Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 03:20 AM EDT

PDB ID	:	1JZ4
Title	:	E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-DEOXY-GALACTOSYL-ENZYME INTERMEDIATE (Low Bis-Tris)
Authors	:	Juers, D.H.; Matthews, B.W.
Deposited on	:	2001-09-13
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

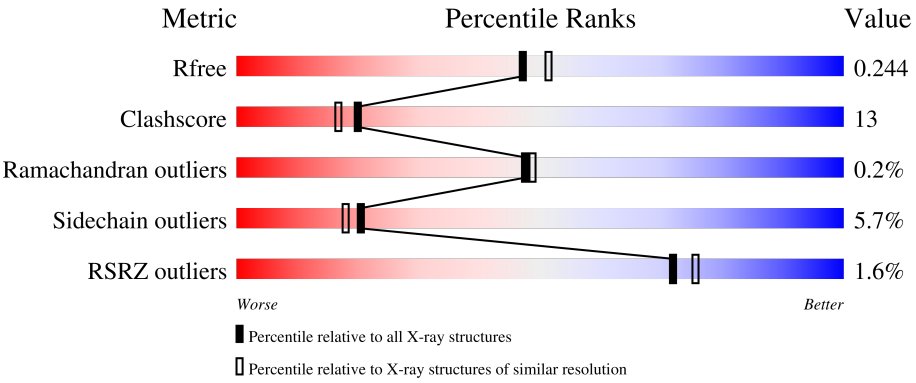
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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% 64% 29% 5% ••
1	B	1023	% 62% 30% 5% ••
1	C	1023	2% 63% 28% 7% ••
1	D	1023	2% 63% 30% 5% ••

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	B	8508	-	X	-	-
5	DMS	C	8506	-	-	X	-
5	DMS	D	8412	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36890 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			

There are 32 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
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
C	1	GLY	THR	cloning artifact	? P00722
C	2	SER	MET	cloning artifact	? P00722
C	3	HIS	ILE	cloning artifact	? P00722
C	4	MET	THR	cloning artifact	? P00722
C	5	LEU	ASP	cloning artifact	? P00722

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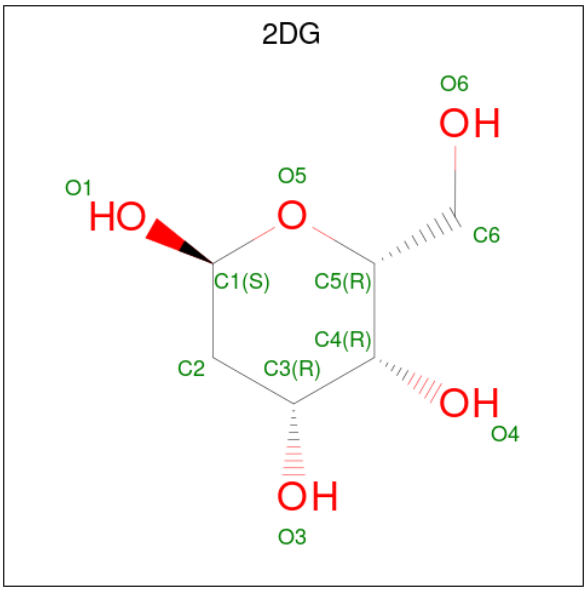
Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLU	SER	cloning artifact	? P00722
C	7	ASP	LEU	cloning artifact	? P00722
C	8	PRO	ALA	cloning artifact	? P00722
D	1	GLY	THR	cloning artifact	? P00722
D	2	SER	MET	cloning artifact	? P00722
D	3	HIS	ILE	cloning artifact	? P00722
D	4	MET	THR	cloning artifact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

- Molecule 2 is 2-deoxy-alpha-D-galactopyranose (three-letter code: 2DG) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	B	1	Total C O 10 6 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0

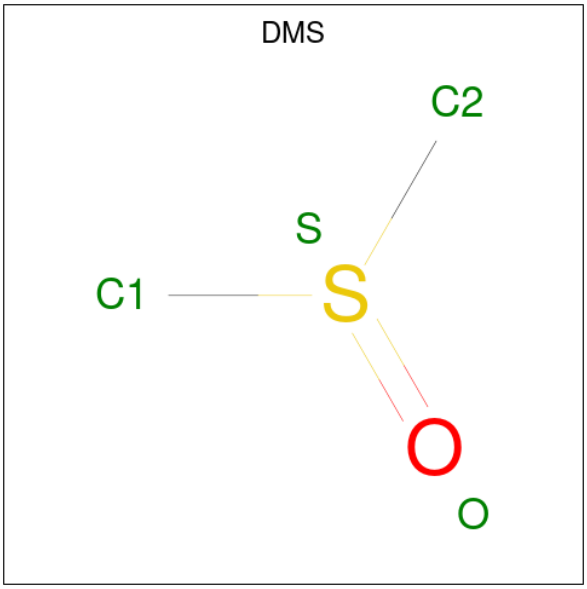
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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



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

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

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

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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	992	Total O 992 992	0	0
6	B	995	Total O 995 995	0	0

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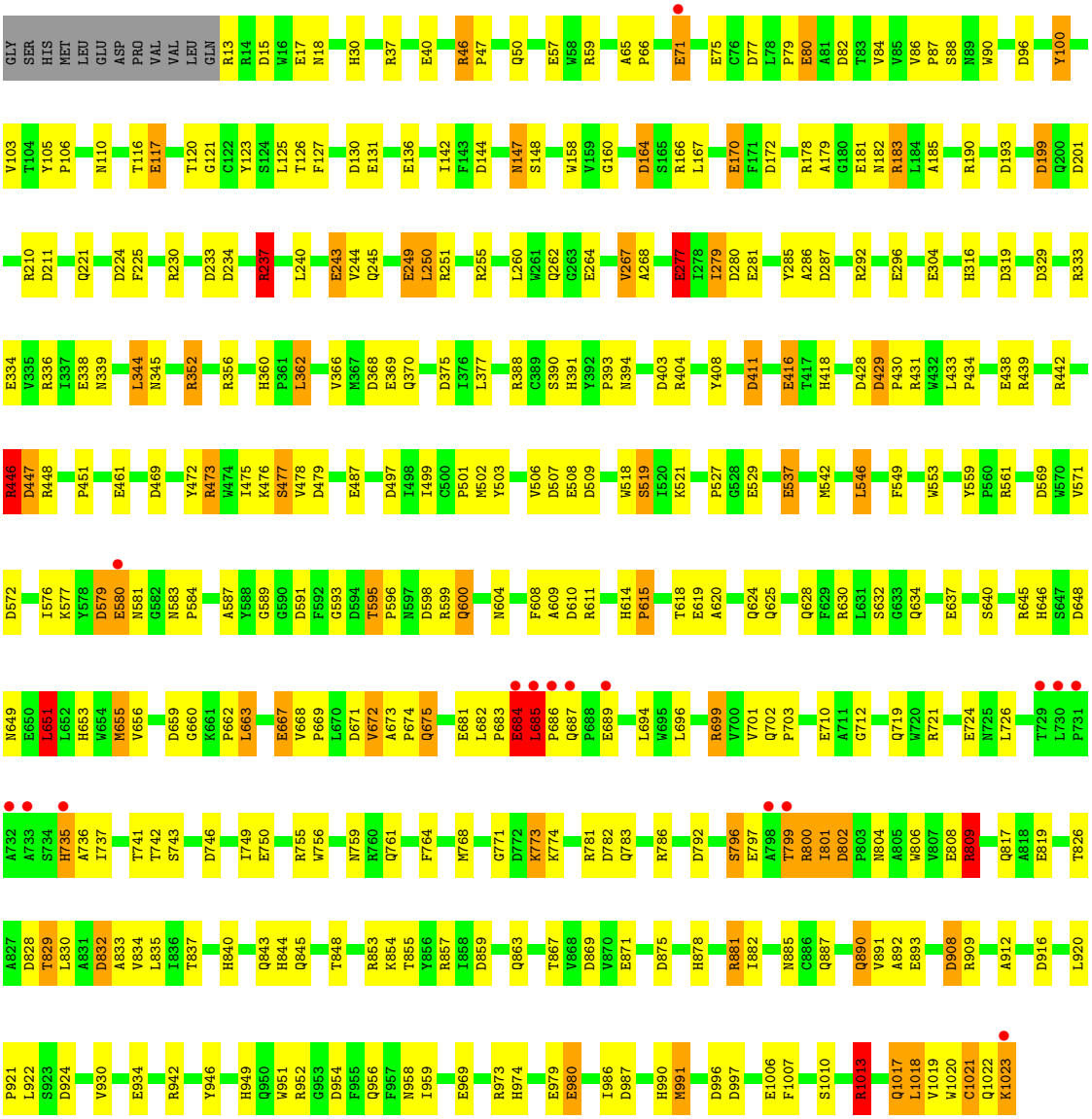
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	946	Total O 946 946	0	0
6	D	980	Total O 980 980	0	0

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.

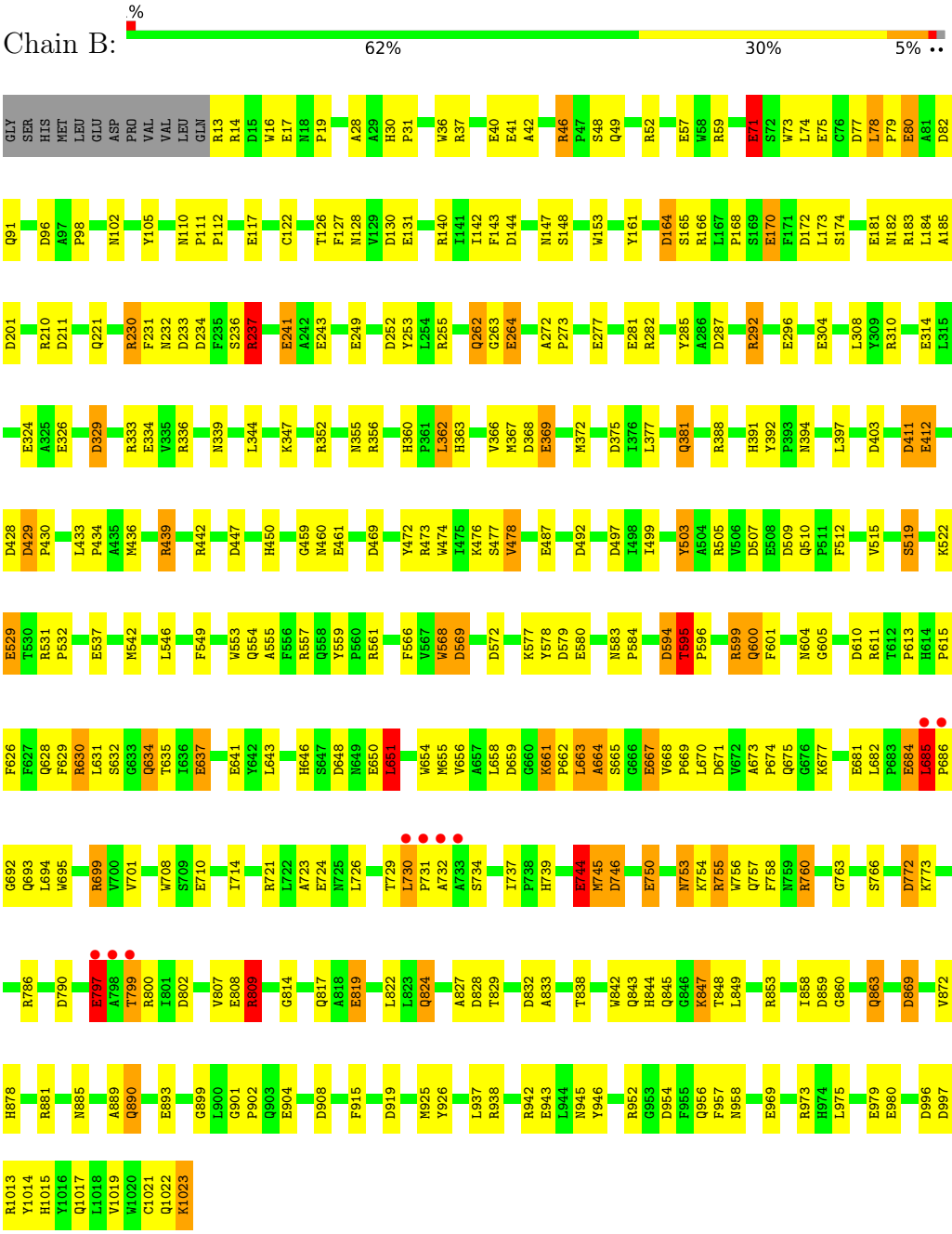
• Molecule 1: Beta-Galactosidase

Chain A:



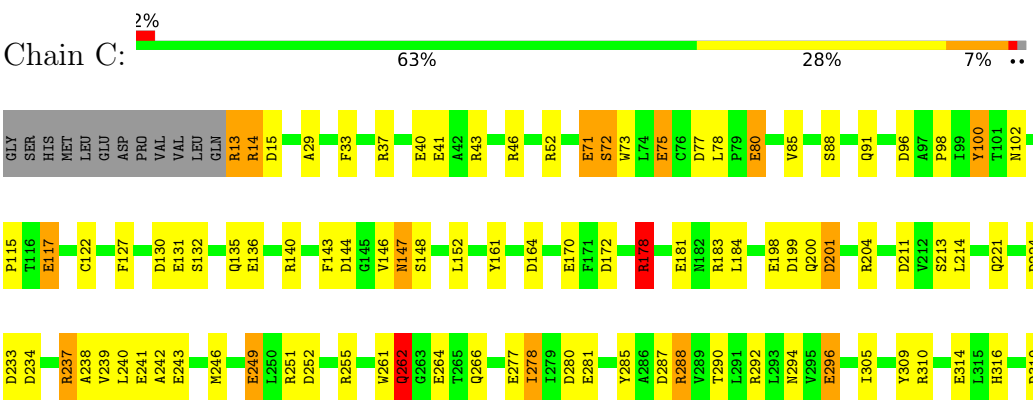
• Molecule 1: Beta-Galactosidase

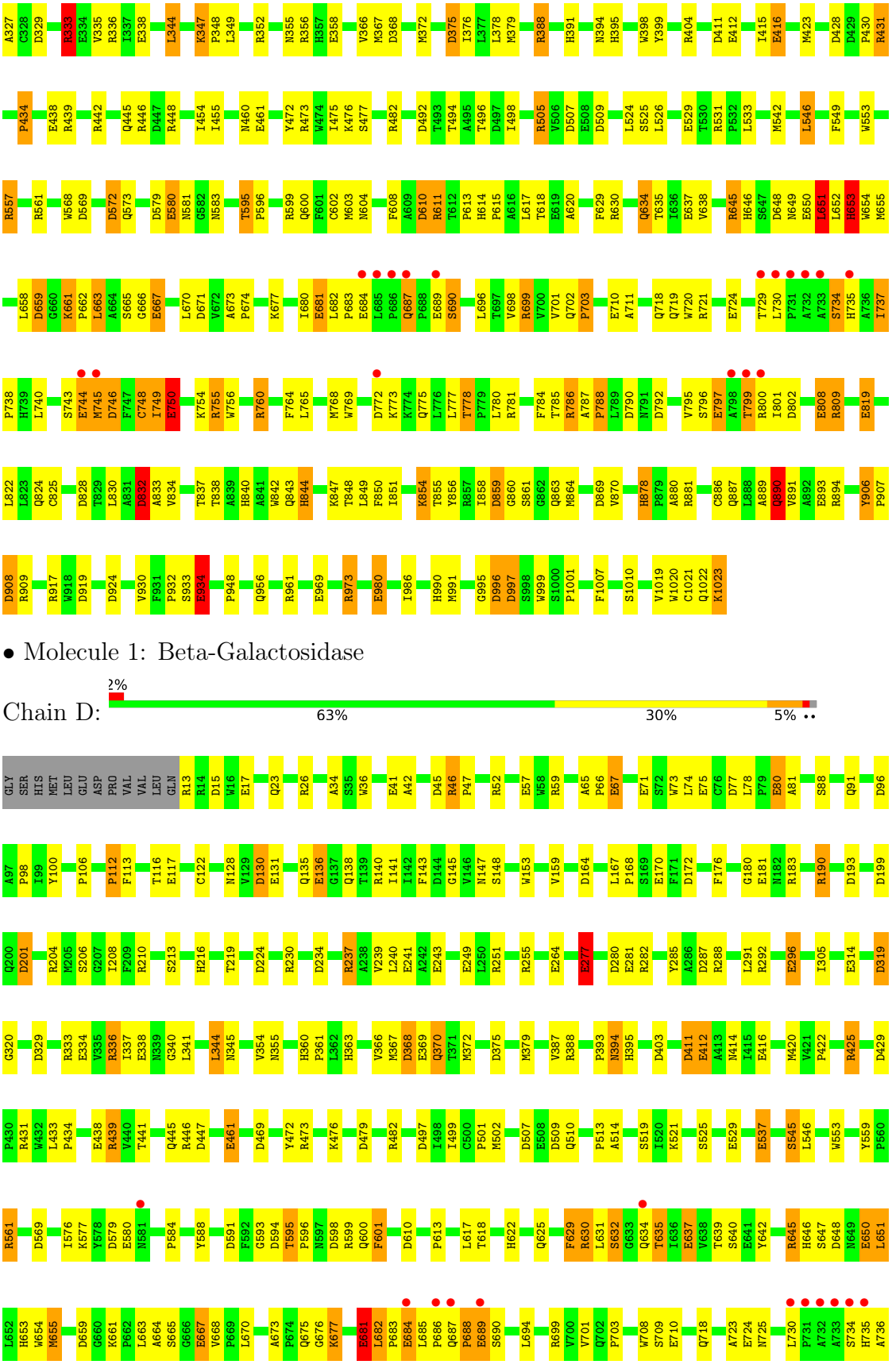
Chain B:



• Molecule 1: Beta-Galactosidase

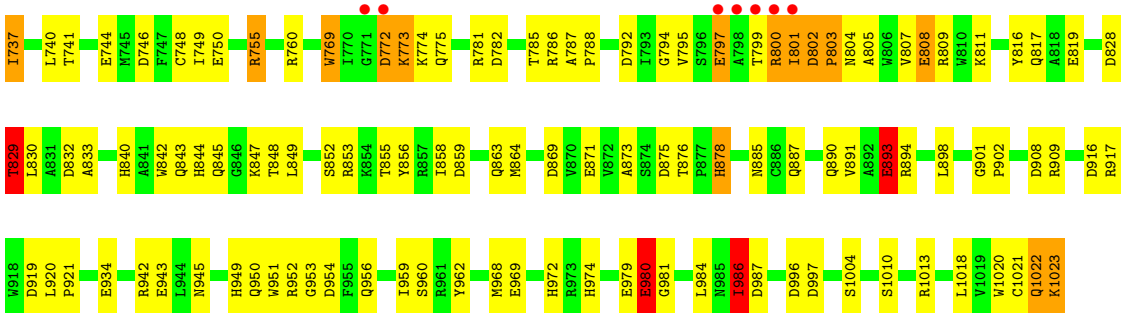
Chain C:





• Molecule 1: Beta-Galactosidase

Chain D:


I737 L740 T741 E744 M745 D746 F747 C748 I749 E750 R755 R760 W769 I770 G771 D772 K773 K774 Q775 R781 D782 T785 R786 A787 P788 D792 I793 G794 V795 S796 E797 A798 T799 R800 I801 D802 P803 N804 A805 W806 V807 E808 R809 W810 K811 Y816 Q817 A818 E819 D828
T829 L830 A831 D832 A833 H840 A841 W842 Q843 H844 Q845 G846 K847 T848 L849 S852 R853 K854 T855 Y856 R857 I858 D859 Q863 M864 D869 V870 E871 V872 A873 S874 D875 T876 P877 H878 N885 C886 Q887 Q890 V891 A892 E893 R894 L898 G901 P902 D908 R909 D916 R917
W918 D919 L920 P921 E934 R942 E943 L944 N945 H949 Q950 W951 R952 G953 D954 F955 Q956 I959 S960 R961 Y962 M968 E969 H972 R973 H974 E979 E980 G981 L984 N985 I986 D987 D996 D997 S1004 S1010 R1013 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	149.50Å 169.00Å 200.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.0 (40.00-2.10) 86.4 (19.99-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.09Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.164 , 0.267 0.152 , 0.244	Depositor DCC
R_{free} test set	3827 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å^2)	11.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 95.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36890	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 36.06 % 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 5.3009e-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, MG, 2DG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.09	43/8367 (0.5%)	1.73	174/11415 (1.5%)
1	B	1.11	48/8367 (0.6%)	1.69	165/11415 (1.4%)
1	C	1.11	42/8367 (0.5%)	1.75	177/11415 (1.6%)
1	D	1.11	48/8367 (0.6%)	1.69	151/11415 (1.3%)
All	All	1.10	181/33468 (0.5%)	1.71	667/45660 (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	B	0	1
1	D	1	0
All	All	1	1

All (181) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	277	GLU	CD-OE2	10.41	1.37	1.25
1	C	281	GLU	CD-OE2	10.15	1.36	1.25
1	D	71	GLU	CD-OE2	10.14	1.36	1.25
1	C	684	GLU	CD-OE2	9.88	1.36	1.25
1	C	296	GLU	CD-OE2	9.86	1.36	1.25
1	A	304	GLU	CD-OE2	9.53	1.36	1.25
1	A	136	GLU	CD-OE2	9.34	1.35	1.25
1	B	461	GLU	CD-OE2	8.92	1.35	1.25
1	D	243	GLU	CD-OE2	8.72	1.35	1.25
1	D	136	GLU	CD-OE2	8.49	1.34	1.25
1	A	537	GLU	CD-OE2	8.29	1.34	1.25
1	A	296	GLU	CD-OE2	8.22	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	281	GLU	CD-OE2	8.19	1.34	1.25
1	B	324	GLU	CD-OE2	7.92	1.34	1.25
1	A	249	GLU	CD-OE2	7.91	1.34	1.25
1	C	980	GLU	CD-OE2	7.74	1.34	1.25
1	D	650	GLU	CD-OE2	7.57	1.33	1.25
1	C	744	GLU	CD-OE2	7.54	1.33	1.25
1	D	681	GLU	CD-OE2	7.54	1.33	1.25
1	A	1006	GLU	CD-OE2	7.54	1.33	1.25
1	D	980	GLU	CD-OE2	7.47	1.33	1.25
1	A	281	GLU	CD-OE2	7.42	1.33	1.25
1	C	819	GLU	CD-OE2	7.40	1.33	1.25
1	D	979	GLU	CD-OE2	7.33	1.33	1.25
1	B	296	GLU	CD-OE2	7.29	1.33	1.25
1	A	243	GLU	CD-OE2	7.26	1.33	1.25
1	B	980	GLU	CD-OE2	7.26	1.33	1.25
1	A	684	GLU	CD-OE2	7.24	1.33	1.25
1	D	41	GLU	CD-OE2	7.20	1.33	1.25
1	A	689	GLU	CD-OE2	7.18	1.33	1.25
1	B	529	GLU	CD-OE2	7.18	1.33	1.25
1	D	580	GLU	CD-OE2	7.12	1.33	1.25
1	B	71	GLU	CD-OE2	7.10	1.33	1.25
1	D	893	GLU	CD-OE2	7.07	1.33	1.25
1	B	650	GLU	CD-OE2	7.03	1.33	1.25
1	B	819	GLU	CD-OE2	7.00	1.33	1.25
1	C	750	GLU	CD-OE2	6.98	1.33	1.25
1	D	969	GLU	CD-OE2	6.98	1.33	1.25
1	B	904	GLU	CD-OE1	-6.97	1.18	1.25
1	C	198	GLU	CD-OE2	6.95	1.33	1.25
1	A	57	GLU	CD-OE2	6.92	1.33	1.25
1	C	893	GLU	CD-OE2	6.89	1.33	1.25
1	B	314	GLU	CD-OE1	-6.88	1.18	1.25
1	A	71	GLU	CD-OE2	6.88	1.33	1.25
1	B	243	GLU	CD-OE2	6.86	1.33	1.25
1	C	170	GLU	CD-OE2	6.85	1.33	1.25
1	C	529	GLU	CD-OE2	6.81	1.33	1.25
1	D	296	GLU	CD-OE2	6.75	1.33	1.25
1	A	338	GLU	CD-OE2	6.73	1.33	1.25
1	A	416	GLU	CD-OE2	6.72	1.33	1.25
1	C	689	GLU	CD-OE2	6.71	1.33	1.25
1	C	710	GLU	CD-OE2	6.66	1.32	1.25
1	C	314	GLU	CD-OE2	6.64	1.32	1.25
1	C	277	GLU	CD-OE2	6.63	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	80	GLU	CD-OE2	6.61	1.32	1.25
1	D	241	GLU	CD-OE2	6.58	1.32	1.25
1	B	710	GLU	CD-OE2	6.58	1.32	1.25
1	B	969	GLU	CD-OE2	6.58	1.32	1.25
1	A	170	GLU	CD-OE2	6.58	1.32	1.25
1	C	667	GLU	CD-OE2	6.55	1.32	1.25
1	D	170	GLU	CD-OE2	6.55	1.32	1.25
1	B	117	GLU	CD-OE2	6.53	1.32	1.25
1	D	808	GLU	CD-OE2	6.50	1.32	1.25
1	C	241	GLU	CD-OE2	6.44	1.32	1.25
1	A	277	GLU	CD-OE2	6.42	1.32	1.25
1	B	580	GLU	CD-OE2	6.42	1.32	1.25
1	C	580	GLU	CD-OE2	6.39	1.32	1.25
1	A	334	GLU	CD-OE2	6.36	1.32	1.25
1	C	650	GLU	CD-OE2	6.36	1.32	1.25
1	B	637	GLU	CD-OE2	6.36	1.32	1.25
1	C	934	GLU	CD-OE2	6.35	1.32	1.25
1	B	689	GLU	CD-OE2	6.34	1.32	1.25
1	D	819	GLU	CD-OE2	6.34	1.32	1.25
1	A	637	GLU	CD-OE2	6.32	1.32	1.25
1	B	943	GLU	CD-OE2	6.31	1.32	1.25
1	A	969	GLU	CD-OE2	6.29	1.32	1.25
1	B	40	GLU	CD-OE2	6.26	1.32	1.25
1	B	684	GLU	CD-OE2	6.26	1.32	1.25
1	C	969	GLU	CD-OE2	6.26	1.32	1.25
1	B	181	GLU	CD-OE2	6.24	1.32	1.25
1	D	117	GLU	CD-OE2	6.24	1.32	1.25
1	B	264	GLU	CD-OE2	6.22	1.32	1.25
1	C	181	GLU	CD-OE2	6.22	1.32	1.25
1	B	41	GLU	CD-OE2	6.19	1.32	1.25
1	C	338	GLU	CD-OE2	6.18	1.32	1.25
1	D	934	GLU	CD-OE2	6.17	1.32	1.25
1	C	136	GLU	CD-OE2	6.14	1.32	1.25
1	C	249	GLU	CD-OE2	6.14	1.32	1.25
1	C	71	GLU	CD-OE2	6.13	1.32	1.25
1	A	117	GLU	CD-OE2	6.13	1.32	1.25
1	B	744	GLU	CD-OE2	6.12	1.32	1.25
1	D	416	GLU	CD-OE2	6.12	1.32	1.25
1	D	281	GLU	CD-OE2	6.10	1.32	1.25
1	A	893	GLU	CD-OE2	6.10	1.32	1.25
1	C	442	ARG	CZ-NH1	6.10	1.41	1.33
1	A	487	GLU	CD-OE2	6.07	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	529	GLU	CD-OE2	6.05	1.32	1.25
1	D	943	GLU	CD-OE1	-6.05	1.19	1.25
1	D	943	GLU	CD-OE2	6.05	1.32	1.25
1	C	416	GLU	CD-OE2	6.04	1.32	1.25
1	D	17	GLU	CD-OE2	6.03	1.32	1.25
1	D	684	GLU	CD-OE2	6.03	1.32	1.25
1	A	80	GLU	CD-OE2	6.02	1.32	1.25
1	D	797	GLU	CD-OE2	6.00	1.32	1.25
1	D	537	GLU	CD-OE2	6.00	1.32	1.25
1	A	819	GLU	CD-OE2	5.98	1.32	1.25
1	C	681	GLU	CD-OE2	5.96	1.32	1.25
1	D	438	GLU	CD-OE2	5.94	1.32	1.25
1	A	580	GLU	CD-OE2	5.92	1.32	1.25
1	D	529	GLU	CD-OE2	5.92	1.32	1.25
1	A	750	GLU	CD-OE2	5.92	1.32	1.25
1	C	461	GLU	CD-OE2	5.91	1.32	1.25
1	C	75	GLU	CD-OE2	5.91	1.32	1.25
1	C	41	GLU	CD-OE2	5.87	1.32	1.25
1	B	334	GLU	CD-OE2	5.86	1.32	1.25
1	D	131	GLU	CD-OE2	5.84	1.32	1.25
1	D	249	GLU	CD-OE2	5.84	1.32	1.25
1	A	710	GLU	CD-OE2	5.84	1.32	1.25
1	B	1006	GLU	CD-OE2	5.84	1.32	1.25
1	B	893	GLU	CD-OE2	5.83	1.32	1.25
1	B	277	GLU	CD-OE2	5.82	1.32	1.25
1	B	724	GLU	CD-OE2	5.80	1.32	1.25
1	B	667	GLU	CD-OE2	5.80	1.32	1.25
1	D	750	GLU	CD-OE2	5.76	1.31	1.25
1	A	980	GLU	CD-OE2	5.76	1.31	1.25
1	B	797	GLU	CD-OE2	5.76	1.31	1.25
1	D	75	GLU	CD-OE2	5.75	1.31	1.25
1	A	369	GLU	CD-OE2	5.75	1.31	1.25
1	C	264	GLU	CD-OE2	5.72	1.31	1.25
1	C	412	GLU	CD-OE2	5.72	1.31	1.25
1	D	264	GLU	CD-OE2	5.71	1.31	1.25
1	A	724	GLU	CD-OE2	5.68	1.31	1.25
1	A	131	GLU	CD-OE2	5.67	1.31	1.25
1	B	241	GLU	CD-OE2	5.65	1.31	1.25
1	B	75	GLU	CD-OE2	5.64	1.31	1.25
1	B	170	GLU	CD-OE2	5.63	1.31	1.25
1	B	487	GLU	CD-OE2	5.61	1.31	1.25
1	B	326	GLU	CD-OE2	5.57	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	369	GLU	CD-OE2	5.57	1.31	1.25
1	D	710	GLU	CD-OE2	5.57	1.31	1.25
1	C	358	GLU	CD-OE2	5.57	1.31	1.25
1	C	797	GLU	CD-OE2	5.57	1.31	1.25
1	D	744	GLU	CD-OE2	5.57	1.31	1.25
1	A	979	GLU	CD-OE2	5.56	1.31	1.25
1	A	264	GLU	CD-OE2	5.55	1.31	1.25
1	C	243	GLU	CD-OE2	5.55	1.31	1.25
1	D	314	GLU	CD-OE2	5.54	1.31	1.25
1	D	338	GLU	CD-OE2	5.53	1.31	1.25
1	B	249	GLU	CD-OE2	5.52	1.31	1.25
1	B	80	GLU	CD-OE2	5.51	1.31	1.25
1	B	57	GLU	CD-OE2	5.46	1.31	1.25
1	D	461	GLU	CD-OE2	5.46	1.31	1.25
1	B	979	GLU	CD-OE2	5.44	1.31	1.25
1	D	871	GLU	CD-OE2	5.43	1.31	1.25
1	A	508	GLU	CD-OE2	5.39	1.31	1.25
1	A	681	GLU	CD-OE2	5.37	1.31	1.25
1	A	461	GLU	CD-OE2	5.36	1.31	1.25
1	D	667	GLU	CD-OE2	5.35	1.31	1.25
1	A	369	GLU	CD-OE1	-5.34	1.19	1.25
1	B	17	GLU	CD-OE1	-5.29	1.19	1.25
1	D	369	GLU	CD-OE2	5.27	1.31	1.25
1	A	667	GLU	CD-OE2	5.25	1.31	1.25
1	A	934	GLU	CD-OE2	5.23	1.31	1.25
1	D	637	GLU	CD-OE2	5.20	1.31	1.25
1	B	750	GLU	CD-OE2	5.16	1.31	1.25
1	B	304	GLU	CD-OE1	-5.15	1.20	1.25
1	A	40	GLU	CD-OE2	5.14	1.31	1.25
1	C	438	GLU	CD-OE2	5.14	1.31	1.25
1	D	689	GLU	CD-OE1	-5.14	1.20	1.25
1	D	57	GLU	CD-OE2	5.13	1.31	1.25
1	C	808	GLU	CD-OE2	5.13	1.31	1.25
1	C	80	GLU	CD-OE2	5.12	1.31	1.25
1	A	181	GLU	CD-OE2	5.11	1.31	1.25
1	A	334	GLU	CD-OE1	-5.11	1.20	1.25
1	D	181	GLU	CD-OE2	5.08	1.31	1.25
1	C	324	GLU	CD-OE2	5.08	1.31	1.25
1	B	131	GLU	CD-OE2	5.05	1.31	1.25
1	C	117	GLU	CD-OE2	5.03	1.31	1.25
1	D	412	GLU	CD-OE2	5.01	1.31	1.25
1	B	561	ARG	NE-CZ	5.01	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	GLU	CD-OE2	5.00	1.31	1.25

All (667) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	809	ARG	NE-CZ-NH1	19.72	130.16	120.30
1	C	442	ARG	NE-CZ-NH2	-17.27	111.67	120.30
1	C	786	ARG	NE-CZ-NH1	15.02	127.81	120.30
1	C	721	ARG	NE-CZ-NH1	15.00	127.80	120.30
1	A	46	ARG	NE-CZ-NH1	15.00	127.80	120.30
1	B	881	ARG	NE-CZ-NH1	14.60	127.60	120.30
1	D	561	ARG	NE-CZ-NH1	12.89	126.74	120.30
1	C	43	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	D	630	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	D	172	ASP	CB-CG-OD2	-12.37	107.17	118.30
1	A	280	ASP	CB-CG-OD2	-12.26	107.26	118.30
1	C	280	ASP	CB-CG-OD2	-12.24	107.29	118.30
1	C	630	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	D	224	ASP	CB-CG-OD1	11.97	129.07	118.30
1	C	611	ARG	NE-CZ-NH1	11.93	126.26	120.30
1	C	786	ARG	NE-CZ-NH2	-11.91	114.35	120.30
1	B	252	ASP	CB-CG-OD2	-11.85	107.64	118.30
1	A	37	ARG	NE-CZ-NH1	11.76	126.18	120.30
1	C	204	ARG	NE-CZ-NH1	11.65	126.12	120.30
1	A	699	ARG	NE-CZ-NH2	-11.63	114.48	120.30
1	D	802	ASP	C-N-CD	-11.56	95.17	120.60
1	C	809	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	A	909	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	A	699	ARG	NE-CZ-NH1	11.38	125.99	120.30
1	D	429	ASP	CB-CG-OD1	11.37	128.53	118.30
1	C	230	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	C	310	ARG	NE-CZ-NH1	11.21	125.91	120.30
1	A	497	ASP	CB-CG-OD1	11.20	128.38	118.30
1	B	772	ASP	CB-CG-OD2	-11.13	108.28	118.30
1	D	172	ASP	CB-CG-OD1	11.09	128.28	118.30
1	D	255	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	A	497	ASP	CB-CG-OD2	-10.84	108.54	118.30
1	B	193	ASP	CB-CG-OD1	10.80	128.02	118.30
1	B	772	ASP	CB-CG-OD1	10.73	127.96	118.30
1	C	973	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	A	144	ASP	CB-CG-OD1	10.68	127.92	118.30
1	A	37	ARG	NE-CZ-NH2	-10.52	115.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	287	ASP	CB-CG-OD1	10.48	127.73	118.30
1	B	869	ASP	CB-CG-OD1	10.40	127.66	118.30
1	D	336	ARG	NE-CZ-NH1	10.40	125.50	120.30
1	A	439	ARG	NE-CZ-NH1	10.36	125.48	120.30
1	D	786	ARG	NE-CZ-NH2	-10.31	115.15	120.30
1	A	292	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	B	336	ARG	NE-CZ-NH1	10.23	125.41	120.30
1	B	572	ASP	CB-CG-OD2	-10.19	109.13	118.30
1	C	439	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	C	140	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	A	509	ASP	CB-CG-OD2	-10.09	109.22	118.30
1	C	85	VAL	CA-CB-CG2	-10.02	95.88	110.90
1	C	909	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	A	166	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	D	368	ASP	CB-CG-OD2	-9.86	109.43	118.30
1	C	336	ARG	NE-CZ-NH1	9.85	125.22	120.30
1	B	671	ASP	CB-CG-OD2	-9.80	109.47	118.30
1	C	996	ASP	CB-CG-OD2	-9.77	109.51	118.30
1	C	411	ASP	CB-CG-OD2	-9.76	109.51	118.30
1	C	310	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	A	997	ASP	CB-CG-OD2	-9.72	109.55	118.30
1	D	193	ASP	CB-CG-OD1	9.71	127.03	118.30
1	D	594	ASP	CB-CG-OD2	-9.67	109.59	118.30
1	D	782	ASP	CB-CG-OD2	-9.67	109.60	118.30
1	D	429	ASP	CB-CG-OD2	-9.66	109.61	118.30
1	A	201	ASP	CB-CG-OD2	-9.66	109.61	118.30
1	D	853	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	403	ASP	CB-CG-OD2	-9.61	109.66	118.30
1	B	721	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	A	916	ASP	CB-CG-OD2	-9.58	109.68	118.30
1	A	224	ASP	CB-CG-OD1	9.55	126.89	118.30
1	B	172	ASP	CB-CG-OD1	9.53	126.88	118.30
1	C	233	ASP	CB-CG-OD2	-9.48	109.77	118.30
1	B	492	ASP	CB-CG-OD1	9.48	126.83	118.30
1	A	439	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	B	329	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	A	987	ASP	CB-CG-OD2	-9.37	109.87	118.30
1	A	916	ASP	CB-CG-OD1	9.37	126.73	118.30
1	D	507	ASP	CB-CG-OD2	-9.36	109.88	118.30
1	C	973	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	166	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	A	233	ASP	CB-CG-OD1	9.32	126.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	403	ASP	CB-CG-OD1	9.32	126.69	118.30
1	A	610	ASP	CB-CG-OD1	9.31	126.68	118.30
1	D	45	ASP	CB-CG-OD1	9.26	126.63	118.30
1	A	755	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	D	699	ARG	NE-CZ-NH1	9.25	124.92	120.30
1	B	687	GLN	C-N-CD	-9.24	100.27	120.60
1	C	288	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	A	356	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	561	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	D	329	ASP	CB-CG-OD2	-9.19	110.03	118.30
1	B	469	ASP	CB-CG-OD1	9.15	126.54	118.30
1	C	375	ASP	CB-CG-OD1	9.11	126.50	118.30
1	C	531	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	C	172	ASP	CB-CG-OD1	9.08	126.47	118.30
1	B	881	ARG	NE-CZ-NH2	-9.06	115.77	120.30
1	B	755	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	D	287	ASP	CB-CG-OD2	-9.05	110.16	118.30
1	A	859	ASP	CB-CG-OD1	9.02	126.41	118.30
1	C	333	ARG	NE-CZ-NH1	-9.02	115.79	120.30
1	A	46	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	C	13	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	D	439	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	A	509	ASP	CB-CG-OD1	8.99	126.39	118.30
1	A	442	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	B	319	ASP	CB-CG-OD2	-8.97	110.22	118.30
1	C	448	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	D	507	ASP	CB-CG-OD1	8.95	126.36	118.30
1	C	199	ASP	CB-CG-OD1	8.84	126.25	118.30
1	D	829	THR	N-CA-CB	8.83	127.08	110.30
1	C	579	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	D	781	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	C	645	ARG	NE-CZ-NH2	-8.75	115.93	120.30
1	D	792	ASP	CB-CG-OD1	8.74	126.17	118.30
1	D	800	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	C	748	CYS	CA-CB-SG	-8.70	98.34	114.00
1	A	782	ASP	CB-CG-OD2	-8.60	110.56	118.30
1	B	630	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	411	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	A	130	ASP	CB-CG-OD1	8.54	125.99	118.30
1	B	942	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	C	553	TRP	CA-CB-CG	-8.53	97.50	113.70
1	B	659	ASP	CB-CG-OD2	-8.52	110.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	233	ASP	CB-CG-OD1	8.48	125.94	118.30
1	A	908	ASP	CB-CG-OD1	8.45	125.91	118.30
1	D	15	ASP	CB-CG-OD2	-8.45	110.69	118.30
1	B	166	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	172	ASP	CB-CG-OD1	8.44	125.90	118.30
1	D	224	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	A	319	ASP	CB-CG-OD2	-8.44	110.70	118.30
1	A	987	ASP	CB-CG-OD1	8.42	125.88	118.30
1	D	193	ASP	CB-CG-OD2	-8.42	110.72	118.30
1	D	875	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	D	786	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	B	287	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	A	853	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	D	648	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	C	645	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	A	721	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	531	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	869	ASP	CB-CG-OD2	-8.25	110.87	118.30
1	B	659	ASP	CB-CG-OD1	8.25	125.72	118.30
1	C	961	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	B	648	ASP	CB-CG-OD1	8.20	125.68	118.30
1	D	439	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	D	952	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	C	368	ASP	CB-CG-OD2	-8.15	110.96	118.30
1	B	869	ASP	CB-CG-OD2	-8.15	110.97	118.30
1	C	599	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	996	ASP	CB-CG-OD2	-8.13	110.99	118.30
1	C	855	THR	N-CA-CB	8.12	125.74	110.30
1	B	319	ASP	CB-CG-OD1	8.12	125.61	118.30
1	D	689	GLU	N-CA-CB	8.12	125.21	110.60
1	C	352	ARG	NE-CZ-NH2	-8.09	116.26	120.30
1	C	428	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	C	505	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	A	611	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	492	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	D	411	ASP	CB-CG-OD2	-8.05	111.06	118.30
1	B	919	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	C	199	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	A	190	ARG	NE-CZ-NH2	-8.03	116.29	120.30
1	D	204	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	B	469	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	C	996	ASP	CB-CG-OD1	7.97	125.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	997	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	D	255	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	233	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	C	572	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	A	287	ASP	CB-CG-OD1	7.95	125.45	118.30
1	A	292	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	D	287	ASP	CB-CG-OD1	7.94	125.44	118.30
1	B	429	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	648	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	77	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	C	442	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	908	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	721	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	C	204	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	D	997	ASP	N-CA-CB	7.78	124.59	110.60
1	C	448	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	507	ASP	CB-CG-OD1	7.76	125.28	118.30
1	C	699	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	C	630	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	632	SER	N-CA-CB	7.74	122.12	110.50
1	A	280	ASP	CB-CG-OD1	7.73	125.25	118.30
1	B	199	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	C	230	ARG	NE-CZ-NH2	-7.73	116.44	120.30
1	A	234	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	201	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	553	TRP	CA-CB-CG	-7.70	99.07	113.70
1	D	875	ASP	CB-CG-OD1	7.70	125.23	118.30
1	B	786	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	469	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	572	ASP	CB-CG-OD2	-7.68	111.38	118.30
1	B	832	ASP	CB-CG-OD1	7.68	125.22	118.30
1	A	267	VAL	CG1-CB-CG2	-7.67	98.63	110.90
1	A	130	ASP	CB-CG-OD2	-7.66	111.40	118.30
1	C	388	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	497	ASP	CB-CG-OD1	7.64	125.17	118.30
1	C	280	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	199	ASP	CB-CG-OD1	7.63	125.17	118.30
1	A	809	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	908	ASP	CB-CG-OD2	-7.59	111.47	118.30
1	D	594	ASP	CB-CG-OD1	7.59	125.13	118.30
1	D	952	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	234	ASP	CB-CG-OD2	-7.58	111.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	997	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	A	741	THR	CA-CB-CG2	-7.56	101.81	112.40
1	B	375	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	287	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	B	28	ALA	CB-CA-C	-7.56	98.77	110.10
1	A	469	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	B	292	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	D	632	SER	N-CA-CB	7.55	121.83	110.50
1	A	234	ASP	CB-CG-OD1	7.54	125.08	118.30
1	C	234	ASP	CB-CG-OD1	7.54	125.08	118.30
1	C	659	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	C	859	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	D	859	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	D	832	ASP	CB-CG-OD1	7.52	125.07	118.30
1	C	224	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	172	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	492	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	D	802	ASP	CB-CG-OD2	-7.48	111.56	118.30
1	A	123	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	C	172	ASP	CB-CG-OD2	-7.47	111.57	118.30
1	C	832	ASP	CB-CG-OD1	7.47	125.02	118.30
1	B	802	ASP	CB-CG-OD1	7.46	125.02	118.30
1	A	786	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	D	659	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	429	ASP	CB-CG-OD1	7.42	124.98	118.30
1	B	611	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	569	ASP	CB-CG-OD1	7.37	124.93	118.30
1	A	404	ARG	NE-CZ-NH1	7.37	123.98	120.30
1	B	164	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	A	755	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	B	356	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	917	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	B	610	ASP	CB-CG-OD1	7.30	124.87	118.30
1	D	96	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	B	82	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	991	MET	CG-SD-CE	7.29	111.86	100.20
1	C	721	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	D	1018	LEU	CB-CA-C	-7.24	96.45	110.20
1	C	144	ASP	CB-CG-OD1	7.24	124.81	118.30
1	B	1013	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	D	403	ASP	CB-CG-OD1	7.23	124.80	118.30
1	A	802	ASP	CB-CG-OD2	-7.22	111.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	594	ASP	CB-CG-OD1	7.22	124.80	118.30
1	B	368	ASP	CB-CG-OD1	7.21	124.79	118.30
1	D	859	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	178	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	599	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	43	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	D	997	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	B	832	ASP	N-CA-CB	-7.16	97.71	110.60
1	A	164	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	C	579	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	15	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	D	46	ARG	NE-CZ-NH1	7.13	123.87	120.30
1	C	505	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	C	961	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	D	645	ARG	NE-CZ-NH1	-7.11	116.74	120.30
1	B	439	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	A	1013	ARG	NE-CZ-NH2	7.11	123.85	120.30
1	A	997	ASP	CB-CG-OD1	7.11	124.70	118.30
1	C	140	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	B	832	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	B	144	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	479	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	B	140	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	D	746	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	648	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	B	411	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	D	553	TRP	CA-CB-CG	-7.03	100.34	113.70
1	A	448	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	D	869	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	B	746	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	D	828	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	B	561	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	368	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	A	859	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	C	428	ASP	CB-CG-OD1	6.95	124.56	118.30
1	A	786	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	659	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	B	375	ASP	CB-CG-OD1	6.93	124.54	118.30
1	D	853	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	368	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	C	659	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	610	ASP	CB-CG-OD2	-6.92	112.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	916	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	C	997	ASP	N-CA-CB	6.92	123.05	110.60
1	A	447	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	A	828	ASP	CB-CG-OD2	-6.89	112.09	118.30
1	A	632	SER	N-CA-CB	6.88	120.83	110.50
1	D	782	ASP	CB-CG-OD1	6.88	124.50	118.30
1	B	356	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	C	164	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	210	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	555	ALA	CB-CA-C	-6.86	99.81	110.10
1	D	190	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	C	997	ASP	CB-CG-OD1	6.84	124.46	118.30
1	D	282	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	B	553	TRP	CA-CB-CG	-6.83	100.73	113.70
1	C	52	ARG	NE-CZ-NH2	6.83	123.71	120.30
1	B	185	ALA	N-CA-CB	6.82	119.64	110.10
1	C	492	ASP	CB-CG-OD1	6.82	124.43	118.30
1	A	579	ASP	CB-CG-OD1	6.81	124.43	118.30
1	D	832	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	C	161	TYR	CB-CG-CD2	-6.77	116.94	121.00
1	A	164	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	926	TYR	CB-CG-CD1	6.76	125.05	121.00
1	B	572	ASP	CB-CG-OD1	6.75	124.38	118.30
1	A	569	ASP	CB-CG-OD1	6.75	124.37	118.30
1	B	519	SER	N-CA-CB	-6.73	100.40	110.50
1	C	144	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	D	319	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	B	958	ASN	N-CA-CB	6.71	122.68	110.60
1	A	952	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	579	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	B	336	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	B	505	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	809	ARG	CD-NE-CZ	6.65	132.91	123.60
1	A	237	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	C	352	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	746	ASP	CB-CG-OD2	-6.63	112.34	118.30
1	D	368	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	368	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	642	TYR	CB-CG-CD2	-6.61	117.04	121.00
1	B	594	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	828	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	D	431	ARG	NE-CZ-NH1	6.60	123.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	ASP	CB-CG-OD1	6.59	124.23	118.30
1	D	569	ASP	CB-CG-OD2	-6.58	112.37	118.30
1	D	201	ASP	CB-CG-OD2	-6.58	112.37	118.30
1	B	595	THR	CA-CB-CG2	-6.58	103.19	112.40
1	D	579	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	B	671	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	210	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	352	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	D	610	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	C	77	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	859	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	B	172	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	411	ASP	CB-CG-OD1	6.50	124.15	118.30
1	D	699	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	D	987	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	473	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	C	399	TYR	CB-CG-CD2	-6.45	117.13	121.00
1	B	144	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	446	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	C	671	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	699	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	B	46	ARG	CD-NE-CZ	-6.41	114.63	123.60
1	B	233	ASP	CB-CG-OD1	6.40	124.06	118.30
1	D	792	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	A	356	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	285	TYR	CB-CG-CD1	-6.39	117.17	121.00
1	A	771	GLY	N-CA-C	-6.38	97.14	113.10
1	C	832	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	B	996	ASP	CB-CG-OD1	6.36	124.02	118.30
1	C	130	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	D	15	ASP	CB-CG-OD1	6.34	124.00	118.30
1	B	285	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	D	411	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	869	ASP	CB-CG-OD1	6.33	124.00	118.30
1	C	924	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	D	77	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	557	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	C	333	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	B	442	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	411	ASP	CB-CG-OD1	6.29	123.97	118.30
1	C	1019	VAL	CA-CB-CG1	-6.29	101.47	110.90
1	C	183	ARG	NE-CZ-NH2	-6.28	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	924	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	997	ASP	N-CA-CB	6.27	121.88	110.60
1	A	285	TYR	CD1-CE1-CZ	-6.27	114.16	119.80
1	A	233	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	C	375	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	A	211	ASP	CB-CG-OD1	6.26	123.93	118.30
1	D	916	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	130	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	A	123	TYR	CB-CG-CD1	6.22	124.73	121.00
1	D	319	ASP	CB-CG-OD1	6.22	123.90	118.30
1	A	782	ASP	CB-CG-OD1	6.22	123.90	118.30
1	C	648	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	288	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	C	890	GLN	N-CA-CB	-6.20	99.44	110.60
1	B	908	ASP	CB-CG-OD1	6.19	123.87	118.30
1	A	375	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	D	469	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	59	ARG	NE-CZ-NH1	-6.17	117.21	120.30
1	C	859	ASP	CB-CG-OD1	6.17	123.86	118.30
1	B	237	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	429	ASP	CB-CG-OD1	6.16	123.85	118.30
1	C	77	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	B	875	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	B	497	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	C	183	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	A	507	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	D	183	ARG	NE-CZ-NH1	-6.14	117.23	120.30
1	C	557	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	225	PHE	N-CA-CB	6.13	121.63	110.60
1	C	399	TYR	CB-CG-CD1	6.12	124.67	121.00
1	B	926	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	C	703	PRO	N-CA-CB	6.11	110.64	103.30
1	A	954	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	B	166	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	D	986	ILE	CG1-CB-CG2	-6.10	97.98	111.40
1	D	908	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	B	210	ARG	N-CA-CB	6.09	121.56	110.60
1	B	52	ARG	CB-CA-C	-6.09	98.22	110.40
1	C	610	ASP	CB-CG-OD1	6.09	123.78	118.30
1	B	412	GLU	OE1-CD-OE2	-6.08	116.00	123.30
1	D	772	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	D	479	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	D	746	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	183	ARG	NE-CZ-NH1	-6.07	117.26	120.30
1	A	958	ASN	N-CA-CB	6.07	121.53	110.60
1	C	699	ARG	CB-CA-C	-6.07	98.26	110.40
1	A	630	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	352	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	D	96	ASP	CB-CG-OD1	6.06	123.75	118.30
1	A	477	SER	N-CA-CB	6.05	119.58	110.50
1	D	394	ASN	N-CA-CB	-6.05	99.71	110.60
1	D	100	TYR	N-CA-CB	6.05	121.49	110.60
1	C	648	ASP	CB-CG-OD1	6.03	123.72	118.30
1	C	482	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	C	894	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	D	190	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	D	855	THR	N-CA-CB	6.00	121.70	110.30
1	A	615	PRO	N-CA-CB	6.00	110.50	103.30
1	B	809	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	853	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	D	787	ALA	N-CA-CB	-5.97	101.74	110.10
1	A	411	ASP	CB-CG-OD1	5.96	123.67	118.30
1	C	772	ASP	CB-CG-OD1	5.96	123.67	118.30
1	D	52	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	40	GLU	CG-CD-OE1	5.96	130.22	118.30
1	D	497	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	809	ARG	N-CA-CB	-5.95	99.89	110.60
1	A	572	ASP	CB-CG-OD1	5.95	123.65	118.30
1	D	431	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	100	TYR	CB-CG-CD2	5.94	124.56	121.00
1	A	875	ASP	CB-CG-OD2	-5.94	112.96	118.30
1	A	802	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	147	ASN	N-CA-CB	-5.92	99.94	110.60
1	D	479	ASP	CB-CG-OD1	5.92	123.63	118.30
1	D	140	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	A	144	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	77	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	329	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	917	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	D	601	PHE	CA-CB-CG	-5.90	99.73	113.90
1	B	321	THR	CA-CB-CG2	-5.90	104.14	112.40
1	B	507	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	329	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	651	LEU	N-CA-CB	5.88	122.15	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	828	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	611	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	782	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	82	ASP	CB-CG-OD1	5.84	123.56	118.30
1	D	234	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	255	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	663	LEU	CB-CA-C	-5.82	99.15	110.20
1	D	996	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	252	ASP	CB-CG-OD1	5.79	123.52	118.30
1	C	294	ASN	CA-CB-CG	-5.79	100.66	113.40
1	C	772	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	D	856	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	C	919	ASP	CB-CG-OD1	5.77	123.50	118.30
1	A	869	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	579	ASP	CB-CG-OD1	5.77	123.49	118.30
1	C	546	LEU	N-CA-CB	5.75	121.91	110.40
1	D	509	ASP	CB-CG-OD1	5.75	123.47	118.30
1	D	199	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	A	1019	VAL	CA-CB-CG2	-5.74	102.29	110.90
1	B	699	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	859	ASP	CB-CG-OD1	5.73	123.46	118.30
1	C	494	THR	CA-CB-CG2	-5.73	104.37	112.40
1	C	909	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	611	ARG	N-CA-CB	5.73	120.91	110.60
1	D	694	LEU	CB-CG-CD1	-5.72	101.28	111.00
1	A	13	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	D	878	HIS	CA-CB-CG	-5.71	103.89	113.60
1	C	792	ASP	CB-CG-OD2	-5.71	113.17	118.30
1	D	420	MET	CG-SD-CE	-5.71	91.07	100.20
1	A	185	ALA	N-CA-CB	5.69	118.07	110.10
1	A	221	GLN	N-CA-CB	-5.69	100.36	110.60
1	C	13	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	610	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	D	71	GLU	CB-CA-C	5.67	121.73	110.40
1	C	509	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	C	431	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	193	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	D	648	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	894	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	C	690	SER	N-CA-CB	-5.64	102.05	110.50
1	C	869	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	790	ASP	CB-CG-OD1	5.63	123.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	428	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	672	VAL	CB-CA-C	-5.60	100.76	111.40
1	B	308	LEU	CB-CA-C	-5.60	99.56	110.20
1	D	319	ASP	N-CA-CB	5.59	120.66	110.60
1	A	211	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	319	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	568	TRP	CA-CB-CG	-5.57	103.11	113.70
1	B	952	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	507	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	881	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	699	ARG	NH1-CZ-NH2	-5.54	113.30	119.40
1	C	844	HIS	CA-CB-CG	-5.54	104.18	113.60
1	D	77	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	34	ALA	N-CA-CB	5.54	117.85	110.10
1	B	211	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	15	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	147	ASN	N-CA-CB	-5.53	100.65	110.60
1	A	408	TYR	CB-CG-CD1	5.53	124.32	121.00
1	C	52	ARG	CB-CA-C	-5.53	99.35	110.40
1	C	908	ASP	CB-CG-OD1	5.53	123.27	118.30
1	D	469	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	651	LEU	N-CA-CB	5.49	121.39	110.40
1	B	721	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	D	802	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	161	TYR	CB-CG-CD1	-5.49	117.71	121.00
1	B	509	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	A	329	ASP	CB-CG-OD1	5.47	123.23	118.30
1	A	292	ARG	CD-NE-CZ	5.47	131.26	123.60
1	C	15	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	439	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	D	130	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	917	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	D	760	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	A	506	VAL	CA-CB-CG1	-5.45	102.72	110.90
1	A	1018	LEU	CB-CA-C	-5.44	99.86	110.20
1	C	659	ASP	N-CA-CB	5.44	120.39	110.60
1	C	446	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	882	ILE	CA-CB-CG1	-5.42	100.70	111.00
1	B	938	ARG	N-CA-CB	5.42	120.36	110.60
1	B	842	TRP	CB-CA-C	-5.42	99.56	110.40
1	A	685	LEU	CB-CA-C	5.42	120.50	110.20
1	B	833	ALA	N-CA-CB	-5.42	102.52	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	VAL	CA-CB-CG1	-5.42	102.78	110.90
1	A	832	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	828	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	878	HIS	CA-CB-CG	-5.41	104.41	113.60
1	D	772	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	1021	CYS	CA-CB-SG	-5.40	104.28	114.00
1	B	78	LEU	C-N-CD	-5.40	108.72	120.60
1	B	629	PHE	CB-CA-C	-5.40	99.61	110.40
1	C	434	PRO	N-CA-CB	5.39	109.77	103.30
1	B	428	ASP	CB-CG-OD1	5.37	123.14	118.30
1	C	745	MET	CB-CA-C	5.37	121.15	110.40
1	C	14	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	287	ASP	CB-CG-OD1	5.37	123.13	118.30
1	C	113	PHE	CB-CG-CD2	-5.36	117.05	120.80
1	B	946	TYR	CB-CG-CD1	5.36	124.22	121.00
1	D	840	HIS	CB-CA-C	-5.36	99.69	110.40
1	D	987	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	B	221	GLN	N-CA-CB	-5.35	100.98	110.60
1	A	996	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	908	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	164	ASP	CB-CG-OD1	5.34	123.10	118.30
1	B	234	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	769	TRP	N-CA-CB	5.33	120.19	110.60
1	D	800	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	A	675	GLN	N-CA-CB	5.33	120.19	110.60
1	B	161	TYR	N-CA-CB	-5.32	101.03	110.60
1	C	319	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	D	659	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	438	GLU	CG-CD-OE2	-5.31	107.68	118.30
1	C	854	LYS	CB-CA-C	-5.30	99.79	110.40
1	D	425	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	A	447	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	244	VAL	CA-CB-CG1	5.29	118.84	110.90
1	C	201	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	A	17	GLU	CG-CD-OE2	-5.29	107.72	118.30
1	B	128	ASN	CB-CA-C	-5.28	99.84	110.40
1	B	760	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	D	80	GLU	CG-CD-OE2	-5.27	107.75	118.30
1	C	33	PHE	CB-CA-C	-5.27	99.86	110.40
1	D	919	ASP	CB-CG-OD1	5.26	123.04	118.30
1	C	131	GLU	CG-CD-OE1	5.26	128.83	118.30
1	D	446	ARG	NE-CZ-NH1	5.26	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	864	MET	CG-SD-CE	5.26	108.61	100.20
1	C	438	GLU	CB-CA-C	-5.26	99.89	110.40
1	A	796	SER	N-CA-CB	5.26	118.39	110.50
1	C	653	HIS	N-CA-CB	5.25	120.06	110.60
1	A	645	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	D	723	ALA	N-CA-CB	5.25	117.45	110.10
1	C	164	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	100	TYR	CB-CG-CD1	-5.24	117.85	121.00
1	B	403	ASP	CB-CA-C	-5.24	99.91	110.40
1	D	800	ARG	CD-NE-CZ	5.24	130.94	123.60
1	A	840	HIS	CB-CA-C	-5.24	99.92	110.40
1	C	262	GLN	N-CA-C	-5.24	96.86	111.00
1	D	320	GLY	C-N-CA	-5.24	108.61	121.70
1	B	753	ASN	CA-CB-CG	-5.23	101.89	113.40
1	B	973	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	C	786	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	853	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	113	PHE	CA-CB-CG	-5.22	101.37	113.90
1	A	179	ALA	N-CA-CB	5.22	117.41	110.10
1	B	559	TYR	CB-CG-CD1	5.22	124.13	121.00
1	C	507	ASP	CB-CG-OD2	-5.22	113.61	118.30
1	D	52	ARG	CB-CA-C	-5.22	99.97	110.40
1	D	199	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	569	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	347	LYS	CB-CA-C	-5.21	99.98	110.40
1	A	96	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	572	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	234	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	C	524	LEU	CB-CG-CD1	-5.20	102.16	111.00
1	A	952	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	253	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	C	721	ARG	CD-NE-CZ	5.20	130.88	123.60
1	C	919	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	D	510	GLN	N-CA-C	-5.19	96.98	111.00
1	A	828	ASP	CB-CG-OD1	5.18	122.96	118.30
1	C	211	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	792	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	C	760	ARG	N-CA-CB	5.17	119.90	110.60
1	A	82	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	D	482	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	261	TRP	CB-CA-C	-5.15	100.09	110.40
1	D	755	ARG	NE-CZ-NH1	5.15	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	559	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	C	100	TYR	CB-CG-CD1	5.14	124.09	121.00
1	D	559	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	B	164	ASP	N-CA-CB	5.14	119.86	110.60
1	C	856	TYR	CG-CD2-CE2	-5.14	117.19	121.30
1	B	381	GLN	CA-CB-CG	-5.14	102.09	113.40
1	B	954	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	598	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	769	TRP	CB-CA-C	-5.12	100.16	110.40
1	A	368	ASP	CB-CG-OD1	5.12	122.90	118.30
1	B	875	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	67	GLU	CG-CD-OE2	-5.11	108.08	118.30
1	A	375	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	363	HIS	CA-CB-CG	-5.09	104.94	113.60
1	B	546	LEU	N-CA-CB	5.09	120.59	110.40
1	A	352	ARG	CG-CD-NE	5.09	122.49	111.80
1	D	629	PHE	CB-CA-C	-5.09	100.22	110.40
1	C	473	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	C	788	PRO	N-CA-CB	5.08	109.40	103.30
1	B	503	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	C	113	PHE	CB-CA-C	-5.07	100.27	110.40
1	A	199	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	B	827	ALA	N-CA-CB	5.06	117.18	110.10
1	B	310	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	B	782	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	B	130	ASP	CB-CG-OD1	5.04	122.83	118.30
1	C	252	ASP	CB-CG-OD2	-5.04	113.77	118.30
1	B	790	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	404	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	C	130	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	239	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	C	906	TYR	CA-CB-CG	-5.03	103.85	113.40
1	D	280	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	B	664	ALA	N-CA-CB	-5.03	103.06	110.10
1	D	954	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	120	THR	CA-CB-CG2	-5.02	105.37	112.40
1	B	651	LEU	CB-CA-C	5.02	119.74	110.20
1	A	503	TYR	CD1-CE1-CZ	-5.02	115.28	119.80
1	D	610	ASP	CB-CG-OD1	5.02	122.82	118.30
1	A	942	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	B	685	LEU	CB-CA-C	5.01	119.72	110.20
1	D	686	PRO	N-CA-CB	5.01	109.31	103.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	689	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	329	ASP	Sidechain

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	8125	0	7716	188	1
1	B	8125	0	7716	201	0
1	C	8125	0	7716	219	0
1	D	8125	0	7716	208	0
2	A	10	0	9	0	0
2	B	10	0	9	1	0
2	C	10	0	9	0	0
2	D	10	0	9	2	0
3	A	3	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	3	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	3	0	0	0	0
5	A	100	0	150	9	0
5	B	108	0	162	10	0
5	C	112	0	168	15	0
5	D	92	0	138	13	0
6	A	992	0	0	21	0
6	B	995	0	0	14	0
6	C	946	0	0	14	1
6	D	980	0	0	18	0
All	All	36890	0	31518	810	1

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 13.

All (810) 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)
1:C:634:GLN:H	1:C:634:GLN:NE2	1.47	1.13
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.33	1.10
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.54	1.05
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.37	1.02
1:B:797:GLU:HG2	1:B:799:THR:HG23	1.35	1.02
1:B:600:GLN:H	1:B:600:GLN:HE21	1.09	0.98
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.30	0.94
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.03	0.93
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.02	0.93
1:D:804:ASN:HA	1:D:809:ARG:HE	1.30	0.93
1:D:653:HIS:HD2	1:D:667:GLU:HB3	1.36	0.91
1:A:600:GLN:H	1:A:600:GLN:HE21	1.17	0.91
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.34	0.91
1:D:651:LEU:CD2	1:D:701:VAL:HB	2.01	0.91
1:D:804:ASN:HD22	1:D:809:ARG:CZ	1.85	0.90
1:B:232:ASN:ND2	1:B:237:ARG:HG3	1.88	0.89
1:B:655:MET:HE2	1:B:665:SER:HB3	1.54	0.89
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.38	0.88
1:D:804:ASN:HA	1:D:809:ARG:NE	1.89	0.85
1:A:735:HIS:ND1	1:A:735:HIS:N	2.24	0.85
1:B:668:VAL:HG12	1:B:669:PRO:HD2	1.57	0.83
1:C:634:GLN:NE2	1:C:634:GLN:N	2.26	0.83
1:A:797:GLU:O	1:A:801:ILE:HD13	1.79	0.82
1:D:843:GLN:HG2	1:D:848:THR:HA	1.61	0.82
1:B:730:LEU:HD12	1:B:730:LEU:H	1.44	0.82
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.29	0.81
1:B:634:GLN:HG2	1:B:682:LEU:O	1.80	0.81
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.62	0.81
1:C:824:GLN:HG2	1:C:825:CYS:N	1.96	0.81
1:A:863:GLN:HG2	1:A:1021:CYS:HB3	1.62	0.80
1:D:804:ASN:CB	1:D:809:ARG:HH21	1.93	0.80
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.17	0.79
1:D:807:VAL:O	1:D:811:LYS:HG3	1.83	0.79
1:D:802:ASP:OD1	1:D:803:PRO:HD2	1.83	0.79
1:C:634:GLN:H	1:C:634:GLN:HE21	1.30	0.79
1:D:651:LEU:HD23	1:D:701:VAL:HB	1.63	0.78
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:SER:HB3	6:C:9337:HOH:O	1.84	0.77
1:C:102:ASN:HD22	5:C:8506:DMS:H13	1.50	0.77
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.67	0.77
1:D:230:ARG:HD3	6:D:9630:HOH:O	1.84	0.76
1:A:646:HIS:ND1	6:A:9408:HOH:O	2.17	0.76
1:C:777:LEU:HG	1:C:889:ALA:HA	1.68	0.76
1:D:797:GLU:O	1:D:801:ILE:HD13	1.85	0.76
1:A:809:ARG:HG2	1:A:809:ARG:HH11	1.50	0.76
1:B:655:MET:HG3	6:B:8989:HOH:O	1.85	0.75
1:B:142:ILE:CG1	1:B:170:GLU:HG2	2.14	0.75
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.67	0.75
1:C:785:THR:O	1:C:881:ARG:HD2	1.88	0.74
1:B:797:GLU:HG2	1:B:799:THR:CG2	2.17	0.74
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.69	0.74
1:A:887:GLN:NE2	1:A:980:GLU:O	2.20	0.74
1:D:237:ARG:NH1	6:D:9257:HOH:O	2.20	0.74
1:B:142:ILE:HG12	1:B:170:GLU:CG	2.18	0.74
1:B:531:ARG:HB3	1:B:532:PRO:HD2	1.70	0.73
1:C:749:ILE:N	1:C:749:ILE:HD12	2.03	0.73
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.04	0.73
1:C:878:HIS:HD2	6:C:8694:HOH:O	1.71	0.73
1:C:687:GLN:HE21	1:C:687:GLN:N	1.86	0.73
1:D:634:GLN:NE2	1:D:682:LEU:O	2.22	0.73
1:D:651:LEU:HD21	1:D:653:HIS:CE1	2.23	0.72
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.69	0.72
1:C:102:ASN:HD22	5:C:8506:DMS:C1	2.03	0.72
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.01	0.72
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.03	0.72
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.69	0.72
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.55	0.71
1:D:749:ILE:HD12	1:D:749:ILE:N	2.04	0.71
1:C:797:GLU:O	1:C:801:ILE:HD13	1.90	0.71
1:B:651:LEU:O	1:B:651:LEU:HD23	1.91	0.71
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.72	0.70
1:C:356:ARG:HD2	1:C:379:MET:CE	2.22	0.70
1:B:772:ASP:OD1	1:B:773:LYS:HD3	1.92	0.70
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.74	0.70
1:C:748:CYS:C	1:C:749:ILE:HD12	2.12	0.70
1:D:112:PRO:HD2	1:D:113:PHE:CE1	2.26	0.69
1:A:84:VAL:HA	5:A:8414:DMS:O	1.92	0.69
1:A:473:ARG:NH1	6:A:9273:HOH:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:LEU:H	1:B:730:LEU:CD1	2.00	0.69
1:B:878:HIS:HD2	6:B:8690:HOH:O	1.74	0.69
1:D:622:HIS:O	1:D:625:GLN:HG3	1.92	0.68
1:A:800:ARG:O	1:A:800:ARG:HG2	1.92	0.68
1:A:749:ILE:HD12	1:A:749:ILE:N	2.08	0.68
1:B:634:GLN:HE22	1:B:684:GLU:HA	1.57	0.68
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.22	0.68
1:A:249:GLU:OE2	1:A:251:ARG:NE	2.23	0.68
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.27	0.68
1:C:651:LEU:HD21	1:C:653:HIS:HE1	1.57	0.68
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.76	0.68
1:C:765:LEU:HD21	1:C:768:MET:CE	2.24	0.68
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.27	0.67
1:D:804:ASN:HD22	1:D:809:ARG:HH21	1.39	0.67
1:A:829:THR:HG23	1:A:834:VAL:HG22	1.77	0.67
1:A:277:GLU:H	1:A:277:GLU:CD	1.98	0.67
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.24	0.67
1:C:651:LEU:CD1	1:C:701:VAL:HB	2.24	0.67
1:B:1022:GLN:HG2	1:B:1023:LYS:N	2.09	0.67
1:D:725:ASN:HB2	6:D:9521:HOH:O	1.94	0.67
1:D:88:SER:HA	1:D:366:VAL:HG21	1.76	0.67
1:D:887:GLN:NE2	1:D:980:GLU:O	2.28	0.66
1:B:651:LEU:HD23	1:B:651:LEU:C	2.15	0.66
1:A:599:ARG:HG3	1:A:600:GLN:NE2	2.10	0.66
1:A:595:THR:HA	1:A:596:PRO:C	2.16	0.66
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.11	0.66
1:B:637:GLU:OE2	1:B:677:LYS:HD3	1.95	0.66
1:C:858:ILE:CD1	1:C:864:MET:HB2	2.26	0.66
1:C:718:GLN:HG2	5:C:8503:DMS:C1	2.26	0.65
1:D:635:THR:HG23	1:D:681:GLU:OE1	1.95	0.65
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.78	0.65
1:B:102:ASN:HD22	5:B:8506:DMS:C1	2.10	0.65
1:B:684:GLU:O	1:B:686:PRO:HD3	1.97	0.65
1:B:634:GLN:NE2	1:B:684:GLU:HA	2.12	0.65
1:C:232:ASN:ND2	1:C:237:ARG:HG3	2.12	0.65
1:D:804:ASN:HA	1:D:809:ARG:CZ	2.26	0.65
1:A:857:ARG:HG2	6:A:9068:HOH:O	1.97	0.64
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.28	0.64
1:B:809:ARG:HG2	1:B:809:ARG:NH1	2.08	0.64
1:D:804:ASN:CA	1:D:809:ARG:HH21	2.09	0.64
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:LEU:O	1:C:661:LYS:HB2	1.98	0.64
1:C:743:SER:O	1:C:760:ARG:NH1	2.28	0.64
1:D:135:GLN:C	1:D:136:GLU:HG2	2.18	0.64
1:D:804:ASN:HA	1:D:809:ARG:NH2	2.13	0.64
1:C:749:ILE:HG13	1:C:834:VAL:HG11	1.81	0.63
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.79	0.63
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.29	0.63
1:C:765:LEU:HD21	1:C:768:MET:HE3	1.81	0.63
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.79	0.63
1:B:945:ASN:HB3	1:B:1023:LYS:HE2	1.78	0.63
1:C:230:ARG:HG3	1:C:230:ARG:NH1	2.04	0.63
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.95	0.63
1:A:1017:GLN:HG3	1:A:1017:GLN:O	1.99	0.63
1:B:367:MET:CE	1:B:372:MET:HG3	2.29	0.63
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.30	0.63
1:B:241:GLU:HG3	1:B:292:ARG:HG3	1.79	0.62
1:C:596:PRO:HB3	6:C:9379:HOH:O	1.98	0.62
1:D:748:CYS:C	1:D:749:ILE:HD12	2.19	0.62
1:D:1022:GLN:HG3	1:D:1023:LYS:N	2.14	0.62
1:B:615:PRO:O	1:B:618:THR:HG22	1.99	0.62
1:C:822:LEU:HD13	1:C:840:HIS:NE2	2.14	0.62
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.81	0.62
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.64	0.62
1:C:292:ARG:HH12	5:C:8412:DMS:C2	2.12	0.62
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.29	0.62
1:B:236:SER:C	1:B:237:ARG:HG2	2.17	0.62
1:A:878:HIS:HD2	6:A:8674:HOH:O	1.83	0.62
1:D:805:ALA:O	1:D:809:ARG:HG3	2.00	0.61
1:C:858:ILE:HD11	1:C:864:MET:HB2	1.81	0.61
1:A:599:ARG:HG3	1:A:600:GLN:HE21	1.65	0.61
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.35	0.61
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.82	0.61
1:D:804:ASN:HA	1:D:809:ARG:HH21	1.65	0.61
1:A:844:HIS:HD2	6:A:9406:HOH:O	1.83	0.61
1:A:431:ARG:HG3	6:A:9338:HOH:O	1.99	0.61
1:C:887:GLN:NE2	1:C:980:GLU:O	2.32	0.61
1:C:454:ILE:HG13	1:C:455:ILE:HG13	1.83	0.61
1:D:795:VAL:HG23	6:D:9473:HOH:O	1.99	0.61
1:D:844:HIS:CE1	1:D:845:GLN:HG2	2.36	0.60
1:D:230:ARG:HH12	1:D:239:VAL:HG11	1.65	0.60
1:D:634:GLN:HB3	1:D:682:LEU:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ASN:CA	1:D:809:ARG:HE	2.07	0.60
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.99	0.60
1:D:804:ASN:HB2	1:D:809:ARG:HH21	1.66	0.60
1:D:472:TYR:O	1:D:476:LYS:HG2	2.02	0.60
1:A:110:ASN:OD1	6:A:9307:HOH:O	2.15	0.60
1:C:745:MET:HA	1:C:745:MET:CE	2.32	0.60
1:B:367:MET:HE2	1:B:372:MET:HG3	1.83	0.59
1:C:88:SER:HA	1:C:366:VAL:HG21	1.83	0.59
1:C:278:ILE:HD13	1:C:278:ILE:N	2.16	0.59
1:D:794:GLY:HA3	6:D:8986:HOH:O	2.01	0.59
1:D:91:GLN:HB3	1:D:98:PRO:HD3	1.84	0.59
1:A:640:SER:O	1:A:675:GLN:HA	2.03	0.59
1:D:128:ASN:HB3	1:D:180:GLY:O	2.03	0.59
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.68	0.59
5:A:8420:DMS:H21	6:D:9470:HOH:O	2.02	0.59
1:A:890:GLN:HG3	1:A:891:VAL:N	2.17	0.59
1:D:473:ARG:NH1	1:D:476:LYS:HB2	2.17	0.58
1:C:237:ARG:HH11	1:C:237:ARG:HB2	1.68	0.58
1:D:795:VAL:HG12	6:D:9678:HOH:O	2.03	0.58
1:B:200:GLN:HG2	1:B:391:HIS:HB2	1.84	0.58
1:A:587:ALA:HB1	1:A:591:ASP:HB2	1.85	0.58
1:C:690:SER:HB2	6:C:9334:HOH:O	2.03	0.58
1:C:744:GLU:O	1:C:760:ARG:HD3	2.03	0.58
1:D:595:THR:HA	1:D:596:PRO:C	2.23	0.58
1:A:832:ASP:OD1	1:A:832:ASP:N	2.33	0.58
1:B:630:ARG:NE	1:B:637:GLU:OE1	2.36	0.58
1:C:796:SER:OG	1:C:802:ASP:N	2.28	0.58
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.39	0.58
1:B:600:GLN:HE21	1:B:600:GLN:N	1.91	0.58
1:B:1022:GLN:HG2	1:B:1023:LYS:O	2.04	0.58
1:D:593:GLY:O	1:D:595:THR:HG22	2.03	0.58
1:D:393:PRO:HD3	1:D:412:GLU:O	2.03	0.58
1:B:631:LEU:HD12	1:B:635:THR:O	2.04	0.58
1:A:687:GLN:HG3	6:A:9416:HOH:O	2.02	0.57
1:C:768:MET:O	1:C:775:GLN:N	2.37	0.57
1:C:778:THR:HG23	1:C:887:GLN:CB	2.34	0.57
1:A:599:ARG:HG3	1:A:600:GLN:H	1.68	0.57
1:D:375:ASP:O	1:D:379:MET:HG3	2.05	0.57
1:C:249:GLU:OE2	1:C:251:ARG:HD3	2.04	0.57
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.85	0.57
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:873:ALA:O	1:D:876:THR:HG22	2.05	0.57
1:D:878:HIS:HD2	6:D:8814:HOH:O	1.88	0.57
1:A:279:ILE:HD11	1:D:422:PRO:HG2	1.86	0.56
1:A:683:PRO:O	1:A:685:LEU:HG	2.04	0.56
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.87	0.56
1:C:781:ARG:NH1	6:C:9326:HOH:O	2.38	0.56
1:C:802:ASP:O	1:C:808:GLU:HG3	2.05	0.56
1:B:577:LYS:O	1:B:584:PRO:HA	2.04	0.56
1:D:240:LEU:HD23	1:D:240:LEU:C	2.25	0.56
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.04	0.56
1:D:682:LEU:HD22	1:D:683:PRO:HD2	1.85	0.56
1:C:651:LEU:HD11	1:C:701:VAL:HB	1.88	0.56
1:C:734:SER:HB3	1:C:860:GLY:C	2.26	0.56
1:C:843:GLN:NE2	1:C:848:THR:OG1	2.37	0.56
1:A:949:HIS:O	1:A:1023:LYS:NZ	2.38	0.56
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.36	0.55
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.40	0.55
1:B:646:HIS:CE1	1:B:673:ALA:HB2	2.42	0.55
1:D:277:GLU:OE1	5:D:8412:DMS:O	2.25	0.55
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.06	0.55
1:A:625:GLN:NE2	6:A:8804:HOH:O	2.39	0.55
1:C:651:LEU:CD2	1:C:653:HIS:HE1	2.19	0.55
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.42	0.55
1:A:653:HIS:CD2	1:A:667:GLU:HG2	2.42	0.55
1:D:629:PHE:O	1:D:630:ARG:NH1	2.35	0.55
1:D:891:VAL:HG23	1:D:981:GLY:HA2	1.89	0.55
1:C:786:ARG:HG2	1:C:880:ALA:HB1	1.89	0.55
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.89	0.55
1:B:634:GLN:HG2	1:B:682:LEU:HB2	1.89	0.55
1:B:655:MET:SD	1:B:656:VAL:N	2.80	0.54
1:C:654:TRP:O	1:C:665:SER:HB2	2.07	0.54
1:C:655:MET:HE2	1:C:665:SER:HB3	1.89	0.54
1:D:128:ASN:HB2	6:D:9631:HOH:O	2.06	0.54
1:B:499:ILE:HD11	1:B:529:GLU:CG	2.36	0.54
1:B:878:HIS:CD2	6:B:8690:HOH:O	2.54	0.54
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.89	0.54
1:A:843:GLN:HG2	1:A:848:THR:HA	1.89	0.54
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.42	0.54
1:B:863:GLN:HG3	1:B:1021:CYS:CB	2.37	0.54
1:A:416:GLU:OE2	1:A:418:HIS:HB2	2.07	0.54
1:D:521:LYS:HE2	6:D:9163:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:759:ASN:OD1	1:A:761:GLN:N	2.38	0.54
1:A:830:LEU:HD12	1:A:833:ALA:HB3	1.90	0.54
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.89	0.54
1:D:340:GLY:O	1:D:561:ARG:HG2	2.08	0.54
1:D:718:GLN:NE2	5:D:8503:DMS:H13	2.23	0.54
1:D:847:LYS:HG3	1:D:848:THR:N	2.18	0.54
1:D:843:GLN:CG	1:D:848:THR:HA	2.35	0.54
1:C:824:GLN:OE1	1:C:837:THR:HG22	2.08	0.54
1:A:764:PHE:CD1	1:A:781:ARG:NH1	2.76	0.54
1:C:890:GLN:HG3	1:C:891:VAL:N	2.22	0.54
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.38	0.53
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.76	0.53
1:D:801:ILE:CG2	1:D:802:ASP:H	2.21	0.53
1:C:652:LEU:HD23	1:C:680:ILE:HD13	1.90	0.53
1:C:832:ASP:OD1	1:C:832:ASP:N	2.41	0.53
1:C:843:GLN:HA	1:C:847:LYS:O	2.07	0.53
1:D:292:ARG:HH12	5:D:8412:DMS:H22	1.71	0.53
1:D:577:LYS:O	1:D:584:PRO:HA	2.08	0.53
1:D:804:ASN:C	1:D:809:ARG:HE	2.12	0.53
1:B:685:LEU:O	1:B:686:PRO:C	2.47	0.53
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.43	0.53
5:B:8601:DMS:H13	6:B:9437:HOH:O	2.07	0.53
1:C:948:PRO:O	1:C:1023:LYS:N	2.34	0.53
1:B:599:ARG:HH11	1:B:600:GLN:NE2	2.05	0.53
1:C:367:MET:HA	1:C:367:MET:CE	2.39	0.53
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.43	0.53
1:D:36:TRP:CD2	1:D:42:ALA:HA	2.43	0.53
1:C:333:ARG:O	1:C:333:ARG:HD3	2.08	0.53
1:C:46:ARG:HG2	6:C:9473:HOH:O	2.07	0.53
1:C:367:MET:HA	1:C:367:MET:HE3	1.91	0.53
1:D:802:ASP:O	1:D:804:ASN:N	2.42	0.53
1:D:843:GLN:HG2	1:D:848:THR:CA	2.36	0.53
1:D:863:GLN:HG2	1:D:1021:CYS:CB	2.39	0.53
1:A:577:LYS:O	1:A:584:PRO:HA	2.09	0.53
1:C:809:ARG:NH2	1:C:1001:PRO:CG	2.72	0.53
1:A:77:ASP:O	1:A:79:PRO:HD3	2.10	0.52
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.90	0.52
1:C:292:ARG:HH12	5:C:8412:DMS:H22	1.74	0.52
1:D:237:ARG:HB3	1:D:237:ARG:NH1	2.17	0.52
1:C:796:SER:HB2	1:C:802:ASP:HB3	1.92	0.52
1:D:986:ILE:O	1:D:986:ILE:HG22	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:GLU:HB3	1:B:800:ARG:H	1.73	0.52
1:C:755:ARG:HG2	1:C:769:TRP:HE3	1.70	0.52
1:B:699:ARG:NH2	5:B:8415:DMS:C1	2.72	0.52
1:C:572:ASP:HB3	1:C:603:MET:HG2	1.91	0.52
1:A:279:ILE:HD11	1:D:422:PRO:CG	2.39	0.52
1:A:527:PRO:HB3	1:B:339:ASN:O	2.09	0.52
1:C:687:GLN:HE21	1:C:687:GLN:H	1.56	0.52
1:B:890:GLN:HB3	6:B:9524:HOH:O	2.09	0.52
1:C:430:PRO:HD3	5:C:8420:DMS:H22	1.92	0.52
1:D:801:ILE:HG22	1:D:802:ASP:N	2.25	0.52
1:A:446:ARG:HG2	1:A:447:ASP:OD1	2.09	0.52
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.22	0.52
1:B:744:GLU:HB2	1:B:745:MET:HE3	1.91	0.52
1:C:78:LEU:HB3	1:C:80:GLU:HG3	1.92	0.52
1:A:268:ALA:HA	5:A:8602:DMS:H22	1.92	0.52
1:C:861:SER:OG	1:C:863:GLN:HG3	2.10	0.52
1:C:750:GLU:OE2	1:C:755:ARG:HB2	2.10	0.52
1:B:863:GLN:CG	1:B:1021:CYS:HB3	2.38	0.51
1:C:600:GLN:HB2	1:C:603:MET:HE2	1.92	0.51
1:D:285:TYR:HB3	1:D:288:ARG:HG3	1.92	0.51
1:D:167:LEU:HB3	1:D:168:PRO:HD2	1.92	0.51
1:A:433:LEU:N	1:A:434:PRO:CD	2.73	0.51
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.45	0.51
1:C:824:GLN:HG2	1:C:825:CYS:H	1.74	0.51
1:D:800:ARG:O	1:D:801:ILE:O	2.29	0.51
1:C:746:ASP:CA	1:C:760:ARG:HG3	2.24	0.51
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.93	0.51
1:D:972:HIS:HB3	1:D:974:HIS:ND1	2.25	0.51
1:B:847:LYS:HG2	1:B:849:LEU:HD23	1.93	0.51
1:C:749:ILE:CG1	1:C:834:VAL:HG11	2.40	0.51
1:A:949:HIS:HB2	1:A:951:TRP:CH2	2.46	0.51
1:B:105:TYR:CE1	1:B:419:GLY:HA3	2.46	0.51
1:B:873:ALA:O	1:B:876:THR:HG22	2.11	0.51
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.93	0.51
1:D:640:SER:O	1:D:675:GLN:HA	2.10	0.51
1:A:250:LEU:HD11	1:A:286:ALA:O	2.11	0.51
1:C:615:PRO:O	1:C:618:THR:HG22	2.11	0.51
1:A:433:LEU:N	1:A:434:PRO:HD2	2.26	0.51
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.93	0.51
1:A:735:HIS:O	1:A:736:ALA:HB2	2.09	0.51
1:C:796:SER:CB	1:C:802:ASP:H	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:THR:HA	1:B:596:PRO:C	2.32	0.50
1:C:114:VAL:HB	1:C:115:PRO:HD2	1.92	0.50
1:C:655:MET:HE3	1:C:662:PRO:HB3	1.93	0.50
1:B:730:LEU:HD12	1:B:730:LEU:N	2.21	0.50
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.36	0.50
1:C:784:PHE:CD1	1:C:850:PHE:CD1	2.99	0.50
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.42	0.50
1:A:352:ARG:HD3	1:A:624:GLN:HB3	1.93	0.50
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.47	0.50
1:B:230:ARG:NH1	1:B:241:GLU:OE1	2.44	0.50
1:B:531:ARG:HB3	1:B:532:PRO:CD	2.41	0.50
1:B:753:ASN:N	1:B:753:ASN:OD1	2.45	0.50
1:C:680:ILE:O	1:C:680:ILE:HG22	2.07	0.50
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.10	0.50
1:D:891:VAL:CG2	1:D:981:GLY:HA2	2.42	0.50
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.23	0.50
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.93	0.50
1:C:833:ALA:HB1	1:C:858:ILE:O	2.11	0.50
1:D:599:ARG:HG3	1:D:600:GLN:H	1.76	0.50
1:A:473:ARG:NH1	1:A:476:LYS:CB	2.74	0.50
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.94	0.50
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.93	0.50
1:C:132:SER:HB2	5:C:8504:DMS:H11	1.94	0.50
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.46	0.50
1:C:847:LYS:NZ	1:D:724:GLU:O	2.45	0.50
1:D:688:PRO:C	1:D:690:SER:H	2.14	0.50
1:A:127:PHE:N	1:A:127:PHE:CD2	2.79	0.50
1:A:167:LEU:HD21	1:A:393:PRO:HG2	1.94	0.50
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.12	0.50
1:D:78:LEU:HD23	6:D:9218:HOH:O	2.11	0.50
1:D:801:ILE:CG2	1:D:802:ASP:N	2.75	0.50
1:B:499:ILE:HD11	1:B:529:GLU:CD	2.32	0.50
1:B:1017:GLN:HB2	6:B:9517:HOH:O	2.12	0.50
1:C:266:GLN:NE2	5:C:8602:DMS:S	2.85	0.50
1:D:513:PRO:O	1:D:514:ALA:HB3	2.12	0.50
1:B:320:GLY:O	5:B:8406:DMS:O	2.29	0.49
1:C:37:ARG:HG3	1:C:37:ARG:HH11	1.77	0.49
1:B:684:GLU:HG2	1:B:685:LEU:N	2.27	0.49
1:C:724:GLU:O	1:D:847:LYS:NZ	2.44	0.49
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.09	0.49
1:A:809:ARG:HH11	1:A:809:ARG:CG	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:450:HIS:HE1	6:B:9574:HOH:O	1.95	0.49
1:B:797:GLU:CG	1:B:799:THR:HG23	2.25	0.49
5:C:8503:DMS:H13	6:C:9034:HOH:O	2.11	0.49
1:D:219:THR:HG21	6:D:9649:HOH:O	2.12	0.49
1:A:663:LEU:HD12	1:A:686:PRO:HG2	1.95	0.49
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.94	0.49
1:B:869:ASP:OD1	1:B:1015:HIS:ND1	2.45	0.49
1:B:142:ILE:HG22	6:B:8857:HOH:O	2.12	0.49
6:B:9363:HOH:O	5:C:8420:DMS:H21	2.12	0.49
1:C:608:PHE:CE1	1:C:614:HIS:CD2	3.00	0.49
1:C:824:GLN:O	1:C:838:THR:HA	2.13	0.49
1:D:441:THR:O	1:D:445:GLN:HG3	2.12	0.49
1:D:829:THR:HG22	1:D:830:LEU:N	2.28	0.49
1:D:945:ASN:OD1	1:D:950:GLN:HG3	2.12	0.49
1:A:624:GLN:NE2	6:A:8624:HOH:O	2.45	0.49
1:D:251:ARG:HD2	5:D:8416:DMS:C1	2.42	0.49
1:B:699:ARG:NH2	5:B:8415:DMS:H11	2.28	0.49
1:C:595:THR:HA	1:C:596:PRO:C	2.32	0.49
1:D:654:TRP:CZ3	1:D:665:SER:HA	2.48	0.49
1:A:518:TRP:O	1:A:519:SER:C	2.51	0.49
1:B:729:THR:HG23	6:B:9217:HOH:O	2.12	0.49
1:B:843:GLN:HA	1:B:847:LYS:O	2.13	0.49
1:C:696:LEU:O	1:C:719:GLN:HA	2.12	0.49
1:D:847:LYS:HG2	1:D:849:LEU:HD23	1.95	0.49
1:B:601:PHE:HB3	6:B:9551:HOH:O	2.13	0.48
1:B:694:LEU:HD12	1:B:723:ALA:HB3	1.94	0.48
1:C:796:SER:OG	1:C:801:ILE:HA	2.13	0.48
1:D:502:MET:HA	1:D:537:GLU:O	2.13	0.48
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.95	0.48
1:A:702:GLN:O	1:A:712:GLY:N	2.43	0.48
1:C:237:ARG:NH1	1:C:237:ARG:CB	2.76	0.48
1:C:285:TYR:HB3	1:C:288:ARG:HG3	1.95	0.48
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.95	0.48
1:A:237:ARG:HH11	1:A:237:ARG:CG	2.26	0.48
1:A:240:LEU:C	1:A:240:LEU:HD23	2.32	0.48
1:B:843:GLN:HG2	1:B:848:THR:HA	1.95	0.48
1:C:781:ARG:HG2	1:C:781:ARG:HH11	1.77	0.48
1:C:844:HIS:HD2	6:C:9418:HOH:O	1.95	0.48
1:D:143:PHE:O	1:D:168:PRO:HA	2.13	0.48
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.95	0.48
1:C:546:LEU:HA	6:C:8749:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:893:GLU:HG3	1:D:894:ARG:CD	2.44	0.48
1:A:587:ALA:HB1	1:A:591:ASP:CB	2.42	0.48
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.81	0.48
1:B:262:GLN:NE2	1:B:263:GLY:N	2.61	0.48
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.49	0.48
1:D:598:ASP:O	1:D:601:PHE:HB2	2.14	0.48
1:B:102:ASN:OD1	1:B:201:ASP:HB2	2.12	0.48
1:C:703:PRO:O	1:C:711:ALA:HB1	2.13	0.48
1:C:740:LEU:HA	1:C:748:CYS:O	2.14	0.48
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.95	0.48
1:C:242:ALA:O	1:C:290:THR:HA	2.14	0.48
1:D:159:VAL:HG22	1:D:176:PHE:CE2	2.48	0.48
1:D:736:ALA:C	1:D:737:ILE:HG22	2.34	0.48
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.13	0.48
1:C:746:ASP:HA	1:C:760:ARG:CG	2.23	0.48
1:D:201:ASP:OD2	2:D:2001:2DG:O4	2.25	0.48
1:D:808:GLU:OE1	1:D:811:LYS:HE3	2.13	0.48
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.14	0.48
1:B:568:TRP:CH2	2:B:2001:2DG:H3	2.49	0.48
1:B:701:VAL:HG22	1:B:714:ILE:HG12	1.96	0.48
1:A:279:ILE:HG23	1:A:279:ILE:HD13	1.62	0.47
1:A:974:HIS:HB3	6:A:9019:HOH:O	2.14	0.47
1:B:14:ARG:HA	1:B:16:TRP:CZ3	2.48	0.47
1:B:36:TRP:CD1	1:B:48:SER:HB2	2.48	0.47
1:D:145:GLY:N	1:D:210:ARG:HB2	2.28	0.47
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.28	0.47
1:D:1020:TRP:HD1	1:D:1021:CYS:N	2.11	0.47
1:D:354:VAL:O	1:D:387:VAL:HA	2.14	0.47
1:A:249:GLU:HG2	1:A:251:ARG:NE	2.29	0.47
1:B:537:GLU:HA	1:B:566:PHE:O	2.14	0.47
1:D:718:GLN:HG2	5:D:8503:DMS:C1	2.44	0.47
1:A:646:HIS:NE2	1:A:671:ASP:OD1	2.40	0.47
1:C:542:MET:HA	1:C:604:ASN:HA	1.95	0.47
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.49	0.47
1:B:646:HIS:CE1	1:B:673:ALA:CB	2.97	0.47
1:C:178:ARG:O	1:C:178:ARG:HG2	2.14	0.47
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.96	0.47
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.97	0.47
1:A:655:MET:HE2	1:A:656:VAL:O	2.14	0.47
1:B:126:THR:HA	1:B:182:ASN:O	2.14	0.47
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:859:ASP:OD1	1:C:861:SER:OG	2.27	0.47
1:D:654:TRP:CZ2	1:D:683:PRO:HG2	2.50	0.47
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.31	0.47
1:B:377:LEU:O	1:B:381:GLN:HG3	2.15	0.47
1:B:807:VAL:CG1	1:B:808:GLU:N	2.76	0.47
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.68	0.47
1:C:780:LEU:HA	1:C:886:CYS:HB3	1.97	0.47
1:D:230:ARG:HH12	1:D:239:VAL:CG1	2.25	0.47
1:D:292:ARG:NH1	5:D:8412:DMS:C2	2.76	0.47
1:D:545:SER:O	1:D:909:ARG:HD3	2.15	0.47
1:D:893:GLU:HG3	1:D:894:ARG:HD2	1.96	0.47
1:B:655:MET:SD	1:B:656:VAL:O	2.72	0.47
1:C:91:GLN:HG2	1:C:98:PRO:HA	1.96	0.47
1:A:871:GLU:OE1	1:B:726:LEU:HD22	2.15	0.47
1:A:628:GLN:HG3	6:A:9028:HOH:O	2.15	0.47
1:A:959:ILE:HG23	1:A:959:ILE:O	2.14	0.47
1:A:1013:ARG:HH11	1:A:1013:ARG:HD3	1.58	0.47
1:B:628:GLN:HE22	5:B:8402:DMS:C2	2.28	0.47
1:C:525:SER:HB3	1:D:525:SER:HB3	1.97	0.47
1:B:807:VAL:HG13	1:B:808:GLU:N	2.31	0.46
1:D:785:THR:HB	1:D:816:TYR:CE2	2.50	0.46
1:A:260:LEU:O	1:A:267:VAL:HG22	2.15	0.46
1:C:749:ILE:O	1:C:755:ARG:HA	2.15	0.46
5:C:8506:DMS:H11	6:C:9396:HOH:O	2.16	0.46
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.79	0.46
1:A:125:LEU:O	1:A:183:ARG:HA	2.15	0.46
1:B:578:TYR:HA	1:B:583:ASN:O	2.15	0.46
1:B:661:LYS:O	1:B:663:LEU:HD23	2.15	0.46
1:C:651:LEU:HD22	1:C:667:GLU:HG2	1.97	0.46
1:D:363:HIS:HD2	6:D:9298:HOH:O	1.97	0.46
1:A:80:GLU:O	1:A:80:GLU:HG2	2.15	0.46
1:B:105:TYR:CD1	1:B:419:GLY:HA3	2.51	0.46
1:D:112:PRO:HD2	1:D:113:PHE:CD1	2.51	0.46
1:D:291:LEU:HD22	1:D:291:LEU:N	2.30	0.46
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.98	0.46
1:D:654:TRP:CZ2	1:D:683:PRO:CG	2.98	0.46
1:A:117:GLU:HG3	6:A:9004:HOH:O	2.16	0.46
1:A:599:ARG:CG	1:A:600:GLN:NE2	2.79	0.46
1:A:806:TRP:CE2	1:A:991:MET:HE3	2.50	0.46
1:A:863:GLN:HG2	1:A:1021:CYS:CB	2.39	0.46
1:B:282:ARG:HB2	1:C:423:MET:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.34	0.46
1:B:519:SER:HB3	1:B:522:LYS:HB3	1.96	0.46
1:C:749:ILE:N	1:C:749:ILE:CD1	2.75	0.46
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.97	0.46
1:A:65:ALA:CB	1:A:66:PRO:HD2	2.39	0.46
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.80	0.46
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.82	0.46
1:B:433:LEU:N	1:B:434:PRO:CD	2.79	0.46
1:B:744:GLU:HB3	1:B:745:MET:HE2	1.98	0.46
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.49	0.46
1:D:65:ALA:HB1	1:D:67:GLU:OE1	2.15	0.46
1:D:972:HIS:HB3	1:D:974:HIS:HD1	1.79	0.46
1:A:106:PRO:O	5:A:8410:DMS:H22	2.16	0.46
1:B:173:LEU:O	1:B:174:SER:C	2.52	0.46
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.98	0.46
1:D:618:THR:HG21	6:D:9054:HOH:O	2.15	0.46
1:B:88:SER:HA	1:B:366:VAL:HG21	1.98	0.46
1:B:183:ARG:NH1	6:B:8921:HOH:O	2.39	0.46
1:C:629:PHE:HA	1:C:637:GLU:O	2.16	0.46
1:C:858:ILE:HD13	1:C:864:MET:HB2	1.97	0.46
1:C:96:ASP:HB2	6:C:8977:HOH:O	2.15	0.46
1:A:59:ARG:HG2	5:A:8502:DMS:C1	2.47	0.45
1:A:158:TRP:CZ2	1:A:160:GLY:HA2	2.50	0.45
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.28	0.45
1:D:344:LEU:O	1:D:345:ASN:C	2.52	0.45
5:A:8502:DMS:H12	6:A:9319:HOH:O	2.15	0.45
1:B:658:LEU:O	1:B:661:LYS:HG3	2.16	0.45
1:B:661:LYS:HA	1:B:662:PRO:HD3	1.48	0.45
1:B:744:GLU:CB	1:B:745:MET:CE	2.95	0.45
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.99	0.45
1:C:475:ILE:HD13	1:C:475:ILE:HG21	1.52	0.45
1:D:664:ALA:O	1:D:665:SER:HB3	2.15	0.45
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.98	0.45
1:B:91:GLN:HG2	1:B:98:PRO:HA	1.98	0.45
1:C:230:ARG:O	1:C:238:ALA:HA	2.17	0.45
1:C:651:LEU:CD2	1:C:653:HIS:CE1	2.99	0.45
1:A:88:SER:HA	1:A:366:VAL:HG21	1.98	0.45
1:A:593:GLY:O	1:A:595:THR:HG22	2.15	0.45
1:B:925:MET:HB3	6:B:8644:HOH:O	2.16	0.45
1:C:581:ASN:HB2	1:C:583:ASN:ND2	2.32	0.45
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ASN:HD22	1:D:809:ARG:NE	2.12	0.45
1:A:802:ASP:O	1:A:808:GLU:HG3	2.17	0.45
1:D:749:ILE:N	1:D:749:ILE:CD1	2.72	0.45
1:A:685:LEU:CB	1:A:686:PRO:CD	2.95	0.45
1:A:921:PRO:O	1:A:922:LEU:C	2.55	0.45
1:B:474:TRP:O	1:B:478:VAL:HG13	2.16	0.45
1:B:734:SER:CB	1:B:860:GLY:HA3	2.47	0.45
1:B:756:TRP:CD2	1:B:858:ILE:HD13	2.51	0.45
1:D:367:MET:HB3	1:D:372:MET:HE2	1.97	0.45
1:D:942:ARG:HA	1:D:953:GLY:O	2.17	0.45
1:B:46:ARG:HH11	1:B:46:ARG:HD2	1.44	0.45
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.52	0.45
1:B:663:LEU:O	1:B:664:ALA:HB2	2.16	0.45
1:C:838:THR:OG1	1:C:854:LYS:HB2	2.17	0.45
1:D:237:ARG:NH1	1:D:237:ARG:CG	2.77	0.45
1:D:473:ARG:HD2	1:D:473:ARG:HA	1.80	0.45
1:D:654:TRP:CE3	1:D:655:MET:HA	2.51	0.45
1:D:667:GLU:C	1:D:668:VAL:HG23	2.36	0.45
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.52	0.45
1:B:822:LEU:HD11	1:B:824:GLN:O	2.17	0.45
1:B:937:LEU:HA	1:B:957:PHE:O	2.16	0.45
1:C:737:ILE:HA	1:C:738:PRO:HD3	1.90	0.45
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.52	0.45
1:B:102:ASN:ND2	5:B:8506:DMS:C1	2.77	0.45
1:B:734:SER:HB2	1:B:860:GLY:HA3	1.99	0.45
1:B:872:VAL:O	1:B:873:ALA:C	2.55	0.45
1:C:809:ARG:HH21	1:C:1001:PRO:HG3	1.81	0.45
1:A:701:VAL:O	1:A:703:PRO:HD3	2.17	0.45
1:A:990:HIS:HD2	1:A:991:MET:O	2.00	0.45
1:B:646:HIS:CE1	1:B:673:ALA:CA	3.00	0.45
1:D:370:GLN:HB2	6:D:9235:HOH:O	2.16	0.45
1:D:639:THR:OG1	1:D:677:LYS:HG3	2.16	0.45
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.52	0.45
1:B:945:ASN:HB3	1:B:1023:LYS:CE	2.46	0.44
1:C:249:GLU:CD	1:C:251:ARG:HD3	2.38	0.44
1:C:756:TRP:CE2	1:C:858:ILE:HD12	2.52	0.44
1:C:777:LEU:HD23	1:C:777:LEU:HA	1.69	0.44
1:A:262:GLN:HG3	6:A:9568:HOH:O	2.17	0.44
1:A:429:ASP:HA	1:A:430:PRO:HD2	1.86	0.44
1:A:472:TYR:O	1:A:476:LYS:HG2	2.18	0.44
1:C:557:ARG:HD2	6:C:8638:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ASN:HA	1:D:148:SER:HA	1.60	0.44
1:B:262:GLN:HE21	1:B:262:GLN:C	2.21	0.44
1:B:814:GLY:HA3	1:B:844:HIS:CG	2.52	0.44
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.99	0.44
1:A:126:THR:HA	1:A:182:ASN:O	2.18	0.44
1:A:577:LYS:HD3	1:A:587:ALA:HB2	1.98	0.44
1:B:347:LYS:HB2	1:B:643:LEU:HD13	1.99	0.44
1:B:674:PRO:O	1:B:675:GLN:HB2	2.18	0.44
1:B:817:GLN:NE2	1:B:817:GLN:HA	2.32	0.44
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.68	0.44
1:B:687:GLN:HA	1:B:688:PRO:HD3	1.69	0.44
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.52	0.44
1:A:59:ARG:HG2	5:A:8502:DMS:H11	1.99	0.44
1:A:90:TRP:CZ3	1:A:121:GLY:HA3	2.53	0.44
1:A:339:ASN:O	1:B:527:PRO:HB3	2.17	0.44
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.52	0.44
1:A:668:VAL:HA	1:A:669:PRO:HD3	1.81	0.44
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.18	0.44
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.99	0.44
1:C:152:LEU:HD11	1:C:184:LEU:HD22	2.00	0.44
1:C:326:GLU:O	1:C:327:ALA:HB2	2.17	0.44
1:C:781:ARG:NH1	1:C:781:ARG:HG2	2.33	0.44
1:B:416:GLU:HA	1:B:460:ASN:O	2.17	0.44
1:C:100:TYR:OH	1:C:201:ASP:OD1	2.26	0.44
1:C:240:LEU:C	1:C:240:LEU:HD23	2.37	0.44
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.36	0.44
1:D:588:TYR:O	1:D:591:ASP:HB2	2.17	0.44
1:D:599:ARG:HG3	1:D:600:GLN:N	2.33	0.44
1:A:600:GLN:HE21	1:A:600:GLN:N	1.99	0.44
1:C:561:ARG:HD3	1:D:525:SER:O	2.18	0.44
1:D:190:ARG:HG3	1:D:206:SER:HB3	2.00	0.44
1:D:368:ASP:O	1:D:372:MET:HG3	2.18	0.44
1:A:178:ARG:HD2	6:A:9436:HOH:O	2.16	0.43
1:A:344:LEU:O	1:A:345:ASN:C	2.56	0.43
1:A:561:ARG:HD3	1:B:525:SER:O	2.18	0.43
1:A:651:LEU:C	1:A:651:LEU:HD12	2.39	0.43
1:A:696:LEU:O	1:A:719:GLN:HA	2.18	0.43
1:B:824:GLN:O	1:B:838:THR:HA	2.18	0.43
1:C:255:ARG:HB2	1:C:316:HIS:CE1	2.53	0.43
1:C:472:TYR:O	1:C:476:LYS:HG2	2.18	0.43
1:D:138:GLN:O	1:D:216:HIS:HA	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:630:ARG:NH1	6:D:9277:HOH:O	2.50	0.43
1:B:255:ARG:HB2	1:B:316:HIS:CE1	2.53	0.43
1:B:847:LYS:HG3	1:B:848:THR:N	2.33	0.43
1:C:505:ARG:HG2	1:C:996:ASP:OD2	2.18	0.43
1:C:638:VAL:O	1:C:677:LYS:HA	2.18	0.43
1:C:842:TRP:O	1:C:849:LEU:N	2.44	0.43
1:C:990:HIS:HD2	1:C:991:MET:O	2.01	0.43
1:B:262:GLN:HE21	1:B:263:GLY:N	2.14	0.43
1:B:613:PRO:HG2	6:B:9240:HOH:O	2.17	0.43
1:B:693:GLN:HG2	1:B:695:TRP:NE1	2.34	0.43
1:C:111:PRO:HA	1:C:112:PRO:HA	1.67	0.43
1:A:742:THR:HG22	1:A:743:SER:N	2.32	0.43
1:B:110:ASN:N	1:B:111:PRO:CD	2.82	0.43
1:C:262:GLN:HB2	1:C:309:TYR:CE2	2.53	0.43
1:D:701:VAL:O	1:D:703:PRO:HD3	2.19	0.43
1:A:608:PHE:CD1	1:A:614:HIS:HD2	2.36	0.43
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.85	0.43
1:C:799:THR:O	1:C:800:ARG:HG2	2.18	0.43
1:D:23:GLN:HB2	1:D:26:ARG:HB2	2.00	0.43
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.48	0.43
1:A:142:ILE:HG23	1:A:170:GLU:HG2	2.00	0.43
1:A:774:LYS:NZ	6:A:9275:HOH:O	2.51	0.43
1:B:369:GLU:HB2	1:B:397:LEU:CD2	2.49	0.43
1:B:427:THR:HG22	1:B:436:MET:SD	2.59	0.43
1:B:599:ARG:HH11	1:B:599:ARG:HG3	1.84	0.43
1:C:375:ASP:O	1:C:379:MET:HG3	2.18	0.43
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.77	0.43
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.54	0.43
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.54	0.43
1:C:344:LEU:CB	1:C:349:LEU:HD21	2.49	0.43
1:C:608:PHE:CZ	1:C:614:HIS:CD2	3.06	0.43
1:C:610:ASP:O	1:C:611:ARG:HB2	2.18	0.43
1:C:663:LEU:HD22	1:C:663:LEU:HA	1.82	0.43
1:C:743:SER:O	1:C:744:GLU:C	2.56	0.43
1:D:833:ALA:HB1	1:D:858:ILE:O	2.18	0.43
1:D:986:ILE:HD13	1:D:986:ILE:HG21	1.51	0.43
1:A:583:ASN:HB3	1:A:584:PRO:HD2	2.00	0.43
1:A:1017:GLN:HE21	1:A:1017:GLN:HB2	1.74	0.43
1:B:626:PHE:O	1:B:641:GLU:N	2.36	0.43
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.54	0.43
1:D:433:LEU:N	1:D:434:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:842:TRP:HZ3	1:D:852:SER:HB3	1.84	0.43
1:A:749:ILE:HD12	1:A:749:ILE:H	1.83	0.43
1:B:377:LEU:HD22	1:B:708:TRP:HA	2.01	0.43
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.49	0.43
1:B:899:GLY:HA2	1:B:915:PHE:CE1	2.54	0.43
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.01	0.43
1:B:37:ARG:NH1	5:B:8504:DMS:C2	2.82	0.43
1:B:143:PHE:O	1:B:168:PRO:HA	2.19	0.43
1:B:360:HIS:CE1	1:B:362:LEU:H	2.36	0.43
1:B:901:GLY:HA3	1:B:902:PRO:HA	1.80	0.43
1:C:431:ARG:NH2	6:C:9033:HOH:O	2.29	0.43
1:C:526:LEU:HD23	1:C:526:LEU:HA	1.78	0.43
1:A:835:LEU:HD11	1:A:855:THR:HB	2.02	0.42
1:B:654:TRP:O	1:B:665:SER:HB2	2.19	0.42
1:D:629:PHE:HA	1:D:637:GLU:O	2.19	0.42
1:A:655:MET:HE2	1:A:656:VAL:H	1.84	0.42
1:C:533:LEU:C	1:C:533:LEU:HD23	2.39	0.42
1:B:797:GLU:O	1:B:800:ARG:N	2.51	0.42
1:B:869:ASP:HA	1:B:1014:TYR:O	2.18	0.42
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.55	0.42
1:C:655:MET:CE	1:C:662:PRO:HB3	2.49	0.42
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.20	0.42
1:A:75:GLU:OE1	1:A:75:GLU:HA	2.18	0.42
1:A:100:TYR:HB3	1:A:589:GLY:HA2	2.01	0.42
1:B:36:TRP:CD2	1:B:42:ALA:HA	2.54	0.42
1:C:237:ARG:NH2	1:C:296:GLU:OE2	2.52	0.42
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.34	0.42
1:C:795:VAL:HG12	5:C:8506:DMS:H22	2.01	0.42
1:C:908:ASP:HB3	1:C:1007:PHE:CG	2.55	0.42
1:C:930:VAL:HA	1:C:973:ARG:HD3	2.01	0.42
1:D:36:TRP:NE1	1:D:46:ARG:O	2.43	0.42
1:D:59:ARG:NH2	1:D:81:ALA:HB3	2.34	0.42
1:D:673:ALA:O	1:D:676:GLY:N	2.40	0.42
1:A:360:HIS:HE1	1:A:362:LEU:HB2	1.84	0.42
1:B:71:GLU:H	1:B:71:GLU:CD	2.22	0.42
1:C:127:PHE:N	1:C:127:PHE:CD2	2.87	0.42
1:C:335:VAL:HG22	1:C:344:LEU:HD12	2.01	0.42
1:C:649:ASN:O	1:C:702:GLN:HG2	2.20	0.42
1:D:959:ILE:O	1:D:960:SER:HB3	2.19	0.42
1:D:962:TYR:CE1	5:D:8508:DMS:H21	2.55	0.42
1:D:984:LEU:HD11	1:D:986:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.54	0.42
1:B:975:LEU:HD23	1:B:975:LEU:HA	1.82	0.42
5:C:8601:DMS:H22	6:C:9543:HOH:O	2.19	0.42
1:D:208:ILE:HG21	1:D:208:ILE:HD13	1.75	0.42
1:A:599:ARG:HG3	1:A:600:GLN:N	2.32	0.42
1:C:720:TRP:HA	5:C:8427:DMS:C1	2.50	0.42
1:C:930:VAL:O	1:C:932:PRO:HD3	2.20	0.42
1:D:830:LEU:N	1:D:833:ALA:O	2.45	0.42
1:A:521:LYS:HE2	6:A:9023:HOH:O	2.19	0.42
1:B:473:ARG:O	1:B:474:TRP:C	2.56	0.42
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.31	0.42
1:C:416:GLU:HA	1:C:460:ASN:O	2.19	0.42
1:D:141:ILE:HD13	1:D:143:PHE:CE1	2.54	0.42
1:D:360:HIS:ND1	1:D:361:PRO:HD2	2.35	0.42
1:A:655:MET:HG3	1:A:656:VAL:N	2.25	0.42
1:A:726:LEU:HD12	1:B:848:THR:HG22	2.01	0.42
1:B:13:ARG:O	1:B:14:ARG:C	2.58	0.42
1:B:658:LEU:HD11	1:B:692:GLY:HA3	2.02	0.42
1:B:777:LEU:HG	1:B:889:ALA:HA	2.01	0.42
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.19	0.42
1:D:613:PRO:HB3	1:D:617:LEU:HD23	2.02	0.42
1:D:898:LEU:HA	1:D:898:LEU:HD12	1.81	0.42
1:A:660:GLY:O	1:A:662:PRO:HD3	2.20	0.42
1:B:86:VAL:HG13	1:B:87:PRO:HA	2.02	0.42
1:C:376:ILE:HG13	1:C:398:TRP:CH2	2.55	0.42
1:D:277:GLU:CD	1:D:277:GLU:H	2.19	0.42
1:D:588:TYR:N	1:D:591:ASP:OD2	2.37	0.42
1:D:788:PRO:HD2	1:D:968:MET:HG3	2.02	0.42
1:A:646:HIS:ND1	1:A:673:ALA:HA	2.34	0.41
5:A:8420:DMS:C2	6:D:9470:HOH:O	2.64	0.41
1:B:757:GLN:HG2	1:B:758:PHE:N	2.27	0.41
1:C:415:ILE:HD13	1:C:415:ILE:HG21	1.87	0.41
1:C:608:PHE:CE1	1:C:614:HIS:HD2	2.37	0.41
1:D:251:ARG:HD2	5:D:8416:DMS:H11	2.02	0.41
1:B:292:ARG:NH1	5:B:8412:DMS:H22	2.35	0.41
1:B:472:TYR:O	1:B:476:LYS:HG2	2.19	0.41
1:C:787:ALA:HA	1:C:788:PRO:HD3	1.95	0.41
1:C:13:ARG:O	1:C:14:ARG:C	2.58	0.41
1:C:147:ASN:HA	1:C:148:SER:HA	1.59	0.41
1:C:661:LYS:HB2	1:C:661:LYS:HE3	1.39	0.41
1:C:995:GLY:O	1:C:996:ASP:C	2.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.55	0.41
1:A:475:ILE:HG21	1:A:475:ILE:HD13	1.80	0.41
1:B:569:ASP:O	1:B:605:GLY:HA2	2.20	0.41
1:C:347:LYS:HB3	1:C:348:PRO:HD2	2.01	0.41
1:A:279:ILE:CD1	1:D:422:PRO:CG	2.98	0.41
1:A:542:MET:HA	1:A:604:ASN:HA	2.02	0.41
1:C:654:TRP:NE1	1:C:666:GLY:HA3	2.34	0.41
1:C:851:ILE:O	1:C:870:VAL:HA	2.20	0.41
1:A:390:SER:HA	1:A:391:HIS:HA	1.88	0.41
1:A:615:PRO:O	1:A:618:THR:HG22	2.20	0.41
1:A:845:GLN:HE21	1:A:845:GLN:HB3	1.62	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.61	0.41
1:D:106:PRO:C	5:D:8419:DMS:H22	2.41	0.41
1:D:646:HIS:CD2	1:D:647:SER:N	2.88	0.41
1:D:801:ILE:HG22	1:D:802:ASP:H	1.85	0.41
1:A:30:HIS:NE2	1:A:170:GLU:OE1	2.53	0.41
1:A:854:LYS:HA	1:A:867:THR:O	2.21	0.41
1:B:542:MET:HA	1:B:604:ASN:HA	2.02	0.41
1:C:658:LEU:O	1:C:659:ASP:C	2.57	0.41
1:C:769:TRP:HA	1:C:773:LYS:O	2.21	0.41
1:D:74:LEU:HD22	1:D:153:TRP:CG	2.55	0.41
1:D:461:GLU:OE1	2:D:2001:2DG:H21	2.21	0.41
1:A:316:HIS:HB2	5:A:8406:DMS:H23	2.02	0.41
1:A:781:ARG:NH1	6:A:9309:HOH:O	2.53	0.41
1:B:19:PRO:HD3	1:B:112:PRO:HB3	2.02	0.41
1:C:143:PHE:HB3	1:C:146:VAL:HG23	2.00	0.41
1:D:414:ASN:ND2	1:D:439:ARG:NH1	2.69	0.41
1:A:50:GLN:CD	1:A:50:GLN:N	2.73	0.41
1:A:147:ASN:HA	1:A:148:SER:HA	1.54	0.41
1:A:571:VAL:CG2	1:A:609:ALA:HA	2.51	0.41
1:A:577:LYS:HB3	1:A:577:LYS:HE3	1.91	0.41
1:A:655:MET:HE2	1:A:656:VAL:N	2.35	0.41
1:A:694:LEU:HD23	1:A:694:LEU:HA	1.89	0.41
1:B:231:PHE:CD1	1:B:231:PHE:N	2.89	0.41
1:B:412:GLU:CG	1:B:459:GLY:HA2	2.50	0.41
1:B:744:GLU:CB	1:B:745:MET:HE3	2.51	0.41
1:C:29:ALA:HB3	1:C:445:GLN:OE1	2.21	0.41
1:C:344:LEU:HB3	1:C:349:LEU:HD21	2.03	0.41
1:C:498:ILE:HD13	1:C:498:ILE:HG21	1.89	0.41
1:C:718:GLN:CG	5:C:8503:DMS:C1	2.97	0.41
1:D:337:ILE:HA	1:D:341:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:LEU:HA	1:B:79:PRO:HD3	1.75	0.41
1:B:232:ASN:C	5:B:8417:DMS:H22	2.40	0.41
1:D:251:ARG:HD2	5:D:8416:DMS:H12	2.03	0.41
1:D:654:TRP:CE3	1:D:665:SER:HA	2.56	0.41
1:D:890:GLN:HG3	1:D:891:VAL:N	2.36	0.41
1:D:949:HIS:HB3	1:D:951:TRP:CH2	2.56	0.41
1:A:370:GLN:HB2	6:A:9098:HOH:O	2.21	0.40
1:A:502:MET:HB2	1:A:537:GLU:HB2	2.02	0.40
1:B:367:MET:HE1	1:B:372:MET:HG3	2.00	0.40
1:B:510:GLN:O	1:B:512:PHE:N	2.49	0.40
1:B:689:GLU:O	1:B:690:SER:CB	2.69	0.40
1:A:352:ARG:HH11	1:A:352:ARG:HG3	1.86	0.40
1:A:908:ASP:HB3	1:A:1007:PHE:CD1	2.56	0.40
1:B:766:SER:HA	1:B:779:PRO:HB3	2.04	0.40
1:C:221:GLN:O	1:C:246:MET:HA	2.22	0.40
1:C:496:THR:O	1:C:496:THR:HG23	2.21	0.40
1:C:765:LEU:CD2	1:C:768:MET:HE3	2.49	0.40
1:D:130:ASP:OD2	5:D:8703:DMS:H22	2.21	0.40
5:D:8413:DMS:H21	6:D:9300:HOH:O	2.20	0.40
1:A:663:LEU:CD1	1:A:686:PRO:HG2	2.51	0.40
1:A:826:THR:OG1	1:A:837:THR:HB	2.21	0.40
1:B:744:GLU:HB3	1:B:745:MET:CE	2.51	0.40
1:D:740:LEU:HD12	1:D:741:THR:N	2.36	0.40
1:A:240:LEU:HD13	1:A:260:LEU:HD13	2.04	0.40
1:A:388:ARG:HH11	1:A:388:ARG:HD3	1.63	0.40
1:A:579:ASP:OD1	1:A:581:ASN:HB2	2.22	0.40
1:B:746:ASP:HA	1:B:760:ARG:HG3	2.04	0.40
1:C:573:GLN:HB2	1:C:602:CYS:O	2.22	0.40
1:C:933:SER:O	1:C:934:GLU:C	2.58	0.40
1:D:576:ILE:HA	1:D:576:ILE:HD13	1.82	0.40
1:A:18:ASN:N	1:A:193:ASP:OD2	2.53	0.40
1:A:546:LEU:HA	6:A:8730:HOH:O	2.20	0.40
1:A:576:ILE:HD13	1:A:576:ILE:HA	1.84	0.40
1:A:684:GLU:HG2	1:A:685:LEU:N	2.34	0.40
1:A:756:TRP:CD1	1:A:768:MET:HG2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LYS:NZ	6:C:9410:HOH:O[3_544]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	964 (96%)	44 (4%)	1 (0%)	51	54
1	B	1009/1023 (99%)	956 (95%)	48 (5%)	5 (0%)	29	26
1	C	1009/1023 (99%)	963 (95%)	46 (5%)	0	100	100
1	D	1009/1023 (99%)	962 (95%)	43 (4%)	4 (0%)	34	32
All	All	4036/4092 (99%)	3845 (95%)	181 (4%)	10 (0%)	47	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	B	731	PRO
1	D	688	PRO
1	D	801	ILE
1	B	688	PRO
1	D	803	PRO
1	B	732	ALA
1	D	164	ASP
1	B	164	ASP
1	A	164	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	816 (94%)	48 (6%)	21	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	864/875 (99%)	815 (94%)	49 (6%)	20	18
1	C	864/875 (99%)	817 (95%)	47 (5%)	22	20
1	D	864/875 (99%)	812 (94%)	52 (6%)	19	16
All	All	3456/3500 (99%)	3260 (94%)	196 (6%)	20	18

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	116	THR
1	A	230	ARG
1	A	237	ARG
1	A	250	LEU
1	A	277	GLU
1	A	279	ILE
1	A	333	ARG
1	A	336	ARG
1	A	344	LEU
1	A	362	LEU
1	A	377	LEU
1	A	394	ASN
1	A	446	ARG
1	A	451	PRO
1	A	477	SER
1	A	478	VAL
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	595	THR
1	A	600	GLN
1	A	634	GLN
1	A	651	LEU
1	A	655	MET
1	A	672	VAL
1	A	682	LEU
1	A	684	GLU
1	A	685	LEU
1	A	699	ARG
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS

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Mol	Chain	Res	Type
1	A	796	SER
1	A	799	THR
1	A	800	ARG
1	A	801	ILE
1	A	809	ARG
1	A	817	GLN
1	A	829	THR
1	A	885	ASN
1	A	890	GLN
1	A	956	GLN
1	A	986	ILE
1	A	1013	ARG
1	A	1017	GLN
1	A	1018	LEU
1	A	1023	LYS
1	B	49	GLN
1	B	71	GLU
1	B	80	GLU
1	B	165	SER
1	B	230	ARG
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU
1	B	392	TYR
1	B	394	ASN
1	B	439	ARG
1	B	477	SER
1	B	478	VAL
1	B	503	TYR
1	B	515	VAL
1	B	554	GLN
1	B	594	ASP
1	B	595	THR
1	B	600	GLN
1	B	634	GLN
1	B	651	LEU
1	B	661	LYS
1	B	663	LEU
1	B	667	GLU

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Mol	Chain	Res	Type
1	B	681	GLU
1	B	685	LEU
1	B	687	GLN
1	B	730	LEU
1	B	737	ILE
1	B	744	GLU
1	B	745	MET
1	B	754	LYS
1	B	755	ARG
1	B	797	GLU
1	B	799	THR
1	B	809	ARG
1	B	819	GLU
1	B	824	GLN
1	B	829	THR
1	B	845	GLN
1	B	847	LYS
1	B	863	GLN
1	B	885	ASN
1	B	890	GLN
1	B	956	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	72	SER
1	C	75	GLU
1	C	117	GLU
1	C	135	GLN
1	C	178	ARG
1	C	213	SER
1	C	214	LEU
1	C	230	ARG
1	C	237	ARG
1	C	262	GLN
1	C	278	ILE
1	C	333	ARG
1	C	344	LEU
1	C	394	ASN
1	C	477	SER
1	C	580	GLU
1	C	595	THR
1	C	634	GLN
1	C	635	THR

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Mol	Chain	Res	Type
1	C	646	HIS
1	C	651	LEU
1	C	653	HIS
1	C	661	LYS
1	C	663	LEU
1	C	681	GLU
1	C	687	GLN
1	C	699	ARG
1	C	729	THR
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	746	ASP
1	C	749	ILE
1	C	750	GLU
1	C	755	ARG
1	C	778	THR
1	C	799	THR
1	C	819	GLU
1	C	830	LEU
1	C	832	ASP
1	C	890	GLN
1	C	934	GLU
1	C	956	GLN
1	C	986	ILE
1	C	1023	LYS
1	D	13	ARG
1	D	80	GLU
1	D	112	PRO
1	D	116	THR
1	D	213	SER
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	425	ARG
1	D	519	SER
1	D	545	SER

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Mol	Chain	Res	Type
1	D	546	LEU
1	D	595	THR
1	D	631	LEU
1	D	632	SER
1	D	635	THR
1	D	651	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	677	LYS
1	D	681	GLU
1	D	682	LEU
1	D	684	GLU
1	D	685	LEU
1	D	687	GLN
1	D	689	GLU
1	D	730	LEU
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	769	TRP
1	D	772	ASP
1	D	773	LYS
1	D	774	LYS
1	D	799	THR
1	D	817	GLN
1	D	829	THR
1	D	885	ASN
1	D	893	GLU
1	D	956	GLN
1	D	980	GLU
1	D	986	ILE
1	D	1004	SER
1	D	1013	ARG
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	558	GLN

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Mol	Chain	Res	Type
1	A	600	GLN
1	A	624	GLN
1	A	653	HIS
1	A	675	GLN
1	A	757	GLN
1	A	761	GLN
1	A	817	GLN
1	A	824	GLN
1	A	844	HIS
1	A	845	GLN
1	A	878	HIS
1	A	977	HIS
1	A	1017	GLN
1	B	102	ASN
1	B	262	GLN
1	B	266	GLN
1	B	363	HIS
1	B	485	GLN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	757	GLN
1	B	817	GLN
1	B	824	GLN
1	B	878	HIS
1	C	102	ASN
1	C	163	GLN
1	C	262	GLN
1	C	266	GLN
1	C	583	ASN
1	C	634	GLN
1	C	653	HIS
1	C	687	GLN
1	C	843	GLN
1	C	844	HIS
1	C	878	HIS
1	D	135	GLN
1	D	163	GLN
1	D	363	HIS
1	D	583	ASN
1	D	624	GLN

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Mol	Chain	Res	Type
1	D	628	GLN
1	D	653	HIS
1	D	804	ASN
1	D	878	HIS
1	D	977	HIS
1	D	1017	GLN
1	D	1022	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 132 ligands modelled in this entry, 25 are monoatomic - leaving 107 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	D	8508	-	3,3,3	0.56	0	3,3,3	0.59	0
5	DMS	A	8504	-	3,3,3	0.35	0	3,3,3	0.42	0
5	DMS	B	8414	-	3,3,3	0.56	0	3,3,3	0.76	0
5	DMS	B	8601	-	3,3,3	0.43	0	3,3,3	0.29	0
5	DMS	D	8412	-	3,3,3	1.49	1 (33%)	3,3,3	0.59	0
5	DMS	C	8401	-	3,3,3	0.88	0	3,3,3	0.76	0
5	DMS	C	8427	-	3,3,3	0.90	0	3,3,3	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	B	8421	-	3,3,3	0.84	0	3,3,3	0.14	0
5	DMS	B	8402	-	3,3,3	1.89	2 (66%)	3,3,3	0.18	0
5	DMS	C	8412	-	3,3,3	0.87	0	3,3,3	0.56	0
5	DMS	C	8425	4	3,3,3	1.48	1 (33%)	3,3,3	1.65	1 (33%)
5	DMS	A	8409	-	3,3,3	2.34	2 (66%)	3,3,3	0.36	0
2	2DG	A	2001	1,4	10,10,11	1.04	1 (10%)	13,13,15	1.89	3 (23%)
5	DMS	C	8417	-	3,3,3	0.86	0	3,3,3	0.52	0
5	DMS	A	8501	-	3,3,3	1.45	1 (33%)	3,3,3	0.32	0
5	DMS	B	8404	-	3,3,3	0.81	0	3,3,3	0.36	0
5	DMS	D	8409	-	3,3,3	2.22	1 (33%)	3,3,3	0.59	0
5	DMS	B	8425	4	3,3,3	1.92	1 (33%)	3,3,3	0.37	0
5	DMS	C	8402	-	3,3,3	2.08	1 (33%)	3,3,3	0.72	0
5	DMS	B	8408	-	3,3,3	1.41	0	3,3,3	0.40	0
5	DMS	C	8504	-	3,3,3	1.11	0	3,3,3	0.23	0
5	DMS	A	8412	-	3,3,3	0.76	0	3,3,3	0.20	0
5	DMS	C	8415	-	3,3,3	1.57	1 (33%)	3,3,3	0.97	0
5	DMS	A	8419	-	3,3,3	0.66	0	3,3,3	0.40	0
5	DMS	A	8405	-	3,3,3	1.50	1 (33%)	3,3,3	0.24	0
5	DMS	C	8501	-	3,3,3	1.53	0	3,3,3	1.19	1 (33%)
5	DMS	B	8403	-	3,3,3	1.46	0	3,3,3	1.25	1 (33%)
5	DMS	B	8405	-	3,3,3	0.89	0	3,3,3	0.39	0
5	DMS	B	8407	-	3,3,3	1.51	0	3,3,3	0.26	0
5	DMS	B	8413	-	3,3,3	2.23	2 (66%)	3,3,3	0.82	0
5	DMS	A	8402	-	3,3,3	1.57	1 (33%)	3,3,3	0.14	0
2	2DG	D	2001	1,4	10,10,11	1.42	2 (20%)	13,13,15	2.35	4 (30%)
5	DMS	C	8404	-	3,3,3	1.29	0	3,3,3	0.68	0
5	DMS	C	8602	-	3,3,3	1.06	0	3,3,3	0.16	0
5	DMS	A	8406	-	3,3,3	1.88	1 (33%)	3,3,3	0.45	0
2	2DG	B	2001	1,4	10,10,11	1.41	1 (10%)	13,13,15	1.27	1 (7%)
5	DMS	D	8414	-	3,3,3	1.22	0	3,3,3	0.08	0
5	DMS	D	8503	-	3,3,3	1.34	1 (33%)	3,3,3	0.78	0
5	DMS	B	8401	-	3,3,3	0.66	0	3,3,3	0.44	0
5	DMS	A	8407	-	3,3,3	1.74	2 (66%)	3,3,3	0.54	0
5	DMS	B	8420	-	3,3,3	1.30	1 (33%)	3,3,3	0.39	0
5	DMS	D	8408	-	3,3,3	1.14	0	3,3,3	0.32	0
5	DMS	A	8413	-	3,3,3	2.03	2 (66%)	3,3,3	0.16	0
5	DMS	C	8419	-	3,3,3	1.40	0	3,3,3	0.19	0
5	DMS	A	8421	-	3,3,3	0.89	0	3,3,3	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	B	8417	-	3,3,3	1.18	0	3,3,3	0.48	0
5	DMS	C	8403	-	3,3,3	0.84	0	3,3,3	0.43	0
5	DMS	B	8409	-	3,3,3	0.71	0	3,3,3	1.28	1 (33%)
5	DMS	C	8420	-	3,3,3	1.29	0	3,3,3	0.66	0
5	DMS	B	8504	-	3,3,3	0.11	0	3,3,3	0.08	0
5	DMS	D	8701	-	3,3,3	2.89	2 (66%)	3,3,3	0.76	0
5	DMS	A	8502	-	3,3,3	1.16	0	3,3,3	1.36	1 (33%)
5	DMS	D	8410	-	3,3,3	1.30	0	3,3,3	0.49	0
5	DMS	A	8425	4	3,3,3	1.42	1 (33%)	3,3,3	0.56	0
5	DMS	C	8407	-	3,3,3	1.16	0	3,3,3	0.11	0
5	DMS	B	8406	-	3,3,3	1.26	1 (33%)	3,3,3	0.26	0
5	DMS	D	8419	-	3,3,3	0.88	0	3,3,3	0.36	0
5	DMS	C	8421	-	3,3,3	0.60	0	3,3,3	0.23	0
5	DMS	A	8411	-	3,3,3	1.56	1 (33%)	3,3,3	0.15	0
5	DMS	C	8423	-	3,3,3	1.30	0	3,3,3	0.31	0
5	DMS	D	8405	-	3,3,3	0.83	0	3,3,3	0.25	0
5	DMS	A	8417	-	3,3,3	1.12	0	3,3,3	0.50	0
5	DMS	D	8403	-	3,3,3	0.52	0	3,3,3	0.31	0
5	DMS	D	8401	-	3,3,3	1.78	1 (33%)	3,3,3	0.33	0
5	DMS	C	8503	-	3,3,3	0.79	0	3,3,3	0.42	0
5	DMS	D	8411	-	3,3,3	0.93	0	3,3,3	0.49	0
5	DMS	C	8409	-	3,3,3	1.58	1 (33%)	3,3,3	0.38	0
5	DMS	D	8416	-	3,3,3	0.77	0	3,3,3	0.23	0
5	DMS	A	8414	-	3,3,3	0.76	0	3,3,3	0.44	0
5	DMS	C	8506	-	3,3,3	1.59	1 (33%)	3,3,3	1.25	1 (33%)
5	DMS	B	8427	-	3,3,3	0.88	0	3,3,3	0.61	0
5	DMS	A	8410	-	3,3,3	0.72	0	3,3,3	0.09	0
5	DMS	D	8417	-	3,3,3	1.27	0	3,3,3	0.72	0
5	DMS	B	8416	-	3,3,3	1.30	0	3,3,3	0.07	0
5	DMS	D	8402	-	3,3,3	1.15	0	3,3,3	0.63	0
5	DMS	A	8415	-	3,3,3	1.94	1 (33%)	3,3,3	0.15	0
5	DMS	D	8421	-	3,3,3	1.03	0	3,3,3	0.08	0
5	DMS	D	8413	-	3,3,3	0.89	0	3,3,3	0.65	0
5	DMS	A	8503	-	3,3,3	0.66	0	3,3,3	0.18	0
5	DMS	A	8602	-	3,3,3	0.87	0	3,3,3	0.83	0
2	2DG	C	2001	1,4	10,10,11	1.28	1 (10%)	13,13,15	1.87	1 (7%)
5	DMS	B	8508	-	3,3,3	2.50	3 (100%)	3,3,3	0.38	0
5	DMS	C	8408	-	3,3,3	0.68	0	3,3,3	0.25	0
5	DMS	A	8403	-	3,3,3	0.97	0	3,3,3	0.74	0
5	DMS	A	8404	-	3,3,3	1.82	1 (33%)	3,3,3	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	D	8406	-	3,3,3	1.02	0	3,3,3	0.38	0
5	DMS	C	8405	-	3,3,3	1.83	1 (33%)	3,3,3	0.26	0
5	DMS	A	8408	-	3,3,3	1.06	0	3,3,3	0.24	0
5	DMS	C	8414	-	3,3,3	1.59	1 (33%)	3,3,3	0.36	0
5	DMS	B	8423	-	3,3,3	0.57	0	3,3,3	0.15	0
5	DMS	C	8601	-	3,3,3	1.09	0	3,3,3	0.61	0
5	DMS	C	8413	-	3,3,3	2.95	2 (66%)	3,3,3	0.43	0
5	DMS	D	8501	-	3,3,3	0.84	0	3,3,3	0.90	0
5	DMS	D	8705	-	3,3,3	1.23	0	3,3,3	0.21	0
5	DMS	A	8420	-	3,3,3	1.57	1 (33%)	3,3,3	1.02	0
5	DMS	A	8401	-	3,3,3	1.94	1 (33%)	3,3,3	0.12	0
5	DMS	B	8411	-	3,3,3	0.36	0	3,3,3	0.76	0
5	DMS	B	8415	-	3,3,3	1.10	0	3,3,3	1.33	1 (33%)
5	DMS	B	8412	-	3,3,3	1.92	1 (33%)	3,3,3	0.18	0
5	DMS	B	8410	-	3,3,3	1.30	0	3,3,3	0.49	0
5	DMS	C	8411	-	3,3,3	1.68	1 (33%)	3,3,3	0.34	0
5	DMS	B	8506	-	3,3,3	1.39	0	3,3,3	0.79	0
5	DMS	C	8410	-	3,3,3	1.10	0	3,3,3	0.36	0
5	DMS	B	8502	-	3,3,3	0.74	0	3,3,3	1.26	1 (33%)
5	DMS	D	8703	-	3,3,3	0.84	0	3,3,3	0.33	0
5	DMS	D	8404	-	3,3,3	1.58	1 (33%)	3,3,3	0.51	0
5	DMS	C	8416	-	3,3,3	1.11	0	3,3,3	0.72	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	2DG	A	2001	1,4	-	1/2/16/18	0/1/1/1
2	2DG	B	2001	1,4	-	1/2/16/18	0/1/1/1
2	2DG	C	2001	1,4	-	1/2/16/18	0/1/1/1
2	2DG	D	2001	1,4	-	1/2/16/18	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8413	DMS	O-S	4.50	1.80	1.50
5	D	8701	DMS	O-S	3.75	1.75	1.50
5	D	8409	DMS	O-S	3.74	1.75	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	2DG	C2-C3	3.40	1.57	1.52
5	A	8409	DMS	O-S	3.29	1.72	1.50
5	A	8406	DMS	C2-S	-3.25	1.51	1.75
5	A	8401	DMS	O-S	3.14	1.71	1.50
5	C	8402	DMS	C2-S	3.12	1.99	1.75
5	B	8508	DMS	C1-S	3.08	1.98	1.75
2	B	2001	2DG	C4-C5	3.02	1.59	1.53
5	A	8415	DMS	C2-S	3.00	1.98	1.75
5	B	8412	DMS	C2-S	2.94	1.97	1.75
5	A	8404	DMS	C2-S	2.88	1.97	1.75
5	B	8425	DMS	O-S	2.82	1.69	1.50
5	D	8701	DMS	C2-S	2.80	1.96	1.75
5	B	8413	DMS	C1-S	2.75	1.96	1.75
5	A	8420	DMS	C2-S	2.68	1.95	1.75
5	C	8405	DMS	O-S	2.63	1.68	1.50
5	A	8413	DMS	C2-S	2.62	1.95	1.75
5	C	8409	DMS	O-S	2.61	1.67	1.50
5	C	8415	DMS	C2-S	2.60	1.95	1.75
5	C	8414	DMS	C1-S	-2.58	1.56	1.75
5	A	8411	DMS	C1-S	2.56	1.94	1.75
5	B	8402	DMS	C2-S	2.54	1.94	1.75
2	C	2001	2DG	C4-C5	2.51	1.58	1.53
5	D	8401	DMS	C2-S	2.47	1.94	1.75
5	D	8404	DMS	C2-S	2.43	1.93	1.75
5	B	8413	DMS	O-S	2.36	1.66	1.50
5	A	8409	DMS	C1-S	2.36	1.93	1.75
5	A	8402	DMS	C2-S	2.35	1.93	1.75
5	A	8405	DMS	O-S	2.30	1.65	1.50
5	A	8413	DMS	O-S	2.28	1.65	1.50
2	A	2001	2DG	C2-C3	2.28	1.55	1.52
5	C	8425	DMS	C2-S	2.27	1.92	1.75
5	A	8501	DMS	C2-S	2.19	1.92	1.75
5	B	8420	DMS	C2-S	2.17	1.92	1.75
5	C	8506	DMS	C2-S	2.16	1.91	1.75
5	B	8508	DMS	C2-S	2.15	1.91	1.75
5	B	8406	DMS	C1-S	2.15	1.91	1.75
5	B	8508	DMS	O-S	2.14	1.64	1.50
5	C	8413	DMS	C2-S	2.14	1.91	1.75
2	D	2001	2DG	C4-C5	2.12	1.57	1.53
5	A	8425	DMS	C2-S	2.11	1.91	1.75
5	A	8407	DMS	C2-S	2.10	1.91	1.75
5	D	8503	DMS	C1-S	2.08	1.91	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8411	DMS	C1-S	2.05	1.91	1.75
5	B	8402	DMS	O-S	2.04	1.64	1.50
5	D	8412	DMS	O-S	2.04	1.64	1.50
5	A	8407	DMS	O-S	2.01	1.63	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	2001	2DG	C3-C4-C5	-5.77	104.22	109.97
2	A	2001	2DG	C3-C4-C5	-4.74	105.25	109.97
2	D	2001	2DG	C1-O5-C5	4.27	119.43	112.01
2	D	2001	2DG	C2-C3-C4	4.25	116.04	111.16
2	D	2001	2DG	C3-C4-C5	-4.21	105.77	109.97
2	A	2001	2DG	C1-C2-C3	-2.92	105.79	110.68
5	C	8425	DMS	C2-S-C1	2.84	113.06	98.44
2	D	2001	2DG	C1-C2-C3	-2.55	106.42	110.68
5	A	8502	DMS	C2-S-C1	2.36	110.59	98.44
5	B	8415	DMS	C2-S-C1	2.28	110.17	98.44
2	A	2001	2DG	O4-C4-C3	-2.27	105.64	109.99
5	B	8409	DMS	C2-S-C1	2.20	109.74	98.44
5	B	8502	DMS	C2-S-C1	2.18	109.65	98.44
5	C	8506	DMS	C2-S-C1	2.16	109.54	98.44
2	B	2001	2DG	O3-C3-C2	-2.10	104.93	109.96
5	B	8403	DMS	C2-S-C1	2.08	109.16	98.44
5	C	8501	DMS	C2-S-C1	-2.03	88.00	98.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

31 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8508	DMS	1	0
5	B	8601	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8412	DMS	4	0
5	C	8427	DMS	1	0
5	B	8402	DMS	1	0
5	C	8412	DMS	2	0
5	C	8504	DMS	1	0
2	D	2001	2DG	2	0
5	C	8602	DMS	1	0
5	A	8406	DMS	1	0
2	B	2001	2DG	1	0
5	D	8503	DMS	2	0
5	B	8417	DMS	1	0
5	C	8420	DMS	2	0
5	B	8504	DMS	1	0
5	A	8502	DMS	3	0
5	B	8406	DMS	1	0
5	D	8419	DMS	1	0
5	C	8503	DMS	3	0
5	D	8416	DMS	3	0
5	A	8414	DMS	1	0
5	C	8506	DMS	4	0
5	A	8410	DMS	1	0
5	D	8413	DMS	1	0
5	A	8602	DMS	1	0
5	C	8601	DMS	1	0
5	A	8420	DMS	2	0
5	B	8415	DMS	2	0
5	B	8412	DMS	1	0
5	B	8506	DMS	2	0
5	D	8703	DMS	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.76	16 (1%)	72	75	5, 15, 44, 98	0
1	B	1011/1023 (98%)	-0.73	11 (1%)	80	84	5, 15, 45, 100	0
1	C	1011/1023 (98%)	-0.70	17 (1%)	70	74	6, 15, 46, 100	0
1	D	1011/1023 (98%)	-0.70	19 (1%)	66	71	4, 16, 46, 99	0
All	All	4044/4092 (98%)	-0.72	63 (1%)	72	75	4, 15, 45, 100	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	731	PRO	8.2
1	A	735	HIS	8.0
1	A	686	PRO	7.8
1	B	731	PRO	7.3
1	D	732	ALA	6.5
1	C	732	ALA	5.8
1	D	735	HIS	5.7
1	B	730	LEU	5.4
1	B	689	GLU	5.3
1	D	799	THR	5.1
1	B	733	ALA	4.9
1	D	686	PRO	4.9
1	B	732	ALA	4.6
1	D	730	LEU	4.6
1	C	689	GLU	4.6
1	A	730	LEU	4.5
1	A	732	ALA	4.5
1	D	800	ARG	4.2
1	C	730	LEU	4.1
1	D	731	PRO	4.0
1	A	731	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	797	GLU	3.8
1	A	689	GLU	3.7
1	D	734	SER	3.6
1	C	733	ALA	3.6
1	C	735	HIS	3.6
1	A	687	GLN	3.5
1	B	687	GLN	3.4
1	A	799	THR	3.4
1	B	799	THR	3.3
1	B	685	LEU	3.2
1	D	689	GLU	3.2
1	C	798	ALA	3.2
1	A	733	ALA	3.2
1	A	685	LEU	3.1
1	D	581	ASN	3.1
1	D	687	GLN	2.9
1	D	684	GLU	2.9
1	C	800	ARG	2.9
1	B	798	ALA	2.8
1	B	686	PRO	2.7
1	C	729	THR	2.7
1	D	771	GLY	2.7
1	A	71	GLU	2.5
1	C	744	GLU	2.5
1	C	687	GLN	2.5
1	A	729	THR	2.4
1	B	797	GLU	2.4
1	C	799	THR	2.4
1	A	684	GLU	2.4
1	C	685	LEU	2.3
1	D	772	ASP	2.3
1	C	686	PRO	2.3
1	D	733	ALA	2.2
1	A	580	GLU	2.2
1	D	634	GLN	2.2
1	A	1023	LYS	2.2
1	C	745	MET	2.2
1	D	801	ILE	2.1
1	C	772	ASP	2.1
1	A	798	ALA	2.1
1	C	684	GLU	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, 95^{th} 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	0.89	0.21	24,53,80,80	0
5	DMS	B	8508	4/4	0.90	0.11	27,31,46,64	0
3	MG	A	3005	1/1	0.90	0.04	36,36,36,36	0
4	NA	D	3103	1/1	0.91	0.11	38,38,38,38	0
5	DMS	B	8406	4/4	0.92	0.19	34,40,61,78	0
5	DMS	B	8413	4/4	0.93	0.15	22,32,35,42	0
5	DMS	B	8427	4/4	0.93	0.10	28,31,42,65	0
5	DMS	A	8502	4/4	0.93	0.12	14,21,75,84	0
5	DMS	A	8417	4/4	0.93	0.17	25,26,61,100	0
5	DMS	B	8408	4/4	0.94	0.17	15,25,43,60	0
5	DMS	A	8415	4/4	0.94	0.10	24,27,28,70	0
5	DMS	C	8419	4/4	0.94	0.14	33,44,54,61	0
5	DMS	D	8417	4/4	0.94	0.14	18,26,39,73	0
5	DMS	B	8415	4/4	0.94	0.12	22,26,33,67	0
5	DMS	B	8407	4/4	0.95	0.17	34,34,63,66	0
5	DMS	A	8425	4/4	0.95	0.15	34,40,45,45	0
5	DMS	C	8413	4/4	0.95	0.16	31,32,34,38	0
5	DMS	C	8415	4/4	0.95	0.11	20,26,33,52	0
5	DMS	C	8417	4/4	0.95	0.10	24,51,57,58	0
4	NA	B	3104	1/1	0.95	0.09	37,37,37,37	0
5	DMS	C	8423	4/4	0.95	0.10	26,27,32,61	0
5	DMS	C	8602	4/4	0.95	0.11	27,32,53,77	0
5	DMS	A	8421	4/4	0.95	0.18	42,43,67,100	0
5	DMS	B	8425	4/4	0.95	0.12	22,30,32,54	0
5	DMS	B	8502	4/4	0.96	0.09	13,30,45,50	0
5	DMS	B	8412	4/4	0.96	0.11	21,33,34,38	0
2	2DG	D	2001	10/11	0.96	0.08	9,15,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	A	8406	4/4	0.96	0.13	7,53,55,100	0
5	DMS	C	8416	4/4	0.96	0.26	31,33,49,64	0
5	DMS	B	8417	4/4	0.96	0.10	26,31,34,63	0
5	DMS	B	8420	4/4	0.96	0.13	36,45,63,100	0
5	DMS	B	8421	4/4	0.96	0.10	14,46,60,85	0
5	DMS	C	8425	4/4	0.96	0.11	33,37,39,48	0
5	DMS	C	8503	4/4	0.96	0.19	20,31,54,100	0
5	DMS	C	8506	4/4	0.96	0.10	15,24,47,89	0
5	DMS	C	8601	4/4	0.96	0.14	31,53,55,100	0
5	DMS	B	8423	4/4	0.96	0.10	28,44,71,87	0
5	DMS	D	8406	4/4	0.96	0.08	18,19,20,34	0
5	DMS	D	8409	4/4	0.96	0.07	25,30,39,53	0
5	DMS	A	8407	4/4	0.96	0.13	28,40,42,43	0
5	DMS	A	8409	4/4	0.96	0.11	24,27,39,42	0
5	DMS	D	8705	4/4	0.96	0.12	24,32,51,51	0
2	2DG	B	2001	10/11	0.97	0.11	13,15,19,24	0
5	DMS	B	8416	4/4	0.97	0.12	35,42,52,88	0
5	DMS	A	8501	4/4	0.97	0.08	12,13,29,33	0
3	MG	D	3005	1/1	0.97	0.05	43,43,43,43	0
5	DMS	A	8503	4/4	0.97	0.20	42,47,48,100	0
2	2DG	C	2001	10/11	0.97	0.08	7,15,26,27	0
5	DMS	A	8413	4/4	0.97	0.12	34,34,53,100	0
4	NA	C	3103	1/1	0.97	0.06	22,22,22,22	0
5	DMS	B	8409	4/4	0.97	0.09	18,32,33,38	0
4	NA	C	3104	1/1	0.97	0.08	26,26,26,26	0
5	DMS	B	8601	4/4	0.97	0.11	36,60,100,100	0
5	DMS	D	8414	4/4	0.97	0.14	17,32,44,92	0
5	DMS	D	8416	4/4	0.97	0.21	16,34,42,89	0
5	DMS	C	8409	4/4	0.97	0.09	23,35,41,41	0
5	DMS	D	8421	4/4	0.97	0.11	36,45,48,52	0
5	DMS	D	8501	4/4	0.97	0.08	16,34,36,46	0
5	DMS	D	8503	4/4	0.97	0.18	33,53,64,100	0
2	2DG	A	2001	10/11	0.97	0.07	10,15,18,25	0
5	DMS	B	8414	4/4	0.97	0.13	24,43,49,100	0
5	DMS	A	8411	4/4	0.98	0.08	24,26,28,100	0
5	DMS	A	8412	4/4	0.98	0.10	24,33,37,37	0
5	DMS	C	8414	4/4	0.98	0.08	17,18,23,39	0
3	MG	B	3001	1/1	0.98	0.06	11,11,11,11	0
5	DMS	B	8410	4/4	0.98	0.09	18,27,41,54	0
5	DMS	A	8414	4/4	0.98	0.10	16,37,47,100	0
4	NA	C	3101	1/1	0.98	0.05	11,11,11,11	0
5	DMS	C	8420	4/4	0.98	0.12	34,36,53,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	C	8421	4/4	0.98	0.11	26,26,41,64	0
3	MG	D	3002	1/1	0.98	0.07	19,19,19,19	0
5	DMS	A	8419	4/4	0.98	0.12	24,26,55,100	0
5	DMS	C	8427	4/4	0.98	0.15	37,43,81,82	0
5	DMS	C	8501	4/4	0.98	0.12	23,23,34,38	0
5	DMS	A	8420	4/4	0.98	0.08	33,35,39,46	0
5	DMS	C	8504	4/4	0.98	0.07	32,34,42,64	0
3	MG	A	3002	1/1	0.98	0.05	14,14,14,14	0
4	NA	A	3101	1/1	0.98	0.05	13,13,13,13	0
5	DMS	A	8402	4/4	0.98	0.07	11,26,30,47	0
5	DMS	D	8402	4/4	0.98	0.07	9,23,27,32	0
4	NA	A	3103	1/1	0.98	0.11	25,25,25,25	0
4	NA	B	3101	1/1	0.98	0.06	13,13,13,13	0
5	DMS	D	8410	4/4	0.98	0.10	22,35,39,100	0
5	DMS	D	8412	4/4	0.98	0.10	15,25,32,33	0
5	DMS	D	8413	4/4	0.98	0.13	21,24,34,35	0
5	DMS	A	8504	4/4	0.98	0.10	23,35,38,100	0
5	DMS	A	8602	4/4	0.98	0.18	42,45,100,100	0
5	DMS	B	8504	4/4	0.98	0.10	31,37,51,52	0
5	DMS	D	8419	4/4	0.98	0.07	18,32,40,44	0
5	DMS	B	8506	4/4	0.98	0.10	31,39,63,100	0
5	DMS	B	8402	4/4	0.98	0.07	8,21,25,29	0
4	NA	B	3102	1/1	0.98	0.06	13,13,13,13	0
5	DMS	D	8508	4/4	0.98	0.08	19,46,50,80	0
5	DMS	D	8701	4/4	0.98	0.09	15,17,22,37	0
5	DMS	C	8407	4/4	0.98	0.11	35,39,51,52	0
5	DMS	C	8408	4/4	0.98	0.09	13,35,46,83	0
4	NA	D	3102	1/1	0.99	0.05	18,18,18,18	0
4	NA	A	3104	1/1	0.99	0.06	21,21,21,21	0
5	DMS	A	8401	4/4	0.99	0.09	6,13,16,19	0
3	MG	D	3001	1/1	0.99	0.02	15,15,15,15	0
5	DMS	A	8403	4/4	0.99	0.09	15,20,21,23	0
5	DMS	A	8404	4/4	0.99	0.06	9,22,22,30	0
5	DMS	A	8405	4/4	0.99	0.05	11,22,25,27	0
3	MG	A	3001	1/1	0.99	0.02	13,13,13,13	0
4	NA	B	3103	1/1	0.99	0.03	19,19,19,19	0
5	DMS	A	8408	4/4	0.99	0.08	14,23,31,82	0
5	DMS	B	8401	4/4	0.99	0.07	13,13,21,22	0
3	MG	B	3002	1/1	0.99	0.04	14,14,14,14	0
5	DMS	B	8403	4/4	0.99	0.12	12,12,18,21	0
5	DMS	D	8401	4/4	0.99	0.06	10,11,20,27	0
5	DMS	B	8404	4/4	0.99	0.07	16,20,30,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	D	8403	4/4	0.99	0.10	21,26,27,45	0
5	DMS	D	8404	4/4	0.99	0.07	14,19,26,80	0
5	DMS	D	8405	4/4	0.99	0.08	18,23,42,100	0
5	DMS	B	8405	4/4	0.99	0.11	23,28,62,71	0
5	DMS	D	8408	4/4	0.99	0.10	14,27,28,36	0
5	DMS	C	8401	4/4	0.99	0.08	10,11,21,30	0
5	DMS	C	8402	4/4	0.99	0.07	6,31,38,40	0
5	DMS	D	8411	4/4	0.99	0.05	11,27,27,100	0
5	DMS	C	8403	4/4	0.99	0.10	10,12,16,19	0
5	DMS	C	8404	4/4	0.99	0.06	11,13,21,21	0
5	DMS	C	8405	4/4	0.99	0.10	16,23,25,38	0
5	DMS	A	8410	4/4	0.99	0.09	28,39,55,58	0
3	MG	C	3001	1/1	0.99	0.03	12,12,12,12	0
4	NA	C	3102	1/1	0.99	0.04	16,16,16,16	0
5	DMS	C	8410	4/4	0.99	0.07	21,35,37,43	0
5	DMS	C	8411	4/4	0.99	0.08	18,20,34,50	0
5	DMS	C	8412	4/4	0.99	0.06	18,31,67,100	0
4	NA	A	3102	1/1	0.99	0.04	15,15,15,15	0
3	MG	C	3002	1/1	0.99	0.06	12,12,12,12	0
5	DMS	B	8411	4/4	0.99	0.05	15,17,32,100	0
4	NA	D	3101	1/1	0.99	0.04	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.