Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:39 PM GMT

PDB ID	:	1PX3
Title	:	E. COLI (LACZ) BETA-GALACTOSIDASE (G794A)
Authors	:	Juers, D.H.; Hakda, S.; Matthews, B.W.; Huber, R.E.
Deposited on	:	2003-07-02
Resolution	:	1.60 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

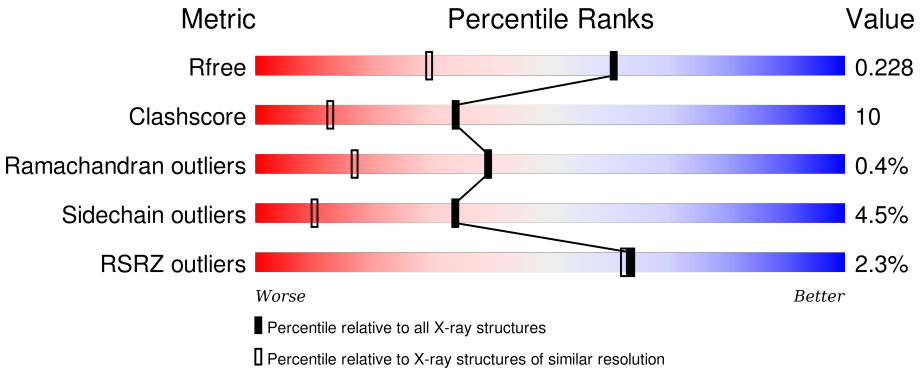
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	3% 69% 25% 5%
1	B	1023	2% 68% 25% 6%
1	C	1023	2% 69% 25%
1	D	1023	2% 68% 24% 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
2	MG	B	3001	-	-	-	X
2	MG	C	3001	-	-	-	X
4	DMS	A	8404	-	-	X	X
4	DMS	A	8406	-	-	-	X
4	DMS	A	8408	-	-	-	X
4	DMS	A	8412	-	-	-	X
4	DMS	A	8417	-	-	-	X
4	DMS	A	8419	-	-	-	X
4	DMS	A	8502	-	-	-	X
4	DMS	B	8404	-	-	-	X
4	DMS	B	8417	-	-	-	X
4	DMS	B	8502	-	-	-	X
4	DMS	B	8508	-	-	-	X
4	DMS	C	8403	-	-	-	X
4	DMS	C	8405	-	-	-	X
4	DMS	C	8417	-	-	-	X
4	DMS	C	8425	-	-	X	X
4	DMS	C	8501	-	-	-	X
4	DMS	C	8503	-	-	-	X
4	DMS	C	8602	-	-	-	X
4	DMS	D	8404	-	-	-	X
4	DMS	D	8417	-	-	-	X
4	DMS	D	8419	-	-	-	X
4	DMS	D	8508	-	-	-	X
4	DMS	D	8703	-	-	X	-
4	DMS	D	8705	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36619 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	1010	Total	C	N	O	S	0	0	0
			8119	5135	1439	1507	38			
1	B	1009	Total	C	N	O	S	0	0	0
			8114	5132	1438	1506	38			
1	C	1007	Total	C	N	O	S	0	0	0
			8095	5120	1433	1504	38			
1	D	1008	Total	C	N	O	S	0	0	0
			8103	5126	1434	1505	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP P00722
A	2	SER	-	CLONING ARTIFACT	UNP P00722
A	3	HIS	-	CLONING ARTIFACT	UNP P00722
A	4	MET	-	CLONING ARTIFACT	UNP P00722
A	5	LEU	-	CLONING ARTIFACT	UNP P00722
A	6	GLU	-	CLONING ARTIFACT	UNP P00722
A	7	ASP	-	CLONING ARTIFACT	UNP P00722
A	8	PRO	-	CLONING ARTIFACT	UNP P00722
A	794	ALA	GLY	ENGINEERED	UNP P00722
B	1	GLY	-	CLONING ARTIFACT	UNP P00722
B	2	SER	-	CLONING ARTIFACT	UNP P00722
B	3	HIS	-	CLONING ARTIFACT	UNP P00722
B	4	MET	-	CLONING ARTIFACT	UNP P00722
B	5	LEU	-	CLONING ARTIFACT	UNP P00722
B	6	GLU	-	CLONING ARTIFACT	UNP P00722
B	7	ASP	-	CLONING ARTIFACT	UNP P00722
B	8	PRO	-	CLONING ARTIFACT	UNP P00722
B	794	ALA	GLY	ENGINEERED	UNP P00722
C	1	GLY	-	CLONING ARTIFACT	UNP P00722
C	2	SER	-	CLONING ARTIFACT	UNP P00722
C	3	HIS	-	CLONING ARTIFACT	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	CLONING ARTIFACT	UNP P00722
C	5	LEU	-	CLONING ARTIFACT	UNP P00722
C	6	GLU	-	CLONING ARTIFACT	UNP P00722
C	7	ASP	-	CLONING ARTIFACT	UNP P00722
C	8	PRO	-	CLONING ARTIFACT	UNP P00722
C	794	ALA	GLY	ENGINEERED	UNP P00722
D	1	GLY	-	CLONING ARTIFACT	UNP P00722
D	2	SER	-	CLONING ARTIFACT	UNP P00722
D	3	HIS	-	CLONING ARTIFACT	UNP P00722
D	4	MET	-	CLONING ARTIFACT	UNP P00722
D	5	LEU	-	CLONING ARTIFACT	UNP P00722
D	6	GLU	-	CLONING ARTIFACT	UNP P00722
D	7	ASP	-	CLONING ARTIFACT	UNP P00722
D	8	PRO	-	CLONING ARTIFACT	UNP P00722
D	794	ALA	GLY	ENGINEERED	UNP P00722

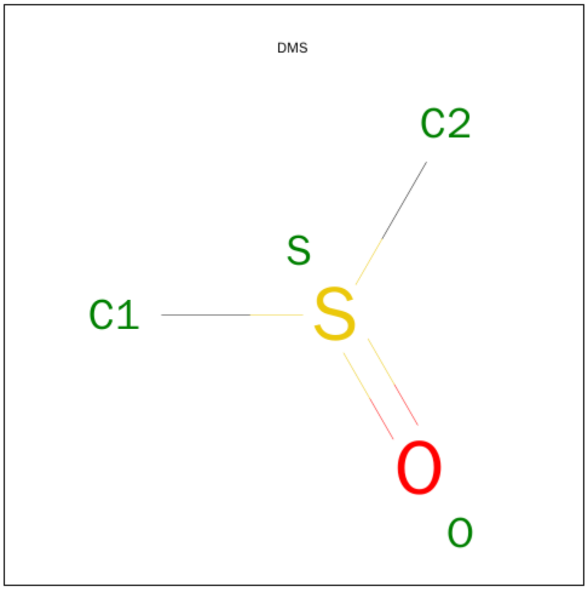
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

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

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

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

- Molecule 5 is water.

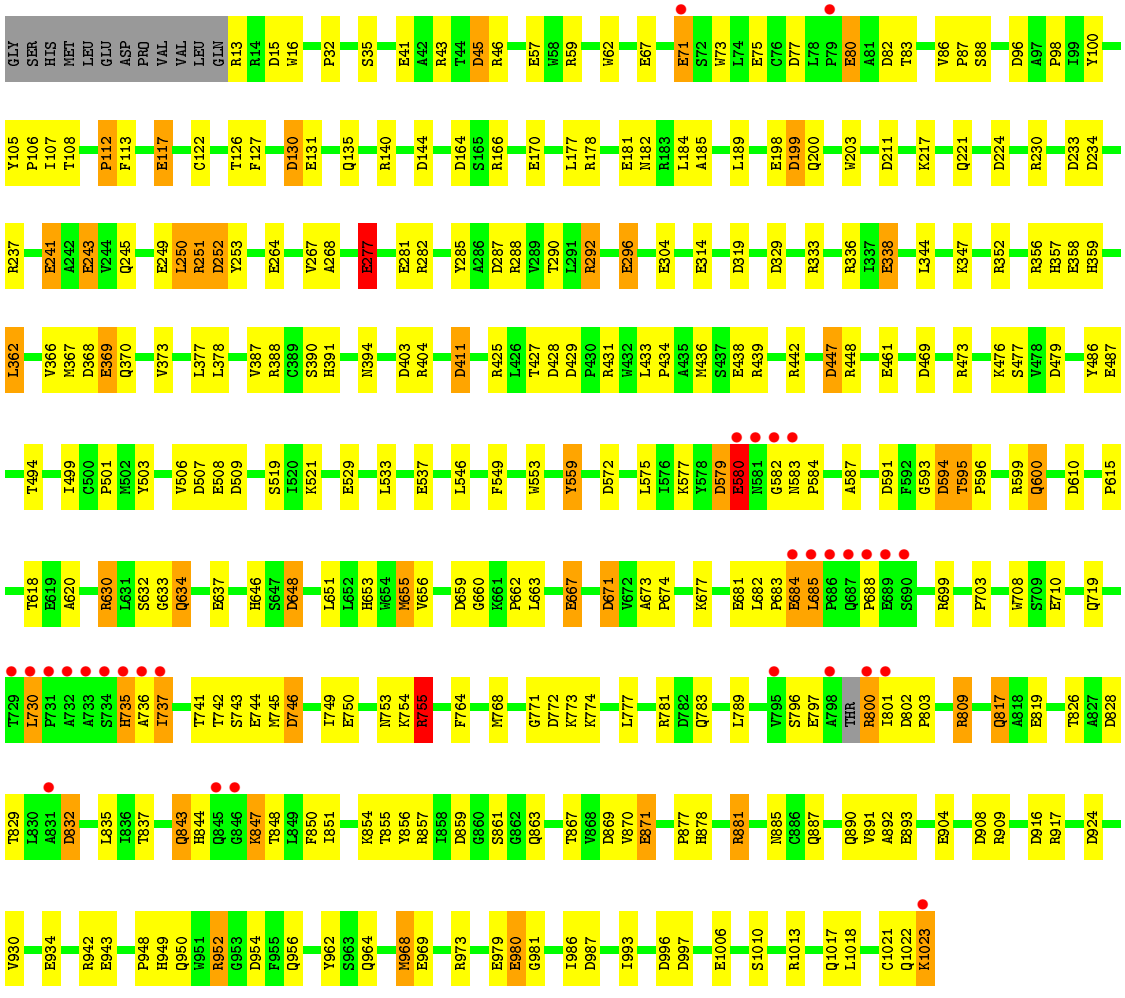
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	916	Total O 916 916	0	0
5	B	985	Total O 985 985	0	0
5	C	935	Total O 935 935	0	0
5	D	984	Total O 984 984	0	0

3 Residue-property plots (i)

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

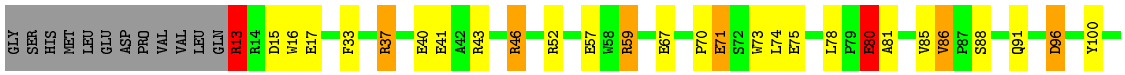
- Molecule 1: beta-galactosidase

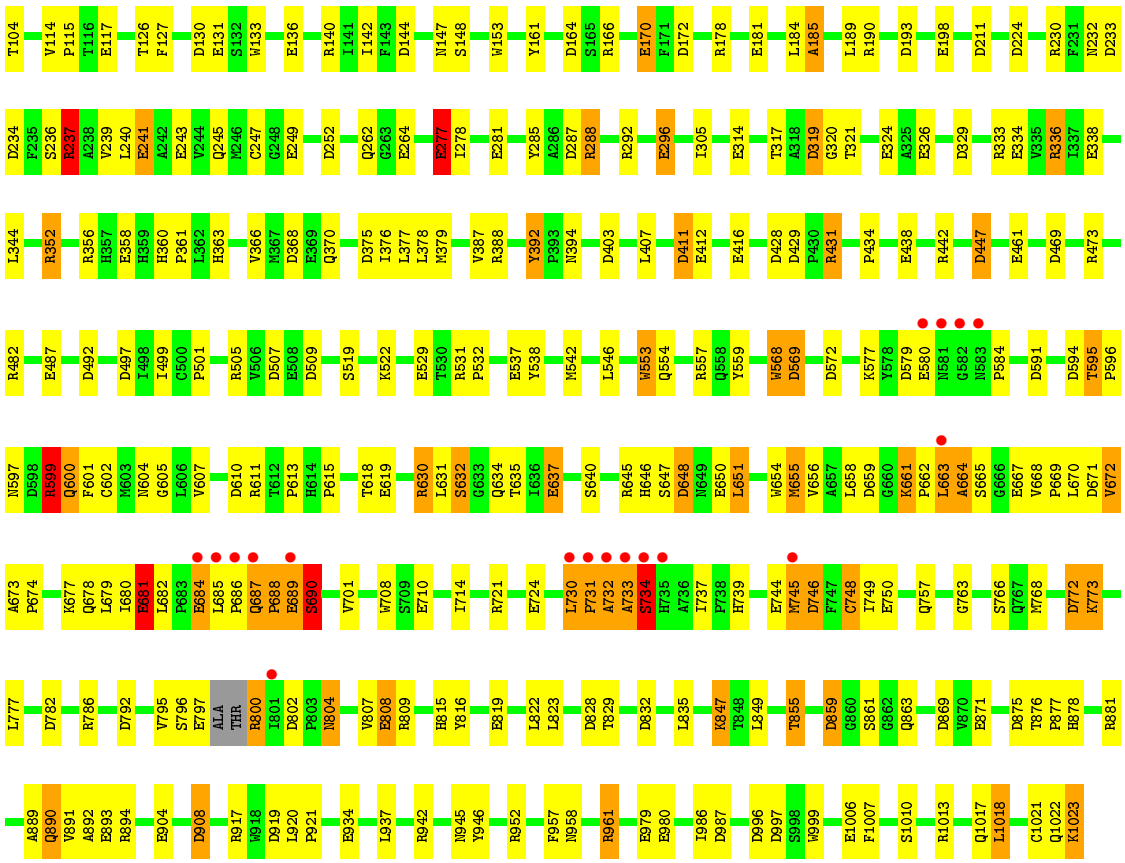
Chain A:



- Molecule 1: beta-galactosidase

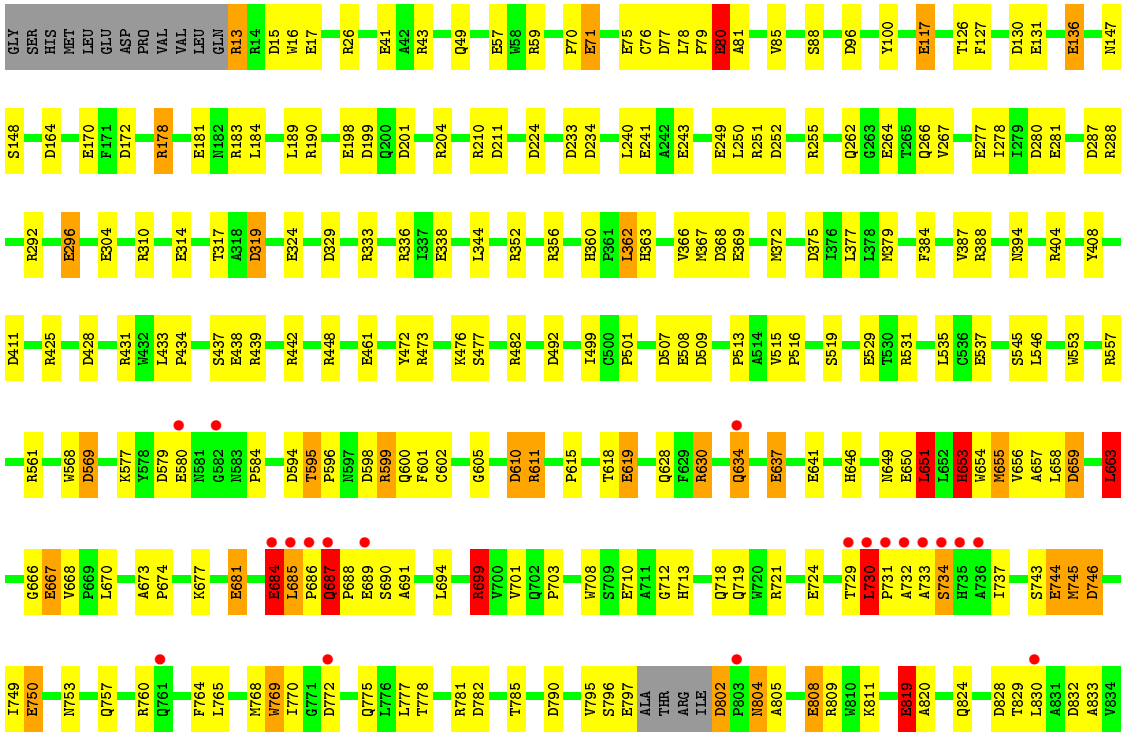
Chain B:

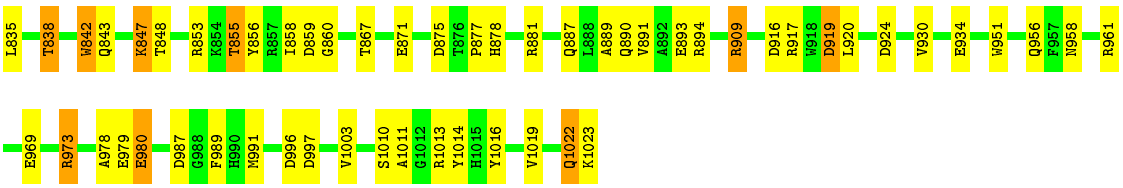




- Molecule 1: beta-galactosidase

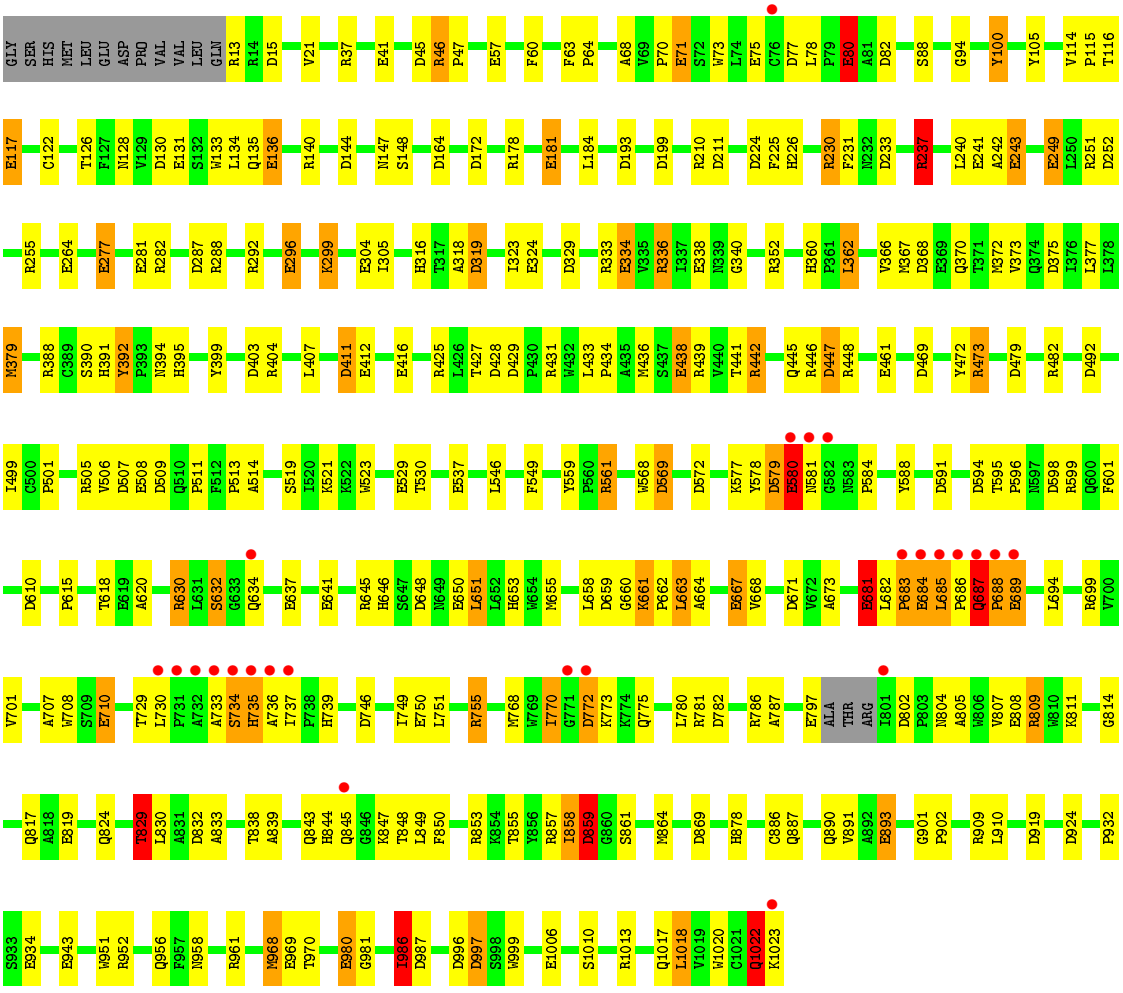
Chain C:





- Molecule 1: beta-galactosidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	149.70Å 168.59Å 200.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.70 – 1.60 21.69 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.1 (21.70-1.60) 88.2 (21.69-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 1.60Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.192 , 0.243 0.180 , 0.228	Depositor DCC
R_{free} test set	8858 reflections (1.54%)	DCC
Wilson B-factor (Å^2)	14.1	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 83.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 610095 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	36619	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.46 % 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 5.8122e-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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.12	44/8360 (0.5%)	1.67	159/11404 (1.4%)
1	B	1.15	55/8355 (0.7%)	1.64	152/11397 (1.3%)
1	C	1.13	50/8336 (0.6%)	1.66	162/11372 (1.4%)
1	D	1.13	45/8344 (0.5%)	1.68	172/11383 (1.5%)
All	All	1.13	194/33395 (0.6%)	1.66	645/45556 (1.4%)

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

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

All (194) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	537	GLU	CD-OE2	9.86	1.36	1.25
1	A	249	GLU	CD-OE2	9.72	1.36	1.25
1	D	136	GLU	CD-OE2	8.94	1.35	1.25
1	D	893	GLU	CD-OE2	8.89	1.35	1.25
1	C	650	GLU	CD-OE2	8.83	1.35	1.25
1	D	681	GLU	CD-OE2	8.80	1.35	1.25
1	C	684	GLU	CD-OE2	8.73	1.35	1.25
1	B	980	GLU	CD-OE2	8.60	1.35	1.25
1	C	170	GLU	CD-OE2	8.51	1.35	1.25
1	D	650	GLU	CD-OE2	8.40	1.34	1.25
1	C	969	GLU	CD-OE2	8.40	1.34	1.25
1	A	537	GLU	CD-OE2	8.21	1.34	1.25
1	A	296	GLU	CD-OE2	8.05	1.34	1.25
1	D	281	GLU	CD-OE2	7.99	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	580	GLU	CD-OE2	7.86	1.34	1.25
1	A	1006	GLU	CD-OE2	7.86	1.34	1.25
1	A	487	GLU	CD-OE2	7.81	1.34	1.25
1	C	819	GLU	CD-OE2	7.64	1.34	1.25
1	B	71	GLU	CD-OE2	7.59	1.34	1.25
1	D	71	GLU	CD-OE2	7.58	1.33	1.25
1	A	304	GLU	CD-OE2	7.55	1.33	1.25
1	D	41	GLU	CD-OE2	7.53	1.33	1.25
1	B	1006	GLU	CD-OE2	7.52	1.33	1.25
1	A	71	GLU	CD-OE2	7.51	1.33	1.25
1	D	296	GLU	CD-OE2	7.51	1.33	1.25
1	C	934	GLU	CD-OE2	7.49	1.33	1.25
1	D	710	GLU	CD-OE2	7.47	1.33	1.25
1	C	75	GLU	CD-OE2	7.42	1.33	1.25
1	A	281	GLU	CD-OE2	7.40	1.33	1.25
1	B	281	GLU	CD-OE2	7.39	1.33	1.25
1	A	980	GLU	CD-OE2	7.36	1.33	1.25
1	D	819	GLU	CD-OE2	7.30	1.33	1.25
1	B	681	GLU	CD-OE2	7.29	1.33	1.25
1	B	461	GLU	CD-OE2	7.27	1.33	1.25
1	C	641	GLU	CD-OE1	-7.26	1.17	1.25
1	A	681	GLU	CD-OE2	7.21	1.33	1.25
1	D	943	GLU	CD-OE2	7.20	1.33	1.25
1	B	689	GLU	CD-OE2	7.15	1.33	1.25
1	A	131	GLU	CD-OE2	7.13	1.33	1.25
1	A	979	GLU	CD-OE2	7.11	1.33	1.25
1	A	667	GLU	CD-OE2	7.09	1.33	1.25
1	A	80	GLU	CD-OE2	7.09	1.33	1.25
1	D	808	GLU	CD-OE2	7.04	1.33	1.25
1	D	243	GLU	CD-OE2	6.97	1.33	1.25
1	C	529	GLU	CD-OE2	6.95	1.33	1.25
1	B	893	GLU	CD-OE2	6.95	1.33	1.25
1	B	243	GLU	CD-OE2	6.94	1.33	1.25
1	C	80	GLU	CD-OE2	6.88	1.33	1.25
1	D	75	GLU	CD-OE2	6.86	1.33	1.25
1	C	667	GLU	CD-OE2	6.84	1.33	1.25
1	C	750	GLU	CD-OE2	6.83	1.33	1.25
1	C	314	GLU	CD-OE1	-6.80	1.18	1.25
1	A	969	GLU	CD-OE2	6.80	1.33	1.25
1	A	241	GLU	CD-OE2	6.79	1.33	1.25
1	C	744	GLU	CD-OE2	6.79	1.33	1.25
1	C	980	GLU	CD-OE2	6.79	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	744	GLU	CD-OE2	6.78	1.33	1.25
1	D	438	GLU	CD-OE2	6.78	1.33	1.25
1	C	131	GLU	CD-OE2	6.77	1.33	1.25
1	C	710	GLU	CD-OE2	6.73	1.33	1.25
1	D	969	GLU	CD-OE2	6.73	1.33	1.25
1	A	508	GLU	CD-OE2	6.73	1.33	1.25
1	C	71	GLU	CD-OE2	6.73	1.33	1.25
1	D	667	GLU	CD-OE2	6.72	1.33	1.25
1	B	170	GLU	CD-OE2	6.66	1.32	1.25
1	C	277	GLU	CD-OE2	6.64	1.32	1.25
1	A	943	GLU	CD-OE2	6.63	1.32	1.25
1	D	338	GLU	CD-OE2	6.63	1.32	1.25
1	C	537	GLU	CD-OE2	6.62	1.32	1.25
1	C	304	GLU	CD-OE2	6.59	1.32	1.25
1	A	684	GLU	CD-OE2	6.58	1.32	1.25
1	D	797	GLU	CD-OE2	6.57	1.32	1.25
1	D	980	GLU	CD-OE2	6.56	1.32	1.25
1	A	710	GLU	CD-OE2	6.55	1.32	1.25
1	B	75	GLU	CD-OE2	6.53	1.32	1.25
1	D	750	GLU	CD-OE2	6.47	1.32	1.25
1	C	893	GLU	CD-OE2	6.45	1.32	1.25
1	D	117	GLU	CD-OE2	6.43	1.32	1.25
1	C	296	GLU	CD-OE2	6.43	1.32	1.25
1	A	819	GLU	CD-OE2	6.42	1.32	1.25
1	B	667	GLU	CD-OE2	6.39	1.32	1.25
1	A	243	GLU	CD-OE2	6.39	1.32	1.25
1	D	684	GLU	CD-OE2	6.37	1.32	1.25
1	B	17	GLU	CD-OE2	6.37	1.32	1.25
1	B	338	GLU	CD-OE2	6.35	1.32	1.25
1	C	681	GLU	CD-OE2	6.35	1.32	1.25
1	A	170	GLU	CD-OE2	6.33	1.32	1.25
1	A	438	GLU	CD-OE2	6.32	1.32	1.25
1	C	797	GLU	CD-OE2	6.31	1.32	1.25
1	B	619	GLU	CD-OE2	6.29	1.32	1.25
1	A	277	GLU	CD-OE2	6.28	1.32	1.25
1	D	304	GLU	CD-OE2	6.27	1.32	1.25
1	B	871	GLU	CD-OE2	6.26	1.32	1.25
1	C	281	GLU	CD-OE2	6.24	1.32	1.25
1	D	241	GLU	CD-OE2	6.23	1.32	1.25
1	A	41	GLU	CD-OE2	6.23	1.32	1.25
1	B	904	GLU	CD-OE1	-6.22	1.18	1.25
1	D	689	GLU	CD-OE2	6.21	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	744	GLU	CD-OE2	6.20	1.32	1.25
1	C	181	GLU	CD-OE2	6.20	1.32	1.25
1	B	117	GLU	CD-OE2	6.19	1.32	1.25
1	D	131	GLU	CD-OE2	6.16	1.32	1.25
1	B	684	GLU	CD-OE2	6.15	1.32	1.25
1	B	808	GLU	CD-OE2	6.15	1.32	1.25
1	A	117	GLU	CD-OE2	6.15	1.32	1.25
1	C	198	GLU	CD-OE2	6.14	1.32	1.25
1	D	249	GLU	CD-OE2	6.14	1.32	1.25
1	C	41	GLU	CD-OE2	6.13	1.32	1.25
1	B	314	GLU	CD-OE1	-6.13	1.19	1.25
1	C	871	GLU	CD-OE2	6.12	1.32	1.25
1	D	277	GLU	CD-OE2	6.12	1.32	1.25
1	B	296	GLU	CD-OE2	6.11	1.32	1.25
1	D	508	GLU	CD-OE1	-6.10	1.19	1.25
1	D	580	GLU	CD-OE2	6.08	1.32	1.25
1	C	619	GLU	CD-OE2	6.04	1.32	1.25
1	B	724	GLU	CD-OE2	6.04	1.32	1.25
1	D	181	GLU	CD-OE2	6.03	1.32	1.25
1	B	487	GLU	CD-OE2	6.02	1.32	1.25
1	C	580	GLU	CD-OE2	6.02	1.32	1.25
1	B	416	GLU	CD-OE2	6.01	1.32	1.25
1	A	264	GLU	CD-OE2	6.00	1.32	1.25
1	C	689	GLU	CD-OE2	6.00	1.32	1.25
1	C	117	GLU	CD-OE2	5.99	1.32	1.25
1	B	438	GLU	CD-OE2	5.99	1.32	1.25
1	D	934	GLU	CD-OE2	5.96	1.32	1.25
1	A	934	GLU	CD-OE2	5.96	1.32	1.25
1	A	750	GLU	CD-OE2	5.93	1.32	1.25
1	B	934	GLU	CD-OE2	5.93	1.32	1.25
1	A	904	GLU	CD-OE2	5.91	1.32	1.25
1	C	17	GLU	CD-OE1	-5.89	1.19	1.25
1	B	131	GLU	CD-OE2	5.83	1.32	1.25
1	A	580	GLU	CD-OE2	5.83	1.32	1.25
1	D	529	GLU	CD-OE2	5.83	1.32	1.25
1	D	57	GLU	CD-OE2	5.82	1.32	1.25
1	C	241	GLU	CD-OE2	5.79	1.32	1.25
1	C	249	GLU	CD-OE2	5.79	1.32	1.25
1	B	40	GLU	CD-OE2	5.79	1.32	1.25
1	B	277	GLU	CD-OE2	5.76	1.31	1.25
1	C	136	GLU	CD-OE2	5.75	1.31	1.25
1	D	264	GLU	CD-OE2	5.75	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	80	GLU	CD-OE2	5.74	1.31	1.25
1	B	650	GLU	CD-OE2	5.73	1.31	1.25
1	B	412	GLU	CD-OE2	5.72	1.31	1.25
1	D	324	GLU	CD-OE2	5.72	1.31	1.25
1	B	819	GLU	CD-OE2	5.68	1.31	1.25
1	D	641	GLU	CD-OE2	5.68	1.31	1.25
1	A	67	GLU	CD-OE2	5.68	1.31	1.25
1	D	637	GLU	CD-OE2	5.66	1.31	1.25
1	B	80	GLU	CD-OE2	5.62	1.31	1.25
1	B	136	GLU	CD-OE2	5.62	1.31	1.25
1	C	482	ARG	CZ-NH1	5.62	1.40	1.33
1	A	893	GLU	CD-OE2	5.58	1.31	1.25
1	B	537	GLU	CD-OE2	5.57	1.31	1.25
1	C	724	GLU	CD-OE2	5.55	1.31	1.25
1	B	979	GLU	CD-OE2	5.54	1.31	1.25
1	B	264	GLU	CD-OE2	5.52	1.31	1.25
1	C	338	GLU	CD-OE2	5.50	1.31	1.25
1	A	871	GLU	CD-OE2	5.49	1.31	1.25
1	B	324	GLU	CD-OE2	5.49	1.31	1.25
1	B	249	GLU	CD-OE2	5.47	1.31	1.25
1	C	57	GLU	CD-OE2	5.45	1.31	1.25
1	C	324	GLU	CD-OE2	5.45	1.31	1.25
1	B	797	GLU	CD-OE2	5.44	1.31	1.25
1	A	797	GLU	CD-OE2	5.43	1.31	1.25
1	D	334	GLU	CD-OE2	5.41	1.31	1.25
1	A	369	GLU	CD-OE2	5.40	1.31	1.25
1	B	326	GLU	CD-OE2	5.39	1.31	1.25
1	C	243	GLU	CD-OE2	5.35	1.31	1.25
1	A	358	GLU	CD-OE2	5.34	1.31	1.25
1	B	334	GLU	CD-OE1	-5.31	1.19	1.25
1	B	241	GLU	CD-OE2	5.29	1.31	1.25
1	C	461	GLU	CD-OE1	-5.27	1.19	1.25
1	C	438	GLU	CD-OE2	5.26	1.31	1.25
1	B	710	GLU	CD-OE2	5.24	1.31	1.25
1	B	41	GLU	CD-OE2	5.24	1.31	1.25
1	B	67	GLU	CD-OE1	-5.24	1.19	1.25
1	B	637	GLU	CD-OE2	5.22	1.31	1.25
1	B	198	GLU	CD-OE2	5.20	1.31	1.25
1	B	57	GLU	CD-OE2	5.19	1.31	1.25
1	D	461	GLU	CD-OE2	5.19	1.31	1.25
1	C	442	ARG	CZ-NH1	5.17	1.39	1.33
1	A	181	GLU	CD-OE2	5.17	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	GLU	CD-OE2	5.16	1.31	1.25
1	B	314	GLU	CD-OE2	5.16	1.31	1.25
1	B	529	GLU	CD-OE2	5.15	1.31	1.25
1	A	529	GLU	CD-OE2	5.12	1.31	1.25
1	C	979	GLU	CD-OE2	5.11	1.31	1.25
1	C	637	GLU	CD-OE2	5.10	1.31	1.25
1	A	461	GLU	CD-OE2	5.09	1.31	1.25
1	D	412	GLU	CD-OE2	5.06	1.31	1.25
1	C	808	GLU	CD-OE2	5.03	1.31	1.25
1	B	358	GLU	CD-OE2	5.02	1.31	1.25
1	D	1006	GLU	CD-OE2	5.01	1.31	1.25
1	A	338	GLU	CD-OE2	5.01	1.31	1.25

All (645) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	699	ARG	NE-CZ-NH1	24.71	132.65	120.30
1	C	699	ARG	NE-CZ-NH2	-20.33	110.14	120.30
1	C	599	ARG	NE-CZ-NH1	16.78	128.69	120.30
1	D	630	ARG	NE-CZ-NH1	16.23	128.41	120.30
1	C	473	ARG	NE-CZ-NH1	16.07	128.33	120.30
1	A	431	ARG	NE-CZ-NH2	-16.02	112.29	120.30
1	A	431	ARG	NE-CZ-NH1	15.68	128.14	120.30
1	C	442	ARG	NE-CZ-NH2	-15.01	112.80	120.30
1	B	557	ARG	NE-CZ-NH2	-14.83	112.89	120.30
1	D	431	ARG	NE-CZ-NH1	14.75	127.67	120.30
1	B	599	ARG	NE-CZ-NH1	14.44	127.52	120.30
1	B	473	ARG	NE-CZ-NH1	13.91	127.25	120.30
1	D	781	ARG	NE-CZ-NH1	13.68	127.14	120.30
1	D	439	ARG	NE-CZ-NH2	-13.64	113.48	120.30
1	A	166	ARG	NE-CZ-NH2	-13.23	113.68	120.30
1	D	630	ARG	NE-CZ-NH2	-13.21	113.70	120.30
1	D	446	ARG	NE-CZ-NH1	13.01	126.81	120.30
1	A	233	ASP	CB-CG-OD2	-12.96	106.63	118.30
1	B	599	ARG	NE-CZ-NH2	-12.83	113.89	120.30
1	A	251	ARG	NE-CZ-NH1	12.71	126.65	120.30
1	C	233	ASP	CB-CG-OD2	-12.70	106.87	118.30
1	D	172	ASP	CB-CG-OD2	-12.58	106.98	118.30
1	B	356	ARG	NE-CZ-NH1	12.57	126.58	120.30
1	A	13	ARG	NE-CZ-NH2	-12.22	114.19	120.30
1	D	439	ARG	NE-CZ-NH1	12.13	126.36	120.30
1	D	15	ASP	CB-CG-OD2	-12.07	107.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	233	ASP	CB-CG-OD1	12.05	129.14	118.30
1	D	857	ARG	NE-CZ-NH1	11.93	126.26	120.30
1	D	473	ARG	NE-CZ-NH1	11.91	126.25	120.30
1	C	853	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	B	557	ARG	NE-CZ-NH1	11.83	126.21	120.30
1	B	746	ASP	CB-CG-OD2	-11.71	107.76	118.30
1	B	166	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	A	442	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	A	13	ARG	NE-CZ-NH1	11.46	126.03	120.30
1	D	687	GLN	C-N-CD	-11.41	95.50	120.60
1	C	721	ARG	NE-CZ-NH1	11.39	125.99	120.30
1	C	43	ARG	NE-CZ-NH1	11.36	125.98	120.30
1	C	224	ASP	CB-CG-OD1	11.11	128.29	118.30
1	D	13	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	D	431	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	D	996	ASP	CB-CG-OD1	10.82	128.04	118.30
1	B	285	TYR	CB-CG-CD2	-10.79	114.52	121.00
1	D	13	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	D	15	ASP	CB-CG-OD1	10.76	127.99	118.30
1	D	594	ASP	CB-CG-OD2	-10.72	108.66	118.30
1	D	172	ASP	CB-CG-OD1	10.66	127.89	118.30
1	B	952	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	C	13	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	C	233	ASP	CB-CG-OD1	10.58	127.82	118.30
1	C	721	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	C	599	ARG	NE-CZ-NH2	-10.49	115.05	120.30
1	A	166	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	B	329	ASP	CB-CG-OD2	-10.47	108.88	118.30
1	A	1013	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	B	388	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	352	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	224	ASP	CB-CG-OD1	9.93	127.24	118.30
1	C	917	ARG	NE-CZ-NH2	9.89	125.24	120.30
1	A	336	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	A	46	ARG	NE-CZ-NH1	9.83	125.21	120.30
1	B	368	ASP	CB-CG-OD1	9.79	127.11	118.30
1	A	987	ASP	CB-CG-OD2	-9.78	109.50	118.30
1	B	224	ASP	CB-CG-OD1	9.70	127.03	118.30
1	B	336	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	A	439	ARG	NE-CZ-NH2	-9.59	115.50	120.30
1	A	428	ASP	CB-CG-OD2	-9.57	109.68	118.30
1	A	292	ARG	NE-CZ-NH1	9.48	125.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	442	ARG	NE-CZ-NH1	9.46	125.03	120.30
1	B	233	ASP	CB-CG-OD1	9.46	126.81	118.30
1	A	996	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	D	473	ARG	NE-CZ-NH2	-9.41	115.59	120.30
1	D	230	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	B	572	ASP	CB-CG-OD2	-9.40	109.84	118.30
1	A	439	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	C	482	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	B	772	ASP	CB-CG-OD2	-9.24	109.99	118.30
1	C	973	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	C	473	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	A	509	ASP	CB-CG-OD2	-9.17	110.05	118.30
1	B	875	ASP	CB-CG-OD1	9.17	126.55	118.30
1	C	473	ARG	CD-NE-CZ	9.15	136.41	123.60
1	C	431	ARG	NE-CZ-NH2	-9.13	115.74	120.30
1	B	996	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	A	425	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	B	319	ASP	CB-CG-OD1	9.09	126.48	118.30
1	A	292	ARG	NE-CZ-NH2	-9.07	115.77	120.30
1	A	828	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	B	411	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	D	699	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	A	997	ASP	CB-CG-OD2	-8.94	110.25	118.30
1	C	859	ASP	CB-CG-OD2	-8.92	110.27	118.30
1	A	509	ASP	CB-CG-OD1	8.92	126.33	118.30
1	D	144	ASP	CB-CG-OD1	8.90	126.31	118.30
1	C	832	ASP	CB-CG-OD2	-8.86	110.33	118.30
1	A	610	ASP	CB-CG-OD1	8.85	126.27	118.30
1	C	199	ASP	CB-CG-OD1	8.84	126.26	118.30
1	A	909	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	D	336	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	D	594	ASP	CB-CG-OD1	8.84	126.25	118.30
1	C	482	ARG	NE-CZ-NH2	-8.82	115.89	120.30
1	C	961	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	B	572	ASP	CB-CG-OD1	8.80	126.22	118.30
1	D	233	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	A	336	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	917	ARG	NE-CZ-NH1	-8.73	115.94	120.30
1	B	630	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	B	429	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	B	594	ASP	CB-CG-OD2	-8.71	110.46	118.30
1	D	282	ARG	NE-CZ-NH2	-8.69	115.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	310	ARG	NE-CZ-NH2	-8.67	115.97	120.30
1	C	996	ASP	CB-CG-OD1	8.67	126.10	118.30
1	D	210	ARG	NE-CZ-NH1	-8.67	115.97	120.30
1	B	13	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	B	442	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	869	ASP	CB-CG-OD1	8.52	125.97	118.30
1	B	952	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	D	482	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	B	329	ASP	CB-CG-OD1	8.50	125.95	118.30
1	A	428	ASP	CB-CG-OD1	8.49	125.94	118.30
1	B	746	ASP	CB-CG-OD1	8.49	125.94	118.30
1	B	287	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	A	771	GLY	N-CA-C	-8.46	91.96	113.10
1	D	996	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	C	428	ASP	CB-CG-OD1	8.41	125.87	118.30
1	D	579	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	D	428	ASP	CB-CG-OD1	8.38	125.84	118.30
1	B	569	ASP	CB-CG-OD2	-8.38	110.76	118.30
1	C	287	ASP	CB-CG-OD2	-8.36	110.77	118.30
1	C	772	ASP	CB-CG-OD2	-8.35	110.79	118.30
1	D	869	ASP	CB-CG-OD1	8.34	125.81	118.30
1	B	648	ASP	CB-CG-OD2	-8.34	110.80	118.30
1	B	233	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	B	43	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	A	954	ASP	CB-CG-OD1	8.32	125.79	118.30
1	A	671	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	A	144	ASP	CB-CG-OD2	-8.31	110.82	118.30
1	B	130	ASP	CB-CG-OD1	8.29	125.76	118.30
1	A	755	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	144	ASP	CB-CG-OD1	8.24	125.71	118.30
1	D	909	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	942	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	C	375	ASP	CB-CG-OD1	8.18	125.66	118.30
1	D	442	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	D	507	ASP	CB-CG-OD1	8.17	125.66	118.30
1	D	388	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	368	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	D	446	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	809	ARG	NE-CZ-NH2	-8.09	116.25	120.30
1	A	954	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	828	ASP	CB-CG-OD1	8.08	125.57	118.30
1	D	997	ASP	CB-CG-OD2	-8.07	111.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	987	ASP	CB-CG-OD1	8.04	125.54	118.30
1	B	786	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	D	482	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	D	987	ASP	CB-CG-OD1	8.01	125.51	118.30
1	C	909	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	C	802	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	B	509	ASP	CB-CG-OD1	7.99	125.49	118.30
1	A	507	ASP	CB-CG-OD2	-7.98	111.11	118.30
1	C	924	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	D	469	ASP	CB-CG-OD1	7.94	125.45	118.30
1	B	431	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	D	572	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	832	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	D	352	ARG	NE-CZ-NH1	7.91	124.25	120.30
1	D	648	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	A	140	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	D	45	ASP	CB-CG-OD1	7.90	125.41	118.30
1	C	557	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	A	288	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	D	591	ASP	CB-CG-OD1	7.86	125.37	118.30
1	C	802	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	211	ASP	CB-CG-OD1	7.79	125.31	118.30
1	A	411	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	C	832	ASP	CB-CG-OD1	7.76	125.28	118.30
1	C	772	ASP	CB-CG-OD1	7.74	125.27	118.30
1	B	469	ASP	CB-CG-OD1	7.74	125.27	118.30
1	C	859	ASP	CB-CG-OD1	7.74	125.27	118.30
1	A	659	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	D	251	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	B	442	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	C	352	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	A	908	ASP	CB-CG-OD1	7.68	125.21	118.30
1	C	961	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	B	648	ASP	CB-CG-OD1	7.58	125.12	118.30
1	C	183	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	C	287	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	809	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	C	352	ARG	NE-CZ-NH2	-7.52	116.54	120.30
1	D	224	ASP	CB-CG-OD1	7.52	125.06	118.30
1	A	856	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	D	116	THR	CA-CB-CG2	-7.51	101.88	112.40
1	D	288	ARG	NE-CZ-NH1	7.51	124.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	630	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	130	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	B	287	ASP	CB-CG-OD1	7.50	125.05	118.30
1	C	750	GLU	N-CA-CB	7.49	124.08	110.60
1	C	599	ARG	CD-NE-CZ	7.49	134.09	123.60
1	C	996	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	A	388	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	D	507	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	B	569	ASP	CB-CG-OD1	7.47	125.02	118.30
1	C	699	ARG	CD-NE-CZ	7.45	134.03	123.60
1	D	252	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	D	659	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	B	919	ASP	CB-CG-OD2	-7.44	111.61	118.30
1	B	859	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	252	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	D	130	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	C	611	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	D	579	ASP	CB-CG-OD1	7.41	124.97	118.30
1	B	288	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	B	804	ASN	N-CA-CB	7.38	123.89	110.60
1	C	853	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	C	411	ASP	CB-CG-OD1	7.34	124.91	118.30
1	B	428	ASP	CB-CG-OD1	7.33	124.90	118.30
1	C	329	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	A	77	ASP	CB-CG-OD2	-7.32	111.72	118.30
1	B	15	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	A	282	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	C	234	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	C	630	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	659	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	D	561	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	C	594	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	D	193	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	469	ASP	CB-CG-OD1	7.22	124.80	118.30
1	D	857	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	D	919	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	B	828	ASP	CB-CG-OD1	7.21	124.78	118.30
1	B	832	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	267	VAL	CA-CB-CG2	-7.20	100.11	110.90
1	D	469	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	C	77	ASP	CB-CG-OD1	7.17	124.75	118.30
1	D	233	ASP	CB-CG-OD1	7.17	124.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	980	GLU	C-N-CA	-7.17	107.25	122.30
1	A	45	ASP	CB-CG-OD1	7.16	124.74	118.30
1	D	403	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	224	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	C	579	ASP	CB-CG-OD1	7.13	124.72	118.30
1	B	13	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	130	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	A	997	ASP	N-CA-CB	7.09	123.37	110.60
1	D	428	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	610	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	D	429	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	B	610	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	D	559	TYR	CB-CG-CD2	-7.06	116.77	121.00
1	C	958	ASN	N-CA-CB	7.05	123.30	110.60
1	C	411	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	96	ASP	CB-CG-OD1	7.05	124.65	118.30
1	C	178	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	828	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	D	287	ASP	CB-CG-OD1	7.03	124.63	118.30
1	B	473	ARG	CD-NE-CZ	7.02	133.43	123.60
1	D	448	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	D	659	ASP	CB-CG-OD1	7.01	124.61	118.30
1	C	782	ASP	CB-CG-OD1	7.00	124.60	118.30
1	D	509	ASP	CB-CG-OD1	7.00	124.59	118.30
1	B	1018	LEU	CB-CA-C	-6.99	96.92	110.20
1	C	368	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	A	579	ASP	CB-CG-OD1	6.97	124.58	118.30
1	B	875	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	B	859	ASP	CB-CG-OD1	6.96	124.56	118.30
1	C	1016	TYR	CB-CG-CD2	-6.95	116.83	121.00
1	A	579	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	404	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	447	ASP	CB-CG-OD1	6.93	124.54	118.30
1	D	319	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	A	942	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	C	255	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	C	987	ASP	CB-CG-OD1	6.91	124.52	118.30
1	B	190	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	C	252	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	D	388	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	172	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	C	404	ARG	NE-CZ-NH2	-6.87	116.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	193	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	C	190	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	772	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	561	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	B	579	ASP	CB-CG-OD1	6.79	124.41	118.30
1	B	829	THR	CA-CB-CG2	-6.77	102.92	112.40
1	B	881	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	671	ASP	CB-CG-OD1	6.77	124.39	118.30
1	D	802	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	A	319	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	D	829	THR	N-CA-CB	6.75	123.13	110.30
1	D	997	ASP	N-CA-CB	6.75	122.75	110.60
1	B	492	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	B	559	TYR	CD1-CE1-CZ	-6.74	113.74	119.80
1	C	557	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	253	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	D	392	TYR	CB-CG-CD2	6.72	125.03	121.00
1	C	894	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	469	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	D	429	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	509	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	B	59	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	D	404	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	916	ASP	CB-CG-OD1	6.65	124.28	118.30
1	C	76	CYS	N-CA-CB	-6.65	98.63	110.60
1	C	288	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	D	140	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	108	THR	CA-CB-CG2	-6.64	103.11	112.40
1	B	958	ASN	N-CA-CB	6.64	122.55	110.60
1	A	252	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	B	388	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	C	569	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	875	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	1022	GLN	N-CA-CB	6.60	122.48	110.60
1	D	144	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	C	425	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	782	ASP	CB-CG-OD1	6.57	124.21	118.30
1	B	611	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	D	781	ARG	CD-NE-CZ	6.57	132.79	123.60
1	B	288	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	D	632	SER	N-CA-CB	6.55	120.32	110.50
1	A	82	ASP	CB-CG-OD1	6.54	124.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	411	ASP	CB-CG-OD1	6.54	124.19	118.30
1	C	43	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	D	375	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	B	239	VAL	CA-CB-CG2	-6.52	101.12	110.90
1	A	594	ASP	CB-CG-OD1	6.50	124.16	118.30
1	D	986	ILE	CG1-CB-CG2	-6.50	97.10	111.40
1	C	909	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	D	569	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	C	733	ALA	N-CA-CB	6.49	119.18	110.10
1	B	172	ASP	CB-CG-OD1	6.48	124.13	118.30
1	D	809	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	1013	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	A	952	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	559	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	C	199	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	D	598	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	D	569	ASP	CB-CG-OD1	6.46	124.11	118.30
1	D	591	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	B	96	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	D	838	THR	CA-CB-CG2	-6.45	103.37	112.40
1	B	482	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	D	425	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	234	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	178	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	D	336	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	C	439	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	671	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	D	237	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	368	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	448	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	C	442	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	B	507	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	A	648	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	255	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	199	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	594	ASP	CB-CG-OD1	6.32	123.98	118.30
1	B	816	TYR	CB-CG-CD2	-6.31	117.21	121.00
1	C	164	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	859	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	C	280	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	D	352	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	C	531	ARG	NE-CZ-NH1	6.30	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	578	TYR	CB-CG-CD2	-6.29	117.22	121.00
1	C	492	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	A	869	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	B	285	TYR	CB-CG-CD1	6.27	124.76	121.00
1	B	997	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	A	996	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	968	MET	N-CA-CB	-6.26	99.33	110.60
1	B	507	ASP	CB-CG-OD1	6.25	123.93	118.30
1	B	792	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	43	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	768	MET	CA-CB-CG	6.24	123.92	113.30
1	A	429	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	D	509	ASP	CB-CG-OD2	-6.23	112.69	118.30
1	C	917	ARG	CD-NE-CZ	-6.23	114.88	123.60
1	B	579	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	247	CYS	CA-CB-SG	-6.22	102.80	114.00
1	D	802	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	591	ASP	CB-CG-OD1	6.22	123.90	118.30
1	D	630	ARG	CD-NE-CZ	6.21	132.30	123.60
1	A	178	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	26	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	772	ASP	CB-CG-OD1	6.20	123.88	118.30
1	B	497	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	184	LEU	CB-CA-C	-6.16	98.49	110.20
1	C	553	TRP	CA-CB-CG	-6.16	101.99	113.70
1	B	178	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	C	130	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	A	594	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	D	130	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	404	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	319	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	15	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	319	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	D	987	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	881	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	D	448	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	D	100	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	D	997	ASP	CB-CG-OD1	6.07	123.76	118.30
1	D	287	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	C	507	ASP	CB-CG-OD1	6.05	123.74	118.30
1	D	224	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	D	199	ASP	CB-CG-OD1	6.04	123.74	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	82	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	429	ASP	CB-CG-OD1	6.03	123.73	118.30
1	C	594	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	431	ARG	CD-NE-CZ	6.02	132.03	123.60
1	A	730	LEU	CB-CA-C	6.01	121.61	110.20
1	C	598	ASP	CB-CG-OD1	6.00	123.70	118.30
1	D	505	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	230	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	A	447	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	D	251	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	D	832	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	C	13	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	D	319	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	610	ASP	CB-CG-OD1	5.97	123.68	118.30
1	B	144	ASP	CB-CG-OD1	5.96	123.67	118.30
1	C	431	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	719	GLN	CB-CA-C	-5.92	98.56	110.40
1	C	828	ASP	CB-CG-OD1	5.91	123.62	118.30
1	B	997	ASP	N-CA-CB	5.91	121.24	110.60
1	D	958	ASN	N-CA-CB	5.91	121.23	110.60
1	C	782	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	D	850	PHE	CB-CA-C	-5.90	98.60	110.40
1	A	553	TRP	CA-CB-CG	-5.90	102.50	113.70
1	A	997	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	772	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	942	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	D	37	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	B	908	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	15	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	C	369	GLU	CG-CD-OE2	-5.87	106.56	118.30
1	A	648	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	164	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	469	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	C	867	THR	CA-CB-CG2	-5.85	104.21	112.40
1	A	1018	LEU	CB-CA-C	-5.85	99.09	110.20
1	B	211	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	C	997	ASP	N-CA-CB	5.83	121.10	110.60
1	A	15	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	1013	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	D	804	ASN	CA-CB-CG	-5.83	100.58	113.40
1	D	699	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	D	416	GLU	CG-CD-OE1	5.80	129.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	782	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	C	659	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	508	GLU	N-CA-CB	-5.79	100.17	110.60
1	C	255	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	802	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	671	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	997	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	33	PHE	CB-CA-C	-5.78	98.84	110.40
1	C	201	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	224	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	B	869	ASP	CB-CG-OD1	5.77	123.49	118.30
1	D	610	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	664	ALA	CB-CA-C	-5.76	101.47	110.10
1	D	598	ASP	CB-CG-OD1	5.75	123.48	118.30
1	D	329	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	796	SER	N-CA-CB	5.75	119.12	110.50
1	C	856	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	D	588	TYR	CZ-CE2-CD2	-5.75	114.63	119.80
1	B	568	TRP	CA-CB-CG	-5.75	102.78	113.70
1	A	741	THR	CA-CB-CG2	-5.74	104.36	112.40
1	D	859	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	C	224	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	287	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	112	PRO	N-CA-CB	-5.69	96.34	102.60
1	B	352	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	D	46	ARG	NE-CZ-NH1	-5.69	117.46	120.30
1	D	1013	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	691	ALA	CB-CA-C	-5.68	101.58	110.10
1	A	285	TYR	CB-CG-CD2	-5.67	117.59	121.00
1	C	997	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	D	178	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	803	PRO	N-CA-CB	5.66	110.09	103.30
1	D	919	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	790	ASP	CB-CG-OD1	5.64	123.38	118.30
1	C	842	TRP	CG-CD2-CE3	-5.64	128.82	133.90
1	B	46	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	505	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	C	280	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	832	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	C	919	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	429	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	388	ARG	NE-CZ-NH2	-5.61	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	161	TYR	N-CA-CB	-5.61	100.51	110.60
1	C	733	ALA	CB-CA-C	5.60	118.50	110.10
1	B	961	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	919	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	344	LEU	CA-CB-CG	-5.58	102.46	115.30
1	C	85	VAL	CA-CB-CG2	-5.58	102.53	110.90
1	C	126	THR	CA-CB-CG2	-5.58	104.58	112.40
1	A	75	GLU	CB-CA-C	5.58	121.56	110.40
1	B	721	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	C	428	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	314	GLU	OE1-CD-OE2	-5.57	116.62	123.30
1	A	599	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	908	ASP	CB-CG-OD1	5.56	123.30	118.30
1	B	519	SER	N-CA-CB	-5.56	102.17	110.50
1	A	486	TYR	CG-CD2-CE2	-5.54	116.86	121.30
1	B	403	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	403	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	C	164	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	368	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	D	968	MET	N-CA-CB	-5.54	100.63	110.60
1	D	770	ILE	N-CA-C	-5.53	96.06	111.00
1	D	772	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	B	126	THR	CA-CB-CG2	-5.52	104.67	112.40
1	C	1013	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	D	299	LYS	CA-CB-CG	-5.51	101.28	113.40
1	D	681	GLU	CB-CA-C	5.51	121.42	110.40
1	C	204	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	634	GLN	CB-CG-CD	5.50	125.91	111.60
1	C	234	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	15	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	962	TYR	CB-CG-CD2	5.49	124.29	121.00
1	D	673	ALA	N-CA-CB	-5.48	102.43	110.10
1	B	52	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	B	86	VAL	CG1-CB-CG2	-5.47	102.14	110.90
1	C	653	HIS	N-CA-CB	5.46	120.44	110.60
1	D	379	MET	CG-SD-CE	-5.46	91.46	100.20
1	D	746	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	A	486	TYR	CZ-CE2-CD2	5.46	124.71	119.80
1	B	193	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	425	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	D	77	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	D	395	HIS	N-CA-CB	-5.45	100.79	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	TYR	N-CA-CB	5.45	120.40	110.60
1	A	924	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	234	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	B	659	ASP	CB-CG-OD1	5.43	123.19	118.30
1	D	855	THR	N-CA-CB	5.43	120.62	110.30
1	D	479	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	553	TRP	CA-CB-CG	-5.42	103.39	113.70
1	C	96	ASP	N-CA-CB	5.42	120.35	110.60
1	B	782	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	987	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	A	503	TYR	CG-CD1-CE1	5.40	125.62	121.30
1	C	172	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	479	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	909	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	C	368	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	37	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	15	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	D	411	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	62	TRP	CB-CG-CD2	5.37	133.59	126.60
1	A	861	SER	CB-CA-C	-5.37	99.90	110.10
1	A	802	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	996	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	352	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	329	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	755	ARG	N-CA-CB	5.35	120.23	110.60
1	A	251	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
1	C	730	LEU	C-N-CD	-5.34	108.86	120.60
1	A	802	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	D	399	TYR	CD1-CE1-CZ	-5.34	115.00	119.80
1	C	729	THR	N-CA-CB	5.33	120.43	110.30
1	C	651	LEU	N-CA-CB	5.32	121.03	110.40
1	D	492	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	A	329	ASP	CB-CG-OD2	-5.31	113.53	118.30
1	D	211	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	B	140	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	572	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	746	ASP	CB-CA-C	-5.29	99.82	110.40
1	B	894	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	237	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	D	472	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	A	221	GLN	N-CA-CB	-5.27	101.11	110.60
1	B	640	SER	CB-CA-C	-5.26	100.11	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	721	ARG	CD-NE-CZ	5.25	130.96	123.60
1	D	853	ARG	NE-CZ-NH2	5.25	122.93	120.30
1	B	505	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	A	632	SER	CB-CA-C	5.25	120.07	110.10
1	A	477	SER	N-CA-CB	5.25	118.37	110.50
1	C	431	ARG	CA-CB-CG	-5.24	101.87	113.40
1	C	408	TYR	CD1-CE1-CZ	-5.24	115.09	119.80
1	C	855	THR	N-CA-CB	5.24	120.25	110.30
1	A	96	ASP	N-CA-CB	5.24	120.03	110.60
1	C	211	ASP	CB-CG-OD2	-5.23	113.60	118.30
1	C	1013	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	136	GLU	CB-CA-C	-5.22	99.96	110.40
1	B	185	ALA	N-CA-CB	5.21	117.40	110.10
1	C	336	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	769	TRP	CB-CA-C	-5.21	99.98	110.40
1	D	288	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	277	GLU	CG-CD-OE1	5.21	128.71	118.30
1	A	211	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	748	CYS	CA-CB-SG	-5.20	104.65	114.00
1	B	591	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	416	GLU	CG-CD-OE2	-5.19	107.92	118.30
1	D	184	LEU	CB-CA-C	-5.18	100.35	110.20
1	B	632	SER	N-CA-CB	5.18	118.26	110.50
1	C	13	ARG	N-CA-CB	5.17	119.90	110.60
1	C	719	GLN	CB-CA-C	-5.17	100.07	110.40
1	C	978	ALA	CB-CA-C	-5.17	102.35	110.10
1	B	538	TYR	CG-CD2-CE2	5.17	125.43	121.30
1	D	924	ASP	CB-CG-OD1	5.16	122.95	118.30
1	B	855	THR	N-CA-CB	5.16	120.10	110.30
1	C	384	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	B	952	ARG	CD-NE-CZ	5.15	130.81	123.60
1	C	477	SER	N-CA-CB	-5.14	102.78	110.50
1	D	403	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	A	857	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	746	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	185	ALA	N-CA-CB	5.13	117.28	110.10
1	B	392	TYR	CG-CD2-CE2	5.12	125.39	121.30
1	A	329	ASP	CB-CG-OD1	5.12	122.90	118.30
1	C	210	ARG	N-CA-CB	5.11	119.80	110.60
1	C	916	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	523	TRP	CE3-CZ3-CH2	-5.10	115.59	121.20
1	A	177	LEU	CB-CG-CD1	-5.10	102.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	170	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	A	447	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	431	ARG	CD-NE-CZ	5.09	130.73	123.60
1	D	21	VAL	CA-CB-CG2	-5.07	103.30	110.90
1	C	610	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	D	782	ASP	CB-CG-OD1	5.07	122.86	118.30
1	B	746	ASP	CB-CA-C	-5.06	100.28	110.40
1	A	772	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	230	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	356	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	319	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	D	786	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	234	ASP	CB-CG-OD1	5.06	122.85	118.30
1	D	707	ALA	CB-CA-C	-5.05	102.52	110.10
1	C	663	LEU	CB-CA-C	-5.05	100.60	110.20
1	D	869	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	A	282	ARG	NE-CZ-NH1	5.05	122.82	120.30
1	D	447	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	962	TYR	CB-CG-CD1	-5.04	117.97	121.00
1	A	892	ALA	CB-CA-C	5.04	117.66	110.10
1	C	509	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	82	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	324	GLU	N-CA-CB	5.03	119.66	110.60
1	A	267	VAL	CG1-CB-CG2	-5.02	102.86	110.90
1	A	746	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	C	448	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	334	GLU	OE1-CD-OE2	-5.01	117.28	123.30
1	B	659	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	D	559	TYR	CB-CG-CD1	5.01	124.01	121.00
1	C	838	THR	CA-CB-CG2	-5.01	105.39	112.40
1	D	100	TYR	N-CA-CB	5.00	119.61	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	733	ALA	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8119	0	7710	160	0
1	B	8114	0	7705	173	0
1	C	8095	0	7681	156	0
1	D	8103	0	7692	154	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	88	0	132	19	0
4	B	72	0	108	7	0
4	C	84	0	126	17	0
4	D	96	0	144	15	0
5	A	916	0	0	20	0
5	B	985	0	0	15	0
5	C	935	0	0	14	0
5	D	984	0	0	17	0
All	All	36619	0	31298	645	0

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

All (645) 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)
4:B:8601:DMS:C2	4:B:8601:DMS:S	2.03	1.47
1:B:376:ILE:HA	1:B:379:MET:HE2	1.26	1.12
1:C:649:ASN:HA	4:C:8425:DMS:H12	1.37	1.06
1:B:232:ASN:ND2	1:B:237:ARG:HG3	1.84	0.92
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.01	0.91
1:B:599:ARG:HH11	1:B:599:ARG:HG3	1.39	0.88
1:B:684:GLU:O	1:B:686:PRO:HD3	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:ARG:HD2	5:A:9418:HOH:O	1.75	0.86
1:D:1017:GLN:HG2	1:D:1018:LEU:N	1.90	0.86
1:B:376:ILE:HA	1:B:379:MET:CE	2.07	0.84
1:C:808:GLU:HA	1:C:811:LYS:HZ3	1.42	0.84
1:D:829:THR:O	1:D:830:LEU:HD23	1.78	0.84
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.08	0.83
1:A:600:GLN:H	1:A:600:GLN:HE21	1.26	0.83
1:B:13:ARG:HG3	1:C:13:ARG:NH2	1.92	0.83
1:B:600:GLN:H	1:B:600:GLN:HE21	1.24	0.83
1:C:687:GLN:HB3	1:C:688:PRO:HD2	1.60	0.82
1:D:858:ILE:CD1	1:D:864:MET:HG3	2.09	0.82
1:C:367:MET:HB3	1:C:372:MET:HE2	1.62	0.81
1:B:847:LYS:HD3	1:B:849:LEU:HD23	1.63	0.81
1:D:807:VAL:O	1:D:811:LYS:HD3	1.79	0.81
1:B:599:ARG:NH1	1:B:599:ARG:HG3	1.89	0.81
1:D:316:HIS:HA	1:D:323:ILE:HD12	1.63	0.80
1:C:703:PRO:HG2	4:C:8425:DMS:H13	1.64	0.80
1:D:787:ALA:HA	1:D:968:MET:HE2	1.64	0.80
1:A:655:MET:HE2	1:A:662:PRO:HA	1.62	0.80
1:A:653:HIS:CD2	1:A:667:GLU:HG3	2.17	0.79
1:B:651:LEU:O	1:B:651:LEU:HD23	1.82	0.79
1:D:843:GLN:HG2	1:D:848:THR:HA	1.64	0.79
1:A:843:GLN:HG3	1:A:848:THR:HA	1.63	0.79
1:C:808:GLU:HA	1:C:811:LYS:NZ	1.96	0.79
1:D:634:GLN:HB2	1:D:682:LEU:HB2	1.64	0.78
1:C:765:LEU:HD21	1:C:768:MET:CE	2.13	0.78
1:C:809:ARG:NH1	1:C:877:PRO:HB3	1.99	0.78
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.66	0.78
1:B:379:MET:HE3	1:B:407:LEU:HD11	1.66	0.77
1:B:1022:GLN:HG3	1:B:1023:LYS:O	1.85	0.77
1:A:863:GLN:CG	1:A:1021:CYS:HB3	2.14	0.77
1:B:678:GLN:NE2	1:B:680:ILE:HD11	1.99	0.77
1:C:745:MET:HG2	5:C:9388:HOH:O	1.83	0.77
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.67	0.77
1:C:703:PRO:HD2	4:C:8425:DMS:H11	1.66	0.76
1:C:599:ARG:HG3	1:C:600:GLN:OE1	1.85	0.76
1:A:634:GLN:HB3	1:A:682:LEU:HB2	1.66	0.76
1:C:78:LEU:HD22	1:C:80:GLU:OE1	1.86	0.76
1:D:858:ILE:HD11	1:D:864:MET:HG3	1.65	0.76
4:A:8416:DMS:H11	5:A:9210:HOH:O	1.86	0.75
5:C:9488:HOH:O	1:D:530:THR:HG22	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:LEU:C	1:B:680:ILE:HD12	2.07	0.75
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.69	0.75
1:B:986:ILE:CD1	1:B:1018:LEU:HD21	2.17	0.75
1:D:685:LEU:HD23	1:D:686:PRO:HD2	1.68	0.74
1:C:684:GLU:OE2	1:C:686:PRO:HB3	1.88	0.74
1:C:649:ASN:HA	4:C:8425:DMS:C1	2.17	0.74
1:C:599:ARG:NH2	1:C:795:VAL:HB	2.03	0.73
1:C:835:LEU:HD11	1:C:855:THR:HB	1.70	0.73
1:B:679:LEU:O	1:B:680:ILE:HD12	1.89	0.73
1:A:277:GLU:H	1:A:277:GLU:CD	1.90	0.73
1:B:687:GLN:HE21	1:B:687:GLN:N	1.85	0.73
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.21	0.73
1:A:241:GLU:OE1	1:A:292:ARG:NE	2.21	0.73
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.24	0.73
1:B:658:LEU:O	1:B:661:LYS:HD2	1.88	0.73
1:B:745:MET:H	1:B:745:MET:CE	2.02	0.73
1:A:32:PRO:HB2	4:A:8404:DMS:H13	1.71	0.72
1:A:583:ASN:OD1	1:A:584:PRO:HD2	1.89	0.72
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.71	0.72
1:D:664:ALA:HB3	1:D:685:LEU:HD21	1.71	0.71
1:C:770:ILE:HD12	1:C:775:GLN:CD	2.10	0.71
1:B:890:GLN:HG3	1:B:891:VAL:N	2.03	0.71
1:C:745:MET:CE	1:C:745:MET:HA	2.20	0.71
4:D:8421:DMS:H11	5:D:9329:HOH:O	1.90	0.71
1:C:802:ASP:OD1	1:C:804:ASN:HB2	1.90	0.71
1:D:651:LEU:HD13	1:D:651:LEU:C	2.11	0.71
1:A:746:ASP:HB2	5:A:9486:HOH:O	1.90	0.71
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.72	0.70
1:B:278:ILE:HD12	5:B:9153:HOH:O	1.92	0.70
1:B:1022:GLN:HG3	1:B:1023:LYS:N	2.04	0.70
1:D:843:GLN:CG	1:D:848:THR:HA	2.22	0.70
1:B:319:ASP:OD1	1:B:321:THR:N	2.22	0.70
1:A:651:LEU:CD1	1:A:667:GLU:HG2	2.22	0.69
1:B:772:ASP:OD1	1:B:773:LYS:HD3	1.92	0.69
1:B:655:MET:CE	1:B:662:PRO:HB3	2.22	0.69
4:C:8410:DMS:H13	5:C:8970:HOH:O	1.91	0.69
1:A:737:ILE:O	1:A:737:ILE:HD13	1.91	0.69
1:A:863:GLN:HG3	1:A:1021:CYS:HB3	1.74	0.69
1:A:80:GLU:N	1:A:80:GLU:OE1	2.23	0.69
4:C:8413:DMS:H12	5:C:9181:HOH:O	1.93	0.68
1:D:634:GLN:NE2	1:D:682:LEU:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:8411:DMS:H21	5:B:9552:HOH:O	1.92	0.68
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.26	0.68
1:D:952:ARG:O	1:D:1018:LEU:HD22	1.93	0.68
1:D:134:LEU:HA	4:D:8705:DMS:H22	1.74	0.68
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.58	0.68
1:D:595:THR:HA	1:D:596:PRO:C	2.13	0.68
1:C:684:GLU:HG3	1:C:684:GLU:O	1.94	0.68
1:D:135:GLN:C	1:D:136:GLU:HG2	2.13	0.68
1:D:133:TRP:HE1	4:D:8703:DMS:H23	1.57	0.68
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.29	0.68
1:C:703:PRO:HG2	4:C:8425:DMS:C1	2.24	0.67
1:A:749:ILE:N	1:A:749:ILE:HD12	2.09	0.67
1:B:687:GLN:NE2	1:B:687:GLN:N	2.43	0.67
1:B:634:GLN:HG2	1:B:682:LEU:O	1.94	0.67
1:C:730:LEU:HD23	1:C:730:LEU:N	2.09	0.67
1:A:494:THR:HB	1:D:473:ARG:NH2	2.10	0.67
1:A:32:PRO:HB2	4:A:8404:DMS:C1	2.25	0.66
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.11	0.66
1:D:887:GLN:NE2	1:D:980:GLU:O	2.28	0.66
1:D:230:ARG:HD3	5:D:9609:HOH:O	1.95	0.66
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.60	0.66
1:A:887:GLN:NE2	1:A:980:GLU:O	2.26	0.66
1:D:687:GLN:OE1	1:D:688:PRO:HD2	1.95	0.66
1:C:890:GLN:HG3	1:C:891:VAL:N	2.11	0.65
1:D:117:GLU:HB2	5:D:9146:HOH:O	1.96	0.65
1:A:847:LYS:NZ	5:A:9292:HOH:O	2.30	0.65
1:B:678:GLN:HE21	1:B:680:ILE:HD11	1.61	0.65
1:D:237:ARG:NH1	5:D:9254:HOH:O	2.29	0.65
1:D:658:LEU:O	1:D:661:LYS:HG3	1.96	0.64
1:D:579:ASP:HA	5:D:9220:HOH:O	1.97	0.64
1:A:863:GLN:HG2	1:A:1021:CYS:HB3	1.78	0.64
1:C:599:ARG:NH1	5:C:8969:HOH:O	2.30	0.64
1:B:986:ILE:HD13	1:B:1018:LEU:HD21	1.78	0.64
1:C:599:ARG:HH21	1:C:795:VAL:CG1	2.11	0.64
1:A:630:ARG:HA	4:A:8503:DMS:O	1.98	0.63
1:A:106:PRO:O	4:A:8410:DMS:H22	1.99	0.63
1:D:858:ILE:HD12	1:D:864:MET:HG3	1.79	0.63
1:B:847:LYS:HD3	1:B:849:LEU:CD2	2.27	0.63
1:A:579:ASP:O	1:A:582:GLY:N	2.26	0.63
1:C:878:HIS:HD2	5:C:8701:HOH:O	1.79	0.63
1:A:832:ASP:OD1	1:A:832:ASP:N	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.29	0.63
1:D:859:ASP:CG	1:D:861:SER:H	2.02	0.62
1:C:367:MET:HB3	1:C:372:MET:CE	2.28	0.62
1:D:859:ASP:OD2	1:D:861:SER:N	2.29	0.62
1:B:730:LEU:CB	1:B:731:PRO:HD2	2.29	0.62
1:B:655:MET:HE3	1:B:662:PRO:HB3	1.80	0.62
1:D:878:HIS:HD2	5:D:8818:HOH:O	1.83	0.62
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.35	0.62
1:A:112:PRO:HD2	1:A:113:PHE:CE1	2.33	0.62
1:C:830:LEU:N	1:C:830:LEU:HD23	2.14	0.61
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.30	0.61
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.34	0.61
1:B:730:LEU:HB2	1:B:731:PRO:HD2	1.83	0.61
1:D:577:LYS:O	1:D:584:PRO:HA	2.01	0.61
1:A:800:ARG:HD3	1:A:801:ILE:N	2.15	0.61
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.82	0.61
1:D:829:THR:C	1:D:830:LEU:HD23	2.20	0.61
1:B:890:GLN:CG	1:B:891:VAL:N	2.63	0.61
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.82	0.60
1:B:986:ILE:HD11	1:B:1018:LEU:HD21	1.82	0.60
1:D:681:GLU:HG2	5:D:9421:HOH:O	1.99	0.60
1:D:237:ARG:HG2	1:D:237:ARG:HH11	1.66	0.60
1:A:660:GLY:O	1:A:662:PRO:HD3	2.02	0.60
1:B:277:GLU:HG2	5:B:9401:HOH:O	2.01	0.60
1:D:438:GLU:HG2	1:D:442:ARG:HD2	1.83	0.60
1:C:651:LEU:HD12	1:C:701:VAL:O	2.01	0.60
1:C:684:GLU:O	1:C:686:PRO:HD3	2.01	0.60
1:B:685:LEU:O	1:B:687:GLN:NE2	2.35	0.60
1:C:743:SER:O	1:C:760:ARG:NH1	2.27	0.60
1:B:379:MET:CE	1:B:407:LEU:HD11	2.32	0.60
1:D:126:THR:CG2	1:D:181:GLU:HG2	2.32	0.59
1:A:135:GLN:NE2	5:A:9437:HOH:O	2.35	0.59
1:D:133:TRP:HE1	4:D:8703:DMS:C2	2.15	0.59
1:B:878:HIS:HD2	5:B:8690:HOH:O	1.85	0.59
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.37	0.59
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.38	0.59
4:D:8703:DMS:H23	5:D:9600:HOH:O	2.03	0.59
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.85	0.59
1:A:890:GLN:HG3	1:A:891:VAL:N	2.18	0.59
1:B:387:VAL:HG22	5:B:9493:HOH:O	2.02	0.59
1:D:373:VAL:O	1:D:377:LEU:HG	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:795:VAL:HG12	5:B:9500:HOH:O	2.03	0.58
1:D:770:ILE:HD12	1:D:775:GLN:CD	2.23	0.58
1:D:379:MET:HE1	1:D:407:LEU:HD13	1.84	0.58
1:A:655:MET:HG2	5:A:8968:HOH:O	2.01	0.58
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.16	0.58
1:C:278:ILE:HD13	1:C:278:ILE:N	2.16	0.58
1:C:595:THR:HA	1:C:596:PRO:C	2.24	0.58
1:C:296:GLU:HA	1:C:296:GLU:OE1	2.02	0.58
1:B:597:ASN:OD1	1:B:599:ARG:HD3	2.04	0.58
1:D:68:ALA:O	1:D:70:PRO:HD3	2.03	0.58
1:C:599:ARG:HH21	1:C:795:VAL:HB	1.68	0.58
1:D:859:ASP:OD2	1:D:861:SER:HB3	2.03	0.58
1:C:599:ARG:HG3	1:C:600:GLN:H	1.69	0.57
1:D:126:THR:HG23	1:D:181:GLU:HG2	1.86	0.57
1:C:734:SER:CB	1:C:860:GLY:HA3	2.34	0.57
1:A:347:LYS:HE3	5:A:9435:HOH:O	2.04	0.57
1:C:745:MET:HE3	1:C:745:MET:HA	1.86	0.57
1:A:683:PRO:O	1:A:685:LEU:HG	2.04	0.57
1:C:824:GLN:O	1:C:838:THR:HA	2.04	0.57
1:C:688:PRO:HG3	1:C:694:LEU:HD11	1.86	0.57
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.69	0.57
1:A:494:THR:CB	1:D:473:ARG:HH22	2.17	0.57
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.86	0.57
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.85	0.57
1:D:805:ALA:O	1:D:809:ARG:HG3	2.05	0.57
1:C:765:LEU:HD21	1:C:768:MET:HE1	1.85	0.57
1:B:236:SER:C	1:B:237:ARG:HG2	2.25	0.56
1:D:710:GLU:HG2	5:D:9085:HOH:O	2.05	0.56
1:B:678:GLN:HG2	1:B:680:ILE:CD1	2.34	0.56
1:B:431:ARG:HG2	5:C:9420:HOH:O	2.05	0.56
1:A:730:LEU:HD21	1:B:823:LEU:HB3	1.87	0.56
1:C:240:LEU:HD23	1:C:240:LEU:C	2.25	0.56
1:C:615:PRO:O	1:C:618:THR:HG22	2.05	0.56
1:C:730:LEU:CB	1:C:731:PRO:HD2	2.35	0.56
1:A:595:THR:HA	1:A:596:PRO:C	2.24	0.56
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.88	0.56
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.06	0.56
1:C:757:GLN:OE1	1:C:769:TRP:HH2	1.87	0.56
1:B:637:GLU:CD	1:B:677:LYS:HE2	2.25	0.55
1:C:317:THR:OG1	1:C:319:ASP:OD1	2.24	0.55
1:D:1022:GLN:HG3	1:D:1023:LYS:N	2.01	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:890:GLN:HG3	1:D:891:VAL:N	2.21	0.55
1:C:805:ALA:HB3	1:C:808:GLU:HG2	1.89	0.55
1:B:78:LEU:HB3	1:B:80:GLU:CG	2.36	0.55
1:B:655:MET:HE1	1:B:662:PRO:HB3	1.88	0.55
1:B:890:GLN:HG2	5:B:9553:HOH:O	2.06	0.55
1:C:991:MET:HE2	1:C:1003:VAL:HG21	1.89	0.55
1:B:363:HIS:HD2	5:B:9171:HOH:O	1.89	0.55
1:C:809:ARG:CZ	1:C:877:PRO:HB3	2.36	0.54
4:D:8406:DMS:O	5:D:9596:HOH:O	2.18	0.54
1:C:745:MET:HE2	1:C:745:MET:HA	1.88	0.54
1:A:32:PRO:HB3	4:A:8404:DMS:H11	1.88	0.54
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.89	0.54
1:A:494:THR:HB	1:D:473:ARG:HH22	1.72	0.54
1:D:292:ARG:HH12	4:D:8412:DMS:C2	2.19	0.54
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.42	0.54
1:B:655:MET:SD	1:B:656:VAL:N	2.80	0.54
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.71	0.54
1:A:32:PRO:CB	4:A:8404:DMS:H11	2.37	0.54
1:A:878:HIS:HD2	5:A:8676:HOH:O	1.90	0.54
1:A:703:PRO:HG2	4:A:8425:DMS:H11	1.90	0.54
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.90	0.54
1:D:951:TRP:HB3	1:D:1018:LEU:HD11	1.89	0.54
1:A:817:GLN:HG2	5:A:8938:HOH:O	2.08	0.54
1:A:648:ASP:OD2	5:A:9405:HOH:O	2.19	0.54
4:A:8502:DMS:H12	5:A:9284:HOH:O	2.07	0.54
1:B:859:ASP:OD1	1:B:861:SER:OG	2.23	0.54
1:D:843:GLN:HG2	1:D:848:THR:CA	2.36	0.53
1:B:945:ASN:HB3	1:B:1023:LYS:HE2	1.89	0.53
1:A:863:GLN:HG3	1:A:1021:CYS:CB	2.38	0.53
1:A:237:ARG:HG2	1:A:296:GLU:OE1	2.08	0.53
1:B:687:GLN:HE21	1:B:687:GLN:H	1.53	0.53
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.90	0.53
1:D:237:ARG:HG2	1:D:237:ARG:NH1	2.23	0.53
1:D:379:MET:HE2	1:D:407:LEU:HD11	1.91	0.53
1:B:615:PRO:O	1:B:618:THR:HG22	2.08	0.53
1:B:70:PRO:HG2	1:B:78:LEU:HD21	1.91	0.53
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.90	0.53
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.38	0.53
1:D:292:ARG:HH12	4:D:8412:DMS:H21	1.74	0.53
1:C:513:PRO:HG2	5:C:8615:HOH:O	2.08	0.53
1:D:615:PRO:O	1:D:618:THR:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:ALA:O	1:B:734:SER:O	2.28	0.52
1:D:580:GLU:OE1	1:D:580:GLU:O	2.27	0.52
1:D:687:GLN:CD	1:D:688:PRO:HD2	2.30	0.52
1:A:809:ARG:HH21	1:A:877:PRO:HB3	1.74	0.52
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.90	0.52
1:D:237:ARG:NH1	1:D:296:GLU:OE1	2.43	0.52
1:B:78:LEU:HB3	1:B:80:GLU:HG3	1.92	0.52
1:C:599:ARG:NH2	1:C:795:VAL:CB	2.72	0.52
1:B:658:LEU:HD21	1:B:690:SER:HB3	1.92	0.52
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.27	0.52
1:C:730:LEU:HB3	1:C:731:PRO:HD2	1.91	0.52
1:A:107:ILE:HG22	4:A:8410:DMS:H22	1.91	0.52
1:D:708:TRP:CZ2	4:D:8403:DMS:H12	2.45	0.52
1:B:748:CYS:C	1:B:749:ILE:HD12	2.31	0.52
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.91	0.52
1:C:703:PRO:CD	4:C:8425:DMS:H11	2.40	0.51
1:A:32:PRO:CB	4:A:8404:DMS:C1	2.88	0.51
1:D:299:LYS:NZ	5:D:9387:HOH:O	2.23	0.51
1:B:595:THR:HA	1:B:596:PRO:C	2.31	0.51
1:A:533:LEU:C	1:A:533:LEU:HD23	2.30	0.51
1:B:749:ILE:N	1:B:749:ILE:HD12	2.25	0.51
1:A:637:GLU:OE2	1:A:677:LYS:HE3	2.10	0.51
1:B:59:ARG:NH2	1:B:81:ALA:HB3	2.25	0.51
1:B:240:LEU:HD23	1:B:240:LEU:C	2.30	0.51
1:B:632:SER:O	1:B:635:THR:N	2.37	0.51
1:A:742:THR:HG22	1:A:743:SER:N	2.24	0.51
1:D:729:THR:HG23	5:D:9324:HOH:O	2.11	0.51
1:D:773:LYS:HG2	1:D:775:GLN:NE2	2.26	0.51
1:B:296:GLU:OE1	1:B:296:GLU:HA	2.11	0.51
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.26	0.50
1:B:631:LEU:HD12	1:B:635:THR:O	2.11	0.50
1:C:637:GLU:OE2	1:C:677:LYS:NZ	2.42	0.50
1:D:1022:GLN:HG3	1:D:1023:LYS:HG2	1.91	0.50
1:B:542:MET:HA	1:B:604:ASN:HA	1.93	0.50
1:A:252:ASP:OD1	4:A:8416:DMS:H11	2.11	0.50
1:A:378:LEU:HD11	5:A:8867:HOH:O	2.11	0.50
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.80	0.50
1:D:114:VAL:HB	1:D:115:PRO:CD	2.42	0.50
1:C:833:ALA:HB1	1:C:858:ILE:O	2.11	0.50
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.92	0.50
1:B:375:ASP:O	1:B:379:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:GLN:CG	1:A:891:VAL:N	2.75	0.50
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.47	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.92	0.50
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.93	0.50
1:A:88:SER:HA	1:A:366:VAL:HG21	1.94	0.50
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.94	0.50
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.94	0.50
1:C:699:ARG:NH2	5:C:9404:HOH:O	2.45	0.50
1:A:45:ASP:OD2	5:A:9168:HOH:O	2.20	0.50
1:A:662:PRO:O	1:A:663:LEU:HD23	2.12	0.50
1:B:16:TRP:CG	1:B:189:LEU:CD1	2.94	0.50
1:A:737:ILE:HD13	1:A:737:ILE:C	2.31	0.49
1:B:777:LEU:HG	1:B:889:ALA:HA	1.94	0.49
1:A:559:TYR:CE2	1:B:522:LYS:HA	2.47	0.49
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.80	0.49
1:A:655:MET:CE	1:A:662:PRO:HA	2.37	0.49
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.24	0.49
1:D:318:ALA:HB3	5:D:9568:HOH:O	2.12	0.49
1:A:703:PRO:HG2	4:A:8425:DMS:C1	2.43	0.49
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.30	0.49
1:D:651:LEU:HD12	1:D:653:HIS:CE1	2.47	0.49
1:C:777:LEU:HG	1:C:889:ALA:HA	1.95	0.49
1:A:851:ILE:O	1:A:870:VAL:HA	2.13	0.49
1:C:847:LYS:HE2	5:C:9333:HOH:O	2.12	0.49
1:B:807:VAL:CG1	1:B:808:GLU:N	2.75	0.49
1:A:633:GLY:O	1:A:634:GLN:OE1	2.30	0.49
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.47	0.48
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.95	0.48
1:D:651:LEU:CD1	1:D:653:HIS:CE1	2.97	0.48
1:D:379:MET:HE1	1:D:407:LEU:CD1	2.42	0.48
1:D:240:LEU:C	1:D:240:LEU:HD23	2.33	0.48
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.96	0.48
1:C:599:ARG:HH21	1:C:795:VAL:CB	2.25	0.48
1:D:687:GLN:CG	1:D:688:PRO:HD2	2.43	0.48
1:C:819:GLU:H	1:C:819:GLU:HG2	1.45	0.48
1:D:60:PHE:HA	1:D:122:CYS:O	2.14	0.48
1:A:59:ARG:HG2	4:A:8502:DMS:C1	2.43	0.48
1:C:811:LYS:HB2	1:C:811:LYS:NZ	2.29	0.48
1:D:682:LEU:C	1:D:683:PRO:O	2.49	0.48
1:C:79:PRO:HD2	1:C:80:GLU:OE2	2.14	0.48
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:GLY:O	1:D:561:ARG:HG2	2.14	0.48
1:B:730:LEU:HG	1:B:730:LEU:H	1.50	0.48
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.49	0.48
1:C:887:GLN:NE2	1:C:980:GLU:O	2.46	0.48
1:D:660:GLY:O	1:D:662:PRO:HD3	2.14	0.48
1:C:919:ASP:O	1:C:920:LEU:HD23	2.14	0.48
1:A:600:GLN:N	1:A:600:GLN:HE21	2.03	0.48
1:C:651:LEU:HD12	1:C:651:LEU:N	2.28	0.48
1:A:735:HIS:CD2	1:A:735:HIS:N	2.81	0.48
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.49	0.47
1:C:651:LEU:HD13	1:C:653:HIS:CE1	2.50	0.47
1:D:893:GLU:HG2	1:D:893:GLU:O	2.13	0.47
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.95	0.47
1:C:387:VAL:HG22	5:C:9470:HOH:O	2.13	0.47
1:C:687:GLN:CB	1:C:688:PRO:HD2	2.32	0.47
1:D:379:MET:CE	1:D:407:LEU:HD11	2.45	0.47
1:B:645:ARG:NH2	1:B:648:ASP:OD1	2.47	0.47
1:A:754:LYS:NZ	5:A:9390:HOH:O	2.47	0.47
1:A:835:LEU:HD11	1:A:855:THR:HB	1.95	0.47
1:C:655:MET:HG3	1:C:655:MET:O	2.14	0.47
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.96	0.47
1:C:147:ASN:HA	1:C:148:SER:HA	1.64	0.47
1:B:663:LEU:HD22	1:B:663:LEU:C	2.35	0.47
1:A:433:LEU:N	1:A:434:PRO:CD	2.77	0.47
1:D:513:PRO:O	1:D:514:ALA:HB3	2.14	0.47
1:A:844:HIS:HD2	5:A:9350:HOH:O	1.98	0.47
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.49	0.47
1:C:989:PHE:N	1:C:989:PHE:CD1	2.83	0.47
1:D:664:ALA:HB3	1:D:685:LEU:CD2	2.40	0.47
1:A:241:GLU:OE2	1:A:292:ARG:NH2	2.48	0.47
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.15	0.47
1:A:521:LYS:HE2	5:A:9021:HOH:O	2.13	0.47
1:C:356:ARG:HD2	1:C:379:MET:CE	2.45	0.47
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.50	0.47
1:A:506:VAL:CG1	1:A:521:LYS:HE3	2.45	0.47
1:C:292:ARG:HH12	4:C:8412:DMS:C2	2.27	0.47
1:A:826:THR:OG1	1:A:837:THR:HB	2.15	0.47
1:C:634:GLN:H	1:C:634:GLN:CD	2.13	0.47
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.96	0.47
1:B:241:GLU:OE1	1:B:292:ARG:HG2	2.15	0.47
1:B:319:ASP:OD1	1:B:320:GLY:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:TRP:NE1	4:D:8703:DMS:C2	2.78	0.46
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.15	0.46
1:A:369:GLU:O	1:A:373:VAL:HG23	2.15	0.46
1:D:231:PHE:O	4:D:8417:DMS:H22	2.14	0.46
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.97	0.46
1:B:796:SER:HB3	1:B:999:TRP:HB3	1.97	0.46
1:D:521:LYS:HE2	5:D:9164:HOH:O	2.15	0.46
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.50	0.46
1:C:599:ARG:NH2	1:C:795:VAL:CG1	2.78	0.46
1:C:829:THR:C	1:C:830:LEU:HD23	2.35	0.46
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.97	0.46
1:A:126:THR:HA	1:A:182:ASN:O	2.15	0.46
4:B:8409:DMS:O	5:B:9107:HOH:O	2.21	0.46
1:C:78:LEU:HB3	1:C:80:GLU:CD	2.35	0.46
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.46
1:D:843:GLN:HA	1:D:847:LYS:O	2.15	0.46
1:C:296:GLU:HG2	4:C:8601:DMS:C1	2.46	0.46
1:A:809:ARG:NH2	1:A:877:PRO:HB3	2.30	0.46
1:C:610:ASP:O	1:C:611:ARG:HB2	2.16	0.46
1:A:387:VAL:HG22	5:A:9450:HOH:O	2.15	0.46
1:D:858:ILE:CD1	1:D:858:ILE:N	2.79	0.46
1:D:133:TRP:NE1	4:D:8703:DMS:H23	2.27	0.46
1:D:961:ARG:NE	1:D:981:GLY:O	2.49	0.46
1:A:59:ARG:HG2	4:A:8502:DMS:H11	1.97	0.46
1:C:718:GLN:HG2	4:C:8503:DMS:H11	1.98	0.46
1:A:774:LYS:HE2	1:A:774:LYS:HB2	1.61	0.46
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.51	0.46
1:C:651:LEU:H	1:C:651:LEU:HD12	1.80	0.46
1:A:593:GLY:O	1:A:595:THR:HG22	2.14	0.46
1:C:843:GLN:HA	1:C:847:LYS:O	2.16	0.46
1:C:619:GLU:HG2	1:C:909:ARG:HG3	1.98	0.46
1:A:127:PHE:N	1:A:127:PHE:CD2	2.81	0.46
1:D:986:ILE:HD12	1:D:986:ILE:HG21	1.49	0.46
1:D:682:LEU:O	1:D:683:PRO:O	2.34	0.46
1:A:107:ILE:HG22	4:A:8410:DMS:C2	2.45	0.46
1:A:890:GLN:OE1	1:A:948:PRO:HD3	2.16	0.46
1:B:637:GLU:OE2	1:B:677:LYS:HE2	2.15	0.46
1:C:843:GLN:HG2	1:C:848:THR:HA	1.97	0.46
1:D:736:ALA:HB3	1:D:751:LEU:HD11	1.98	0.46
1:C:730:LEU:HD23	1:C:730:LEU:H	1.78	0.46
1:B:376:ILE:CA	1:B:379:MET:HE2	2.19	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLN:HE21	1:A:685:LEU:HD11	1.80	0.45
1:A:890:GLN:HG3	1:A:891:VAL:H	1.78	0.45
1:C:266:GLN:NE2	4:C:8602:DMS:S	2.90	0.45
1:D:88:SER:HA	1:D:366:VAL:HG21	1.98	0.45
1:C:703:PRO:HD2	4:C:8425:DMS:C1	2.42	0.45
1:C:16:TRP:CG	1:C:189:LEU:CD1	2.99	0.45
1:A:290:THR:HB	4:A:8412:DMS:H22	1.98	0.45
1:D:80:GLU:H	1:D:80:GLU:HG3	1.58	0.45
1:A:362:LEU:HD22	1:A:362:LEU:HA	1.68	0.45
1:A:651:LEU:HD13	1:A:667:GLU:HG2	1.96	0.45
1:A:843:GLN:HG3	1:A:848:THR:CA	2.38	0.45
1:C:687:GLN:CB	1:C:688:PRO:CD	2.94	0.45
1:B:655:MET:SD	1:B:664:ALA:O	2.74	0.45
1:D:770:ILE:HD12	1:D:775:GLN:NE2	2.31	0.45
1:A:730:LEU:HD12	1:A:730:LEU:N	2.32	0.45
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.51	0.45
1:A:580:GLU:OE1	1:A:580:GLU:O	2.35	0.45
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.98	0.45
1:B:701:VAL:HG22	1:B:714:ILE:HG12	1.98	0.45
1:B:731:PRO:HB2	1:B:732:ALA:H	1.64	0.45
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.51	0.45
1:B:292:ARG:NH1	4:B:8412:DMS:C2	2.79	0.45
1:B:796:SER:OG	1:B:800:ARG:NH2	2.49	0.45
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.33	0.45
1:D:105:TYR:O	4:D:8419:DMS:O	2.34	0.45
1:A:646:HIS:NE2	1:A:671:ASP:OD2	2.44	0.45
1:C:749:ILE:HD12	1:C:749:ILE:N	2.31	0.45
1:A:268:ALA:HA	4:A:8602:DMS:H22	1.99	0.45
1:D:833:ALA:HB1	1:D:858:ILE:O	2.16	0.45
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.47	0.45
1:D:441:THR:O	1:D:445:GLN:HG3	2.17	0.45
1:B:85:VAL:HG12	1:B:86:VAL:N	2.28	0.45
1:B:651:LEU:C	1:B:651:LEU:HD23	2.36	0.45
1:D:844:HIS:O	1:D:845:GLN:HB2	2.17	0.45
1:D:824:GLN:HB3	1:D:839:ALA:HB3	1.98	0.45
1:B:379:MET:HE3	1:B:407:LEU:CD1	2.41	0.45
1:A:843:GLN:HA	1:A:847:LYS:O	2.17	0.45
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.51	0.45
1:B:678:GLN:HG2	1:B:680:ILE:HD11	1.99	0.45
1:B:745:MET:SD	1:B:745:MET:N	2.88	0.45
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:LEU:O	1:C:251:ARG:HD3	2.16	0.45
1:B:731:PRO:O	1:B:732:ALA:HB2	2.16	0.45
1:C:569:ASP:O	1:C:605:GLY:HA2	2.17	0.45
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.52	0.45
1:A:338:GLU:OE1	5:A:9270:HOH:O	2.21	0.44
1:B:668:VAL:HG12	1:B:669:PRO:O	2.17	0.44
1:D:147:ASN:HA	1:D:148:SER:HA	1.68	0.44
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.52	0.44
1:C:656:VAL:O	1:C:663:LEU:HB2	2.18	0.44
1:D:859:ASP:OD1	1:D:861:SER:OG	2.26	0.44
1:C:785:THR:O	1:C:881:ARG:HD2	2.16	0.44
1:C:601:PHE:CD1	1:C:796:SER:HA	2.51	0.44
1:C:651:LEU:HD13	1:C:653:HIS:HE1	1.82	0.44
1:D:932:PRO:HD2	1:D:970:THR:O	2.17	0.44
1:C:78:LEU:HB3	1:C:80:GLU:OE2	2.18	0.44
1:B:142:ILE:HG12	1:B:170:GLU:HG2	2.00	0.44
1:B:680:ILE:N	1:B:680:ILE:HD12	2.31	0.44
1:B:745:MET:N	1:B:745:MET:CE	2.77	0.44
1:B:80:GLU:HG2	1:B:80:GLU:H	1.18	0.44
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	2.00	0.44
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.53	0.44
1:B:835:LEU:HD11	1:B:855:THR:HB	1.98	0.44
1:A:250:LEU:C	1:A:251:ARG:HG2	2.38	0.44
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.33	0.44
1:B:88:SER:HA	1:B:366:VAL:HG21	2.00	0.44
1:A:577:LYS:O	1:A:584:PRO:HA	2.18	0.44
1:B:920:LEU:HB3	1:B:921:PRO:HD2	2.00	0.44
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.53	0.44
1:C:744:GLU:O	1:C:760:ARG:HD3	2.18	0.44
1:A:742:THR:CG2	1:A:743:SER:N	2.81	0.44
1:A:850:PHE:HA	1:A:871:GLU:O	2.18	0.44
1:C:951:TRP:HA	1:C:1019:VAL:O	2.18	0.44
1:A:745:MET:HE2	1:A:745:MET:HB3	1.71	0.43
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.98	0.43
1:B:600:GLN:N	1:B:600:GLN:HE21	2.03	0.43
1:C:835:LEU:CD1	1:C:855:THR:HB	2.44	0.43
1:B:654:TRP:CE3	1:B:665:SER:HA	2.54	0.43
4:D:8503:DMS:O	5:D:8975:HOH:O	2.20	0.43
1:B:745:MET:HE1	1:B:745:MET:H	1.79	0.43
1:B:687:GLN:HA	1:B:688:PRO:HD3	1.69	0.43
1:C:628:GLN:NE2	4:C:8402:DMS:O	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:HIS:O	1:A:736:ALA:HB2	2.18	0.43
1:A:362:LEU:O	1:A:362:LEU:HD13	2.18	0.43
1:D:845:GLN:HA	1:D:845:GLN:OE1	2.18	0.43
1:D:100:TYR:OH	1:D:601:PHE:HB3	2.19	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.01	0.43
1:D:433:LEU:N	1:D:434:PRO:CD	2.82	0.43
1:B:961:ARG:NH1	5:B:9162:HOH:O	2.33	0.43
1:B:73:TRP:CZ2	1:B:185:ALA:HB1	2.54	0.43
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.54	0.43
1:B:773:LYS:CD	1:B:773:LYS:N	2.79	0.43
1:C:651:LEU:HD13	1:C:701:VAL:HB	2.01	0.43
1:B:601:PHE:CD1	1:B:796:SER:HA	2.54	0.43
1:B:147:ASN:HA	1:B:148:SER:HA	1.54	0.43
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.35	0.43
1:A:682:LEU:HD23	1:A:682:LEU:HA	1.83	0.43
1:B:730:LEU:CB	1:B:731:PRO:CD	2.97	0.43
1:A:587:ALA:HB1	1:A:591:ASP:HB2	2.01	0.43
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.54	0.43
1:A:655:MET:CE	1:A:662:PRO:HB3	2.47	0.43
1:D:94:GLY:HA3	4:D:8421:DMS:H22	2.01	0.43
1:D:237:ARG:CG	1:D:237:ARG:NH1	2.79	0.43
1:D:986:ILE:HD13	1:D:986:ILE:HG23	1.47	0.43
1:B:669:PRO:CB	5:B:9418:HOH:O	2.66	0.43
1:A:427:THR:HG22	1:A:436:MET:SD	2.59	0.43
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.83	0.43
1:B:647:SER:OG	1:B:672:VAL:HG23	2.18	0.43
1:D:581:ASN:N	1:D:581:ASN:OD1	2.51	0.43
1:D:305:ILE:HD11	1:D:645:ARG:HB3	2.01	0.42
1:C:730:LEU:CD2	1:C:730:LEU:N	2.81	0.42
1:A:949:HIS:O	1:A:1023:LYS:NZ	2.53	0.42
1:D:226:HIS:O	1:D:242:ALA:HA	2.18	0.42
1:C:820:ALA:HB2	1:C:842:TRP:CE2	2.54	0.42
1:D:427:THR:HG22	1:D:436:MET:SD	2.59	0.42
1:C:367:MET:CB	1:C:372:MET:HE2	2.39	0.42
1:A:749:ILE:N	1:A:749:ILE:CD1	2.79	0.42
1:A:494:THR:CB	1:D:473:ARG:NH2	2.75	0.42
1:D:379:MET:CE	1:D:407:LEU:CD1	2.97	0.42
1:C:545:SER:O	1:C:909:ARG:HD3	2.19	0.42
1:B:336:ARG:HD3	5:B:9199:HOH:O	2.19	0.42
1:B:815:HIS:CD2	1:B:849:LEU:HD13	2.55	0.42
1:A:655:MET:HE3	1:A:656:VAL:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:577:LYS:O	1:B:584:PRO:HA	2.18	0.42
1:B:661:LYS:HA	1:B:662:PRO:HD3	1.52	0.42
1:C:655:MET:SD	1:C:657:ALA:HB2	2.60	0.42
1:A:854:LYS:HA	1:A:867:THR:O	2.19	0.42
1:C:658:LEU:O	1:C:659:ASP:C	2.55	0.42
1:B:773:LYS:HD3	1:B:773:LYS:N	2.35	0.42
1:A:781:ARG:NH1	5:A:9274:HOH:O	2.53	0.42
1:C:49:GLN:HG2	5:C:9432:HOH:O	2.19	0.42
1:D:780:LEU:HA	1:D:886:CYS:HB3	2.02	0.42
1:B:104:THR:HB	5:B:9533:HOH:O	2.19	0.42
1:B:569:ASP:O	1:B:605:GLY:HA2	2.19	0.42
1:B:127:PHE:N	1:B:127:PHE:CD2	2.88	0.42
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.55	0.42
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.51	0.42
1:A:357:HIS:CD2	5:A:9479:HOH:O	2.72	0.42
1:A:57:GLU:HB3	1:A:83:THR:CG2	2.50	0.42
4:B:8403:DMS:H23	5:B:8899:HOH:O	2.19	0.42
1:A:950:GLN:OE1	1:A:952:ARG:NE	2.37	0.42
1:D:664:ALA:CB	1:D:685:LEU:HD21	2.44	0.42
1:A:473:ARG:HD3	5:D:8713:HOH:O	2.18	0.42
1:A:390:SER:HA	1:A:391:HIS:HA	1.85	0.42
1:D:78:LEU:HA	1:D:78:LEU:HD23	1.75	0.42
1:C:387:VAL:HG13	5:C:9470:HOH:O	2.19	0.42
1:C:718:GLN:HG2	4:C:8503:DMS:C1	2.50	0.42
1:D:667:GLU:C	1:D:668:VAL:HG23	2.39	0.42
1:D:768:MET:HE1	1:D:1020:TRP:CE2	2.54	0.42
1:A:35:SER:HB2	1:A:217:LYS:HD3	2.02	0.42
1:D:739:HIS:O	1:D:749:ILE:HA	2.19	0.42
1:B:937:LEU:HA	1:B:957:PHE:O	2.20	0.41
1:A:753:ASN:N	1:A:753:ASN:OD1	2.51	0.41
1:B:379:MET:HB2	1:B:379:MET:HE2	1.93	0.41
1:C:770:ILE:HD12	1:C:775:GLN:CG	2.50	0.41
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.83	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.94	0.41
1:C:59:ARG:NH2	1:C:81:ALA:HB3	2.34	0.41
1:B:607:VAL:HG12	1:B:613:PRO:HA	2.02	0.41
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.55	0.41
1:A:843:GLN:HG2	1:A:847:LYS:C	2.41	0.41
1:D:379:MET:HB3	1:D:379:MET:HE3	1.46	0.41
1:C:363:HIS:HD2	5:C:9179:HOH:O	2.02	0.41
1:C:745:MET:CA	1:C:745:MET:CE	2.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.52	0.41
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.02	0.41
1:D:663:LEU:HD22	1:D:694:LEU:HD21	2.02	0.41
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.39	0.41
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.02	0.41
1:B:181:GLU:OE2	5:B:9427:HOH:O	2.22	0.41
1:D:599:ARG:HH11	1:D:599:ARG:HD2	1.66	0.41
1:D:878:HIS:HE1	5:D:9360:HOH:O	2.02	0.41
1:C:515:VAL:N	1:C:516:PRO:CD	2.83	0.41
1:B:531:ARG:HB3	1:B:532:PRO:HD2	2.01	0.41
1:C:472:TYR:OH	1:C:476:LYS:HE2	2.21	0.41
1:B:687:GLN:NE2	1:B:687:GLN:CA	2.83	0.41
1:B:777:LEU:HD23	1:B:777:LEU:HA	1.90	0.41
1:D:506:VAL:CG1	1:D:521:LYS:HE3	2.51	0.41
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.56	0.41
1:B:773:LYS:HD2	1:B:773:LYS:HA	1.68	0.41
1:B:85:VAL:CG1	1:B:86:VAL:N	2.82	0.41
1:C:753:ASN:OD1	1:C:753:ASN:N	2.52	0.41
1:C:577:LYS:HE3	1:C:577:LYS:HB3	1.91	0.41
1:A:964:GLN:O	1:A:968:MET:HB2	2.21	0.41
1:C:667:GLU:C	1:C:668:VAL:HG23	2.41	0.41
1:B:13:ARG:HD3	1:B:13:ARG:HA	1.78	0.41
1:A:764:PHE:CD1	1:A:781:ARG:NH1	2.89	0.41
1:A:708:TRP:CZ2	4:A:8403:DMS:H12	2.56	0.41
1:C:712:GLY:O	1:C:713:HIS:C	2.57	0.41
1:A:699:ARG:HH11	1:A:699:ARG:HD2	1.74	0.41
1:D:225:PHE:HA	1:D:243:GLU:O	2.21	0.41
1:B:681:GLU:H	1:B:681:GLU:HG2	1.67	0.41
1:C:1022:GLN:HE21	1:C:1022:GLN:HB3	1.57	0.41
1:D:843:GLN:HG3	1:D:848:THR:HA	2.02	0.40
1:B:1022:GLN:NE2	1:B:1023:LYS:O	2.52	0.40
1:B:654:TRP:O	1:B:665:SER:HB2	2.20	0.40
1:A:594:ASP:C	1:A:595:THR:HG22	2.41	0.40
1:B:807:VAL:HG13	1:B:808:GLU:N	2.35	0.40
1:A:359:HIS:N	1:A:367:MET:HE1	2.36	0.40
1:A:241:GLU:CD	1:A:292:ARG:NH2	2.74	0.40
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.56	0.40
1:B:37:ARG:HH12	4:B:8504:DMS:H23	1.86	0.40
1:D:733:ALA:O	1:D:735:HIS:ND1	2.53	0.40
1:D:367:MET:HE2	1:D:372:MET:HG3	2.03	0.40
1:A:952:ARG:NH2	1:A:1021:CYS:SG	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLN:NE2	1:A:682:LEU:HD12	2.36	0.40
1:D:687:GLN:HA	1:D:688:PRO:HD3	1.61	0.40
1:C:296:GLU:HG2	4:C:8601:DMS:H12	2.03	0.40
1:C:781:ARG:HG2	1:C:781:ARG:HH11	1.85	0.40
1:C:634:GLN:OE1	1:C:681:GLU:HG2	2.21	0.40
1:C:16:TRP:CD2	1:C:189:LEU:CD1	3.04	0.40
1:A:200:GLN:HG2	1:A:391:HIS:HB2	2.02	0.40
1:A:615:PRO:O	1:A:618:THR:HG22	2.22	0.40
1:B:46:ARG:HH11	1:B:46:ARG:HD2	1.78	0.40
1:B:114:VAL:HB	1:B:115:PRO:CD	2.51	0.40
1:C:100:TYR:CE2	1:C:602:CYS:HB3	2.56	0.40
1:B:133:TRP:CD1	4:B:8504:DMS:C1	3.04	0.40
1:C:584:PRO:O	4:C:8411:DMS:H22	2.21	0.40
1:C:654:TRP:NE1	1:C:666:GLY:HA3	2.35	0.40
1:A:575:LEU:HA	1:A:575:LEU:HD23	1.69	0.40
1:B:379:MET:CE	1:B:407:LEU:CD1	2.99	0.40
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.47	0.40
1:A:891:VAL:HG23	1:A:981:GLY:HA2	2.02	0.40
1:D:379:MET:HB2	1:D:379:MET:HE2	1.77	0.40
1:B:16:TRP:CD2	1:B:189:LEU:CD1	3.04	0.40
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.85	0.40
1:B:378:LEU:HA	1:B:378:LEU:HD23	1.96	0.40
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1006/1023 (98%)	972 (97%)	33 (3%)	1 (0%)	56 31
1	B	1005/1023 (98%)	962 (96%)	36 (4%)	7 (1%)	26 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	1003/1023 (98%)	968 (96%)	32 (3%)	3 (0%)	46 23
1	D	1004/1023 (98%)	961 (96%)	39 (4%)	4 (0%)	39 17
All	All	4018/4092 (98%)	3863 (96%)	140 (4%)	15 (0%)	39 17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	B	731	PRO
1	B	732	ALA
1	B	734	SER
1	D	688	PRO
1	C	734	SER
1	D	734	SER
1	A	688	PRO
1	B	688	PRO
1	B	733	ALA
1	D	164	ASP
1	B	164	ASP
1	C	687	GLN
1	C	732	ALA
1	D	683	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	863/875 (99%)	831 (96%)	32 (4%)	41 13
1	B	863/875 (99%)	821 (95%)	42 (5%)	31 8
1	C	861/875 (98%)	824 (96%)	37 (4%)	35 11
1	D	862/875 (98%)	819 (95%)	43 (5%)	30 7
All	All	3449/3500 (98%)	3295 (96%)	154 (4%)	34 10

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	117	GLU
1	A	130	ASP
1	A	250	LEU
1	A	277	GLU
1	A	333	ARG
1	A	362	LEU
1	A	370	GLN
1	A	377	LEU
1	A	394	ASN
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	595	THR
1	A	600	GLN
1	A	655	MET
1	A	684	GLU
1	A	685	LEU
1	A	735	HIS
1	A	737	ILE
1	A	755	ARG
1	A	773	LYS
1	A	800	ARG
1	A	817	GLN
1	A	829	THR
1	A	843	GLN
1	A	847	LYS
1	A	885	ASN
1	A	956	GLN
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	13	ARG
1	B	71	GLU
1	B	80	GLU
1	B	230	ARG
1	B	237	ARG
1	B	262	GLN
1	B	277	GLU
1	B	333	ARG
1	B	344	LEU
1	B	370	GLN
1	B	392	TYR

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Mol	Chain	Res	Type
1	B	394	ASN
1	B	546	LEU
1	B	554	GLN
1	B	595	THR
1	B	599	ARG
1	B	600	GLN
1	B	630	ARG
1	B	646	HIS
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	663	LEU
1	B	672	VAL
1	B	681	GLU
1	B	687	GLN
1	B	689	GLU
1	B	690	SER
1	B	730	LEU
1	B	734	SER
1	B	737	ILE
1	B	745	MET
1	B	766	SER
1	B	768	MET
1	B	773	LYS
1	B	800	ARG
1	B	804	ASN
1	B	847	LYS
1	B	890	GLN
1	B	917	ARG
1	B	1017	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	80	GLU
1	C	117	GLU
1	C	136	GLU
1	C	178	ARG
1	C	262	GLN
1	C	264	GLU
1	C	333	ARG
1	C	344	LEU
1	C	362	LEU
1	C	394	ASN

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Mol	Chain	Res	Type
1	C	437	SER
1	C	519	SER
1	C	535	LEU
1	C	546	LEU
1	C	595	THR
1	C	630	ARG
1	C	634	GLN
1	C	651	LEU
1	C	653	HIS
1	C	655	MET
1	C	663	LEU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	690	SER
1	C	699	ARG
1	C	730	LEU
1	C	737	ILE
1	C	745	MET
1	C	750	GLU
1	C	804	ASN
1	C	819	GLU
1	C	847	LYS
1	C	956	GLN
1	C	1022	GLN
1	C	1023	LYS
1	D	71	GLU
1	D	80	GLU
1	D	128	ASN
1	D	237	ARG
1	D	249	GLU
1	D	277	GLU
1	D	319	ASP
1	D	333	ARG
1	D	362	LEU
1	D	370	GLN
1	D	392	TYR
1	D	394	ASN
1	D	511	PRO
1	D	519	SER
1	D	546	LEU
1	D	580	GLU

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Mol	Chain	Res	Type
1	D	630	ARG
1	D	632	SER
1	D	651	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	681	GLU
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	772	ASP
1	D	817	GLN
1	D	829	THR
1	D	849	LEU
1	D	858	ILE
1	D	859	ASP
1	D	910	LEU
1	D	956	GLN
1	D	986	ILE
1	D	1018	LEU
1	D	1022	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	363	HIS
1	A	600	GLN
1	A	634	GLN
1	A	653	HIS
1	A	735	HIS
1	A	739	HIS
1	A	817	GLN
1	A	824	GLN
1	A	844	HIS
1	A	878	HIS

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Mol	Chain	Res	Type
1	B	262	GLN
1	B	363	HIS
1	B	554	GLN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	675	GLN
1	B	687	GLN
1	B	757	GLN
1	B	878	HIS
1	B	977	HIS
1	C	363	HIS
1	C	624	GLN
1	C	646	HIS
1	C	653	HIS
1	C	687	GLN
1	C	824	GLN
1	C	878	HIS
1	C	977	HIS
1	C	1022	GLN
1	D	128	ASN
1	D	135	GLN
1	D	163	GLN
1	D	624	GLN
1	D	628	GLN
1	D	634	GLN
1	D	704	ASN
1	D	761	GLN
1	D	824	GLN
1	D	878	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 113 ligands modelled in this entry, 28 are monoatomic - leaving 85 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	DMS	A	8401	-	3,3,3	1.18	0	3,3,3	0.51	0
4	DMS	A	8402	-	3,3,3	1.17	0	3,3,3	0.75	0
4	DMS	A	8403	-	3,3,3	1.73	1 (33%)	3,3,3	0.62	0
4	DMS	A	8404	-	3,3,3	1.43	1 (33%)	3,3,3	0.56	0
4	DMS	A	8405	-	3,3,3	1.27	1 (33%)	3,3,3	0.43	0
4	DMS	A	8406	-	3,3,3	1.70	1 (33%)	3,3,3	0.41	0
4	DMS	A	8408	-	3,3,3	0.53	0	3,3,3	0.34	0
4	DMS	A	8409	-	3,3,3	2.30	1 (33%)	3,3,3	0.50	0
4	DMS	A	8410	-	3,3,3	0.57	0	3,3,3	0.55	0
4	DMS	A	8411	-	3,3,3	1.46	0	3,3,3	0.48	0
4	DMS	A	8412	-	3,3,3	2.03	1 (33%)	3,3,3	0.44	0
4	DMS	A	8414	-	3,3,3	0.38	0	3,3,3	0.20	0
4	DMS	A	8416	-	3,3,3	1.96	2 (66%)	3,3,3	0.61	0
4	DMS	A	8417	-	3,3,3	0.97	0	3,3,3	0.79	0
4	DMS	A	8419	-	3,3,3	1.08	0	3,3,3	0.40	0
4	DMS	A	8421	-	3,3,3	0.96	0	3,3,3	0.77	0
4	DMS	A	8425	3	3,3,3	1.19	0	3,3,3	0.70	0
4	DMS	A	8501	-	3,3,3	0.75	0	3,3,3	0.43	0
4	DMS	A	8502	-	3,3,3	2.02	1 (33%)	3,3,3	0.99	0
4	DMS	A	8503	-	3,3,3	1.04	0	3,3,3	0.73	0
4	DMS	A	8504	-	3,3,3	0.88	0	3,3,3	0.41	0
4	DMS	A	8602	-	3,3,3	0.70	0	3,3,3	0.22	0
4	DMS	B	8401	-	3,3,3	0.95	0	3,3,3	0.41	0
4	DMS	B	8402	-	3,3,3	1.76	1 (33%)	3,3,3	1.26	1 (33%)
4	DMS	B	8403	-	3,3,3	1.09	0	3,3,3	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DMS	B	8404	-	3,3,3	0.96	0	3,3,3	0.51	0
4	DMS	B	8405	-	3,3,3	2.18	1 (33%)	3,3,3	0.27	0
4	DMS	B	8408	-	3,3,3	1.22	0	3,3,3	0.06	0
4	DMS	B	8409	-	3,3,3	2.63	1 (33%)	3,3,3	0.51	0
4	DMS	B	8411	-	3,3,3	0.54	0	3,3,3	0.81	0
4	DMS	B	8412	-	3,3,3	0.87	0	3,3,3	0.25	0
4	DMS	B	8414	-	3,3,3	0.96	0	3,3,3	0.39	0
4	DMS	B	8416	-	3,3,3	0.99	0	3,3,3	0.23	0
4	DMS	B	8417	-	3,3,3	0.80	0	3,3,3	0.51	0
4	DMS	B	8421	-	3,3,3	0.58	0	3,3,3	0.37	0
4	DMS	B	8425	3	3,3,3	1.11	0	3,3,3	0.40	0
4	DMS	B	8502	-	3,3,3	1.46	0	3,3,3	1.22	1 (33%)
4	DMS	B	8504	-	3,3,3	0.34	0	3,3,3	0.12	0
4	DMS	B	8508	-	3,3,3	2.00	1 (33%)	3,3,3	0.80	0
4	DMS	B	8601	-	3,3,3	2.41	1 (33%)	3,3,3	0.79	0
4	DMS	C	8401	-	3,3,3	1.69	1 (33%)	3,3,3	0.34	0
4	DMS	C	8402	-	3,3,3	2.16	1 (33%)	3,3,3	0.17	0
4	DMS	C	8403	-	3,3,3	1.40	1 (33%)	3,3,3	0.32	0
4	DMS	C	8404	-	3,3,3	1.26	0	3,3,3	1.10	0
4	DMS	C	8405	-	3,3,3	2.56	2 (66%)	3,3,3	0.26	0
4	DMS	C	8408	-	3,3,3	0.74	0	3,3,3	1.09	0
4	DMS	C	8409	-	3,3,3	2.11	1 (33%)	3,3,3	0.32	0
4	DMS	C	8410	-	3,3,3	0.67	0	3,3,3	0.16	0
4	DMS	C	8411	-	3,3,3	1.10	0	3,3,3	0.30	0
4	DMS	C	8412	-	3,3,3	1.19	0	3,3,3	1.37	1 (33%)
4	DMS	C	8413	-	3,3,3	0.70	0	3,3,3	0.29	0
4	DMS	C	8414	-	3,3,3	1.69	1 (33%)	3,3,3	1.18	0
4	DMS	C	8416	-	3,3,3	0.66	0	3,3,3	0.31	0
4	DMS	C	8417	-	3,3,3	0.26	0	3,3,3	0.41	0
4	DMS	C	8421	-	3,3,3	1.21	0	3,3,3	0.57	0
4	DMS	C	8425	3	3,3,3	1.02	0	3,3,3	0.12	0
4	DMS	C	8501	-	3,3,3	1.48	1 (33%)	3,3,3	0.76	0
4	DMS	C	8503	-	3,3,3	0.82	0	3,3,3	1.41	1 (33%)
4	DMS	C	8504	-	3,3,3	1.20	0	3,3,3	1.08	0
4	DMS	C	8601	-	3,3,3	0.64	0	3,3,3	0.52	0
4	DMS	C	8602	-	3,3,3	0.53	0	3,3,3	0.20	0
4	DMS	D	8401	-	3,3,3	1.62	1 (33%)	3,3,3	0.12	0
4	DMS	D	8402	-	3,3,3	1.33	0	3,3,3	0.22	0
4	DMS	D	8403	-	3,3,3	1.26	0	3,3,3	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DMS	D	8404	-	3,3,3	1.15	0	3,3,3	0.51	0
4	DMS	D	8405	-	3,3,3	0.78	0	3,3,3	0.47	0
4	DMS	D	8406	-	3,3,3	0.83	0	3,3,3	0.51	0
4	DMS	D	8408	-	3,3,3	1.28	0	3,3,3	0.26	0
4	DMS	D	8409	-	3,3,3	1.92	1 (33%)	3,3,3	1.38	1 (33%)
4	DMS	D	8410	-	3,3,3	1.88	1 (33%)	3,3,3	0.21	0
4	DMS	D	8411	-	3,3,3	1.33	0	3,3,3	0.22	0
4	DMS	D	8412	-	3,3,3	1.60	1 (33%)	3,3,3	0.53	0
4	DMS	D	8413	-	3,3,3	0.78	0	3,3,3	0.03	0
4	DMS	D	8414	-	3,3,3	0.39	0	3,3,3	0.54	0
4	DMS	D	8416	-	3,3,3	0.24	0	3,3,3	0.53	0
4	DMS	D	8417	-	3,3,3	0.44	0	3,3,3	0.21	0
4	DMS	D	8419	-	3,3,3	0.59	0	3,3,3	0.50	0
4	DMS	D	8421	-	3,3,3	0.32	0	3,3,3	0.48	0
4	DMS	D	8425	3	3,3,3	0.89	0	3,3,3	0.36	0
4	DMS	D	8501	-	3,3,3	0.83	0	3,3,3	0.36	0
4	DMS	D	8503	-	3,3,3	0.66	0	3,3,3	0.78	0
4	DMS	D	8508	-	3,3,3	1.36	0	3,3,3	0.89	0
4	DMS	D	8701	-	3,3,3	1.47	1 (33%)	3,3,3	0.45	0
4	DMS	D	8703	-	3,3,3	0.81	0	3,3,3	0.27	0
4	DMS	D	8705	-	3,3,3	1.87	1 (33%)	3,3,3	0.29	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8416	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	A	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8503	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8602	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8421	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	C	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8503	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8419	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	D	8501	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8503	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8508	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8705	-	-	0/0/0/0	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	8406	DMS	C2-S	-2.87	1.53	1.75
4	A	8416	DMS	O-S	-2.74	1.31	1.50
4	D	8705	DMS	C1-S	-2.58	1.55	1.75
4	C	8414	DMS	O-S	-2.22	1.34	1.50
4	C	8501	DMS	C1-S	-2.14	1.59	1.75
4	A	8404	DMS	O-S	-2.06	1.35	1.50
4	A	8416	DMS	C1-S	-2.01	1.60	1.75
4	D	8412	DMS	O-S	2.04	1.64	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8401	DMS	O-S	2.08	1.64	1.50
4	D	8701	DMS	C1-S	2.11	1.92	1.75
4	C	8405	DMS	C1-S	2.13	1.92	1.75
4	A	8405	DMS	O-S	2.18	1.65	1.50
4	D	8410	DMS	C2-S	2.27	1.93	1.75
4	C	8403	DMS	O-S	2.28	1.65	1.50
4	C	8401	DMS	C2-S	2.29	1.93	1.75
4	B	8402	DMS	C2-S	2.59	1.95	1.75
4	A	8403	DMS	C2-S	2.63	1.96	1.75
4	B	8508	DMS	C1-S	2.79	1.97	1.75
4	D	8409	DMS	O-S	2.84	1.69	1.50
4	A	8412	DMS	C1-S	2.93	1.98	1.75
4	C	8402	DMS	C2-S	3.07	1.99	1.75
4	A	8502	DMS	C1-S	3.21	2.00	1.75
4	A	8409	DMS	O-S	3.30	1.72	1.50
4	B	8405	DMS	O-S	3.47	1.74	1.50
4	C	8409	DMS	O-S	3.60	1.75	1.50
4	B	8601	DMS	C2-S	3.65	2.03	1.75
4	C	8405	DMS	O-S	3.86	1.76	1.50
4	B	8409	DMS	O-S	4.52	1.81	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	8502	DMS	C2-S-C1	2.10	109.32	98.46
4	B	8402	DMS	C2-S-C1	2.15	109.55	98.46
4	C	8412	DMS	C2-S-C1	2.33	110.50	98.46
4	D	8409	DMS	C2-S-C1	2.35	110.58	98.46
4	C	8503	DMS	C2-S-C1	2.38	110.74	98.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

33 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8403	DMS	1	0
4	A	8404	DMS	5	0
4	A	8410	DMS	3	0
4	A	8412	DMS	1	0
4	A	8416	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8425	DMS	2	0
4	A	8502	DMS	3	0
4	A	8503	DMS	1	0
4	A	8602	DMS	1	0
4	B	8403	DMS	1	0
4	B	8409	DMS	1	0
4	B	8411	DMS	1	0
4	B	8412	DMS	1	0
4	B	8504	DMS	2	0
4	B	8601	DMS	1	0
4	C	8402	DMS	1	0
4	C	8410	DMS	1	0
4	C	8411	DMS	1	0
4	C	8412	DMS	1	0
4	C	8413	DMS	1	0
4	C	8425	DMS	7	0
4	C	8503	DMS	2	0
4	C	8601	DMS	2	0
4	C	8602	DMS	1	0
4	D	8403	DMS	1	0
4	D	8406	DMS	1	0
4	D	8412	DMS	2	0
4	D	8417	DMS	1	0
4	D	8419	DMS	1	0
4	D	8421	DMS	2	0
4	D	8503	DMS	1	0
4	D	8703	DMS	5	0
4	D	8705	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	1010/1023 (98%)	-0.35	30 (2%)	54	51	9, 18, 47, 97	0
1	B	1009/1023 (98%)	-0.38	18 (1%)	71	70	9, 17, 44, 94	0
1	C	1007/1023 (98%)	-0.38	20 (1%)	68	67	8, 17, 45, 99	0
1	D	1008/1023 (98%)	-0.38	25 (2%)	61	58	9, 17, 46, 94	0
All	All	4034/4092 (98%)	-0.37	93 (2%)	64	62	8, 17, 45, 99	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	733	ALA	7.9
1	A	730	LEU	7.3
1	C	732	ALA	7.2
1	B	733	ALA	7.1
1	B	731	PRO	6.9
1	A	735	HIS	6.7
1	C	731	PRO	6.3
1	B	730	LEU	6.1
1	C	687	GLN	5.9
1	C	730	LEU	5.7
1	A	689	GLU	5.7
1	A	731	PRO	5.6
1	D	732	ALA	5.6
1	D	733	ALA	5.4
1	C	689	GLU	5.3
1	D	735	HIS	5.2
1	A	686	PRO	5.2
1	B	732	ALA	5.0
1	D	730	LEU	4.7
1	D	731	PRO	4.6
1	C	735	HIS	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	689	GLU	4.4
1	C	686	PRO	4.4
1	A	580	GLU	4.3
1	B	689	GLU	4.3
1	D	684	GLU	4.3
1	D	734	SER	4.2
1	C	685	LEU	4.1
1	A	798	ALA	4.1
1	A	687	GLN	4.1
1	A	732	ALA	4.0
1	A	733	ALA	4.0
1	D	686	PRO	3.9
1	D	687	GLN	3.8
1	D	771	GLY	3.8
1	A	801	ILE	3.8
1	B	735	HIS	3.7
1	B	687	GLN	3.6
1	B	686	PRO	3.6
1	A	685	LEU	3.5
1	B	685	LEU	3.4
1	C	684	GLU	3.4
1	D	580	GLU	3.4
1	D	76	CYS	3.3
1	A	795	VAL	3.2
1	A	729	THR	3.2
1	D	683	PRO	3.2
1	B	580	GLU	3.2
1	C	580	GLU	3.2
1	B	745	MET	3.1
1	A	734	SER	3.1
1	C	634	GLN	3.0
1	A	581	ASN	3.0
1	A	1023	LYS	3.0
1	A	688	PRO	3.0
1	D	845	GLN	3.0
1	B	801	ILE	3.0
1	A	800	ARG	2.9
1	D	688	PRO	2.9
1	D	736	ALA	2.9
1	B	684	GLU	2.9
1	D	581	ASN	2.9
1	B	734	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	685	LEU	2.7
1	A	582	GLY	2.6
1	C	736	ALA	2.6
1	D	737	ILE	2.6
1	B	583	ASN	2.5
1	D	634	GLN	2.5
1	D	801	ILE	2.4
1	B	581	ASN	2.4
1	A	736	ALA	2.3
1	C	803	PRO	2.3
1	D	582	GLY	2.3
1	C	761	GLN	2.3
1	D	772	ASP	2.3
1	B	663	LEU	2.2
1	C	830	LEU	2.2
1	C	582	GLY	2.2
1	A	737	ILE	2.2
1	A	583	ASN	2.2
1	A	71	GLU	2.2
1	B	582	GLY	2.2
1	A	684	GLU	2.2
1	C	729	THR	2.2
1	D	1023	LYS	2.2
1	A	79	PRO	2.1
1	A	845	GLN	2.1
1	A	690	SER	2.1
1	A	831	ALA	2.1
1	A	846	GLY	2.1
1	C	772	ASP	2.1
1	C	734	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
4	DMS	A	8419	4/4	0.91	0.19	6.81	65,67,69,100	0
4	DMS	C	8602	4/4	0.91	0.14	4.97	25,45,68,100	0
4	DMS	A	8404	4/4	0.94	0.10	4.89	19,26,41,49	0
4	DMS	D	8419	4/4	0.88	0.20	4.80	54,72,74,95	0
4	DMS	C	8425	4/4	0.96	0.21	4.63	44,50,66,88	0
4	DMS	B	8508	4/4	0.91	0.12	4.63	36,41,50,64	0
4	DMS	C	8403	4/4	0.99	0.12	4.46	16,21,24,30	0
4	DMS	C	8503	4/4	0.83	0.16	4.25	30,35,46,59	0
4	DMS	A	8417	4/4	0.94	0.12	4.06	26,26,68,100	0
4	DMS	A	8406	4/4	0.95	0.12	3.96	12,45,59,77	0
4	DMS	B	8417	4/4	0.91	0.16	3.89	31,39,48,62	0
4	DMS	B	8404	4/4	0.94	0.11	3.55	24,29,41,100	0
4	DMS	D	8404	4/4	0.97	0.09	3.54	22,27,43,76	0
4	DMS	C	8417	4/4	0.93	0.10	3.43	33,36,45,63	0
4	DMS	B	8502	4/4	0.96	0.10	2.94	22,27,37,41	0
2	MG	B	3001	1/1	1.00	0.08	2.93	14,14,14,14	0
4	DMS	A	8502	4/4	0.92	0.17	2.75	23,38,48,83	0
4	DMS	C	8501	4/4	0.95	0.10	2.47	27,31,39,56	0
4	DMS	C	8405	4/4	0.97	0.10	2.34	28,31,31,36	0
4	DMS	D	8508	4/4	0.93	0.11	2.31	39,47,52,59	0
4	DMS	D	8417	4/4	0.89	0.13	2.23	26,32,41,100	0
4	DMS	A	8408	4/4	0.97	0.10	2.20	21,34,39,80	0
2	MG	C	3001	1/1	1.00	0.09	2.17	15,15,15,15	0
4	DMS	D	8705	4/4	0.90	0.16	2.08	18,50,52,67	0
4	DMS	A	8412	4/4	0.96	0.14	2.07	28,33,41,100	0
4	DMS	B	8425	4/4	0.86	0.13	1.92	32,33,41,56	0
4	DMS	A	8401	4/4	0.99	0.10	1.91	12,15,15,17	0
4	DMS	D	8406	4/4	0.97	0.09	1.83	21,25,26,42	0
4	DMS	B	8408	4/4	0.98	0.11	1.79	33,34,35,100	0
4	DMS	B	8405	4/4	0.98	0.11	1.74	31,36,37,40	0
4	DMS	B	8504	4/4	0.97	0.09	1.67	30,33,44,82	0
3	NA	B	3104	1/1	0.96	0.12	1.67	33,33,33,33	0
4	DMS	C	8412	4/4	0.98	0.10	1.65	30,37,38,41	0
4	DMS	C	8408	4/4	0.97	0.09	1.60	26,28,34,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	DMS	A	8504	4/4	0.98	0.08	1.45	23,40,44,77	0
4	DMS	D	8403	4/4	0.98	0.07	1.29	21,26,28,31	0
4	DMS	B	8401	4/4	0.98	0.09	1.25	16,19,21,23	0
3	NA	D	3103	1/1	0.95	0.10	1.14	36,36,36,36	0
4	DMS	D	8411	4/4	0.98	0.11	1.08	31,33,34,100	0
4	DMS	C	8411	4/4	0.98	0.11	1.01	25,31,31,100	0
3	NA	A	3103	1/1	0.95	0.10	0.97	38,38,38,38	0
4	DMS	C	8404	4/4	0.97	0.07	0.89	17,23,30,37	0
3	NA	A	3104	1/1	0.97	0.09	0.83	29,29,29,29	0
4	DMS	D	8701	4/4	0.98	0.09	0.81	15,18,24,53	0
4	DMS	D	8501	4/4	0.93	0.08	0.77	25,33,43,59	0
4	DMS	D	8425	4/4	0.90	0.15	0.68	16,27,33,36	4
4	DMS	A	8425	4/4	0.93	0.14	0.67	29,37,46,51	0
4	DMS	B	8403	4/4	0.99	0.08	0.63	22,23,28,30	0
4	DMS	A	8411	4/4	0.97	0.10	0.60	25,34,36,44	0
3	NA	B	3101	1/1	0.97	0.07	0.55	17,17,17,17	0
3	NA	C	3104	1/1	0.96	0.08	0.50	28,28,28,28	0
3	NA	A	3101	1/1	0.99	0.07	0.44	23,23,23,23	0
4	DMS	A	8501	4/4	0.96	0.08	0.30	20,25,41,42	0
4	DMS	B	8411	4/4	0.99	0.10	0.27	33,34,34,46	0
3	NA	D	3104	1/1	0.91	0.09	0.27	35,35,35,35	0
4	DMS	D	8401	4/4	0.99	0.07	0.14	14,17,19,20	0
4	DMS	A	8403	4/4	0.99	0.06	0.08	21,23,28,29	0
3	NA	C	3103	1/1	0.99	0.08	0.00	27,27,27,27	0
3	NA	D	3101	1/1	0.97	0.07	-0.13	24,24,24,24	0
4	DMS	B	8402	4/4	0.98	0.06	-0.29	16,16,21,22	0
4	DMS	D	8405	4/4	0.99	0.06	-0.35	24,25,39,45	0
4	DMS	A	8405	4/4	0.99	0.06	-0.37	25,25,26,29	0
4	DMS	D	8412	4/4	0.99	0.06	-0.41	27,27,35,100	0
4	DMS	C	8402	4/4	0.99	0.05	-0.50	16,16,23,25	0
4	DMS	B	8412	4/4	0.98	0.06	-0.59	26,29,33,36	0
3	NA	C	3101	1/1	0.99	0.05	-0.95	18,18,18,18	0
3	NA	B	3103	1/1	0.98	0.07	-0.96	26,26,26,26	0
4	DMS	A	8402	4/4	0.99	0.05	-0.99	15,17,23,36	0
4	DMS	D	8402	4/4	0.99	0.05	-1.09	12,20,21,23	0
3	NA	B	3102	1/1	1.00	0.06	-1.12	13,13,13,13	0
4	DMS	C	8401	4/4	0.99	0.05	-1.59	14,15,19,20	0
3	NA	C	3102	1/1	0.99	0.05	-1.60	14,14,14,14	0
3	NA	A	3102	1/1	0.99	0.04	-1.71	12,12,12,12	0
2	MG	B	3002	1/1	0.99	0.04	-1.91	15,15,15,15	0
2	MG	A	3002	1/1	0.99	0.04	-2.10	17,17,17,17	0
4	DMS	D	8408	4/4	0.99	0.06	-2.14	18,30,35,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	MG	D	3001	1/1	0.99	0.03	-2.17	14,14,14,14	0
3	NA	D	3102	1/1	0.99	0.04	-2.59	12,12,12,12	0
2	MG	C	3002	1/1	0.99	0.03	-2.88	13,13,13,13	0
2	MG	A	3001	1/1	0.99	0.04	-3.05	17,17,17,17	0
2	MG	D	3002	1/1	0.99	0.03	-4.84	16,16,16,16	0
4	DMS	D	8414	4/4	0.96	0.15	-	33,50,100,100	0
4	DMS	B	8416	4/4	0.96	0.12	-	32,33,42,49	0
4	DMS	D	8703	4/4	0.90	0.19	-	37,58,59,100	0
4	DMS	C	8413	4/4	0.86	0.21	-	42,69,100,100	0
4	DMS	C	8416	4/4	0.96	0.25	-	44,51,52,100	0
4	DMS	C	8410	4/4	0.98	0.11	-	26,40,42,49	0
4	DMS	D	8413	4/4	0.88	0.16	-	28,56,73,100	0
4	DMS	C	8601	4/4	0.93	0.14	-	49,50,73,100	0
4	DMS	C	8409	4/4	0.95	0.08	-	29,30,33,36	0
4	DMS	A	8421	4/4	0.87	0.26	-	35,58,84,100	0
4	DMS	D	8409	4/4	0.92	0.11	-	24,33,33,40	0
4	DMS	D	8503	4/4	0.90	0.19	-	43,44,59,100	0
2	MG	D	3005	1/1	0.96	0.09	-	26,26,26,26	0
2	MG	C	3004	1/1	0.79	0.10	-	52,52,52,52	0
4	DMS	C	8414	4/4	0.95	0.11	-	23,25,34,42	0
2	MG	A	3005	1/1	0.74	0.12	-	42,42,42,42	0
4	DMS	A	8503	4/4	0.92	0.19	-	41,50,94,100	0
2	MG	C	3006	1/1	0.97	0.09	-	31,31,31,31	0
4	DMS	B	8414	4/4	0.98	0.13	-	25,36,42,46	0
4	DMS	A	8416	4/4	0.95	0.18	-	20,39,63,71	0
4	DMS	D	8421	4/4	0.92	0.20	-	42,61,71,100	0
4	DMS	B	8421	4/4	0.95	0.11	-	32,60,64,68	0
4	DMS	D	8410	4/4	0.96	0.10	-	40,52,57,60	0
4	DMS	A	8414	4/4	0.96	0.13	-	22,43,69,100	0
4	DMS	A	8602	4/4	0.98	0.15	-	35,49,98,100	0
4	DMS	B	8409	4/4	0.94	0.09	-	21,26,39,44	0
4	DMS	D	8416	4/4	0.90	0.16	-	25,43,52,77	0
4	DMS	A	8410	4/4	0.97	0.11	-	41,49,78,100	0
4	DMS	C	8504	4/4	0.81	0.14	-	36,68,72,73	0
4	DMS	A	8409	4/4	0.96	0.09	-	23,25,28,41	0
4	DMS	B	8601	4/4	0.95	0.13	-	33,36,39,39	0
4	DMS	C	8421	4/4	0.96	0.17	-	41,44,60,65	0

6.5 Other polymers

There are no such residues in this entry.