Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 09:33 PM EDT

PDB ID	:	1JYW
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 (i) 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 (i)) were used in the production of this report:

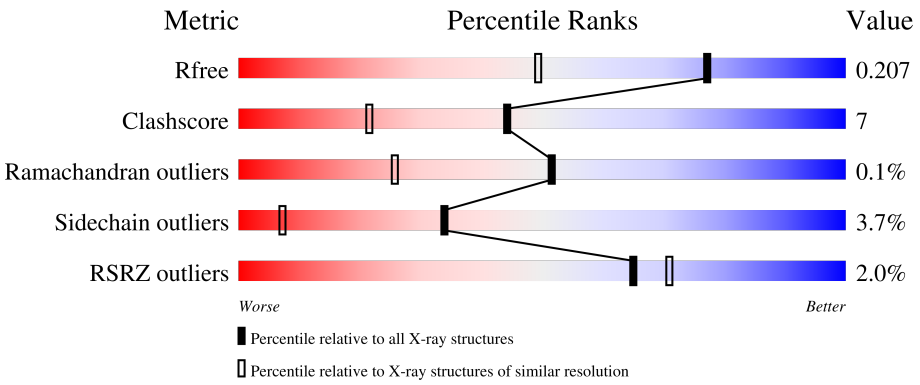
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	1483 (1.56-1.56)
Clashscore	141614	1529 (1.56-1.56)
Ramachandran outliers	138981	1498 (1.56-1.56)
Sidechain outliers	138945	1495 (1.56-1.56)
RSRZ outliers	127900	1465 (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 <=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	2% 75% 20%
1	B	1023	% 74% 21%
1	C	1023	2% 74% 22%
1	D	1023	3% 73% 21%

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	-	-
5	DMS	B	8508	-	X	-	-
5	DMS	C	8402	-	-	X	-
5	DMS	D	8407	-	X	-	-
5	DMS	D	8416	-	-	X	-

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	1011	8127	5139	1441	1509	38	0	2	0
1	B	1011	8128	5139	1442	1509	38	0	2	0
1	C	1011	8128	5139	1442	1509	38	0	2	0
1	D	1011	8128	5139	1442	1509	38	0	2	0

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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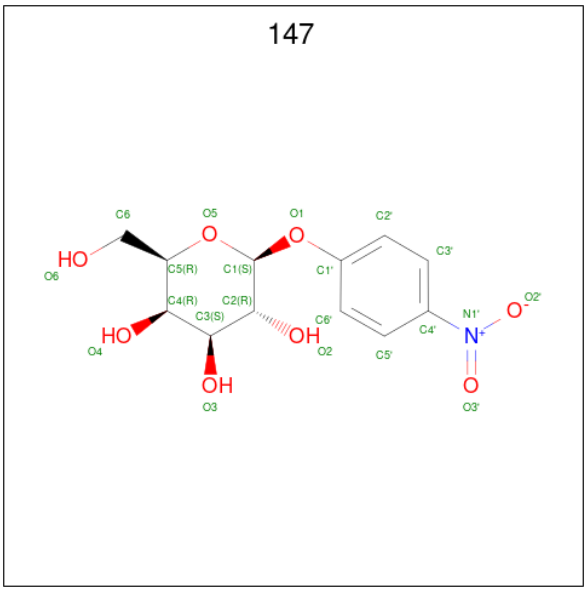
Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	THR	cloning artifact	? P00722
C	5	LEU	ASP	cloning artifact	? P00722
C	6	GLU	SER	cloning artifact	? P00722
C	7	ASP	LEU	cloning artifact	? P00722
C	8	PRO	ALA	cloning artifact	? P00722
C	537	GLN	GLU	engineered mutation	? P00722
D	1	GLY	THR	cloning 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 (three-letter code: 147) (formula: $C_{12}H_{15}NO_8$).



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

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

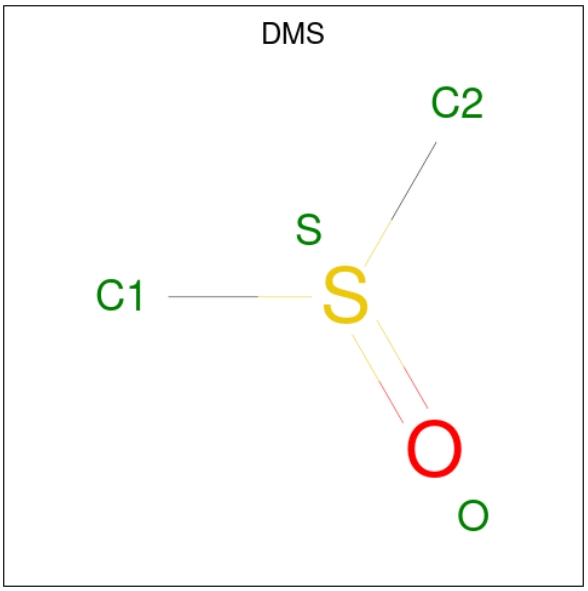
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

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

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

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

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

- Molecule 6 is water.

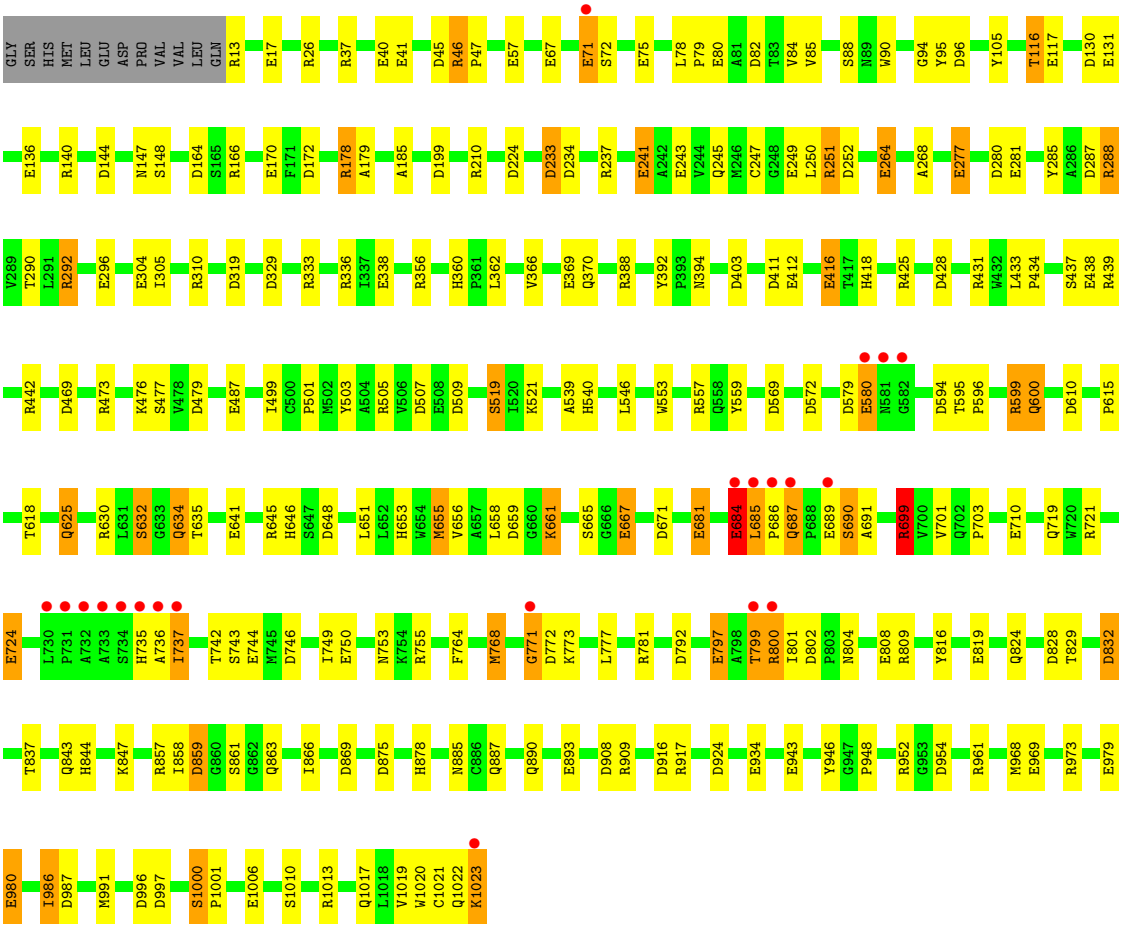
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	1112	1112	1112	0	0
			Total	O		
6	B	1128	1128	1128	0	0
			Total	O		
6	C	1104	1104	1104	0	0
			Total	O		
6	D	1118	1118	1118	0	0

3 Residue-property plots (i)

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.

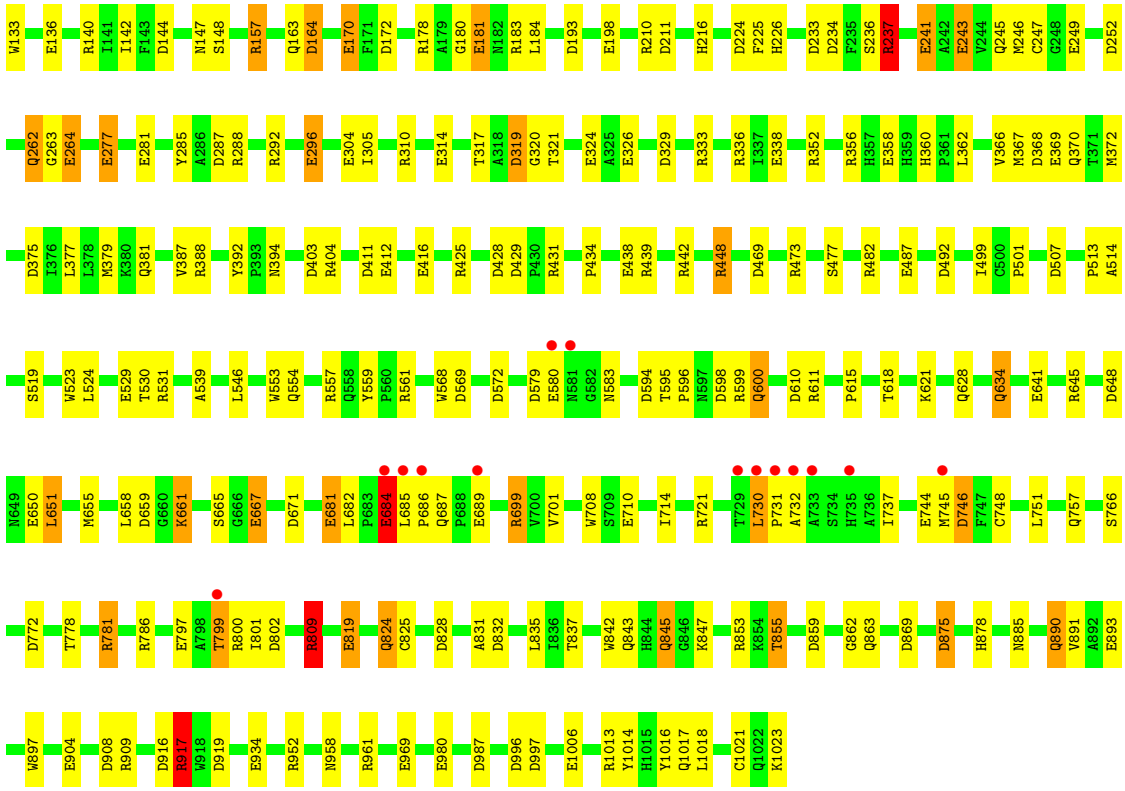
• Molecule 1: Beta-Galactosidase

Chain A:



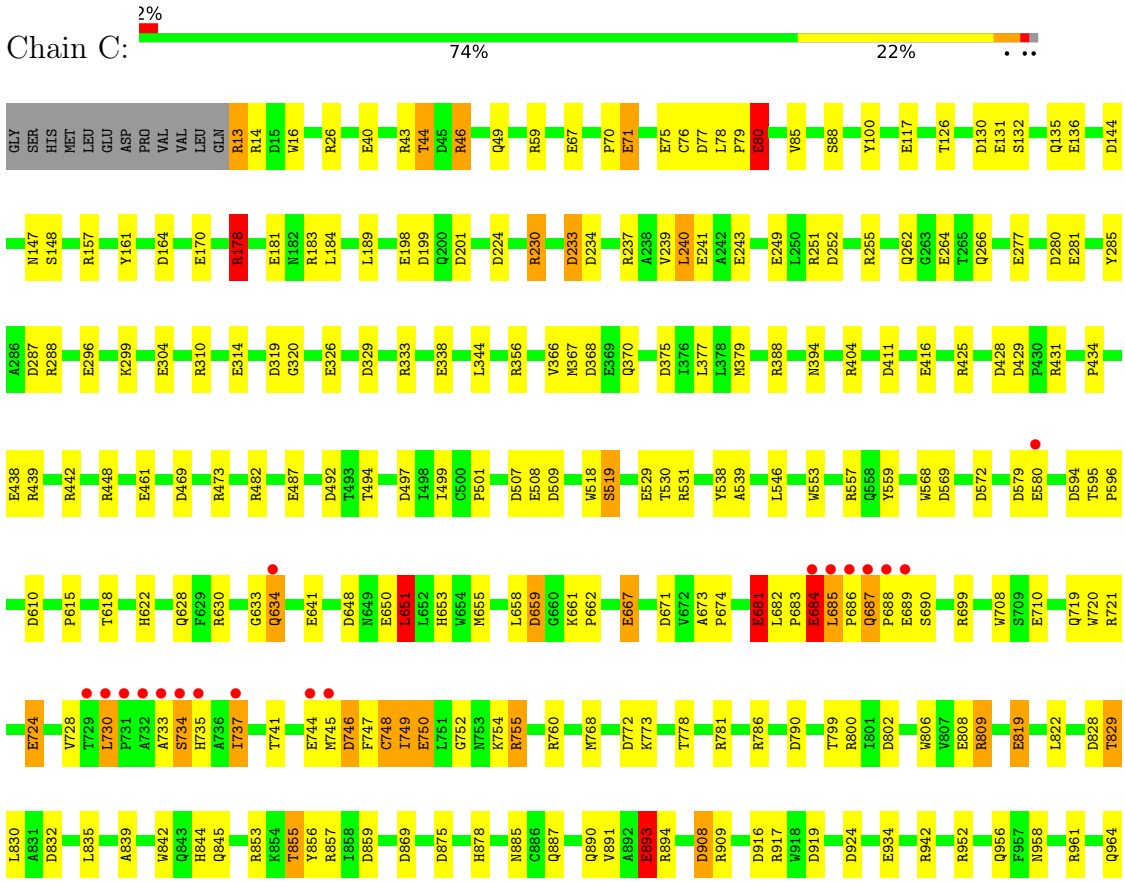
• Molecule 1: Beta-Galactosidase

Chain B:



- Molecule 1: Beta-Galactosidase

Chain C:



Q965 N968 E969 R973 E979 E980 D987 D996 D997 S1000 P1001 F1007 R1013 Q1017 C1021 Q1022 K1023

• Molecule 1: Beta-Galactosidase

Chain D: 3% 73% 21%

GLY SER HIS MET LEU GLU ASP PRO VAL VAL LEU GLN R13 R14 D15 W16 E17 R37 E41 D45 R46 P47 E67 E71 S72 W73 L74 E75 C76 D77 E80 V85 V86 P87 S88 D96 P111 P112 F113 T116 E117 C122 N128 V129 D130 E131 L134

Q135 E136 R140 D144 N147 S148 R157 D164 S165 R166 E170 F171 D172 F176 L177 R178 A179 G180 E181 N182 R183 D193 D224 R230 D233 D234 R237 L240 E241 A242 E243 E249 L250 R251 D252 Y253 L254 R255 E264 V267 E277 D280

E281 D287 R292 E296 E304 I305 E314 D319 E324 A325 E326 D329 R333 E334 E338 N339 G340 L344 R352 R356 H360 P361 L362 H363 V366 M367 D368 E369 Q370 T371 M372 V373 L377 N394 H395 D403 D411 E416 R425

D428 D429 P430 R431 W432 L433 P434 R439 R442 R446 D447 R448 E461 D469 Y472 R473 K476 D479 R482 E487 D492 I499 C500 P501 D507 E508 D509 P513 A514 S519 Y538 A539 L546 Y559 P560 R561 D569 D572

K577 Y578 D579 E580 N581 G582 N583 P584 Y588 D591 D594 T595 P596 D610 T618 E619 Q625 F629 R630 L631 S632 G633 Q634 E637 V638 T639 S640 E641 R645 D648 N649 E650 L651 L652 H653 L658 D659 G660 K661 P662 L663 E667 L670 Q675 G676 K677

E681 L682 P683 E684 L685 P686 Q687 P688 E689 S690 R699 V700 V701 E710 W717 Q718 Q719 E724 L730 P731 A732 A733 S734 H735 A736 I737 P738 H739 D746 I749 E750 L751 K754 R755 R760 M768 W769 T770 G771 D772 K773 K774 Q775 T778 R781 D792

E797 A798 T799 R800 I801 D802 P803 N804 E808 R809 G814 Q817 A818 E819 T829 L830 A831 D832 H840 Q843 H844 Q845 C846 K847 T848 L849 F850 I858 D859 G860 Q863 D869 H878 N885 C886 Q887 Q890 V891 A892 E893 R894 D908 R909 L910 D916

R917 W918 D919 D924 M925 Y926 R942 E943 R952 G953 D954 N958 R961 Y962 R973 E979 E980 I986 D987 D996 D997 L1018 V1019 W1020 C1021 Q1022 K1023

4 Data and refinement statistics (i)

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 28.75 – 1.55	Depositor EDS
% Data completeness (in resolution range)	98.3 (28.80-1.55) 91.2 (28.75-1.55)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 1.54Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.180 , 0.229 0.164 , 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)	0.34 , 84.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.21	49/8382 (0.6%)	1.67	163/11435 (1.4%)
1	B	1.23	51/8383 (0.6%)	1.65	169/11437 (1.5%)
1	C	1.21	46/8383 (0.5%)	1.71	180/11437 (1.6%)
1	D	1.22	47/8383 (0.6%)	1.61	161/11437 (1.4%)
All	All	1.22	193/33531 (0.6%)	1.66	673/45746 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

All (193) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1006	GLU	CD-OE2	10.08	1.36	1.25
1	D	681	GLU	CD-OE2	9.79	1.36	1.25
1	D	893	GLU	CD-OE2	9.79	1.36	1.25
1	B	71	GLU	CD-OE2	9.33	1.35	1.25
1	B	689	GLU	CD-OE2	9.25	1.35	1.25
1	B	1006	GLU	CD-OE2	8.94	1.35	1.25
1	B	650	GLU	CD-OE2	8.87	1.35	1.25
1	C	243	GLU	CD-OE2	8.81	1.35	1.25
1	D	650	GLU	CD-OE2	8.72	1.35	1.25
1	A	243	GLU	CD-OE2	8.56	1.35	1.25
1	C	80	GLU	CD-OE2	8.56	1.35	1.25
1	C	684	GLU	CD-OE2	8.40	1.34	1.25
1	C	304	GLU	CD-OE2	8.27	1.34	1.25
1	A	170	GLU	CD-OE2	8.21	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	667	GLU	CD-OE2	8.20	1.34	1.25
1	C	71	GLU	CD-OE2	8.18	1.34	1.25
1	A	80	GLU	CD-OE2	8.10	1.34	1.25
1	D	170	GLU	CD-OE2	8.05	1.34	1.25
1	A	580	GLU	CD-OE2	8.04	1.34	1.25
1	C	689	GLU	CD-OE2	8.05	1.34	1.25
1	D	75	GLU	CD-OE2	7.93	1.34	1.25
1	C	338	GLU	CD-OE2	7.86	1.34	1.25
1	A	241	GLU	CD-OE2	7.85	1.34	1.25
1	A	249	GLU	CD-OE2	7.83	1.34	1.25
1	B	819	GLU	CD-OE2	7.78	1.34	1.25
1	D	17	GLU	CD-OE2	7.76	1.34	1.25
1	C	75	GLU	CD-OE2	7.76	1.34	1.25
1	B	667	GLU	CD-OE2	7.75	1.34	1.25
1	C	281	GLU	CD-OE2	7.68	1.34	1.25
1	D	689	GLU	CD-OE2	7.68	1.34	1.25
1	C	819	GLU	CD-OE2	7.67	1.34	1.25
1	A	681	GLU	CD-OE2	7.59	1.33	1.25
1	B	296	GLU	CD-OE2	7.59	1.33	1.25
1	A	281	GLU	CD-OE2	7.57	1.33	1.25
1	C	934	GLU	CD-OE2	7.52	1.33	1.25
1	A	979	GLU	CD-OE2	7.50	1.33	1.25
1	D	580	GLU	CD-OE2	7.50	1.33	1.25
1	A	487	GLU	CD-OE2	7.50	1.33	1.25
1	A	969	GLU	CD-OE2	7.43	1.33	1.25
1	D	326	GLU	CD-OE2	7.41	1.33	1.25
1	C	131	GLU	CD-OE2	7.39	1.33	1.25
1	B	684	GLU	CD-OE2	7.39	1.33	1.25
1	D	281	GLU	CD-OE2	7.38	1.33	1.25
1	C	67	GLU	CD-OE2	7.38	1.33	1.25
1	D	243	GLU	CD-OE2	7.37	1.33	1.25
1	D	296	GLU	CD-OE2	7.34	1.33	1.25
1	B	249	GLU	CD-OE2	7.33	1.33	1.25
1	A	980	GLU	CD-OE2	7.32	1.33	1.25
1	D	819	GLU	CD-OE2	7.30	1.33	1.25
1	B	40	GLU	CD-OE2	7.29	1.33	1.25
1	A	438	GLU	CD-OE2	7.28	1.33	1.25
1	B	980	GLU	CD-OE2	7.28	1.33	1.25
1	B	338	GLU	CD-OE2	7.19	1.33	1.25
1	C	241	GLU	CD-OE2	7.19	1.33	1.25
1	B	314	GLU	CD-OE2	7.18	1.33	1.25
1	C	264	GLU	CD-OE2	7.17	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	744	GLU	CD-OE2	7.16	1.33	1.25
1	A	689	GLU	CD-OE2	7.14	1.33	1.25
1	C	170	GLU	CD-OE2	7.12	1.33	1.25
1	A	684	GLU	CD-OE2	7.11	1.33	1.25
1	D	80	GLU	CD-OE2	7.10	1.33	1.25
1	C	198	GLU	CD-OE2	7.10	1.33	1.25
1	B	580	GLU	CD-OE2	7.08	1.33	1.25
1	D	241	GLU	CD-OE2	6.99	1.33	1.25
1	B	487	GLU	CD-OE2	6.94	1.33	1.25
1	D	684	GLU	CD-OE2	6.91	1.33	1.25
1	A	71	GLU	CD-OE2	6.90	1.33	1.25
1	D	136	GLU	CD-OE2	6.88	1.33	1.25
1	A	296	GLU	CD-OE2	6.85	1.33	1.25
1	D	277	GLU	CD-OE2	6.83	1.33	1.25
1	D	637	GLU	CD-OE2	6.83	1.33	1.25
1	C	326	GLU	CD-OE2	6.82	1.33	1.25
1	B	281	GLU	CD-OE2	6.78	1.33	1.25
1	D	338	GLU	CD-OE2	6.75	1.33	1.25
1	B	529	GLU	CD-OE2	6.74	1.33	1.25
1	D	724	GLU	CD-OE2	6.74	1.33	1.25
1	B	934	GLU	CD-OE2	6.72	1.33	1.25
1	D	71	GLU	CD-OE2	6.71	1.33	1.25
1	C	893	GLU	CD-OE2	6.71	1.33	1.25
1	A	943	GLU	CD-OE2	6.68	1.32	1.25
1	A	277	GLU	CD-OE2	6.61	1.32	1.25
1	C	529	GLU	CD-OE2	6.61	1.32	1.25
1	C	136	GLU	CD-OE2	6.58	1.32	1.25
1	C	969	GLU	CD-OE2	6.52	1.32	1.25
1	B	117	GLU	CD-OE2	6.51	1.32	1.25
1	C	277	GLU	CD-OE2	6.49	1.32	1.25
1	C	710	GLU	CD-OE2	6.47	1.32	1.25
1	C	979	GLU	CD-OE2	6.46	1.32	1.25
1	D	979	GLU	CD-OE2	6.46	1.32	1.25
1	A	136	GLU	CD-OE2	6.43	1.32	1.25
1	A	710	GLU	CD-OE2	6.43	1.32	1.25
1	A	744	GLU	CD-OE2	6.42	1.32	1.25
1	C	750	GLU	CD-OE2	6.40	1.32	1.25
1	A	117	GLU	CD-OE2	6.39	1.32	1.25
1	D	67	GLU	CD-OE2	6.39	1.32	1.25
1	D	334	GLU	CD-OE2	6.38	1.32	1.25
1	D	264	GLU	CD-OE2	6.37	1.32	1.25
1	B	243	GLU	CD-OE2	6.34	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	304	GLU	CD-OE2	6.34	1.32	1.25
1	C	117	GLU	CD-OE2	6.33	1.32	1.25
1	D	943	GLU	CD-OE2	6.30	1.32	1.25
1	B	710	GLU	CD-OE2	6.30	1.32	1.25
1	C	808	GLU	CD-OE2	6.28	1.32	1.25
1	D	710	GLU	CD-OE2	6.28	1.32	1.25
1	A	57	GLU	CD-OE1	-6.26	1.18	1.25
1	C	980	GLU	CD-OE2	6.25	1.32	1.25
1	D	117	GLU	CD-OE2	6.23	1.32	1.25
1	A	75	GLU	CD-OE2	6.22	1.32	1.25
1	A	797	GLU	CD-OE1	-6.22	1.18	1.25
1	C	681	GLU	CD-OE2	6.20	1.32	1.25
1	B	744	GLU	CD-OE2	6.20	1.32	1.25
1	D	750	GLU	CD-OE2	6.19	1.32	1.25
1	C	296	GLU	CD-OE2	6.19	1.32	1.25
1	A	667	GLU	CD-OE2	6.16	1.32	1.25
1	C	487	GLU	CD-OE2	6.16	1.32	1.25
1	A	369	GLU	CD-OE2	6.15	1.32	1.25
1	A	338	GLU	CD-OE2	6.14	1.32	1.25
1	B	416	GLU	CD-OE2	6.11	1.32	1.25
1	B	681	GLU	CD-OE2	6.11	1.32	1.25
1	D	667	GLU	CD-OE2	6.09	1.32	1.25
1	B	136	GLU	CD-OE2	6.09	1.32	1.25
1	B	75	GLU	CD-OE2	6.03	1.32	1.25
1	B	181	GLU	CD-OE2	6.03	1.32	1.25
1	B	893	GLU	CD-OE2	6.01	1.32	1.25
1	D	41	GLU	CD-OE2	6.01	1.32	1.25
1	A	131	GLU	CD-OE2	6.00	1.32	1.25
1	D	131	GLU	CD-OE2	6.00	1.32	1.25
1	B	277	GLU	CD-OE2	5.99	1.32	1.25
1	B	170	GLU	CD-OE2	5.99	1.32	1.25
1	B	241	GLU	CD-OE2	5.94	1.32	1.25
1	A	724	GLU	CD-OE2	5.91	1.32	1.25
1	B	243	GLU	CD-OE1	-5.89	1.19	1.25
1	B	969	GLU	CD-OE1	-5.88	1.19	1.25
1	D	461	GLU	CD-OE2	5.87	1.32	1.25
1	B	80	GLU	CD-OE2	5.86	1.32	1.25
1	D	808	GLU	CD-OE2	5.82	1.32	1.25
1	A	819	GLU	CD-OE2	5.80	1.32	1.25
1	A	505	ARG	CZ-NH2	5.80	1.40	1.33
1	C	416	GLU	CD-OE2	5.80	1.32	1.25
1	B	442	ARG	CZ-NH1	5.78	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	GLU	CD-OE2	5.77	1.31	1.25
1	A	412	GLU	CD-OE2	5.76	1.31	1.25
1	D	304	GLU	CD-OE2	5.75	1.31	1.25
1	B	369	GLU	CD-OE2	5.71	1.31	1.25
1	B	641	GLU	CD-OE1	-5.71	1.19	1.25
1	B	198	GLU	CD-OE2	5.68	1.31	1.25
1	C	230	ARG	NE-CZ	5.68	1.40	1.33
1	C	249	GLU	CD-OE2	5.66	1.31	1.25
1	A	264	GLU	CD-OE2	5.65	1.31	1.25
1	D	249	GLU	CD-OE2	5.63	1.31	1.25
1	D	181	GLU	CD-OE2	5.62	1.31	1.25
1	A	893	GLU	CD-OE2	5.62	1.31	1.25
1	C	580	GLU	CD-OE2	5.62	1.31	1.25
1	A	934	GLU	CD-OE2	5.61	1.31	1.25
1	B	264	GLU	CD-OE2	5.61	1.31	1.25
1	D	487	GLU	CD-OE2	5.61	1.31	1.25
1	C	461	GLU	CD-OE2	5.57	1.31	1.25
1	B	131	GLU	CD-OE2	5.57	1.31	1.25
1	B	969	GLU	CD-OE2	5.56	1.31	1.25
1	C	650	GLU	CD-OE2	5.49	1.31	1.25
1	C	508	GLU	CD-OE2	5.48	1.31	1.25
1	C	641	GLU	CD-OE1	-5.47	1.19	1.25
1	B	412	GLU	CD-OE2	5.42	1.31	1.25
1	B	904	GLU	CD-OE1	-5.41	1.19	1.25
1	D	508	GLU	CD-OE2	5.40	1.31	1.25
1	D	314	GLU	CD-OE2	5.38	1.31	1.25
1	A	41	GLU	CD-OE2	5.33	1.31	1.25
1	B	641	GLU	CD-OE2	5.31	1.31	1.25
1	C	314	GLU	CD-OE2	5.30	1.31	1.25
1	A	67	GLU	CD-OE2	5.26	1.31	1.25
1	C	482	ARG	CZ-NH1	5.25	1.39	1.33
1	D	619	GLU	CD-OE2	5.24	1.31	1.25
1	A	750	GLU	CD-OE2	5.22	1.31	1.25
1	D	980	GLU	CD-OE2	5.22	1.31	1.25
1	B	326	GLU	CD-OE2	5.20	1.31	1.25
1	A	808	GLU	CD-OE2	5.19	1.31	1.25
1	B	324	GLU	CD-OE1	-5.18	1.20	1.25
1	C	492	ASP	CG-OD2	5.17	1.37	1.25
1	D	425	ARG	NE-CZ	5.15	1.39	1.33
1	A	243	GLU	CD-OE1	-5.11	1.20	1.25
1	D	641	GLU	CD-OE2	5.08	1.31	1.25
1	A	17	GLU	CD-OE2	5.08	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	324	GLU	CD-OE1	-5.07	1.20	1.25
1	A	437	SER	CB-OG	-5.07	1.35	1.42
1	C	724	GLU	CD-OE2	5.06	1.31	1.25
1	B	57	GLU	CD-OE2	5.06	1.31	1.25
1	B	897	TRP	CD2-CE2	5.06	1.47	1.41
1	A	416	GLU	CD-OE2	5.04	1.31	1.25
1	B	781	ARG	CZ-NH2	5.03	1.39	1.33
1	A	310	ARG	CZ-NH2	5.02	1.39	1.33
1	A	641	GLU	CD-OE1	-5.01	1.20	1.25
1	B	67	GLU	CD-OE2	5.01	1.31	1.25
1	D	717	TRP	CD2-CE2	5.01	1.47	1.41

All (673) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	230	ARG	NE-CZ-NH1	33.80	137.20	120.30
1	C	630	ARG	NE-CZ-NH2	-20.87	109.87	120.30
1	C	721	ARG	NE-CZ-NH1	19.65	130.13	120.30
1	A	755	ARG	NE-CZ-NH1	17.36	128.98	120.30
1	A	431	ARG	NE-CZ-NH2	-16.56	112.02	120.30
1	C	442	ARG	NE-CZ-NH2	-16.22	112.19	120.30
1	C	630	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	A	755	ARG	NE-CZ-NH2	-14.84	112.88	120.30
1	C	230	ARG	CD-NE-CZ	14.15	143.41	123.60
1	A	233	ASP	CB-CG-OD1	14.14	131.03	118.30
1	B	46	ARG	NE-CZ-NH2	-13.96	113.32	120.30
1	C	230	ARG	NE-CZ-NH2	-13.72	113.44	120.30
1	B	442	ARG	NE-CZ-NH1	13.57	127.08	120.30
1	A	431	ARG	NE-CZ-NH1	13.34	126.97	120.30
1	A	233	ASP	CB-CG-OD2	-13.27	106.35	118.30
1	B	786	ARG	NE-CZ-NH2	-13.17	113.71	120.30
1	C	579	ASP	CB-CG-OD2	-13.13	106.48	118.30
1	B	425	ARG	NE-CZ-NH2	-12.95	113.82	120.30
1	A	800	ARG	NE-CZ-NH1	12.37	126.48	120.30
1	C	224	ASP	CB-CG-OD1	12.15	129.24	118.30
1	A	166	ARG	NE-CZ-NH2	-11.99	114.31	120.30
1	A	251	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	D	172	ASP	CB-CG-OD2	-11.72	107.75	118.30
1	B	46	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	C	809	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	C	832	ASP	CB-CG-OD1	11.61	128.75	118.30
1	C	832	ASP	CB-CG-OD2	-11.54	107.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	579	ASP	CB-CG-OD1	11.54	128.69	118.30
1	B	832	ASP	CB-CG-OD1	11.39	128.55	118.30
1	C	178	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	D	630	ARG	NE-CZ-NH1	11.27	125.93	120.30
1	D	13	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	B	832	ASP	CB-CG-OD2	-11.01	108.40	118.30
1	A	610	ASP	CB-CG-OD1	10.96	128.16	118.30
1	D	446	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	A	224	ASP	CB-CG-OD1	10.91	128.12	118.30
1	A	336	ARG	NE-CZ-NH1	10.67	125.64	120.30
1	D	446	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	D	183	ARG	NE-CZ-NH1	-10.59	115.00	120.30
1	A	599	ARG	NE-CZ-NH1	-10.43	115.09	120.30
1	B	853	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	B	233	ASP	CB-CG-OD1	10.14	127.43	118.30
1	C	996	ASP	CB-CG-OD2	-10.14	109.17	118.30
1	C	473	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	B	482	ARG	NE-CZ-NH1	10.09	125.35	120.30
1	D	233	ASP	CB-CG-OD1	10.00	127.30	118.30
1	B	442	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	D	832	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	A	411	ASP	CB-CG-OD2	-9.69	109.58	118.30
1	A	442	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	C	234	ASP	CB-CG-OD1	9.61	126.95	118.30
1	A	909	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	D	233	ASP	CB-CG-OD2	-9.57	109.69	118.30
1	D	429	ASP	CB-CG-OD2	-9.55	109.71	118.30
1	D	996	ASP	CB-CG-OD1	9.50	126.85	118.30
1	B	234	ASP	CB-CG-OD1	9.48	126.83	118.30
1	A	144	ASP	CB-CG-OD1	9.44	126.80	118.30
1	D	594	ASP	CB-CG-OD1	9.43	126.78	118.30
1	D	996	ASP	CB-CG-OD2	-9.38	109.86	118.30
1	D	659	ASP	CB-CG-OD1	9.32	126.69	118.30
1	C	659	ASP	CB-CG-OD1	9.31	126.68	118.30
1	B	13	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	B	336	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	C	43	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	D	429	ASP	CB-CG-OD1	9.24	126.62	118.30
1	C	199	ASP	CB-CG-OD1	9.21	126.59	118.30
1	D	45	ASP	CB-CG-OD1	9.21	126.59	118.30
1	B	952	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	C	961	ARG	NE-CZ-NH1	9.19	124.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	172	ASP	CB-CG-OD1	9.16	126.54	118.30
1	C	230	ARG	NH1-CZ-NH2	-9.16	109.33	119.40
1	A	26	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	A	172	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	A	356	ARG	NE-CZ-NH1	9.09	124.85	120.30
1	B	919	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	B	425	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	C	875	ASP	CB-CG-OD1	9.04	126.44	118.30
1	C	961	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	A	800	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	C	46	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	B	252	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	D	15	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	A	802	ASP	CB-CG-OD1	8.98	126.39	118.30
1	B	909	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	A	45	ASP	CB-CG-OD1	8.94	126.34	118.30
1	A	594	ASP	CB-CG-OD1	8.93	126.33	118.30
1	A	924	ASP	CB-CG-OD1	8.89	126.30	118.30
1	D	144	ASP	CB-CG-OD1	8.88	126.29	118.30
1	B	448	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	329	ASP	CB-CG-OD2	-8.85	110.34	118.30
1	B	648	ASP	CB-CG-OD2	-8.82	110.36	118.30
1	C	428	ASP	CB-CG-OD1	8.81	126.22	118.30
1	C	509	ASP	CB-CG-OD1	8.78	126.20	118.30
1	B	77	ASP	CB-CG-OD1	8.77	126.19	118.30
1	D	746	ASP	CB-CG-OD2	-8.76	110.42	118.30
1	A	610	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	699	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	96	ASP	CB-CG-OD1	8.68	126.11	118.30
1	A	411	ASP	CB-CG-OD1	8.67	126.10	118.30
1	D	507	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	C	786	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	A	46	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	C	233	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	C	13	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	D	368	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	B	352	ARG	NE-CZ-NH2	-8.59	116.00	120.30
1	A	632	SER	N-CA-CB	8.59	123.38	110.50
1	C	178	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	B	746	ASP	CB-CG-OD2	-8.56	110.60	118.30
1	B	233	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	C	234	ASP	CB-CG-OD2	-8.54	110.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	507	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	C	473	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	D	869	ASP	CB-CG-OD1	8.51	125.96	118.30
1	D	224	ASP	CB-CG-OD1	8.51	125.96	118.30
1	B	388	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	C	859	ASP	CB-CG-OD1	8.46	125.91	118.30
1	A	917	ARG	NE-CZ-NH1	-8.46	116.07	120.30
1	C	721	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	D	755	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	C	869	ASP	CB-CG-OD1	8.38	125.84	118.30
1	D	425	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	B	539[A]	ALA	CB-CA-C	-8.35	97.57	110.10
1	B	539[B]	ALA	CB-CA-C	-8.35	97.57	110.10
1	A	559	TYR	CB-CG-CD2	-8.33	116.00	121.00
1	C	659	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	B	802	ASP	CB-CG-OD1	8.33	125.80	118.30
1	A	509	ASP	CB-CG-OD1	8.31	125.78	118.30
1	D	172	ASP	CB-CG-OD1	8.27	125.74	118.30
1	A	832	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	D	439	ARG	NE-CZ-NH2	-8.25	116.18	120.30
1	B	77	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	B	492	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	234	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	D	166	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	B	368	ASP	CB-CG-OD2	-8.17	110.95	118.30
1	A	816	TYR	CB-CG-CD1	-8.16	116.10	121.00
1	D	909	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	428	ASP	CB-CG-OD1	8.16	125.65	118.30
1	A	924	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	D	193	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	A	572	ASP	CB-CG-OD1	8.14	125.63	118.30
1	D	403	ASP	CB-CG-OD1	8.14	125.62	118.30
1	D	909	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	B	572	ASP	CB-CG-OD1	8.07	125.56	118.30
1	C	233	ASP	CB-CG-OD1	8.06	125.55	118.30
1	D	916	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	329	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	B	594	ASP	CB-CG-OD1	8.01	125.51	118.30
1	D	809	ARG	CD-NE-CZ	7.99	134.79	123.60
1	B	183	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	B	411	ASP	CB-CG-OD2	-7.98	111.11	118.30
1	C	853	ARG	NE-CZ-NH2	-7.96	116.32	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	469	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	B	875	ASP	CB-CG-OD1	7.95	125.46	118.30
1	A	954	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	C	908	ASP	CB-CG-OD1	7.93	125.44	118.30
1	D	193	ASP	CB-CG-OD1	7.93	125.44	118.30
1	D	578	TYR	CB-CG-CD2	-7.93	116.24	121.00
1	B	611	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	D	859	ASP	CB-CG-OD1	7.89	125.40	118.30
1	D	319	ASP	CB-CG-OD1	7.86	125.37	118.30
1	A	909	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	C	594	ASP	CB-CG-OD1	7.83	125.34	118.30
1	A	973	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	B	172	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	961	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	C	630	ARG	CD-NE-CZ	7.75	134.45	123.60
1	C	996	ASP	CB-CG-OD1	7.74	125.26	118.30
1	C	610	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	178	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	C	431	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	329	ASP	CB-CG-OD1	7.70	125.23	118.30
1	D	428	ASP	CB-CG-OD1	7.69	125.22	118.30
1	B	746	ASP	CB-CG-OD1	7.68	125.21	118.30
1	B	671	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	671	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	C	319	ASP	CB-CG-OD2	-7.63	111.44	118.30
1	A	946	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	D	924	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	B	285	TYR	CB-CG-CD2	-7.62	116.43	121.00
1	D	579	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	431	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	329	ASP	CB-CG-OD1	7.60	125.14	118.30
1	B	439	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	B	659	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	B	908	ASP	CB-CG-OD1	7.57	125.11	118.30
1	D	942	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	D	492	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	A	442	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	C	13	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	D	559	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	D	578	TYR	CB-CG-CD1	7.51	125.51	121.00
1	B	853	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	C	255	ARG	NE-CZ-NH1	7.48	124.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	659	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	D	411	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	A	439	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	D	469	ASP	CB-CG-OD1	7.45	125.01	118.30
1	A	559	TYR	CG-CD2-CE2	-7.44	115.35	121.30
1	A	425	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	746	ASP	CB-CG-OD2	-7.43	111.61	118.30
1	C	492	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	A	659	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	D	539[A]	ALA	CB-CA-C	-7.40	99.00	110.10
1	D	539[B]	ALA	CB-CA-C	-7.40	99.00	110.10
1	D	980	GLU	C-N-CA	-7.40	106.77	122.30
1	C	183	ARG	NE-CZ-NH1	7.39	123.99	120.30
1	D	431	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	A	116	THR	CA-CB-CG2	-7.39	102.06	112.40
1	C	507	ASP	CB-CG-OD1	7.36	124.92	118.30
1	B	473	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	D	482	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	A	428	ASP	CB-CG-OD1	7.34	124.90	118.30
1	A	859	ASP	CB-CG-OD2	-7.34	111.70	118.30
1	B	594	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	C	917	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	D	15	ASP	CB-CG-OD1	7.33	124.89	118.30
1	D	329	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	C	733	ALA	N-CA-CB	7.29	120.31	110.10
1	D	509	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	287	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	C	183	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	C	368	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	D	116	THR	CA-CB-CG2	-7.23	102.28	112.40
1	B	319	ASP	CB-CG-OD1	7.23	124.80	118.30
1	A	869	ASP	CB-CG-OD1	7.22	124.80	118.30
1	D	987	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	448	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	234	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	539[A]	ALA	CB-CA-C	-7.19	99.32	110.10
1	A	539[B]	ALA	CB-CA-C	-7.19	99.32	110.10
1	A	292	ARG	NE-CZ-NH2	-7.19	116.71	120.30
1	C	733	ALA	CB-CA-C	7.18	120.88	110.10
1	A	130	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	869	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	392	TYR	CG-CD1-CE1	-7.16	115.58	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	157	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	224	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	B	43	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	D	77	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	832	ASP	CB-CG-OD1	7.12	124.70	118.30
1	B	611	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	234	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	76	CYS	CA-CB-SG	-7.10	101.22	114.00
1	D	859	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	368	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	802	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	C	539[A]	ALA	CB-CA-C	-7.07	99.50	110.10
1	C	539[B]	ALA	CB-CA-C	-7.07	99.50	110.10
1	D	356	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	C	439	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	610	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	828	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	952	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	D	579	ASP	CB-CG-OD1	7.01	124.61	118.30
1	D	845	GLN	C-N-CA	-7.01	107.58	122.30
1	D	924	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	772	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	C	425	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	531	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	D	352	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	14	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	699	ARG	NE-CZ-NH2	6.95	123.77	120.30
1	C	859	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	D	319	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	772	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	954	ASP	CB-CG-OD1	6.91	124.52	118.30
1	D	632	SER	N-CA-CB	6.89	120.84	110.50
1	B	869	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	610	ASP	CB-CG-OD1	6.89	124.50	118.30
1	C	958	ASN	N-CA-CB	6.89	122.99	110.60
1	B	319	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	D	287	ASP	CB-CG-OD1	6.87	124.48	118.30
1	B	572	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	579	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	D	561	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	572	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	C	85	VAL	CA-CB-CG2	-6.83	100.66	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	916	ASP	CB-CG-OD1	6.82	124.43	118.30
1	C	438	GLU	CG-CD-OE2	-6.82	104.67	118.30
1	D	252	ASP	CB-CG-OD1	6.82	124.43	118.30
1	A	987	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	368	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	771	GLY	N-CA-C	-6.78	96.14	113.10
1	C	987	ASP	CB-CG-OD1	6.77	124.39	118.30
1	B	569	ASP	CB-CG-OD1	6.76	124.39	118.30
1	A	721	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	1018	LEU	CB-CA-C	-6.76	97.36	110.20
1	C	594	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	C	802	ASP	CB-CG-OD1	6.74	124.36	118.30
1	D	368	ASP	CB-CG-OD1	6.74	124.36	118.30
1	A	507	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	A	987	ASP	CB-CG-OD1	6.72	124.35	118.30
1	D	411	ASP	CB-CG-OD1	6.72	124.35	118.30
1	C	136	GLU	CB-CA-C	-6.71	96.98	110.40
1	B	561	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	C	144	ASP	CB-CG-OD1	6.71	124.34	118.30
1	D	287	ASP	CB-CG-OD2	-6.71	112.27	118.30
1	D	781	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	952	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	A	356	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	D	507	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	356	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	B	599	ARG	NE-CZ-NH2	6.65	123.62	120.30
1	C	809	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	C	916	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	288	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	C	659	ASP	CB-CA-C	6.63	123.66	110.40
1	D	130	ASP	CB-CG-OD1	6.63	124.27	118.30
1	C	44	THR	CA-CB-CG2	-6.63	103.12	112.40
1	D	952	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	D	919	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	809	ARG	NE-CZ-NH1	6.61	123.60	120.30
1	B	519	SER	N-CA-CB	-6.60	100.59	110.50
1	B	140	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	772	ASP	CB-CG-OD1	6.59	124.24	118.30
1	A	144	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	B	507	ASP	CB-CG-OD1	6.56	124.20	118.30
1	D	144	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	A	579	ASP	CB-CG-OD2	-6.54	112.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	224	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	B	15	ASP	CB-CG-OD2	-6.53	112.43	118.30
1	B	919	ASP	CB-CG-OD1	6.53	124.17	118.30
1	A	95	TYR	CG-CD2-CE2	-6.52	116.08	121.30
1	B	310	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	C	507	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	D	403	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	82	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	917	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	C	329	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	D	832	ASP	CB-CG-OD1	6.47	124.13	118.30
1	A	540[A]	HIS	N-CA-CB	-6.47	98.95	110.60
1	A	540[B]	HIS	N-CA-CB	-6.47	98.95	110.60
1	C	748	CYS	CA-CB-SG	-6.47	102.35	114.00
1	B	987	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	916	ASP	CB-CG-OD1	6.47	124.12	118.30
1	B	952	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	859	ASP	CB-CG-OD1	6.46	124.12	118.30
1	B	211	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	1019	VAL	CA-CB-CG2	-6.45	101.22	110.90
1	D	746	ASP	CB-CG-OD1	6.45	124.10	118.30
1	A	477	SER	N-CA-CB	6.43	120.14	110.50
1	C	280	ASP	CB-CG-OD1	6.43	124.09	118.30
1	D	800	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	B	828	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	492	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	755	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	D	329	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	952	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	D	479	ASP	CB-CG-OD1	6.38	124.05	118.30
1	B	287	ASP	CB-CG-OD1	6.38	124.04	118.30
1	D	255	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	280	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	14	ARG	N-CA-CB	6.35	122.04	110.60
1	B	557	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	996	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	B	659	ASP	CB-CG-OD1	6.33	123.99	118.30
1	B	786	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	842	TRP	CH2-CZ2-CE2	-6.32	111.08	117.40
1	D	1018	LEU	CB-CA-C	-6.32	98.20	110.20
1	B	144	ASP	CB-CG-OD1	6.32	123.98	118.30
1	C	924	ASP	CB-CG-OD1	6.31	123.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	338	GLU	CG-CD-OE2	-6.29	105.72	118.30
1	D	845	GLN	CB-CA-C	-6.27	97.85	110.40
1	D	267	VAL	CG1-CB-CG2	-6.26	100.88	110.90
1	D	802	ASP	CB-CG-OD1	6.26	123.93	118.30
1	D	625	GLN	CG-CD-OE1	-6.25	109.09	121.60
1	A	319	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	D	439	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	A	1021	CYS	CA-CB-SG	-6.25	102.75	114.00
1	C	799	THR	CA-CB-CG2	-6.24	103.66	112.40
1	C	610	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	D	252	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	D	919	ASP	CB-CG-OD1	6.23	123.91	118.30
1	B	958	ASN	N-CA-CB	6.22	121.81	110.60
1	D	973	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	C	404	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	B	438	GLU	CG-CD-OE2	-6.20	105.91	118.30
1	A	968	MET	CA-CB-CG	6.19	123.82	113.30
1	B	224	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	519	SER	N-CA-CB	-6.18	101.23	110.50
1	C	559	TYR	CD1-CE1-CZ	-6.18	114.24	119.80
1	D	770	ILE	N-CA-C	-6.18	94.33	111.00
1	B	429	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	625	GLN	CG-CD-OE1	-6.16	109.28	121.60
1	D	719	GLN	CB-CA-C	-6.16	98.08	110.40
1	D	809	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	469	ASP	CB-CG-OD1	6.16	123.84	118.30
1	B	482	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	792	ASP	CB-CG-OD1	6.15	123.84	118.30
1	C	280	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	859	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	D	448	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	747	PHE	CB-CG-CD2	6.12	125.09	120.80
1	B	247	CYS	CA-CB-SG	-6.11	103.00	114.00
1	D	492	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	568	TRP	CA-CB-CG	-6.11	102.09	113.70
1	B	855	THR	N-CA-CB	6.10	121.88	110.30
1	C	469	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	234	ASP	CB-CG-OD1	6.09	123.78	118.30
1	C	829	THR	CA-CB-CG2	-6.09	103.88	112.40
1	C	857	ARG	NE-CZ-NH1	-6.09	117.26	120.30
1	D	681	GLU	CB-CA-C	6.09	122.57	110.40
1	D	130	ASP	CB-CG-OD2	-6.08	112.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	442	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	292	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	D	594	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	B	859	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	828	ASP	CB-CG-OD1	6.05	123.74	118.30
1	C	404	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	792	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	388	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	B	439	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	832	ASP	N-CA-CB	-6.03	99.75	110.60
1	D	572	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	D	416	GLU	CG-CD-OE1	6.03	130.36	118.30
1	C	310	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	509	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	C	439	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	255	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	D	324	GLU	N-CA-CB	6.01	121.42	110.60
1	A	288	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	164	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	49	GLN	CB-CG-CD	6.00	127.20	111.60
1	D	588	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	D	472	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	C	411	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	D	746	ASP	CB-CA-C	-5.95	98.49	110.40
1	A	285	TYR	CD1-CE1-CZ	-5.95	114.45	119.80
1	B	917	ARG	CD-NE-CZ	-5.94	115.28	123.60
1	C	252	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	A	997	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	C	917	ARG	CD-NE-CZ	-5.93	115.30	123.60
1	C	572	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	13	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	B	237	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	179	ALA	N-CA-CB	5.89	118.35	110.10
1	B	157	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	B	157	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	D	85	VAL	CA-CB-CG2	-5.88	102.08	110.90
1	C	494	THR	CA-CB-CG2	-5.87	104.19	112.40
1	A	252	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	D	442	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	875	ASP	CB-CG-OD1	5.85	123.56	118.30
1	C	239	VAL	CA-CB-CG2	-5.83	102.15	110.90
1	A	237	ARG	NE-CZ-NH1	5.83	123.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	310	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	916	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	45	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	37	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	598	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	857	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	D	251	ARG	CG-CD-NE	-5.81	99.60	111.80
1	C	319	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	572	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	721	ARG	CD-NE-CZ	5.80	131.72	123.60
1	C	648	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	991	MET	CG-SD-CE	5.80	109.48	100.20
1	B	579	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	1014	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	B	997	ASP	N-CA-CB	5.77	120.99	110.60
1	B	52	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	829	THR	CA-CB-CG2	-5.76	104.33	112.40
1	B	105	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	D	482	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	746	ASP	CB-CA-C	-5.76	98.89	110.40
1	C	199	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	288	ARG	NH1-CZ-NH2	5.74	125.71	119.40
1	B	819	GLU	CB-CA-C	5.74	121.88	110.40
1	D	253	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	A	13	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	14	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	D	958	ASN	N-CA-CB	5.73	120.91	110.60
1	A	746	ASP	CB-CG-OD1	5.73	123.45	118.30
1	D	395	HIS	N-CA-CB	-5.72	100.30	110.60
1	B	721	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	845	GLN	C-N-CA	-5.72	110.29	122.30
1	D	96	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	748	CYS	CA-CB-SG	-5.71	103.72	114.00
1	B	996	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	569	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	164	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	C	750	GLU	N-CA-CB	5.68	120.82	110.60
1	D	255	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	319	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	746	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	B	26	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	D	610	ASP	CB-CG-OD1	5.66	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	B	172	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	C	164	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	D	908	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	A	772	ASP	CB-CG-OD1	5.65	123.39	118.30
1	C	482	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	648	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	691	ALA	CB-CA-C	-5.64	101.64	110.10
1	D	178	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	246	MET	CG-SD-CE	-5.61	91.22	100.20
1	C	856	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	B	559	TYR	CD1-CE1-CZ	-5.59	114.76	119.80
1	C	919	ASP	CB-CG-OD1	5.58	123.33	118.30
1	A	559	TYR	CD1-CE1-CZ	-5.58	114.78	119.80
1	B	469	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	843	GLN	O-C-N	5.57	131.62	122.70
1	A	1000	SER	N-CA-CB	5.57	118.86	110.50
1	C	157	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	648	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	559	TYR	CG-CD2-CE2	-5.57	116.85	121.30
1	C	438	GLU	CG-CD-OE1	5.56	129.43	118.30
1	C	497	ASP	CB-CG-OD1	5.56	123.30	118.30
1	C	557	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	800	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	372	MET	CG-SD-CE	5.54	109.06	100.20
1	A	996	ASP	CB-CG-OD1	5.53	123.28	118.30
1	C	130	ASP	CB-CG-OD1	5.53	123.27	118.30
1	A	95	TYR	CD1-CE1-CZ	-5.52	114.83	119.80
1	B	553	TRP	CA-CB-CG	-5.51	103.22	113.70
1	D	140	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	D	280	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	699	ARG	CD-NE-CZ	5.51	131.31	123.60
1	C	924	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	689	GLU	C-N-CA	5.49	135.43	121.70
1	A	671	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	288	ARG	CG-CD-NE	-5.48	100.28	111.80
1	A	746	ASP	CB-CA-C	-5.48	99.44	110.40
1	D	682	LEU	CB-CA-C	-5.48	99.79	110.20
1	A	503	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	C	839	ALA	N-CA-CB	5.48	117.77	110.10
1	D	469	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	D	591	ASP	CB-CG-OD1	5.47	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	249	GLU	OE1-CD-OE2	5.46	129.86	123.30
1	C	699	ARG	CD-NE-CZ	-5.46	115.96	123.60
1	A	719	GLN	CB-CA-C	-5.46	99.49	110.40
1	C	569	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	251	ARG	CD-NE-CZ	5.45	131.23	123.60
1	C	59	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	379	MET	CG-SD-CE	5.43	108.89	100.20
1	C	429	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	C	828	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	367	MET	CG-SD-CE	5.41	108.86	100.20
1	C	741	THR	CA-CB-CG2	-5.41	104.82	112.40
1	D	760	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	C	719	GLN	CB-CA-C	-5.40	99.59	110.40
1	D	878	HIS	CA-CB-CG	-5.40	104.41	113.60
1	C	909	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	86	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	D	538	TYR	CB-CG-CD2	5.40	124.24	121.00
1	D	850	PHE	CB-CA-C	-5.40	99.61	110.40
1	C	790	ASP	CB-CG-OD1	5.39	123.15	118.30
1	A	768	MET	CG-SD-CE	5.39	108.82	100.20
1	D	916	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	A	96	ASP	N-CA-CB	5.38	120.28	110.60
1	B	819	GLU	N-CA-CB	-5.37	100.93	110.60
1	B	96	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	A	388	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	C	942	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	553	TRP	CA-CB-CG	-5.34	103.55	113.70
1	C	752	GLY	O-C-N	5.34	131.25	122.70
1	A	507	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	687	GLN	N-CA-CB	5.34	120.21	110.60
1	C	240	LEU	CA-CB-CG	-5.34	103.02	115.30
1	C	388	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	842	TRP	CH2-CZ2-CE2	-5.34	112.06	117.40
1	A	247	CYS	CA-CB-SG	-5.34	104.39	114.00
1	B	523	TRP	CG-CD2-CE3	-5.33	129.10	133.90
1	C	100	TYR	CG-CD2-CE2	-5.33	117.03	121.30
1	A	800	ARG	CD-NE-CZ	5.32	131.05	123.60
1	B	82	ASP	CB-CG-OD1	5.32	123.09	118.30
1	C	77	ASP	CB-CG-OD1	5.32	123.09	118.30
1	B	1016	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	C	184	LEU	CB-CA-C	-5.31	100.10	110.20
1	C	285	TYR	CB-CG-CD2	-5.31	117.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	404	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	D	781	ARG	CD-NE-CZ	5.30	131.02	123.60
1	C	126	THR	CA-CB-CG2	-5.30	104.98	112.40
1	C	26	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	D	926	TYR	CB-CG-CD1	5.29	124.18	121.00
1	B	477	SER	N-CA-CB	-5.29	102.56	110.50
1	A	961	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	52	ARG	CB-CA-C	-5.29	99.82	110.40
1	D	46	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	D	164	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	249	GLU	CG-CD-OE2	-5.28	107.75	118.30
1	D	917	ARG	NE-CZ-NH2	-5.27	117.66	120.30
1	D	809	ARG	CG-CD-NE	-5.27	100.73	111.80
1	C	857	ARG	CD-NE-CZ	-5.27	116.23	123.60
1	A	439	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	802	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	594	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	A	252	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	690	SER	N-CA-CB	-5.24	102.64	110.50
1	A	185	ALA	N-CA-CB	5.24	117.44	110.10
1	A	1000	SER	CA-CB-OG	-5.24	97.05	111.20
1	C	973	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	136	GLU	N-CA-CB	-5.24	101.17	110.60
1	B	288	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	857	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	B	82	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	A	164	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	832	ASP	N-CA-CB	-5.21	101.22	110.60
1	A	908	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	77	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	671	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	1000	SER	N-CA-CB	5.20	118.30	110.50
1	C	633	GLY	C-N-CA	5.20	134.69	121.70
1	C	856	TYR	CG-CD2-CE2	-5.20	117.14	121.30
1	C	553	TRP	CA-CB-CG	-5.18	103.85	113.70
1	C	875	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	B	969	GLU	CA-CB-CG	-5.17	102.02	113.40
1	B	524	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	A	140	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	C	968	MET	CG-SD-CE	-5.17	91.94	100.20
1	A	569	ASP	CB-CG-OD1	5.16	122.95	118.30
1	C	519	SER	N-CA-CB	-5.16	102.77	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	822	LEU	CB-CG-CD2	-5.16	102.24	111.00
1	C	997	ASP	N-CA-CB	5.15	119.86	110.60
1	C	919	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	599	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	144	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	C	538	TYR	CB-CG-CD1	-5.14	117.92	121.00
1	B	164	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	358	GLU	CG-CD-OE2	-5.12	108.06	118.30
1	C	161	TYR	N-CA-CB	-5.12	101.38	110.60
1	D	817	GLN	CB-CG-CD	-5.12	98.29	111.60
1	B	193	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	746	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	855	THR	N-CA-CB	5.11	120.00	110.30
1	A	403	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	568	TRP	CA-CB-CG	-5.10	104.01	113.70
1	D	961	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	C	721	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	B	699	ARG	CB-CG-CD	5.09	124.84	111.60
1	C	651	LEU	N-CA-CB	5.09	120.58	110.40
1	A	630	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	479	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	280	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	375	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	557	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	210	ARG	N-CA-CB	5.08	119.74	110.60
1	C	917	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	210	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	559	TYR	CB-CG-CD1	5.07	124.05	121.00
1	C	40	GLU	CG-CD-OE1	5.07	128.44	118.30
1	C	181	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	D	840	HIS	CB-CA-C	-5.07	100.27	110.40
1	A	428	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	A	648	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	D	37	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	755	ARG	CD-NE-CZ	5.05	130.68	123.60
1	B	163	GLN	N-CA-CB	5.05	119.70	110.60
1	B	1013	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	C	518	TRP	CE3-CZ3-CH2	-5.05	115.64	121.20
1	C	531	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	D	778	THR	CA-CB-CG2	-5.05	105.33	112.40
1	B	778	THR	CA-CB-CG2	-5.04	105.34	112.40
1	B	546	LEU	N-CA-CB	5.04	120.48	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	375	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	403	ASP	CB-CG-OD1	5.04	122.84	118.30
1	D	634	GLN	N-CA-CB	5.04	119.67	110.60
1	A	277	GLU	CG-CD-OE1	5.03	128.36	118.30
1	C	842	TRP	CB-CA-C	-5.03	100.34	110.40
1	C	287	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	A	40	GLU	CG-CD-OE1	5.03	128.36	118.30
1	C	43	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	C	819	GLU	N-CA-CB	-5.03	101.55	110.60
1	D	954	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	201	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	D	997	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	D	699	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	C	411	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	392	TYR	CD1-CG-CD2	5.01	123.41	117.90
1	C	894	ARG	CB-CA-C	-5.00	100.39	110.40

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	104	0
1	B	8128	0	7712	89	0
1	C	8128	0	7712	93	0
1	D	8128	0	7712	120	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
4	D	4	0	0	0	0
5	A	108	0	162	17	0
5	B	108	0	162	14	0
5	C	112	0	168	14	0
5	D	108	0	162	19	0
6	A	1112	0	0	16	3
6	B	1128	0	0	15	0
6	C	1104	0	0	16	3
6	D	1118	0	0	27	0
All	All	37524	0	31553	427	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 7.

All (427) 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: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:B:655:MET:HE2	1:B:665:SER:HB3	1.42	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:A:699:ARG:HG3	1:A:699:ARG:HH11	1.36	0.91
1:A:655:MET:HE2	1:A:656:VAL:N	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:268:ALA:HA	5:A:8602:DMS:H22	1.59	0.84
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: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:A:290:THR:HB	5:A:8412:DMS:C2	2.12	0.80
1:C:530:THR:HG22	6:D:8752:HOH:O	1.82	0.80
1:D:131:GLU:OE2	1:D:135:GLN:HG3	1.83	0.79
1:A:797:GLU:O	1:A:801:ILE:HD13	1.83	0.78
1:A:685:LEU:HD12	1:A:686:PRO:CD	2.14	0.78
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.48	0.77
1:D:134:LEU:HA	5:D:8705:DMS:H22	1.65	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: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:C:748:CYS:C	1:C:749:ILE:HD12	2.06	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
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
5:D:8417:DMS:H12	6:D:9774:HOH:O	1.87	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:773:LYS:HD2	1:D:774:LYS:O	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:LEU:O	5:D:8705:DMS:H21	1.90	0.72
1:B:845:GLN:OE1	1:B:845:GLN:HA	1.89	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: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:A:290:THR:HB	5:A:8412:DMS:H22	1.74	0.70
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.07	0.70
1:D:581:ASN:HD22	1:D:583:ASN:HD22	1.40	0.69
1:D:292:ARG:HH12	5:D:8412:DMS:H22	1.58	0.69
1:C:367:MET:HE1	6:C:9644:HOH:O	1.92	0.68
1:D:887:GLN:NE2	1:D:980:GLU:O	2.25	0.68
5:B:8411:DMS:H21	6:B:9633:HOH:O	1.94	0.68
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.20	0.68
5:D:8416:DMS:H22	6:D:9410:HOH:O	1.93	0.68
1:A:233:ASP:HA	5:A:8417:DMS:C1	2.24	0.68
1:B:730:LEU:H	1:B:730:LEU:CD1	1.99	0.68
1:B:655:MET:HE2	1:B:665:SER:CB	2.21	0.67
5:A:8420:DMS:H21	6:D:9524:HOH:O	1.94	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:134:LEU:HA	5:D:8705:DMS:C2	2.25	0.66
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:A:634:GLN:HA	1:A:634:GLN:NE2	2.06	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
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:878:HIS:HD2	6:A:8674:HOH:O	1.79	0.66
1:A:655:MET:HE2	1:A:656:VAL:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:646:HIS:ND1	6:A:9438:HOH:O	2.22	0.65
1:A:290:THR:HB	5:A:8412:DMS:H21	1.79	0.64
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: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:C:356:ARG:HD2	1:C:379:MET:HE1	1.79	0.64
1:C:687:GLN:HE21	1:C:687:GLN:HA	1.61	0.64
1:D:878:HIS:HD2	6:D:8825:HOH:O	1.80	0.63
1:D:595:THR:HA	1:D:596:PRO:C	2.17	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:B:75:GLU:HA	1:B:75:GLU:OE1	2.00	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:D:372:MET:HE1	1:D:395:HIS:HB3	1.82	0.61
1:A:84:VAL:HB	5:A:8414:DMS:O	2.01	0.61
1:A:277:GLU:H	1:A:277:GLU:CD	2.03	0.61
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: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:800:ARG:HG2	6:A:9380:HOH:O	2.02	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H21	6:C:9067:HOH:O	2.03	0.59
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.85	0.59
5:D:8409:DMS:O	6:D:9258:HOH:O	2.16	0.59
1:B:178:ARG:HG3	1:B:178:ARG:O	2.03	0.58
1:D:363:HIS:HD2	6:D:9334:HOH:O	1.86	0.58
1:B:600:GLN:HE21	1:B:600:GLN:N	1.97	0.58
1:B:824:GLN:HG2	1:B:825:CYS:N	2.18	0.58
5:C:8406:DMS:H13	6:C:9698:HOH:O	2.03	0.58
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.11	0.58
1:A:233:ASP:HA	5:A:8417:DMS:H12	1.86	0.58
1:A:737:ILE:C	1:A:737:ILE:HD13	2.24	0.58
1:D:847:LYS:HG3	1:D:848:THR:N	2.19	0.58
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
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.38	0.57
1:D:230:ARG:HD3	6:D:9706:HOH:O	2.02	0.57
1:B:236:SER:C	1:B:237:ARG:HG2	2.25	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
5:D:8427:DMS:H12	6:D:9169:HOH:O	2.05	0.56
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.85	0.56
5:D:8406:DMS:H21	6:D:9684:HOH:O	2.05	0.56
1:A:655:MET:CB	1:A:699:ARG:HH22	2.17	0.56
1:A:241:GLU:CD	1:A:292:ARG:HE	2.08	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:B:651:LEU:HD23	1:B:651:LEU:C	2.25	0.55
1:A:245:GLN:CD	1:A:288:ARG:HE	2.10	0.55
1:C:595:THR:HA	1:C:596:PRO:C	2.26	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:A:595:THR:HA	1:A:596:PRO:C	2.27	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:C:240:LEU:C	1:C:240:LEU:HD23	2.28	0.54
1:B:890:GLN:HB3	6:B:9568:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:MET:CE	1:C:662:PRO:HB3	2.38	0.54
1:A:94:GLY:HA3	5:A:8421:DMS:H23	1.90	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:B:699:ARG:HH21	5:B:8415:DMS:C1	2.20	0.54
1:A:699:ARG:HG3	1:A:699:ARG:NH1	2.13	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:C:367:MET:HE3	1:C:367:MET:HA	1.90	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
1:A:288:ARG:NH1	6:A:9036:HOH:O	2.28	0.53
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:D:240:LEU:HD23	1:D:240:LEU:C	2.29	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:B:595:THR:HA	1:B:596:PRO:C	2.30	0.52
1:D:754:LYS:C	1:D:755:ARG:HG2	2.30	0.52
1:D:618:THR:HG21	6:D:9065:HOH:O	2.09	0.52
1:A:735:HIS:O	1:A:736:ALA:HB2	2.10	0.51
1:D:651:LEU:HD12	1:D:701:VAL:HB	1.92	0.51
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.28	0.51
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:ILE:HD13	1:A:737:ILE:O	2.11	0.51
1:B:133:TRP:CD1	5:B:8504:DMS:C1	2.94	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: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: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
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.92	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:367:MET:HB3	1:D:372:MET:HE2	1.94	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
5:B:8417:DMS:H23	6:D:9785:HOH:O	2.12	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:D:250:LEU:O	5:D:8416:DMS:H21	2.12	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: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
5:C:8506:DMS:H21	6:C:9496:HOH:O	2.12	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:C:829:THR:HG22	1:C:830:LEU:N	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.48	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: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:A:768:MET:HE3	1:A:1020:TRP:CZ2	2.48	0.48
1:D:135:GLN:C	1:D:136:GLU:HG2	2.34	0.48
1:D:737:ILE:HD12	1:D:832:ASP:HA	1.95	0.48
5:D:8427:DMS:H11	6:D:8960:HOH:O	2.14	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
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:251:ARG:HH11	5:A:8416:DMS:C2	2.27	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:251:ARG:HA	5:D:8416:DMS:H22	1.95	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:847:LYS:HE2	1:B:875:ASP:OD1	2.15	0.47
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.98	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: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: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: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: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:804:ASN:ND2	1:D:809:ARG:CZ	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:88:SER:HA	1:D:366:VAL:HG21	1.98	0.46
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.98	0.46
1:B:13:ARG:O	1:B:14:ARG:C	2.55	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:B:699:ARG:NH2	5:B:8415:DMS:C1	2.79	0.45
1:B:781:ARG:HD3	6:B:9687:HOH:O	2.16	0.45
1:B:890:GLN:CG	1:B:891:VAL:N	2.73	0.45
1:C:13:ARG:O	1:C:14:ARG:C	2.54	0.45
1:C:952:ARG:NH2	1:C:1021:CYS:SG	2.88	0.45
1:D:367:MET:HB3	1:D:372:MET:CE	2.46	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
1:A:655:MET:HE3	1:A:665:SER:HB3	1.97	0.45
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.99	0.45
1:D:962:TYR:CE1	5:D:8508:DMS:H12	2.52	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
6:B:9393:HOH:O	5:C:8420:DMS:H21	2.17	0.44
5:B:8421:DMS:H22	6:B:9134:HOH:O	2.16	0.44
1:C:266:GLN:NE2	5:C:8602:DMS:S	2.91	0.44
1:C:1000:SER:O	1:C:1001:PRO:C	2.56	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:C:233:ASP:HA	5:C:8417:DMS:S	2.57	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:A:8419:DMS:H23	6:A:9367:HOH:O	2.18	0.44
1:C:684:GLU:HG2	1:C:685:LEU:N	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PRO:O	6:B:9658:HOH:O	2.21	0.43
1:D:130:ASP:OD2	5:D:8703:DMS:H22	2.19	0.43
1:D:688:PRO:C	1:D:690:SER:H	2.21	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: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:C:749:ILE:N	1:C:749:ILE:CD1	2.82	0.43
1:C:768:MET:HB2	1:C:768:MET:HE3	1.80	0.43
1:C:844:HIS:HD2	6:C:9477:HOH:O	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:132:SER:HB2	5:C:8504:DMS:H11	2.01	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:D:893:GLU:O	1:D:893:GLU:HG3	2.19	0.42
1:A:866:ILE:O	1:A:1017:GLN:HG2	2.19	0.42
1:A:233:ASP:HA	5:A:8417:DMS:H13	1.96	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
1:D:768:MET:HE2	1:D:1020:TRP:CZ2	2.54	0.42
1:C:595:THR:HG23	1:C:595:THR:O	2.19	0.42
1:A:753:ASN:HB2	1:A:771:GLY:HA2	2.02	0.42
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.34	0.42
1:D:1022:GLN:HE21	1:D:1022:GLN:C	2.23	0.42
1:A:986:ILE:HG23	1:A:986:ILE:HD13	1.77	0.42
1:B:133:TRP:CD1	5:B:8504:DMS:H11	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:251:ARG:HH11	5:A:8416:DMS:H23	1.84	0.41
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.18	0.41
1:D:538:TYR:C	1:D:539[B]:ALA:O	2.57	0.41
1:D:661:LYS:HG3	1:D:661:LYS:H	1.57	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:A:1000:SER:O	1:A:1001:PRO:C	2.57	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: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:A:655:MET:HE2	1:A:655:MET:C	2.38	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: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
1:A:859:ASP:OD1	1:A:861:SER:OG	2.26	0.41
5:A:8409:DMS:O	6:A:9105:HOH:O	2.22	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:684:GLU:CG	1:C:685:LEU:N	2.80	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:513:PRO:O	1:B:514:ALA:HB3	2.20	0.40
1:D:651:LEU:CD1	1:D:651:LEU:C	2.90	0.40
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.56	0.40
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.56	0.40
1:C:70:PRO:HG2	1:C:78:LEU:HD21	2.03	0.40
1:D:893:GLU:HG2	1:D:894:ARG:HG2	2.03	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:C:968:MET:HB2	1:C:968:MET:HE2	1.66	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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	1011/1023 (99%)	974 (96%)	37 (4%)	0	100	100
1	B	1011/1023 (99%)	978 (97%)	30 (3%)	3 (0%)	41	19
1	C	1011/1023 (99%)	974 (96%)	36 (4%)	1 (0%)	51	26
1	D	1011/1023 (99%)	971 (96%)	38 (4%)	2 (0%)	47	23
All	All	4044/4092 (99%)	3897 (96%)	141 (4%)	6 (0%)	51	26

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 (i)

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	864/875 (99%)	839 (97%)	25 (3%)	42 13
1	B	865/875 (99%)	834 (96%)	31 (4%)	35 8
1	C	865/875 (99%)	827 (96%)	38 (4%)	28 4
1	D	865/875 (99%)	831 (96%)	34 (4%)	32 6
All	All	3459/3500 (99%)	3331 (96%)	128 (4%)	34 7

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	TRP
1	A	116	THR
1	A	250	LEU
1	A	333	ARG
1	A	394	ASN
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	600	GLN
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	737	ILE
1	A	773	LYS
1	A	799	THR
1	A	885	ASN
1	A	986	ILE
1	A	1013	ARG
1	A	1023	LYS
1	B	71	GLU
1	B	80	GLU
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	277	GLU

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Mol	Chain	Res	Type
1	B	333	ARG
1	B	370	GLN
1	B	392	TYR
1	B	394	ASN
1	B	554	GLN
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	745	MET
1	B	766	SER
1	B	799	THR
1	B	809	ARG
1	B	819	GLU
1	B	824	GLN
1	B	845	GLN
1	B	885	ASN
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	262	GLN
1	C	299	LYS
1	C	333	ARG
1	C	344	LEU
1	C	370	GLN
1	C	394	ASN
1	C	519	SER
1	C	546	LEU
1	C	634	GLN
1	C	651	LEU

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Mol	Chain	Res	Type
1	C	659	ASP
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	735	HIS
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	956	GLN
1	C	968	MET
1	C	1013	ARG
1	C	1017	GLN
1	C	1022	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	112	PRO
1	D	237	ARG
1	D	277	GLU
1	D	319	ASP
1	D	333	ARG
1	D	344	LEU
1	D	370	GLN
1	D	394	ASN
1	D	519	SER
1	D	546	LEU
1	D	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

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Mol	Chain	Res	Type
1	D	734	SER
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	910	LEU
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 (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	GLN
1	A	614	HIS
1	A	624	GLN
1	A	634	GLN
1	A	653	HIS
1	A	675	GLN
1	A	824	GLN
1	A	844	HIS
1	A	878	HIS
1	B	262	GLN
1	B	363	HIS
1	B	510	GLN
1	B	583	ASN
1	B	600	GLN
1	B	614	HIS
1	B	624	GLN
1	B	628	GLN
1	B	878	HIS
1	B	890	GLN
1	B	1017	GLN
1	C	363	HIS
1	C	624	GLN
1	C	634	GLN
1	C	687	GLN
1	C	824	GLN

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Mol	Chain	Res	Type
1	C	878	HIS
1	C	977	HIS
1	D	135	GLN
1	D	363	HIS
1	D	583	ASN
1	D	624	GLN
1	D	628	GLN
1	D	634	GLN
1	D	653	HIS
1	D	704	ASN
1	D	804	ASN
1	D	878	HIS
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 monosaccharides 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	C	8412	-	3,3,3	1.68	1 (33%)	3,3,3	0.30	0
5	DMS	A	8504	-	3,3,3	0.28	0	3,3,3	0.51	0
5	DMS	C	8415	-	3,3,3	1.68	0	3,3,3	0.49	0
5	DMS	B	8417	-	3,3,3	1.47	1 (33%)	3,3,3	0.58	0
5	DMS	C	8421	-	3,3,3	0.80	0	3,3,3	1.08	0
5	DMS	C	8409	-	3,3,3	2.39	1 (33%)	3,3,3	0.88	0
5	DMS	C	8404	-	3,3,3	1.29	0	3,3,3	0.67	0
5	DMS	C	8601	-	3,3,3	1.40	1 (33%)	3,3,3	0.63	0
5	DMS	C	8420	-	3,3,3	2.36	1 (33%)	3,3,3	0.91	0
5	DMS	D	8417	-	3,3,3	0.81	0	3,3,3	0.14	0
5	DMS	B	8412	-	3,3,3	0.93	0	3,3,3	0.17	0
5	DMS	C	8413	-	3,3,3	2.31	1 (33%)	3,3,3	0.60	0
5	DMS	C	8425	4	3,3,3	1.61	1 (33%)	3,3,3	0.56	0
5	DMS	D	8703	-	3,3,3	1.00	0	3,3,3	0.55	0
5	DMS	A	8421	-	3,3,3	0.75	0	3,3,3	0.27	0
5	DMS	C	8504	-	3,3,3	0.79	0	3,3,3	0.49	0
5	DMS	B	8421	-	3,3,3	0.78	0	3,3,3	1.08	0
2	147	D	2001	4	21,22,22	0.86	1 (4%)	29,31,31	1.38	1 (3%)
5	DMS	D	8419	-	3,3,3	0.45	0	3,3,3	0.46	0
5	DMS	B	8420	-	3,3,3	1.50	1 (33%)	3,3,3	0.17	0
5	DMS	D	8705	-	3,3,3	1.23	0	3,3,3	0.15	0
5	DMS	D	8410	-	3,3,3	1.40	1 (33%)	3,3,3	0.48	0
5	DMS	A	8409	-	3,3,3	2.40	1 (33%)	3,3,3	0.63	0
5	DMS	A	8407	-	3,3,3	3.26	2 (66%)	3,3,3	0.46	0
5	DMS	B	8407	-	3,3,3	2.25	1 (33%)	3,3,3	0.46	0
5	DMS	A	8402	-	3,3,3	2.21	1 (33%)	3,3,3	0.33	0
5	DMS	C	8602	-	3,3,3	0.27	0	3,3,3	0.60	0
5	DMS	D	8427	-	3,3,3	1.07	0	3,3,3	0.20	0
5	DMS	A	8416	-	3,3,3	1.12	0	3,3,3	0.42	0
5	DMS	C	8414	-	3,3,3	1.89	2 (66%)	3,3,3	0.83	0
5	DMS	B	8601	-	3,3,3	1.86	2 (66%)	3,3,3	0.68	0
5	DMS	D	8406	-	3,3,3	0.67	0	3,3,3	0.36	0
5	DMS	A	8401	-	3,3,3	0.93	0	3,3,3	0.27	0
5	DMS	C	8419	-	3,3,3	1.12	0	3,3,3	0.27	0
5	DMS	C	8402	-	3,3,3	2.48	1 (33%)	3,3,3	0.38	0
5	DMS	A	8417	-	3,3,3	0.96	0	3,3,3	0.56	0
5	DMS	C	8416	-	3,3,3	1.75	1 (33%)	3,3,3	0.34	0
5	DMS	C	8427	-	3,3,3	0.94	0	3,3,3	0.61	0
5	DMS	D	8412	-	3,3,3	1.44	0	3,3,3	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DMS	C	8401	-	3,3,3	0.78	0	3,3,3	0.23	0
5	DMS	D	8701	-	3,3,3	2.71	2 (66%)	3,3,3	0.50	0
5	DMS	D	8401	-	3,3,3	1.22	0	3,3,3	0.95	0
5	DMS	D	8501	-	3,3,3	1.20	0	3,3,3	0.41	0
5	DMS	A	8411	-	3,3,3	0.81	0	3,3,3	0.26	0
5	DMS	D	8421	-	3,3,3	0.49	0	3,3,3	0.33	0
5	DMS	A	8405	-	3,3,3	1.37	1 (33%)	3,3,3	0.74	0
2	147	B	2001	4	21,22,22	0.83	1 (4%)	29,31,31	1.68	9 (31%)
5	DMS	B	8411	-	3,3,3	1.61	0	3,3,3	0.56	0
5	DMS	D	8404	-	3,3,3	1.90	1 (33%)	3,3,3	0.46	0
5	DMS	A	8423	-	3,3,3	1.49	0	3,3,3	0.24	0
5	DMS	D	8409	-	3,3,3	2.22	1 (33%)	3,3,3	1.04	0
5	DMS	C	8506	-	3,3,3	2.29	1 (33%)	3,3,3	0.23	0
2	147	C	2001	4	21,22,22	0.84	0	29,31,31	1.27	1 (3%)
5	DMS	A	8415	-	3,3,3	2.68	3 (100%)	3,3,3	0.30	0
5	DMS	B	8416	-	3,3,3	1.20	0	3,3,3	0.57	0
5	DMS	D	8405	-	3,3,3	1.29	0	3,3,3	0.50	0
5	DMS	C	8407	-	3,3,3	1.61	1 (33%)	3,3,3	0.16	0
5	DMS	D	8408	-	3,3,3	1.29	0	3,3,3	0.34	0
5	DMS	B	8427	-	3,3,3	0.65	0	3,3,3	0.28	0
5	DMS	D	8411	-	3,3,3	0.76	0	3,3,3	0.21	0
5	DMS	B	8414	-	3,3,3	0.58	0	3,3,3	1.41	1 (33%)
5	DMS	C	8501	-	3,3,3	1.11	0	3,3,3	0.79	0
5	DMS	C	8405	-	3,3,3	1.99	1 (33%)	3,3,3	0.33	0
5	DMS	A	8410	-	3,3,3	0.78	0	3,3,3	0.94	0
5	DMS	B	8425	4	3,3,3	1.74	1 (33%)	3,3,3	0.33	0
5	DMS	A	8427	-	3,3,3	0.78	0	3,3,3	0.17	0
5	DMS	C	8408	-	3,3,3	1.33	0	3,3,3	0.82	0
5	DMS	B	8413	-	3,3,3	2.18	1 (33%)	3,3,3	0.99	0
5	DMS	D	8423	-	3,3,3	1.63	1 (33%)	3,3,3	0.44	0
5	DMS	C	8406	-	3,3,3	1.68	0	3,3,3	0.40	0
5	DMS	D	8403	-	3,3,3	1.35	0	3,3,3	0.78	0
5	DMS	A	8425	4	3,3,3	2.14	2 (66%)	3,3,3	0.72	0
5	DMS	D	8407	-	3,3,3	2.14	3 (100%)	3,3,3	0.51	0
5	DMS	A	8413	-	3,3,3	3.00	3 (100%)	3,3,3	0.74	0
5	DMS	D	8413	-	3,3,3	1.40	1 (33%)	3,3,3	0.48	0
5	DMS	B	8405	-	3,3,3	1.37	1 (33%)	3,3,3	0.99	0
5	DMS	B	8408	-	3,3,3	1.23	0	3,3,3	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DMS	B	8508	-	3,3,3	2.66	3 (100%)	3,3,3	0.30	0
5	DMS	A	8420	-	3,3,3	1.61	0	3,3,3	0.58	0
5	DMS	C	8417	-	3,3,3	0.80	0	3,3,3	1.05	0
5	DMS	A	8501	-	3,3,3	1.65	1 (33%)	3,3,3	0.37	0
5	DMS	A	8408	-	3,3,3	1.13	0	3,3,3	1.14	0
5	DMS	D	8402	-	3,3,3	2.06	1 (33%)	3,3,3	0.62	0
5	DMS	D	8508	-	3,3,3	1.68	1 (33%)	3,3,3	0.44	0
5	DMS	D	8416	-	3,3,3	0.74	0	3,3,3	0.61	0
5	DMS	A	8414	-	3,3,3	0.94	0	3,3,3	0.20	0
5	DMS	D	8425	4	3,3,3	0.96	0	3,3,3	0.91	0
5	DMS	B	8423	-	3,3,3	0.79	0	3,3,3	0.89	0
5	DMS	C	8411	-	3,3,3	1.37	0	3,3,3	0.29	0
5	DMS	B	8403	-	3,3,3	1.87	2 (66%)	3,3,3	0.57	0
5	DMS	B	8406	-	3,3,3	1.19	0	3,3,3	0.89	0
5	DMS	B	8401	-	3,3,3	0.87	0	3,3,3	0.54	0
5	DMS	A	8419	-	3,3,3	0.70	0	3,3,3	0.62	0
5	DMS	B	8410	-	3,3,3	1.73	1 (33%)	3,3,3	0.41	0
5	DMS	B	8504	-	3,3,3	1.01	0	3,3,3	0.58	0
5	DMS	B	8502	-	3,3,3	1.42	1 (33%)	3,3,3	1.95	1 (33%)
5	DMS	A	8412	-	3,3,3	2.22	1 (33%)	3,3,3	0.29	0
5	DMS	B	8404	-	3,3,3	1.53	1 (33%)	3,3,3	0.14	0
5	DMS	A	8602	-	3,3,3	1.32	0	3,3,3	0.65	0
5	DMS	D	8415	-	3,3,3	3.17	2 (66%)	3,3,3	0.21	0
5	DMS	A	8406	3	3,3,3	0.46	0	3,3,3	0.24	0
5	DMS	B	8409	-	3,3,3	2.84	2 (66%)	3,3,3	0.78	0
5	DMS	C	8410	-	3,3,3	1.18	0	3,3,3	0.39	0
5	DMS	B	8415	-	3,3,3	2.91	2 (66%)	3,3,3	1.89	1 (33%)
5	DMS	B	8506	-	3,3,3	1.91	1 (33%)	3,3,3	0.59	0
5	DMS	C	8403	-	3,3,3	1.95	1 (33%)	3,3,3	0.36	0
5	DMS	A	8502	-	3,3,3	2.18	2 (66%)	3,3,3	1.70	1 (33%)
5	DMS	C	8423	-	3,3,3	0.83	0	3,3,3	0.27	0
5	DMS	D	8414	-	3,3,3	0.54	0	3,3,3	0.47	0
5	DMS	A	8404	-	3,3,3	1.66	1 (33%)	3,3,3	0.35	0
2	147	A	2001	4	21,22,22	0.74	0	29,31,31	1.56	4 (13%)
5	DMS	B	8402	-	3,3,3	2.58	3 (100%)	3,3,3	0.82	0
5	DMS	A	8403	-	3,3,3	2.39	1 (33%)	3,3,3	0.39	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	D	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

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8407	DMS	O-S	4.88	1.83	1.50
5	B	8409	DMS	O-S	4.14	1.78	1.50
5	C	8409	DMS	O-S	4.04	1.77	1.50
5	A	8409	DMS	O-S	3.90	1.76	1.50
5	B	8415	DMS	C2-S	3.89	2.04	1.75
5	D	8415	DMS	O-S	3.86	1.76	1.50
5	C	8402	DMS	C2-S	3.81	2.04	1.75
5	C	8420	DMS	O-S	3.79	1.75	1.50
5	A	8403	DMS	C2-S	3.72	2.03	1.75
5	B	8508	DMS	C1-S	3.58	2.02	1.75
5	D	8701	DMS	O-S	3.56	1.74	1.50
5	D	8415	DMS	C1-S	3.49	2.01	1.75
5	D	8409	DMS	O-S	3.45	1.73	1.50
5	A	8413	DMS	C2-S	3.44	2.01	1.75
5	A	8402	DMS	C2-S	3.33	2.00	1.75
5	C	8413	DMS	O-S	3.32	1.72	1.50
5	A	8412	DMS	C1-S	3.28	2.00	1.75
5	B	8402	DMS	C2-S	3.26	2.00	1.75
5	B	8407	DMS	C2-S	3.22	1.99	1.75
5	C	8405	DMS	O-S	3.04	1.70	1.50
5	A	8415	DMS	O-S	3.03	1.70	1.50
5	B	8413	DMS	O-S	3.01	1.70	1.50
5	D	8404	DMS	C2-S	2.94	1.97	1.75
5	C	8506	DMS	C1-S	2.94	1.97	1.75
5	B	8506	DMS	C2-S	2.93	1.97	1.75
5	A	8502	DMS	C1-S	2.93	1.97	1.75
5	D	8701	DMS	C2-S	2.83	1.96	1.75
5	B	8410	DMS	C1-S	2.83	1.96	1.75
5	D	8402	DMS	C2-S	2.81	1.96	1.75
5	A	8413	DMS	C1-S	2.80	1.96	1.75
5	D	8508	DMS	O-S	2.71	1.68	1.50
5	A	8413	DMS	O-S	2.69	1.68	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8425	DMS	O-S	2.69	1.68	1.50
5	A	8415	DMS	C2-S	2.65	1.95	1.75
5	B	8415	DMS	O-S	2.61	1.67	1.50
5	A	8501	DMS	O-S	2.58	1.67	1.50
5	C	8416	DMS	C2-S	2.56	1.94	1.75
5	C	8425	DMS	O-S	2.54	1.67	1.50
5	B	8420	DMS	C2-S	2.52	1.94	1.75
5	B	8601	DMS	C2-S	2.49	1.94	1.75
2	B	2001	147	C5'-C4'	-2.45	1.34	1.38
5	C	8412	DMS	O-S	2.44	1.66	1.50
5	A	8407	DMS	C2-S	2.39	1.93	1.75
5	B	8417	DMS	O-S	2.39	1.66	1.50
5	C	8414	DMS	C1-S	-2.38	1.58	1.75
5	A	8425	DMS	C1-S	2.37	1.93	1.75
5	B	8409	DMS	C1-S	2.35	1.93	1.75
5	B	8404	DMS	C2-S	2.35	1.93	1.75
5	D	8413	DMS	O-S	2.34	1.66	1.50
5	B	8403	DMS	C1-S	2.33	1.93	1.75
5	A	8502	DMS	C2-S	2.32	1.93	1.75
5	A	8415	DMS	C1-S	2.31	1.93	1.75
5	C	8601	DMS	C2-S	2.31	1.93	1.75
5	C	8407	DMS	O-S	2.21	1.65	1.50
5	D	8407	DMS	C1-S	2.21	1.92	1.75
5	A	8404	DMS	O-S	2.20	1.65	1.50
5	D	8407	DMS	C2-S	2.20	1.92	1.75
5	A	8425	DMS	C2-S	2.19	1.92	1.75
5	B	8402	DMS	C1-S	-2.18	1.59	1.75
2	D	2001	147	O3-C3	2.17	1.48	1.43
5	B	8405	DMS	O-S	2.14	1.64	1.50
5	B	8402	DMS	O-S	2.14	1.64	1.50
5	C	8414	DMS	C2-S	2.12	1.91	1.75
5	A	8405	DMS	O-S	2.09	1.64	1.50
5	D	8423	DMS	C1-S	2.08	1.91	1.75
5	D	8410	DMS	C1-S	2.08	1.91	1.75
5	B	8403	DMS	C2-S	2.08	1.91	1.75
5	B	8508	DMS	C2-S	2.05	1.91	1.75
5	B	8508	DMS	O-S	2.04	1.64	1.50
5	C	8403	DMS	O-S	2.03	1.63	1.50
5	B	8601	DMS	C1-S	2.03	1.90	1.75
5	D	8407	DMS	O-S	2.03	1.63	1.50
5	B	8502	DMS	C1-S	2.02	1.90	1.75

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	147	C3'-C4'-N1'	-4.55	115.95	119.38
2	B	2001	147	C5'-C4'-N1'	-3.80	116.52	119.38
2	D	2001	147	C5'-C4'-N1'	-3.76	116.55	119.38
2	C	2001	147	O1-C1-C2	-3.48	102.08	107.14
5	B	8502	DMS	C2-S-C1	3.37	115.76	98.44
2	B	2001	147	C6'-C5'-C4'	-3.29	115.51	120.08
2	A	2001	147	C5'-C4'-C3'	3.02	124.84	119.86
5	B	8415	DMS	C2-S-C1	2.94	113.57	98.44
5	A	8502	DMS	C2-S-C1	2.91	113.41	98.44
2	A	2001	147	C3-C4-C5	-2.67	105.48	110.24
2	A	2001	147	C1-C2-C3	2.45	115.10	110.00
2	B	2001	147	C5'-C6'-C1'	2.39	122.66	119.73
2	B	2001	147	C3'-C2'-C1'	-2.34	116.87	119.73
5	B	8414	DMS	C2-S-C1	2.34	110.49	98.44
2	B	2001	147	C1'-O1-C1	2.24	121.07	117.79
2	B	2001	147	C6-C5-C4	2.19	118.13	113.00
2	B	2001	147	O1-C1-C2	-2.11	104.08	107.14
2	B	2001	147	O2-C2-C1	-2.09	104.98	110.05
2	B	2001	147	C5'-C4'-C3'	2.03	123.22	119.86

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.

37 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8417	DMS	1	0
5	C	8420	DMS	1	0
5	D	8417	DMS	1	0
5	B	8412	DMS	1	0
5	D	8703	DMS	1	0
5	A	8421	DMS	1	0
5	C	8504	DMS	1	0
5	B	8421	DMS	1	0
5	D	8705	DMS	3	0

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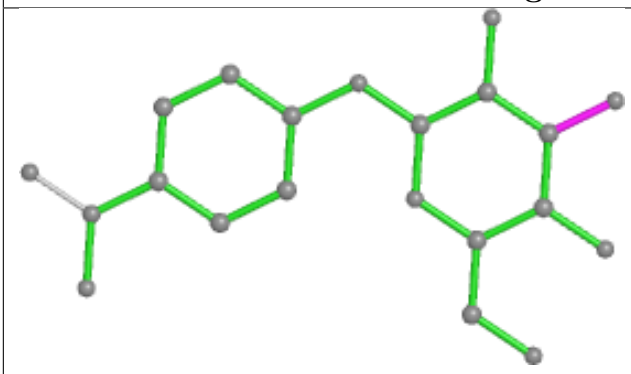
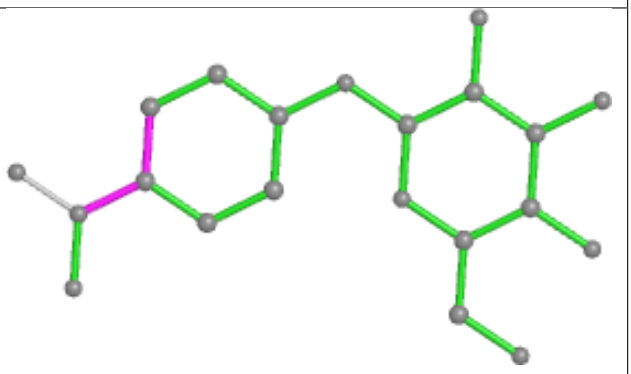
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8409	DMS	1	0
5	C	8602	DMS	1	0
5	D	8427	DMS	2	0
5	A	8416	DMS	2	0
5	D	8406	DMS	2	0
5	C	8402	DMS	4	0
5	A	8417	DMS	3	0
5	C	8427	DMS	2	0
5	D	8412	DMS	2	0
5	B	8411	DMS	1	0
5	D	8409	DMS	1	0
5	C	8506	DMS	2	0
5	C	8406	DMS	2	0
5	B	8508	DMS	1	0
5	A	8420	DMS	1	0
5	C	8417	DMS	1	0
5	D	8508	DMS	1	0
5	D	8416	DMS	4	0
5	A	8414	DMS	2	0
5	B	8406	DMS	2	0
5	A	8419	DMS	1	0
5	B	8504	DMS	3	0
5	A	8412	DMS	3	0
5	A	8602	DMS	1	0
5	D	8415	DMS	2	0
5	B	8415	DMS	3	0
5	B	8402	DMS	1	0
5	A	8403	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 then 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.

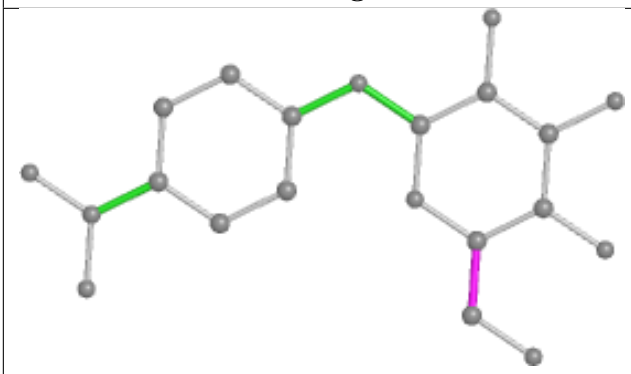
Ligand 147 D 2001



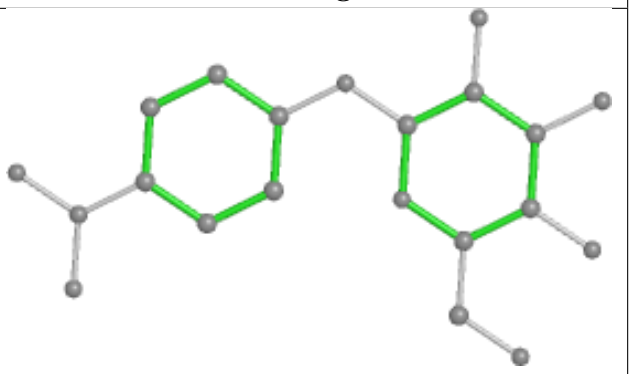
Bond lengths



Bond angles

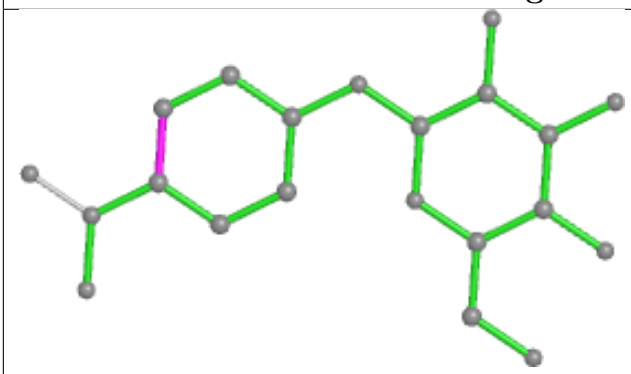


Torsions

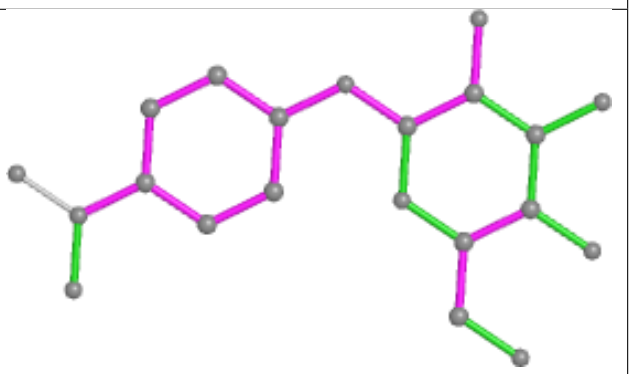


Rings

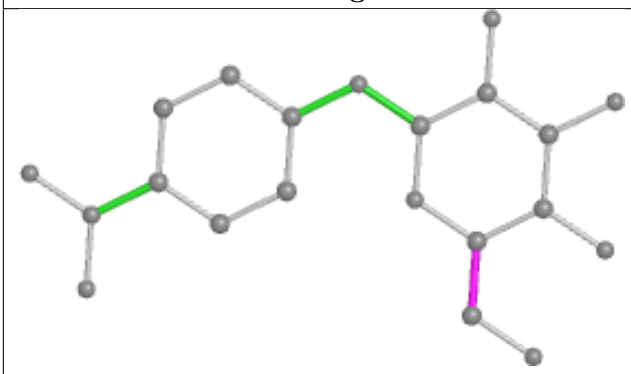
Ligand 147 B 2001



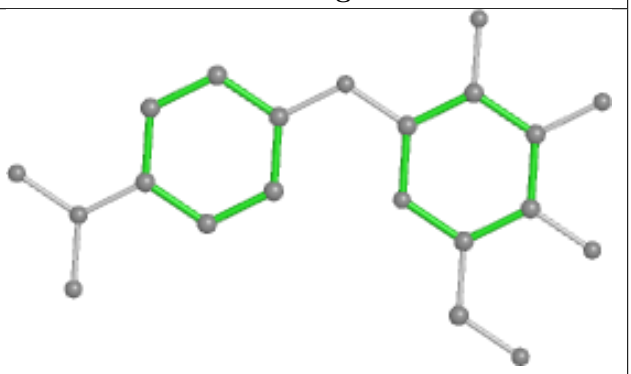
Bond lengths



Bond angles

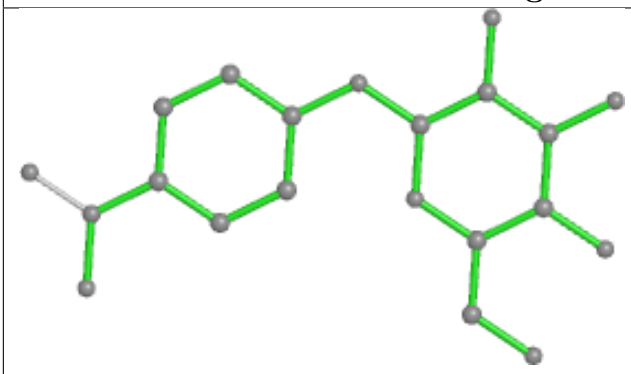


Torsions

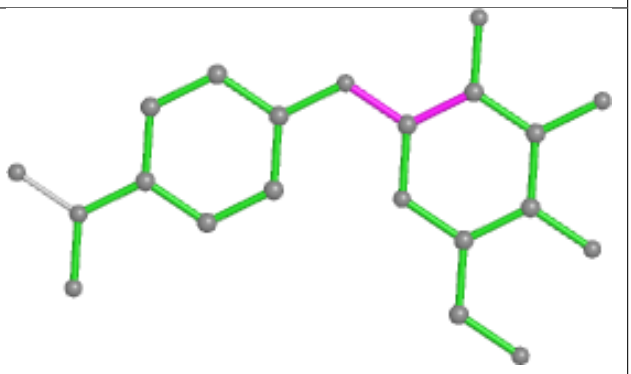


Rings

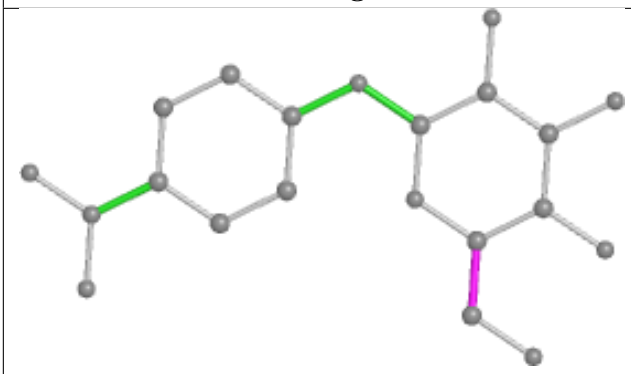
Ligand 147 C 2001



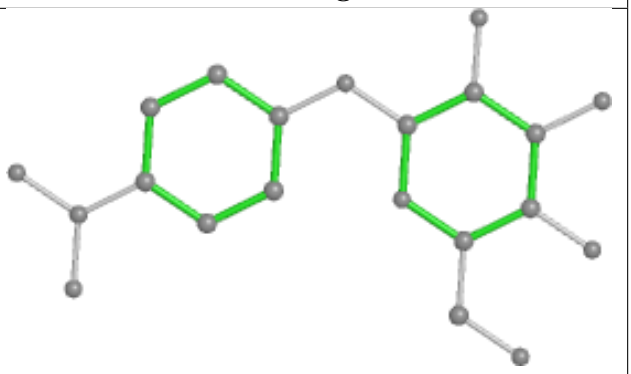
Bond lengths



Bond angles

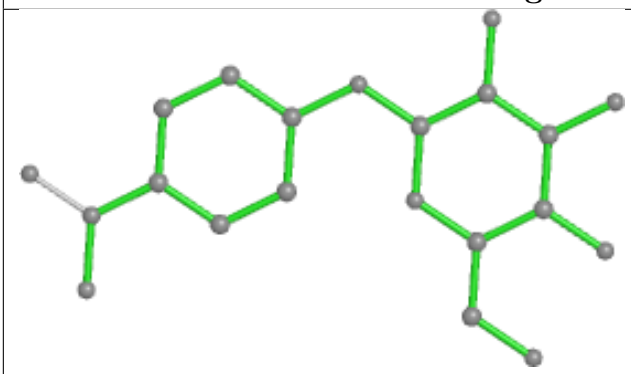


Torsions

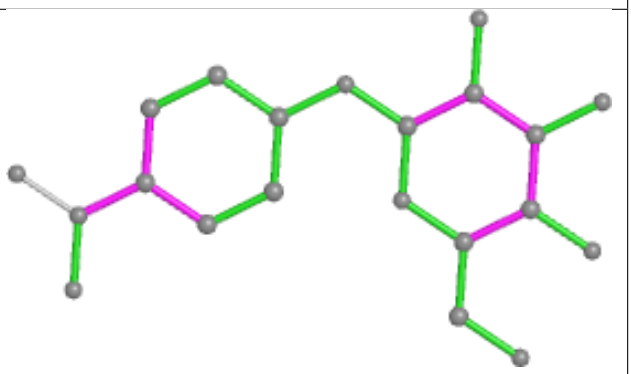


Rings

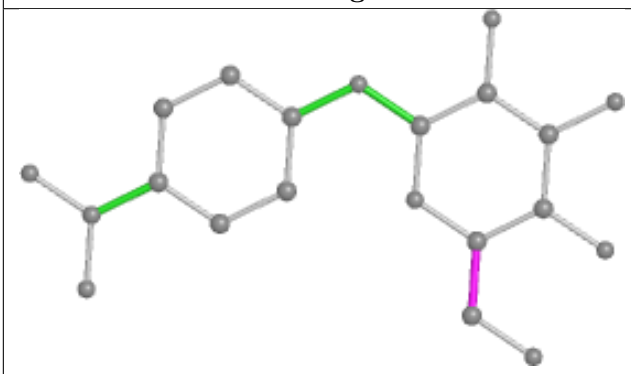
Ligand 147 A 2001



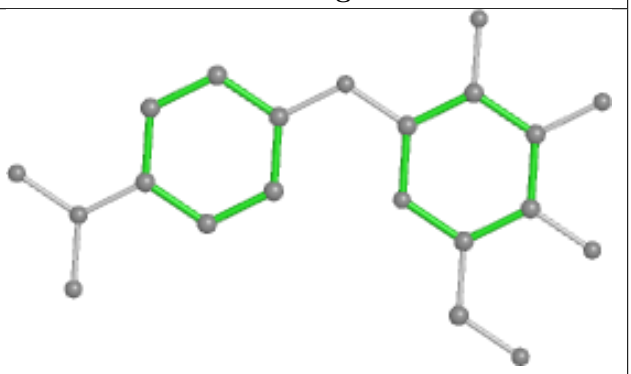
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1011/1023 (98%)	-0.50	21 (2%)	63	69	8, 15, 45, 100	0
1	B	1011/1023 (98%)	-0.50	14 (1%)	75	80	8, 15, 43, 94	0
1	C	1011/1023 (98%)	-0.49	18 (1%)	68	74	8, 15, 47, 100	0
1	D	1011/1023 (98%)	-0.49	27 (2%)	54	62	9, 16, 46, 95	0
All	All	4044/4092 (98%)	-0.50	80 (1%)	65	71	8, 15, 46, 100	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	11.0
1	D	735	HIS	10.0
1	A	735	HIS	9.2
1	B	730	LEU	8.1
1	C	732	ALA	8.1
1	C	730	LEU	8.0
1	B	731	PRO	7.2
1	D	732	ALA	6.9
1	C	731	PRO	6.7
1	C	733	ALA	6.4
1	B	732	ALA	5.9
1	D	689	GLU	5.8
1	A	733	ALA	5.7
1	A	687	GLN	5.7
1	D	734	SER	5.5
1	C	735	HIS	5.4
1	D	686	PRO	5.4
1	B	733	ALA	5.2
1	A	731	PRO	5.2
1	A	730	LEU	5.2
1	D	733	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	730	LEU	5.0
1	A	580	GLU	4.8
1	D	731	PRO	4.4
1	A	689	GLU	4.4
1	D	581	ASN	4.0
1	D	580	GLU	3.9
1	A	737	ILE	3.8
1	B	689	GLU	3.8
1	B	580	GLU	3.6
1	B	684	GLU	3.4
1	B	735	HIS	3.4
1	A	732	ALA	3.4
1	D	687	GLN	3.3
1	D	684	GLU	3.3
1	A	581	ASN	3.2
1	B	685	LEU	3.1
1	C	745	MET	3.0
1	C	634	GLN	2.9
1	B	799	THR	2.9
1	D	1023	LYS	2.8
1	A	71	GLU	2.8
1	A	684	GLU	2.7
1	C	687	GLN	2.7
1	D	634	GLN	2.7
1	C	689	GLU	2.7
1	D	688	PRO	2.7
1	C	685	LEU	2.7
1	C	686	PRO	2.6
1	A	685	LEU	2.6
1	A	1023	LYS	2.6
1	D	683	PRO	2.6
1	D	845	GLN	2.6
1	A	734	SER	2.6
1	B	729	THR	2.5
1	D	737	ILE	2.5
1	C	734	SER	2.5
1	D	582	GLY	2.5
1	A	582	GLY	2.4
1	B	686	PRO	2.4
1	A	799	THR	2.4
1	A	771	GLY	2.4
1	C	580	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	772	ASP	2.3
1	C	684	GLU	2.3
1	D	771	GLY	2.3
1	D	736	ALA	2.1
1	C	737	ILE	2.1
1	B	745	MET	2.1
1	D	800	ARG	2.1
1	C	744	GLU	2.1
1	A	800	ARG	2.1
1	D	663	LEU	2.1
1	D	799	THR	2.1
1	A	736	ALA	2.1
1	D	681	GLU	2.0
1	C	729	THR	2.0
1	B	581	ASN	2.0
1	C	688	PRO	2.0
1	D	798	ALA	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 monosaccharides 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(Å^2)	Q<0.9
5	DMS	D	8703	4/4	0.78	0.26	47,73,77,81	0
5	DMS	C	8419	4/4	0.80	0.20	41,46,50,67	0
5	DMS	D	8427	4/4	0.81	0.16	47,51,59,75	0
5	DMS	A	8427	4/4	0.84	0.14	41,54,55,100	0
5	DMS	D	8423	4/4	0.86	0.17	38,53,100,100	0
5	DMS	D	8407	4/4	0.87	0.16	29,47,53,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	B	8427	4/4	0.87	0.14	35,40,68,100	0
5	DMS	D	8705	4/4	0.87	0.15	20,47,58,71	0
5	DMS	B	8420	4/4	0.89	0.16	41,60,65,69	0
5	DMS	C	8602	4/4	0.89	0.20	21,74,91,100	0
5	DMS	C	8417	4/4	0.89	0.13	24,30,54,74	0
5	DMS	D	8417	4/4	0.89	0.16	26,31,47,100	0
5	DMS	B	8406	4/4	0.90	0.16	35,52,87,100	0
5	DMS	B	8504	4/4	0.91	0.10	35,40,58,63	0
5	DMS	C	8406	4/4	0.91	0.16	37,38,46,94	0
5	DMS	A	8407	4/4	0.91	0.10	23,32,33,45	0
5	DMS	A	8417	4/4	0.91	0.18	23,27,96,100	0
5	DMS	C	8427	4/4	0.91	0.12	49,51,56,65	0
5	DMS	A	8406	4/4	0.91	0.21	13,59,73,100	0
5	DMS	C	8504	4/4	0.92	0.10	35,54,63,66	0
3	MG	A	3105	1/1	0.92	0.11	21,21,21,21	1
5	DMS	C	8423	4/4	0.93	0.13	28,64,100,100	0
5	DMS	A	8421	4/4	0.93	0.21	55,56,68,100	0
5	DMS	A	8423	4/4	0.93	0.12	30,46,74,100	0
3	MG	D	3105	1/1	0.93	0.12	24,24,24,24	1
5	DMS	B	8508	4/4	0.93	0.11	27,35,48,62	0
5	DMS	D	8416	4/4	0.93	0.19	29,53,77,80	0
5	DMS	A	8419	4/4	0.93	0.10	33,46,49,50	0
5	DMS	C	8416	4/4	0.93	0.20	38,50,52,100	0
5	DMS	B	8407	4/4	0.93	0.12	28,32,33,38	0
5	DMS	D	8501	4/4	0.93	0.09	24,30,34,48	0
5	DMS	B	8417	4/4	0.93	0.15	25,28,70,73	0
5	DMS	C	8420	4/4	0.93	0.14	35,55,58,100	0
5	DMS	A	8502	4/4	0.94	0.09	22,26,54,58	0
5	DMS	A	8420	4/4	0.94	0.10	39,45,45,47	0
5	DMS	D	8425	4/4	0.94	0.14	16,19,24,24	4
5	DMS	B	8423	4/4	0.94	0.09	33,34,66,100	0
5	DMS	D	8404	4/4	0.94	0.12	20,23,41,63	0
5	DMS	D	8508	4/4	0.94	0.12	36,52,53,53	0
5	DMS	C	8421	4/4	0.94	0.10	32,46,55,57	0
3	MG	C	3105	1/1	0.94	0.12	19,19,19,19	1
3	MG	A	3005	1/1	0.95	0.05	33,33,33,33	0
5	DMS	D	8406	4/4	0.95	0.10	26,26,28,41	0
5	DMS	B	8421	4/4	0.95	0.09	31,35,46,73	0
5	DMS	A	8412	4/4	0.95	0.19	38,46,51,100	0
5	DMS	A	8414	4/4	0.95	0.12	24,43,84,100	0
5	DMS	B	8502	4/4	0.95	0.10	28,30,43,49	0
5	DMS	B	8415	4/4	0.95	0.10	21,29,32,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	B	8416	4/4	0.95	0.14	34,36,47,90	0
5	DMS	C	8501	4/4	0.95	0.08	20,29,37,51	0
5	DMS	A	8501	4/4	0.95	0.10	17,27,37,39	0
5	DMS	C	8506	4/4	0.95	0.12	26,40,47,52	0
5	DMS	C	8407	4/4	0.95	0.13	27,30,40,42	0
5	DMS	B	8414	4/4	0.96	0.12	30,39,41,100	0
5	DMS	D	8409	4/4	0.96	0.11	29,30,31,34	0
5	DMS	D	8415	4/4	0.96	0.10	20,37,42,100	0
5	DMS	A	8404	4/4	0.96	0.08	18,30,31,39	0
5	DMS	A	8409	4/4	0.96	0.09	26,31,34,40	0
5	DMS	B	8601	4/4	0.96	0.09	30,37,41,45	0
5	DMS	A	8602	4/4	0.96	0.19	38,53,74,100	0
5	DMS	A	8425	4/4	0.96	0.10	33,38,38,44	0
5	DMS	C	8412	4/4	0.96	0.11	28,31,36,100	0
5	DMS	A	8416	4/4	0.96	0.20	22,38,73,100	0
5	DMS	B	8409	4/4	0.96	0.09	25,26,33,34	0
5	DMS	B	8413	4/4	0.96	0.14	27,31,35,39	0
4	NA	C	3104	1/1	0.97	0.08	21,21,21,21	0
5	DMS	B	8402	4/4	0.97	0.07	19,19,28,33	0
5	DMS	B	8404	4/4	0.97	0.07	18,20,31,37	0
5	DMS	C	8601	4/4	0.97	0.09	35,40,42,57	0
4	NA	D	3103	1/1	0.97	0.06	27,27,27,27	0
5	DMS	D	8402	4/4	0.97	0.07	17,28,31,33	0
2	147	A	2001	21/21	0.97	0.06	10,13,21,30	0
5	DMS	B	8408	4/4	0.97	0.09	31,34,38,100	0
5	DMS	C	8402	4/4	0.97	0.08	19,29,34,51	0
2	147	B	2001	21/21	0.97	0.05	9,11,20,35	0
5	DMS	D	8414	4/4	0.97	0.09	24,40,87,100	0
5	DMS	B	8410	4/4	0.97	0.09	19,28,32,38	0
5	DMS	B	8412	4/4	0.97	0.08	27,37,37,43	0
5	DMS	C	8414	4/4	0.97	0.08	22,39,41,49	0
5	DMS	D	8419	4/4	0.97	0.09	33,43,46,48	0
5	DMS	D	8421	4/4	0.97	0.12	49,51,52,52	0
3	MG	C	3006	1/1	0.97	0.12	20,20,20,20	1
5	DMS	A	8408	4/4	0.97	0.08	22,34,35,36	0
2	147	C	2001	21/21	0.97	0.06	10,12,25,50	0
3	MG	D	3005	1/1	0.97	0.07	27,27,27,27	0
5	DMS	A	8413	4/4	0.97	0.10	30,33,34,35	0
2	147	D	2001	21/21	0.97	0.06	11,13,27,32	0
5	DMS	A	8504	4/4	0.97	0.09	22,43,50,100	0
4	NA	B	3104	1/1	0.98	0.06	20,20,20,20	0
3	MG	B	3105	1/1	0.98	0.07	18,18,18,18	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	C	8404	4/4	0.98	0.07	18,19,26,29	0
5	DMS	C	8405	4/4	0.98	0.09	27,27,28,32	0
4	NA	A	3103	1/1	0.98	0.06	23,23,23,23	0
5	DMS	D	8403	4/4	0.98	0.07	18,26,28,29	0
5	DMS	B	8403	4/4	0.98	0.09	21,22,28,30	0
5	DMS	C	8408	4/4	0.98	0.06	18,29,30,31	0
5	DMS	C	8409	4/4	0.98	0.07	24,31,33,34	0
5	DMS	D	8408	4/4	0.98	0.08	18,31,36,39	0
5	DMS	C	8410	4/4	0.98	0.09	22,24,33,34	0
5	DMS	D	8412	4/4	0.98	0.08	27,27,33,100	0
5	DMS	D	8413	4/4	0.98	0.11	28,31,31,100	0
4	NA	D	3104	1/1	0.98	0.06	28,28,28,28	0
5	DMS	C	8413	4/4	0.98	0.14	31,33,34,36	0
5	DMS	B	8405	4/4	0.98	0.10	27,30,30,34	0
5	DMS	C	8415	4/4	0.98	0.06	21,26,32,45	0
5	DMS	A	8410	4/4	0.98	0.10	22,31,40,44	0
5	DMS	A	8411	4/4	0.98	0.05	22,26,26,43	0
5	DMS	B	8425	4/4	0.98	0.07	19,25,27,29	0
5	DMS	A	8402	4/4	0.98	0.07	15,29,30,47	0
5	DMS	A	8403	4/4	0.98	0.07	23,23,25,31	0
4	NA	A	3104	1/1	0.98	0.09	23,23,23,23	0
5	DMS	C	8425	4/4	0.98	0.09	27,29,29,100	0
5	DMS	D	8701	4/4	0.98	0.09	16,17,22,44	0
5	DMS	B	8506	4/4	0.98	0.07	27,34,43,44	0
5	DMS	A	8415	4/4	0.98	0.08	19,36,37,46	0
4	NA	B	3101	1/1	0.99	0.03	12,12,12,12	0
5	DMS	D	8410	4/4	0.99	0.07	20,29,30,34	0
5	DMS	D	8411	4/4	0.99	0.05	19,24,26,71	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
5	DMS	A	8405	4/4	0.99	0.09	21,24,25,32	0
4	NA	C	3102	1/1	0.99	0.03	12,12,12,12	0
5	DMS	B	8411	4/4	0.99	0.06	21,23,25,33	0
5	DMS	C	8411	4/4	0.99	0.10	22,23,23,28	0
4	NA	C	3103	1/1	0.99	0.04	21,21,21,21	0
5	DMS	B	8401	4/4	0.99	0.05	14,17,18,18	0
5	DMS	D	8401	4/4	0.99	0.05	13,15,17,20	0
4	NA	A	3101	1/1	0.99	0.04	13,13,13,13	0
3	MG	D	3002	1/1	0.99	0.03	14,14,14,14	0
5	DMS	C	8401	4/4	0.99	0.04	14,15,18,18	0
5	DMS	D	8405	4/4	0.99	0.07	24,30,30,34	0
3	MG	A	3002	1/1	0.99	0.04	14,14,14,14	0

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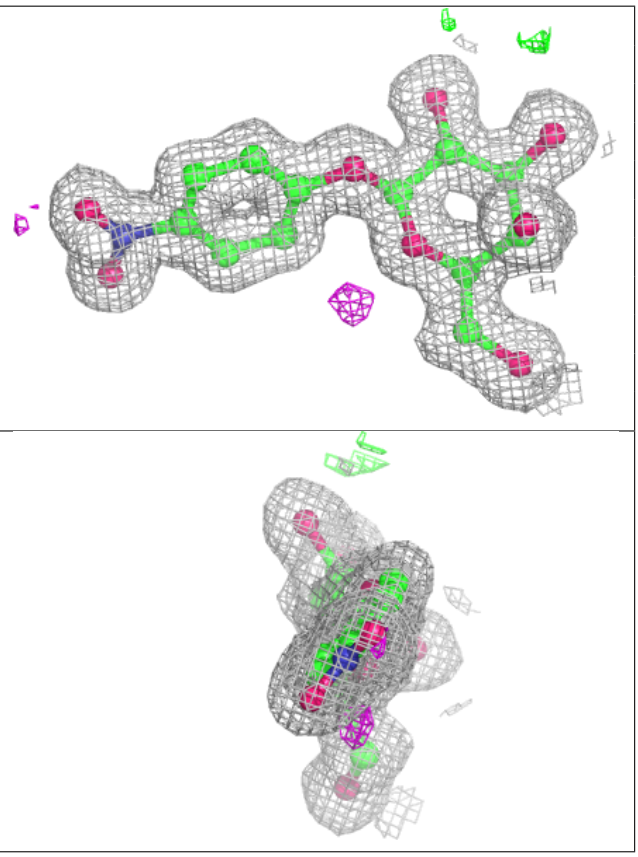
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	C	8403	4/4	0.99	0.06	22,24,25,26	0
5	DMS	A	8401	4/4	0.99	0.06	11,13,14,15	0
4	NA	B	3102	1/1	1.00	0.03	11,11,11,11	0
3	MG	B	3002	1/1	1.00	0.03	14,14,14,14	0
3	MG	B	3001	1/1	1.00	0.02	10,10,10,10	0
4	NA	C	3101	1/1	1.00	0.03	11,11,11,11	0
4	NA	A	3102	1/1	1.00	0.02	12,12,12,12	0
3	MG	D	3001	1/1	1.00	0.03	12,12,12,12	0
3	MG	C	3001	1/1	1.00	0.03	10,10,10,10	0
4	NA	D	3101	1/1	1.00	0.04	13,13,13,13	0
4	NA	D	3102	1/1	1.00	0.04	11,11,11,11	0
3	MG	C	3002	1/1	1.00	0.02	13,13,13,13	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.

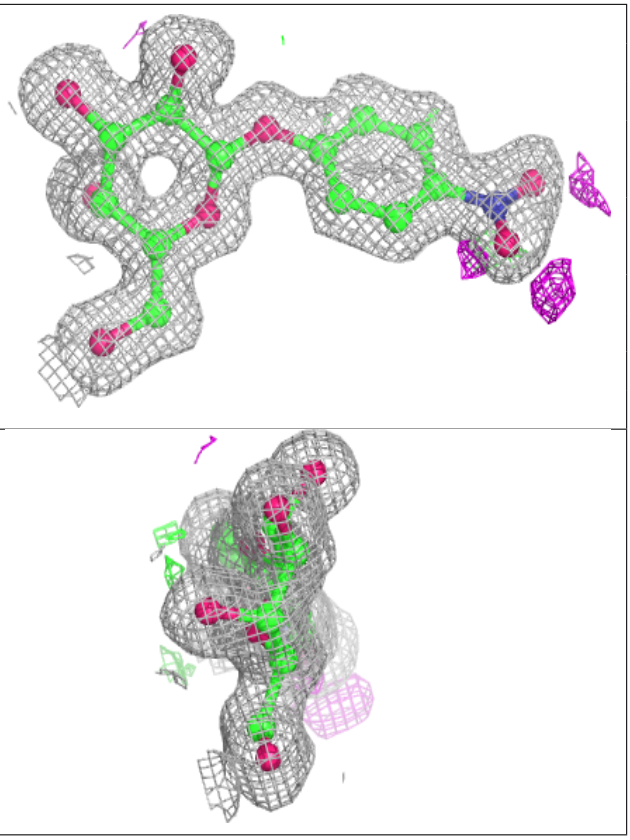
Electron density around 147 A 2001:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



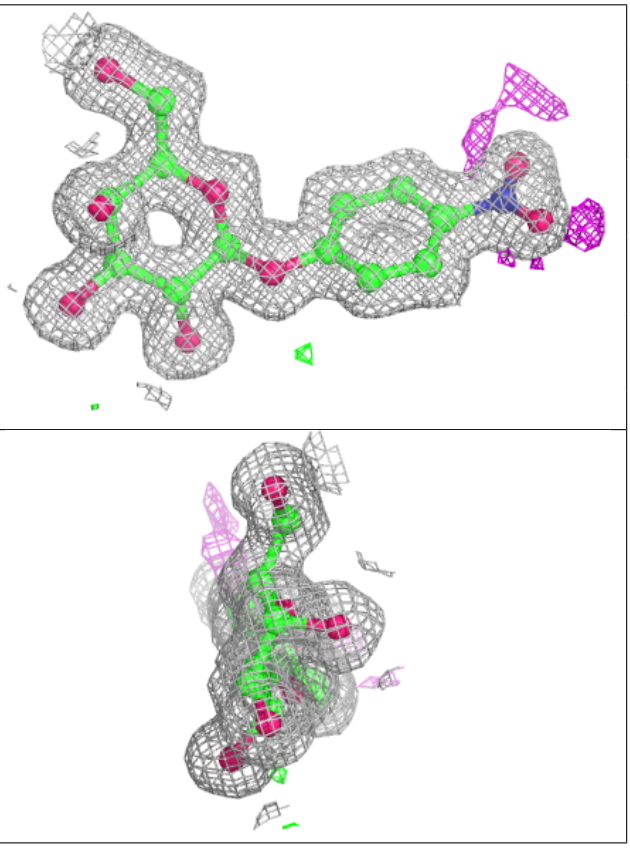
Electron density around 147 B 2001:

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



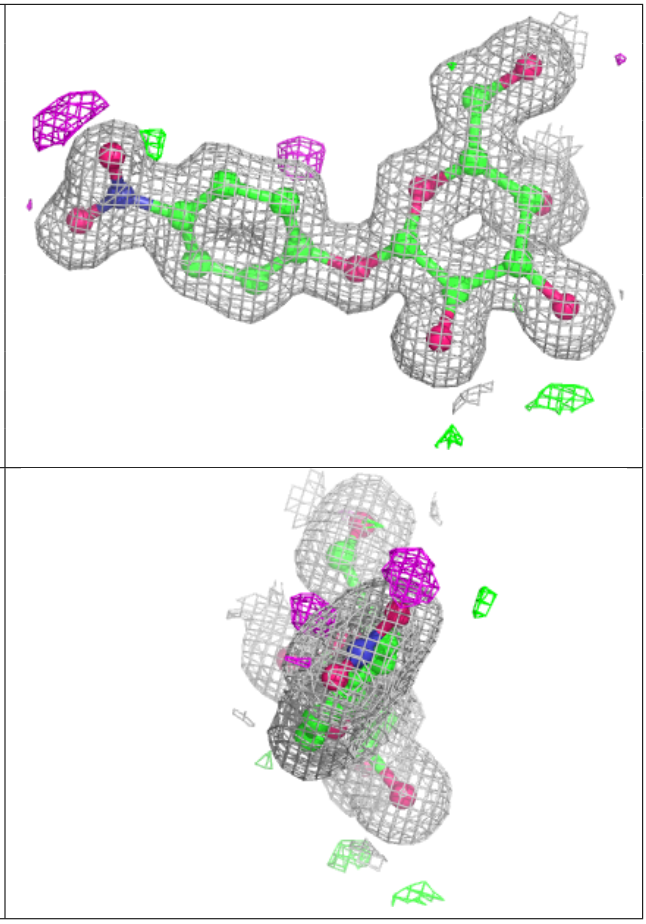
Electron density around 147 C 2001:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.