



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:38 PM UTC

PDB ID : 1JYW / pdb_00001jyw
Title : E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH PNPG
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.55 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

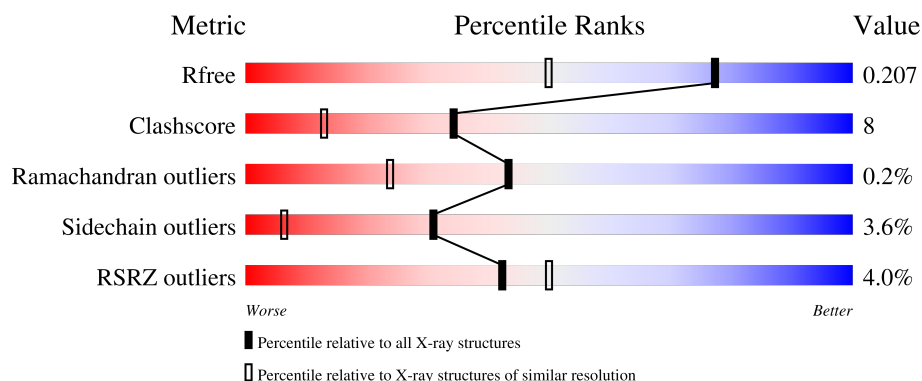
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	4% 78% 17% ..
1	B	1023	4% 78% 18% ..
1	C	1023	3% 77% 17% ..
1	D	1023	4% 77% 17% ..

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	8413	-	X	-	-
5	DMS	A	8415	-	X	-	-
5	DMS	A	8502	-	X	-	-
5	DMS	B	8402	-	X	-	-
5	DMS	B	8415	-	X	X	-
5	DMS	B	8508	-	X	-	-
5	DMS	C	8402	-	-	X	-
5	DMS	C	8427	-	-	X	-
5	DMS	D	8407	-	X	-	-
5	DMS	D	8705	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37524 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
			8127	5139	1441	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:

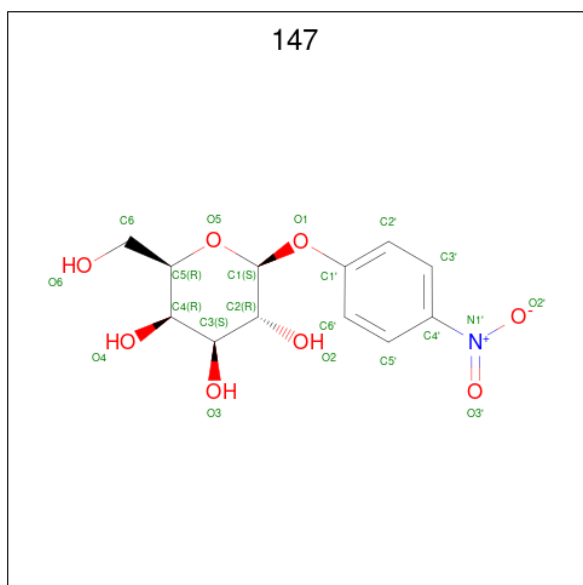
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	cloning artifact	? P00722
A	2	SER	MET	cloning artifact	? P00722
A	3	HIS	ILE	cloning artifact	? P00722
A	4	MET	THR	cloning artifact	? P00722
A	5	LEU	ASP	cloning artifact	? P00722
A	6	GLU	SER	cloning artifact	? P00722
A	7	ASP	LEU	cloning artifact	? 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 4-nitrophenyl beta-D-galactopyranoside (CCD ID: 147) (formula: $C_{12}H_{15}NO_8$).



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

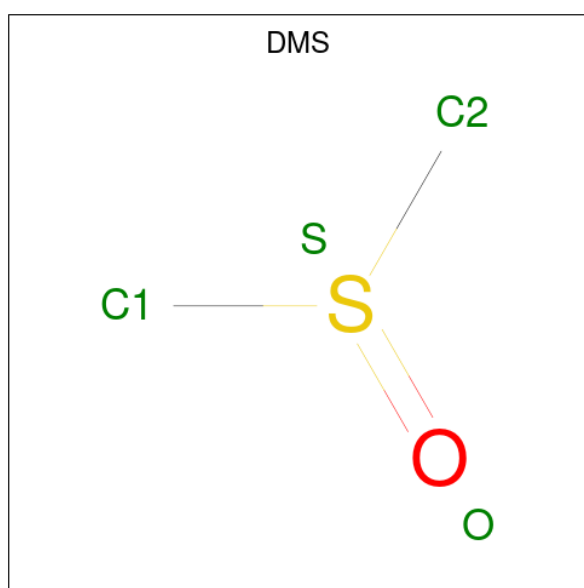
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- 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		

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

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

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

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

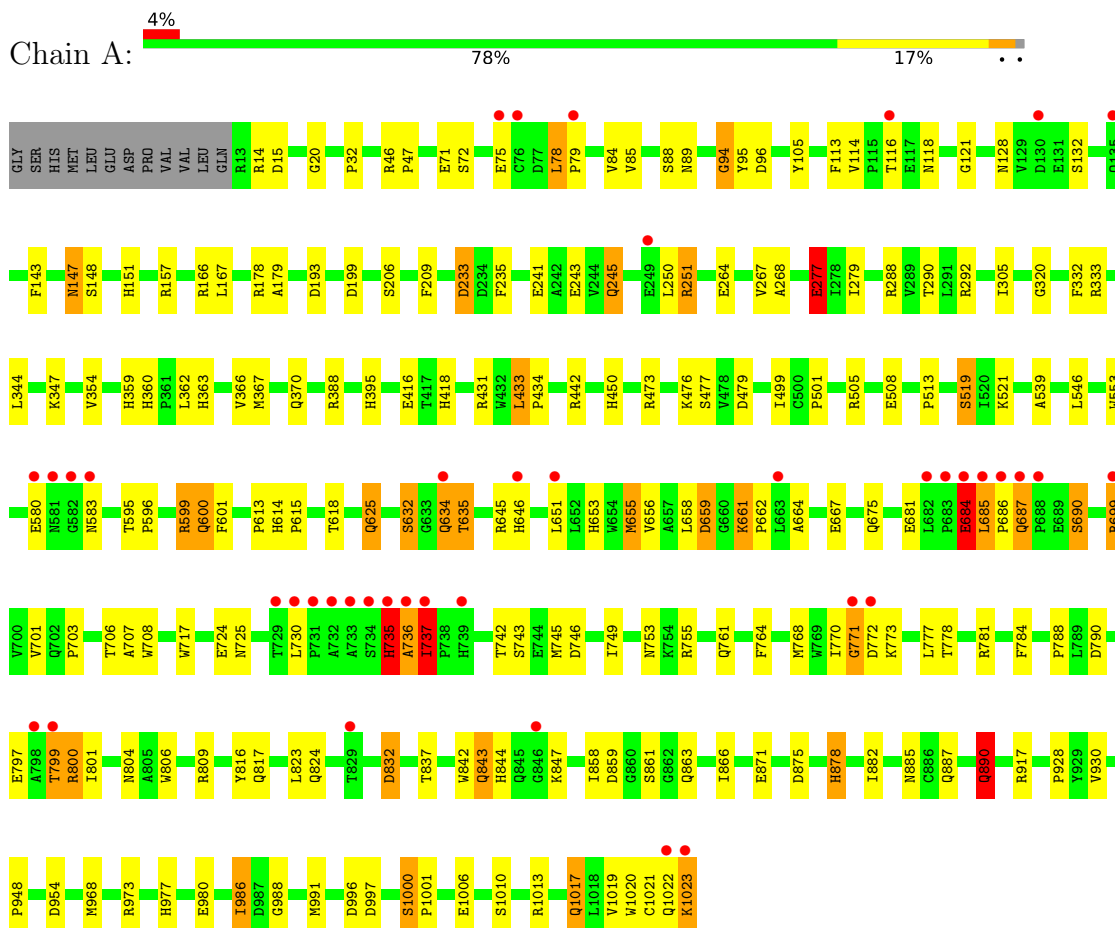
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1112	Total 1112	O 1112	0	0
6	B	1128	Total 1128	O 1128	0	0
6	C	1104	Total 1104	O 1104	0	0
6	D	1118	Total 1118	O 1118	0	0

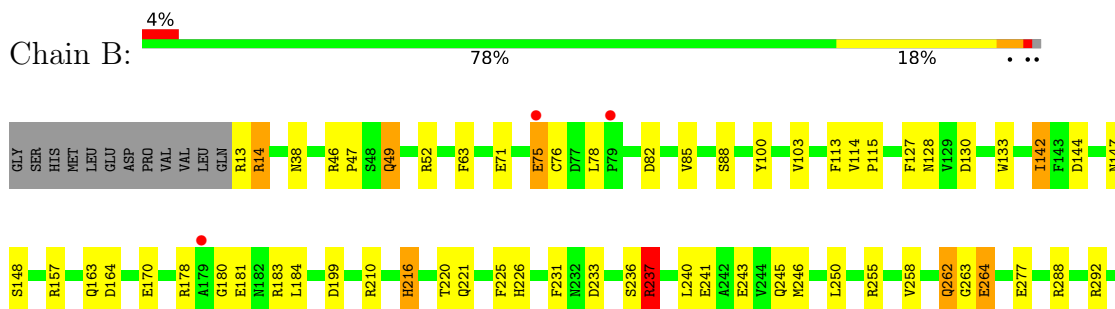
3 Residue-property plots

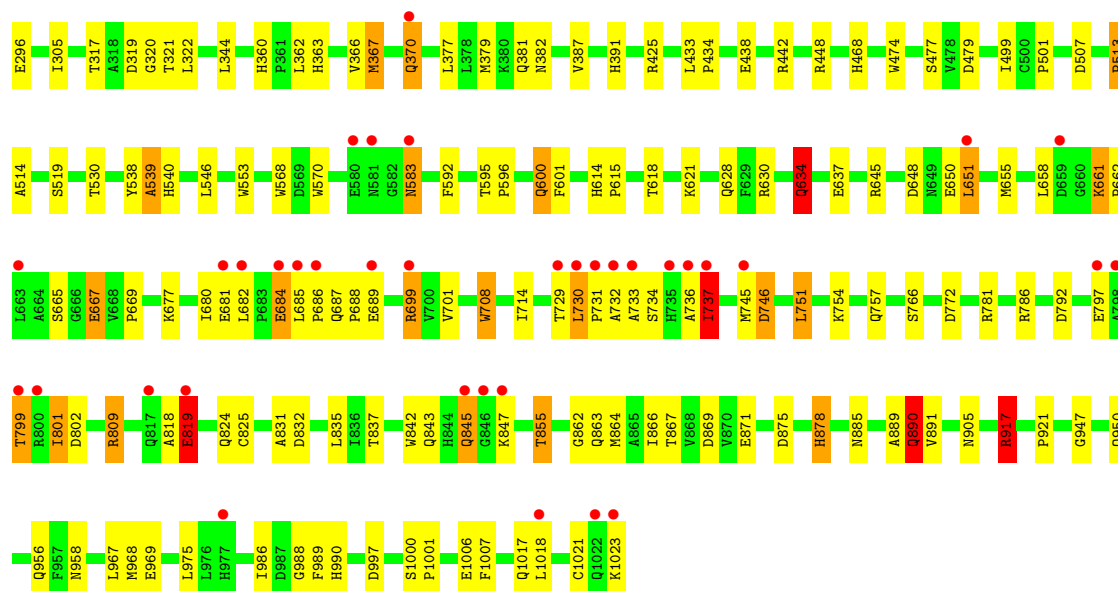
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-Galactosidase

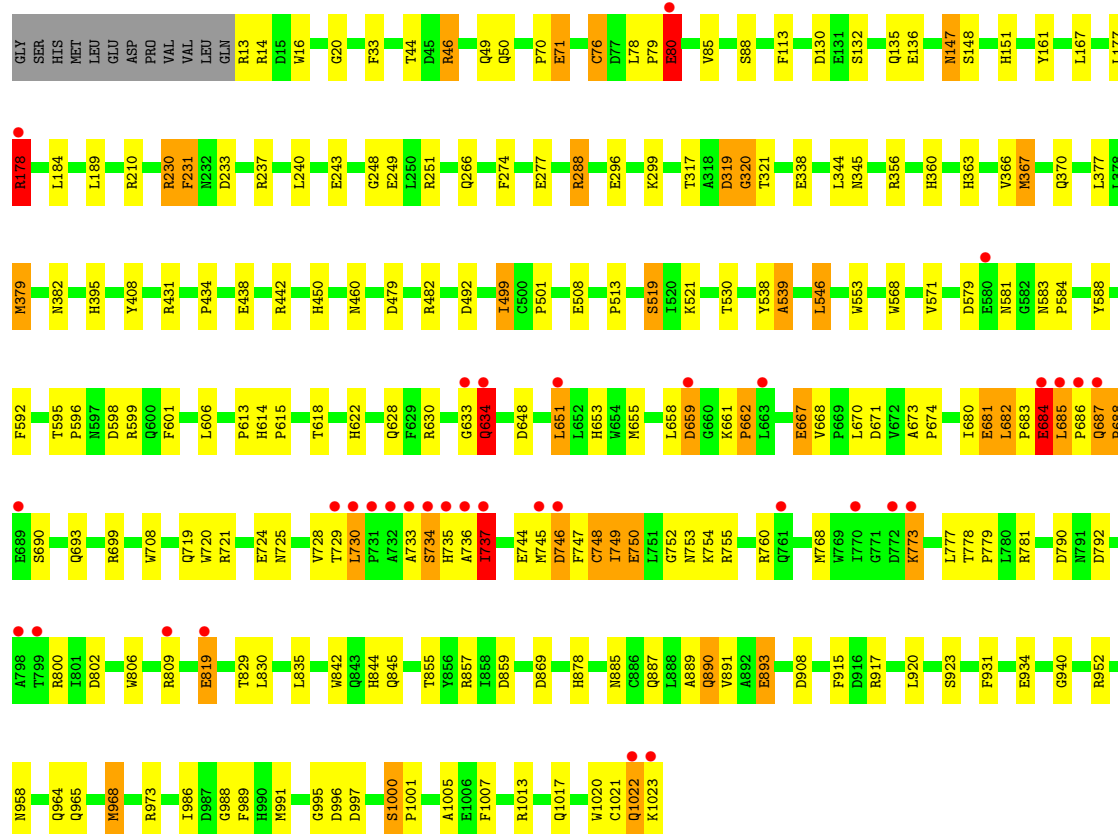
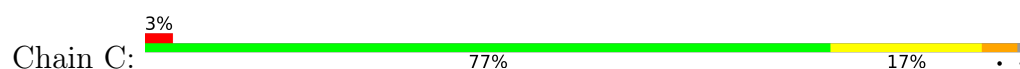


• Molecule 1: Beta-Galactosidase

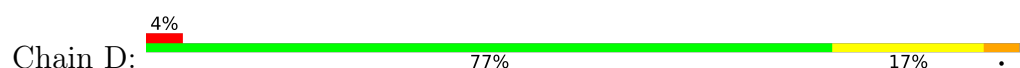


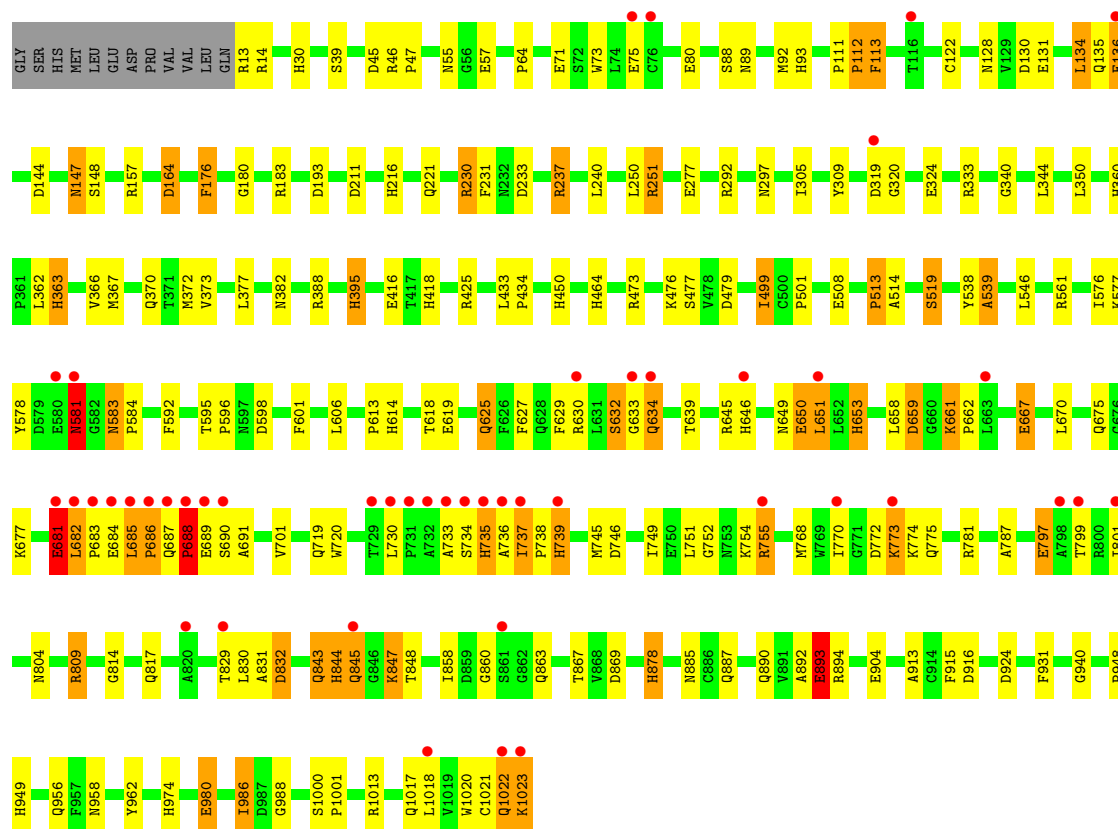


• Molecule 1: Beta-Galactosidase



• Molecule 1: Beta-Galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.68Å 168.60Å 201.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.80 – 1.55 28.80 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.3 (28.80-1.55) 91.5 (28.80-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 1.54Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.180 , 0.229 (Not available) , 0.207	Depositor DCC
R_{free} test set	10463 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 81.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	37524	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4252e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DMS, NA, 147, MG

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	1.43	17/8382 (0.2%)	1.77	117/11435 (1.0%)
1	B	1.45	21/8383 (0.3%)	1.76	113/11437 (1.0%)
1	C	1.43	21/8383 (0.3%)	1.79	140/11437 (1.2%)
1	D	1.44	17/8383 (0.2%)	1.75	120/11437 (1.0%)
All	All	1.44	76/33531 (0.2%)	1.77	490/45746 (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	1	0

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	297	ASN	C-O	-8.61	1.19	1.23
1	A	479	ASP	C-N	-8.41	1.26	1.33
1	C	588	TYR	C-N	7.26	1.39	1.33
1	C	230	ARG	NE-CZ	6.71	1.40	1.33
1	C	151	HIS	CG-CD2	6.60	1.43	1.35
1	D	30	HIS	CG-ND1	6.40	1.45	1.38
1	C	492	ASP	CG-OD2	6.25	1.37	1.25
1	D	418	HIS	CE1-NE2	6.25	1.38	1.32
1	D	425	ARG	NE-CZ	6.09	1.39	1.33
1	B	990	HIS	CE1-NE2	6.08	1.38	1.32
1	A	1006	GLU	CD-OE2	5.99	1.36	1.25
1	B	968	MET	SD-CE	5.99	1.94	1.79
1	B	708	TRP	CA-CB	5.97	1.62	1.53
1	B	199	ASP	CG-OD2	5.90	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	920	LEU	CA-CB	5.87	1.61	1.54
1	D	893	GLU	CD-OE2	5.83	1.36	1.25
1	D	681	GLU	CD-OE2	5.82	1.36	1.25
1	D	450	HIS	ND1-CE1	5.81	1.38	1.32
1	C	450	HIS	ND1-CE1	5.80	1.38	1.32
1	A	333	ARG	CD-NE	5.75	1.54	1.46
1	D	30	HIS	CD2-NE2	5.68	1.44	1.37
1	C	167	LEU	N-CA	5.68	1.50	1.45
1	B	142	ILE	C-O	5.62	1.30	1.24
1	B	442	ARG	CZ-NH1	5.58	1.40	1.32
1	A	450	HIS	ND1-CE1	5.58	1.38	1.32
1	A	151	HIS	CE1-NE2	5.57	1.38	1.32
1	B	71	GLU	CD-OE2	5.56	1.35	1.25
1	A	354	VAL	C-O	5.55	1.30	1.23
1	B	950	GLN	C-O	5.52	1.30	1.23
1	D	904	GLU	C-O	5.52	1.30	1.23
1	B	689	GLU	CD-OE2	5.51	1.35	1.25
1	A	167	LEU	N-CA	5.51	1.50	1.45
1	A	388	ARG	NE-CZ	5.50	1.39	1.33
1	A	505	ARG	CZ-NH2	5.49	1.40	1.33
1	D	662	PRO	CA-C	-5.44	1.46	1.52
1	B	950	GLN	C-N	5.42	1.40	1.33
1	C	662	PRO	CA-C	-5.39	1.46	1.52
1	C	546	LEU	C-N	5.37	1.38	1.33
1	B	737	ILE	CA-CB	-5.36	1.50	1.54
1	B	1006	GLU	CD-OE2	5.34	1.35	1.25
1	D	388	ARG	NE-CZ	5.32	1.39	1.33
1	D	333	ARG	NE-CZ	5.32	1.38	1.33
1	B	792	ASP	CG-OD2	5.31	1.35	1.25
1	C	210	ARG	NE-CZ	5.29	1.38	1.33
1	B	650	GLU	CD-OE2	5.29	1.35	1.25
1	C	792	ASP	CG-OD2	5.28	1.35	1.25
1	C	151	HIS	CE1-NE2	5.27	1.37	1.32
1	B	391	HIS	ND1-CE1	5.27	1.37	1.32
1	C	243	GLU	CD-OE2	5.26	1.35	1.25
1	B	322	LEU	C-N	5.21	1.38	1.33
1	D	650	GLU	CD-OE2	5.21	1.35	1.25
1	A	206	SER	N-CA	5.20	1.52	1.46
1	A	442	ARG	NE-CZ	5.19	1.38	1.33
1	B	540[A]	HIS	ND1-CE1	5.19	1.37	1.32
1	B	540[B]	HIS	ND1-CE1	5.19	1.37	1.32
1	B	258	VAL	C-O	5.15	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	PHE	C-O	5.13	1.30	1.23
1	D	233	ASP	CG-OD2	5.13	1.35	1.25
1	A	243	GLU	CD-OE2	5.11	1.35	1.25
1	C	80	GLU	CD-OE2	5.11	1.35	1.25
1	B	905	ASN	C-N	5.10	1.39	1.32
1	D	211	ASP	CG-OD2	5.09	1.35	1.25
1	C	482	ARG	CZ-NH1	5.08	1.39	1.32
1	B	468	HIS	CE1-NE2	5.08	1.37	1.32
1	C	479	ASP	C-N	-5.08	1.28	1.34
1	C	450	HIS	CE1-NE2	5.07	1.37	1.32
1	A	157	ARG	NE-CZ	5.07	1.38	1.33
1	C	460	ASN	CA-C	5.07	1.58	1.52
1	D	350	LEU	C-O	5.06	1.29	1.23
1	C	379	MET	CA-CB	5.03	1.61	1.53
1	A	928	PRO	N-CA	-5.03	1.41	1.47
1	C	684	GLU	CD-OE2	5.02	1.34	1.25
1	A	114	VAL	CA-C	5.02	1.58	1.52
1	D	940	GLY	CA-C	5.02	1.56	1.51
1	A	151	HIS	CG-ND1	5.02	1.43	1.38
1	C	50	GLN	CA-C	5.02	1.59	1.52

All (490) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	ARG	NE-CZ-NH1	15.70	137.20	121.50
1	C	230	ARG	CD-NE-CZ	13.58	143.41	124.40
1	D	845	GLN	CA-C-N	-10.47	107.58	122.86
1	D	845	GLN	C-N-CA	-10.47	107.58	122.86
1	C	630	ARG	NE-CZ-NH2	-10.37	109.87	119.20
1	D	689	GLU	CA-C-N	9.74	135.43	121.02
1	D	689	GLU	C-N-CA	9.74	135.43	121.02
1	D	845	GLN	CB-CA-C	-9.55	97.85	111.80
1	D	878	HIS	CA-CB-CG	-9.39	104.41	113.80
1	D	770	ILE	N-CA-C	-8.81	94.33	107.37
1	D	297	ASN	O-C-N	-8.68	117.54	121.53
1	C	721	ARG	NE-CZ-NH1	8.63	130.13	121.50
1	B	49	GLN	CB-CG-CD	8.59	127.20	112.60
1	D	817	GLN	CB-CG-CD	-8.42	98.29	112.60
1	C	845	GLN	CA-C-N	-8.34	110.29	122.46
1	C	845	GLN	C-N-CA	-8.34	110.29	122.46
1	D	893	GLU	CB-CG-CD	8.31	126.72	112.60
1	C	659	ASP	CB-CA-C	8.29	123.66	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	683	PRO	CB-CA-C	-8.18	100.57	111.12
1	A	431	ARG	NE-CZ-NH2	-7.98	112.02	119.20
1	D	736	ALA	N-CA-C	7.98	122.57	109.96
1	A	725	ASN	CA-CB-CG	-7.98	104.62	112.60
1	C	274	PHE	CA-CB-CG	-7.91	105.89	113.80
1	A	735	HIS	CA-CB-CG	-7.80	106.00	113.80
1	D	659	ASP	CA-CB-CG	7.80	120.40	112.60
1	C	442	ARG	NE-CZ-NH2	-7.79	112.19	119.20
1	D	581	ASN	CA-CB-CG	7.75	120.35	112.60
1	D	625	GLN	OE1-CD-NE2	7.71	130.31	122.60
1	C	230	ARG	NH1-CZ-NH2	-7.67	109.33	119.30
1	A	687	GLN	CA-C-N	7.59	127.63	119.89
1	A	687	GLN	C-N-CA	7.59	127.63	119.89
1	B	889	ALA	CA-C-N	-7.53	109.58	123.05
1	B	889	ALA	C-N-CA	-7.53	109.58	123.05
1	C	363	HIS	CA-CB-CG	-7.50	106.30	113.80
1	A	755	ARG	NE-CZ-NH1	7.48	128.98	121.50
1	D	809	ARG	CD-NE-CZ	7.42	134.79	124.40
1	A	279	ILE	N-CA-C	-7.42	105.89	111.90
1	B	363	HIS	CA-CB-CG	-7.41	106.39	113.80
1	C	729	THR	CA-C-N	7.35	130.65	120.65
1	C	729	THR	C-N-CA	7.35	130.65	120.65
1	C	633	GLY	CA-C-N	7.30	134.69	122.79
1	C	633	GLY	C-N-CA	7.30	134.69	122.79
1	D	633	GLY	CA-C-N	-7.24	111.15	122.67
1	D	633	GLY	C-N-CA	-7.24	111.15	122.67
1	D	733	ALA	N-CA-C	7.21	120.84	110.24
1	A	14	ARG	N-CA-CB	-7.20	101.74	110.53
1	A	771	GLY	N-CA-C	-7.19	96.14	113.18
1	A	632	SER	N-CA-CB	7.19	123.38	110.95
1	C	630	ARG	CD-NE-CZ	7.18	134.45	124.40
1	D	681	GLU	CB-CA-C	7.13	122.57	110.81
1	C	592	PHE	CA-CB-CG	-7.12	106.68	113.80
1	A	832	ASP	N-CA-CB	-7.11	101.22	111.54
1	A	78	LEU	CA-C-O	7.09	125.48	119.66
1	C	680	ILE	CA-C-N	-7.08	112.95	122.72
1	C	680	ILE	C-N-CA	-7.08	112.95	122.72
1	B	832	ASP	N-CA-CB	-7.08	99.75	111.49
1	D	297	ASN	CB-CA-C	-7.07	106.18	111.20
1	A	1000	SER	CA-CB-OG	-7.03	97.05	111.10
1	A	755	ARG	NE-CZ-NH2	-7.02	112.88	119.20
1	A	684	GLU	CB-CG-CD	7.02	124.53	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	844	HIS	CA-CB-CG	-6.97	106.83	113.80
1	D	309	TYR	N-CA-C	-6.95	99.68	109.69
1	A	583	ASN	CA-CB-CG	-6.93	105.67	112.60
1	B	871	GLU	CB-CG-CD	-6.92	100.84	112.60
1	C	633	GLY	O-C-N	6.91	129.96	123.19
1	A	816	TYR	CA-C-N	-6.89	111.75	122.37
1	A	816	TYR	C-N-CA	-6.89	111.75	122.37
1	A	770	ILE	N-CA-CB	6.88	120.59	111.64
1	D	113	PHE	CA-CB-CG	-6.87	106.93	113.80
1	B	14	ARG	N-CA-CB	6.79	122.04	111.71
1	B	255	ARG	CA-C-N	-6.78	113.71	123.06
1	B	255	ARG	C-N-CA	-6.78	113.71	123.06
1	D	739	HIS	CA-CB-CG	-6.77	107.03	113.80
1	A	477	SER	N-CA-CB	6.77	120.14	110.13
1	C	1005	ALA	N-CA-C	6.74	119.49	111.33
1	C	725	ASN	CA-CB-CG	-6.72	105.88	112.60
1	A	684	GLU	N-CA-C	-6.71	100.36	110.28
1	B	370	GLN	CB-CG-CD	6.70	123.99	112.60
1	C	248	GLY	CA-C-N	-6.68	113.28	122.30
1	C	248	GLY	C-N-CA	-6.68	113.28	122.30
1	B	130	ASP	CA-CB-CG	-6.67	105.94	112.60
1	D	144	ASP	CA-CB-CG	-6.64	105.96	112.60
1	B	819	GLU	CB-CG-CD	6.63	123.87	112.60
1	C	76	CYS	N-CA-C	6.60	119.21	109.24
1	C	752	GLY	O-C-N	6.58	131.25	122.70
1	D	136	GLU	N-CA-C	6.57	117.81	108.74
1	B	819	GLU	CB-CA-C	6.55	121.88	109.37
1	B	867	THR	CA-CB-OG1	-6.55	99.78	109.60
1	B	519	SER	N-CA-C	-6.54	101.02	110.24
1	B	890	GLN	N-CA-C	6.54	119.75	110.14
1	B	46	ARG	NE-CZ-NH2	-6.53	113.32	119.20
1	C	630	ARG	NE-CZ-NH1	6.53	128.03	121.50
1	A	433	LEU	CA-C-O	6.52	124.66	118.34
1	A	477	SER	CA-CB-OG	-6.52	98.07	111.10
1	B	917	ARG	CD-NE-CZ	-6.51	115.28	124.40
1	B	843	GLN	O-C-N	6.51	131.62	123.15
1	C	917	ARG	CD-NE-CZ	-6.50	115.30	124.40
1	C	958	ASN	N-CA-CB	6.50	122.99	111.69
1	D	183	ARG	NE-CZ-NH1	-6.50	115.00	121.50
1	C	988	GLY	N-CA-C	-6.48	104.47	112.77
1	C	773	LYS	N-CA-C	6.48	119.26	108.96
1	D	915	PHE	CA-CB-CG	-6.47	107.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	681	GLU	CB-CG-CD	6.46	123.58	112.60
1	A	89	ASN	OD1-CG-ND2	6.46	129.06	122.60
1	B	539[A]	ALA	CB-CA-C	-6.46	97.57	110.42
1	B	539[B]	ALA	CB-CA-C	-6.46	97.57	110.42
1	C	659	ASP	CA-CB-CG	6.46	119.06	112.60
1	D	614	HIS	N-CA-C	-6.45	101.72	110.36
1	C	513	PRO	CB-CA-C	-6.44	102.65	111.21
1	A	599	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	C	230	ARG	NE-CZ-NH2	-6.40	113.44	119.20
1	B	433	LEU	CA-C-O	6.39	124.54	118.34
1	C	249	GLU	N-CA-C	6.39	119.13	108.96
1	B	82	ASP	CA-CB-CG	-6.39	106.21	112.60
1	D	646	HIS	ND1-CG-CD2	6.39	112.49	106.10
1	A	977	HIS	CA-CB-CG	6.37	120.17	113.80
1	A	737	ILE	N-CA-CB	6.36	120.11	111.21
1	B	869	ASP	CA-CB-CG	-6.36	106.25	112.60
1	A	209	PHE	CA-CB-CG	-6.34	107.46	113.80
1	D	735	HIS	CA-CB-CG	-6.33	107.47	113.80
1	C	1000	SER	CA-CB-OG	-6.33	98.44	111.10
1	B	513	PRO	CB-CA-C	-6.32	103.31	111.46
1	C	684	GLU	CB-CG-CD	6.31	123.33	112.60
1	C	521	LYS	CG-CD-CE	6.31	125.81	111.30
1	B	736	ALA	N-CA-C	6.30	118.12	109.18
1	C	598	ASP	CA-CB-CG	-6.29	106.31	112.60
1	D	931	PHE	CA-CB-CG	-6.28	107.52	113.80
1	A	613	PRO	CB-CA-C	-6.28	102.75	110.98
1	C	682	LEU	CA-C-N	6.27	126.18	119.85
1	C	682	LEU	C-N-CA	6.27	126.18	119.85
1	C	136	GLU	CB-CA-C	-6.27	96.98	110.45
1	D	662	PRO	CA-C-O	-6.26	114.54	121.23
1	C	71	GLU	CB-CG-CD	6.25	123.22	112.60
1	A	954	ASP	CA-CB-CG	-6.23	106.37	112.60
1	A	788	PRO	N-CA-CB	6.19	108.84	103.27
1	D	988	GLY	N-CA-C	-6.18	104.85	112.77
1	C	802	ASP	CA-CB-CG	-6.18	106.42	112.60
1	C	583	ASN	CA-CB-CG	-6.18	106.42	112.60
1	C	746	ASP	N-CA-C	6.17	118.56	109.24
1	C	277	GLU	N-CA-CB	-6.17	101.92	110.38
1	D	395	HIS	N-CA-CB	-6.17	100.30	109.98
1	A	687	GLN	CB-CA-C	6.17	119.99	109.82
1	C	634	GLN	N-CA-C	-6.16	103.18	111.87
1	D	980	GLU	CA-C-N	-6.16	106.77	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	980	GLU	C-N-CA	-6.16	106.77	120.99
1	D	682	LEU	CB-CA-C	-6.13	99.79	109.42
1	D	64	PRO	O-C-N	6.12	130.62	122.30
1	D	363	HIS	CA-CB-CG	-6.12	107.68	113.80
1	C	940	GLY	O-C-N	6.11	127.45	122.51
1	A	20	GLY	N-CA-C	-6.10	107.09	114.66
1	A	736	ALA	N-CA-C	6.10	117.82	108.42
1	B	85	VAL	CB-CA-C	-6.10	102.68	111.34
1	D	847	LYS	CA-C-N	-6.10	114.07	122.30
1	D	847	LYS	C-N-CA	-6.10	114.07	122.30
1	B	786	ARG	NE-CZ-NH2	-6.09	113.71	119.20
1	C	395	HIS	ND1-CE1-NE2	6.09	114.50	108.40
1	B	614	HIS	N-CA-CB	6.09	116.80	109.74
1	A	746	ASP	CA-CB-CG	-6.06	106.54	112.60
1	D	176	PHE	CA-CB-CG	-6.06	107.74	113.80
1	C	753	ASN	CA-C-N	-6.06	112.63	122.81
1	C	753	ASN	C-N-CA	-6.06	112.63	122.81
1	B	568	TRP	CA-CB-CG	-6.05	102.09	113.60
1	A	790	ASP	CA-CB-CG	-6.04	106.56	112.60
1	D	869	ASP	CA-CB-CG	-6.04	106.56	112.60
1	B	969	GLU	CA-CB-CG	-6.04	102.02	114.10
1	B	878	HIS	CA-CB-CG	-6.04	107.76	113.80
1	C	601	PHE	CA-CB-CG	-6.04	107.76	113.80
1	C	699	ARG	CD-NE-CZ	-6.03	115.96	124.40
1	A	513	PRO	CB-CA-C	-6.02	103.20	111.21
1	C	890	GLN	N-CA-C	6.02	119.39	110.48
1	D	136	GLU	N-CA-CB	-6.01	101.17	111.21
1	D	583	ASN	CA-CB-CG	-6.01	106.58	112.60
1	D	843	GLN	CA-C-N	-6.01	113.49	122.39
1	D	843	GLN	C-N-CA	-6.01	113.49	122.39
1	B	855	THR	N-CA-CB	6.01	121.88	111.00
1	D	619	GLU	N-CA-C	-6.01	104.64	111.07
1	C	614	HIS	N-CA-C	-6.00	102.33	110.36
1	B	425	ARG	NE-CZ-NH2	-5.97	113.82	119.20
1	B	78	LEU	CA-C-O	5.97	125.07	119.76
1	C	438	GLU	CG-CD-OE2	-5.97	104.67	118.40
1	B	997	ASP	N-CA-CB	5.97	120.99	111.56
1	D	773	LYS	N-CA-C	5.96	118.43	108.96
1	B	648	ASP	N-CA-C	5.95	119.60	112.93
1	A	359	HIS	ND1-CG-CD2	5.95	112.05	106.10
1	B	680	ILE	CA-C-N	-5.94	113.81	122.19
1	B	680	ILE	C-N-CA	-5.94	113.81	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	736	ALA	N-CA-C	5.92	119.18	110.59
1	C	737	ILE	N-CA-CB	5.92	119.51	111.21
1	B	989	PHE	CA-CB-CG	-5.91	107.89	113.80
1	B	570	TRP	N-CA-C	5.91	117.59	111.03
1	D	592	PHE	CA-CB-CG	-5.91	107.89	113.80
1	A	245	GLN	CB-CG-CD	5.91	122.64	112.60
1	B	382	ASN	CA-CB-CG	-5.90	106.70	112.60
1	A	128	ASN	OD1-CG-ND2	5.89	128.49	122.60
1	B	997	ASP	CA-CB-CG	-5.89	106.71	112.60
1	B	699	ARG	CB-CG-CD	5.89	124.84	111.30
1	B	75	GLU	CA-C-N	-5.88	111.57	121.75
1	B	75	GLU	C-N-CA	-5.88	111.57	121.75
1	C	779	PRO	N-CA-CB	5.87	108.91	103.39
1	A	601	PHE	CA-CB-CG	-5.87	107.93	113.80
1	D	324	GLU	N-CA-CB	5.87	121.42	111.57
1	D	625	GLN	CG-CD-OE1	-5.86	109.09	120.80
1	D	578	TYR	CA-C-O	-5.85	114.38	120.70
1	C	648	ASP	CA-CB-CG	-5.84	106.76	112.60
1	C	857	ARG	CD-NE-CZ	-5.84	116.23	124.40
1	A	635	THR	N-CA-C	5.84	118.75	109.24
1	B	669	PRO	CB-CA-C	-5.83	103.45	111.21
1	B	890	GLN	OE1-CD-NE2	5.83	128.43	122.60
1	D	147	ASN	OD1-CG-ND2	5.83	128.43	122.60
1	D	93	HIS	N-CA-C	-5.83	105.75	112.92
1	D	974	HIS	CA-CB-CG	-5.82	107.98	113.80
1	A	778	THR	CA-CB-OG1	-5.82	100.87	109.60
1	A	614	HIS	N-CA-C	-5.82	102.57	110.36
1	C	519	SER	O-C-N	-5.82	115.87	122.97
1	B	958	ASN	N-CA-CB	5.81	121.81	111.69
1	C	733	ALA	N-CA-CB	5.81	120.31	110.49
1	D	867	THR	CA-C-O	-5.80	114.09	120.36
1	B	63	PHE	CA-CB-CG	-5.80	108.00	113.80
1	A	784	PHE	CA-CB-CG	-5.80	108.00	113.80
1	A	875	ASP	CA-CB-CG	-5.80	106.80	112.60
1	B	220	THR	CA-CB-OG1	-5.78	100.93	109.60
1	D	948	PRO	CB-CA-C	-5.78	102.31	111.04
1	A	14	ARG	CA-CB-CG	-5.78	102.54	114.10
1	C	859	ASP	CA-C-N	5.78	127.36	120.14
1	C	859	ASP	C-N-CA	5.78	127.36	120.14
1	A	707	ALA	CA-C-N	-5.78	113.48	122.37
1	A	707	ALA	C-N-CA	-5.78	113.48	122.37
1	C	519	SER	N-CA-C	-5.77	102.11	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	598	ASP	CA-CB-CG	-5.77	106.83	112.60
1	B	1007	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	625	GLN	CG-CD-OE1	-5.76	109.28	120.80
1	B	662	PRO	N-CA-CB	5.76	108.69	103.34
1	B	688	PRO	CA-C-N	5.75	129.05	120.31
1	B	688	PRO	C-N-CA	5.75	129.05	120.31
1	C	819	GLU	N-CA-CB	-5.75	101.55	110.57
1	A	842	TRP	CE2-CD2-CE3	5.74	124.54	118.80
1	D	539[A]	ALA	CB-CA-C	-5.74	99.00	110.42
1	D	539[B]	ALA	CB-CA-C	-5.74	99.00	110.42
1	B	76	CYS	CA-CB-SG	-5.73	101.22	114.40
1	C	320	GLY	CA-C-N	-5.73	114.11	122.19
1	C	320	GLY	C-N-CA	-5.73	114.11	122.19
1	A	96	ASP	N-CA-CB	5.73	120.28	111.46
1	C	85	VAL	CA-CB-CG2	-5.73	100.66	110.40
1	B	519	SER	N-CA-CB	-5.72	100.59	109.69
1	D	632	SER	N-CA-CB	5.72	120.84	110.95
1	B	772	ASP	CA-CB-CG	5.72	118.32	112.60
1	C	147	ASN	CA-C-O	-5.71	114.19	120.30
1	C	46	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	D	787	ALA	N-CA-C	-5.70	99.60	109.58
1	A	519	SER	N-CA-C	-5.70	102.20	110.24
1	B	890	GLN	N-CA-CB	-5.70	102.21	110.70
1	A	890	GLN	N-CA-CB	-5.69	101.64	110.29
1	B	819	GLU	N-CA-CB	-5.69	100.93	110.83
1	D	519	SER	N-CA-C	-5.68	102.23	110.24
1	D	147	ASN	N-CA-CB	-5.68	101.63	110.55
1	C	408	TYR	CA-C-N	-5.66	115.25	123.06
1	C	408	TYR	C-N-CA	-5.66	115.25	123.06
1	D	479	ASP	CA-CB-CG	-5.66	106.94	112.60
1	D	134	LEU	N-CA-C	-5.66	105.87	112.89
1	B	614	HIS	N-CA-C	-5.66	102.78	110.36
1	C	113	PHE	CA-CB-CG	-5.66	108.14	113.80
1	D	477	SER	CB-CA-C	-5.66	101.28	110.79
1	A	659	ASP	CA-C-N	-5.65	114.61	122.86
1	A	659	ASP	C-N-CA	-5.65	114.61	122.86
1	A	75	GLU	N-CA-CB	5.65	118.72	110.47
1	B	975	LEU	N-CA-CB	-5.64	102.14	110.49
1	A	179	ALA	N-CA-CB	5.64	118.35	109.83
1	A	687	GLN	N-CA-CB	5.64	120.21	109.44
1	D	251	ARG	CG-CD-NE	-5.63	99.60	112.00
1	C	177	LEU	CB-CA-C	-5.62	100.72	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	843	GLN	OE1-CD-NE2	5.62	128.22	122.60
1	C	296	GLU	CB-CG-CD	-5.62	103.05	112.60
1	B	592	PHE	CA-CB-CG	-5.61	108.19	113.80
1	B	801	ILE	O-C-N	-5.61	116.95	122.67
1	A	996	ASP	N-CA-C	-5.60	105.27	111.71
1	B	479	ASP	CA-CB-CG	-5.60	107.00	112.60
1	A	843	GLN	CA-C-N	-5.60	113.01	121.86
1	A	843	GLN	C-N-CA	-5.60	113.01	121.86
1	D	832	ASP	CA-CB-CG	-5.59	107.01	112.60
1	B	442	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	A	539[A]	ALA	CB-CA-C	-5.58	99.32	110.42
1	A	539[B]	ALA	CB-CA-C	-5.58	99.32	110.42
1	B	729	THR	N-CA-CB	5.58	118.96	109.87
1	D	1013	ARG	CA-CB-CG	-5.57	102.97	114.10
1	A	235	PHE	CA-CB-CG	-5.56	108.24	113.80
1	D	746	ASP	CB-CA-C	-5.56	98.49	110.45
1	C	184	LEU	CB-CA-C	-5.56	100.10	109.50
1	B	264	GLU	CA-C-O	5.55	126.00	119.28
1	D	686	PRO	CB-CA-C	-5.55	102.94	110.60
1	B	986	ILE	CB-CG1-CD1	-5.55	102.14	113.80
1	C	319	ASP	CA-C-N	-5.55	114.50	122.00
1	C	319	ASP	C-N-CA	-5.55	114.50	122.00
1	D	689	GLU	O-C-N	5.54	129.96	122.59
1	A	251	ARG	N-CA-CB	-5.54	102.06	111.69
1	D	1017	GLN	CB-CG-CD	5.53	122.01	112.60
1	A	917	ARG	CD-NE-CZ	-5.53	116.66	124.40
1	C	382	ASN	CA-CB-CG	-5.53	107.07	112.60
1	C	613	PRO	CB-CA-C	-5.53	103.73	110.98
1	B	583	ASN	CB-CA-C	5.52	116.81	108.86
1	D	89	ASN	N-CA-C	-5.52	100.24	109.24
1	B	113	PHE	CA-CB-CG	-5.52	108.28	113.80
1	A	871	GLU	CB-CG-CD	-5.51	103.23	112.60
1	C	338	GLU	CG-CD-OE2	-5.51	105.72	118.40
1	B	733	ALA	N-CA-C	5.50	118.56	110.30
1	C	20	GLY	N-CA-C	-5.50	108.11	115.32
1	D	14	ARG	N-CA-CB	-5.50	104.19	110.35
1	B	1018	LEU	CB-CA-C	-5.49	97.36	109.56
1	A	233	ASP	CB-CG-OD1	5.49	131.03	118.40
1	D	1017	GLN	OE1-CD-NE2	-5.49	117.11	122.60
1	C	539[A]	ALA	CB-CA-C	-5.49	99.50	110.42
1	C	539[B]	ALA	CB-CA-C	-5.49	99.50	110.42
1	C	288	ARG	CD-NE-CZ	-5.48	116.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	76	CYS	N-CA-C	5.48	117.40	109.07
1	A	279	ILE	N-CA-CB	-5.48	102.67	111.82
1	C	581	ASN	CA-CB-CG	-5.47	107.13	112.60
1	D	513	PRO	CB-CA-C	-5.47	104.40	111.46
1	A	431	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	D	634	GLN	N-CA-CB	5.47	119.67	110.92
1	D	601	PHE	CA-CB-CG	-5.47	108.33	113.80
1	B	553	TRP	CA-CB-CG	-5.46	103.22	113.60
1	D	752	GLY	CA-C-N	-5.45	113.95	122.73
1	D	752	GLY	C-N-CA	-5.45	113.95	122.73
1	C	161	TYR	N-CA-CB	-5.45	101.38	111.52
1	D	216	HIS	ND1-CG-CD2	5.45	111.55	106.10
1	A	320	GLY	N-CA-C	5.45	122.63	114.95
1	C	662	PRO	N-CA-CB	5.45	108.15	103.36
1	C	499	ILE	CA-C-N	-5.44	116.79	122.89
1	C	499	ILE	C-N-CA	-5.44	116.79	122.89
1	B	988	GLY	N-CA-C	-5.44	105.81	112.77
1	D	382	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	166	ARG	NE-CZ-NH2	-5.44	114.31	119.20
1	B	438	GLU	CG-CD-OE2	-5.43	105.91	118.40
1	A	917	ARG	NE-CZ-NH1	-5.43	116.07	121.50
1	C	750	GLU	N-CA-CB	5.43	120.82	111.00
1	B	507	ASP	CA-CB-CG	-5.42	107.17	112.60
1	C	842	TRP	CB-CA-C	-5.42	100.34	109.72
1	A	817	GLN	CB-CG-CD	-5.42	103.39	112.60
1	C	599	ARG	N-CA-C	5.41	116.53	108.31
1	D	719	GLN	CB-CA-C	-5.41	98.08	109.38
1	C	395	HIS	ND1-CG-CD2	5.41	111.51	106.10
1	A	823	LEU	N-CA-C	-5.40	107.05	113.97
1	A	1019	VAL	CA-CB-CG2	-5.40	101.22	110.40
1	A	15	ASP	CA-CB-CG	-5.40	107.20	112.60
1	B	630	ARG	CA-C-N	-5.39	113.99	122.73
1	B	630	ARG	C-N-CA	-5.39	113.99	122.73
1	C	989	PHE	CA-CB-CG	-5.39	108.41	113.80
1	B	802	ASP	CA-CB-CG	-5.39	107.21	112.60
1	A	625	GLN	OE1-CD-NE2	5.39	127.99	122.60
1	B	746	ASP	CB-CA-C	-5.38	98.89	110.45
1	D	193	ASP	N-CA-C	-5.38	105.98	112.54
1	D	688	PRO	CB-CA-C	-5.37	102.69	111.56
1	C	634	GLN	CA-C-O	5.37	127.26	120.65
1	C	693	GLN	CB-CA-C	-5.36	100.91	109.75
1	B	103	VAL	CB-CA-C	-5.35	105.48	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	747	PHE	CA-CB-CG	5.35	119.15	113.80
1	D	913	ALA	CA-C-O	-5.35	115.73	121.56
1	D	39	SER	N-CA-C	5.35	118.02	111.82
1	D	613	PRO	CB-CA-C	-5.35	103.97	110.98
1	D	231	PHE	CA-CB-CG	-5.34	108.46	113.80
1	B	667	GLU	CB-CG-CD	-5.34	103.52	112.60
1	B	917	ARG	CA-CB-CG	-5.33	103.43	114.10
1	A	583	ASN	CA-C-O	5.33	124.03	119.66
1	A	128	ASN	CA-CB-CG	-5.33	107.27	112.60
1	B	288	ARG	CG-CD-NE	-5.33	100.28	112.00
1	A	968	MET	N-CA-CB	-5.32	102.03	110.28
1	A	519	SER	N-CA-CB	-5.32	101.23	109.69
1	B	921	PRO	N-CA-CB	5.32	107.98	103.35
1	B	52	ARG	CB-CA-C	-5.31	99.82	109.38
1	C	890	GLN	N-CA-CB	-5.31	102.22	110.29
1	D	685	LEU	N-CA-C	5.31	117.35	110.40
1	D	958	ASN	N-CA-CB	5.30	120.91	111.69
1	C	917	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	553	TRP	CA-CB-CG	-5.29	103.55	113.60
1	C	931	PHE	CA-CB-CG	-5.29	108.51	113.80
1	C	744	GLU	CB-CA-C	-5.29	102.02	110.79
1	A	772	ASP	CB-CA-C	5.28	119.58	111.02
1	B	889	ALA	CA-C-O	5.27	126.03	119.97
1	B	986	ILE	CB-CA-C	5.26	118.24	110.77
1	C	735	HIS	N-CA-CB	5.26	118.04	110.20
1	C	670	LEU	CA-C-N	-5.26	113.71	122.92
1	C	670	LEU	C-N-CA	-5.26	113.71	122.92
1	D	499	ILE	N-CA-C	-5.26	101.90	108.84
1	C	997	ASP	N-CA-CB	5.25	119.86	111.56
1	C	733	ALA	CB-CA-C	5.25	120.88	110.42
1	C	345	ASN	CA-CB-CG	-5.25	107.36	112.60
1	C	777	LEU	N-CA-C	-5.24	107.01	113.41
1	A	233	ASP	CB-CG-OD2	-5.24	106.35	118.40
1	A	988	GLY	N-CA-C	-5.24	106.06	112.77
1	C	748	CYS	CA-CB-SG	-5.24	102.35	114.40
1	D	75	GLU	CA-C-N	-5.24	112.69	121.75
1	D	75	GLU	C-N-CA	-5.24	112.69	121.75
1	D	627	PHE	CA-CB-CG	-5.24	108.56	113.80
1	C	721	ARG	CD-NE-CZ	5.23	131.72	124.40
1	C	130	ASP	CA-CB-CG	-5.23	107.37	112.60
1	B	210	ARG	N-CA-CB	5.23	119.74	111.43
1	B	237	ARG	CA-CB-CG	-5.22	103.65	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	GLY	O-C-N	-5.22	120.06	123.35
1	B	216	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	118	ASN	N-CA-CB	-5.21	102.53	111.39
1	C	360	HIS	CA-CB-CG	-5.21	108.59	113.80
1	A	193	ASP	N-CA-C	-5.21	106.19	112.54
1	B	163	GLN	N-CA-CB	5.20	119.70	111.43
1	B	842	TRP	CB-CA-C	-5.20	101.66	110.19
1	D	416	GLU	CG-CD-OE1	5.20	130.36	118.40
1	B	71	GLU	CB-CG-CD	5.19	121.43	112.60
1	B	183	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	C	431	ARG	CA-CB-CG	-5.19	103.72	114.10
1	D	685	LEU	N-CA-CB	5.19	117.25	109.88
1	B	100	TYR	CA-CB-CG	-5.18	104.57	113.90
1	C	579	ASP	CB-CG-OD2	-5.18	106.48	118.40
1	C	231	PHE	CA-CB-CG	-5.18	108.62	113.80
1	D	464	HIS	CA-CB-CG	-5.18	108.62	113.80
1	C	869	ASP	CA-CB-CG	-5.18	107.42	112.60
1	D	956	GLN	N-CA-C	-5.17	101.44	109.72
1	C	33	PHE	CA-CB-CG	5.17	118.97	113.80
1	A	675	GLN	CB-CA-C	-5.17	102.81	111.23
1	A	771	GLY	CA-C-N	-5.16	114.39	122.49
1	A	771	GLY	C-N-CA	-5.16	114.39	122.49
1	B	221	GLN	N-CA-CB	-5.16	103.41	111.56
1	B	144	ASP	CA-CB-CG	-5.15	107.45	112.60
1	B	751	LEU	N-CA-CB	5.14	118.58	110.71
1	C	321	THR	CA-CB-OG1	-5.14	101.89	109.60
1	D	320	GLY	N-CA-C	5.14	123.14	115.64
1	C	482	ARG	CB-CA-C	-5.14	101.50	109.20
1	C	606	LEU	N-CA-C	-5.14	106.52	112.89
1	B	477	SER	N-CA-CB	-5.13	102.56	110.16
1	A	477	SER	CB-CA-C	-5.13	102.17	110.79
1	C	735	HIS	CA-CB-CG	5.13	118.93	113.80
1	D	164	ASP	CA-CB-CG	-5.13	107.47	112.60
1	A	662	PRO	N-CA-CB	5.13	107.89	103.27
1	A	1017	GLN	CA-CB-CG	-5.13	103.84	114.10
1	B	885	ASN	O-C-N	5.13	129.10	123.25
1	C	553	TRP	CA-CB-CG	-5.13	103.85	113.60
1	A	118	ASN	O-C-N	5.13	125.70	121.44
1	A	930	VAL	N-CA-CB	5.13	116.55	110.55
1	A	94	GLY	O-C-N	-5.13	116.45	122.45
1	A	690	SER	N-CA-CB	-5.12	102.64	110.42
1	A	746	ASP	CB-CA-C	-5.12	99.44	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	809	ARG	CG-CD-NE	-5.12	100.73	112.00
1	D	1018	LEU	CB-CA-C	-5.12	98.20	109.56
1	B	634	GLN	CA-C-N	-5.12	115.66	122.72
1	B	634	GLN	C-N-CA	-5.12	115.66	122.72
1	A	878	HIS	CA-CB-CG	-5.11	108.69	113.80
1	C	584	PRO	CB-CA-C	-5.11	104.29	110.98
1	D	576	ILE	CB-CA-C	-5.10	104.51	111.15
1	B	38	ASN	CA-CB-CG	-5.10	107.50	112.60
1	D	606	LEU	N-CA-C	-5.09	106.33	112.54
1	D	691	ALA	N-CA-C	5.09	117.27	110.35
1	C	915	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	730	LEU	CB-CA-C	5.09	117.41	109.42
1	C	85	VAL	N-CA-CB	-5.09	103.29	110.26
1	C	499	ILE	N-CA-C	-5.08	102.13	108.84
1	A	147	ASN	N-CA-CB	-5.08	102.72	110.65
1	B	699	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	C	571	VAL	N-CA-C	5.08	116.03	108.46
1	D	45	ASP	CA-CB-CG	-5.08	107.52	112.60
1	C	923	SER	N-CA-C	5.08	117.55	111.71
1	D	949	HIS	N-CA-C	5.08	118.40	110.32
1	B	474	TRP	CA-C-N	-5.08	114.16	120.56
1	B	474	TRP	C-N-CA	-5.08	114.16	120.56
1	D	916	ASP	CA-C-O	-5.07	115.66	120.94
1	A	113	PHE	CA-CB-CG	-5.07	108.73	113.80
1	B	729	THR	O-C-N	5.07	129.25	123.02
1	A	1021	CYS	CA-CB-SG	-5.07	102.75	114.40
1	B	956	GLN	N-CA-C	-5.07	101.62	109.72
1	A	95	TYR	N-CA-C	5.06	117.69	111.82
1	B	967	LEU	O-C-N	5.06	127.48	122.12
1	D	221	GLN	OE1-CD-NE2	-5.06	117.54	122.60
1	C	568	TRP	CA-CB-CG	-5.05	104.01	113.60
1	A	997	ASP	CA-CB-CG	-5.05	107.55	112.60
1	C	178	ARG	NE-CZ-NH2	-5.04	114.66	119.20
1	A	882	ILE	CA-CB-CG1	-5.04	101.84	110.40
1	C	889	ALA	CA-C-O	5.03	125.76	119.97
1	A	143	PHE	CB-CA-C	-5.03	102.59	110.79
1	A	395	HIS	CA-C-O	5.03	125.40	120.17
1	D	653	HIS	ND1-CG-CD2	5.03	111.13	106.10
1	D	924	ASP	CA-CB-CG	-5.03	107.57	112.60
1	A	706	THR	CA-C-N	-5.03	112.34	121.14
1	A	706	THR	C-N-CA	-5.03	112.34	121.14
1	A	772	ASP	N-CA-CB	-5.03	102.91	111.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	688	PRO	CA-C-N	5.02	127.94	120.31
1	C	688	PRO	C-N-CA	5.02	127.94	120.31
1	D	57	GLU	N-CA-C	5.02	117.80	109.46
1	C	790	ASP	CA-CB-CG	-5.02	107.58	112.60
1	A	118	ASN	OD1-CG-ND2	5.02	127.62	122.60
1	C	671	ASP	CB-CA-C	5.02	119.22	111.95
1	A	363	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	277	GLU	CB-CG-CD	5.01	121.13	112.60
1	B	947	GLY	O-C-N	-5.01	116.76	121.77
1	C	395	HIS	N-CA-CB	-5.01	102.39	109.75

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	733	ALA	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8127	0	7711	119	0
1	B	8128	0	7712	106	0
1	C	8128	0	7712	107	0
1	D	8128	0	7712	134	0
2	A	21	0	13	0	0
2	B	21	0	13	0	0
2	C	21	0	13	0	0
2	D	21	0	13	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	4	0	0	0	0
5	A	108	0	162	25	0
5	B	108	0	162	21	0
5	C	112	0	168	22	0
5	D	108	0	162	25	0
6	A	1112	0	0	17	3
6	B	1128	0	0	17	0
6	C	1104	0	0	17	3
6	D	1118	0	0	26	0
All	All	37524	0	31553	489	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (489) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:8415:DMS:S	5:D:8415:DMS:C1	2.01	1.48
5:B:8508:DMS:C1	5:B:8508:DMS:S	2.02	1.47
5:A:8403:DMS:C2	5:A:8403:DMS:S	2.03	1.46
5:B:8415:DMS:C2	5:B:8415:DMS:S	2.04	1.45
5:C:8402:DMS:S	5:C:8402:DMS:C2	2.04	1.44
1:C:634:GLN:H	1:C:634:GLN:NE2	1.33	1.25
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.39	1.20
1:A:290:THR:HB	5:A:8412:DMS:H23	1.23	1.16
1:A:233:ASP:HA	5:A:8417:DMS:H13	1.33	1.09
1:D:134:LEU:HA	5:D:8705:DMS:H23	1.42	1.02
1:B:730:LEU:HD12	1:B:730:LEU:H	1.21	1.01
1:A:634:GLN:HA	1:A:634:GLN:HE21	1.27	0.99
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.45	0.98
1:C:634:GLN:H	1:C:634:GLN:HE21	1.11	0.97
1:A:685:LEU:HD12	1:A:686:PRO:HD3	1.42	0.96
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.29	0.95
1:C:634:GLN:NE2	1:C:634:GLN:N	2.15	0.94
1:B:634:GLN:HG2	1:B:682:LEU:O	1.67	0.93
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.05	0.92
1:A:699:ARG:HG3	1:A:699:ARG:HH11	1.36	0.91
1:B:600:GLN:H	1:B:600:GLN:HE21	1.18	0.89
1:D:629:PHE:O	1:D:630:ARG:HD3	1.72	0.89
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.04	0.88
1:A:264:GLU:HG3	6:A:9484:HOH:O	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:GLN:H	1:A:600:GLN:HE21	1.22	0.87
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.54	0.87
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.40	0.84
1:A:655:MET:HB3	1:A:699:ARG:HH22	1.40	0.84
1:C:964:GLN:O	1:C:968:MET:HG2	1.77	0.83
1:D:658:LEU:O	1:D:661:LYS:HG3	1.79	0.83
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.24	0.83
1:D:134:LEU:CA	5:D:8705:DMS:H23	2.08	0.82
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.60	0.82
1:D:681:GLU:HG2	6:D:9469:HOH:O	1.79	0.81
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.45	0.81
1:D:634:GLN:HB2	1:D:682:LEU:HB2	1.60	0.81
1:B:655:MET:CE	1:B:665:SER:HB3	2.12	0.80
1:C:748:CYS:C	1:C:749:ILE:HD12	2.06	0.80
1:C:530:THR:HG22	6:D:8752:HOH:O	1.82	0.80
1:A:251:ARG:HH11	5:A:8416:DMS:H23	1.47	0.80
1:C:973:ARG:O	5:C:8423:DMS:H12	1.82	0.79
5:D:8416:DMS:H23	6:D:9410:HOH:O	1.81	0.79
5:C:8417:DMS:H22	6:C:9245:HOH:O	1.82	0.79
1:D:130:ASP:OD2	5:D:8703:DMS:H23	1.83	0.79
1:D:131:GLU:OE2	1:D:135:GLN:HG3	1.83	0.79
1:B:655:MET:HE2	1:B:665:SER:HB3	1.66	0.78
5:A:8420:DMS:H22	6:D:9524:HOH:O	1.83	0.78
1:B:699:ARG:NH2	5:B:8415:DMS:H11	1.99	0.78
1:A:797:GLU:O	1:A:801:ILE:HD13	1.83	0.78
1:A:973:ARG:O	5:A:8423:DMS:H12	1.84	0.78
1:A:685:LEU:HD12	1:A:686:PRO:CD	2.14	0.78
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.19	0.77
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.48	0.77
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.67	0.77
1:B:890:GLN:HG2	1:B:891:VAL:N	1.94	0.77
1:A:658:LEU:O	1:A:661:LYS:HG3	1.84	0.77
1:A:290:THR:HB	5:A:8412:DMS:C2	2.12	0.75
1:B:658:LEU:O	1:B:661:LYS:HG3	1.85	0.75
1:C:658:LEU:O	1:C:661:LYS:HE3	1.86	0.75
1:B:699:ARG:HH21	5:B:8415:DMS:H11	1.48	0.75
1:D:847:LYS:NZ	6:D:9500:HOH:O	2.19	0.75
1:B:890:GLN:HG3	6:B:9636:HOH:O	1.86	0.75
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.49	0.75
1:D:653:HIS:HD2	1:D:667:GLU:HB3	1.51	0.74
1:B:157:ARG:HD3	6:B:9466:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:LEU:H	1:C:730:LEU:HD23	1.52	0.74
1:B:651:LEU:O	1:B:651:LEU:HD23	1.87	0.74
1:A:687:GLN:NE2	6:A:9446:HOH:O	2.20	0.73
6:A:9690:HOH:O	1:B:530:THR:HG22	1.86	0.73
1:D:685:LEU:HB3	1:D:686:PRO:CD	2.19	0.72
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.01	0.72
1:D:962:TYR:OH	5:D:8508:DMS:H11	1.88	0.72
1:D:773:LYS:HD2	1:D:774:LYS:O	1.90	0.72
1:B:845:GLN:OE1	1:B:845:GLN:HA	1.89	0.72
1:B:233:ASP:HA	5:B:8417:DMS:H13	1.72	0.72
1:D:473:ARG:NH1	1:D:476:LYS:HB2	2.03	0.72
1:A:887:GLN:NE2	1:A:980:GLU:O	2.21	0.71
1:B:878:HIS:HD2	6:B:8697:HOH:O	1.73	0.71
1:A:655:MET:HE2	1:A:656:VAL:O	1.91	0.71
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.72	0.71
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.04	0.71
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.72	0.71
1:D:804:ASN:HA	1:D:809:ARG:HH21	1.54	0.71
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.06	0.70
1:B:1017:GLN:HB2	6:B:9559:HOH:O	1.91	0.70
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.07	0.70
5:D:8421:DMS:H12	6:D:9371:HOH:O	1.93	0.69
1:D:581:ASN:HD22	1:D:583:ASN:HD22	1.40	0.69
1:D:595:THR:HA	1:D:596:PRO:C	2.17	0.68
1:D:887:GLN:NE2	1:D:980:GLU:O	2.25	0.68
5:B:8411:DMS:H22	6:B:9633:HOH:O	1.94	0.68
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.20	0.68
1:D:720:TRP:HA	5:D:8427:DMS:H12	1.75	0.68
1:B:730:LEU:H	1:B:730:LEU:CD1	1.99	0.68
1:A:268:ALA:HA	5:A:8602:DMS:H23	1.75	0.67
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.24	0.67
1:D:797:GLU:O	1:D:801:ILE:HD13	1.95	0.67
1:D:804:ASN:HD22	1:D:809:ARG:HH21	1.41	0.67
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.75	0.67
1:D:508:GLU:OE2	5:D:8407:DMS:H11	1.95	0.67
1:C:878:HIS:HD2	6:C:8704:HOH:O	1.77	0.66
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.78	0.66
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.28	0.66
1:D:237:ARG:NH1	6:D:9286:HOH:O	2.25	0.66
1:B:181:GLU:OE2	6:B:9502:HOH:O	2.13	0.66
1:B:245:GLN:NE2	6:B:9680:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:LEU:HD23	1:C:730:LEU:N	2.09	0.66
1:D:634:GLN:NE2	1:D:682:LEU:O	2.29	0.66
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.77	0.66
1:A:277:GLU:H	1:A:277:GLU:CD	2.03	0.66
1:A:878:HIS:HD2	6:A:8674:HOH:O	1.79	0.66
5:D:8406:DMS:O	6:D:9684:HOH:O	2.12	0.65
1:A:861:SER:OG	1:A:863:GLN:HG3	1.95	0.65
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.32	0.65
1:A:646:HIS:ND1	6:A:9438:HOH:O	2.22	0.65
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.11	0.64
1:C:730:LEU:H	1:C:730:LEU:CD2	2.06	0.64
1:D:130:ASP:CG	5:D:8703:DMS:H23	2.23	0.64
1:A:708:TRP:CZ2	5:A:8403:DMS:H13	2.32	0.64
1:C:367:MET:HE3	1:C:367:MET:HA	1.79	0.64
1:D:128:ASN:HB3	1:D:180:GLY:O	1.97	0.64
1:B:319:ASP:OD1	1:B:321:THR:N	2.29	0.64
1:C:634:GLN:HE21	1:C:634:GLN:N	1.87	0.64
1:A:290:THR:CB	5:A:8412:DMS:H23	2.15	0.64
1:C:687:GLN:HE21	1:C:687:GLN:HA	1.61	0.64
1:C:768:MET:HE1	1:C:1020:TRP:CZ2	2.32	0.64
1:D:649:ASN:HA	5:D:8425:DMS:H12	1.80	0.63
1:A:634:GLN:HA	1:A:634:GLN:NE2	2.06	0.63
1:A:267:VAL:O	5:A:8602:DMS:H23	1.98	0.63
1:D:878:HIS:HD2	6:D:8825:HOH:O	1.80	0.63
5:B:8410:DMS:H22	6:B:8882:HOH:O	1.99	0.63
5:D:8427:DMS:H11	6:D:8960:HOH:O	1.98	0.63
1:C:745:MET:HG2	6:C:9471:HOH:O	1.99	0.63
1:B:13:ARG:NH1	6:B:9618:HOH:O	2.29	0.62
1:A:890:GLN:OE1	1:A:948:PRO:HD3	1.98	0.62
1:D:844:HIS:HD2	6:D:9787:HOH:O	1.81	0.62
1:B:730:LEU:HD12	1:B:730:LEU:N	2.05	0.62
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.34	0.62
1:A:737:ILE:C	1:A:737:ILE:HD13	2.24	0.62
1:A:737:ILE:HD11	6:A:9651:HOH:O	1.98	0.62
1:D:1022:GLN:O	1:D:1022:GLN:HG3	1.99	0.62
1:C:965:GLN:HA	1:C:968:MET:SD	2.39	0.61
1:D:135:GLN:O	1:D:136:GLU:HG2	2.00	0.61
1:A:717:TRP:CH2	5:A:8415:DMS:H12	2.35	0.61
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.00	0.61
1:B:236:SER:C	1:B:237:ARG:HG2	2.25	0.61
1:A:84:VAL:HB	5:A:8414:DMS:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.83	0.61
1:C:356:ARG:HD2	1:C:379:MET:CE	2.29	0.61
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.16	0.61
1:B:651:LEU:HD23	1:B:651:LEU:C	2.25	0.61
1:D:292:ARG:HH12	5:D:8412:DMS:H23	1.64	0.61
1:D:581:ASN:HD22	1:D:583:ASN:ND2	1.98	0.61
1:C:46:ARG:HG2	6:C:9538:HOH:O	2.00	0.60
1:A:241:GLU:CD	1:A:292:ARG:HE	2.08	0.60
1:A:800:ARG:HG2	6:A:9380:HOH:O	2.02	0.60
1:B:708:TRP:CZ2	5:B:8403:DMS:H13	2.37	0.60
1:C:178:ARG:HD3	6:C:9502:HOH:O	2.02	0.60
1:A:724:GLU:O	1:B:847:LYS:NZ	2.30	0.60
1:D:773:LYS:HG3	1:D:775:GLN:HE21	1.66	0.60
1:D:250:LEU:O	5:D:8416:DMS:H22	2.01	0.60
1:C:749:ILE:HD12	1:C:749:ILE:N	2.16	0.60
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.01	0.60
1:D:844:HIS:CD2	6:D:9787:HOH:O	2.54	0.60
1:A:245:GLN:CD	1:A:288:ARG:HE	2.10	0.60
1:C:595:THR:HA	1:C:596:PRO:C	2.26	0.59
1:A:655:MET:HA	1:A:655:MET:HE3	1.84	0.59
1:C:687:GLN:HA	1:C:687:GLN:NE2	2.15	0.59
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.83	0.59
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.31	0.59
1:D:739:HIS:ND1	6:D:8745:HOH:O	2.31	0.59
5:C:8427:DMS:H11	6:C:8841:HOH:O	2.02	0.59
5:C:8427:DMS:H22	6:C:9067:HOH:O	2.03	0.59
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.85	0.59
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.37	0.59
1:B:864:MET:HE3	1:B:866:ILE:HD11	1.85	0.59
1:D:134:LEU:HA	5:D:8705:DMS:C2	2.25	0.59
5:D:8409:DMS:O	6:D:9258:HOH:O	2.16	0.59
1:C:240:LEU:C	1:C:240:LEU:HD23	2.28	0.58
1:A:595:THR:HA	1:A:596:PRO:C	2.27	0.58
1:B:178:ARG:O	1:B:178:ARG:HG3	2.03	0.58
1:D:363:HIS:HD2	6:D:9334:HOH:O	1.86	0.58
1:D:367:MET:HB3	1:D:372:MET:HE3	1.86	0.58
1:B:600:GLN:HE21	1:B:600:GLN:N	1.97	0.58
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.11	0.58
1:A:233:ASP:CA	5:A:8417:DMS:H13	2.22	0.57
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.34	0.57
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.38	0.57
1:D:240:LEU:HD23	1:D:240:LEU:C	2.29	0.57
1:D:230:ARG:HD3	6:D:9706:HOH:O	2.02	0.57
1:C:79:PRO:HD2	1:C:80:GLU:OE2	2.05	0.57
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.86	0.57
1:D:754:LYS:C	1:D:755:ARG:HG2	2.30	0.57
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.85	0.56
1:B:595:THR:HA	1:B:596:PRO:C	2.30	0.56
1:A:655:MET:CB	1:A:699:ARG:HH22	2.17	0.56
1:A:655:MET:HE3	1:A:655:MET:CA	2.36	0.56
1:C:720:TRP:HA	5:C:8427:DMS:C1	2.36	0.56
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.74	0.55
1:C:719:GLN:O	5:C:8427:DMS:H13	2.06	0.55
1:A:94:GLY:HA3	5:A:8421:DMS:H21	1.89	0.55
1:A:824:GLN:NE2	1:A:837:THR:HG22	2.21	0.55
1:D:237:ARG:HB3	1:D:237:ARG:NH1	2.19	0.55
1:D:804:ASN:HA	1:D:809:ARG:HE	1.72	0.55
1:C:320:GLY:O	5:C:8406:DMS:H12	2.06	0.55
1:C:724:GLU:O	1:D:847:LYS:NZ	2.39	0.55
1:C:634:GLN:NE2	1:C:634:GLN:CA	2.71	0.54
1:D:754:LYS:HE2	1:D:1022:GLN:HG2	1.90	0.54
1:A:88:SER:HA	1:A:366:VAL:HG21	1.88	0.54
1:B:890:GLN:HB3	6:B:9568:HOH:O	2.07	0.54
1:C:655:MET:CE	1:C:662:PRO:HB3	2.38	0.54
1:A:653:HIS:CD2	1:A:701:VAL:HG21	2.42	0.54
1:B:292:ARG:HH12	5:B:8412:DMS:C2	2.20	0.54
1:B:685:LEU:HB3	1:B:686:PRO:HD2	1.89	0.54
1:A:749:ILE:HD13	1:A:858:ILE:HD12	1.89	0.54
1:B:226:HIS:CE1	1:B:448:ARG:NH1	2.75	0.54
1:A:699:ARG:HG3	1:A:699:ARG:NH1	2.13	0.54
1:C:367:MET:HE1	6:C:9644:HOH:O	2.08	0.54
1:D:131:GLU:OE2	1:D:131:GLU:O	2.25	0.53
1:B:360:HIS:HE1	1:B:362:LEU:HD12	1.73	0.53
1:C:320:GLY:HA2	5:C:8406:DMS:O	2.07	0.53
1:D:80:GLU:OE1	1:D:80:GLU:N	2.36	0.53
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.89	0.53
1:C:728:VAL:O	1:C:730:LEU:HD23	2.09	0.53
1:B:835:LEU:HD11	1:B:855:THR:HB	1.90	0.53
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.42	0.53
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.29	0.53
1:D:781:ARG:NH1	6:D:9479:HOH:O	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ARG:NH1	6:A:9036:HOH:O	2.28	0.53
1:D:768:MET:HE1	1:D:1020:TRP:CE2	2.44	0.53
1:D:135:GLN:C	1:D:136:GLU:HG2	2.34	0.52
1:D:804:ASN:HD22	1:D:809:ARG:CZ	2.15	0.52
1:A:832:ASP:OD1	1:A:832:ASP:N	2.42	0.52
1:A:684:GLU:O	1:A:685:LEU:HD13	2.09	0.52
1:A:844:HIS:HD2	6:A:9436:HOH:O	1.91	0.52
1:B:634:GLN:HB3	1:B:681:GLU:OE2	2.10	0.52
1:D:577:LYS:O	1:D:584:PRO:HA	2.09	0.52
1:D:157:ARG:HG2	1:D:176:PHE:HE2	1.74	0.52
1:B:797:GLU:HG2	1:B:799:THR:HG23	1.92	0.52
1:D:618:THR:HG23	6:D:9081:HOH:O	2.09	0.52
1:D:675:GLN:HG3	6:D:9580:HOH:O	2.10	0.52
1:A:132:SER:HB2	5:A:8504:DMS:H21	1.92	0.52
1:D:618:THR:HG21	6:D:9065:HOH:O	2.09	0.52
5:B:8421:DMS:H23	6:B:9134:HOH:O	2.09	0.51
1:D:651:LEU:HD12	1:D:701:VAL:HB	1.92	0.51
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.38	0.51
1:D:847:LYS:HG3	1:D:848:THR:N	2.19	0.51
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.92	0.51
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.38	0.51
1:A:737:ILE:HD13	1:A:737:ILE:O	2.11	0.51
1:B:655:MET:HE1	1:B:665:SER:HB3	1.92	0.51
1:A:651:LEU:CD2	1:A:703:PRO:HG3	2.41	0.51
1:C:835:LEU:HD11	1:C:855:THR:HB	1.92	0.51
1:C:288:ARG:NH1	6:C:9069:HOH:O	2.27	0.51
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.28	0.51
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.94	0.51
1:B:628:GLN:HE22	5:B:8402:DMS:C2	2.24	0.51
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.25	0.51
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.41	0.51
1:A:615:PRO:O	1:A:618:THR:HG22	2.11	0.50
1:A:245:GLN:OE1	1:A:288:ARG:NE	2.43	0.50
1:A:600:GLN:HE21	1:A:600:GLN:N	2.02	0.50
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.93	0.50
1:B:13:ARG:O	1:B:14:ARG:C	2.55	0.50
1:C:628:GLN:NE2	5:C:8402:DMS:O	2.43	0.50
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.46	0.50
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.41	0.50
1:C:651:LEU:HD11	1:C:653:HIS:HE1	1.77	0.50
1:B:320:GLY:O	5:B:8406:DMS:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.92	0.50
1:C:13:ARG:O	1:C:14:ARG:C	2.54	0.50
1:C:890:GLN:HG3	1:C:891:VAL:N	2.27	0.50
1:A:85:VAL:N	5:A:8414:DMS:O	2.42	0.50
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.93	0.50
1:D:734:SER:OG	1:D:860:GLY:HA3	2.12	0.50
5:A:8403:DMS:C2	5:A:8403:DMS:C1	2.90	0.50
1:B:824:GLN:HG2	1:B:825:CYS:N	2.18	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.93	0.50
1:A:685:LEU:O	1:A:687:GLN:OE1	2.29	0.49
1:B:379:MET:HE1	1:B:387:VAL:HB	1.93	0.49
1:C:44:THR:OG1	1:C:46:ARG:HD3	2.13	0.49
1:D:80:GLU:HG3	6:D:9758:HOH:O	2.11	0.49
1:A:508:GLU:OE2	5:A:8407:DMS:H11	2.12	0.49
1:A:735:HIS:O	1:A:736:ALA:HB2	2.10	0.49
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.95	0.49
1:B:684:GLU:HG2	1:B:685:LEU:N	2.24	0.49
1:C:1000:SER:O	1:C:1001:PRO:C	2.56	0.49
1:D:630:ARG:NH1	6:D:9312:HOH:O	2.44	0.49
1:D:829:THR:O	1:D:830:LEU:HD23	2.13	0.49
1:A:147:ASN:HA	1:A:148:SER:HA	1.59	0.49
1:A:625:GLN:NE2	6:A:8800:HOH:O	2.34	0.49
1:A:655:MET:HE2	1:A:656:VAL:N	2.27	0.49
1:C:829:THR:HG22	1:C:830:LEU:N	2.27	0.49
1:B:367:MET:HA	1:B:367:MET:HE3	1.95	0.49
1:C:508:GLU:OE2	5:C:8407:DMS:H11	2.12	0.49
1:D:843:GLN:HA	1:D:847:LYS:O	2.13	0.49
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.27	0.49
1:D:92:MET:HA	1:D:92:MET:HE2	1.95	0.48
1:D:134:LEU:C	5:D:8705:DMS:H23	2.37	0.48
1:D:373:VAL:O	1:D:377:LEU:HG	2.14	0.48
1:D:804:ASN:HA	1:D:809:ARG:NH2	2.26	0.48
1:B:615:PRO:O	1:B:618:THR:HG22	2.13	0.48
1:C:317:THR:OG1	1:C:319:ASP:OD1	2.29	0.48
1:C:655:MET:HE1	1:C:662:PRO:HB3	1.95	0.48
1:D:688:PRO:C	1:D:690:SER:H	2.21	0.48
1:D:625:GLN:NE2	6:D:8952:HOH:O	2.39	0.48
1:D:738:PRO:HG3	1:D:751:LEU:HD13	1.95	0.48
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.48	0.48
1:C:147:ASN:HA	1:C:148:SER:HA	1.64	0.48
1:D:745:MET:HE2	1:D:745:MET:HB2	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:737:ILE:HD12	1:D:832:ASP:HA	1.95	0.48
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.74	0.48
1:B:600:GLN:H	1:B:600:GLN:NE2	2.00	0.48
1:B:699:ARG:HE	1:B:714:ILE:HD13	1.79	0.48
1:C:615:PRO:O	1:C:618:THR:HG22	2.14	0.48
1:C:367:MET:HE3	1:C:367:MET:CA	2.43	0.47
5:C:8506:DMS:C2	6:C:9496:HOH:O	2.62	0.47
5:D:8415:DMS:C1	5:D:8415:DMS:C2	2.92	0.47
1:A:600:GLN:H	1:A:600:GLN:NE2	2.03	0.47
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.48	0.47
1:D:659:ASP:HA	6:D:9797:HOH:O	2.14	0.47
1:C:622:HIS:CE1	5:C:8402:DMS:C1	2.97	0.47
1:B:699:ARG:HH21	5:B:8415:DMS:C1	2.20	0.47
1:B:847:LYS:HE2	1:B:875:ASP:OD1	2.15	0.47
1:B:147:ASN:HA	1:B:148:SER:HA	1.57	0.47
1:C:634:GLN:OE1	1:C:681:GLU:HG2	2.14	0.47
1:C:708:TRP:CZ2	5:C:8403:DMS:H13	2.50	0.47
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.97	0.47
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.50	0.47
1:B:292:ARG:HH12	5:B:8412:DMS:H23	1.80	0.47
1:D:737:ILE:HD13	1:D:831:ALA:O	2.15	0.47
1:D:749:ILE:CD1	1:D:858:ILE:HD12	2.45	0.47
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.96	0.47
1:D:1022:GLN:HE21	1:D:1022:GLN:C	2.23	0.47
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.97	0.47
1:C:653:HIS:CE1	1:C:667:GLU:CG	2.98	0.47
1:C:690:SER:HB2	6:C:9380:HOH:O	2.15	0.47
1:C:965:GLN:O	1:C:968:MET:HG3	2.14	0.47
1:A:233:ASP:HA	5:A:8417:DMS:C1	2.24	0.46
1:B:387:VAL:HG22	6:B:9693:HOH:O	2.14	0.46
1:B:681:GLU:OE1	1:B:681:GLU:HA	2.15	0.46
1:C:653:HIS:ND1	1:C:667:GLU:CG	2.79	0.46
1:D:538:TYR:C	1:D:539[B]:ALA:O	2.57	0.46
1:A:717:TRP:CZ2	5:A:8415:DMS:H12	2.51	0.46
1:B:655:MET:HE2	1:B:665:SER:CB	2.42	0.46
1:D:804:ASN:ND2	1:D:809:ARG:CZ	2.77	0.46
1:A:521:LYS:HE2	6:A:9025:HOH:O	2.15	0.46
1:D:986:ILE:HD12	1:D:986:ILE:HG21	1.63	0.46
1:A:742:THR:HG22	1:A:743:SER:N	2.30	0.46
1:B:88:SER:HA	1:B:366:VAL:HG21	1.98	0.46
1:B:809:ARG:HG2	1:B:809:ARG:NH1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:SER:HA	1:D:366:VAL:HG21	1.98	0.46
1:A:1000:SER:O	1:A:1001:PRO:C	2.57	0.46
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.98	0.46
1:B:601:PHE:CD2	5:B:8506:DMS:H12	2.51	0.46
1:C:634:GLN:HB2	1:C:682:LEU:HB2	1.98	0.46
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.27	0.46
1:A:655:MET:CE	1:A:656:VAL:N	2.80	0.45
1:B:781:ARG:HD3	6:B:9687:HOH:O	2.16	0.45
1:D:651:LEU:CD1	1:D:651:LEU:C	2.90	0.45
1:D:962:TYR:CZ	5:D:8508:DMS:H11	2.51	0.45
1:C:634:GLN:C	1:C:634:GLN:CD	2.85	0.45
1:C:952:ARG:NH2	1:C:1021:CYS:SG	2.88	0.45
1:A:781:ARG:NH1	6:A:9332:HOH:O	2.50	0.45
1:C:49:GLN:HG2	6:C:9326:HOH:O	2.16	0.45
5:C:8506:DMS:H22	6:C:9496:HOH:O	2.16	0.45
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.99	0.45
1:B:246:MET:HE3	1:B:250:LEU:HD23	1.99	0.45
1:A:685:LEU:HD13	1:A:685:LEU:HA	1.62	0.45
1:C:893:GLU:HG2	6:C:9145:HOH:O	2.17	0.45
1:D:360:HIS:HE1	1:D:362:LEU:HD12	1.82	0.45
1:A:651:LEU:CD1	1:A:653:HIS:CE1	2.99	0.45
1:B:262:GLN:NE2	1:B:263:GLY:N	2.65	0.45
1:C:667:GLU:C	1:C:668:VAL:HG23	2.42	0.45
1:D:372:MET:HE1	1:D:395:HIS:CG	2.52	0.45
1:A:655:MET:HE2	1:A:656:VAL:C	2.41	0.44
1:C:266:GLN:NE2	5:C:8602:DMS:S	2.91	0.44
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.00	0.44
1:C:16:TRP:CG	1:C:189:LEU:HD13	2.52	0.44
1:D:55:ASN:O	5:D:8408:DMS:H21	2.18	0.44
1:B:655:MET:HE2	1:B:655:MET:HB2	1.44	0.44
1:A:859:ASP:OD1	1:A:861:SER:OG	2.26	0.44
1:B:708:TRP:CH2	5:B:8403:DMS:H13	2.53	0.44
1:C:233:ASP:HA	5:C:8417:DMS:S	2.57	0.44
1:C:538:TYR:C	1:C:539[B]:ALA:O	2.59	0.44
1:C:673:ALA:HB1	1:C:674:PRO:HD2	2.00	0.44
1:D:251:ARG:HA	5:D:8416:DMS:C2	2.47	0.44
1:D:890:GLN:HE21	1:D:892:ALA:HB2	1.83	0.44
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.18	0.44
5:B:8427:DMS:H13	6:B:9709:HOH:O	2.17	0.44
1:C:684:GLU:HG2	1:C:685:LEU:N	2.13	0.44
1:D:292:ARG:NH1	5:D:8412:DMS:H23	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:8705:DMS:H22	6:D:9781:HOH:O	2.16	0.44
1:A:71:GLU:HG3	1:A:72:SER:N	2.33	0.44
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.82	0.44
1:B:818:ALA:C	1:B:819:GLU:HG2	2.29	0.44
1:D:367:MET:HB3	1:D:372:MET:CE	2.46	0.44
1:B:240:LEU:C	1:B:240:LEU:HD23	2.43	0.44
5:A:8419:DMS:H21	6:A:9367:HOH:O	2.18	0.43
1:B:47:PRO:O	6:B:9658:HOH:O	2.21	0.43
1:A:655:MET:HE3	1:A:664:ALA:O	2.18	0.43
1:B:381:GLN:O	1:B:621:LYS:HE3	2.19	0.43
1:B:797:GLU:O	1:B:801:ILE:HD13	2.18	0.43
5:C:8402:DMS:C2	5:C:8402:DMS:C1	2.94	0.43
1:D:651:LEU:HD12	1:D:651:LEU:O	2.18	0.43
1:A:658:LEU:O	1:A:659:ASP:C	2.59	0.43
1:B:128:ASN:HA	1:B:180:GLY:O	2.18	0.43
1:B:237:ARG:HD2	1:B:296:GLU:OE1	2.18	0.43
1:C:829:THR:HG22	1:C:830:LEU:O	2.18	0.43
1:D:1000:SER:O	1:D:1001:PRO:C	2.61	0.43
1:A:745:MET:HE1	1:A:761:GLN:HB2	2.01	0.43
1:C:749:ILE:N	1:C:749:ILE:CD1	2.82	0.43
1:C:844:HIS:HD2	6:C:9477:HOH:O	2.00	0.43
1:A:32:PRO:HB2	5:A:8404:DMS:H13	2.00	0.43
1:A:178:ARG:CD	6:A:9467:HOH:O	2.66	0.43
1:D:659:ASP:O	6:D:9319:HOH:O	2.21	0.43
1:B:917:ARG:HH11	1:B:917:ARG:HD3	1.55	0.43
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.19	0.43
1:C:781:ARG:NH1	6:C:9371:HOH:O	2.52	0.43
1:D:111:PRO:HA	1:D:112:PRO:HA	1.80	0.43
1:A:416:GLU:OE2	1:A:418:HIS:HB2	2.19	0.43
1:C:231:PHE:O	5:C:8417:DMS:H12	2.19	0.43
1:B:1000:SER:O	1:B:1001:PRO:C	2.61	0.43
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.98	0.43
1:D:473:ARG:NH1	1:D:476:LYS:CB	2.79	0.43
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.99	0.42
1:B:133:TRP:CZ3	1:B:216:HIS:HB2	2.54	0.42
1:C:356:ARG:NH2	6:C:9644:HOH:O	2.24	0.42
1:D:863:GLN:HG2	1:D:1021:CYS:CB	2.48	0.42
1:B:824:GLN:OE1	1:B:837:THR:HG22	2.19	0.42
1:A:866:ILE:O	1:A:1017:GLN:HG2	2.19	0.42
1:A:433:LEU:N	1:A:434:PRO:CD	2.82	0.42
1:C:806:TRP:HA	1:C:809:ARG:HE	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ASN:HB2	1:A:771:GLY:HA2	2.02	0.42
1:B:538:TYR:C	1:B:539[B]:ALA:O	2.60	0.42
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.34	0.42
1:A:986:ILE:HG23	1:A:986:ILE:HD13	1.77	0.42
1:C:737:ILE:O	1:C:737:ILE:HG13	2.14	0.42
1:D:639:THR:OG1	1:D:677:LYS:HE2	2.20	0.42
1:B:601:PHE:CE2	5:B:8506:DMS:H12	2.54	0.42
1:B:737:ILE:HD13	1:B:831:ALA:O	2.19	0.42
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.32	0.42
1:D:237:ARG:NH1	1:D:237:ARG:CG	2.80	0.42
1:D:433:LEU:N	1:D:434:PRO:CD	2.83	0.42
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.18	0.41
1:D:629:PHE:C	1:D:630:ARG:HD3	2.40	0.41
6:B:9393:HOH:O	5:C:8420:DMS:H22	2.20	0.41
1:C:806:TRP:CD2	1:C:991:MET:HE1	2.55	0.41
1:D:661:LYS:HG3	1:D:661:LYS:H	1.57	0.41
1:C:132:SER:HB2	5:C:8504:DMS:H12	2.02	0.41
1:B:225:PHE:HA	1:B:243:GLU:O	2.21	0.41
1:C:750:GLU:HG2	1:C:755:ARG:HG3	2.01	0.41
1:B:114:VAL:HB	1:B:115:PRO:HD2	2.02	0.41
1:D:681:GLU:HG2	1:D:681:GLU:H	1.65	0.41
1:A:367:MET:HA	1:A:367:MET:HE2	2.02	0.41
1:D:147:ASN:HA	1:D:148:SER:HA	1.69	0.41
1:A:473:ARG:NH1	1:A:476:LYS:CB	2.81	0.41
1:B:49:GLN:HG2	6:B:9314:HOH:O	2.21	0.41
1:B:305:ILE:HD11	1:B:645:ARG:HB3	2.02	0.41
1:C:595:THR:O	1:C:595:THR:HG23	2.19	0.41
1:D:112:PRO:HD2	1:D:113:PHE:CE1	2.55	0.41
1:A:370:GLN:HG3	6:A:9074:HOH:O	2.20	0.41
5:A:8409:DMS:O	6:A:9105:HOH:O	2.22	0.41
1:B:231:PHE:O	5:B:8417:DMS:H23	2.21	0.41
1:B:751:LEU:HD23	1:B:862:GLY:HA2	2.01	0.41
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.03	0.41
1:C:622:HIS:CE1	5:C:8402:DMS:H12	2.55	0.41
1:D:340:GLY:O	1:D:561:ARG:HG2	2.21	0.41
1:A:78:LEU:HA	1:A:79:PRO:HD3	1.73	0.41
1:B:262:GLN:NE2	1:B:262:GLN:C	2.79	0.40
1:B:513:PRO:O	1:B:514:ALA:HB3	2.20	0.40
1:D:658:LEU:O	1:D:659:ASP:C	2.63	0.40
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.56	0.40
5:A:8410:DMS:H11	6:A:8942:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.56	0.40
1:B:637:GLU:CD	1:B:677:LYS:HE3	2.46	0.40
1:C:70:PRO:HG2	1:C:78:LEU:HD21	2.03	0.40
1:C:356:ARG:CD	1:C:379:MET:HE1	2.46	0.40
1:C:995:GLY:O	1:C:996:ASP:C	2.64	0.40
1:D:893:GLU:HG2	1:D:894:ARG:HG2	2.03	0.40
1:A:806:TRP:CD2	1:A:991:MET:HE1	2.56	0.40
1:B:320:GLY:HA2	5:B:8406:DMS:O	2.22	0.40
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.03	0.40
1:D:513:PRO:O	1:D:514:ALA:HB3	2.22	0.40
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.57	0.40
1:A:843:GLN:HA	1:A:847:LYS:O	2.22	0.40
1:C:965:GLN:HA	1:C:968:MET:CG	2.51	0.40
1:D:372:MET:HE1	1:D:395:HIS:HB3	2.03	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:9652:HOH:O	6:C:9432:HOH:O[3_544]	2.15	0.05
6:A:9694:HOH:O	6:C:9467:HOH:O[3_544]	2.16	0.04
6:A:9697:HOH:O	6:C:9628:HOH:O[2_554]	2.19	0.01

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	611/1023 (60%)	585 (96%)	26 (4%)	0	100	100
1	B	1011/1023 (99%)	978 (97%)	30 (3%)	3 (0%)	36	18
1	C	1011/1023 (99%)	974 (96%)	36 (4%)	1 (0%)	48	26
1	D	1011/1023 (99%)	971 (96%)	38 (4%)	2 (0%)	43	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3644/4092 (89%)	3508 (96%)	130 (4%)	6 (0%)	43 24

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	731	PRO
1	B	732	ALA
1	C	734	SER
1	D	688	PRO
1	B	164	ASP
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	864/875 (99%)	836 (97%)	28 (3%)	34 8
1	B	865/875 (99%)	836 (97%)	29 (3%)	32 7
1	C	865/875 (99%)	828 (96%)	37 (4%)	26 4
1	D	865/875 (99%)	834 (96%)	31 (4%)	31 6
All	All	3459/3500 (99%)	3334 (96%)	125 (4%)	31 6

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	THR
1	A	250	LEU
1	A	277	GLU
1	A	344	LEU
1	A	347	LYS
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	632	SER
1	A	634	GLN
1	A	655	MET
1	A	661	LYS
1	A	667	GLU
1	A	684	GLU
1	A	685	LEU
1	A	690	SER
1	A	699	ARG
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	799	THR
1	A	800	ARG
1	A	885	ASN
1	A	890	GLN
1	A	986	ILE
1	A	1013	ARG
1	A	1023	LYS
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	277	GLU
1	B	344	LEU
1	B	367	MET
1	B	370	GLN
1	B	546	LEU
1	B	583	ASN
1	B	600	GLN
1	B	634	GLN
1	B	651	LEU
1	B	661	LYS
1	B	667	GLU
1	B	684	GLU
1	B	687	GLN
1	B	730	LEU
1	B	734	SER
1	B	737	ILE
1	B	745	MET
1	B	754	LYS
1	B	766	SER
1	B	799	THR

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Mol	Chain	Res	Type
1	B	809	ARG
1	B	819	GLU
1	B	845	GLN
1	B	890	GLN
1	B	917	ARG
1	B	1023	LYS
1	C	71	GLU
1	C	76	CYS
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG
1	C	230	ARG
1	C	251	ARG
1	C	299	LYS
1	C	344	LEU
1	C	367	MET
1	C	370	GLN
1	C	519	SER
1	C	546	LEU
1	C	634	GLN
1	C	651	LEU
1	C	659	ASP
1	C	667	GLU
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	730	LEU
1	C	734	SER
1	C	737	ILE
1	C	749	ILE
1	C	773	LYS
1	C	800	ARG
1	C	819	GLU
1	C	885	ASN
1	C	893	GLU
1	C	934	GLU
1	C	968	MET
1	C	986	ILE
1	C	1013	ARG
1	C	1017	GLN
1	C	1022	GLN

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Mol	Chain	Res	Type
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	112	PRO
1	D	230	ARG
1	D	237	ARG
1	D	277	GLU
1	D	319	ASP
1	D	344	LEU
1	D	370	GLN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	632	SER
1	D	651	LEU
1	D	661	LYS
1	D	667	GLU
1	D	681	GLU
1	D	684	GLU
1	D	687	GLN
1	D	730	LEU
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	772	ASP
1	D	797	GLU
1	D	799	THR
1	D	885	ASN
1	D	893	GLU
1	D	986	ILE
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	49	GLN
1	A	163	GLN
1	A	445	GLN
1	A	485	GLN
1	A	600	GLN

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Mol	Chain	Res	Type
1	A	614	HIS
1	A	624	GLN
1	A	634	GLN
1	A	653	HIS
1	A	704	ASN
1	A	843	GLN
1	A	844	HIS
1	A	878	HIS
1	A	885	ASN
1	B	163	GLN
1	B	226	HIS
1	B	245	GLN
1	B	262	GLN
1	B	363	HIS
1	B	445	GLN
1	B	485	GLN
1	B	583	ASN
1	B	600	GLN
1	B	614	HIS
1	B	624	GLN
1	B	628	GLN
1	B	653	HIS
1	B	687	GLN
1	B	863	GLN
1	B	878	HIS
1	B	885	ASN
1	B	890	GLN
1	B	945	ASN
1	B	950	GLN
1	B	965	GLN
1	B	977	HIS
1	B	1017	GLN
1	C	128	ASN
1	C	163	GLN
1	C	226	HIS
1	C	245	GLN
1	C	266	GLN
1	C	363	HIS
1	C	485	GLN
1	C	634	GLN
1	C	687	GLN
1	C	704	ASN

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Mol	Chain	Res	Type
1	C	824	GLN
1	C	843	GLN
1	C	878	HIS
1	C	977	HIS
1	D	135	GLN
1	D	163	GLN
1	D	245	GLN
1	D	266	GLN
1	D	363	HIS
1	D	485	GLN
1	D	583	ASN
1	D	624	GLN
1	D	634	GLN
1	D	653	HIS
1	D	775	GLN
1	D	804	ASN
1	D	843	GLN
1	D	878	HIS
1	D	890	GLN
1	D	903	GLN
1	D	977	HIS
1	D	1022	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 144 ligands modelled in this entry, 31 are monoatomic - leaving 113 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	B	8414	-	3,3,3	0.59	0	3,3,3	1.41	1 (33%)
5	DMS	A	8502	-	3,3,3	2.24	2 (66%)	3,3,3	1.71	1 (33%)
5	DMS	B	8413	-	3,3,3	2.23	1 (33%)	3,3,3	1.00	0
5	DMS	B	8411	-	3,3,3	1.64	1 (33%)	3,3,3	0.57	0
5	DMS	D	8421	-	3,3,3	0.52	0	3,3,3	0.33	0
5	DMS	B	8420	-	3,3,3	1.54	1 (33%)	3,3,3	0.17	0
5	DMS	D	8414	-	3,3,3	0.56	0	3,3,3	0.48	0
5	DMS	B	8405	-	3,3,3	1.40	1 (33%)	3,3,3	0.99	0
5	DMS	A	8406	3	3,3,3	0.49	0	3,3,3	0.25	0
5	DMS	D	8423	-	3,3,3	1.66	1 (33%)	3,3,3	0.45	0
5	DMS	B	8408	-	3,3,3	1.27	0	3,3,3	0.16	0
5	DMS	D	8705	-	3,3,3	1.28	0	3,3,3	0.16	0
5	DMS	C	8501	-	3,3,3	1.15	0	3,3,3	0.79	0
5	DMS	B	8415	-	3,3,3	2.99	2 (66%)	3,3,3	1.90	1 (33%)
5	DMS	A	8415	-	3,3,3	2.75	3 (100%)	3,3,3	0.31	0
5	DMS	B	8601	-	3,3,3	1.92	2 (66%)	3,3,3	0.69	0
5	DMS	A	8403	-	3,3,3	2.46	1 (33%)	3,3,3	0.39	0
5	DMS	D	8419	-	3,3,3	0.45	0	3,3,3	0.46	0
5	DMS	A	8410	-	3,3,3	0.80	0	3,3,3	0.94	0
5	DMS	D	8401	-	3,3,3	1.24	0	3,3,3	0.95	0
5	DMS	A	8427	-	3,3,3	0.80	0	3,3,3	0.18	0
5	DMS	B	8427	-	3,3,3	0.67	0	3,3,3	0.27	0
5	DMS	D	8425	4	3,3,3	0.98	0	3,3,3	0.92	0
5	DMS	D	8413	-	3,3,3	1.43	1 (33%)	3,3,3	0.48	0
5	DMS	A	8425	4	3,3,3	2.19	2 (66%)	3,3,3	0.73	0
5	DMS	C	8403	-	3,3,3	1.99	2 (66%)	3,3,3	0.37	0
5	DMS	C	8413	-	3,3,3	2.37	1 (33%)	3,3,3	0.60	0
5	DMS	D	8410	-	3,3,3	1.43	1 (33%)	3,3,3	0.49	0
5	DMS	C	8504	-	3,3,3	0.82	0	3,3,3	0.48	0
5	DMS	B	8410	-	3,3,3	1.78	1 (33%)	3,3,3	0.42	0
5	DMS	C	8402	-	3,3,3	2.55	2 (66%)	3,3,3	0.38	0
5	DMS	D	8402	-	3,3,3	2.12	2 (66%)	3,3,3	0.62	0
5	DMS	C	8423	-	3,3,3	0.85	0	3,3,3	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8406	-	3,3,3	1.72	0	3,3,3	0.40	0
2	147	D	2001	4	22,22,22	0.96	2 (9%)	29,31,31	1.34	2 (6%)
2	147	B	2001	4	22,22,22	0.99	2 (9%)	29,31,31	1.67	9 (31%)
5	DMS	B	8409	-	3,3,3	2.91	2 (66%)	3,3,3	0.79	0
5	DMS	B	8504	-	3,3,3	1.05	0	3,3,3	0.58	0
5	DMS	C	8421	-	3,3,3	0.81	0	3,3,3	1.08	0
5	DMS	D	8417	-	3,3,3	0.83	0	3,3,3	0.14	0
5	DMS	D	8407	-	3,3,3	2.20	3 (100%)	3,3,3	0.51	0
5	DMS	B	8425	4	3,3,3	1.79	1 (33%)	3,3,3	0.33	0
5	DMS	D	8508	-	3,3,3	1.72	1 (33%)	3,3,3	0.46	0
5	DMS	D	8416	-	3,3,3	0.75	0	3,3,3	0.61	0
5	DMS	A	8402	-	3,3,3	2.27	1 (33%)	3,3,3	0.34	0
5	DMS	B	8406	-	3,3,3	1.22	0	3,3,3	0.89	0
5	DMS	A	8414	-	3,3,3	0.96	0	3,3,3	0.20	0
5	DMS	B	8502	-	3,3,3	1.46	1 (33%)	3,3,3	1.96	1 (33%)
5	DMS	C	8416	-	3,3,3	1.80	1 (33%)	3,3,3	0.34	0
5	DMS	C	8425	4	3,3,3	1.65	1 (33%)	3,3,3	0.57	0
5	DMS	B	8421	-	3,3,3	0.81	0	3,3,3	1.08	0
5	DMS	A	8420	-	3,3,3	1.64	0	3,3,3	0.58	0
5	DMS	D	8404	-	3,3,3	1.95	1 (33%)	3,3,3	0.46	0
5	DMS	A	8401	-	3,3,3	0.95	0	3,3,3	0.26	0
5	DMS	C	8411	-	3,3,3	1.40	0	3,3,3	0.28	0
5	DMS	C	8409	-	3,3,3	2.45	1 (33%)	3,3,3	0.89	0
5	DMS	D	8408	-	3,3,3	1.33	0	3,3,3	0.35	0
5	DMS	C	8417	-	3,3,3	0.82	0	3,3,3	1.06	0
5	DMS	A	8602	-	3,3,3	1.35	1 (33%)	3,3,3	0.65	0
5	DMS	B	8401	-	3,3,3	0.88	0	3,3,3	0.54	0
5	DMS	C	8407	-	3,3,3	1.65	1 (33%)	3,3,3	0.17	0
5	DMS	D	8411	-	3,3,3	0.77	0	3,3,3	0.20	0
5	DMS	B	8423	-	3,3,3	0.80	0	3,3,3	0.90	0
5	DMS	C	8419	-	3,3,3	1.14	0	3,3,3	0.27	0
5	DMS	C	8401	-	3,3,3	0.79	0	3,3,3	0.25	0
5	DMS	C	8405	-	3,3,3	2.04	1 (33%)	3,3,3	0.33	0
5	DMS	A	8409	-	3,3,3	2.46	1 (33%)	3,3,3	0.63	0
5	DMS	B	8416	-	3,3,3	1.23	1 (33%)	3,3,3	0.57	0
5	DMS	D	8415	-	3,3,3	3.26	2 (66%)	3,3,3	0.21	0
5	DMS	A	8417	-	3,3,3	0.98	0	3,3,3	0.56	0
5	DMS	D	8703	-	3,3,3	1.02	0	3,3,3	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8414	-	3,3,3	1.96	2 (66%)	3,3,3	0.84	0
5	DMS	C	8404	-	3,3,3	1.32	0	3,3,3	0.67	0
5	DMS	A	8416	-	3,3,3	1.15	0	3,3,3	0.42	0
5	DMS	B	8403	-	3,3,3	1.92	2 (66%)	3,3,3	0.58	0
5	DMS	C	8410	-	3,3,3	1.20	0	3,3,3	0.39	0
5	DMS	D	8427	-	3,3,3	1.09	0	3,3,3	0.19	0
5	DMS	D	8701	-	3,3,3	2.78	2 (66%)	3,3,3	0.50	0
5	DMS	A	8405	-	3,3,3	1.39	1 (33%)	3,3,3	0.74	0
5	DMS	B	8404	-	3,3,3	1.57	1 (33%)	3,3,3	0.13	0
5	DMS	A	8411	-	3,3,3	0.82	0	3,3,3	0.26	0
5	DMS	B	8402	-	3,3,3	2.66	3 (100%)	3,3,3	0.83	0
5	DMS	D	8405	-	3,3,3	1.31	0	3,3,3	0.50	0
5	DMS	C	8506	-	3,3,3	2.36	1 (33%)	3,3,3	0.22	0
5	DMS	A	8419	-	3,3,3	0.74	0	3,3,3	0.62	0
5	DMS	D	8412	-	3,3,3	1.47	0	3,3,3	0.77	0
2	147	A	2001	4	22,22,22	0.89	1 (4%)	29,31,31	1.50	4 (13%)
5	DMS	A	8413	-	3,3,3	3.08	3 (100%)	3,3,3	0.75	0
5	DMS	A	8504	-	3,3,3	0.30	0	3,3,3	0.52	0
5	DMS	D	8501	-	3,3,3	1.24	0	3,3,3	0.41	0
5	DMS	A	8423	-	3,3,3	1.52	0	3,3,3	0.25	0
5	DMS	C	8408	-	3,3,3	1.36	0	3,3,3	0.82	0
5	DMS	C	8412	-	3,3,3	1.71	1 (33%)	3,3,3	0.31	0
5	DMS	B	8417	-	3,3,3	1.50	1 (33%)	3,3,3	0.59	0
5	DMS	D	8406	-	3,3,3	0.68	0	3,3,3	0.36	0
5	DMS	D	8409	-	3,3,3	2.28	1 (33%)	3,3,3	1.05	0
5	DMS	B	8407	-	3,3,3	2.31	1 (33%)	3,3,3	0.46	0
5	DMS	D	8403	-	3,3,3	1.39	1 (33%)	3,3,3	0.79	0
5	DMS	B	8508	-	3,3,3	2.73	3 (100%)	3,3,3	0.30	0
5	DMS	A	8421	-	3,3,3	0.76	0	3,3,3	0.27	0
5	DMS	C	8601	-	3,3,3	1.44	1 (33%)	3,3,3	0.64	0
5	DMS	A	8407	-	3,3,3	3.34	2 (66%)	3,3,3	0.47	0
5	DMS	A	8404	-	3,3,3	1.70	1 (33%)	3,3,3	0.35	0
5	DMS	C	8602	-	3,3,3	0.29	0	3,3,3	0.60	0
2	147	C	2001	4	22,22,22	1.01	1 (4%)	29,31,31	1.27	1 (3%)
5	DMS	C	8427	-	3,3,3	0.96	0	3,3,3	0.62	0
5	DMS	A	8412	-	3,3,3	2.28	1 (33%)	3,3,3	0.29	0
5	DMS	C	8420	-	3,3,3	2.42	1 (33%)	3,3,3	0.92	0
5	DMS	A	8408	-	3,3,3	1.17	0	3,3,3	1.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8501	-	3,3,3	1.69	1 (33%)	3,3,3	0.37	0
5	DMS	C	8415	-	3,3,3	1.72	0	3,3,3	0.50	0
5	DMS	B	8412	-	3,3,3	0.95	0	3,3,3	0.17	0
5	DMS	B	8506	-	3,3,3	1.96	1 (33%)	3,3,3	0.60	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	147	C	2001	4	-	1/8/30/30	0/2/2/2
2	147	A	2001	4	-	1/8/30/30	0/2/2/2
2	147	B	2001	4	-	1/8/30/30	0/2/2/2
2	147	D	2001	4	-	1/8/30/30	0/2/2/2

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8407	DMS	O-S	5.00	1.83	1.50
5	B	8409	DMS	O-S	4.24	1.78	1.50
5	C	8409	DMS	O-S	4.14	1.77	1.50
5	B	8415	DMS	C2-S	4.01	2.04	1.76
5	A	8409	DMS	O-S	3.99	1.76	1.50
5	D	8415	DMS	O-S	3.95	1.76	1.50
5	C	8402	DMS	C2-S	3.93	2.04	1.76
5	C	8420	DMS	O-S	3.88	1.75	1.50
5	A	8403	DMS	C2-S	3.84	2.03	1.76
5	B	8508	DMS	C1-S	3.69	2.02	1.76
5	D	8701	DMS	O-S	3.64	1.74	1.50
5	D	8415	DMS	C1-S	3.60	2.01	1.76
5	A	8413	DMS	C2-S	3.55	2.01	1.76
5	D	8409	DMS	O-S	3.53	1.73	1.50
5	A	8402	DMS	C2-S	3.43	2.00	1.76
5	C	8413	DMS	O-S	3.40	1.72	1.50
5	A	8412	DMS	C1-S	3.38	2.00	1.76
5	B	8402	DMS	C2-S	3.36	2.00	1.76
5	B	8407	DMS	C2-S	3.32	1.99	1.76
5	C	8405	DMS	O-S	3.11	1.70	1.50
5	A	8415	DMS	O-S	3.10	1.70	1.50
5	B	8413	DMS	O-S	3.08	1.70	1.50
5	D	8404	DMS	C2-S	3.03	1.97	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8506	DMS	C1-S	3.03	1.97	1.76
5	B	8506	DMS	C2-S	3.02	1.97	1.76
5	A	8502	DMS	C1-S	3.02	1.97	1.76
5	D	8701	DMS	C2-S	2.92	1.96	1.76
5	B	8410	DMS	C1-S	2.91	1.96	1.76
5	D	8402	DMS	C2-S	2.89	1.96	1.76
5	A	8413	DMS	C1-S	2.88	1.96	1.76
5	D	8508	DMS	O-S	2.77	1.68	1.50
5	A	8413	DMS	O-S	2.75	1.68	1.50
5	B	8425	DMS	O-S	2.75	1.68	1.50
5	A	8415	DMS	C2-S	2.73	1.95	1.76
5	B	8415	DMS	O-S	2.67	1.67	1.50
5	A	8501	DMS	O-S	2.64	1.67	1.50
5	C	8416	DMS	C2-S	2.63	1.94	1.76
5	C	8425	DMS	O-S	2.60	1.67	1.50
5	B	8420	DMS	C2-S	2.59	1.94	1.76
2	B	2001	147	C5'-C4'	-2.58	1.34	1.38
5	B	8601	DMS	C2-S	2.56	1.94	1.76
2	C	2001	147	O2'-N1'	-2.52	1.18	1.35
5	C	8412	DMS	O-S	2.50	1.66	1.50
5	C	8414	DMS	C1-S	-2.48	1.58	1.76
5	A	8407	DMS	C2-S	2.46	1.93	1.76
5	A	8425	DMS	C1-S	2.44	1.93	1.76
2	B	2001	147	O2'-N1'	-2.44	1.19	1.35
5	B	8417	DMS	O-S	2.44	1.66	1.50
5	B	8409	DMS	C1-S	2.41	1.93	1.76
5	B	8404	DMS	C2-S	2.41	1.93	1.76
2	A	2001	147	O2'-N1'	-2.41	1.19	1.35
5	B	8403	DMS	C1-S	2.40	1.93	1.76
5	D	8413	DMS	O-S	2.39	1.66	1.50
5	A	8502	DMS	C2-S	2.39	1.93	1.76
5	A	8415	DMS	C1-S	2.38	1.93	1.76
5	C	8601	DMS	C2-S	2.38	1.93	1.76
5	B	8402	DMS	C1-S	-2.28	1.59	1.76
5	D	8407	DMS	C1-S	2.27	1.92	1.76
5	C	8407	DMS	O-S	2.26	1.65	1.50
5	D	8407	DMS	C2-S	2.26	1.92	1.76
5	A	8425	DMS	C2-S	2.25	1.92	1.76
5	A	8404	DMS	O-S	2.25	1.65	1.50
2	D	2001	147	O2'-N1'	-2.19	1.20	1.35
5	B	8405	DMS	O-S	2.19	1.64	1.50
5	B	8402	DMS	O-S	2.19	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8414	DMS	C2-S	2.18	1.91	1.76
5	D	8423	DMS	C1-S	2.14	1.91	1.76
5	D	8410	DMS	C1-S	2.14	1.91	1.76
5	A	8405	DMS	O-S	2.13	1.64	1.50
5	B	8403	DMS	C2-S	2.13	1.91	1.76
5	B	8508	DMS	C2-S	2.11	1.91	1.76
5	B	8601	DMS	C1-S	2.09	1.90	1.76
5	B	8508	DMS	O-S	2.08	1.64	1.50
5	B	8502	DMS	C1-S	2.08	1.90	1.76
2	D	2001	147	O3-C3	2.08	1.48	1.43
5	C	8403	DMS	O-S	2.08	1.63	1.50
5	D	8407	DMS	O-S	2.07	1.63	1.50
5	D	8403	DMS	C2-S	2.05	1.90	1.76
5	D	8402	DMS	O-S	2.03	1.63	1.50
5	C	8402	DMS	O-S	2.03	1.63	1.50
5	A	8602	DMS	C2-S	2.02	1.90	1.76
5	B	8416	DMS	O-S	2.02	1.63	1.50
5	C	8403	DMS	C2-S	2.01	1.90	1.76
5	B	8411	DMS	C2-S	2.00	1.90	1.76

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	147	C3'-C4'-N1'	-3.88	115.95	119.34
2	C	2001	147	O1-C1-C2	-3.48	102.08	107.16
2	B	2001	147	C6'-C5'-C4'	-3.45	115.51	120.08
5	B	8502	DMS	C2-S-C1	3.38	115.76	98.42
2	B	2001	147	C5'-C4'-N1'	-3.23	116.52	119.34
2	D	2001	147	C5'-C4'-N1'	-3.19	116.55	119.34
2	A	2001	147	C5'-C4'-C3'	3.09	124.84	119.88
5	B	8415	DMS	C2-S-C1	2.96	113.57	98.42
5	A	8502	DMS	C2-S-C1	2.92	113.41	98.42
2	A	2001	147	C3-C4-C5	-2.62	105.48	110.23
2	B	2001	147	C5'-C6'-C1'	2.56	122.66	119.73
2	B	2001	147	C3'-C2'-C1'	-2.50	116.87	119.73
2	A	2001	147	C1-C2-C3	2.42	115.10	110.01
5	B	8414	DMS	C2-S-C1	2.35	110.49	98.42
2	B	2001	147	C1'-O1-C1	2.31	121.07	117.82
2	B	2001	147	O2-C2-C1	-2.14	104.98	110.08
2	B	2001	147	O1-C1-C2	-2.11	104.08	107.16
2	B	2001	147	C6-C5-C4	2.08	118.13	113.02
2	B	2001	147	C5'-C4'-C3'	2.08	123.22	119.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	147	O3'-N1'-C4'	-2.05	116.00	118.82

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	147	O5-C5-C6-O6
2	A	2001	147	O5-C5-C6-O6
2	D	2001	147	O5-C5-C6-O6
2	C	2001	147	O5-C5-C6-O6

There are no ring outliers.

53 monomers are involved in 93 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8411	DMS	1	0
5	D	8421	DMS	1	0
5	D	8705	DMS	5	0
5	B	8415	DMS	4	0
5	A	8415	DMS	2	0
5	A	8403	DMS	3	0
5	A	8410	DMS	1	0
5	B	8427	DMS	1	0
5	D	8425	DMS	1	0
5	C	8403	DMS	1	0
5	C	8504	DMS	1	0
5	B	8410	DMS	1	0
5	C	8402	DMS	5	0
5	C	8423	DMS	1	0
5	C	8406	DMS	2	0
5	B	8504	DMS	1	0
5	D	8407	DMS	1	0
5	D	8508	DMS	2	0
5	D	8416	DMS	3	0
5	B	8406	DMS	2	0
5	A	8414	DMS	2	0
5	B	8421	DMS	1	0
5	A	8420	DMS	1	0
5	D	8408	DMS	1	0
5	C	8417	DMS	3	0
5	A	8602	DMS	2	0

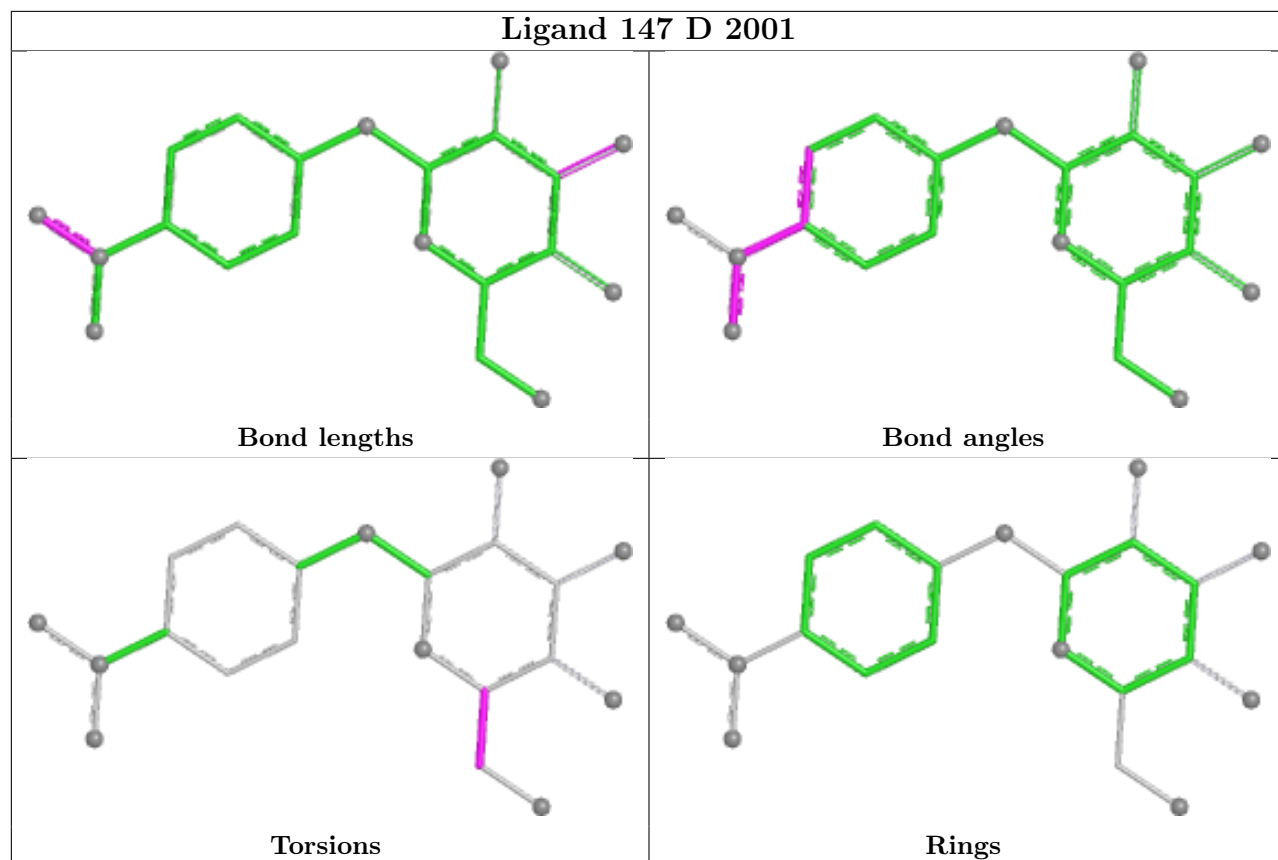
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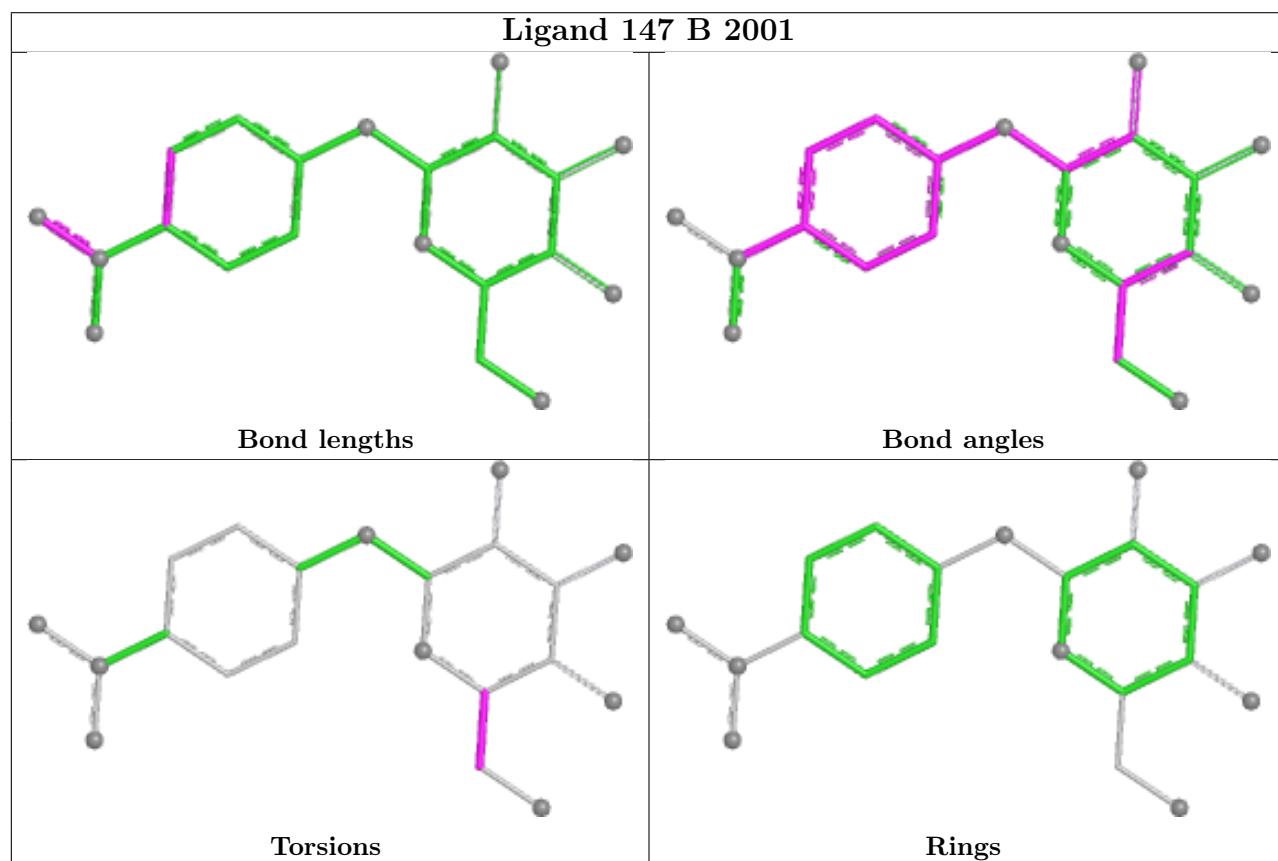
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8407	DMS	1	0
5	A	8409	DMS	1	0
5	D	8415	DMS	2	0
5	A	8417	DMS	3	0
5	D	8703	DMS	2	0
5	A	8416	DMS	1	0
5	B	8403	DMS	2	0
5	D	8427	DMS	2	0
5	B	8402	DMS	1	0
5	C	8506	DMS	2	0
5	A	8419	DMS	1	0
5	D	8412	DMS	3	0
5	A	8504	DMS	1	0
5	A	8423	DMS	1	0
5	B	8417	DMS	2	0
5	D	8406	DMS	1	0
5	D	8409	DMS	1	0
5	B	8508	DMS	1	0
5	A	8421	DMS	1	0
5	A	8407	DMS	1	0
5	A	8404	DMS	1	0
5	C	8602	DMS	1	0
5	C	8427	DMS	4	0
5	A	8412	DMS	3	0
5	C	8420	DMS	1	0
5	B	8412	DMS	2	0
5	B	8506	DMS	2	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.

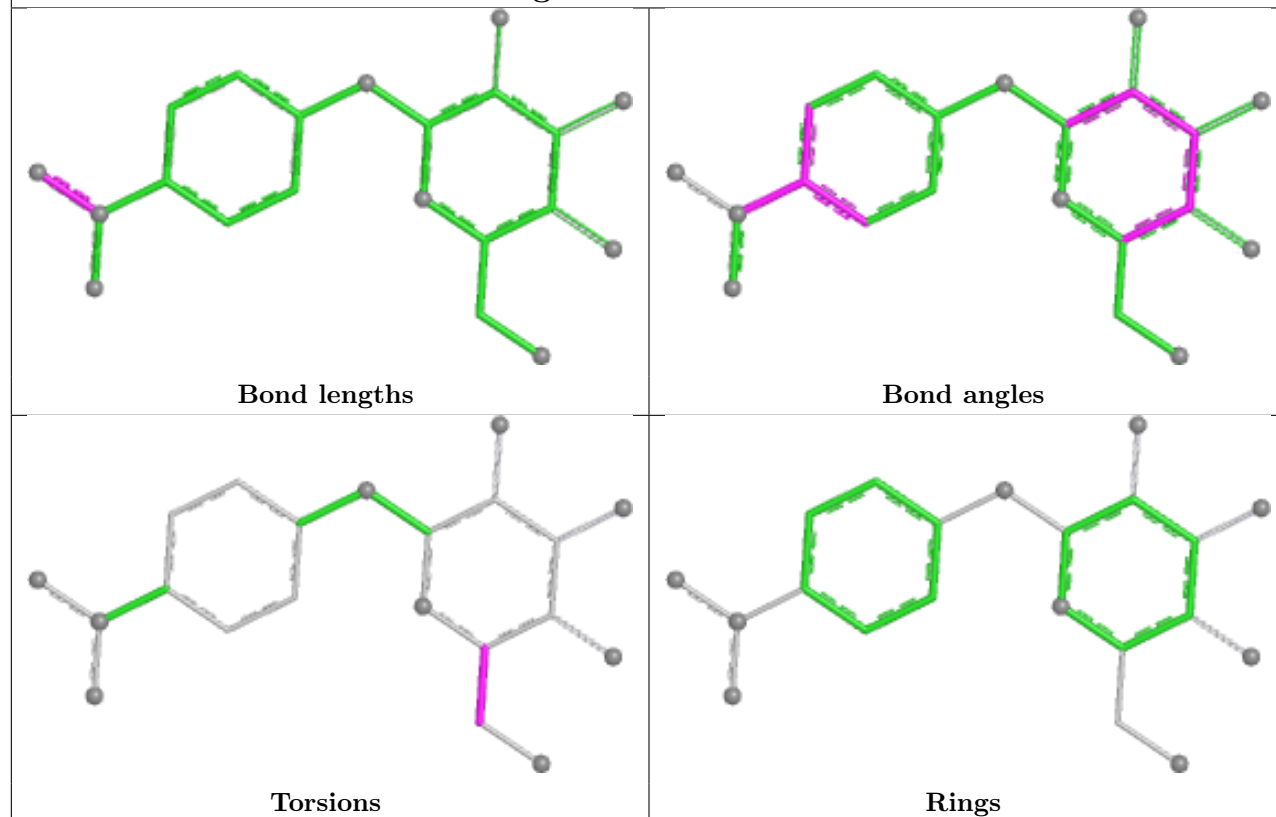
Ligand 147 D 2001



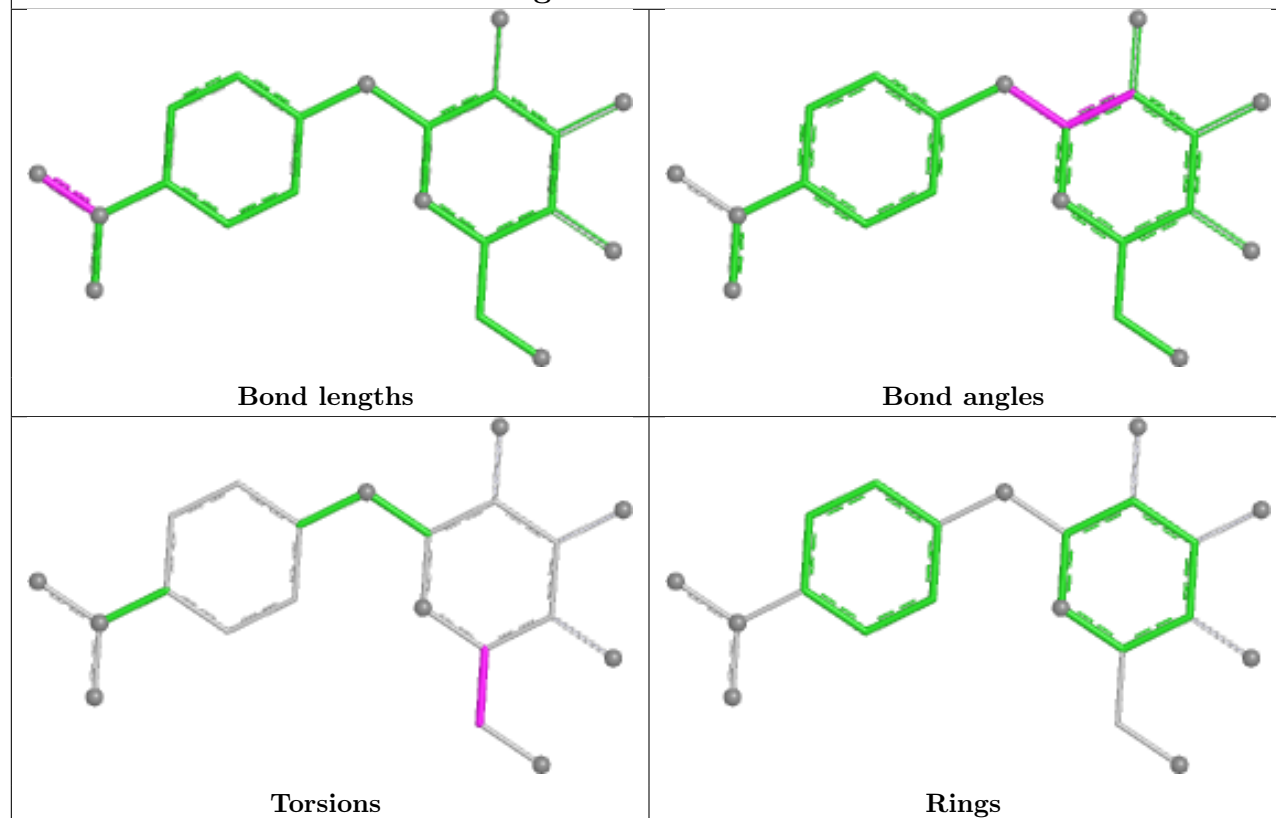
Ligand 147 B 2001



Ligand 147 A 2001



Ligand 147 C 2001



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.27	41 (4%)	41	49	8, 15, 45, 100	1 (0%)
1	B	1011/1023 (98%)	-0.30	39 (3%)	43	51	8, 15, 43, 94	1 (0%)
1	C	1011/1023 (98%)	-0.28	34 (3%)	48	56	8, 15, 47, 100	1 (0%)
1	D	1011/1023 (98%)	-0.23	46 (4%)	38	46	9, 16, 46, 95	1 (0%)
All	All	4044/4092 (98%)	-0.27	160 (3%)	42	50	8, 15, 46, 100	4 (0%)

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	8.5
1	A	730	LEU	7.5
1	B	730	LEU	5.5
1	D	686	PRO	5.4
1	C	730	LEU	5.3
1	D	737	ILE	5.1
1	D	733	ALA	5.1
1	A	771	GLY	4.8
1	A	737	ILE	4.8
1	C	736	ALA	4.7
1	D	735	HIS	4.7
1	A	731	PRO	4.6
1	D	688	PRO	4.5
1	D	734	SER	4.4
1	A	687	GLN	4.4
1	A	732	ALA	4.4
1	B	732	ALA	4.4
1	D	732	ALA	4.3
1	B	651	LEU	4.1
1	D	730	LEU	4.1
1	A	699	ARG	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	799	THR	4.0
1	D	76	CYS	4.0
1	D	685	LEU	4.0
1	C	737	ILE	4.0
1	C	798	ALA	4.0
1	A	829	THR	4.0
1	A	798	ALA	3.9
1	B	1018	LEU	3.9
1	D	651	LEU	3.9
1	D	736	ALA	3.8
1	A	1023	LYS	3.8
1	A	735	HIS	3.8
1	A	733	ALA	3.8
1	D	799	THR	3.8
1	B	686	PRO	3.7
1	C	731	PRO	3.7
1	D	634	GLN	3.7
1	A	646	HIS	3.7
1	C	732	ALA	3.6
1	C	733	ALA	3.6
1	B	685	LEU	3.6
1	D	731	PRO	3.5
1	A	772	ASP	3.4
1	C	686	PRO	3.4
1	B	745	MET	3.4
1	B	729	THR	3.3
1	C	1023	LYS	3.3
1	A	135	GLN	3.3
1	D	581	ASN	3.3
1	B	733	ALA	3.3
1	D	1023	LYS	3.2
1	C	1022	GLN	3.2
1	C	687	GLN	3.2
1	A	736	ALA	3.2
1	A	249	GLU	3.1
1	C	772	ASP	3.1
1	A	634	GLN	3.1
1	C	734	SER	3.1
1	B	179	ALA	3.1
1	B	731	PRO	3.1
1	B	737	ILE	3.1
1	D	689	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	682	LEU	3.0
1	D	646	HIS	3.0
1	B	845	GLN	3.0
1	C	633	GLY	3.0
1	B	735	HIS	3.0
1	D	829	THR	3.0
1	D	773	LYS	2.9
1	B	819	GLU	2.9
1	C	651	LEU	2.9
1	C	634	GLN	2.9
1	B	580	GLU	2.9
1	C	735	HIS	2.9
1	C	761	GLN	2.8
1	C	659	ASP	2.8
1	A	799	THR	2.8
1	B	684	GLU	2.8
1	A	581	ASN	2.8
1	B	79	PRO	2.7
1	C	663	LEU	2.7
1	D	690	SER	2.7
1	A	729	THR	2.7
1	D	729	THR	2.7
1	A	651	LEU	2.7
1	C	178	ARG	2.7
1	D	755	ARG	2.7
1	D	687	GLN	2.6
1	D	681	GLU	2.6
1	D	319	ASP	2.6
1	A	682	LEU	2.6
1	D	861	SER	2.6
1	B	689	GLU	2.6
1	D	75	GLU	2.6
1	D	845	GLN	2.6
1	D	580	GLU	2.6
1	A	683	PRO	2.5
1	A	688	PRO	2.5
1	A	734	SER	2.5
1	B	736	ALA	2.5
1	C	746	ASP	2.5
1	C	580	GLU	2.5
1	A	76	CYS	2.4
1	C	819	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	582	GLY	2.4
1	A	116	THR	2.4
1	A	685	LEU	2.4
1	D	739	HIS	2.4
1	B	699	ARG	2.4
1	D	633	GLY	2.4
1	A	684	GLU	2.4
1	C	770	ILE	2.4
1	B	682	LEU	2.4
1	C	685	LEU	2.4
1	C	773	LYS	2.4
1	C	799	THR	2.4
1	B	846	GLY	2.4
1	B	659	ASP	2.3
1	B	1023	LYS	2.3
1	A	580	GLU	2.3
1	B	75	GLU	2.3
1	B	681	GLU	2.3
1	B	370	GLN	2.3
1	D	663	LEU	2.3
1	D	770	ILE	2.3
1	D	116	THR	2.3
1	B	663	LEU	2.3
1	B	798	ALA	2.2
1	B	583	ASN	2.2
1	D	683	PRO	2.2
1	B	800	ARG	2.2
1	C	689	GLU	2.2
1	A	663	LEU	2.2
1	D	630	ARG	2.2
1	D	798	ALA	2.2
1	A	739	HIS	2.2
1	B	1022	GLN	2.2
1	A	75	GLU	2.2
1	D	820	ALA	2.2
1	A	79	PRO	2.2
1	A	130	ASP	2.2
1	B	977	HIS	2.2
1	D	1018	LEU	2.1
1	D	801	ILE	2.1
1	B	581	ASN	2.1
1	C	80	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	136	GLU	2.1
1	B	817	GLN	2.1
1	D	1022	GLN	2.1
1	C	729	THR	2.1
1	A	1022	GLN	2.1
1	A	583	ASN	2.1
1	A	846	GLY	2.1
1	B	847	LYS	2.0
1	C	809	ARG	2.0
1	B	797	GLU	2.0
1	D	684	GLU	2.0
1	C	684	GLU	2.0
1	C	745	MET	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	D	8703	4/4	0.73	0.28	47,73,77,81	0
5	DMS	B	8406	4/4	0.79	0.25	35,52,87,100	0
5	DMS	D	8423	4/4	0.80	0.25	38,53,100,100	0
5	DMS	B	8420	4/4	0.80	0.22	41,60,65,69	0
5	DMS	A	8427	4/4	0.84	0.18	41,54,55,100	0
5	DMS	D	8407	4/4	0.85	0.23	29,47,53,100	0
5	DMS	A	8421	4/4	0.85	0.21	55,56,68,100	0
5	DMS	D	8427	4/4	0.85	0.18	47,51,59,75	0
5	DMS	C	8419	4/4	0.85	0.17	41,46,50,67	0
5	DMS	B	8423	4/4	0.86	0.22	33,34,66,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	B	8427	4/4	0.86	0.21	35,40,68,100	0
5	DMS	C	8417	4/4	0.86	0.15	24,30,54,74	0
5	DMS	A	8406	4/4	0.86	0.19	13,59,73,100	0
5	DMS	D	8417	4/4	0.87	0.17	26,31,47,100	0
5	DMS	A	8407	4/4	0.87	0.16	23,32,33,45	0
5	DMS	C	8423	4/4	0.87	0.25	28,64,100,100	0
5	DMS	A	8423	4/4	0.87	0.19	30,46,74,100	0
5	DMS	D	8705	4/4	0.87	0.16	20,47,58,71	0
5	DMS	C	8420	4/4	0.88	0.21	35,55,58,100	0
5	DMS	A	8417	4/4	0.88	0.21	23,27,96,100	0
5	DMS	C	8427	4/4	0.88	0.15	49,51,56,65	0
5	DMS	C	8602	4/4	0.88	0.23	21,74,91,100	0
5	DMS	A	8602	4/4	0.88	0.19	38,53,74,100	0
5	DMS	C	8406	4/4	0.89	0.20	37,38,46,94	0
5	DMS	A	8416	4/4	0.89	0.17	22,38,73,100	0
5	DMS	D	8416	4/4	0.89	0.18	29,53,77,80	0
5	DMS	A	8412	4/4	0.89	0.18	38,46,51,100	0
5	DMS	B	8414	4/4	0.90	0.21	30,39,41,100	0
5	DMS	A	8502	4/4	0.90	0.15	22,26,54,58	0
5	DMS	D	8501	4/4	0.90	0.12	24,30,34,48	0
5	DMS	B	8504	4/4	0.90	0.12	35,40,58,63	0
5	DMS	C	8506	4/4	0.90	0.15	26,40,47,52	0
5	DMS	B	8417	4/4	0.91	0.14	25,28,70,73	0
3	MG	A	3105	1/1	0.91	0.09	21,21,21,21	1
5	DMS	D	8414	4/4	0.91	0.22	24,40,87,100	0
5	DMS	B	8421	4/4	0.91	0.14	31,35,46,73	0
5	DMS	A	8420	4/4	0.91	0.13	39,45,45,47	0
5	DMS	C	8421	4/4	0.91	0.14	32,46,55,57	0
5	DMS	B	8407	4/4	0.91	0.16	28,32,33,38	0
5	DMS	B	8502	4/4	0.91	0.13	28,30,43,49	0
5	DMS	D	8508	4/4	0.91	0.15	36,52,53,53	0
5	DMS	C	8504	4/4	0.91	0.14	35,54,63,66	0
3	MG	C	3105	1/1	0.91	0.07	19,19,19,19	1
5	DMS	D	8425	4/4	0.92	0.14	16,19,24,24	4
5	DMS	C	8407	4/4	0.92	0.13	27,30,40,42	0
5	DMS	C	8416	4/4	0.92	0.16	38,50,52,100	0
5	DMS	A	8414	4/4	0.92	0.20	24,43,84,100	0
5	DMS	D	8421	4/4	0.92	0.14	49,51,52,52	0
5	DMS	B	8416	4/4	0.92	0.15	34,36,47,90	0
5	DMS	A	8419	4/4	0.93	0.14	33,46,49,50	0
5	DMS	D	8415	4/4	0.93	0.18	20,37,42,100	0
5	DMS	C	8601	4/4	0.93	0.13	35,40,42,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	B	8508	4/4	0.93	0.14	27,35,48,62	0
5	DMS	D	8404	4/4	0.93	0.12	20,23,41,63	0
5	DMS	A	8501	4/4	0.93	0.11	17,27,37,39	0
5	DMS	C	8414	4/4	0.94	0.12	22,39,41,49	0
3	MG	D	3105	1/1	0.94	0.09	24,24,24,24	1
5	DMS	A	8425	4/4	0.94	0.14	33,38,38,44	0
5	DMS	B	8409	4/4	0.94	0.10	25,26,33,34	0
5	DMS	B	8412	4/4	0.94	0.11	27,37,37,43	0
5	DMS	B	8413	4/4	0.94	0.12	27,31,35,39	0
5	DMS	A	8504	4/4	0.94	0.15	22,43,50,100	0
5	DMS	B	8415	4/4	0.94	0.13	21,29,32,37	0
5	DMS	B	8601	4/4	0.94	0.12	30,37,41,45	0
5	DMS	C	8402	4/4	0.94	0.13	19,29,34,51	0
3	MG	A	3005	1/1	0.94	0.07	33,33,33,33	0
5	DMS	B	8402	4/4	0.94	0.12	19,19,28,33	0
5	DMS	C	8412	4/4	0.94	0.16	28,31,36,100	0
5	DMS	D	8419	4/4	0.95	0.10	33,43,46,48	0
5	DMS	A	8413	4/4	0.95	0.11	30,33,34,35	0
5	DMS	D	8406	4/4	0.95	0.13	26,26,28,41	0
5	DMS	C	8501	4/4	0.95	0.10	20,29,37,51	0
5	DMS	D	8409	4/4	0.95	0.11	29,30,31,34	0
5	DMS	B	8408	4/4	0.95	0.13	31,34,38,100	0
5	DMS	C	8413	4/4	0.95	0.11	31,33,34,36	0
5	DMS	A	8408	4/4	0.95	0.10	22,34,35,36	0
5	DMS	B	8410	4/4	0.95	0.10	19,28,32,38	0
5	DMS	D	8412	4/4	0.96	0.14	27,27,33,100	0
5	DMS	D	8413	4/4	0.96	0.14	28,31,31,100	0
4	NA	C	3104	1/1	0.96	0.09	21,21,21,21	0
5	DMS	C	8425	4/4	0.96	0.14	27,29,29,100	0
5	DMS	C	8409	4/4	0.96	0.09	24,31,33,34	0
5	DMS	C	8410	4/4	0.96	0.10	22,24,33,34	0
5	DMS	B	8403	4/4	0.96	0.08	21,22,28,30	0
5	DMS	B	8404	4/4	0.96	0.09	18,20,31,37	0
5	DMS	A	8409	4/4	0.96	0.09	26,31,34,40	0
5	DMS	B	8506	4/4	0.96	0.10	27,34,43,44	0
5	DMS	D	8402	4/4	0.96	0.11	17,28,31,33	0
5	DMS	A	8404	4/4	0.96	0.12	18,30,31,39	0
3	MG	B	3105	1/1	0.96	0.05	18,18,18,18	1
4	NA	A	3103	1/1	0.96	0.07	23,23,23,23	0
5	DMS	A	8415	4/4	0.96	0.10	19,36,37,46	0
3	MG	D	3005	1/1	0.97	0.08	27,27,27,27	0
5	DMS	C	8404	4/4	0.97	0.08	18,19,26,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	D	3103	1/1	0.97	0.09	27,27,27,27	0
4	NA	D	3104	1/1	0.97	0.07	28,28,28,28	0
5	DMS	D	8403	4/4	0.97	0.07	18,26,28,29	0
5	DMS	B	8405	4/4	0.97	0.11	27,30,30,34	0
5	DMS	A	8402	4/4	0.97	0.13	15,29,30,47	0
5	DMS	A	8410	4/4	0.97	0.09	22,31,40,44	0
5	DMS	D	8408	4/4	0.97	0.08	18,31,36,39	0
5	DMS	A	8403	4/4	0.97	0.07	23,23,25,31	0
5	DMS	D	8410	4/4	0.97	0.08	20,29,30,34	0
5	DMS	D	8701	4/4	0.97	0.11	16,17,22,44	0
4	NA	A	3104	1/1	0.97	0.11	23,23,23,23	0
5	DMS	C	8415	4/4	0.97	0.09	21,26,32,45	0
5	DMS	A	8405	4/4	0.98	0.07	21,24,25,32	0
2	147	D	2001	21/21	0.98	0.05	11,13,27,32	0
5	DMS	C	8411	4/4	0.98	0.07	22,23,23,28	0
2	147	A	2001	21/21	0.98	0.04	10,13,21,30	0
2	147	B	2001	21/21	0.98	0.05	9,11,20,35	0
2	147	C	2001	21/21	0.98	0.05	10,12,25,50	0
3	MG	C	3006	1/1	0.98	0.05	20,20,20,20	1
5	DMS	A	8411	4/4	0.98	0.08	22,26,26,43	0
5	DMS	C	8403	4/4	0.98	0.07	22,24,25,26	0
5	DMS	D	8405	4/4	0.98	0.09	24,30,30,34	0
4	NA	B	3104	1/1	0.98	0.05	20,20,20,20	0
5	DMS	C	8405	4/4	0.98	0.09	27,27,28,32	0
5	DMS	B	8411	4/4	0.98	0.08	21,23,25,33	0
5	DMS	B	8425	4/4	0.98	0.07	19,25,27,29	0
5	DMS	C	8408	4/4	0.98	0.07	18,29,30,31	0
5	DMS	D	8411	4/4	0.98	0.09	19,24,26,71	0
4	NA	C	3102	1/1	0.99	0.03	12,12,12,12	0
4	NA	C	3103	1/1	0.99	0.08	21,21,21,21	0
4	NA	A	3101	1/1	0.99	0.04	13,13,13,13	0
5	DMS	C	8401	4/4	0.99	0.06	14,15,18,18	0
4	NA	D	3102	1/1	0.99	0.03	11,11,11,11	0
3	MG	D	3002	1/1	0.99	0.04	14,14,14,14	0
3	MG	A	3002	1/1	0.99	0.04	14,14,14,14	0
5	DMS	B	8401	4/4	0.99	0.06	14,17,18,18	0
5	DMS	A	8401	4/4	0.99	0.04	11,13,14,15	0
5	DMS	D	8401	4/4	0.99	0.06	13,15,17,20	0
4	NA	B	3103	1/1	0.99	0.03	19,19,19,19	0
3	MG	A	3001	1/1	0.99	0.03	11,11,11,11	0
4	NA	B	3102	1/1	1.00	0.05	11,11,11,11	0
3	MG	C	3002	1/1	1.00	0.04	13,13,13,13	0

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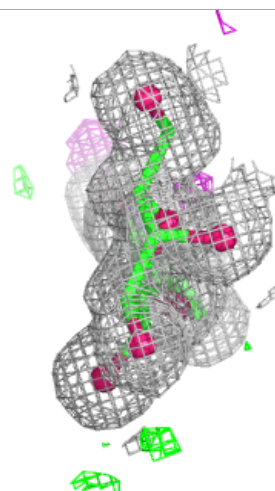
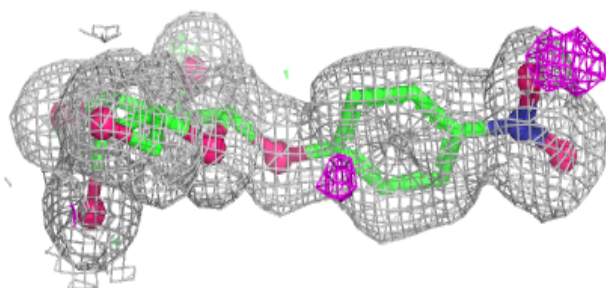
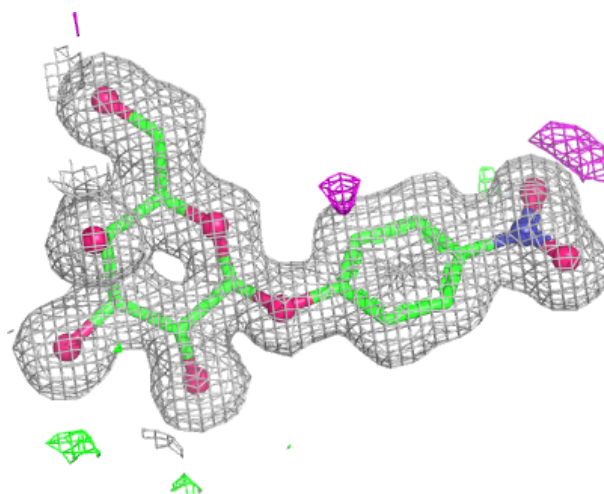
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	B	3002	1/1	1.00	0.03	14,14,14,14	0
4	NA	C	3101	1/1	1.00	0.02	11,11,11,11	0
3	MG	B	3001	1/1	1.00	0.03	10,10,10,10	0
4	NA	A	3102	1/1	1.00	0.03	12,12,12,12	0
3	MG	D	3001	1/1	1.00	0.02	12,12,12,12	0
4	NA	D	3101	1/1	1.00	0.03	13,13,13,13	0
3	MG	C	3001	1/1	1.00	0.02	10,10,10,10	0
4	NA	B	3101	1/1	1.00	0.03	12,12,12,12	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.

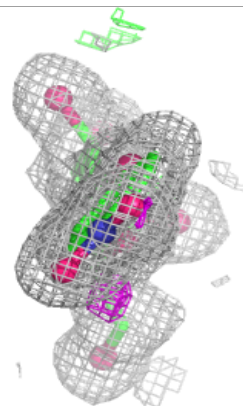
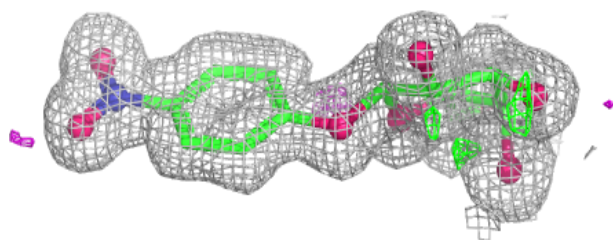
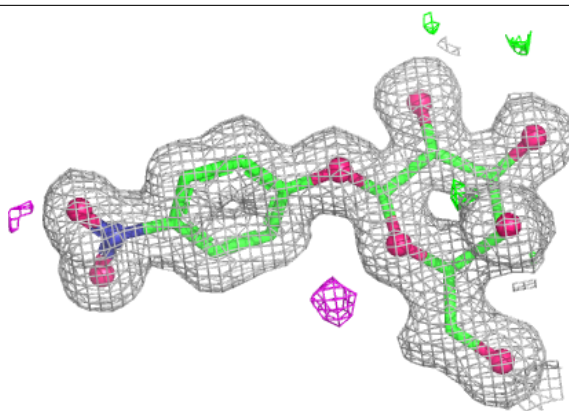
Electron density around 147 D 2001:

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

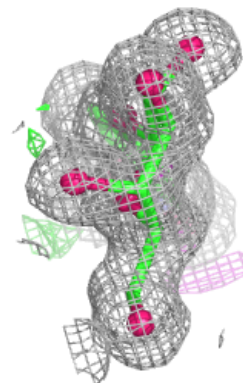
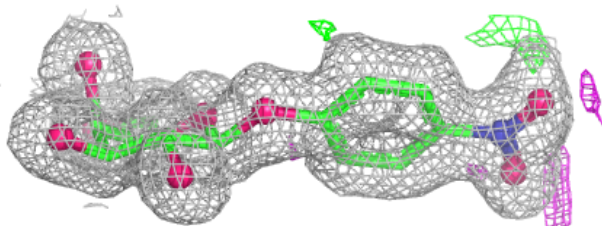
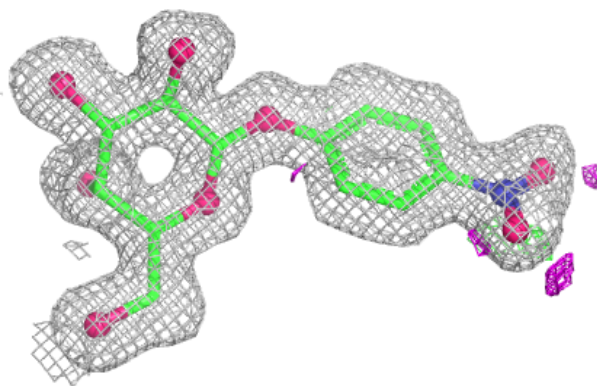


Electron density around 147 A 2001:

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

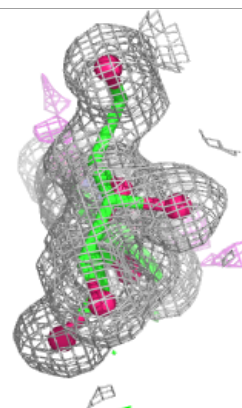
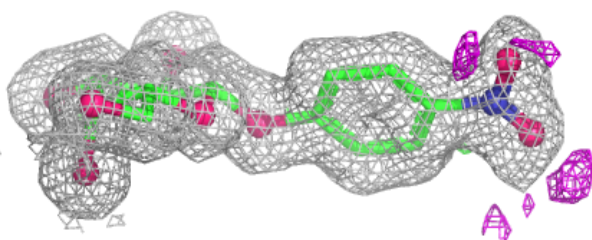
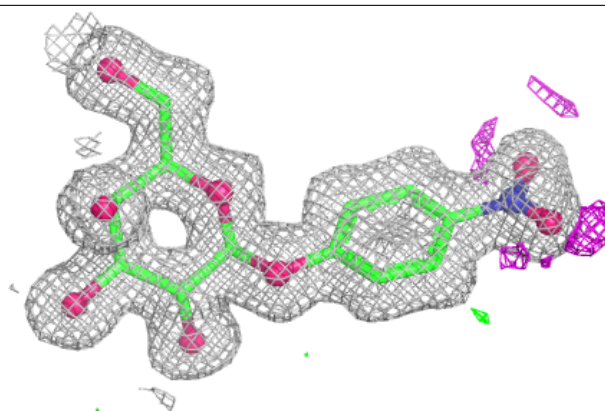
**Electron density around 147 B 2001:**

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



Electron density around 147 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.