Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 09:03 AM EDT

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

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

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

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

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

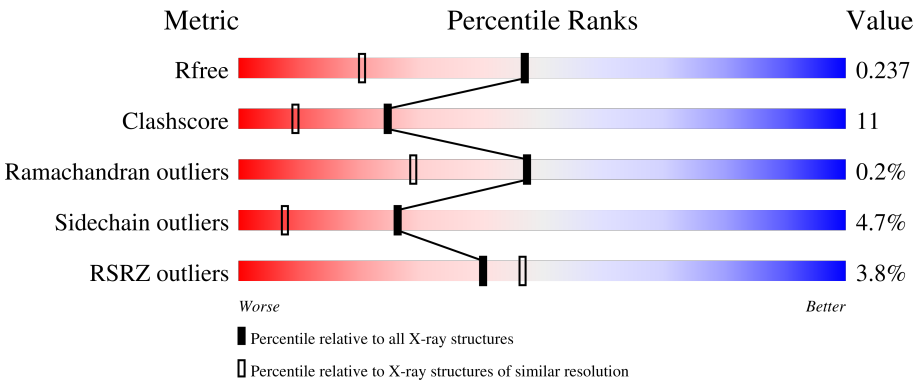
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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

Mol	Chain	Length	Quality of chain
1	A	1023	4% 68% 26%
1	B	1023	3% 67% 25% 6%
1	C	1023	3% 73% 22%
1	D	1023	4% 69% 26%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	B	8407	-	X	-	-
5	DMS	C	8506	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Beta-Galactosidase.

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

There are 32 discrepancies between the modelled and reference sequences:

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

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

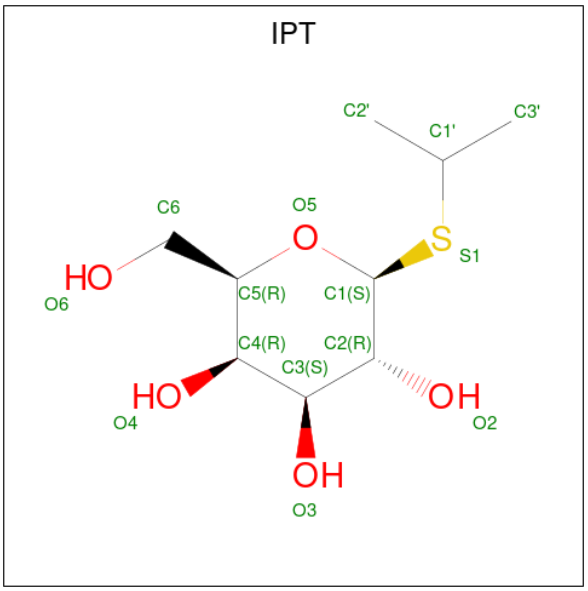
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

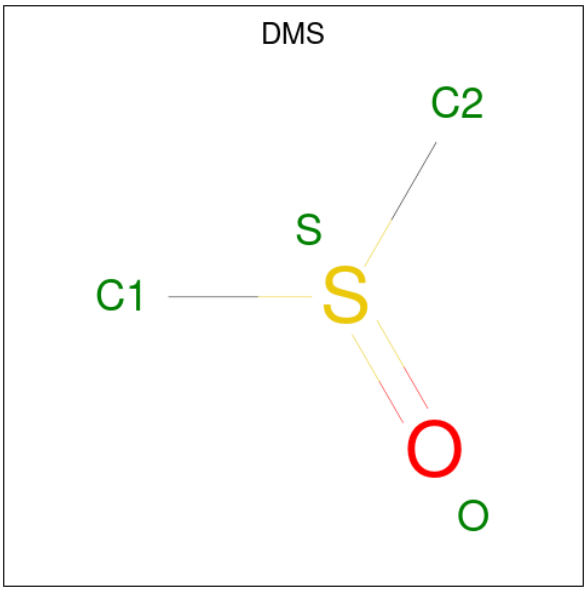
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Na 3 3	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	3	Total Na 3 3	0	0

- Molecule 4 is 1-methylethyl 1-thio-beta-D-galactopyranoside (three-letter code: IPT) (formula: $C_9H_{18}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	15	9	5	1	0	0
			Total	C	O	S		
4	A	1	15	9	5	1	0	0
			Total	C	O	S		
4	B	1	15	9	5	1	0	0
			Total	C	O	S		
4	C	1	15	9	5	1	0	0
			Total	C	O	S		
4	D	1	15	9	5	1	0	0
			Total	C	O	S		
4	D	1	15	9	5	1	0	0

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



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

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

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	865	865	865	0	0

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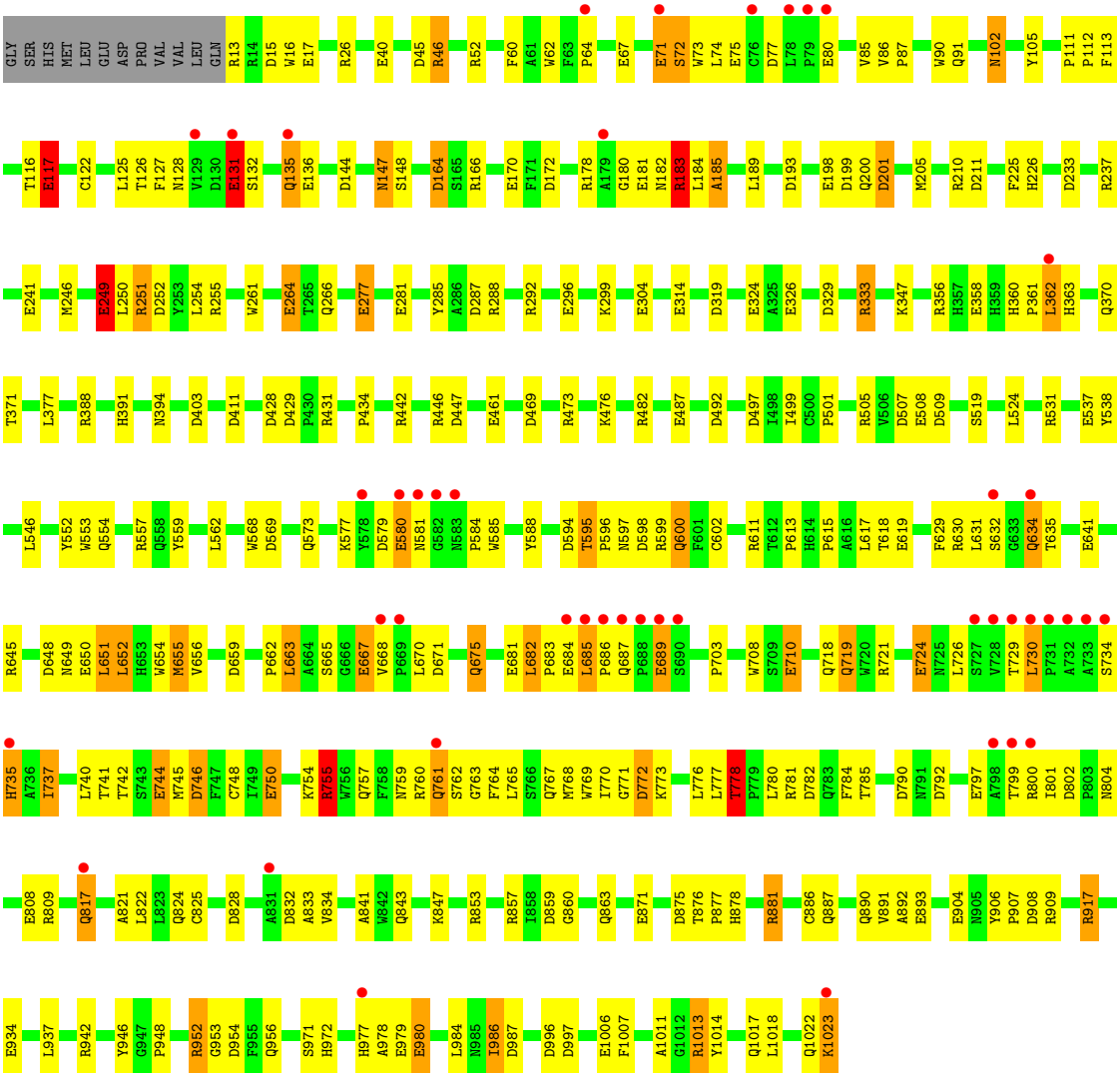
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	B	935	935	935	0	0
			Total	O		
6	C	922	922	922	0	0
			Total	O		
6	D	885	885	885	0	0

3 Residue-property plots (i)

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

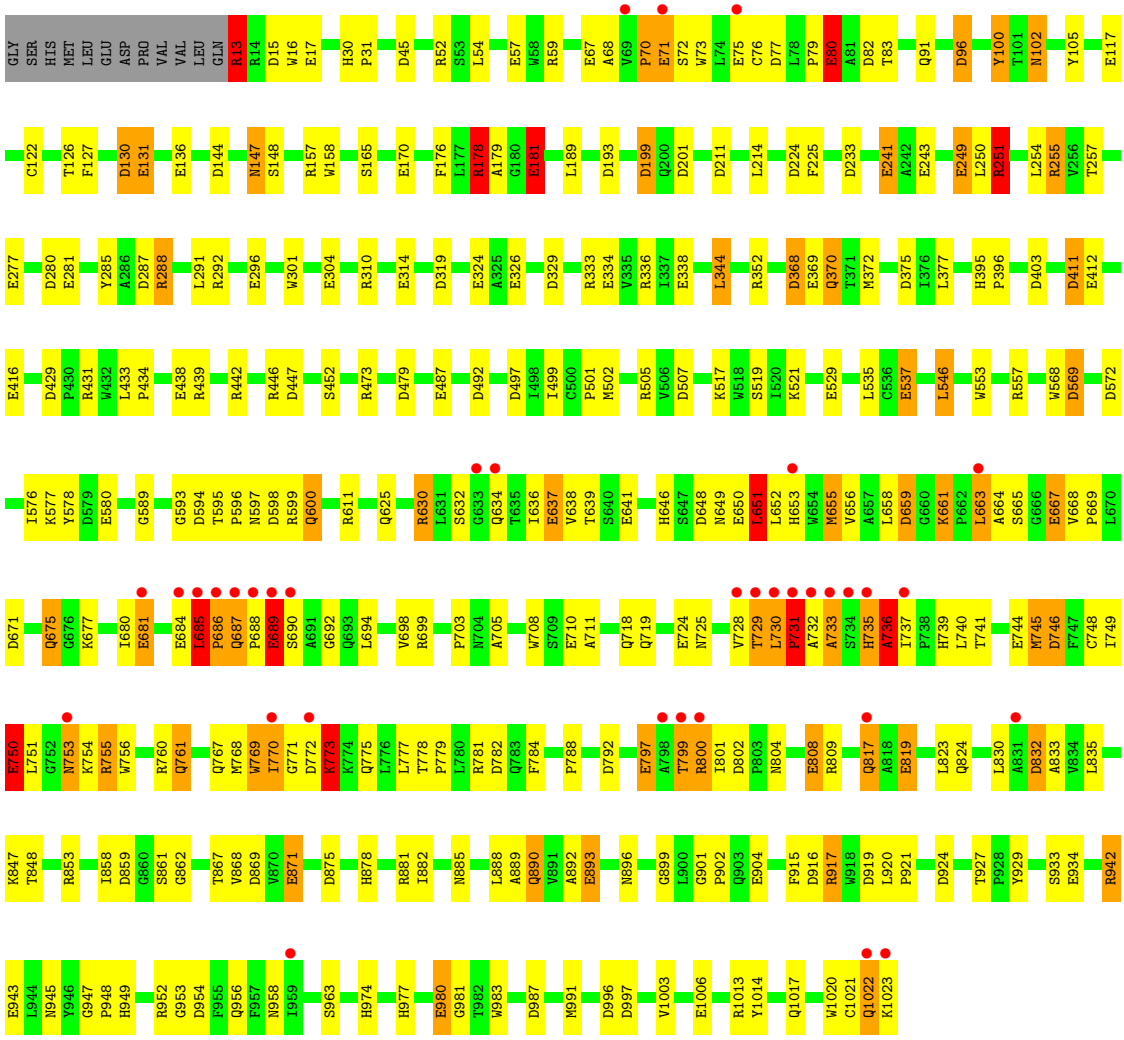
• Molecule 1: Beta-Galactosidase

Chain A:



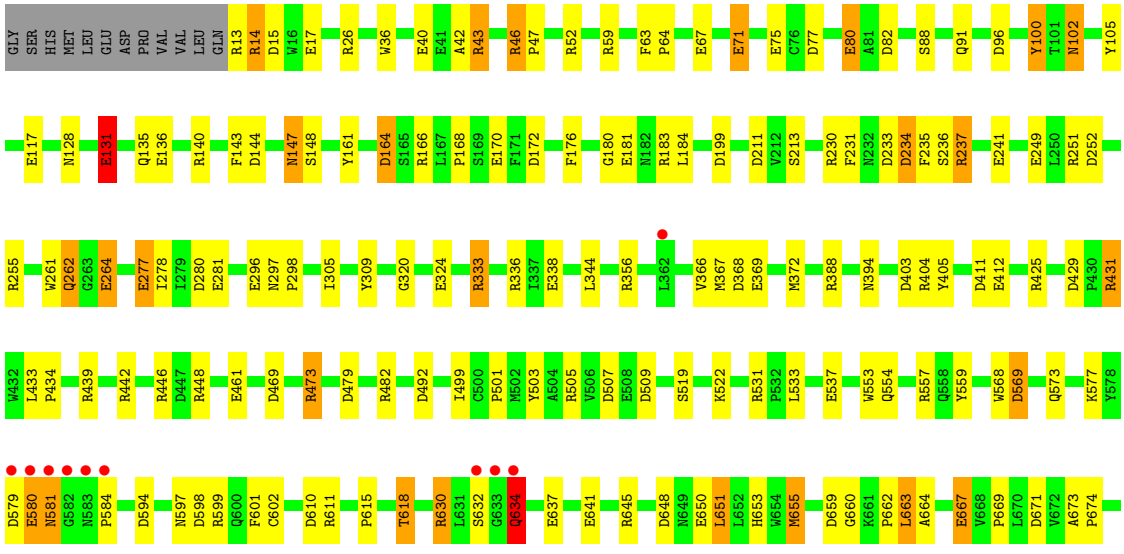
• Molecule 1: Beta-Galactosidase

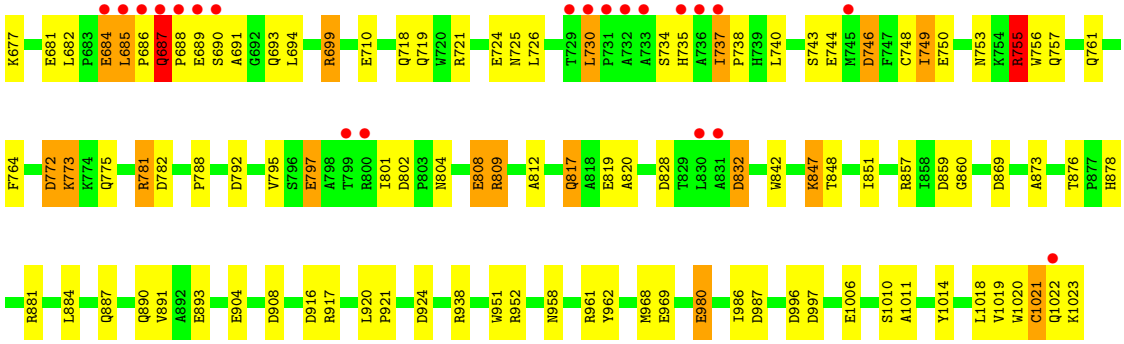
Chain B:



• Molecule 1: Beta-Galactosidase

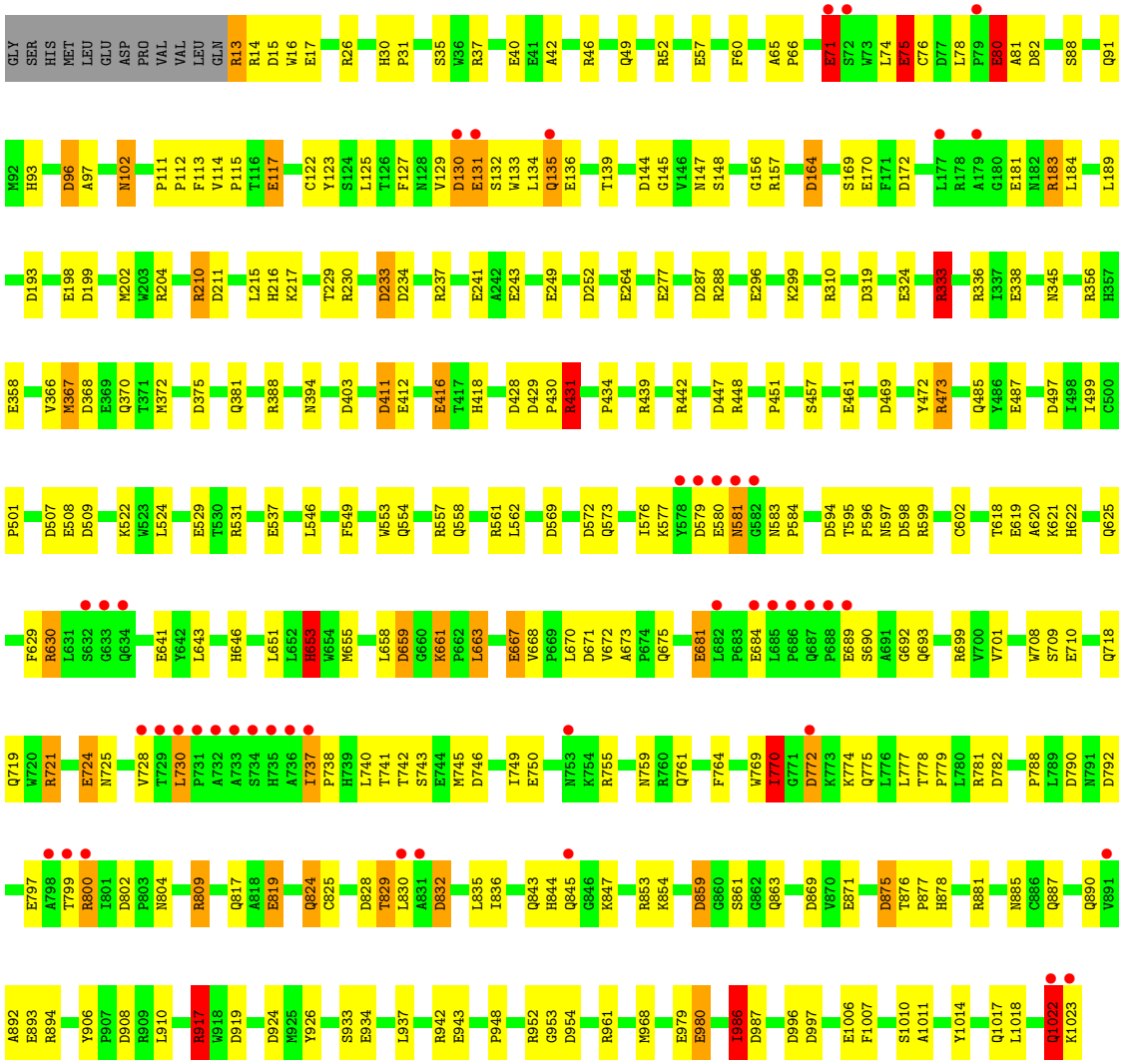
Chain C:





- Molecule 1: Beta-Galactosidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	151.77Å 161.19Å 202.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.00 – 1.75 17.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	89.6 (27.00-1.75) 89.7 (17.00-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.75Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.168 , 0.244 0.172 , 0.237	Depositor DCC
R_{free} test set	6397 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 98.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	36516	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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 37.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0575e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	1.03	45/8367 (0.5%)	1.57	134/11415 (1.2%)
1	B	1.06	51/8367 (0.6%)	1.56	154/11415 (1.3%)
1	C	1.06	41/8367 (0.5%)	1.59	137/11415 (1.2%)
1	D	1.03	46/8367 (0.5%)	1.56	152/11415 (1.3%)
All	All	1.04	183/33468 (0.5%)	1.57	577/45660 (1.3%)

All (183) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	GLU	CD-OE2	9.35	1.35	1.25
1	D	40	GLU	CD-OE2	8.65	1.35	1.25
1	C	684	GLU	CD-OE2	8.60	1.35	1.25
1	A	358	GLU	CD-OE2	8.38	1.34	1.25
1	C	338	GLU	CD-OE2	8.26	1.34	1.25
1	B	684	GLU	CD-OE2	8.16	1.34	1.25
1	C	1006	GLU	CD-OE2	7.99	1.34	1.25
1	C	296	GLU	CD-OE2	7.74	1.34	1.25
1	D	71	GLU	CD-OE2	7.55	1.33	1.25
1	C	324	GLU	CD-OE2	7.48	1.33	1.25
1	B	136	GLU	CD-OE2	7.39	1.33	1.25
1	A	131	GLU	CD-OE2	7.39	1.33	1.25
1	D	980	GLU	CD-OE2	7.39	1.33	1.25
1	D	684	GLU	CD-OE2	7.33	1.33	1.25
1	B	529	GLU	CD-OE2	7.28	1.33	1.25
1	C	689	GLU	CD-OE2	7.24	1.33	1.25
1	B	641	GLU	CD-OE1	-7.24	1.17	1.25
1	A	667	GLU	CD-OE2	7.21	1.33	1.25
1	B	181	GLU	CD-OE2	7.19	1.33	1.25
1	B	71	GLU	CD-OE2	7.15	1.33	1.25
1	A	684	GLU	CD-OE2	7.12	1.33	1.25
1	B	681	GLU	CD-OE2	7.10	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	131	GLU	CD-OE2	7.07	1.33	1.25
1	C	980	GLU	CD-OE2	7.07	1.33	1.25
1	D	487	GLU	CD-OE2	7.06	1.33	1.25
1	A	71	GLU	CD-OE2	7.05	1.33	1.25
1	B	689	GLU	CD-OE2	7.02	1.33	1.25
1	D	117	GLU	CD-OE2	7.01	1.33	1.25
1	B	241	GLU	CD-OE2	7.01	1.33	1.25
1	D	537	GLU	CD-OE2	6.99	1.33	1.25
1	B	304	GLU	CD-OE2	6.98	1.33	1.25
1	D	1006	GLU	CD-OE2	6.92	1.33	1.25
1	B	819	GLU	CD-OE2	6.91	1.33	1.25
1	C	277	GLU	CD-OE2	6.89	1.33	1.25
1	C	750	GLU	CD-OE2	6.87	1.33	1.25
1	D	819	GLU	CD-OE2	6.85	1.33	1.25
1	D	580	GLU	CD-OE2	6.85	1.33	1.25
1	A	744	GLU	CD-OE2	6.83	1.33	1.25
1	C	281	GLU	CD-OE2	6.81	1.33	1.25
1	A	487	GLU	CD-OE2	6.79	1.33	1.25
1	A	508	GLU	CD-OE2	6.78	1.33	1.25
1	D	529	GLU	CD-OE2	6.78	1.33	1.25
1	D	170	GLU	CD-OE2	6.72	1.33	1.25
1	B	667	GLU	CD-OE2	6.72	1.33	1.25
1	A	537	GLU	CD-OE2	6.71	1.33	1.25
1	A	979	GLU	CD-OE2	6.70	1.33	1.25
1	D	412	GLU	CD-OE2	6.67	1.32	1.25
1	B	17	GLU	CD-OE2	6.65	1.32	1.25
1	B	537	GLU	CD-OE2	6.64	1.32	1.25
1	A	75	GLU	CD-OE2	6.63	1.32	1.25
1	C	744	GLU	CD-OE2	6.61	1.32	1.25
1	D	724	GLU	CD-OE2	6.57	1.32	1.25
1	B	710	GLU	CD-OE2	6.56	1.32	1.25
1	C	170	GLU	CD-OE2	6.55	1.32	1.25
1	D	619	GLU	CD-OE2	6.55	1.32	1.25
1	A	580	GLU	CD-OE2	6.55	1.32	1.25
1	A	710	GLU	CD-OE2	6.54	1.32	1.25
1	B	580	GLU	CD-OE2	6.49	1.32	1.25
1	C	412	GLU	CD-OE2	6.49	1.32	1.25
1	D	296	GLU	CD-OE2	6.49	1.32	1.25
1	B	326	GLU	CD-OE2	6.46	1.32	1.25
1	B	744	GLU	CD-OE2	6.45	1.32	1.25
1	A	650	GLU	CD-OE2	6.45	1.32	1.25
1	D	75	GLU	CD-OE2	6.43	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	681	GLU	CD-OE2	6.42	1.32	1.25
1	A	181	GLU	CD-OE2	6.42	1.32	1.25
1	A	17	GLU	CD-OE2	6.41	1.32	1.25
1	A	681	GLU	CD-OE2	6.41	1.32	1.25
1	A	296	GLU	CD-OE2	6.40	1.32	1.25
1	A	136	GLU	CD-OE2	6.39	1.32	1.25
1	D	131	GLU	CD-OE2	6.37	1.32	1.25
1	D	750	GLU	CD-OE2	6.36	1.32	1.25
1	C	808	GLU	CD-OE2	6.34	1.32	1.25
1	D	241	GLU	CD-OE2	6.32	1.32	1.25
1	A	249	GLU	CD-OE2	6.31	1.32	1.25
1	C	580	GLU	CD-OE2	6.30	1.32	1.25
1	B	412	GLU	CD-OE2	6.29	1.32	1.25
1	C	819	GLU	CD-OE2	6.29	1.32	1.25
1	D	277	GLU	CD-OE2	6.29	1.32	1.25
1	D	358	GLU	CD-OE2	6.25	1.32	1.25
1	B	369	GLU	CD-OE2	6.24	1.32	1.25
1	A	980	GLU	CD-OE2	6.22	1.32	1.25
1	B	131	GLU	CD-OE2	6.21	1.32	1.25
1	B	1006	GLU	CD-OE2	6.21	1.32	1.25
1	D	416	GLU	CD-OE2	6.20	1.32	1.25
1	C	797	GLU	CD-OE2	6.20	1.32	1.25
1	A	797	GLU	CD-OE2	6.20	1.32	1.25
1	C	264	GLU	CD-OE2	6.19	1.32	1.25
1	D	689	GLU	CD-OE2	6.18	1.32	1.25
1	A	117	GLU	CD-OE2	6.17	1.32	1.25
1	A	619	GLU	CD-OE2	6.17	1.32	1.25
1	B	893	GLU	CD-OE2	6.17	1.32	1.25
1	B	281	GLU	CD-OE2	6.17	1.32	1.25
1	C	75	GLU	CD-OE2	6.16	1.32	1.25
1	A	170	GLU	CD-OE2	6.16	1.32	1.25
1	A	40	GLU	CD-OE2	6.15	1.32	1.25
1	A	277	GLU	CD-OE2	6.10	1.32	1.25
1	D	943	GLU	CD-OE2	6.10	1.32	1.25
1	A	304	GLU	CD-OE2	6.08	1.32	1.25
1	C	136	GLU	CD-OE2	6.06	1.32	1.25
1	A	689	GLU	CD-OE2	6.04	1.32	1.25
1	B	980	GLU	CD-OE2	6.04	1.32	1.25
1	C	17	GLU	CD-OE2	6.04	1.32	1.25
1	C	80	GLU	CD-OE2	6.02	1.32	1.25
1	C	117	GLU	CD-OE2	6.02	1.32	1.25
1	D	667	GLU	CD-OE2	5.99	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	181	GLU	CD-OE2	5.98	1.32	1.25
1	C	537	GLU	CD-OE2	5.97	1.32	1.25
1	B	80	GLU	CD-OE2	5.95	1.32	1.25
1	B	904	GLU	CD-OE2	5.95	1.32	1.25
1	B	277	GLU	CD-OE2	5.93	1.32	1.25
1	B	117	GLU	CD-OE2	5.93	1.32	1.25
1	B	650	GLU	CD-OE2	5.92	1.32	1.25
1	A	324	GLU	CD-OE2	5.89	1.32	1.25
1	D	249	GLU	CD-OE2	5.89	1.32	1.25
1	D	797	GLU	CD-OE2	5.88	1.32	1.25
1	C	710	GLU	CD-OE2	5.87	1.32	1.25
1	D	338	GLU	CD-OE2	5.86	1.32	1.25
1	B	67	GLU	CD-OE2	5.83	1.32	1.25
1	B	296	GLU	CD-OE2	5.83	1.32	1.25
1	C	904	GLU	CD-OE2	5.82	1.32	1.25
1	D	80	GLU	CD-OE2	5.82	1.32	1.25
1	D	681	GLU	CD-OE2	5.81	1.32	1.25
1	B	416	GLU	CD-OE2	5.81	1.32	1.25
1	A	934	GLU	CD-OE2	5.79	1.32	1.25
1	B	750	GLU	CD-OE2	5.79	1.32	1.25
1	B	438	GLU	CD-OE2	5.78	1.32	1.25
1	A	461	GLU	CD-OE2	5.77	1.31	1.25
1	A	750	GLU	CD-OE2	5.77	1.31	1.25
1	D	57	GLU	CD-OE2	5.76	1.31	1.25
1	D	264	GLU	CD-OE2	5.75	1.31	1.25
1	B	249	GLU	CD-OE2	5.75	1.31	1.25
1	C	969	GLU	CD-OE2	5.74	1.31	1.25
1	B	314	GLU	CD-OE1	-5.74	1.19	1.25
1	C	71	GLU	CD-OE2	5.73	1.31	1.25
1	B	324	GLU	CD-OE2	5.71	1.31	1.25
1	D	979	GLU	CD-OE2	5.68	1.31	1.25
1	B	338	GLU	CD-OE2	5.67	1.31	1.25
1	C	893	GLU	CD-OE2	5.67	1.31	1.25
1	A	198	GLU	CD-OE2	5.67	1.31	1.25
1	D	710	GLU	CD-OE2	5.66	1.31	1.25
1	B	943	GLU	CD-OE2	5.65	1.31	1.25
1	D	871	GLU	CD-OE2	5.65	1.31	1.25
1	D	893	GLU	CD-OE2	5.63	1.31	1.25
1	A	326	GLU	CD-OE2	5.62	1.31	1.25
1	B	334	GLU	CD-OE2	5.61	1.31	1.25
1	B	57	GLU	CD-OE2	5.61	1.31	1.25
1	D	136	GLU	CD-OE2	5.61	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	904	GLU	CD-OE2	5.58	1.31	1.25
1	C	67	GLU	CD-OE2	5.57	1.31	1.25
1	A	724	GLU	CD-OE2	5.56	1.31	1.25
1	C	667	GLU	CD-OE2	5.52	1.31	1.25
1	A	871	GLU	CD-OE2	5.51	1.31	1.25
1	D	17	GLU	CD-OE2	5.50	1.31	1.25
1	D	198	GLU	CD-OE2	5.47	1.31	1.25
1	C	641	GLU	CD-OE1	-5.45	1.19	1.25
1	C	650	GLU	CD-OE2	5.45	1.31	1.25
1	C	241	GLU	CD-OE2	5.44	1.31	1.25
1	C	249	GLU	CD-OE2	5.44	1.31	1.25
1	B	75	GLU	CD-OE2	5.44	1.31	1.25
1	D	641	GLU	CD-OE1	-5.44	1.19	1.25
1	A	893	GLU	CD-OE2	5.42	1.31	1.25
1	A	264	GLU	CD-OE2	5.41	1.31	1.25
1	D	324	GLU	CD-OE2	5.40	1.31	1.25
1	A	67	GLU	CD-OE2	5.34	1.31	1.25
1	A	314	GLU	CD-OE2	5.33	1.31	1.25
1	B	170	GLU	CD-OE2	5.25	1.31	1.25
1	C	181	GLU	CD-OE2	5.24	1.31	1.25
1	B	416	GLU	CD-OE1	-5.24	1.19	1.25
1	B	797	GLU	CD-OE2	5.23	1.31	1.25
1	B	637	GLU	CD-OE2	5.19	1.31	1.25
1	C	461	GLU	CD-OE2	5.19	1.31	1.25
1	A	80	GLU	CD-OE2	5.17	1.31	1.25
1	D	243	GLU	CD-OE2	5.15	1.31	1.25
1	D	508	GLU	CD-OE2	5.13	1.31	1.25
1	A	641	GLU	CD-OE1	-5.11	1.20	1.25
1	D	461	GLU	CD-OE1	-5.10	1.20	1.25
1	B	487	GLU	CD-OE2	5.09	1.31	1.25
1	A	281	GLU	CD-OE2	5.08	1.31	1.25
1	B	871	GLU	CD-OE2	5.06	1.31	1.25
1	C	369	GLU	CD-OE2	5.06	1.31	1.25
1	B	808	GLU	CD-OE1	-5.04	1.20	1.25
1	B	724	GLU	CD-OE2	5.01	1.31	1.25

All (577) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	630	ARG	NE-CZ-NH1	13.65	127.12	120.30
1	A	442	ARG	NE-CZ-NH2	-13.52	113.54	120.30
1	C	442	ARG	NE-CZ-NH2	-12.71	113.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	442	ARG	NE-CZ-NH1	12.61	126.61	120.30
1	A	772	ASP	CB-CG-OD2	-12.61	106.95	118.30
1	B	442	ARG	NE-CZ-NH2	-12.53	114.04	120.30
1	A	442	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	C	439	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	D	144	ASP	CB-CG-OD1	11.51	128.66	118.30
1	B	442	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	C	924	ASP	CB-CG-OD2	-11.26	108.17	118.30
1	A	13	ARG	NE-CZ-NH1	11.15	125.88	120.30
1	D	336	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	C	507	ASP	CB-CG-OD2	-11.00	108.40	118.30
1	C	333	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	C	531	ARG	NE-CZ-NH2	-10.67	114.96	120.30
1	C	881	ARG	NE-CZ-NH1	10.63	125.62	120.30
1	A	183	ARG	NE-CZ-NH1	10.49	125.55	120.30
1	A	428	ASP	CB-CG-OD1	10.39	127.65	118.30
1	D	594	ASP	CB-CG-OD2	-10.35	108.98	118.30
1	A	255	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	531	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	B	869	ASP	CB-CG-OD1	10.17	127.45	118.30
1	A	45	ASP	CB-CG-OD1	10.12	127.41	118.30
1	B	648	ASP	CB-CG-OD2	-10.05	109.26	118.30
1	A	193	ASP	CB-CG-OD2	-10.04	109.26	118.30
1	C	952	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	760	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	C	630	ARG	NE-CZ-NH2	-9.92	115.34	120.30
1	B	772	ASP	CB-CG-OD1	9.85	127.17	118.30
1	B	310	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	C	439	ARG	NE-CZ-NH2	-9.76	115.42	120.30
1	A	233	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	C	77	ASP	CB-CG-OD1	9.70	127.03	118.30
1	B	942	ARG	NE-CZ-NH1	9.68	125.14	120.30
1	C	411	ASP	CB-CG-OD1	9.68	127.01	118.30
1	C	356	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	A	996	ASP	CB-CG-OD2	-9.59	109.67	118.30
1	A	772	ASP	CB-CG-OD1	9.53	126.88	118.30
1	B	233	ASP	CB-CG-OD2	-9.51	109.75	118.30
1	C	557	ARG	NE-CZ-NH2	-9.48	115.56	120.30
1	B	201	ASP	CB-CG-OD2	-9.45	109.79	118.30
1	D	144	ASP	CB-CG-OD2	-9.42	109.83	118.30
1	D	204	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	A	287	ASP	CB-CG-OD1	9.33	126.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	594	ASP	CB-CG-OD1	9.30	126.67	118.30
1	B	952	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	C	482	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	D	96	ASP	CB-CG-OD2	-9.24	109.98	118.30
1	D	809	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	A	881	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	594	ASP	CB-CG-OD1	9.22	126.60	118.30
1	D	37	ARG	NE-CZ-NH1	-9.21	115.70	120.30
1	D	439	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	D	46	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	172	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	B	869	ASP	CB-CG-OD2	-9.09	110.12	118.30
1	D	428	ASP	CB-CG-OD1	9.08	126.47	118.30
1	D	82	ASP	CB-CG-OD2	-9.02	110.19	118.30
1	A	469	ASP	CB-CG-OD1	8.98	126.38	118.30
1	C	772	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	A	802	ASP	CB-CG-OD2	-8.78	110.40	118.30
1	C	809	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	D	792	ASP	CB-CG-OD1	8.78	126.20	118.30
1	B	431	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	C	140	ARG	NE-CZ-NH2	-8.76	115.92	120.30
1	C	46	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	D	288	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	D	233	ASP	CB-CG-OD1	8.60	126.04	118.30
1	B	336	ARG	NE-CZ-NH1	8.55	124.58	120.30
1	D	699	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	760	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	C	166	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	C	469	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	B	611	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	D	356	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	D	792	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	B	288	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	A	233	ASP	CB-CG-OD1	8.43	125.89	118.30
1	C	507	ASP	CB-CG-OD1	8.43	125.89	118.30
1	C	917	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	B	924	ASP	CB-CG-OD2	-8.43	110.71	118.30
1	D	82	ASP	CB-CG-OD1	8.42	125.88	118.30
1	D	598	ASP	CB-CG-OD1	8.42	125.88	118.30
1	B	233	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	952	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	A	287	ASP	CB-CG-OD2	-8.34	110.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	881	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	D	13	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	594	ASP	CB-CG-OD1	8.25	125.72	118.30
1	C	594	ASP	CB-CG-OD2	-8.23	110.89	118.30
1	A	557	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	429	ASP	CB-CG-OD1	8.22	125.70	118.30
1	D	164	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	D	46	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	C	166	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	A	809	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	319	ASP	CB-CG-OD1	8.14	125.62	118.30
1	D	987	ASP	CB-CG-OD1	8.10	125.59	118.30
1	C	598	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	D	782	ASP	CB-CG-OD1	8.08	125.58	118.30
1	B	201	ASP	CB-CG-OD1	7.95	125.46	118.30
1	B	997	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	D	130	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	D	310	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	B	875	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	D	924	ASP	CB-CG-OD2	-7.89	111.19	118.30
1	D	234	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	C	446	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	C	924	ASP	CB-CG-OD1	7.87	125.38	118.30
1	A	996	ASP	CB-CG-OD1	7.86	125.38	118.30
1	B	671	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	A	15	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	B	859	ASP	CB-CG-OD1	7.78	125.30	118.30
1	C	755	ARG	NE-CZ-NH1	7.78	124.19	120.30
1	B	755	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	D	671	ASP	CB-CG-OD1	7.75	125.28	118.30
1	B	224	ASP	CB-CG-OD1	7.74	125.26	118.30
1	B	952	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	D	287	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	987	ASP	CB-CG-OD1	7.66	125.19	118.30
1	B	52	ARG	CB-CA-C	-7.66	95.09	110.40
1	C	411	ASP	CB-CG-OD2	-7.66	111.41	118.30
1	D	439	ARG	NE-CZ-NH1	7.65	124.12	120.30
1	D	853	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	B	997	ASP	N-CA-CB	7.63	124.33	110.60
1	B	1013	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	C	52	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	C	952	ARG	NE-CZ-NH1	7.61	124.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	336	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	699	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	A	211	ASP	CB-CG-OD1	7.54	125.08	118.30
1	B	255	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	B	632	SER	N-CA-CB	7.51	121.77	110.50
1	B	375	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	C	802	ASP	CB-CG-OD1	7.49	125.04	118.30
1	C	368	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	A	446	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	C	598	ASP	CB-CG-OD1	7.47	125.02	118.30
1	A	429	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	D	996	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	D	469	ASP	CB-CG-OD1	7.44	125.00	118.30
1	D	442	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	D	429	ASP	CB-CG-OD1	7.44	124.99	118.30
1	C	59	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	D	388	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	428	ASP	CB-CG-OD2	-7.41	111.64	118.30
1	C	425	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	D	721	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	C	431	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	A	505	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	D	130	ASP	CB-CG-OD1	7.38	124.95	118.30
1	C	569	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	B	96	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	D	924	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	594	ASP	CB-CG-OD1	7.32	124.89	118.30
1	C	531	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	B	1013	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	A	252	ASP	CB-CG-OD2	-7.30	111.73	118.30
1	B	473	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	D	431	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	782	ASP	CB-CG-OD1	7.26	124.83	118.30
1	C	233	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	832	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	C	161	TYR	CB-CG-CD1	-7.24	116.66	121.00
1	B	996	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	859	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	B	859	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	B	630	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	C	368	ASP	CB-CG-OD1	7.21	124.79	118.30
1	C	144	ASP	CB-CG-OD1	7.21	124.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	772	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	D	375	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	800	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	517	LYS	N-CA-CB	7.19	123.55	110.60
1	B	997	ASP	CB-CG-OD1	7.19	124.77	118.30
1	C	336	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	D	671	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	A	46	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	C	183	ARG	NE-CZ-NH1	-7.11	116.74	120.30
1	A	859	ASP	CB-CG-OD1	7.11	124.70	118.30
1	A	482	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	13	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	C	469	ASP	CB-CG-OD1	7.09	124.68	118.30
1	C	233	ASP	CB-CG-OD2	-7.08	111.92	118.30
1	D	772	ASP	CB-CG-OD1	7.08	124.67	118.30
1	D	356	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	B	772	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	B	853	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	B	130	ASP	CB-CG-OD2	-7.06	111.95	118.30
1	B	919	ASP	CB-CG-OD1	7.05	124.64	118.30
1	C	164	ASP	CB-CG-OD1	7.05	124.64	118.30
1	D	919	ASP	CB-CG-OD1	7.05	124.64	118.30
1	C	997	ASP	N-CA-CB	7.04	123.28	110.60
1	B	211	ASP	CB-CG-OD1	7.04	124.64	118.30
1	C	553	TRP	CA-CB-CG	-7.04	100.32	113.70
1	A	255	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	13	ARG	CD-NE-CZ	7.04	133.45	123.60
1	B	13	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	15	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	916	ASP	CB-CG-OD1	7.00	124.60	118.30
1	D	319	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	721	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	C	255	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	659	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	C	746	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	B	507	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	D	233	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	C	792	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	193	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	15	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	482	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	375	ASP	CB-CG-OD1	6.87	124.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	917	ARG	CD-NE-CZ	-6.87	113.98	123.60
1	C	859	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	771	GLY	N-CA-C	-6.85	95.97	113.10
1	B	648	ASP	CB-CG-OD1	6.85	124.47	118.30
1	C	962	TYR	CB-CG-CD1	-6.85	116.89	121.00
1	B	987	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	B	431	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	D	411	ASP	CB-CG-OD1	6.84	124.45	118.30
1	D	853	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	352	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	A	237	ARG	CB-CA-C	-6.81	96.78	110.40
1	B	919	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	164	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	875	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	557	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	C	772	ASP	CB-CG-OD1	6.77	124.39	118.30
1	D	429	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	D	569	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	C	781	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	594	ASP	CB-CG-OD2	-6.73	112.24	118.30
1	C	82	ASP	CB-CG-OD1	6.73	124.36	118.30
1	B	916	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	C	43	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	13	ARG	CD-NE-CZ	6.68	132.96	123.60
1	C	505	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	924	ASP	CB-CG-OD1	6.67	124.30	118.30
1	B	255	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	D	172	ASP	CB-CG-OD2	-6.66	112.30	118.30
1	A	659	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	C	255	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	280	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	B	319	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	411	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	D	859	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	552	TYR	CB-CG-CD1	-6.63	117.02	121.00
1	A	594	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	B	598	ASP	CB-CG-OD1	6.62	124.26	118.30
1	B	15	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	B	144	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	987	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	329	ASP	CB-CG-OD2	-6.59	112.36	118.30
1	C	82	ASP	CB-CG-OD2	-6.59	112.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	986	ILE	CG1-CB-CG2	-6.59	96.90	111.40
1	C	987	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	B	429	ASP	CB-CG-OD1	6.55	124.20	118.30
1	D	579	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	A	531	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	A	997	ASP	N-CA-CB	6.54	122.37	110.60
1	B	987	ASP	CB-CG-OD1	6.54	124.18	118.30
1	A	446	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	B	439	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	671	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	671	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	26	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	C	403	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	D	828	ASP	CB-CG-OD2	-6.48	112.46	118.30
1	A	954	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	C	405	TYR	CB-CG-CD2	-6.48	117.11	121.00
1	A	687	GLN	C-N-CD	-6.47	106.36	120.60
1	C	792	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	B	329	ASP	CB-CG-OD1	6.47	124.12	118.30
1	D	431	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	736	ALA	N-CA-CB	6.45	119.12	110.10
1	D	557	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	792	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	329	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	B	211	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	D	997	ASP	N-CA-CB	6.42	122.15	110.60
1	B	505	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	C	859	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	C	916	ASP	CB-CG-OD1	6.39	124.05	118.30
1	D	954	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	172	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	761	GLN	N-CA-CB	6.38	122.09	110.60
1	A	210	ARG	NE-CZ-NH2	-6.37	117.12	120.30
1	B	782	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	A	980	GLU	C-N-CA	-6.36	108.94	122.30
1	C	473	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	853	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	D	497	ASP	CB-CG-OD1	6.35	124.02	118.30
1	D	790	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	588	TYR	CB-CG-CD1	6.34	124.80	121.00
1	A	917	ARG	CD-NE-CZ	-6.33	114.73	123.60
1	A	588	TYR	CB-CG-CD2	-6.33	117.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	503	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	C	958	ASN	N-CA-CB	6.33	121.98	110.60
1	D	367	MET	CG-SD-CE	6.32	110.31	100.20
1	A	403	ASP	CB-CG-OD1	6.32	123.98	118.30
1	D	403	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	492	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	77	ASP	CB-CG-OD1	6.29	123.97	118.30
1	A	116	THR	CA-CB-CG2	-6.27	103.62	112.40
1	D	509	ASP	CB-CG-OD1	6.27	123.95	118.30
1	A	579	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	C	734	SER	N-CA-CB	6.24	119.86	110.50
1	A	538	TYR	CB-CG-CD2	6.22	124.73	121.00
1	C	211	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	15	ASP	CB-CG-OD1	6.21	123.88	118.30
1	D	790	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	356	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	D	252	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	B	446	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	D	954	ASP	CB-CG-OD1	6.17	123.86	118.30
1	B	257	THR	CA-CB-CG2	-6.14	103.80	112.40
1	A	746	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	371	THR	CA-CB-CG2	-6.14	103.81	112.40
1	D	431	ARG	CA-CB-CG	-6.14	99.90	113.40
1	D	96	ASP	CB-CG-OD1	6.12	123.81	118.30
1	B	199	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	832	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	557	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	D	288	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	45	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	B	45	ASP	CB-CG-OD1	6.07	123.77	118.30
1	C	618	THR	CA-CB-CG2	-6.07	103.90	112.40
1	D	237	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	996	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	C	184	LEU	CB-CA-C	-6.04	98.72	110.20
1	B	927	THR	CA-CB-CG2	-6.03	103.96	112.40
1	D	204	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	B	685	LEU	C-N-CD	-6.02	107.35	120.60
1	A	507	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	D	451	PRO	N-CA-CB	6.02	110.52	103.30
1	C	446	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	832	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	C	802	ASP	CB-CG-OD2	-5.99	112.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	336	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	431	ARG	CA-CB-CG	-5.98	100.23	113.40
1	D	287	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	D	368	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	832	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C	388	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	193	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	561	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	52	ARG	CB-CA-C	-5.96	98.49	110.40
1	C	828	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	D	980	GLU	C-N-CA	-5.94	109.83	122.30
1	A	833	ALA	CB-CA-C	-5.94	101.19	110.10
1	D	598	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	D	123	TYR	CB-CG-CD1	5.92	124.55	121.00
1	D	881	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	961	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	D	336	ARG	CD-NE-CZ	5.91	131.88	123.60
1	B	411	ASP	CB-CG-OD1	5.91	123.61	118.30
1	D	569	ASP	CB-CG-OD1	5.91	123.61	118.30
1	D	368	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	185	ALA	N-CA-CB	5.90	118.36	110.10
1	D	725	ASN	CA-CB-CG	-5.90	100.42	113.40
1	A	509	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	D	875	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	572	ASP	CB-CG-OD1	5.88	123.59	118.30
1	D	193	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	671	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	954	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	D	572	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	C	908	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	C	46	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	B	746	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	429	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	C	634	GLN	CB-CA-C	5.84	122.08	110.40
1	D	211	ASP	CB-CG-OD1	5.84	123.56	118.30
1	C	832	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	D	509	ASP	CB-CG-OD2	-5.82	113.07	118.30
1	B	782	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	598	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	553	TRP	CA-CB-CG	-5.81	102.66	113.70
1	C	579	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	D	919	ASP	CB-CG-OD2	-5.81	113.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	B	929	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	D	770	ILE	CA-CB-CG1	5.78	121.99	111.00
1	C	213	SER	CB-CA-C	-5.78	99.11	110.10
1	B	479	ASP	CB-CG-OD1	5.78	123.50	118.30
1	D	832	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	648	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	B	497	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	D	926	TYR	CB-CG-CD1	5.77	124.46	121.00
1	C	812	ALA	N-CA-CB	5.76	118.17	110.10
1	D	894	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	D	996	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	630	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	C	252	ASP	CA-CB-CG	-5.74	100.77	113.40
1	D	403	ASP	CB-CG-OD1	5.74	123.47	118.30
1	A	875	ASP	CB-CG-OD1	5.74	123.47	118.30
1	C	634	GLN	N-CA-CB	5.74	120.94	110.60
1	C	333	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	C	917	ARG	CD-NE-CZ	-5.74	115.56	123.60
1	B	781	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	183	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	B	668	VAL	CB-CA-C	-5.71	100.55	111.40
1	A	790	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	D	15	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	97	ALA	CB-CA-C	-5.70	101.55	110.10
1	D	473	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	280	ASP	CB-CG-OD1	5.70	123.43	118.30
1	B	368	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	144	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	A	252	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	77	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	144	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	D	164	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	733	ALA	N-CA-C	5.66	126.28	111.00
1	C	671	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	C	987	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	388	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	769	TRP	CB-CA-C	-5.62	99.15	110.40
1	C	1018	LEU	CB-CA-C	-5.62	99.52	110.20
1	C	632	SER	N-CA-CB	5.62	118.92	110.50
1	C	659	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	448	ARG	NE-CZ-NH1	5.61	123.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	869	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	144	ASP	CB-CG-OD1	5.61	123.34	118.30
1	A	986	ILE	CG1-CB-CG2	-5.60	99.08	111.40
1	B	57	GLU	CA-CB-CG	-5.59	101.10	113.40
1	B	507	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	743	SER	N-CA-CB	5.59	118.88	110.50
1	A	952	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	333	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	579	ASP	CB-CG-OD1	5.58	123.32	118.30
1	D	746	ASP	CB-CG-OD2	-5.58	113.27	118.30
1	D	42	ALA	CB-CA-C	-5.57	101.74	110.10
1	C	388	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	719	GLN	CB-CA-C	-5.57	99.26	110.40
1	B	59	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	853	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	C	848	THR	CA-CB-CG2	-5.56	104.61	112.40
1	A	246	MET	CG-SD-CE	-5.55	91.31	100.20
1	A	507	ASP	CB-CG-OD1	5.55	123.30	118.30
1	D	832	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	721	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	D	431	ARG	CD-NE-CZ	5.55	131.37	123.60
1	D	553	TRP	CA-CB-CG	-5.54	103.17	113.70
1	B	375	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	578	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	C	237	ARG	CA-CB-CG	-5.54	101.22	113.40
1	A	778	THR	N-CA-CB	5.53	120.81	110.30
1	B	569	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	447	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	82	ASP	CB-CG-OD1	5.51	123.26	118.30
1	B	479	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	D	869	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	782	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	687	GLN	C-N-CD	-5.49	108.52	120.60
1	C	961	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	D	430	PRO	N-CA-CB	5.49	109.88	103.30
1	D	13	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	653	HIS	CA-CB-CG	5.48	122.92	113.60
1	B	52	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	868	VAL	CA-CB-CG2	5.47	119.11	110.90
1	D	234	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C	404	ARG	NE-CZ-NH2	5.47	123.03	120.30
1	D	980	GLU	O-C-N	-5.47	113.90	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	368	ASP	CB-CG-OD2	-5.46	113.39	118.30
1	A	1013	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	509	ASP	CB-CG-OD1	5.45	123.21	118.30
1	C	938	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	908	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	492	ASP	CB-CG-OD1	5.43	123.19	118.30
1	B	403	ASP	CB-CG-OD1	5.43	123.18	118.30
1	B	773	LYS	N-CA-CB	-5.42	100.83	110.60
1	A	469	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	731	PRO	N-CA-CB	5.42	109.81	103.30
1	A	147	ASN	N-CA-CB	-5.42	100.85	110.60
1	B	199	ASP	CB-CG-OD1	5.41	123.17	118.30
1	B	792	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	D	854	LYS	CB-CA-C	-5.40	99.60	110.40
1	C	996	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	802	ASP	CB-CG-OD1	5.38	123.14	118.30
1	D	802	ASP	CB-CG-OD2	-5.37	113.46	118.30
1	A	755	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	100	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	C	908	ASP	CB-CG-OD1	5.36	123.12	118.30
1	C	710	GLU	CB-CA-C	-5.34	99.71	110.40
1	C	26	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	211	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	B	497	ASP	CB-CG-OD1	5.34	123.10	118.30
1	D	859	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	A	648	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	659	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	755	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	472	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	D	202	MET	CG-SD-CE	5.30	108.68	100.20
1	A	782	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	344	LEU	CA-CB-CG	-5.29	103.14	115.30
1	C	448	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	15	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	183	ARG	CD-NE-CZ	5.28	131.00	123.60
1	B	147	ASN	N-CA-CB	-5.28	101.09	110.60
1	A	166	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	C	172	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	B	611	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	C	721	ARG	CB-CA-C	-5.25	99.91	110.40
1	B	319	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	828	ASP	CB-CG-OD1	5.23	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	234	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	553	TRP	CA-CB-CG	-5.22	103.79	113.70
1	D	770	ILE	N-CA-C	-5.19	96.97	111.00
1	D	755	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	802	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	509	ASP	CB-CG-OD1	5.18	122.97	118.30
1	B	735	HIS	CB-CA-C	5.18	120.75	110.40
1	B	165	SER	CB-CA-C	-5.17	100.28	110.10
1	B	403	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	D	1022	GLN	N-CA-CB	5.16	119.89	110.60
1	A	834	VAL	CA-CB-CG2	-5.16	103.16	110.90
1	B	178	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	909	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	225	PHE	N-CA-CB	5.15	119.88	110.60
1	A	319	ASP	N-CA-CB	5.15	119.87	110.60
1	D	229	THR	CA-CB-CG2	-5.15	105.19	112.40
1	B	659	ASP	CB-CG-OD1	5.15	122.93	118.30
1	C	176	PHE	N-CA-CB	-5.14	101.34	110.60
1	D	14	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	126	THR	CA-CB-CG2	-5.14	105.20	112.40
1	D	324	GLU	N-CA-CB	5.13	119.83	110.60
1	B	287	ASP	CB-CG-OD1	5.13	122.92	118.30
1	B	885	ASN	N-CA-CB	5.12	119.81	110.60
1	D	828	ASP	CB-CG-OD1	5.12	122.90	118.30
1	A	166	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	D	199	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	158	TRP	CE3-CZ3-CH2	-5.10	115.59	121.20
1	B	521	LYS	CA-CB-CG	-5.10	102.18	113.40
1	A	201	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	333	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	14	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	210	ARG	N-CA-CB	5.09	119.77	110.60
1	A	635	THR	CA-CB-CG2	-5.09	105.27	112.40
1	A	333	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	C	492	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	A	164	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	A	509	ASP	CB-CA-C	-5.08	100.24	110.40
1	D	123	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	572	ASP	CB-CG-OD1	5.08	122.87	118.30
1	B	746	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	531	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	52	ARG	CB-CA-C	-5.08	100.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	917	ARG	CD-NE-CZ	-5.07	116.50	123.60
1	B	310	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	147	ASN	N-CA-CB	-5.06	101.48	110.60
1	A	746	ASP	CB-CG-OD1	5.06	122.86	118.30
1	B	100	TYR	N-CA-CB	5.06	119.70	110.60
1	A	559	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	C	746	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	792	ASP	CB-CG-OD1	5.05	122.84	118.30
1	B	251	ARG	CD-NE-CZ	-5.05	116.53	123.60
1	C	726	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	D	388	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	958	ASN	N-CA-CB	5.04	119.66	110.60
1	C	1021	CYS	CA-CB-SG	-5.03	104.94	114.00
1	A	629	PHE	CB-CA-C	-5.03	100.34	110.40
1	B	83	THR	CA-CB-CG2	-5.03	105.36	112.40
1	B	942	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	D	630	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	829	THR	N-CA-CB	5.02	119.84	110.30
1	B	651	LEU	N-CA-CB	5.02	120.44	110.40
1	B	224	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	D	448	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	569	ASP	CB-CG-OD1	5.01	122.81	118.30
1	D	81	ALA	CB-CA-C	-5.01	102.59	110.10
1	A	497	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	611	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	D	507	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	A	907	PRO	N-CA-CB	5.00	109.31	103.30
1	C	479	ASP	CB-CG-OD1	5.00	122.80	118.30

There are no chirality outliers.

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	8125	0	7716	174	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	8125	0	7716	216	0
1	C	8125	0	7716	158	0
1	D	8125	0	7716	158	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
4	A	30	0	35	2	0
4	B	15	0	17	0	0
4	C	15	0	17	0	0
4	D	30	0	35	0	0
5	A	72	0	108	7	0
5	B	72	0	108	3	0
5	C	84	0	126	11	0
5	D	68	0	102	5	0
6	A	865	0	0	25	0
6	B	935	0	0	20	0
6	C	922	0	0	13	0
6	D	885	0	0	19	0
All	All	36516	0	31412	701	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 11.

All (701) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.40	1.18
1:B:730:LEU:HD12	1:B:731:PRO:HD3	1.24	1.16
1:B:804:ASN:ND2	1:B:809:ARG:HH21	1.40	1.15
1:D:581:ASN:ND2	1:D:583:ASN:HD22	1.46	1.12
1:D:863:GLN:HE22	1:D:952:ARG:NH2	1.49	1.10
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.26	1.08
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.29	1.08
1:D:581:ASN:HD22	1:D:583:ASN:ND2	1.50	1.07
1:A:634:GLN:H	1:A:634:GLN:NE2	1.56	1.01
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.60	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:ASN:HD22	1:B:809:ARG:NH2	1.61	0.97
1:A:597:ASN:HD22	1:A:599:ARG:H	1.14	0.95
1:A:600:GLN:H	1:A:600:GLN:HE21	1.14	0.94
1:A:634:GLN:HE21	1:A:634:GLN:N	1.65	0.94
1:B:730:LEU:HD12	1:B:730:LEU:H	1.33	0.92
1:C:737:ILE:HD12	1:C:738:PRO:CD	2.01	0.90
1:B:600:GLN:H	1:B:600:GLN:HE21	1.06	0.90
1:C:597:ASN:HD22	1:C:599:ARG:H	1.14	0.90
1:B:597:ASN:HD22	1:B:599:ARG:H	1.13	0.89
1:A:656:VAL:HG21	1:A:685:LEU:CD2	2.04	0.88
1:A:817:GLN:HE21	1:A:817:GLN:N	1.70	0.87
1:B:251:ARG:HH11	1:B:251:ARG:HB3	1.40	0.87
1:A:651:LEU:HD11	1:A:667:GLU:HB2	1.56	0.86
1:B:1022:GLN:HG2	1:B:1023:LYS:N	1.91	0.86
1:A:682:LEU:HB3	1:A:683:PRO:HD2	1.57	0.85
1:D:597:ASN:HD22	1:D:599:ARG:H	1.21	0.85
1:B:685:LEU:HD23	1:B:686:PRO:HD2	1.58	0.85
1:B:664:ALA:HB3	1:B:685:LEU:HD11	1.59	0.85
1:C:890:GLN:HG3	1:C:891:VAL:N	1.92	0.84
1:B:368:ASP:HB2	1:B:370:GLN:HE22	1.42	0.83
1:D:718:GLN:HE21	1:D:719:GLN:H	1.23	0.83
1:B:687:GLN:HB3	1:B:688:PRO:HD2	1.60	0.83
1:B:730:LEU:CD1	1:B:731:PRO:HD3	2.05	0.83
1:D:643:LEU:HD23	1:D:675:GLN:HE21	1.42	0.83
1:A:599:ARG:HB2	1:A:600:GLN:HE21	1.44	0.83
1:D:863:GLN:NE2	1:D:952:ARG:NH2	2.26	0.83
1:A:817:GLN:N	1:A:817:GLN:NE2	2.26	0.82
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.59	0.82
1:D:863:GLN:HE22	1:D:952:ARG:HH22	1.23	0.81
1:A:778:THR:HG23	1:A:887:GLN:HB3	1.60	0.81
1:D:804:ASN:HD22	1:D:809:ARG:HH21	0.86	0.81
1:B:804:ASN:HD22	1:B:809:ARG:HH21	0.82	0.81
1:C:251:ARG:NH1	1:C:251:ARG:HB3	1.97	0.80
1:C:730:LEU:HD12	1:C:730:LEU:H	1.46	0.80
1:B:1022:GLN:HG2	1:B:1023:LYS:H	1.46	0.80
1:C:795:VAL:HG12	5:C:8506:DMS:H22	1.62	0.80
1:A:718:GLN:HE21	1:A:719:GLN:H	1.30	0.80
1:C:634:GLN:H	1:C:634:GLN:HE21	1.30	0.79
1:B:804:ASN:ND2	1:B:809:ARG:NH2	2.25	0.79
1:B:770:ILE:HG21	1:B:1022:GLN:HE21	1.47	0.78
1:C:277:GLU:HG2	6:C:9299:HOH:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:VAL:HG21	1:A:685:LEU:HD22	1.66	0.78
1:B:705:ALA:HB1	6:B:9360:HOH:O	1.84	0.78
1:B:830:LEU:HD11	1:B:835:LEU:HB2	1.66	0.78
1:A:662:PRO:C	1:A:663:LEU:HD23	2.03	0.77
1:D:863:GLN:NE2	1:D:952:ARG:HH22	1.82	0.77
1:A:580:GLU:OE2	1:A:580:GLU:HA	1.85	0.77
1:B:777:LEU:HD21	1:B:889:ALA:HA	1.67	0.77
5:D:8410:DMS:H12	6:D:9305:HOH:O	1.84	0.77
1:D:49:GLN:HG2	6:D:9356:HOH:O	1.84	0.77
1:B:797:GLU:HB3	1:B:799:THR:HG23	1.66	0.76
1:A:651:LEU:HG	1:A:652:LEU:N	2.01	0.75
1:C:773:LYS:CD	1:C:775:GLN:HE22	2.00	0.75
1:B:749:ILE:N	1:B:749:ILE:HD12	2.01	0.75
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.00	0.75
1:B:1017:GLN:HB2	6:B:9309:HOH:O	1.85	0.75
1:D:770:ILE:HD13	1:D:775:GLN:CG	2.17	0.75
1:C:773:LYS:HG2	1:C:775:GLN:NE2	2.02	0.75
1:C:630:ARG:HB3	1:C:630:ARG:HH11	1.52	0.74
1:D:651:LEU:O	1:D:651:LEU:HD12	1.87	0.73
5:A:8420:DMS:H22	6:A:9462:HOH:O	1.88	0.73
1:B:778:THR:HG23	1:B:779:PRO:HD2	1.70	0.73
1:C:804:ASN:OD1	1:C:809:ARG:NH2	2.21	0.73
1:A:656:VAL:HG21	1:A:685:LEU:HD21	1.71	0.73
1:A:685:LEU:HD23	1:A:686:PRO:CD	2.19	0.73
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.70	0.72
1:C:685:LEU:HD23	1:C:686:PRO:HD2	1.71	0.72
1:D:878:HIS:HD2	6:D:8809:HOH:O	1.73	0.72
1:D:658:LEU:O	1:D:661:LYS:HG3	1.90	0.71
1:C:669:PRO:HA	6:C:9344:HOH:O	1.90	0.71
1:A:817:GLN:NE2	6:A:8941:HOH:O	2.20	0.71
1:C:857:ARG:HG2	1:C:857:ARG:HH11	1.56	0.71
1:C:773:LYS:HD3	1:C:775:GLN:HE22	1.55	0.71
1:B:656:VAL:HG21	1:B:685:LEU:HD13	1.73	0.71
1:A:730:LEU:HD21	1:B:823:LEU:HB3	1.73	0.70
1:B:949:HIS:O	1:B:1023:LYS:HE2	1.91	0.70
1:B:646:HIS:HB3	6:B:9265:HOH:O	1.90	0.70
1:D:139:THR:OG1	1:D:216:HIS:HD2	1.75	0.70
1:B:653:HIS:HD2	1:B:667:GLU:HG3	1.55	0.70
1:B:730:LEU:H	1:B:730:LEU:CD1	1.97	0.70
1:C:749:ILE:N	1:C:749:ILE:HD12	2.06	0.70
1:B:370:GLN:H	1:B:370:GLN:CD	1.94	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:685:LEU:O	1:B:687:GLN:N	2.25	0.69
1:A:599:ARG:HB2	1:A:600:GLN:NE2	2.07	0.69
1:B:753:ASN:N	1:B:753:ASN:OD1	2.25	0.69
1:D:863:GLN:HE22	1:D:952:ARG:HH21	1.39	0.69
1:D:1022:GLN:NE2	1:D:1023:LYS:HG3	2.08	0.69
1:A:654:TRP:CZ3	1:A:665:SER:HA	2.28	0.69
1:C:718:GLN:HE21	1:C:719:GLN:H	1.38	0.69
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.25	0.69
1:D:675:GLN:HG3	6:D:9443:HOH:O	1.94	0.68
1:C:797:GLU:O	1:C:801:ILE:HD13	1.93	0.68
1:A:597:ASN:ND2	1:A:599:ARG:H	1.90	0.68
1:A:685:LEU:HD23	1:A:686:PRO:HD2	1.73	0.68
1:D:581:ASN:HD22	1:D:583:ASN:HD22	0.74	0.68
1:A:183:ARG:HG2	6:A:8905:HOH:O	1.93	0.68
1:A:878:HIS:HD2	6:A:8676:HOH:O	1.76	0.68
1:D:78:LEU:HB3	1:D:80:GLU:OE2	1.93	0.68
1:A:887:GLN:NE2	1:A:980:GLU:O	2.27	0.68
1:C:251:ARG:HB3	1:C:251:ARG:HH11	1.57	0.68
1:C:795:VAL:HG12	5:C:8506:DMS:C2	2.23	0.68
1:A:876:THR:OG1	1:A:877:PRO:HD2	1.94	0.68
1:A:615:PRO:O	1:A:618:THR:HG22	1.94	0.68
1:A:800:ARG:NH1	1:A:800:ARG:HB2	2.09	0.68
1:B:755:ARG:HD3	6:B:9342:HOH:O	1.92	0.67
1:B:241:GLU:HG3	1:B:292:ARG:CG	2.18	0.67
1:B:653:HIS:HD2	1:B:667:GLU:CG	2.07	0.67
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.15	0.67
1:C:429:ASP:OD1	1:C:431:ARG:HG3	1.95	0.66
1:C:634:GLN:HE21	1:C:634:GLN:N	1.91	0.66
1:B:251:ARG:HB3	1:B:251:ARG:NH1	2.09	0.66
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.77	0.66
1:D:71:GLU:H	1:D:71:GLU:CD	1.98	0.66
1:A:663:LEU:HD23	1:A:663:LEU:N	2.08	0.66
1:A:634:GLN:H	1:A:634:GLN:HE21	0.79	0.66
1:C:687:GLN:CB	1:C:688:PRO:HD2	2.26	0.66
1:A:431:ARG:HB2	6:A:9430:HOH:O	1.94	0.66
1:B:948:PRO:O	1:B:1023:LYS:N	2.27	0.66
1:A:737:ILE:O	1:A:737:ILE:HD13	1.95	0.65
1:D:643:LEU:CD2	1:D:675:GLN:HE21	2.06	0.65
1:D:781:ARG:NH1	6:D:9387:HOH:O	2.28	0.65
1:C:554:GLN:NE2	6:C:8683:HOH:O	2.30	0.65
1:D:887:GLN:NE2	1:D:980:GLU:O	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASP:OD1	1:B:370:GLN:NE2	2.29	0.65
1:C:857:ARG:HG2	1:C:857:ARG:NH1	2.09	0.65
1:A:890:GLN:HG3	1:A:891:VAL:N	2.12	0.65
1:B:777:LEU:CD2	1:B:889:ALA:HA	2.27	0.65
1:C:738:PRO:HD3	1:C:860:GLY:HA2	1.79	0.64
1:C:847:LYS:HE3	6:C:8855:HOH:O	1.96	0.64
1:C:878:HIS:HD2	6:C:8600:HOH:O	1.80	0.64
1:B:685:LEU:CD2	1:B:686:PRO:HD2	2.27	0.64
1:B:974:HIS:HD2	6:B:8610:HOH:O	1.79	0.64
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.80	0.64
1:C:688:PRO:HG3	1:C:725:ASN:HD21	1.63	0.64
1:B:658:LEU:HD11	1:B:692:GLY:HA3	1.80	0.64
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.63	0.64
1:C:102:ASN:C	1:C:102:ASN:HD22	2.02	0.64
1:D:299:LYS:NZ	6:D:9263:HOH:O	2.28	0.64
1:A:724:GLU:O	1:B:847:LYS:NZ	2.28	0.63
1:B:251:ARG:HH11	1:B:251:ARG:CB	2.08	0.63
1:C:651:LEU:HD12	1:C:651:LEU:C	2.18	0.63
1:C:687:GLN:HB3	1:C:688:PRO:HD2	1.79	0.63
1:D:91:GLN:HG3	1:D:96:ASP:OD1	1.99	0.63
1:D:618:THR:HG21	6:D:9043:HOH:O	1.99	0.63
1:D:948:PRO:HA	1:D:1023:LYS:HG3	1.80	0.63
1:B:13:ARG:HG3	1:C:13:ARG:NH1	2.13	0.63
1:A:685:LEU:CD2	1:A:686:PRO:HD2	2.28	0.63
1:A:655:MET:HG3	1:A:656:VAL:N	2.04	0.63
1:B:847:LYS:HG3	1:B:848:THR:N	2.14	0.63
1:B:797:GLU:O	1:B:801:ILE:HD13	1.99	0.62
1:A:250:LEU:C	1:A:251:ARG:HG2	2.18	0.62
1:B:13:ARG:NH2	1:C:13:ARG:HB2	2.14	0.62
1:C:730:LEU:HD12	1:C:730:LEU:N	2.13	0.62
1:B:79:PRO:HD2	1:B:80:GLU:OE2	1.99	0.62
1:C:664:ALA:HB3	1:C:685:LEU:HD21	1.81	0.62
1:C:801:ILE:HD12	1:C:808:GLU:OE2	1.99	0.62
1:A:347:LYS:HE3	6:A:9165:HOH:O	1.99	0.61
1:B:241:GLU:CG	1:B:292:ARG:HG2	2.20	0.61
1:C:473:ARG:NH1	6:C:9190:HOH:O	2.30	0.61
1:B:768:MET:HE1	6:B:9340:HOH:O	2.00	0.61
1:A:750:GLU:HG3	1:A:755:ARG:HD3	1.82	0.61
1:C:597:ASN:ND2	1:C:599:ARG:H	1.94	0.61
1:A:117:GLU:HG3	6:A:9006:HOH:O	2.00	0.61
1:A:800:ARG:HB2	1:A:800:ARG:CZ	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:GLU:CD	1:B:292:ARG:HE	2.04	0.61
1:C:740:LEU:HD12	1:C:748:CYS:O	2.00	0.61
1:B:718:GLN:HE21	1:B:719:GLN:H	1.47	0.61
1:B:1022:GLN:HB2	6:B:9340:HOH:O	2.00	0.61
1:D:800:ARG:HG3	1:D:800:ARG:HH11	1.64	0.61
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.00	0.60
1:A:226:HIS:ND1	6:A:9109:HOH:O	2.31	0.60
1:B:685:LEU:HD23	1:B:686:PRO:CD	2.30	0.60
1:A:772:ASP:C	1:A:773:LYS:HD3	2.22	0.60
1:A:634:GLN:NE2	1:A:634:GLN:N	2.36	0.60
1:D:749:ILE:HD11	1:D:836:ILE:HD11	1.83	0.60
1:B:867:THR:HG22	6:B:8921:HOH:O	2.01	0.60
1:B:730:LEU:HD12	1:B:730:LEU:N	2.12	0.60
1:B:770:ILE:HG21	1:B:1022:GLN:NE2	2.15	0.60
1:C:43:ARG:NH1	1:C:264:GLU:OE2	2.30	0.60
1:B:878:HIS:HD2	6:B:8589:HOH:O	1.85	0.59
1:A:817:GLN:NE2	1:A:817:GLN:H	1.99	0.59
1:A:742:THR:HG21	6:A:9241:HOH:O	2.01	0.59
1:B:599:ARG:HB2	1:B:600:GLN:HE21	1.65	0.59
1:C:13:ARG:O	1:C:14:ARG:C	2.39	0.59
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.02	0.59
1:C:832:ASP:OD1	1:C:832:ASP:N	2.35	0.59
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.37	0.59
1:D:890:GLN:HE21	1:D:892:ALA:HB2	1.67	0.59
1:D:1022:GLN:HE21	1:D:1023:LYS:N	2.01	0.59
1:C:691:ALA:HA	1:C:725:ASN:HB2	1.84	0.59
1:C:601:PHE:CE1	5:C:8506:DMS:H22	2.38	0.59
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.38	0.58
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.85	0.58
1:D:131:GLU:OE2	1:D:135:GLN:HG2	2.02	0.58
1:D:595:THR:HA	1:D:596:PRO:C	2.23	0.58
1:C:685:LEU:CD2	1:C:686:PRO:HD2	2.32	0.58
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.86	0.58
1:A:577:LYS:NZ	6:A:9249:HOH:O	2.37	0.58
1:D:215:LEU:HD21	1:D:217:LYS:HD3	1.86	0.58
1:A:277:GLU:H	1:A:277:GLU:CD	2.07	0.58
1:C:688:PRO:CG	1:C:725:ASN:HD21	2.17	0.58
1:B:600:GLN:HE21	1:B:600:GLN:N	1.90	0.58
1:A:759:ASN:OD1	1:A:762:SER:N	2.30	0.57
1:D:26:ARG:HD2	1:D:169:SER:HA	1.86	0.57
1:D:830:LEU:HD11	1:D:835:LEU:HB2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:LEU:HD23	1:A:686:PRO:HD3	1.86	0.57
1:B:687:GLN:HB3	1:B:688:PRO:CD	2.33	0.57
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.84	0.57
1:C:748:CYS:C	1:C:749:ILE:HD12	2.25	0.57
1:D:693:GLN:NE2	1:D:721:ARG:HD3	2.20	0.57
1:B:833:ALA:HB1	1:B:858:ILE:O	2.04	0.57
1:D:381:GLN:O	1:D:621:LYS:HE3	2.05	0.57
1:D:651:LEU:HD11	1:D:701:VAL:HB	1.86	0.57
1:B:1020:TRP:HD1	1:B:1021:CYS:N	2.03	0.57
1:C:773:LYS:HD3	1:C:775:GLN:NE2	2.20	0.56
1:A:662:PRO:O	1:A:663:LEU:HD23	2.05	0.56
1:B:675:GLN:HG3	6:B:8773:HOH:O	2.04	0.56
1:D:431:ARG:HG3	6:D:9405:HOH:O	2.04	0.56
1:B:770:ILE:HD12	1:B:1022:GLN:HG3	1.87	0.56
1:D:1022:GLN:HE22	1:D:1023:LYS:HG3	1.68	0.56
1:A:577:LYS:O	1:A:584:PRO:HA	2.06	0.56
1:A:102:ASN:C	1:A:102:ASN:HD22	2.08	0.56
1:A:781:ARG:NH1	6:A:9263:HOH:O	2.33	0.56
1:A:71:GLU:O	1:A:74:LEU:N	2.33	0.56
1:A:431:ARG:O	1:A:431:ARG:HG2	2.06	0.56
1:B:663:LEU:HD12	1:B:685:LEU:HD22	1.88	0.56
1:A:299:LYS:HD2	6:A:9406:HOH:O	2.05	0.56
1:C:737:ILE:CD1	1:C:738:PRO:HD2	2.17	0.56
1:A:201:ASP:OD2	4:A:2001:IPT:H62	2.05	0.55
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.42	0.55
1:C:615:PRO:O	1:C:618:THR:HG22	2.07	0.55
1:D:781:ARG:NH2	6:D:9457:HOH:O	2.39	0.55
1:A:131:GLU:O	1:A:135:GLN:HG2	2.07	0.55
1:C:664:ALA:CB	1:C:685:LEU:HD21	2.36	0.55
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.37	0.55
1:C:46:ARG:HB3	1:C:47:PRO:HD2	1.88	0.55
1:C:688:PRO:HG3	1:C:725:ASN:ND2	2.21	0.55
1:B:847:LYS:HE3	6:B:8840:HOH:O	2.06	0.55
1:B:102:ASN:HD22	1:B:102:ASN:C	2.09	0.55
1:A:759:ASN:OD1	1:A:761:GLN:N	2.40	0.55
1:B:947:GLY:O	1:B:1023:LYS:NZ	2.28	0.55
1:C:584:PRO:HG2	5:C:8411:DMS:H23	1.88	0.55
1:D:629:PHE:O	1:D:630:ARG:HD2	2.07	0.54
1:C:688:PRO:CG	1:C:725:ASN:ND2	2.70	0.54
1:A:241:GLU:HG3	1:A:292:ARG:CG	2.37	0.54
1:B:595:THR:HA	1:B:596:PRO:C	2.27	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.88	0.54
1:D:800:ARG:HG3	1:D:800:ARG:NH1	2.21	0.54
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.42	0.54
1:D:847:LYS:NZ	1:D:875:ASP:OD2	2.34	0.54
1:B:797:GLU:CB	1:B:799:THR:HG23	2.37	0.54
1:D:581:ASN:ND2	1:D:583:ASN:ND2	2.28	0.54
1:B:739:HIS:O	1:B:750:GLU:OE2	2.24	0.54
1:C:847:LYS:NZ	1:D:724:GLU:O	2.40	0.54
1:D:230:ARG:HB3	6:D:9535:HOH:O	2.07	0.54
1:D:622:HIS:O	1:D:625:GLN:HG3	2.08	0.54
1:D:718:GLN:HE21	1:D:719:GLN:N	1.99	0.54
1:A:984:LEU:HD11	1:A:986:ILE:HG12	1.90	0.54
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.23	0.54
1:A:737:ILE:HD13	1:A:737:ILE:C	2.27	0.54
1:B:599:ARG:HB2	1:B:600:GLN:NE2	2.23	0.54
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.37	0.53
1:C:686:PRO:O	1:C:687:GLN:O	2.26	0.53
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.43	0.53
1:B:181:GLU:HG3	6:B:9314:HOH:O	2.07	0.53
1:C:773:LYS:CG	1:C:775:GLN:HE22	2.22	0.53
1:D:573:GLN:HB2	1:D:602:CYS:O	2.08	0.53
5:A:8410:DMS:H12	6:A:9182:HOH:O	2.07	0.53
1:A:112:PRO:HD2	1:A:113:PHE:CE1	2.43	0.53
1:B:291:LEU:N	1:B:291:LEU:HD22	2.24	0.53
1:B:639:THR:OG1	1:B:677:LYS:HE2	2.09	0.53
1:C:730:LEU:H	1:C:730:LEU:CD1	2.03	0.53
1:B:686:PRO:O	1:B:687:GLN:O	2.26	0.53
1:D:16:TRP:CG	1:D:189:LEU:HD13	2.44	0.53
1:C:431:ARG:HD2	6:C:9247:HOH:O	2.09	0.53
1:D:948:PRO:HB2	1:D:1022:GLN:NE2	2.24	0.53
1:D:861:SER:OG	1:D:863:GLN:HG3	2.09	0.53
1:A:524:LEU:HD11	1:A:562:LEU:HG	1.90	0.52
1:D:770:ILE:HD13	1:D:775:GLN:HG3	1.89	0.52
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.06	0.52
1:B:739:HIS:HB3	1:B:750:GLU:OE2	2.08	0.52
1:B:788:PRO:HD2	6:B:8719:HOH:O	2.08	0.52
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.74	0.52
1:A:718:GLN:NE2	6:A:9223:HOH:O	2.42	0.52
1:C:653:HIS:NE2	1:C:667:GLU:OE2	2.43	0.52
1:D:737:ILE:HD13	1:D:738:PRO:HD2	1.91	0.52
1:D:890:GLN:HB2	6:D:9434:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.22	0.52
1:B:730:LEU:N	1:B:731:PRO:CD	2.73	0.52
1:A:362:LEU:HD12	1:A:363:HIS:CE1	2.44	0.52
5:C:8408:DMS:H13	6:C:9398:HOH:O	2.08	0.52
1:D:1022:GLN:NE2	1:D:1023:LYS:HB2	2.25	0.52
1:C:262:GLN:HG3	1:C:309:TYR:CE2	2.44	0.52
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.90	0.51
1:B:599:ARG:HD2	1:B:600:GLN:HE22	1.75	0.51
1:C:685:LEU:CG	1:C:686:PRO:HD2	2.39	0.51
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.45	0.51
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.23	0.51
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.92	0.51
1:D:718:GLN:NE2	6:D:9346:HOH:O	2.43	0.51
1:B:178:ARG:HG3	1:B:179:ALA:O	2.11	0.51
1:C:920:LEU:HB3	1:C:921:PRO:CD	2.34	0.51
1:D:416:GLU:OE2	1:D:418:HIS:HB2	2.10	0.51
1:B:658:LEU:HD22	1:B:688:PRO:CB	2.40	0.51
1:A:757:GLN:O	1:A:765:LEU:HD12	2.11	0.51
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.10	0.51
1:A:261:TRP:CH2	1:A:266:GLN:HB2	2.46	0.51
1:A:599:ARG:HD2	1:A:600:GLN:NE2	2.25	0.51
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.26	0.51
1:B:655:MET:CE	1:B:665:SER:HB3	2.41	0.51
1:C:773:LYS:CG	1:C:775:GLN:NE2	2.74	0.51
1:C:1020:TRP:HD1	1:C:1021:CYS:N	2.08	0.51
1:A:241:GLU:HG3	1:A:292:ARG:HG3	1.92	0.51
1:A:249:GLU:HG3	1:A:251:ARG:NH1	2.26	0.51
1:B:651:LEU:HD22	1:B:651:LEU:C	2.31	0.51
1:B:658:LEU:HD11	1:B:692:GLY:CA	2.41	0.50
1:B:546:LEU:HA	6:B:8644:HOH:O	2.12	0.50
1:B:739:HIS:CD2	1:B:740:LEU:N	2.79	0.50
1:A:91:GLN:OE1	1:A:205:MET:HB3	2.11	0.50
1:B:368:ASP:CB	1:B:370:GLN:HE22	2.19	0.50
1:B:784:PHE:HA	1:B:881:ARG:O	2.11	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.92	0.50
1:A:573:GLN:HB2	1:A:602:CYS:O	2.11	0.50
1:C:699:ARG:HH11	1:C:699:ARG:HG2	1.77	0.50
1:C:573:GLN:HB2	1:C:602:CYS:O	2.12	0.50
1:C:630:ARG:HH11	1:C:630:ARG:CB	2.24	0.50
1:B:770:ILE:O	1:B:771:GLY:C	2.49	0.50
1:C:655:MET:SD	1:C:699:ARG:NH2	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:LEU:O	1:D:183:ARG:HA	2.11	0.50
1:D:618:THR:HG23	6:D:9056:HOH:O	2.11	0.50
1:D:778:THR:HG23	1:D:779:PRO:HD2	1.92	0.50
1:A:735:HIS:ND1	1:A:735:HIS:N	2.60	0.50
1:B:767:GLN:HG3	1:B:768:MET:N	2.27	0.50
1:B:770:ILE:HG13	1:B:775:GLN:NE2	2.26	0.50
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.80	0.50
1:C:820:ALA:HB2	1:C:842:TRP:CE2	2.46	0.50
1:A:824:GLN:HG3	1:A:825:CYS:N	2.27	0.49
1:B:649:ASN:OD1	1:B:703:PRO:HD2	2.12	0.49
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.71	0.49
1:D:35:SER:HB2	1:D:217:LYS:HD2	1.93	0.49
1:B:685:LEU:HD23	1:B:685:LEU:C	2.32	0.49
1:B:777:LEU:HD21	1:B:889:ALA:CA	2.40	0.49
1:D:643:LEU:HD23	1:D:675:GLN:NE2	2.19	0.49
1:A:655:MET:SD	1:A:662:PRO:HB3	2.52	0.49
1:C:128:ASN:HA	1:C:180:GLY:O	2.12	0.49
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.93	0.49
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.94	0.49
1:B:755:ARG:HG2	1:B:769:TRP:CE3	2.48	0.49
1:D:75:GLU:CD	1:D:156:GLY:HA3	2.32	0.49
1:B:656:VAL:HG21	1:B:685:LEU:CD1	2.41	0.49
1:D:770:ILE:CD1	1:D:775:GLN:HG3	2.43	0.49
1:B:658:LEU:HB2	1:B:694:LEU:CD2	2.42	0.49
1:D:742:THR:HG22	1:D:743:SER:N	2.27	0.49
1:D:667:GLU:C	1:D:668:VAL:HG23	2.33	0.49
1:A:347:LYS:NZ	6:A:9136:HOH:O	2.45	0.49
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.48	0.49
1:A:843:GLN:HA	1:A:847:LYS:O	2.13	0.49
1:A:784:PHE:HA	1:A:881:ARG:O	2.13	0.49
1:D:651:LEU:HD12	1:D:651:LEU:C	2.32	0.49
1:A:125:LEU:O	1:A:183:ARG:HA	2.12	0.48
1:C:46:ARG:HB3	1:C:47:PRO:CD	2.43	0.48
1:A:977:HIS:O	1:A:978:ALA:C	2.50	0.48
5:B:8410:DMS:H21	6:B:8775:HOH:O	2.12	0.48
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.48	0.48
1:B:745:MET:SD	1:B:745:MET:N	2.86	0.48
1:C:634:GLN:CA	1:C:634:GLN:NE2	2.77	0.48
1:B:102:ASN:C	1:B:102:ASN:ND2	2.66	0.48
6:B:9083:HOH:O	5:C:8420:DMS:H12	2.14	0.48
1:C:102:ASN:C	1:C:102:ASN:ND2	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ARG:HB3	6:C:9335:HOH:O	2.13	0.48
1:D:948:PRO:CB	1:D:1022:GLN:NE2	2.77	0.48
1:B:16:TRP:CG	1:B:189:LEU:HD13	2.49	0.48
1:B:899:GLY:HA2	1:B:915:PHE:CE1	2.49	0.48
1:C:320:GLY:HA2	5:C:8406:DMS:O	2.13	0.48
1:C:684:GLU:HG2	1:C:685:LEU:N	2.29	0.48
1:B:13:ARG:HH22	1:C:13:ARG:HB2	1.79	0.48
1:B:502:MET:HB2	1:B:537:GLU:HB2	1.96	0.48
1:C:71:GLU:HG2	6:C:9230:HOH:O	2.12	0.48
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.28	0.48
1:C:951:TRP:HA	1:C:1019:VAL:O	2.13	0.48
5:C:8408:DMS:H22	6:C:9206:HOH:O	2.13	0.48
1:C:581:ASN:OD1	1:C:581:ASN:N	2.45	0.48
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.94	0.48
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.29	0.47
1:B:687:GLN:O	1:B:689:GLU:OE2	2.32	0.47
1:B:974:HIS:CD2	6:B:8610:HOH:O	2.61	0.47
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.77	0.47
1:C:367:MET:HE2	1:C:372:MET:HG3	1.96	0.47
1:A:767:GLN:HG3	1:A:768:MET:N	2.29	0.47
1:B:625:GLN:NE2	6:B:8717:HOH:O	2.42	0.47
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.49	0.47
1:C:663:LEU:HA	1:C:663:LEU:HD22	1.38	0.47
1:D:651:LEU:HD13	1:D:653:HIS:ND1	2.29	0.47
1:D:986:ILE:HG23	1:D:986:ILE:HD13	1.45	0.47
1:A:71:GLU:O	1:A:72:SER:C	2.51	0.47
1:B:669:PRO:HB3	6:B:9280:HOH:O	2.14	0.47
1:B:741:THR:HB	1:B:748:CYS:HB3	1.97	0.47
1:A:654:TRP:CE3	1:A:665:SER:HA	2.49	0.47
1:B:735:HIS:O	1:B:736:ALA:HB3	2.15	0.47
1:B:801:ILE:HD12	1:B:808:GLU:OE2	2.14	0.47
1:C:851:ILE:HD11	1:D:728:VAL:HG12	1.96	0.47
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.95	0.47
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.48	0.47
1:B:597:ASN:ND2	1:B:599:ARG:H	1.96	0.47
1:A:132:SER:HA	1:A:135:GLN:CG	2.44	0.47
1:A:778:THR:HG23	1:A:887:GLN:CB	2.37	0.47
1:A:799:THR:OG1	1:A:800:ARG:N	2.47	0.47
1:A:948:PRO:CB	1:A:1022:GLN:HE21	2.27	0.47
1:B:733:ALA:HB3	1:B:735:HIS:CE1	2.49	0.47
1:B:733:ALA:CB	1:B:735:HIS:CE1	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:PHE:CZ	5:C:8506:DMS:H22	2.50	0.47
1:D:659:ASP:O	6:D:9261:HOH:O	2.20	0.47
1:D:737:ILE:HD11	1:D:832:ASP:HA	1.97	0.47
1:A:60:PHE:HA	1:A:122:CYS:O	2.15	0.47
1:A:102:ASN:ND2	1:A:201:ASP:HB2	2.29	0.47
1:B:16:TRP:CG	1:B:189:LEU:CD1	2.97	0.47
1:C:693:GLN:HE22	1:C:724:GLU:HB2	1.79	0.47
1:C:746:ASP:CG	1:C:757:GLN:HE21	2.18	0.47
1:A:595:THR:HA	1:A:596:PRO:C	2.36	0.47
1:C:147:ASN:HA	1:C:148:SER:HA	1.55	0.47
1:D:93:HIS:CD2	5:D:8414:DMS:C2	2.98	0.47
1:A:734:SER:OG	1:A:860:GLY:HA3	2.15	0.46
1:B:630:ARG:CZ	1:B:637:GLU:OE1	2.63	0.46
1:B:658:LEU:HD22	1:B:688:PRO:HB2	1.98	0.46
1:B:739:HIS:CD2	1:B:740:LEU:H	2.32	0.46
1:D:1022:GLN:NE2	1:D:1023:LYS:CB	2.78	0.46
1:B:249:GLU:HG2	1:B:251:ARG:HD3	1.96	0.46
1:B:942:ARG:HA	1:B:953:GLY:O	2.14	0.46
1:C:749:ILE:O	1:C:755:ARG:HA	2.15	0.46
1:D:131:GLU:HA	1:D:134:LEU:HD12	1.97	0.46
1:B:656:VAL:O	1:B:663:LEU:HB2	2.16	0.46
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.50	0.46
1:B:663:LEU:HD12	1:B:685:LEU:CD2	2.45	0.46
1:C:660:GLY:O	1:C:662:PRO:HD3	2.15	0.46
1:D:764:PHE:CE1	1:D:781:ARG:NH1	2.83	0.46
1:A:741:THR:HG22	6:A:9224:HOH:O	2.14	0.46
1:C:788:PRO:HD2	1:C:968:MET:HB2	1.97	0.46
1:C:817:GLN:HE21	1:C:817:GLN:HB3	1.46	0.46
1:A:804:ASN:HB3	6:A:8764:HOH:O	2.15	0.46
1:C:131:GLU:OE1	1:C:135:GLN:NE2	2.49	0.46
1:A:62:TRP:CH2	1:A:64:PRO:HA	2.51	0.46
1:B:751:LEU:HD23	1:B:862:GLY:HA2	1.98	0.46
1:B:1020:TRP:CD1	1:B:1020:TRP:C	2.88	0.46
1:D:147:ASN:HA	1:D:148:SER:HA	1.75	0.46
1:D:708:TRP:CZ2	5:D:8403:DMS:H12	2.51	0.46
1:A:745:MET:HE3	6:A:9319:HOH:O	2.16	0.45
1:B:655:MET:HE2	1:B:664:ALA:O	2.16	0.45
1:C:231:PHE:CD1	1:C:231:PHE:N	2.84	0.45
1:C:693:GLN:NE2	1:C:724:GLU:HB2	2.31	0.45
1:C:804:ASN:HB3	6:C:8686:HOH:O	2.16	0.45
1:A:971:SER:HG	1:A:972:HIS:CE1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLU:HB2	1:B:179:ALA:HB2	1.99	0.45
1:B:896:ASN:HB3	1:B:945:ASN:HB2	1.98	0.45
1:C:637:GLU:OE2	1:C:677:LYS:NZ	2.43	0.45
1:D:730:LEU:H	1:D:730:LEU:HG	1.45	0.45
1:D:742:THR:CG2	1:D:743:SER:N	2.79	0.45
1:A:46:ARG:HH11	1:A:46:ARG:HD3	1.50	0.45
1:A:948:PRO:HB2	1:A:1022:GLN:HE21	1.81	0.45
1:B:901:GLY:HA3	1:B:902:PRO:HA	1.75	0.45
1:C:131:GLU:HG3	1:C:135:GLN:NE2	2.31	0.45
1:D:986:ILE:HD12	1:D:986:ILE:HG21	1.43	0.45
1:B:890:GLN:OE1	1:B:947:GLY:HA3	2.16	0.45
1:C:630:ARG:CB	1:C:630:ARG:NH1	2.80	0.45
1:B:749:ILE:C	1:B:750:GLU:HG3	2.36	0.45
1:C:753:ASN:OD1	1:C:753:ASN:N	2.50	0.45
1:D:367:MET:HB3	1:D:372:MET:CE	2.47	0.45
1:A:85:VAL:CG1	1:A:86:VAL:N	2.79	0.45
1:C:688:PRO:HD3	1:C:694:LEU:HD11	1.99	0.45
1:C:749:ILE:N	1:C:749:ILE:CD1	2.79	0.45
1:D:102:ASN:C	1:D:102:ASN:HD22	2.19	0.45
1:D:233:ASP:HA	5:D:8417:DMS:C1	2.46	0.45
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.81	0.45
1:A:473:ARG:NH1	1:A:476:LYS:CB	2.80	0.45
1:B:285:TYR:HB3	1:B:288:ARG:HG3	1.98	0.45
1:B:890:GLN:OE1	1:B:892:ALA:HB2	2.17	0.45
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.52	0.45
1:D:1017:GLN:HG2	1:D:1018:LEU:N	2.32	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.61	0.45
1:A:292:ARG:NH1	5:A:8412:DMS:C2	2.80	0.45
1:B:832:ASP:N	1:B:832:ASP:OD1	2.50	0.45
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.99	0.45
1:A:85:VAL:HG12	1:A:86:VAL:N	2.30	0.44
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.51	0.44
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.98	0.44
1:B:225:PHE:HA	1:B:243:GLU:O	2.17	0.44
1:B:593:GLY:O	5:B:8413:DMS:H22	2.17	0.44
1:B:888:LEU:O	1:B:981:GLY:HA3	2.17	0.44
1:C:433:LEU:N	1:C:434:PRO:CD	2.80	0.44
1:D:524:LEU:HD11	1:D:562:LEU:HG	1.99	0.44
1:A:135:GLN:HG2	1:A:135:GLN:H	1.29	0.44
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.98	0.44
5:A:8502:DMS:O	6:A:9101:HOH:O	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:LYS:HA	1:B:769:TRP:O	2.18	0.44
1:A:377:LEU:HD22	1:A:708:TRP:HA	2.00	0.44
1:A:631:LEU:HG	1:A:632:SER:N	2.32	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.69	0.44
1:C:737:ILE:HD12	1:C:738:PRO:N	2.32	0.44
1:D:76:CYS:O	6:D:9200:HOH:O	2.21	0.44
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.99	0.44
1:B:728:VAL:HG23	1:B:729:THR:N	2.31	0.44
1:B:1023:LYS:HB2	1:B:1023:LYS:HE3	1.47	0.44
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.18	0.44
1:C:234:ASP:O	1:C:235:PHE:HB2	2.18	0.44
1:D:658:LEU:O	1:D:659:ASP:C	2.56	0.44
1:A:264:GLU:HG3	6:A:9345:HOH:O	2.17	0.44
1:A:769:TRP:HA	1:A:773:LYS:O	2.18	0.44
1:B:13:ARG:CG	1:C:13:ARG:NH1	2.80	0.44
1:B:100:TYR:HB3	1:B:589:GLY:HA2	2.00	0.44
1:B:777:LEU:CD1	1:B:980:GLU:HB3	2.47	0.44
1:A:200:GLN:HG2	1:A:391:HIS:HB2	1.99	0.44
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.99	0.44
1:C:630:ARG:HB3	1:C:630:ARG:NH1	2.27	0.44
1:C:685:LEU:HG	1:C:686:PRO:HD2	1.98	0.44
1:C:755:ARG:HG2	1:C:756:TRP:N	2.32	0.44
1:D:670:LEU:HA	1:D:670:LEU:HD23	1.69	0.44
1:D:843:GLN:HA	1:D:847:LYS:O	2.18	0.44
1:A:360:HIS:ND1	1:A:361:PRO:HD2	2.32	0.44
1:A:654:TRP:O	1:A:665:SER:HB2	2.17	0.44
1:B:127:PHE:CD2	1:B:127:PHE:N	2.85	0.44
1:B:254:LEU:O	1:B:255:ARG:HD3	2.17	0.44
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.44
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.35	0.44
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.53	0.44
1:A:285:TYR:HB3	1:A:288:ARG:HG3	1.99	0.44
1:A:599:ARG:HB2	1:A:600:GLN:H	1.51	0.44
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.99	0.44
1:D:457:SER:HA	1:D:485:GLN:O	2.18	0.44
1:D:740:LEU:HD12	1:D:741:THR:N	2.32	0.44
1:D:917:ARG:HH11	1:D:917:ARG:HD3	1.39	0.44
1:A:740:LEU:HD12	1:A:748:CYS:O	2.18	0.43
1:B:933:SER:O	1:B:934:GLU:C	2.53	0.43
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.53	0.43
1:A:942:ARG:HA	1:A:953:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:ASP:HB2	1:B:370:GLN:NE2	2.22	0.43
1:B:600:GLN:H	1:B:600:GLN:NE2	1.91	0.43
1:C:986:ILE:HG21	1:C:986:ILE:HD13	1.53	0.43
1:A:16:TRP:CD2	1:A:189:LEU:HD13	2.53	0.43
1:B:68:ALA:O	1:B:70:PRO:HD3	2.18	0.43
1:B:652:LEU:HD22	1:B:680:ILE:HD12	2.00	0.43
1:B:730:LEU:O	1:B:731:PRO:O	2.34	0.43
1:B:890:GLN:HE21	1:B:890:GLN:HB2	1.18	0.43
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.99	0.43
1:C:773:LYS:CD	1:C:775:GLN:NE2	2.77	0.43
1:D:1022:GLN:NE2	1:D:1023:LYS:CG	2.78	0.43
1:B:770:ILE:CD1	1:B:1022:GLN:HG3	2.47	0.43
1:C:601:PHE:CE2	5:C:8506:DMS:H23	2.54	0.43
1:D:933:SER:O	1:D:934:GLU:C	2.56	0.43
1:A:128:ASN:HA	1:A:180:GLY:O	2.19	0.43
1:B:250:LEU:O	1:B:251:ARG:HD3	2.18	0.43
1:B:655:MET:HE3	1:B:655:MET:HB2	1.83	0.43
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.52	0.43
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.99	0.43
1:D:145:GLY:N	1:D:210:ARG:HB2	2.33	0.43
1:D:473:ARG:HA	1:D:473:ARG:HD2	1.88	0.43
1:D:737:ILE:HD11	1:D:832:ASP:CA	2.48	0.43
1:D:759:ASN:OD1	1:D:761:GLN:HB3	2.17	0.43
1:D:824:GLN:HG2	1:D:825:CYS:N	2.33	0.43
1:C:887:GLN:NE2	1:C:980:GLU:O	2.51	0.43
1:A:986:ILE:HD12	1:A:986:ILE:HG21	1.70	0.43
5:A:8410:DMS:H21	6:A:9111:HOH:O	2.18	0.43
1:B:595:THR:HG22	5:B:8413:DMS:S	2.58	0.43
1:A:111:PRO:HA	1:A:112:PRO:HA	1.69	0.43
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.68	0.43
1:B:751:LEU:HD23	1:B:862:GLY:CA	2.49	0.43
1:B:777:LEU:CG	1:B:889:ALA:HA	2.49	0.43
1:C:297:ASN:N	1:C:298:PRO:CD	2.82	0.43
1:D:60:PHE:HA	1:D:122:CYS:O	2.17	0.43
1:D:88:SER:HA	1:D:366:VAL:HG21	2.00	0.43
1:D:692:GLY:N	6:D:9430:HOH:O	2.50	0.43
1:B:13:ARG:HG2	1:C:13:ARG:CZ	2.49	0.43
1:B:746:ASP:HA	1:B:760:ARG:HG3	2.00	0.43
1:C:651:LEU:C	1:C:651:LEU:CD1	2.87	0.43
1:A:630:ARG:HH11	1:A:630:ARG:HD2	1.59	0.43
1:B:178:ARG:HD2	1:B:181:GLU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ARG:NH1	1:B:251:ARG:CG	2.79	0.43
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.37	0.43
1:A:770:ILE:HD13	1:A:1022:GLN:HG3	2.01	0.42
1:B:576:ILE:HD12	1:B:576:ILE:HG23	1.67	0.42
1:B:770:ILE:CG2	1:B:1022:GLN:NE2	2.79	0.42
1:D:942:ARG:HA	1:D:953:GLY:O	2.18	0.42
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.87	0.42
1:A:292:ARG:HH11	5:A:8412:DMS:H22	1.84	0.42
1:A:362:LEU:HD22	1:A:362:LEU:HA	1.81	0.42
1:B:661:LYS:HE3	1:B:661:LYS:HB2	1.57	0.42
1:B:685:LEU:CG	1:B:686:PRO:HD2	2.48	0.42
1:C:577:LYS:O	1:C:584:PRO:HA	2.19	0.42
1:D:829:THR:HG21	6:D:9526:HOH:O	2.19	0.42
1:A:73:TRP:CZ2	1:A:185:ALA:HB1	2.54	0.42
1:B:653:HIS:HD2	1:B:667:GLU:HG2	1.83	0.42
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.19	0.42
1:A:667:GLU:C	1:A:668:VAL:HG23	2.39	0.42
1:B:54:LEU:HD11	1:B:214:LEU:HG	2.02	0.42
1:B:599:ARG:HD2	1:B:600:GLN:NE2	2.34	0.42
1:B:730:LEU:H	1:B:731:PRO:HD3	1.84	0.42
1:B:890:GLN:O	1:B:890:GLN:HG3	2.12	0.42
1:C:597:ASN:HD22	1:C:599:ARG:N	1.97	0.42
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.19	0.42
1:D:859:ASP:OD1	1:D:861:SER:N	2.46	0.42
1:D:906:TYR:CZ	1:D:937:LEU:HB2	2.55	0.42
1:A:126:THR:HA	1:A:182:ASN:O	2.19	0.42
1:A:183:ARG:HG2	1:A:183:ARG:HH11	1.85	0.42
1:B:770:ILE:HD12	1:B:1022:GLN:HE21	1.83	0.42
1:A:729:THR:HG23	6:A:9174:HOH:O	2.18	0.42
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.88	0.42
1:A:863:GLN:HE22	1:A:952:ARG:NH2	2.18	0.42
1:B:658:LEU:HD22	1:B:688:PRO:HB3	2.02	0.42
1:B:730:LEU:N	1:B:731:PRO:HD3	2.34	0.42
1:D:431:ARG:HB3	6:D:9558:HOH:O	2.19	0.42
1:C:634:GLN:HE21	1:C:634:GLN:CA	2.31	0.42
1:C:873:ALA:O	1:C:876:THR:HG22	2.20	0.42
1:D:333:ARG:HA	1:D:345:ASN:OD1	2.20	0.42
1:B:663:LEU:HD22	1:B:663:LEU:HA	1.70	0.42
1:D:74:LEU:HA	1:D:74:LEU:HD23	1.68	0.42
1:D:830:LEU:CD1	1:D:835:LEU:HB2	2.48	0.42
1:A:906:TYR:CZ	1:A:937:LEU:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:LYS:HA	1:B:773:LYS:HD3	1.74	0.42
1:A:754:LYS:NZ	6:A:9351:HOH:O	2.28	0.42
1:A:1006:GLU:HG2	1:A:1007:PHE:CD1	2.55	0.42
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.55	0.41
1:A:645:ARG:CZ	4:A:2002:IPT:H1'	2.50	0.41
1:A:773:LYS:HD3	1:A:773:LYS:N	2.35	0.41
1:B:687:GLN:CB	1:B:688:PRO:CD	2.94	0.41
1:C:63:PHE:HB3	1:C:64:PRO:HD2	2.01	0.41
1:C:143:PHE:O	1:C:168:PRO:HA	2.20	0.41
1:A:1013:ARG:NH1	6:A:9150:HOH:O	2.40	0.41
1:B:291:LEU:N	1:B:291:LEU:CD2	2.82	0.41
1:B:817:GLN:OE1	6:B:8928:HOH:O	2.21	0.41
1:C:782:ASP:HA	1:C:884:LEU:HD23	2.03	0.41
1:D:643:LEU:CD2	1:D:675:GLN:NE2	2.79	0.41
1:A:675:GLN:HG3	6:A:8862:HOH:O	2.20	0.41
1:A:776:LEU:C	1:A:777:LEU:HD23	2.41	0.41
1:A:785:THR:O	1:A:881:ARG:HD2	2.20	0.41
1:A:801:ILE:HD13	1:A:808:GLU:OE2	2.21	0.41
1:B:882:ILE:CD1	1:B:1014:TYR:CD1	3.03	0.41
1:C:100:TYR:O	1:C:597:ASN:HA	2.21	0.41
1:A:613:PRO:HB3	1:A:617:LEU:HD23	2.03	0.41
1:B:577:LYS:HB3	1:B:577:LYS:HE3	1.95	0.41
1:B:703:PRO:O	1:B:711:ALA:HB1	2.20	0.41
1:B:991:MET:HE2	1:B:1003:VAL:HG21	2.03	0.41
5:C:8408:DMS:C2	6:C:9206:HOH:O	2.69	0.41
1:D:132:SER:HA	1:D:135:GLN:HG3	2.02	0.41
1:D:133:TRP:N	1:D:133:TRP:CD1	2.87	0.41
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.56	0.41
1:C:36:TRP:CD2	1:C:42:ALA:HA	2.56	0.41
1:C:682:LEU:HD23	1:C:682:LEU:HA	1.91	0.41
1:D:130:ASP:OD1	1:D:132:SER:N	2.43	0.41
1:D:625:GLN:NE2	6:D:8936:HOH:O	2.47	0.41
1:D:908:ASP:HB3	1:D:1007:PHE:CD1	2.55	0.41
1:A:131:GLU:HG2	1:A:135:GLN:OE1	2.20	0.41
1:B:749:ILE:N	1:B:749:ILE:CD1	2.77	0.41
1:C:264:GLU:OE2	1:C:264:GLU:HA	2.21	0.41
1:D:663:LEU:HD22	1:D:663:LEU:HA	1.77	0.41
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.56	0.41
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.82	0.41
1:D:111:PRO:HA	1:D:112:PRO:HA	1.82	0.41
1:D:112:PRO:HD2	1:D:113:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:LEU:HD22	1:B:871:GLU:OE1	2.20	0.41
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.95	0.41
1:B:301:TRP:CH2	1:B:452:SER:HA	2.56	0.41
1:B:636:ILE:HD13	1:B:698:VAL:HG11	2.03	0.41
1:D:102:ASN:C	1:D:102:ASN:ND2	2.74	0.41
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.56	0.41
1:D:910:LEU:HD12	1:D:910:LEU:C	2.41	0.41
1:A:292:ARG:HH11	5:A:8412:DMS:C2	2.34	0.41
1:B:977:HIS:CD2	1:B:977:HIS:O	2.74	0.41
1:D:576:ILE:HD13	1:D:576:ILE:HA	1.83	0.41
1:B:157:ARG:NH1	1:B:176:PHE:HA	2.36	0.40
1:C:610:ASP:O	1:C:611:ARG:HB2	2.21	0.40
1:D:576:ILE:HD12	1:D:576:ILE:HG23	1.78	0.40
1:D:708:TRP:CZ2	5:D:8403:DMS:C1	3.05	0.40
1:D:844:HIS:N	1:D:847:LYS:O	2.47	0.40
1:A:102:ASN:C	1:A:102:ASN:ND2	2.71	0.40
1:A:250:LEU:HA	1:A:250:LEU:HD23	1.82	0.40
1:A:577:LYS:O	1:A:585:TRP:N	2.54	0.40
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.52	0.40
1:C:236:SER:C	1:C:237:ARG:HG3	2.37	0.40
1:C:688:PRO:HG2	1:C:725:ASN:ND2	2.37	0.40
1:D:646:HIS:CD2	1:D:673:ALA:HA	2.57	0.40
1:D:777:LEU:HD23	1:D:777:LEU:HA	1.83	0.40
1:B:377:LEU:HD22	1:B:708:TRP:HA	2.03	0.40
1:C:522:LYS:HD2	1:D:558:GLN:HG2	2.04	0.40
1:D:800:ARG:HH11	1:D:800:ARG:CG	2.31	0.40
1:A:821:ALA:N	1:A:841:ALA:O	2.53	0.40
1:B:638:VAL:O	1:B:677:LYS:HA	2.22	0.40
1:C:533:LEU:C	1:C:533:LEU:HD23	2.42	0.40
1:D:745:MET:HE3	1:D:745:MET:HB2	1.86	0.40
1:B:13:ARG:CG	1:C:13:ARG:CZ	2.99	0.40
1:B:688:PRO:HG2	1:B:725:ASN:ND2	2.36	0.40
1:B:767:GLN:CG	1:B:768:MET:N	2.84	0.40
1:C:559:TYR:CE2	1:D:522:LYS:HA	2.57	0.40
1:D:577:LYS:O	1:D:584:PRO:HA	2.22	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	1009/1023 (99%)	971 (96%)	37 (4%)	1 (0%)	51	33
1	B	1009/1023 (99%)	971 (96%)	33 (3%)	5 (0%)	29	12
1	C	1009/1023 (99%)	968 (96%)	38 (4%)	3 (0%)	41	22
1	D	1009/1023 (99%)	971 (96%)	37 (4%)	1 (0%)	51	33
All	All	4036/4092 (99%)	3881 (96%)	145 (4%)	10 (0%)	47	29

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	686	PRO
1	B	687	GLN
1	B	731	PRO
1	C	687	GLN
1	B	732	ALA
1	B	736	ALA
1	C	690	SER
1	A	164	ASP
1	C	164	ASP
1	D	164	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	821 (95%)	43 (5%)	24	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	864/875 (99%)	815 (94%)	49 (6%)	20 5
1	C	864/875 (99%)	833 (96%)	31 (4%)	35 13
1	D	864/875 (99%)	826 (96%)	38 (4%)	28 8
All	All	3456/3500 (99%)	3295 (95%)	161 (5%)	26 7

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	A	90	TRP
1	A	102	ASN
1	A	117	GLU
1	A	131	GLU
1	A	135	GLN
1	A	178	ARG
1	A	183	ARG
1	A	249	GLU
1	A	251	ARG
1	A	333	ARG
1	A	362	LEU
1	A	370	GLN
1	A	394	ASN
1	A	519	SER
1	A	546	LEU
1	A	554	GLN
1	A	581	ASN
1	A	595	THR
1	A	600	GLN
1	A	634	GLN
1	A	651	LEU
1	A	652	LEU
1	A	655	MET
1	A	663	LEU
1	A	675	GLN
1	A	682	LEU
1	A	685	LEU
1	A	689	GLU
1	A	710	GLU
1	A	730	LEU
1	A	735	HIS
1	A	737	ILE

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Mol	Chain	Res	Type
1	A	744	GLU
1	A	746	ASP
1	A	755	ARG
1	A	761	GLN
1	A	778	THR
1	A	817	GLN
1	A	857	ARG
1	A	917	ARG
1	A	956	GLN
1	A	1023	LYS
1	B	13	ARG
1	B	70	PRO
1	B	71	GLU
1	B	72	SER
1	B	76	CYS
1	B	80	GLU
1	B	102	ASN
1	B	130	ASP
1	B	178	ARG
1	B	181	GLU
1	B	251	ARG
1	B	333	ARG
1	B	344	LEU
1	B	370	GLN
1	B	519	SER
1	B	535	LEU
1	B	546	LEU
1	B	600	GLN
1	B	634	GLN
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	663	LEU
1	B	675	GLN
1	B	681	GLU
1	B	685	LEU
1	B	689	GLU
1	B	690	SER
1	B	729	THR
1	B	730	LEU
1	B	737	ILE
1	B	745	MET

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Mol	Chain	Res	Type
1	B	750	GLU
1	B	753	ASN
1	B	756	TRP
1	B	761	GLN
1	B	770	ILE
1	B	773	LYS
1	B	799	THR
1	B	800	ARG
1	B	817	GLN
1	B	819	GLU
1	B	824	GLN
1	B	861	SER
1	B	890	GLN
1	B	893	GLU
1	B	917	ARG
1	B	956	GLN
1	B	1022	GLN
1	C	80	GLU
1	C	102	ASN
1	C	131	GLU
1	C	230	ARG
1	C	262	GLN
1	C	278	ILE
1	C	333	ARG
1	C	344	LEU
1	C	394	ASN
1	C	519	SER
1	C	580	GLU
1	C	581	ASN
1	C	634	GLN
1	C	651	LEU
1	C	655	MET
1	C	663	LEU
1	C	685	LEU
1	C	687	GLN
1	C	699	ARG
1	C	730	LEU
1	C	735	HIS
1	C	737	ILE
1	C	749	ILE
1	C	755	ARG
1	C	761	GLN

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Mol	Chain	Res	Type
1	C	772	ASP
1	C	773	LYS
1	C	817	GLN
1	C	847	LYS
1	C	1022	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	75	GLU
1	D	80	GLU
1	D	102	ASN
1	D	117	GLU
1	D	129	VAL
1	D	135	GLN
1	D	157	ARG
1	D	183	ARG
1	D	333	ARG
1	D	370	GLN
1	D	394	ASN
1	D	431	ARG
1	D	546	LEU
1	D	554	GLN
1	D	581	ASN
1	D	653	HIS
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	672	VAL
1	D	681	GLU
1	D	690	SER
1	D	730	LEU
1	D	737	ILE
1	D	770	ILE
1	D	772	ASP
1	D	799	THR
1	D	800	ARG
1	D	817	GLN
1	D	819	GLU
1	D	824	GLN
1	D	845	GLN
1	D	885	ASN
1	D	917	ARG

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Mol	Chain	Res	Type
1	D	986	ILE
1	D	1022	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	363	HIS
1	A	597	ASN
1	A	600	GLN
1	A	628	GLN
1	A	634	GLN
1	A	653	HIS
1	A	675	GLN
1	A	693	GLN
1	A	718	GLN
1	A	817	GLN
1	A	843	GLN
1	A	878	HIS
1	A	977	HIS
1	A	1022	GLN
1	B	50	GLN
1	B	102	ASN
1	B	370	GLN
1	B	394	ASN
1	B	597	ASN
1	B	600	GLN
1	B	653	HIS
1	B	693	GLN
1	B	718	GLN
1	B	725	ASN
1	B	735	HIS
1	B	739	HIS
1	B	757	GLN
1	B	775	GLN
1	B	804	ASN
1	B	824	GLN
1	B	878	HIS
1	B	890	GLN
1	B	974	HIS
1	B	977	HIS
1	B	1022	GLN

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Mol	Chain	Res	Type
1	C	102	ASN
1	C	135	GLN
1	C	554	GLN
1	C	581	ASN
1	C	597	ASN
1	C	628	GLN
1	C	634	GLN
1	C	693	GLN
1	C	718	GLN
1	C	725	ASN
1	C	775	GLN
1	C	817	GLN
1	C	824	GLN
1	C	878	HIS
1	C	977	HIS
1	D	102	ASN
1	D	163	GLN
1	D	216	HIS
1	D	294	ASN
1	D	581	ASN
1	D	597	ASN
1	D	646	HIS
1	D	675	GLN
1	D	693	GLN
1	D	718	GLN
1	D	804	ASN
1	D	817	GLN
1	D	824	GLN
1	D	863	GLN
1	D	878	HIS
1	D	1022	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 103 ligands modelled in this entry, 23 are monoatomic - leaving 80 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	IPT	A	2001	3	14,15,15	0.50	0	18,21,21	1.44	3 (16%)
5	DMS	C	8406	-	3,3,3	1.22	0	3,3,3	0.91	0
5	DMS	C	8414	-	3,3,3	0.28	0	3,3,3	0.31	0
5	DMS	C	8422	-	3,3,3	1.22	0	3,3,3	0.33	0
5	DMS	D	8405	-	3,3,3	0.41	0	3,3,3	0.28	0
5	DMS	D	8501	-	3,3,3	1.07	0	3,3,3	0.44	0
5	DMS	A	8409	-	3,3,3	1.74	1 (33%)	3,3,3	0.32	0
5	DMS	B	8410	-	3,3,3	1.19	0	3,3,3	0.21	0
5	DMS	C	8411	-	3,3,3	1.79	1 (33%)	3,3,3	0.60	0
5	DMS	A	8410	-	3,3,3	1.02	0	3,3,3	0.92	0
5	DMS	C	8403	-	3,3,3	1.21	0	3,3,3	0.49	0
5	DMS	C	8506	-	3,3,3	1.45	1 (33%)	3,3,3	0.29	0
5	DMS	A	8412	-	3,3,3	1.00	0	3,3,3	0.72	0
5	DMS	C	8503	-	3,3,3	0.96	0	3,3,3	0.64	0
5	DMS	A	8502	-	3,3,3	1.70	1 (33%)	3,3,3	1.09	0
5	DMS	A	8407	-	3,3,3	1.40	1 (33%)	3,3,3	0.61	0
5	DMS	B	8421	-	3,3,3	0.94	0	3,3,3	0.19	0
5	DMS	C	8402	-	3,3,3	1.42	1 (33%)	3,3,3	1.08	0
5	DMS	A	8404	-	3,3,3	1.24	1 (33%)	3,3,3	1.58	1 (33%)
5	DMS	C	8412	-	3,3,3	0.84	0	3,3,3	0.47	0
5	DMS	B	8402	-	3,3,3	1.08	0	3,3,3	0.26	0
5	DMS	C	8420	-	3,3,3	1.78	1 (33%)	3,3,3	0.56	0
5	DMS	A	8420	-	3,3,3	0.93	0	3,3,3	0.38	0
5	DMS	C	8501	-	3,3,3	0.80	0	3,3,3	0.33	0
5	DMS	C	8404	-	3,3,3	0.86	0	3,3,3	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DMS	D	8413	-	3,3,3	1.45	0	3,3,3	0.50	0
4	IPT	D	2001	3	14,15,15	0.43	0	18,21,21	1.97	5 (27%)
5	DMS	A	8415	-	3,3,3	1.55	1 (33%)	3,3,3	0.51	0
5	DMS	A	8602	-	3,3,3	0.92	0	3,3,3	0.29	0
5	DMS	B	8403	-	3,3,3	2.01	2 (66%)	3,3,3	0.20	0
5	DMS	C	8405	-	3,3,3	0.58	0	3,3,3	0.59	0
5	DMS	B	8404	-	3,3,3	0.28	0	3,3,3	1.02	0
4	IPT	A	2002	-	14,15,15	0.71	0	18,21,21	1.20	2 (11%)
5	DMS	D	8401	-	3,3,3	0.87	0	3,3,3	0.49	0
5	DMS	D	8411	-	3,3,3	0.54	0	3,3,3	0.29	0
5	DMS	B	8409	-	3,3,3	1.74	1 (33%)	3,3,3	0.85	0
5	DMS	C	8408	-	3,3,3	1.77	1 (33%)	3,3,3	0.74	0
5	DMS	B	8502	-	3,3,3	1.46	1 (33%)	3,3,3	0.48	0
5	DMS	D	8414	-	3,3,3	0.43	0	3,3,3	0.18	0
5	DMS	A	8405	-	3,3,3	0.15	0	3,3,3	0.63	0
5	DMS	A	8501	-	3,3,3	1.08	0	3,3,3	0.43	0
5	DMS	B	8420	-	3,3,3	1.63	0	3,3,3	0.29	0
5	DMS	B	8406	-	3,3,3	1.62	1 (33%)	3,3,3	0.38	0
4	IPT	B	2001	3	14,15,15	0.47	0	18,21,21	1.75	3 (16%)
5	DMS	B	8408	-	3,3,3	0.42	0	3,3,3	0.66	0
5	DMS	C	8401	-	3,3,3	0.34	0	3,3,3	0.90	0
5	DMS	A	8408	-	3,3,3	0.31	0	3,3,3	0.50	0
5	DMS	B	8401	-	3,3,3	0.23	0	3,3,3	0.66	0
5	DMS	C	8421	-	3,3,3	0.67	0	3,3,3	0.21	0
5	DMS	D	8408	-	3,3,3	0.92	0	3,3,3	0.46	0
5	DMS	A	8403	-	3,3,3	1.55	1 (33%)	3,3,3	0.45	0
5	DMS	D	8403	-	3,3,3	1.58	0	3,3,3	0.57	0
5	DMS	D	8410	-	3,3,3	1.62	1 (33%)	3,3,3	1.03	0
5	DMS	C	8407	-	3,3,3	1.67	0	3,3,3	0.76	0
5	DMS	A	8413	-	3,3,3	1.32	0	3,3,3	0.36	0
5	DMS	D	8415	-	3,3,3	1.22	0	3,3,3	0.57	0
5	DMS	D	8412	-	3,3,3	0.36	0	3,3,3	0.43	0
5	DMS	D	8407	-	3,3,3	1.70	0	3,3,3	0.96	0
5	DMS	A	8411	-	3,3,3	1.11	0	3,3,3	0.02	0
5	DMS	C	8425	3	3,3,3	1.92	1 (33%)	3,3,3	0.08	0
5	DMS	B	8411	-	3,3,3	0.72	0	3,3,3	0.34	0
5	DMS	D	8404	-	3,3,3	1.63	1 (33%)	3,3,3	0.39	0
5	DMS	B	8412	-	3,3,3	0.50	0	3,3,3	0.12	0
5	DMS	A	8402	-	3,3,3	1.11	0	3,3,3	0.14	0
5	DMS	D	8417	-	3,3,3	1.26	1 (33%)	3,3,3	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DMS	D	8409	-	3,3,3	1.78	1 (33%)	3,3,3	1.18	0
5	DMS	B	8413	-	3,3,3	1.88	1 (33%)	3,3,3	0.07	0
5	DMS	B	8501	-	3,3,3	1.87	1 (33%)	3,3,3	0.44	0
4	IPT	C	2001	3	14,15,15	0.59	0	18,21,21	1.91	5 (27%)
5	DMS	B	8407	-	3,3,3	2.04	2 (66%)	3,3,3	1.31	1 (33%)
5	DMS	C	8409	-	3,3,3	2.05	1 (33%)	3,3,3	0.56	0
5	DMS	B	8425	3	3,3,3	0.65	0	3,3,3	0.24	0
5	DMS	A	8421	-	3,3,3	0.68	0	3,3,3	0.17	0
5	DMS	C	8415	-	3,3,3	1.43	0	3,3,3	0.36	0
5	DMS	A	8401	-	3,3,3	0.71	0	3,3,3	0.36	0
5	DMS	C	8410	-	3,3,3	0.60	0	3,3,3	0.27	0
5	DMS	D	8704	-	3,3,3	0.46	0	3,3,3	0.10	0
5	DMS	B	8405	-	3,3,3	1.14	0	3,3,3	0.82	0
5	DMS	D	8402	-	3,3,3	0.61	0	3,3,3	0.43	0
4	IPT	D	2002	-	14,15,15	0.54	0	18,21,21	1.78	5 (27%)

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	IPT	D	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	A	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	C	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	D	2002	-	-	0/6/26/26	0/1/1/1
4	IPT	A	2002	-	-	0/6/26/26	0/1/1/1
4	IPT	B	2001	3	-	1/6/26/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8413	DMS	O-S	3.24	1.72	1.50
5	C	8425	DMS	O-S	3.23	1.72	1.50
5	C	8409	DMS	O-S	3.09	1.71	1.50
5	D	8409	DMS	O-S	3.00	1.70	1.50
5	B	8403	DMS	O-S	2.83	1.69	1.50
5	C	8420	DMS	C2-S	2.64	1.95	1.75
5	B	8407	DMS	O-S	2.63	1.68	1.50
5	A	8409	DMS	O-S	2.59	1.67	1.50
5	D	8410	DMS	O-S	2.57	1.67	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8502	DMS	C1-S	2.57	1.94	1.75
5	B	8406	DMS	C2-S	2.51	1.94	1.75
5	A	8415	DMS	O-S	2.50	1.67	1.50
5	B	8501	DMS	C1-S	2.49	1.94	1.75
5	B	8409	DMS	O-S	2.47	1.66	1.50
5	B	8407	DMS	C2-S	2.35	1.93	1.75
5	C	8411	DMS	C1-S	2.32	1.93	1.75
5	C	8408	DMS	O-S	2.30	1.65	1.50
5	C	8506	DMS	O-S	2.24	1.65	1.50
5	C	8402	DMS	O-S	2.21	1.65	1.50
5	A	8407	DMS	O-S	2.14	1.64	1.50
5	A	8403	DMS	C1-S	-2.08	1.60	1.75
5	B	8502	DMS	C1-S	2.07	1.91	1.75
5	D	8417	DMS	O-S	2.02	1.63	1.50
5	A	8404	DMS	C2-S	2.02	1.90	1.75
5	D	8404	DMS	O-S	-2.01	1.36	1.50
5	B	8403	DMS	C2-S	2.00	1.90	1.75

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2001	IPT	C2-C1-S1	-4.61	104.20	111.30
4	D	2001	IPT	C6-C5-C4	4.37	123.24	113.00
4	D	2002	IPT	C6-C5-C4	4.26	122.97	113.00
4	B	2001	IPT	C6-C5-C4	4.11	122.63	113.00
4	B	2001	IPT	C2-C1-S1	-3.69	105.61	111.30
4	D	2002	IPT	O6-C6-C5	3.67	123.89	111.29
4	C	2001	IPT	O2-C2-C1	-3.46	103.90	110.27
4	D	2001	IPT	O5-C5-C6	-3.24	98.37	106.44
4	D	2001	IPT	C2-C1-S1	-3.24	106.31	111.30
4	D	2001	IPT	O6-C6-C5	-3.12	100.59	111.29
4	C	2001	IPT	O5-C5-C6	-2.72	99.67	106.44
4	B	2001	IPT	O6-C6-C5	-2.71	101.99	111.29
4	D	2001	IPT	O2-C2-C1	-2.71	105.29	110.27
4	D	2002	IPT	C2-C1-S1	-2.70	107.14	111.30
5	A	8404	DMS	C2-S-C1	2.69	112.30	98.44
4	A	2002	IPT	C2-C1-S1	-2.49	107.47	111.30
4	A	2001	IPT	C2-C1-S1	-2.45	107.53	111.30
4	A	2001	IPT	O2-C2-C3	-2.41	104.77	110.35
4	D	2002	IPT	C3'-C1'-C2'	-2.41	103.42	111.73
5	B	8407	DMS	C2-S-C1	2.27	110.10	98.44
4	D	2002	IPT	O5-C5-C6	-2.25	100.83	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2001	IPT	C1-C2-C3	-2.21	106.22	110.59
4	C	2001	IPT	C6-C5-C4	2.20	118.15	113.00
4	A	2002	IPT	O3-C3-C2	2.13	115.28	110.35
4	C	2001	IPT	C3'-C1'-C2'	-2.06	104.63	111.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

17 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2001	IPT	1	0
5	C	8406	DMS	1	0
5	B	8410	DMS	1	0
5	C	8411	DMS	1	0
5	A	8410	DMS	2	0
5	C	8506	DMS	5	0
5	A	8412	DMS	3	0
5	A	8502	DMS	1	0
5	C	8420	DMS	1	0
5	A	8420	DMS	1	0
4	A	2002	IPT	1	0
5	C	8408	DMS	3	0
5	D	8414	DMS	1	0
5	D	8403	DMS	2	0
5	D	8410	DMS	1	0
5	D	8417	DMS	1	0
5	B	8413	DMS	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1011/1023 (98%)	0.06	44 (4%)	34	40	11, 22, 50, 98	0
1	B	1011/1023 (98%)	0.05	35 (3%)	44	50	11, 20, 51, 100	0
1	C	1011/1023 (98%)	-0.00	31 (3%)	49	55	11, 19, 50, 99	0
1	D	1011/1023 (98%)	0.06	44 (4%)	34	40	12, 23, 52, 96	0
All	All	4044/4092 (98%)	0.04	154 (3%)	40	47	11, 21, 51, 100	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	731	PRO	11.0
1	B	730	LEU	9.1
1	A	735	HIS	8.8
1	C	733	ALA	8.4
1	C	731	PRO	8.0
1	D	730	LEU	8.0
1	D	735	HIS	7.6
1	B	733	ALA	7.5
1	B	689	GLU	7.3
1	B	732	ALA	7.3
1	A	733	ALA	7.1
1	D	686	PRO	7.0
1	D	733	ALA	6.8
1	A	730	LEU	6.7
1	C	732	ALA	6.7
1	A	685	LEU	6.5
1	D	731	PRO	6.5
1	C	685	LEU	6.4
1	C	730	LEU	6.2
1	D	732	ALA	6.2
1	B	1023	LYS	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	6.1
1	A	732	ALA	6.1
1	C	686	PRO	5.8
1	B	734	SER	5.6
1	B	688	PRO	5.5
1	C	689	GLU	5.2
1	C	580	GLU	5.1
1	C	735	HIS	4.9
1	A	731	PRO	4.9
1	C	581	ASN	4.7
1	D	685	LEU	4.7
1	B	685	LEU	4.7
1	C	633	GLY	4.6
1	B	686	PRO	4.6
1	C	729	THR	4.5
1	A	684	GLU	4.4
1	B	687	GLN	4.3
1	C	687	GLN	4.2
1	B	770	ILE	4.2
1	A	689	GLU	4.1
1	D	131	GLU	4.1
1	D	687	GLN	4.0
1	D	581	ASN	4.0
1	B	729	THR	4.0
1	D	772	ASP	4.0
1	D	799	THR	3.9
1	A	79	PRO	3.9
1	D	689	GLU	3.8
1	A	1023	LYS	3.8
1	A	734	SER	3.8
1	A	580	GLU	3.7
1	D	684	GLU	3.7
1	D	800	ARG	3.7
1	B	798	ALA	3.7
1	B	684	GLU	3.6
1	A	799	THR	3.6
1	A	78	LEU	3.6
1	A	687	GLN	3.5
1	D	729	THR	3.5
1	D	634	GLN	3.5
1	D	798	ALA	3.4
1	D	582	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	817	GLN	3.4
1	C	831	ALA	3.3
1	B	690	SER	3.3
1	A	800	ARG	3.3
1	C	634	GLN	3.3
1	D	688	PRO	3.2
1	C	799	THR	3.2
1	D	734	SER	3.2
1	A	581	ASN	3.2
1	B	663	LEU	3.2
1	B	737	ILE	3.1
1	D	1023	LYS	3.1
1	B	633	GLY	3.1
1	C	736	ALA	3.1
1	A	729	THR	3.0
1	D	753	ASN	3.0
1	A	690	SER	3.0
1	D	1022	GLN	3.0
1	A	798	ALA	3.0
1	B	735	HIS	3.0
1	A	632	SER	2.9
1	C	688	PRO	2.9
1	C	579	ASP	2.9
1	A	129	VAL	2.9
1	D	79	PRO	2.9
1	A	761	GLN	2.9
1	C	582	GLY	2.8
1	D	682	LEU	2.7
1	A	71	GLU	2.7
1	B	71	GLU	2.7
1	B	634	GLN	2.7
1	A	131	GLU	2.7
1	C	1022	GLN	2.7
1	B	728	VAL	2.7
1	A	728	VAL	2.6
1	D	632	SER	2.6
1	D	580	GLU	2.6
1	D	845	GLN	2.6
1	B	831	ALA	2.6
1	D	728	VAL	2.6
1	D	177	LEU	2.6
1	D	578	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	772	ASP	2.5
1	C	632	SER	2.5
1	C	745	MET	2.5
1	C	684	GLU	2.5
1	D	633	GLY	2.5
1	D	831	ALA	2.5
1	D	179	ALA	2.4
1	B	753	ASN	2.4
1	A	688	PRO	2.4
1	A	634	GLN	2.4
1	C	800	ARG	2.4
1	A	669	PRO	2.4
1	B	1022	GLN	2.4
1	B	799	THR	2.4
1	D	891	VAL	2.3
1	B	959	ILE	2.3
1	A	668	VAL	2.3
1	D	579	ASP	2.3
1	C	583	ASN	2.3
1	D	72	SER	2.2
1	A	831	ALA	2.2
1	C	737	ILE	2.2
1	D	135	GLN	2.2
1	A	977	HIS	2.2
1	B	800	ARG	2.2
1	C	830	LEU	2.2
1	D	830	LEU	2.2
1	D	736	ALA	2.2
1	B	69	VAL	2.2
1	A	135	GLN	2.2
1	A	362	LEU	2.2
1	B	681	GLU	2.2
1	A	727	SER	2.1
1	C	690	SER	2.1
1	D	71	GLU	2.1
1	C	362	LEU	2.1
1	D	130	ASP	2.1
1	A	80	GLU	2.1
1	A	179	ALA	2.1
1	A	582	GLY	2.1
1	C	584	PRO	2.1
1	A	76	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	817	GLN	2.0
1	A	64	PRO	2.0
1	B	75	GLU	2.0
1	B	653	HIS	2.0
1	D	737	ILE	2.0
1	A	583	ASN	2.0
1	A	578	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	C	8422	4/4	0.90	0.17	34,42,54,66	0
5	DMS	A	8420	4/4	0.92	0.14	39,40,51,84	0
5	DMS	A	8502	4/4	0.92	0.13	40,41,45,54	0
5	DMS	A	8602	4/4	0.92	0.21	42,52,61,79	0
5	DMS	C	8420	4/4	0.92	0.17	51,51,62,94	0
5	DMS	A	8409	4/4	0.92	0.15	36,38,45,46	0
5	DMS	D	8410	4/4	0.93	0.10	25,39,50,55	0
5	DMS	D	8415	4/4	0.93	0.13	39,41,58,66	0
5	DMS	C	8406	4/4	0.94	0.10	22,46,49,55	0
5	DMS	C	8503	4/4	0.94	0.20	35,41,54,64	0
5	DMS	C	8415	4/4	0.94	0.16	29,55,67,77	0
5	DMS	D	8413	4/4	0.94	0.19	27,40,43,54	0
5	DMS	A	8407	4/4	0.94	0.15	32,34,38,40	0
5	DMS	B	8406	4/4	0.95	0.15	43,44,100,100	0
5	DMS	C	8421	4/4	0.95	0.18	48,57,64,83	0
5	DMS	B	8407	4/4	0.95	0.10	22,33,38,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	B	8413	4/4	0.95	0.21	38,54,55,100	0
5	DMS	C	8506	4/4	0.95	0.20	46,50,76,100	0
5	DMS	D	8407	4/4	0.95	0.12	26,31,33,40	0
5	DMS	D	8408	4/4	0.95	0.13	35,42,49,50	0
5	DMS	B	8420	4/4	0.95	0.13	41,44,49,100	0
4	IPT	D	2002	15/15	0.95	0.11	19,26,33,100	0
5	DMS	A	8421	4/4	0.95	0.23	43,59,69,79	0
4	IPT	A	2001	15/15	0.96	0.10	14,18,23,37	0
5	DMS	B	8409	4/4	0.96	0.11	22,39,41,41	0
4	IPT	B	2001	15/15	0.96	0.08	10,18,24,25	0
4	IPT	C	2001	15/15	0.96	0.09	15,17,26,26	0
5	DMS	B	8425	4/4	0.96	0.14	43,54,64,100	0
5	DMS	C	8404	4/4	0.96	0.08	26,29,35,40	0
5	DMS	A	8413	4/4	0.96	0.17	37,52,80,94	0
5	DMS	C	8407	4/4	0.96	0.08	28,28,31,39	0
5	DMS	C	8408	4/4	0.96	0.10	16,38,39,40	0
5	DMS	A	8415	4/4	0.96	0.12	30,37,54,62	0
5	DMS	D	8417	4/4	0.96	0.14	26,28,64,100	0
5	DMS	D	8501	4/4	0.96	0.09	25,40,41,47	0
5	DMS	B	8410	4/4	0.97	0.10	37,39,40,42	0
5	DMS	A	8408	4/4	0.97	0.10	35,47,48,100	0
5	DMS	A	8501	4/4	0.97	0.09	22,41,53,58	0
5	DMS	C	8425	4/4	0.97	0.16	38,40,44,100	0
5	DMS	C	8501	4/4	0.97	0.09	21,42,47,48	0
3	NA	B	3103	1/1	0.97	0.08	35,35,35,35	0
5	DMS	B	8502	4/4	0.97	0.10	28,29,46,100	0
5	DMS	D	8404	4/4	0.97	0.08	18,27,31,34	0
5	DMS	A	8410	4/4	0.97	0.08	26,45,47,100	0
5	DMS	B	8402	4/4	0.97	0.07	21,28,30,31	0
5	DMS	D	8409	4/4	0.97	0.09	34,34,35,42	0
4	IPT	D	2001	15/15	0.97	0.07	14,18,31,33	0
4	IPT	A	2002	15/15	0.97	0.10	13,21,26,28	15
5	DMS	D	8414	4/4	0.97	0.16	31,61,100,100	0
5	DMS	C	8409	4/4	0.97	0.09	24,37,39,57	0
5	DMS	C	8410	4/4	0.97	0.08	29,36,44,45	0
3	NA	B	3104	1/1	0.97	0.09	28,28,28,28	0
5	DMS	D	8704	4/4	0.97	0.23	32,55,100,100	0
2	MG	D	3002	1/1	0.98	0.07	23,23,23,23	0
3	NA	D	3103	1/1	0.98	0.06	34,34,34,34	0
5	DMS	A	8403	4/4	0.98	0.07	20,24,25,28	0
5	DMS	A	8411	4/4	0.98	0.08	28,32,36,100	0
5	DMS	B	8501	4/4	0.98	0.07	18,19,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	A	8412	4/4	0.98	0.08	29,34,41,100	0
5	DMS	C	8402	4/4	0.98	0.07	21,25,27,28	0
5	DMS	D	8403	4/4	0.98	0.08	28,28,31,38	0
5	DMS	C	8403	4/4	0.98	0.08	21,23,29,30	0
5	DMS	D	8405	4/4	0.98	0.07	23,23,26,27	0
5	DMS	B	8403	4/4	0.98	0.08	26,28,30,42	0
5	DMS	C	8405	4/4	0.98	0.09	23,25,26,29	0
5	DMS	B	8404	4/4	0.98	0.07	21,23,27,35	0
5	DMS	B	8405	4/4	0.98	0.07	23,25,28,31	0
5	DMS	A	8404	4/4	0.98	0.07	21,23,32,36	0
5	DMS	A	8405	4/4	0.98	0.07	26,28,31,34	0
5	DMS	B	8408	4/4	0.98	0.08	40,41,54,100	0
5	DMS	C	8411	4/4	0.98	0.11	24,30,33,100	0
5	DMS	C	8414	4/4	0.98	0.14	27,46,60,76	0
2	MG	B	3007	1/1	0.98	0.17	24,24,24,24	0
2	MG	A	3001	1/1	0.99	0.04	18,18,18,18	0
2	MG	C	3001	1/1	0.99	0.04	17,17,17,17	0
5	DMS	B	8411	4/4	0.99	0.08	34,38,49,100	0
5	DMS	B	8412	4/4	0.99	0.07	22,29,30,34	0
2	MG	D	3001	1/1	0.99	0.04	17,17,17,17	0
2	MG	A	3002	1/1	0.99	0.06	21,21,21,21	0
5	DMS	B	8421	4/4	0.99	0.18	28,38,52,53	0
3	NA	A	3101	1/1	0.99	0.07	18,18,18,18	0
3	NA	A	3103	1/1	0.99	0.07	29,29,29,29	0
5	DMS	D	8401	4/4	0.99	0.07	17,19,21,22	0
5	DMS	D	8402	4/4	0.99	0.06	17,26,28,29	0
3	NA	B	3102	1/1	0.99	0.06	16,16,16,16	0
5	DMS	C	8401	4/4	0.99	0.07	16,18,22,22	0
5	DMS	A	8401	4/4	0.99	0.06	16,19,19,19	0
5	DMS	A	8402	4/4	0.99	0.06	18,23,24,28	0
5	DMS	B	8401	4/4	0.99	0.08	15,16,16,19	0
2	MG	B	3001	1/1	0.99	0.04	18,18,18,18	0
2	MG	B	3002	1/1	0.99	0.06	22,22,22,22	0
5	DMS	D	8411	4/4	0.99	0.06	25,28,37,48	0
5	DMS	D	8412	4/4	0.99	0.06	23,26,32,39	0
3	NA	C	3102	1/1	0.99	0.05	16,16,16,16	0
3	NA	C	3103	1/1	0.99	0.07	30,30,30,30	0
3	NA	C	3104	1/1	0.99	0.05	31,31,31,31	0
3	NA	D	3101	1/1	0.99	0.09	20,20,20,20	0
3	NA	D	3102	1/1	0.99	0.06	16,16,16,16	0
5	DMS	C	8412	4/4	0.99	0.07	24,31,39,43	0
3	NA	B	3101	1/1	1.00	0.05	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NA	C	3101	1/1	1.00	0.05	17,17,17,17	0
3	NA	A	3102	1/1	1.00	0.06	16,16,16,16	0
2	MG	C	3002	1/1	1.00	0.05	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.