DMS	1	0
5	C	8503	DMS	1	0
5	A	8415	DMS	1	0
5	A	8417	DMS	1	0
5	D	8420	DMS	1	0

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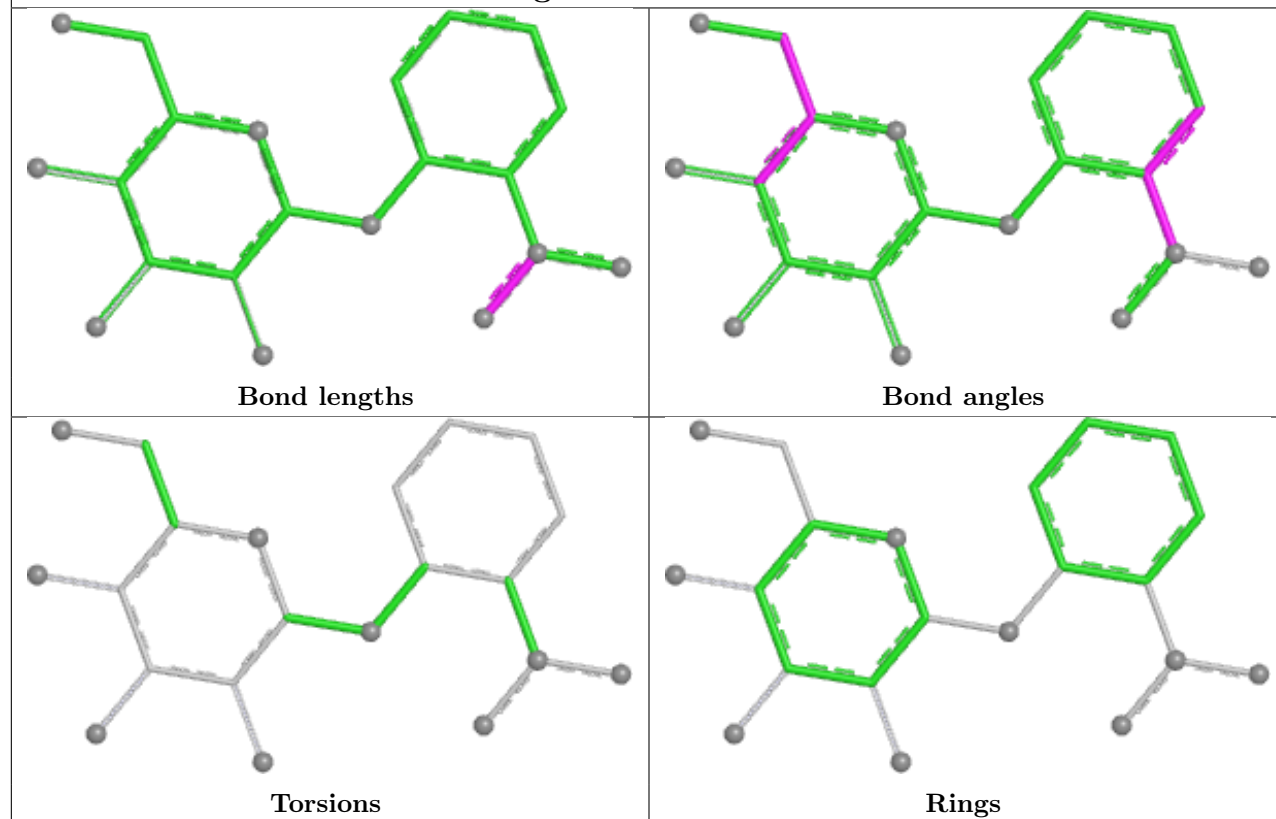
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8508	DMS	1	0
5	B	8423	DMS	1	0
5	C	8423	DMS	1	0
4	A	2001	145	1	0
5	A	8404	DMS	1	0
5	D	8503	DMS	1	0
5	D	8419	DMS	1	0

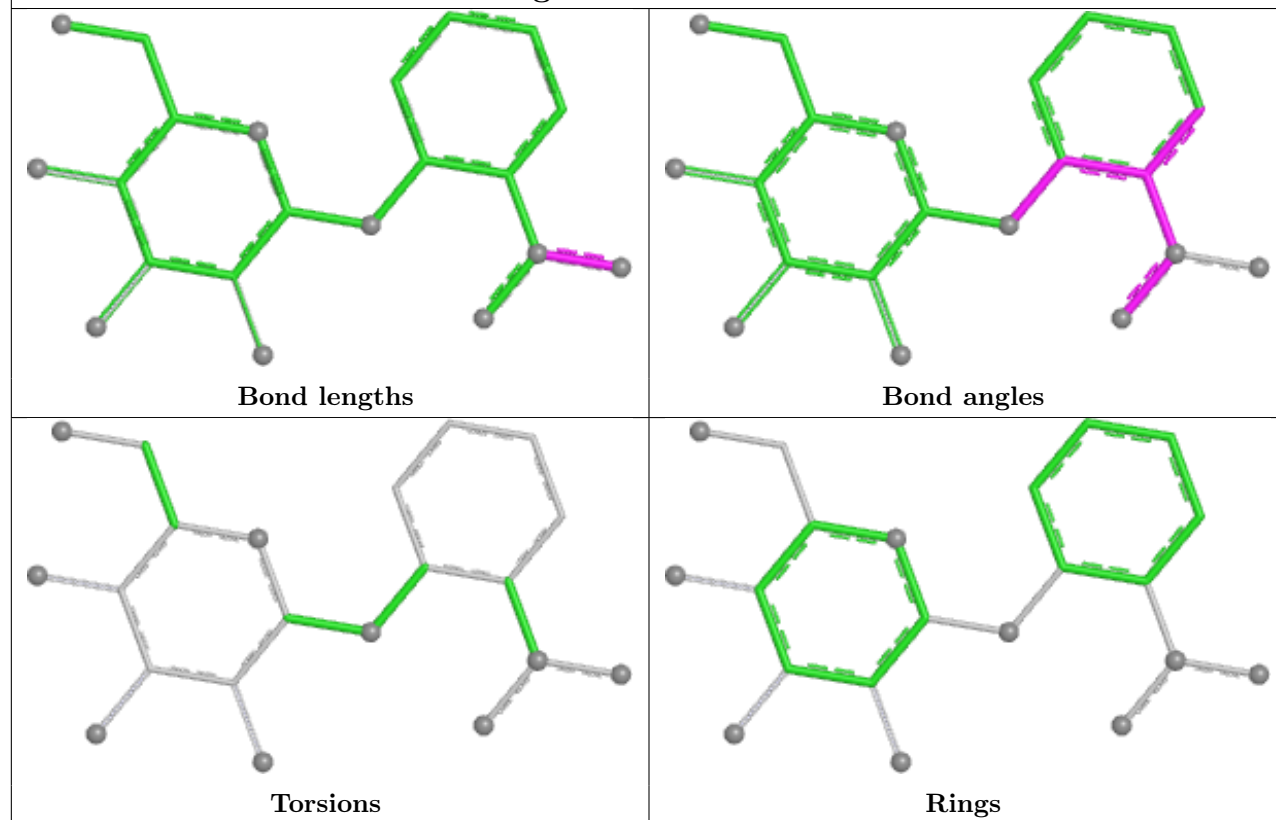
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



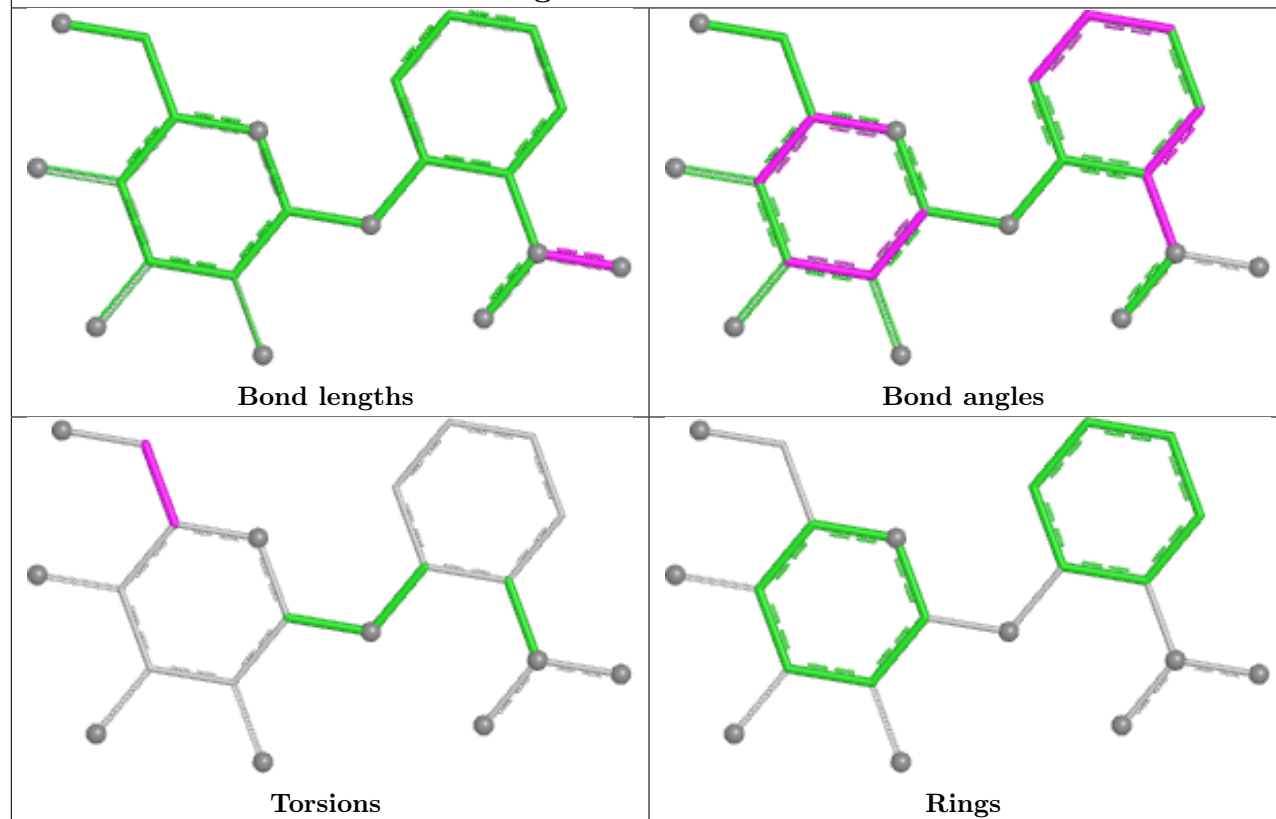
Ligand 145 C 2002



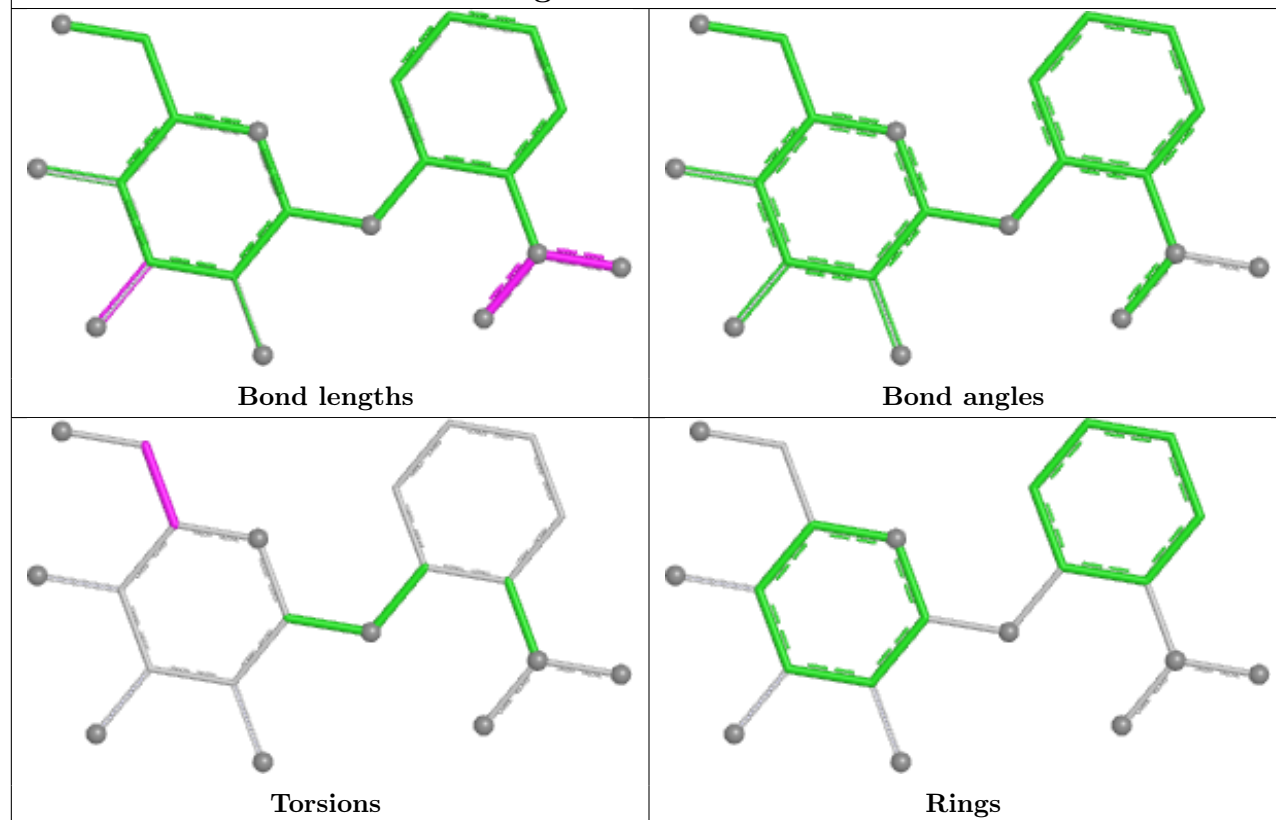
Ligand 145 D 2002



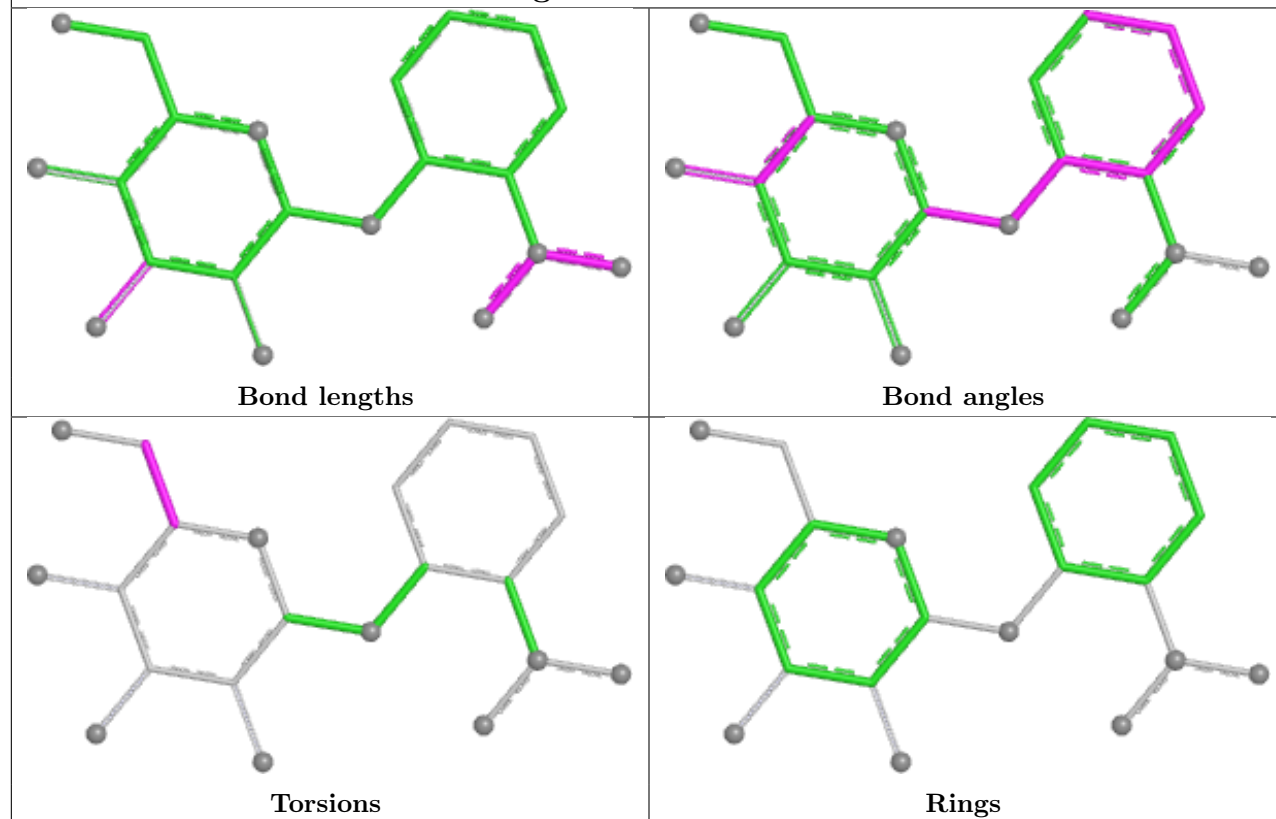
Ligand 145 B 2002



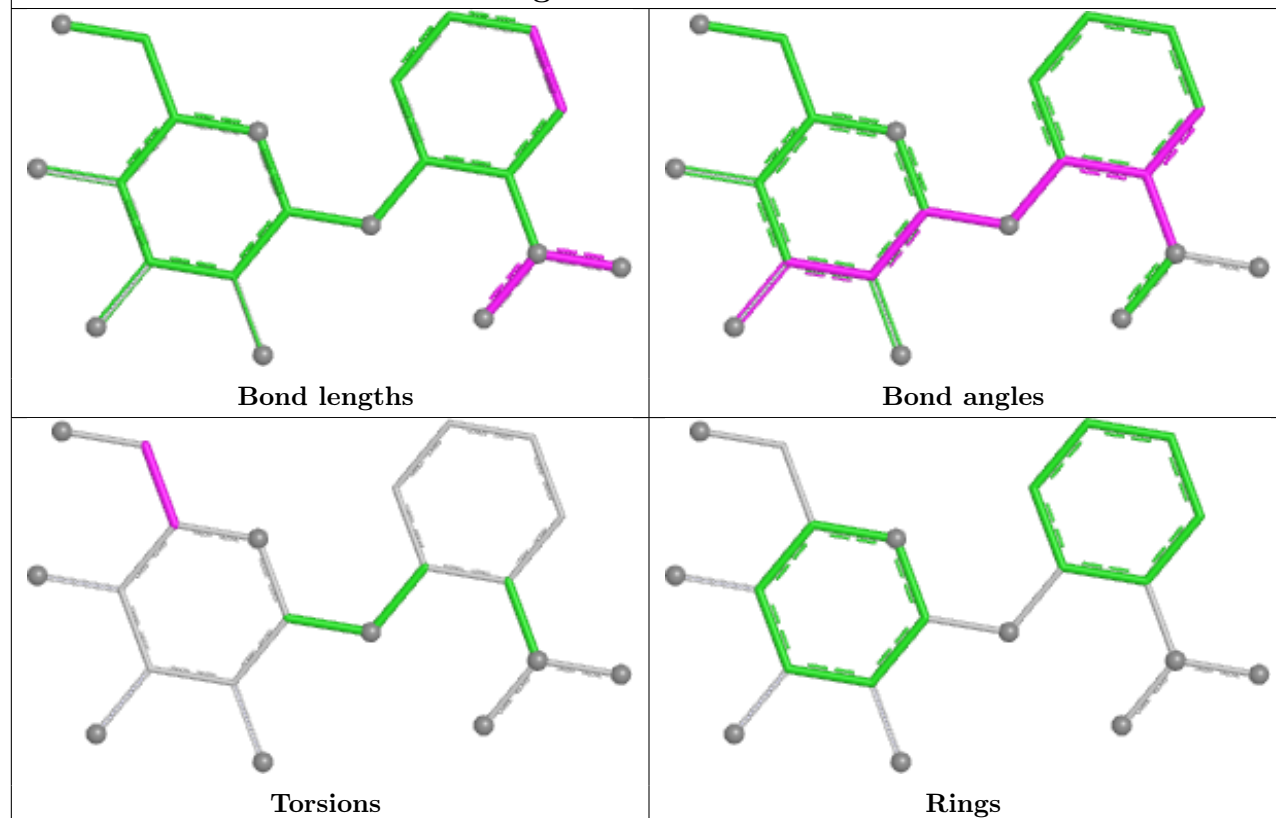
Ligand 145 B 2001

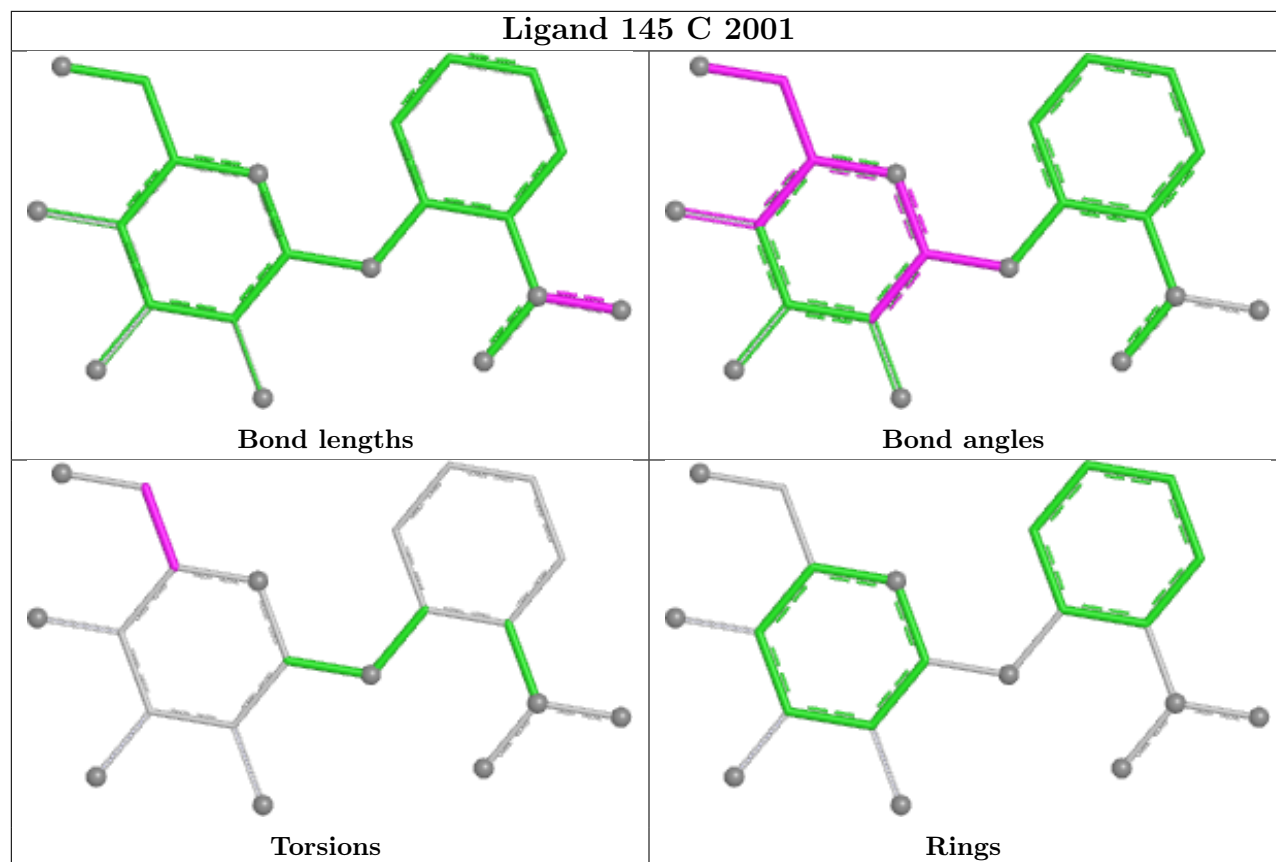


Ligand 145 D 2001



Ligand 145 A 2001





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.44	20 (1%) 65 71	11, 18, 46, 100	1 (0%)
1	B	1011/1023 (98%)	-0.35	24 (2%) 59 66	11, 19, 48, 99	1 (0%)
1	C	1011/1023 (98%)	-0.31	25 (2%) 58 64	11, 20, 51, 100	1 (0%)
1	D	1011/1023 (98%)	-0.37	21 (2%) 63 70	11, 19, 50, 100	1 (0%)
All	All	4044/4092 (98%)	-0.37	90 (2%) 62 69	11, 19, 49, 100	4 (0%)

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	730	LEU	5.6
1	A	730	LEU	5.1
1	B	733	ALA	5.0
1	C	686	PRO	4.8
1	A	686	PRO	4.8
1	B	686	PRO	4.7
1	D	733	ALA	4.6
1	B	685	LEU	4.4
1	A	772	ASP	4.3
1	D	686	PRO	4.2
1	A	735	HIS	4.1
1	B	732	ALA	4.0
1	D	737	ILE	3.9
1	B	737	ILE	3.9
1	C	730	LEU	3.8
1	A	732	ALA	3.8
1	D	732	ALA	3.7
1	C	685	LEU	3.6
1	C	733	ALA	3.6
1	D	663	LEU	3.5
1	D	735	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	685	LEU	3.5
1	A	733	ALA	3.4
1	C	732	ALA	3.4
1	A	1023	LYS	3.4
1	B	730	LEU	3.3
1	B	735	HIS	3.3
1	B	745	MET	3.3
1	D	655	MET	3.3
1	A	829	THR	3.3
1	B	846	GLY	3.2
1	C	1023	LYS	3.2
1	B	729	THR	3.1
1	D	799	THR	3.0
1	A	731	PRO	3.0
1	C	736	ALA	3.0
1	C	735	HIS	3.0
1	D	1023	LYS	3.0
1	A	634	GLN	2.9
1	A	729	THR	2.9
1	A	737	ILE	2.9
1	C	737	ILE	2.8
1	A	799	THR	2.8
1	B	1023	LYS	2.8
1	B	687	GLN	2.8
1	C	830	LEU	2.8
1	C	731	PRO	2.7
1	C	772	ASP	2.7
1	C	1022	GLN	2.7
1	D	736	ALA	2.7
1	D	734	SER	2.6
1	C	829	THR	2.6
1	B	731	PRO	2.6
1	D	731	PRO	2.6
1	D	729	THR	2.6
1	C	734	SER	2.6
1	B	845	GLN	2.6
1	C	634	GLN	2.5
1	D	581	ASN	2.5
1	B	753	ASN	2.5
1	C	761	GLN	2.5
1	A	689	GLU	2.4
1	B	688	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	633	GLY	2.3
1	B	651	LEU	2.3
1	B	734	SER	2.3
1	C	729	THR	2.3
1	A	687	GLN	2.3
1	D	634	GLN	2.2
1	D	688	PRO	2.2
1	B	817	GLN	2.2
1	D	689	GLU	2.2
1	D	829	THR	2.2
1	C	689	GLU	2.2
1	A	739	HIS	2.2
1	B	653	HIS	2.2
1	B	1018	LEU	2.2
1	A	846	GLY	2.1
1	C	663	LEU	2.1
1	A	734	SER	2.1
1	C	135	GLN	2.1
1	C	746	ASP	2.1
1	D	687	GLN	2.1
1	C	683	PRO	2.1
1	A	736	ALA	2.1
1	A	685	LEU	2.1
1	B	699	ARG	2.1
1	B	748	CYS	2.0
1	B	682	LEU	2.0
1	C	739	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	8503	4/4	0.72	0.24	46,82,100,100	0
2	MG	A	3003	1/1	0.74	0.18	61,61,61,61	0
5	DMS	D	8417	4/4	0.76	0.24	26,41,80,100	0
5	DMS	C	8705	4/4	0.82	0.19	35,45,50,100	0
5	DMS	D	8420	4/4	0.84	0.17	27,51,77,94	0
5	DMS	A	8423	4/4	0.85	0.22	36,59,67,100	0
5	DMS	B	8416	4/4	0.85	0.16	46,55,71,100	0
5	DMS	B	8415	4/4	0.86	0.15	30,34,37,73	0
5	DMS	A	8421	4/4	0.87	0.17	51,60,61,74	0
5	DMS	A	8602	4/4	0.87	0.22	54,58,100,100	0
5	DMS	A	8415	4/4	0.88	0.22	24,63,100,100	0
2	MG	B	3003	1/1	0.88	0.14	48,48,48,48	0
5	DMS	B	8421	4/4	0.88	0.17	32,43,53,100	0
5	DMS	B	8423	4/4	0.88	0.17	37,56,72,72	0
5	DMS	B	8417	4/4	0.89	0.12	30,33,36,69	0
5	DMS	C	8416	4/4	0.89	0.19	64,66,100,100	0
5	DMS	A	8416	4/4	0.89	0.18	24,53,80,100	0
5	DMS	D	8503	4/4	0.89	0.19	31,76,100,100	0
5	DMS	B	8504	4/4	0.90	0.16	35,35,69,100	0
5	DMS	D	8407	4/4	0.90	0.14	26,50,53,55	0
5	DMS	B	8407	4/4	0.90	0.16	27,39,40,47	0
5	DMS	C	8423	4/4	0.90	0.13	38,42,44,58	0
5	DMS	A	8503	4/4	0.90	0.21	31,100,100,100	0
5	DMS	D	8703	4/4	0.90	0.17	32,38,49,53	0
5	DMS	A	8502	4/4	0.91	0.15	29,30,54,72	0
5	DMS	D	8416	4/4	0.91	0.14	34,35,54,77	0
5	DMS	C	8419	4/4	0.91	0.12	35,37,40,57	0
5	DMS	A	8407	4/4	0.91	0.12	25,38,39,47	0
5	DMS	B	8414	4/4	0.91	0.15	22,49,74,100	0
5	DMS	C	8415	4/4	0.91	0.14	26,32,41,61	0
5	DMS	C	8504	4/4	0.92	0.13	47,50,51,69	0
5	DMS	C	8407	4/4	0.92	0.14	30,39,40,50	0
5	DMS	B	8413	4/4	0.92	0.16	47,48,50,100	0
5	DMS	D	8415	4/4	0.92	0.18	25,49,64,100	0
5	DMS	B	8419	4/4	0.92	0.13	33,56,58,66	0
5	DMS	C	8417	4/4	0.92	0.10	23,35,47,52	0
4	145	C	2002	21/21	0.92	0.09	24,34,43,47	0
5	DMS	D	8421	4/4	0.92	0.17	32,54,78,100	0
5	DMS	A	8417	4/4	0.92	0.12	25,30,33,100	0
5	DMS	B	8410	4/4	0.92	0.16	29,42,60,100	0
5	DMS	D	8705	4/4	0.92	0.14	26,36,43,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	145	A	2002	21/21	0.93	0.09	20,30,41,43	0
4	145	D	2002	21/21	0.93	0.09	23,35,50,55	0
4	145	B	2002	21/21	0.93	0.09	23,31,41,50	0
5	DMS	B	8508	4/4	0.93	0.10	29,49,50,57	0
5	DMS	C	8425	4/4	0.93	0.15	42,44,49,71	0
5	DMS	A	8414	4/4	0.93	0.15	27,38,66,100	0
5	DMS	D	8425	4/4	0.93	0.18	22,24,28,56	4
5	DMS	C	8409	4/4	0.93	0.12	29,40,45,47	0
5	DMS	D	8508	4/4	0.93	0.11	34,39,44,51	0
5	DMS	C	8602	4/4	0.93	0.16	43,49,52,100	0
5	DMS	B	8420	4/4	0.93	0.13	39,42,46,52	0
5	DMS	C	8421	4/4	0.94	0.12	37,49,62,63	0
3	NA	D	3104	1/1	0.94	0.11	36,36,36,36	0
5	DMS	A	8409	4/4	0.94	0.14	30,41,46,100	0
5	DMS	A	8413	4/4	0.94	0.12	33,35,42,51	0
5	DMS	A	8420	4/4	0.94	0.12	37,44,52,62	0
5	DMS	D	8423	4/4	0.94	0.10	31,39,55,58	0
5	DMS	A	8406	4/4	0.94	0.13	16,52,70,78	0
5	DMS	D	8501	4/4	0.94	0.09	25,31,36,46	0
5	DMS	B	8408	4/4	0.94	0.15	31,36,40,100	0
5	DMS	D	8404	4/4	0.94	0.13	21,31,44,100	0
5	DMS	C	8420	4/4	0.94	0.17	40,41,57,100	0
5	DMS	D	8414	4/4	0.94	0.16	26,44,58,100	0
5	DMS	C	8413	4/4	0.95	0.10	32,33,45,45	0
5	DMS	C	8414	4/4	0.95	0.12	26,35,50,100	0
5	DMS	B	8502	4/4	0.95	0.14	30,31,44,100	0
5	DMS	C	8601	4/4	0.95	0.10	37,38,41,43	0
2	MG	C	3006	1/1	0.95	0.10	41,41,41,41	0
3	NA	C	3104	1/1	0.95	0.10	30,30,30,30	0
5	DMS	B	8601	4/4	0.95	0.10	33,35,37,42	0
5	DMS	A	8501	4/4	0.95	0.09	20,28,34,38	0
5	DMS	D	8409	4/4	0.95	0.14	29,37,43,100	0
5	DMS	C	8408	4/4	0.95	0.13	25,41,48,100	0
5	DMS	B	8425	4/4	0.95	0.09	29,35,36,43	0
3	NA	B	3104	1/1	0.96	0.08	32,32,32,32	0
5	DMS	B	8404	4/4	0.96	0.07	20,21,36,39	0
5	DMS	D	8419	4/4	0.96	0.11	34,36,55,72	0
5	DMS	A	8425	4/4	0.96	0.08	28,32,41,42	0
5	DMS	A	8419	4/4	0.96	0.11	36,44,49,52	0
5	DMS	B	8409	4/4	0.96	0.10	25,34,44,45	0
5	DMS	A	8410	4/4	0.96	0.11	28,36,39,52	0
5	DMS	A	8404	4/4	0.96	0.09	22,27,36,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	8410	4/4	0.96	0.10	24,34,37,39	0
5	DMS	D	8413	4/4	0.96	0.11	31,33,40,55	0
5	DMS	A	8504	4/4	0.96	0.13	21,36,41,87	0
5	DMS	C	8501	4/4	0.96	0.09	18,28,36,48	0
4	145	A	2001	21/21	0.97	0.08	14,17,45,95	0
5	DMS	A	8408	4/4	0.97	0.07	22,35,39,47	0
5	DMS	D	8410	4/4	0.97	0.10	25,34,43,53	0
3	NA	A	3103	1/1	0.97	0.07	25,25,25,25	0
4	145	B	2001	21/21	0.97	0.07	11,15,38,47	0
3	NA	A	3104	1/1	0.97	0.06	25,25,25,25	0
5	DMS	C	8402	4/4	0.97	0.06	18,22,23,28	0
5	DMS	C	8404	4/4	0.97	0.07	21,24,28,31	0
5	DMS	C	8405	4/4	0.97	0.08	27,31,31,32	0
4	145	C	2001	21/21	0.97	0.07	13,17,38,55	0
2	MG	A	3005	1/1	0.97	0.05	31,31,31,31	0
4	145	D	2001	21/21	0.97	0.07	12,19,47,57	0
2	MG	A	3105	1/1	0.97	0.07	31,31,31,31	0
5	DMS	C	8412	4/4	0.97	0.12	26,33,44,100	0
3	NA	D	3103	1/1	0.97	0.08	26,26,26,26	0
5	DMS	D	8402	4/4	0.97	0.07	18,23,24,26	0
2	MG	D	3005	1/1	0.97	0.08	27,27,27,27	0
5	DMS	D	8406	4/4	0.97	0.09	26,27,31,35	0
5	DMS	D	8412	4/4	0.98	0.10	26,28,31,100	0
5	DMS	B	8405	4/4	0.98	0.07	23,28,29,31	0
3	NA	B	3101	1/1	0.98	0.05	16,16,16,16	0
2	MG	C	3105	1/1	0.98	0.06	26,26,26,26	0
5	DMS	A	8402	4/4	0.98	0.06	16,17,22,28	0
5	DMS	C	8411	4/4	0.98	0.06	24,28,30,35	0
5	DMS	A	8403	4/4	0.98	0.06	21,24,27,27	0
5	DMS	B	8411	4/4	0.98	0.11	26,27,31,100	0
5	DMS	B	8412	4/4	0.98	0.08	27,33,35,37	0
5	DMS	A	8412	4/4	0.98	0.09	34,34,37,60	0
3	NA	C	3103	1/1	0.98	0.08	26,26,26,26	0
5	DMS	B	8402	4/4	0.98	0.06	16,21,22,23	0
5	DMS	C	8403	4/4	0.98	0.06	23,24,25,27	0
5	DMS	D	8408	4/4	0.98	0.06	17,31,35,38	0
5	DMS	B	8403	4/4	0.98	0.05	16,21,26,26	0
2	MG	D	3105	1/1	0.98	0.05	31,31,31,31	0
2	MG	B	3001	1/1	0.99	0.03	15,15,15,15	0
3	NA	B	3102	1/1	0.99	0.05	16,16,16,16	0
3	NA	B	3103	1/1	0.99	0.04	25,25,25,25	0
2	MG	D	3001	1/1	0.99	0.03	15,15,15,15	0

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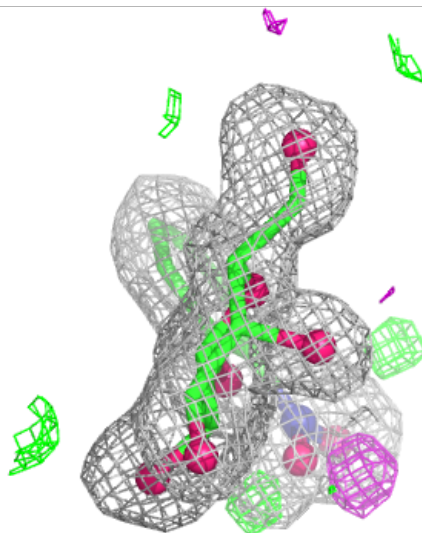
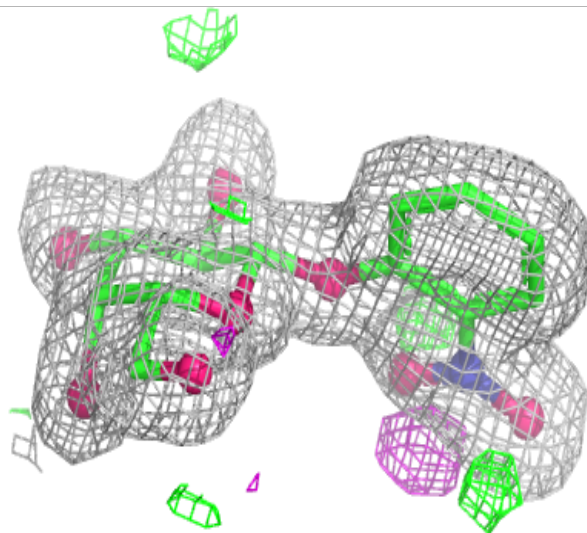
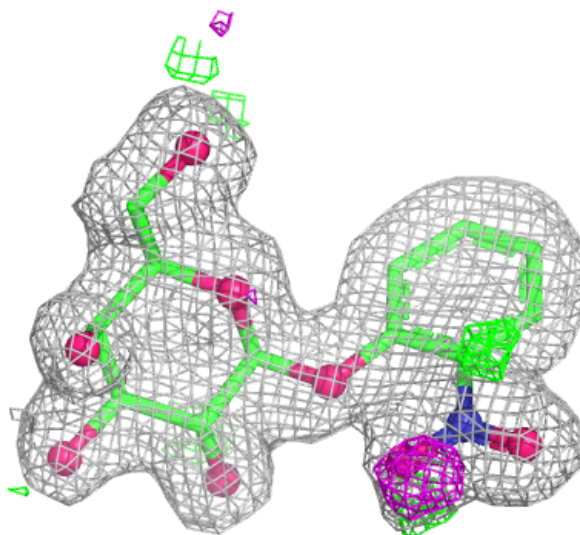
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	3002	1/1	0.99	0.05	17,17,17,17	0
5	DMS	D	8411	4/4	0.99	0.07	23,25,28,59	0
5	DMS	A	8401	4/4	0.99	0.03	12,14,16,18	0
2	MG	B	3002	1/1	0.99	0.03	17,17,17,17	0
5	DMS	C	8401	4/4	0.99	0.03	15,17,21,23	0
3	NA	D	3101	1/1	0.99	0.05	16,16,16,16	0
3	NA	D	3102	1/1	0.99	0.02	15,15,15,15	0
5	DMS	A	8405	4/4	0.99	0.05	20,24,25,27	0
2	MG	A	3002	1/1	0.99	0.04	17,17,17,17	0
3	NA	A	3101	1/1	0.99	0.03	17,17,17,17	0
3	NA	A	3102	1/1	0.99	0.02	15,15,15,15	0
2	MG	B	3105	1/1	0.99	0.03	27,27,27,27	0
2	MG	A	3001	1/1	0.99	0.02	17,17,17,17	0
5	DMS	D	8401	4/4	0.99	0.04	15,16,18,19	0
5	DMS	A	8411	4/4	0.99	0.06	23,24,28,31	0
5	DMS	D	8403	4/4	0.99	0.05	18,25,25,27	0
5	DMS	D	8701	4/4	0.99	0.07	15,16,20,38	0
5	DMS	B	8401	4/4	0.99	0.04	15,17,17,20	0
5	DMS	D	8405	4/4	0.99	0.05	24,25,25,30	0
2	MG	C	3002	1/1	1.00	0.04	15,15,15,15	0
3	NA	C	3101	1/1	1.00	0.05	15,15,15,15	0
3	NA	C	3102	1/1	1.00	0.01	17,17,17,17	0
2	MG	C	3001	1/1	1.00	0.01	15,15,15,15	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

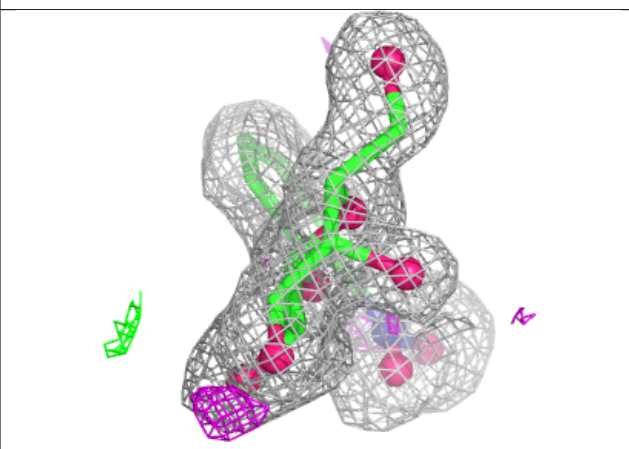
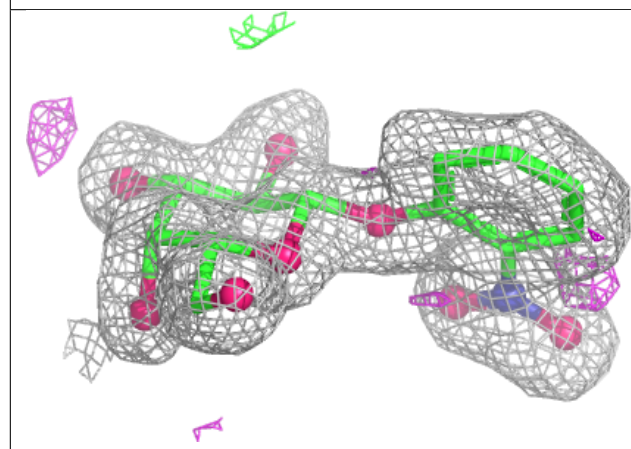
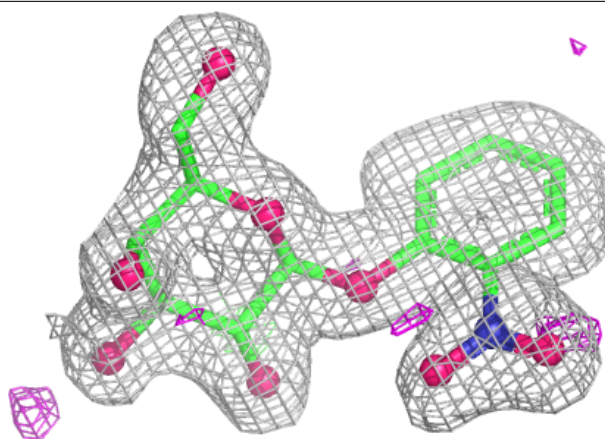
Electron density around 145 C 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



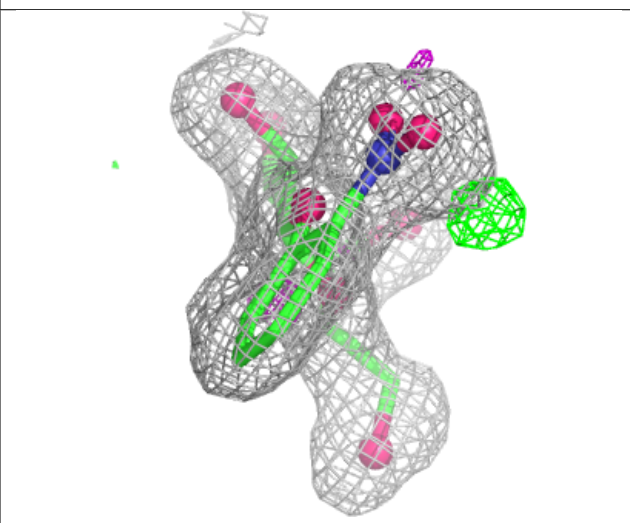
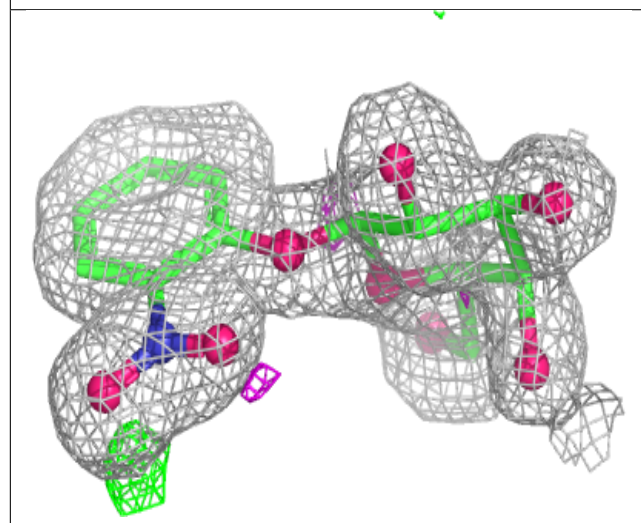
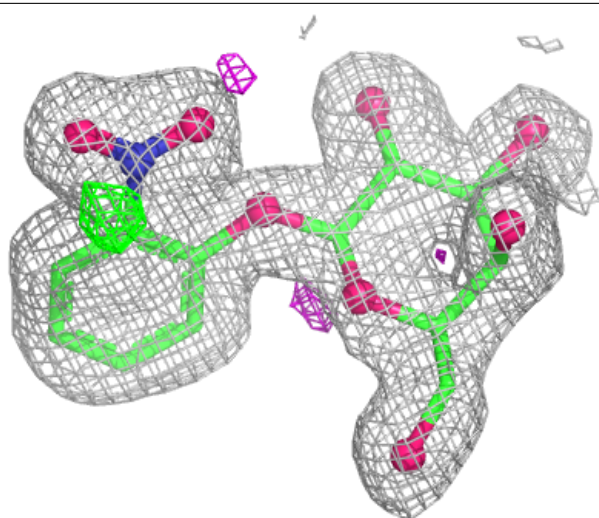
Electron density around 145 Å 2002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



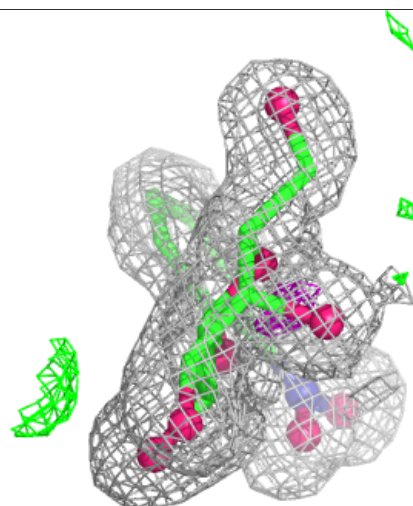
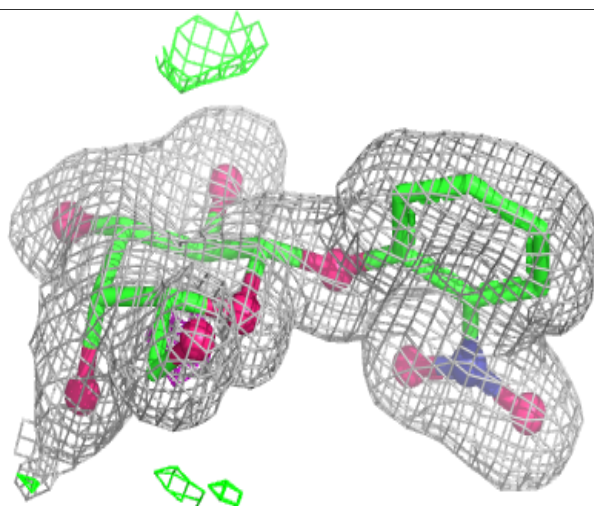
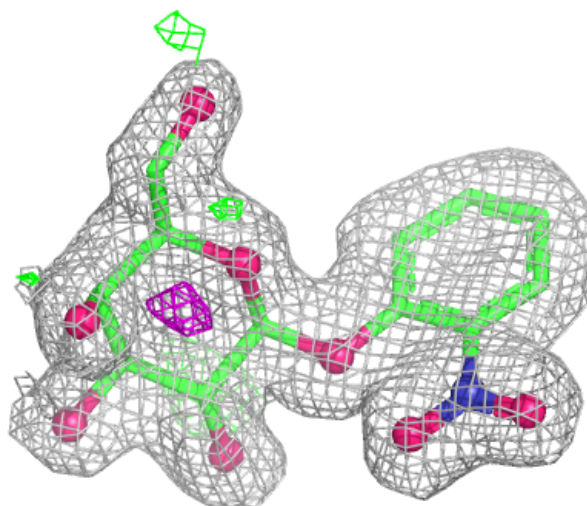
Electron density around 145 D 2002:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



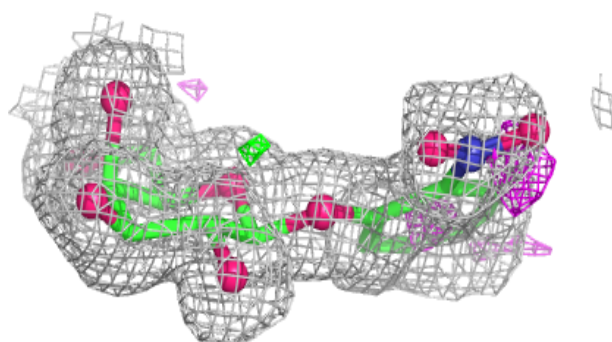
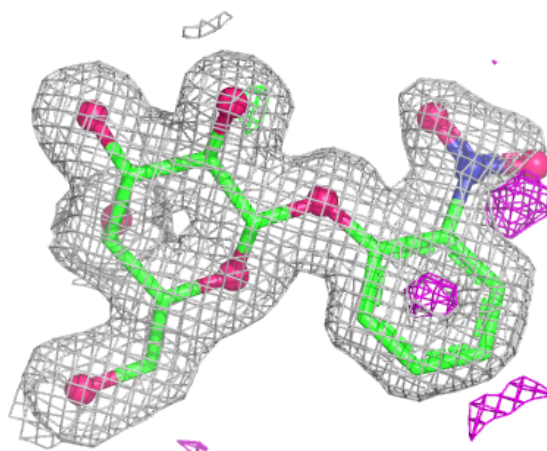
Electron density around 145 B 2002:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



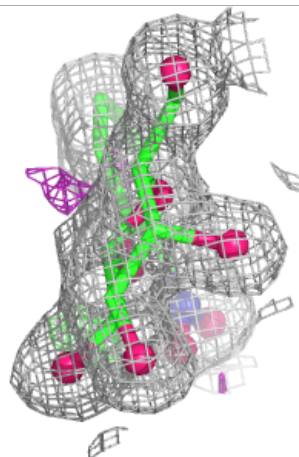
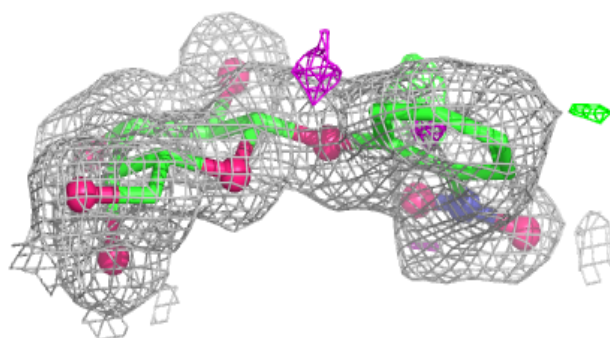
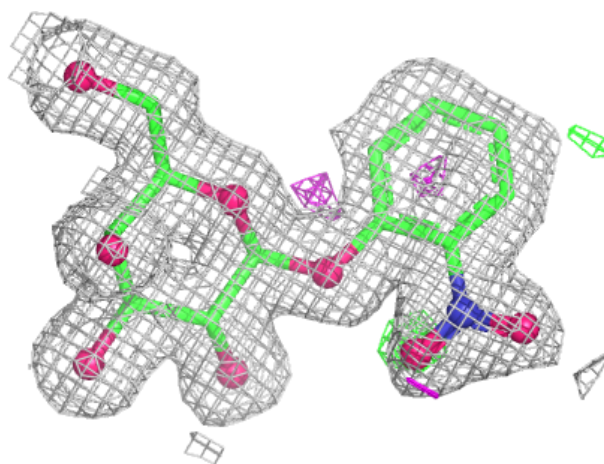
Electron density around 145 Å 2001:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



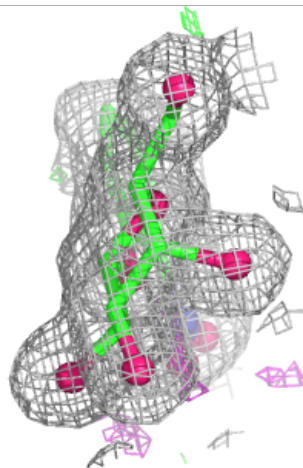
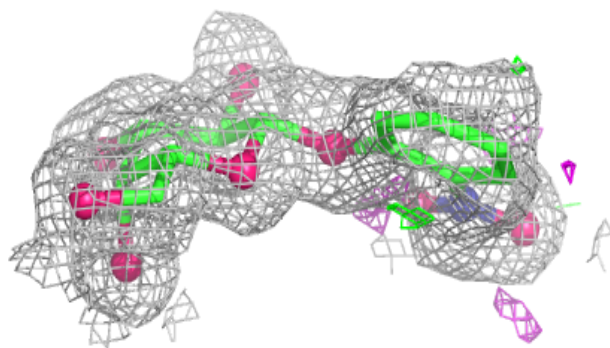
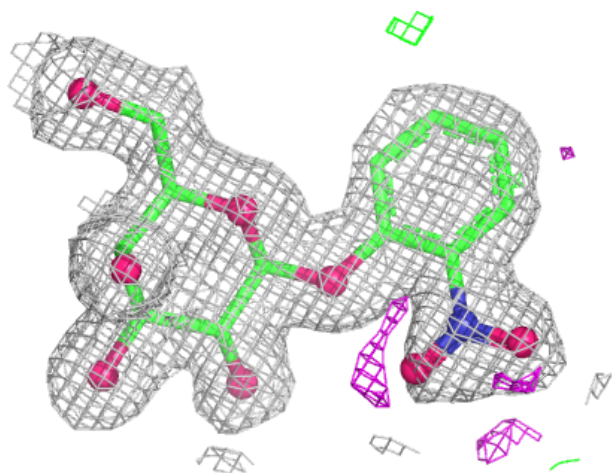
Electron density around 145 B 2001:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



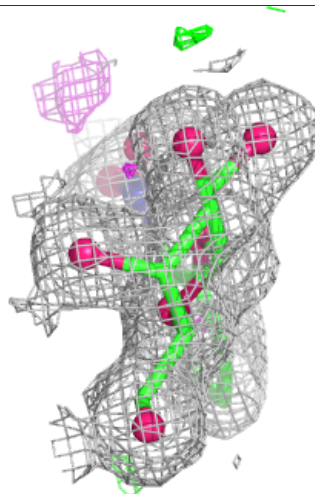
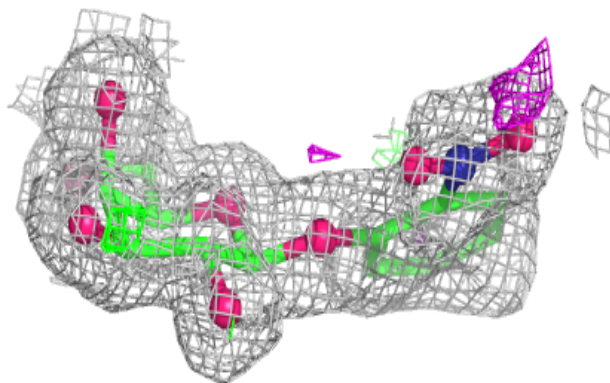
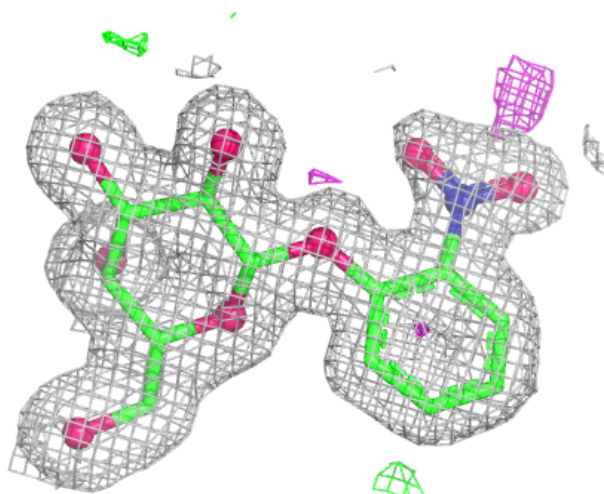
Electron density around 145 C 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 145 D 2001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.