



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 11:21 AM UTC

PDB ID : 1JZ5 / pdb_00001jz5
Title : E. COLI (lacZ) BETA-GALACTOSIDASE IN COMPLEX WITH D-GALCT
OPYRANOSYL-1-ON
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

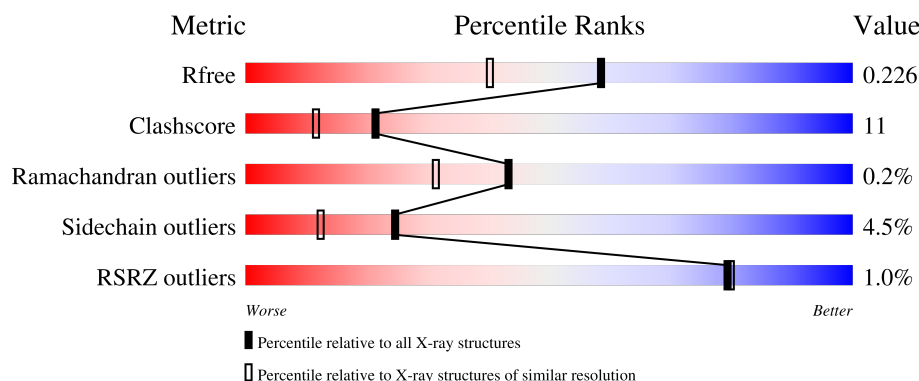
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	1023	70% 24% 5%
1	B	1023	69% 25% 5%
1	C	1023	68% 26% 5%
1	D	1023	70% 23% 5%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	D	8419	-	-	X	-
5	DMS	D	8508	-	-	X	-
5	DMS	D	8701	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36964 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	98	11	0
			8205	5185	1455	1527	38			
1	B	1011	Total	C	N	O	S	64	11	0
			8205	5185	1455	1527	38			
1	C	1011	Total	C	N	O	S	49	11	0
			8205	5185	1455	1527	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			

There are 32 discrepancies between the modelled and reference sequences:

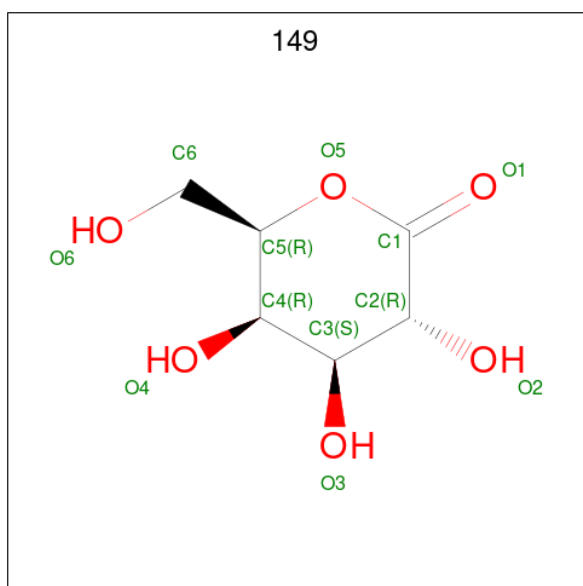
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	cloning artifact	? P00722
A	2	SER	MET	cloning artifact	? P00722
A	3	HIS	ILE	cloning artifact	? P00722
A	4	MET	THR	cloning artifact	? P00722
A	5	LEU	ASP	cloning artifact	? P00722
A	6	GLU	SER	cloning artifact	? P00722
A	7	ASP	LEU	cloning artifact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

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

- Molecule 2 is D-galactonolactone (CCD ID: 149) (formula: $C_6H_{10}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

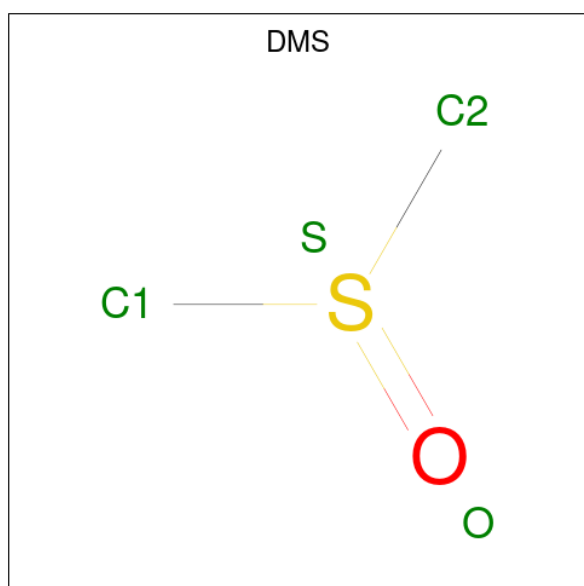
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

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

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

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

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

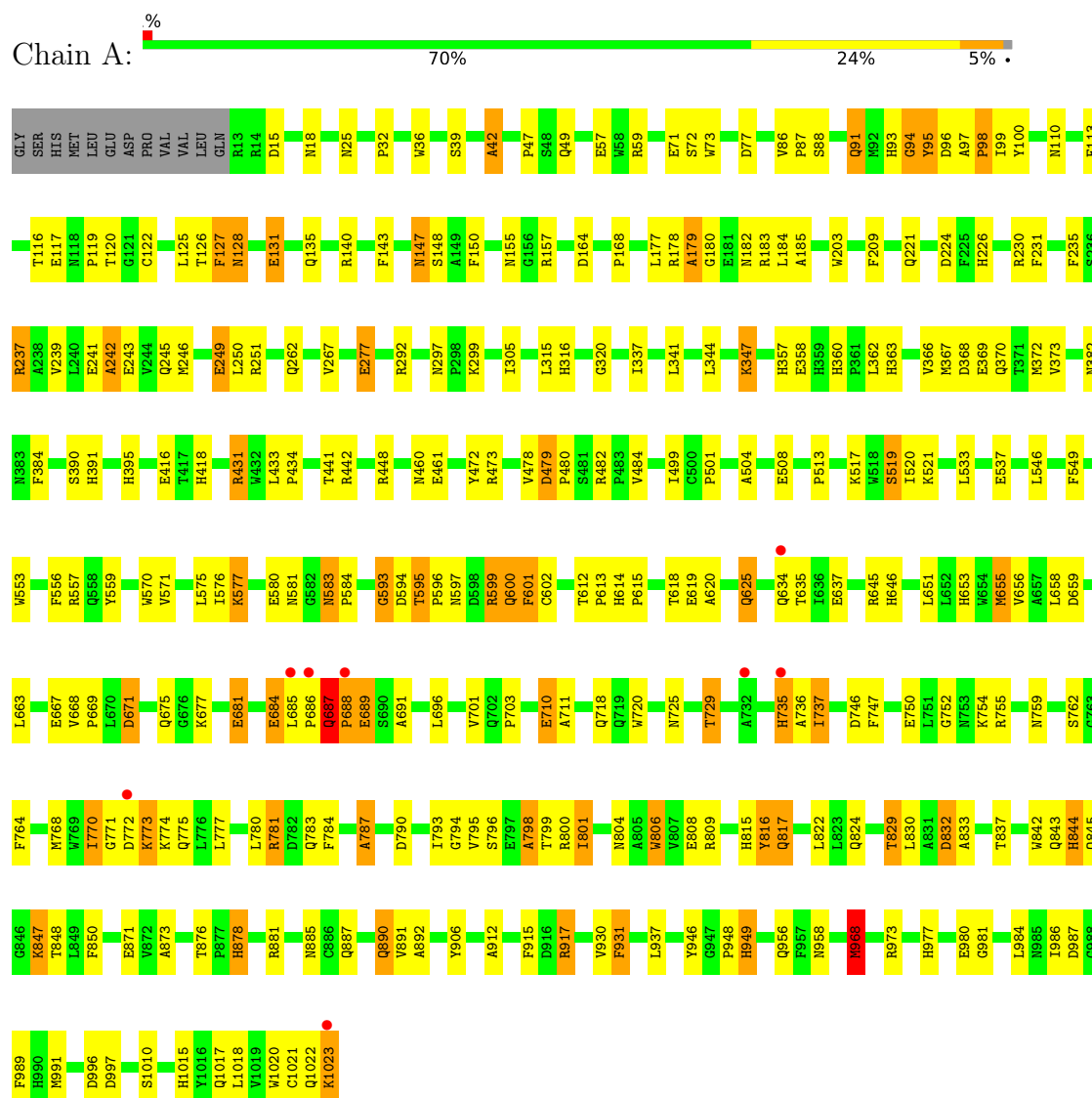
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	953	Total	O	0	0
			953	953		
6	B	937	Total	O	0	0
			937	937		
6	C	952	Total	O	0	0
			952	952		
6	D	959	Total	O	0	0
			959	959		

3 Residue-property plots

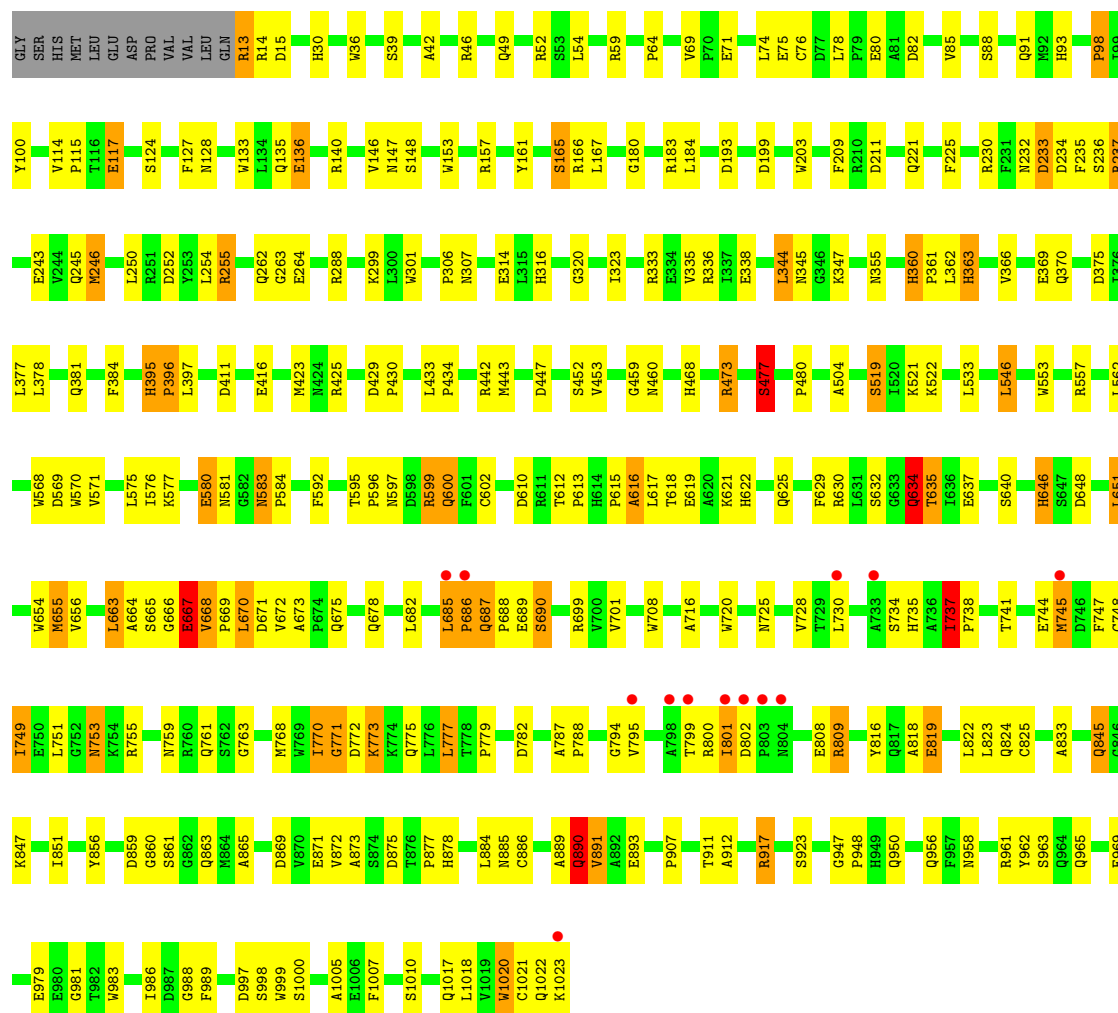
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-Galactosidase

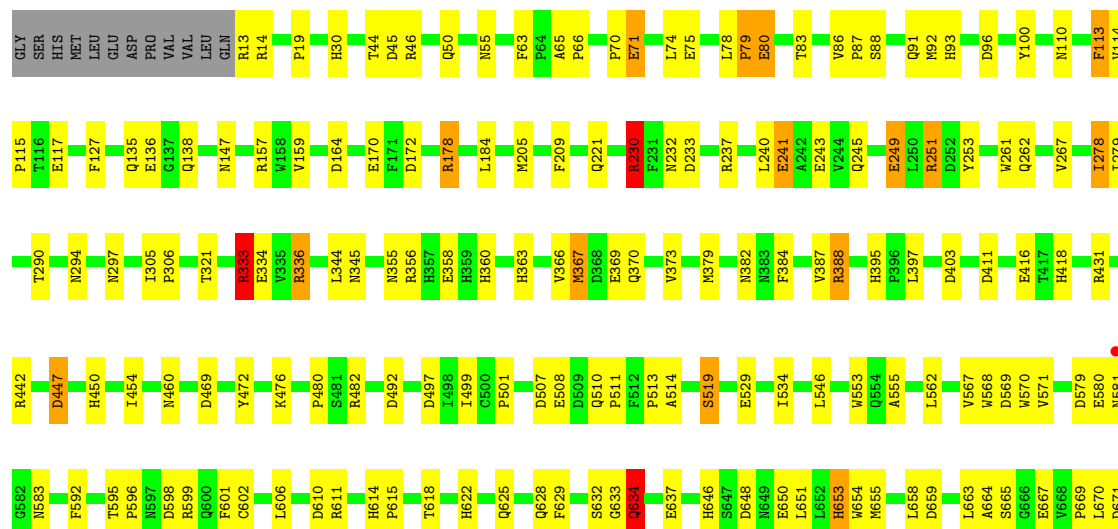


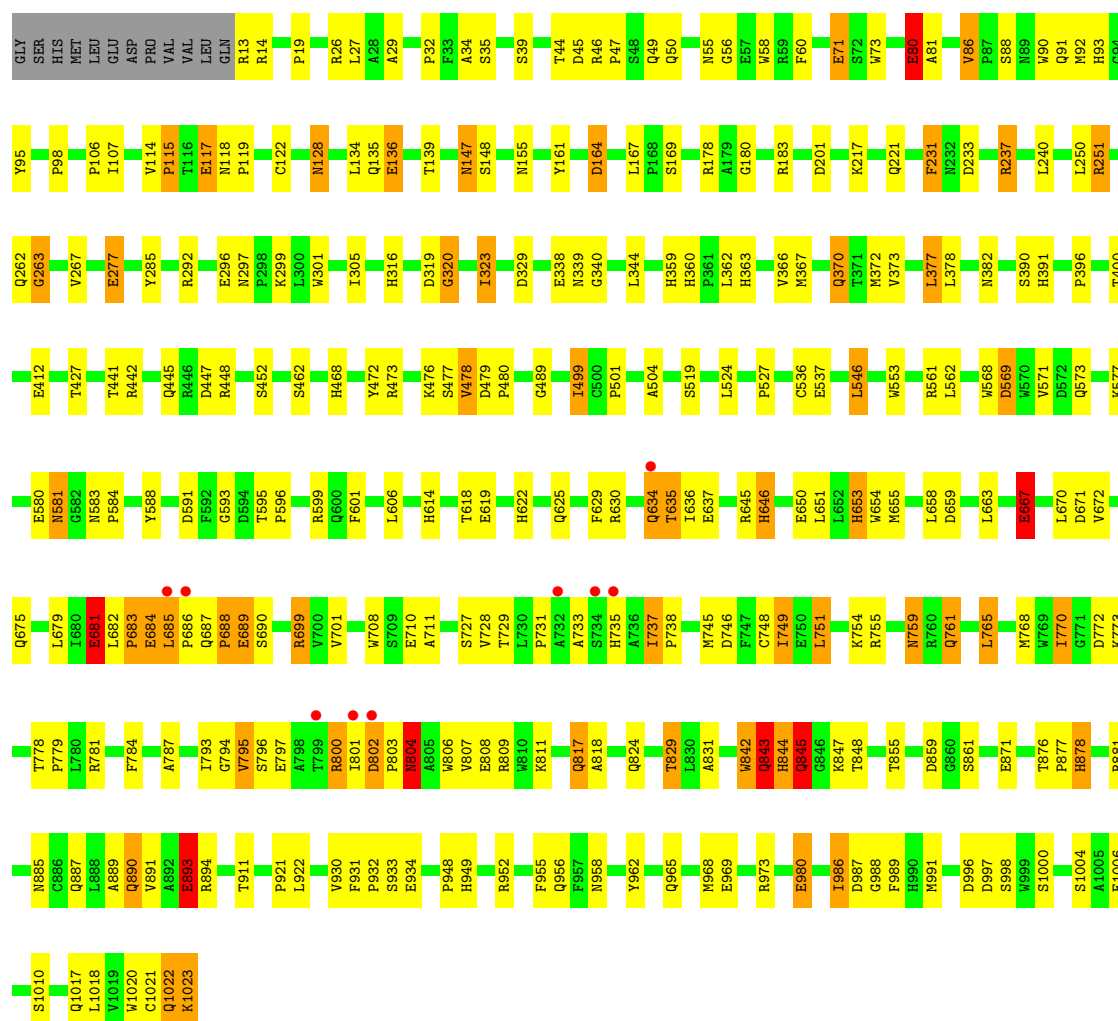
• Molecule 1: Beta-Galactosidase





• Molecule 1: Beta-Galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.69Å 168.02Å 201.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.80 17.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.4 (17.00-1.80) 90.2 (17.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.80Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.160 , 0.231 0.163 , 0.226	Depositor DCC
R_{free} test set	6053 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 108.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36964	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 37.04 % 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 4.5593e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 149, DMS, NA, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.34	9/8448 (0.1%)	1.85	145/11526 (1.3%)
1	B	1.34	12/8448 (0.1%)	1.84	157/11526 (1.4%)
1	C	1.31	15/8448 (0.2%)	1.85	153/11526 (1.3%)
1	D	1.36	22/8367 (0.3%)	1.87	155/11415 (1.4%)
All	All	1.34	58/33711 (0.2%)	1.85	610/45993 (1.3%)

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

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

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	297	ASN	C-O	-7.14	1.20	1.23
1	D	167	LEU	N-CA	6.85	1.51	1.45
1	A	479	ASP	C-N	-6.79	1.26	1.34
1	A	537	GLU	CD-OE2	6.76	1.38	1.25
1	C	418	HIS	CE1-NE2	6.33	1.38	1.32
1	A	681	GLU	CD-OE2	6.26	1.37	1.25
1	A	710	GLU	CD-OE2	6.11	1.36	1.25
1	C	388	ARG	CZ-NH1	6.09	1.41	1.32
1	A	57	GLU	CA-C	-6.03	1.45	1.52
1	D	285	TYR	CA-CB	5.88	1.60	1.53
1	D	86	VAL	CA-CB	-5.88	1.50	1.54
1	C	450	HIS	CE1-NE2	5.85	1.38	1.32
1	D	893	GLU	CD-OE2	5.82	1.36	1.25
1	D	537	GLU	CD-OE2	5.75	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	772	ASP	CG-OD2	5.68	1.36	1.25
1	D	650	GLU	CD-OE2	5.65	1.36	1.25
1	C	719	GLN	CA-C	-5.63	1.45	1.52
1	D	233	ASP	CG-OD2	5.62	1.36	1.25
1	B	770	ILE	CA-CB	-5.60	1.47	1.53
1	B	950	GLN	C-O	5.59	1.30	1.23
1	B	580	GLU	CD-OE2	5.57	1.35	1.25
1	A	249	GLU	CD-OE2	5.56	1.35	1.25
1	D	580	GLU	CD-OE2	5.53	1.35	1.25
1	D	468	HIS	CE1-NE2	5.53	1.38	1.32
1	C	75	GLU	CD-OE2	5.50	1.35	1.25
1	B	668	VAL	C-N	-5.49	1.26	1.33
1	C	511	PRO	N-CA	-5.46	1.43	1.47
1	D	391	HIS	ND1-CE1	5.46	1.38	1.32
1	B	557	ARG	NE-CZ	5.45	1.39	1.33
1	C	893	GLU	CD-OE2	5.44	1.35	1.25
1	C	403	ASP	CG-OD2	5.39	1.35	1.25
1	D	479	ASP	C-O	-5.33	1.18	1.24
1	D	681	GLU	CD-OE2	5.33	1.35	1.25
1	B	947	GLY	C-N	-5.32	1.28	1.33
1	A	242	ALA	C-O	5.29	1.29	1.24
1	D	80	GLU	CD-OE2	5.29	1.35	1.25
1	B	699	ARG	CZ-NH1	5.29	1.40	1.32
1	D	980	GLU	CD-OE2	5.25	1.35	1.25
1	C	980	GLU	CD-OE2	5.23	1.35	1.25
1	C	117	GLU	CD-OE2	5.22	1.35	1.25
1	B	459	GLY	N-CA	5.21	1.51	1.45
1	B	468	HIS	CE1-NE2	5.18	1.37	1.32
1	A	684	GLU	CD-OE2	5.18	1.35	1.25
1	C	447	ASP	CG-OD2	5.17	1.35	1.25
1	D	479	ASP	C-N	-5.17	1.28	1.34
1	C	492	ASP	CG-OD2	5.16	1.35	1.25
1	C	170	GLU	CD-OE2	5.14	1.35	1.25
1	D	71	GLU	CD-OE2	5.12	1.35	1.25
1	D	139	THR	C-O	5.09	1.30	1.24
1	D	167	LEU	CA-CB	5.08	1.60	1.54
1	C	454	ILE	C-O	-5.08	1.19	1.24
1	B	316	HIS	CG-CD2	5.07	1.41	1.35
1	D	684	GLU	CD-OE2	5.07	1.34	1.25
1	C	261	TRP	CA-C	-5.05	1.46	1.52
1	D	117	GLU	CD-OE2	5.05	1.34	1.25
1	B	140	ARG	C-O	5.01	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	ASP	CG-OD2	5.01	1.34	1.25
1	D	569	ASP	CG-OD2	5.01	1.34	1.25

All (610) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	297	ASN	O-C-N	-13.33	115.40	121.53
1	C	725	ASN	CA-CB-CG	-10.91	101.69	112.60
1	A	844	HIS	CA-CB-CG	-10.90	102.89	113.80
1	D	845	GLN	CA-C-N	-10.89	106.56	122.46
1	D	845	GLN	C-N-CA	-10.89	106.56	122.46
1	A	599	ARG	CB-CA-C	-10.49	104.47	116.54
1	C	363	HIS	CA-CB-CG	-10.03	103.77	113.80
1	B	576	ILE	CB-CA-C	-9.80	98.75	110.91
1	B	668	VAL	CB-CA-C	-9.62	99.90	109.33
1	B	699	ARG	NE-CZ-NH1	9.58	131.08	121.50
1	B	363	HIS	CA-CB-CG	-9.17	104.63	113.80
1	A	997	ASP	CA-CB-CG	-9.16	103.44	112.60
1	B	82	ASP	CA-CB-CG	-9.06	103.54	112.60
1	D	893	GLU	CB-CG-CD	9.01	127.92	112.60
1	A	746	ASP	CA-CB-CG	-8.97	103.63	112.60
1	C	680	ILE	CA-C-N	-8.79	110.59	122.72
1	C	680	ILE	C-N-CA	-8.79	110.59	122.72
1	C	294	ASN	CA-CB-CG	-8.76	103.84	112.60
1	B	599	ARG	CB-CA-C	-8.60	106.65	116.54
1	A	790	ASP	CA-CB-CG	-8.53	104.07	112.60
1	A	691	ALA	N-CA-C	8.46	121.86	110.35
1	C	113	PHE	CA-CB-CG	-8.41	105.39	113.80
1	A	816	TYR	CA-C-N	-8.39	109.45	122.37
1	A	816	TYR	C-N-CA	-8.39	109.45	122.37
1	D	1000	SER	N-CA-C	-8.37	100.60	108.13
1	D	90	TRP	N-CA-C	8.37	121.33	111.71
1	B	890	GLN	N-CA-C	8.19	123.12	110.42
1	C	592	PHE	CA-CB-CG	-8.16	105.64	113.80
1	A	97	ALA	N-CA-C	8.14	120.32	110.07
1	C	859	ASP	CA-C-N	8.14	129.15	120.03
1	C	859	ASP	C-N-CA	8.14	129.15	120.03
1	C	360	HIS	CA-CB-CG	-8.00	105.80	113.80
1	A	878	HIS	CA-CB-CG	-7.99	105.81	113.80
1	D	601	PHE	CA-CB-CG	-7.93	105.87	113.80
1	B	670	LEU	CA-C-N	-7.87	109.16	122.92
1	B	670	LEU	C-N-CA	-7.87	109.16	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	699	ARG	NE-CZ-NH2	-7.87	112.12	119.20
1	A	18	ASN	O-C-N	7.84	125.97	121.27
1	A	725	ASN	CA-CB-CG	-7.80	104.80	112.60
1	A	989	PHE	CA-CB-CG	-7.78	106.02	113.80
1	A	231	PHE	CA-CB-CG	-7.78	106.02	113.80
1	D	297	ASN	CA-C-O	7.75	126.46	120.26
1	B	442	ARG	NE-CZ-NH2	-7.70	112.27	119.20
1	D	728	VAL	CA-C-O	7.69	126.07	119.38
1	B	571	VAL	N-CA-C	7.66	119.51	108.48
1	A	583	ASN	CA-CB-CG	-7.65	104.95	112.60
1	C	772	ASP	CA-CB-CG	7.64	120.24	112.60
1	A	968	MET	CA-C-N	-7.62	109.97	122.54
1	A	968	MET	C-N-CA	-7.62	109.97	122.54
1	D	128	ASN	CA-CB-CG	-7.52	105.08	112.60
1	B	670	LEU	CB-CA-C	-7.51	97.36	109.75
1	C	778	THR	CA-C-N	7.51	127.95	119.92
1	C	778	THR	C-N-CA	7.51	127.95	119.92
1	B	646	HIS	CA-CB-CG	-7.50	106.30	113.80
1	B	699	ARG	CD-NE-CZ	7.49	134.89	124.40
1	C	19	PRO	N-CA-CB	7.48	110.44	103.41
1	B	39	SER	CA-CB-OG	-7.43	96.24	111.10
1	B	246	MET	CG-SD-CE	-7.41	84.59	100.90
1	D	221	GLN	N-CA-CB	-7.41	99.61	111.62
1	D	667	GLU	N-CA-CB	7.38	124.34	111.13
1	B	320	GLY	CA-C-N	-7.35	111.82	122.19
1	B	320	GLY	C-N-CA	-7.35	111.82	122.19
1	D	634	GLN	CB-CA-C	7.31	123.07	110.72
1	D	614	HIS	N-CA-C	-7.30	100.57	110.36
1	C	648	ASP	CA-CB-CG	-7.30	105.30	112.60
1	B	635	THR	N-CA-C	7.29	120.61	108.73
1	C	958	ASN	N-CA-CB	7.28	124.61	111.37
1	A	777	LEU	N-CA-C	-7.27	104.94	113.88
1	D	844	HIS	CA-CB-CG	-7.25	106.55	113.80
1	C	279	ILE	CB-CA-C	-7.21	104.38	111.30
1	D	878	HIS	CA-CB-CG	-7.21	106.59	113.80
1	D	323	ILE	N-CA-C	-7.20	104.76	111.45
1	B	788	PRO	N-CA-C	7.15	122.05	111.03
1	A	689	GLU	CA-C-N	7.15	130.90	120.82
1	A	689	GLU	C-N-CA	7.15	130.90	120.82
1	D	746	ASP	N-CA-C	7.14	120.30	109.23
1	B	71	GLU	CB-CG-CD	7.10	124.67	112.60
1	A	997	ASP	N-CA-CB	7.09	122.76	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	728	VAL	CA-C-O	7.08	126.79	119.35
1	A	448	ARG	N-CA-C	7.07	121.01	112.38
1	D	614	HIS	N-CA-CB	7.07	117.94	109.74
1	D	447	ASP	N-CA-C	7.07	122.07	113.38
1	D	802	ASP	CA-CB-CG	-7.06	105.54	112.60
1	A	977	HIS	CA-CB-CG	7.05	120.86	113.80
1	B	360	HIS	CA-CB-CG	-7.05	106.75	113.80
1	A	95	TYR	N-CA-C	7.04	119.81	111.71
1	C	917	ARG	CD-NE-CZ	-7.03	114.56	124.40
1	A	787	ALA	CA-C-N	7.02	127.06	119.90
1	A	787	ALA	C-N-CA	7.02	127.06	119.90
1	D	804	ASN	CA-CB-CG	-7.00	105.59	112.60
1	A	687	GLN	C-N-CD	-6.98	96.40	125.00
1	D	770	ILE	N-CA-CB	6.97	120.69	111.90
1	C	30	HIS	CA-CB-CG	-6.96	106.84	113.80
1	A	599	ARG	N-CA-C	6.96	118.88	108.31
1	D	134	LEU	N-CA-C	-6.94	104.28	112.89
1	B	632	SER	N-CA-CB	6.94	121.32	110.71
1	C	480	PRO	CB-CA-C	-6.91	101.00	111.44
1	D	988	GLY	N-CA-C	-6.91	103.50	113.86
1	B	85	VAL	CB-CA-C	-6.91	101.75	111.21
1	D	710	GLU	CB-CA-C	-6.90	97.47	110.51
1	D	382	ASN	CA-CB-CG	-6.89	105.71	112.60
1	B	39	SER	N-CA-C	6.88	119.63	111.71
1	A	362	LEU	CB-CA-C	-6.88	98.68	109.34
1	B	630	ARG	CA-C-N	-6.87	112.64	122.94
1	B	630	ARG	C-N-CA	-6.87	112.64	122.94
1	A	91	GLN	O-C-N	-6.87	114.19	122.22
1	D	634	GLN	N-CA-CB	6.86	121.36	110.73
1	B	911	THR	N-CA-C	6.85	118.74	111.28
1	A	684	GLU	N-CA-CB	6.85	120.05	109.85
1	D	817	GLN	N-CA-C	6.81	121.76	113.17
1	B	221	GLN	N-CA-CB	-6.81	100.58	111.62
1	A	553	TRP	CA-CB-CG	-6.79	100.70	113.60
1	B	997	ASP	N-CA-CB	6.78	122.27	111.56
1	D	800	ARG	N-CA-C	6.77	120.19	110.10
1	D	581	ASN	CA-CB-CG	6.77	119.37	112.60
1	B	52	ARG	CB-CA-C	-6.75	97.01	109.37
1	D	765	LEU	N-CA-C	-6.73	99.46	109.15
1	B	610	ASP	CA-CB-CG	-6.69	105.91	112.60
1	C	648	ASP	N-CA-C	6.69	120.42	112.93
1	C	997	ASP	N-CA-CB	6.66	122.08	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	570	TRP	N-CA-C	6.64	118.40	111.03
1	C	778	THR	O-C-N	6.64	126.59	121.88
1	D	731	PRO	CB-CA-C	-6.63	102.75	111.23
1	C	249	GLU	N-CA-C	6.62	119.49	108.96
1	D	329	ASP	CA-CB-CG	-6.62	105.98	112.60
1	B	355	ASN	CA-CB-CG	-6.62	105.98	112.60
1	A	357	HIS	CA-CB-CG	-6.61	107.19	113.80
1	C	614	HIS	N-CA-C	-6.61	101.50	110.36
1	C	685	LEU	CA-C-N	6.55	128.03	119.84
1	C	685	LEU	C-N-CA	6.55	128.03	119.84
1	C	571	VAL	N-CA-C	6.54	118.21	108.46
1	A	571	VAL	N-CA-C	6.54	117.54	108.12
1	C	297	ASN	CA-CB-CG	-6.54	106.06	112.60
1	A	931	PHE	CA-C-O	6.51	124.83	119.36
1	A	735	HIS	N-CA-C	-6.47	102.48	111.81
1	A	710	GLU	CB-CA-C	-6.47	99.12	109.80
1	D	606	LEU	N-CA-C	-6.46	104.88	112.89
1	B	473	ARG	CD-NE-CZ	6.45	133.43	124.40
1	D	686	PRO	N-CA-CB	6.45	110.02	103.25
1	A	771	GLY	N-CA-C	-6.44	100.00	110.95
1	D	843	GLN	CA-CB-CG	-6.43	101.24	114.10
1	D	119	PRO	N-CA-CB	6.42	108.96	103.19
1	B	725	ASN	CA-CB-CG	-6.41	106.19	112.60
1	D	19	PRO	N-CA-CB	6.39	109.42	103.41
1	D	527	PRO	CB-CA-C	-6.39	103.53	111.64
1	B	46	ARG	NE-CZ-NH2	-6.38	113.45	119.20
1	B	211	ASP	N-CA-C	6.38	118.54	110.24
1	A	93	HIS	ND1-CE1-NE2	6.37	114.77	108.40
1	C	728	VAL	CA-C-N	-6.37	112.66	122.09
1	C	728	VAL	C-N-CA	-6.37	112.66	122.09
1	C	809	ARG	NE-CZ-NH1	6.35	127.85	121.50
1	D	746	ASP	CA-CB-CG	-6.33	106.27	112.60
1	C	209	PHE	CA-CB-CG	-6.33	107.47	113.80
1	C	669	PRO	CB-CA-C	-6.33	102.80	111.21
1	B	323	ILE	N-CA-C	-6.32	105.57	111.45
1	A	519	SER	N-CA-C	-6.32	101.33	110.24
1	D	14	ARG	N-CA-CB	-6.31	103.28	110.35
1	A	482	ARG	CB-CA-C	-6.31	99.73	109.20
1	C	736	ALA	N-CA-C	6.31	117.81	108.60
1	D	1018	LEU	CB-CA-C	-6.30	96.51	109.94
1	B	741	THR	CA-CB-OG1	-6.29	100.16	109.60
1	A	91	GLN	CA-C-O	6.29	127.20	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	HIS	CA-CB-CG	-6.29	107.51	113.80
1	D	128	ASN	OD1-CG-ND2	6.29	128.89	122.60
1	A	209	PHE	CA-CB-CG	-6.29	107.51	113.80
1	D	667	GLU	CA-CB-CG	6.26	126.63	114.10
1	D	339	ASN	CA-CB-CG	-6.26	106.34	112.60
1	B	477	SER	CB-CA-C	6.24	122.13	110.70
1	B	433	LEU	CA-C-O	6.24	124.85	118.73
1	C	893	GLU	N-CA-C	6.24	119.36	111.69
1	B	54	LEU	N-CA-C	-6.22	105.00	112.59
1	B	443	MET	CA-C-O	6.21	127.10	120.70
1	B	869	ASP	CA-CB-CG	-6.20	106.40	112.60
1	C	232	ASN	N-CA-C	-6.20	101.79	110.35
1	C	249	GLU	CA-C-N	-6.20	112.07	120.87
1	C	249	GLU	C-N-CA	-6.20	112.07	120.87
1	C	747	PHE	CA-CB-CG	6.20	120.00	113.80
1	B	823	LEU	N-CA-C	-6.19	106.26	113.88
1	B	958	ASN	N-CA-CB	6.18	123.02	111.53
1	D	400	THR	CA-CB-OG1	-6.17	100.34	109.60
1	B	779	PRO	N-CA-CB	6.17	109.19	103.39
1	D	478	VAL	CA-C-N	-6.17	116.20	122.74
1	D	478	VAL	C-N-CA	-6.17	116.20	122.74
1	A	442	ARG	NE-CZ-NH2	-6.16	113.66	119.20
1	C	739	HIS	CA-CB-CG	-6.16	107.64	113.80
1	D	546	LEU	N-CA-CB	6.16	120.89	110.49
1	A	736	ALA	N-CA-C	6.15	117.85	108.07
1	B	570	TRP	N-CA-C	6.15	117.85	111.03
1	C	358	GLU	N-CA-CB	-6.13	101.21	110.35
1	C	782	ASP	CA-CB-CG	-6.11	106.49	112.60
1	B	845	GLN	CB-CG-CD	6.11	122.99	112.60
1	B	865	ALA	CA-C-O	6.11	126.90	120.36
1	C	507	ASP	CA-CB-CG	-6.10	106.50	112.60
1	A	593	GLY	CA-C-O	6.09	125.78	119.02
1	C	949	HIS	N-CA-C	6.08	119.73	109.76
1	D	29	ALA	CA-C-O	-6.08	114.64	121.81
1	C	634	GLN	N-CA-C	-6.07	105.71	112.57
1	A	625	GLN	CG-CD-NE2	6.07	125.50	116.40
1	D	553	TRP	CA-CB-CG	-6.06	102.08	113.60
1	D	761	GLN	CA-C-O	6.06	127.40	120.00
1	A	614	HIS	N-CA-C	-6.06	102.24	110.36
1	C	598	ASP	CA-CB-CG	-6.05	106.55	112.60
1	A	441	THR	N-CA-C	6.05	117.88	111.28
1	D	733	ALA	N-CA-C	6.05	118.11	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	944	LEU	CA-C-O	-6.05	113.61	120.32
1	B	575	LEU	CA-C-N	-6.04	114.57	122.37
1	B	575	LEU	C-N-CA	-6.04	114.57	122.37
1	B	384	PHE	CA-CB-CG	-6.04	107.77	113.80
1	B	728	VAL	CA-C-O	6.04	125.46	119.97
1	D	477	SER	CB-CA-C	-6.03	99.67	110.70
1	B	314	GLU	CB-CA-C	-6.03	99.30	109.72
1	A	97	ALA	CA-C-O	6.02	125.25	120.19
1	B	480	PRO	CB-CA-C	-6.02	102.34	111.44
1	B	685	LEU	C-N-CD	-6.01	100.35	125.00
1	A	127	PHE	CA-CB-CG	-6.01	107.79	113.80
1	C	172	ASP	CA-CB-CG	-6.00	106.60	112.60
1	B	209	PHE	N-CA-C	6.00	120.73	113.17
1	A	917	ARG	CD-NE-CZ	-5.99	116.01	124.40
1	C	395	HIS	ND1-CE1-NE2	5.98	114.38	108.40
1	D	147	ASN	N-CA-CB	-5.98	101.32	110.65
1	B	877	PRO	N-CA-CB	5.98	108.63	103.31
1	D	958	ASN	N-CA-CB	5.98	121.95	111.55
1	A	297	ASN	CA-CB-CG	-5.97	106.63	112.60
1	D	221	GLN	OE1-CD-NE2	-5.97	116.63	122.60
1	C	877	PRO	CB-CA-C	-5.96	103.77	111.46
1	A	461	GLU	CA-CB-CG	-5.96	102.19	114.10
1	A	119	PRO	N-CA-CB	5.96	108.55	103.19
1	D	948	PRO	CB-CA-C	-5.95	102.06	111.04
1	B	166	ARG	N-CA-C	5.94	121.32	112.94
1	B	599	ARG	N-CA-C	5.94	117.34	108.31
1	C	384	PHE	CA-CB-CG	-5.94	107.86	113.80
1	A	150	PHE	N-CA-C	5.94	118.14	108.76
1	D	80	GLU	CA-C-N	-5.93	109.91	121.06
1	D	80	GLU	C-N-CA	-5.93	109.91	121.06
1	B	233	ASP	CA-C-N	-5.93	113.24	122.67
1	B	233	ASP	C-N-CA	-5.93	113.24	122.67
1	C	442	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	B	979	GLU	CA-C-N	-5.92	112.46	120.87
1	B	979	GLU	C-N-CA	-5.92	112.46	120.87
1	C	230	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	A	47	PRO	N-CA-CB	5.91	108.49	103.35
1	B	787	ALA	N-CA-C	-5.91	100.82	109.50
1	D	1004	SER	CA-CB-OG	-5.91	99.29	111.10
1	C	321	THR	CA-CB-OG1	-5.90	100.75	109.60
1	A	147	ASN	N-CA-CB	-5.89	101.46	110.65
1	A	996	ASP	N-CA-C	-5.89	104.20	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	93	HIS	N-CA-C	-5.89	105.75	113.17
1	A	433	LEU	CA-C-O	5.88	124.05	118.34
1	C	653	HIS	CA-CB-CG	5.88	119.68	113.80
1	C	553	TRP	CA-CB-CG	-5.87	102.44	113.60
1	B	76	CYS	CA-CB-SG	-5.87	100.90	114.40
1	D	759	ASN	CA-CB-CG	-5.87	106.73	112.60
1	D	889	ALA	CB-CA-C	-5.87	99.77	110.63
1	C	719	GLN	CB-CA-C	-5.87	97.76	109.79
1	B	546	LEU	N-CA-CB	5.87	120.41	110.49
1	C	159	VAL	N-CA-CB	-5.86	104.96	111.41
1	A	39	SER	N-CA-C	5.84	118.42	111.71
1	A	360	HIS	CA-CB-CG	-5.84	107.96	113.80
1	D	890	GLN	N-CA-CB	-5.84	101.42	110.29
1	C	729	THR	CA-C-N	5.83	128.48	120.67
1	C	729	THR	C-N-CA	5.83	128.48	120.67
1	D	711	ALA	CA-C-O	-5.83	114.78	121.19
1	C	209	PHE	N-CA-C	5.82	120.51	113.17
1	B	64	PRO	CB-CA-C	-5.82	102.67	110.88
1	D	479	ASP	CA-C-N	5.82	125.92	119.87
1	D	479	ASP	C-N-CA	5.82	125.92	119.87
1	D	689	GLU	CA-C-N	5.82	129.10	120.95
1	D	689	GLU	C-N-CA	5.82	129.10	120.95
1	D	231	PHE	CA-CB-CG	-5.81	107.99	113.80
1	B	771	GLY	N-CA-C	-5.81	100.17	110.86
1	C	832	ASP	CA-C-N	-5.81	112.46	122.10
1	C	832	ASP	C-N-CA	-5.81	112.46	122.10
1	C	306	PRO	N-CA-CB	5.81	106.31	102.25
1	C	993	ILE	CA-C-O	5.80	124.77	119.20
1	A	277	GLU	N-CA-CB	-5.80	102.06	110.36
1	D	770	ILE	N-CA-C	-5.80	98.06	107.28
1	D	670	LEU	CB-CA-C	-5.80	100.19	109.75
1	B	98	PRO	CB-CA-C	-5.79	103.39	110.98
1	C	747	PHE	N-CA-C	-5.79	99.47	108.90
1	A	94	GLY	O-C-N	-5.78	115.08	122.43
1	A	504	ALA	N-CA-C	-5.78	101.72	110.28
1	B	423	MET	N-CA-C	5.78	118.36	111.71
1	C	687	GLN	CA-C-O	5.77	124.39	119.66
1	D	161	TYR	N-CA-CB	-5.77	100.79	111.53
1	A	184	LEU	CB-CA-C	-5.77	99.64	109.51
1	C	770	ILE	O-C-N	-5.77	117.44	123.03
1	C	71	GLU	CB-CG-CD	5.76	122.39	112.60
1	B	634	GLN	N-CA-C	-5.75	105.85	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	537	GLU	CB-CG-CD	5.74	122.36	112.60
1	C	855	THR	N-CA-CB	5.74	121.41	111.13
1	C	682	LEU	CA-C-N	5.74	125.69	119.78
1	C	682	LEU	C-N-CA	5.74	125.69	119.78
1	B	69	VAL	N-CA-C	5.73	113.56	108.63
1	B	442	ARG	NE-CZ-NH1	5.73	127.23	121.50
1	C	632	SER	N-CA-CB	5.73	120.11	110.77
1	D	829	THR	N-CA-CB	5.72	119.55	110.57
1	A	613	PRO	CB-CA-C	-5.71	102.46	110.63
1	C	74	LEU	CA-C-O	5.71	126.54	119.97
1	B	737	ILE	CB-CA-C	5.71	116.86	110.52
1	A	116	THR	CA-C-N	-5.70	114.83	122.42
1	A	116	THR	C-N-CA	-5.70	114.83	122.42
1	A	369	GLU	CB-CG-CD	-5.70	102.91	112.60
1	B	749	ILE	CA-C-O	-5.70	114.32	120.36
1	B	592	PHE	CA-CB-CG	-5.68	108.12	113.80
1	A	25	ASN	CA-CB-CG	-5.68	106.92	112.60
1	B	167	LEU	O-C-N	5.68	125.91	121.88
1	D	390	SER	CA-C-N	5.68	131.92	121.70
1	D	390	SER	C-N-CA	5.68	131.92	121.70
1	C	988	GLY	N-CA-C	-5.67	105.35	113.86
1	D	619	GLU	N-CA-C	-5.67	105.18	111.36
1	D	796	SER	N-CA-C	-5.67	104.94	113.89
1	B	306	PRO	N-CA-CB	5.65	106.21	102.25
1	A	781	ARG	N-CA-CB	-5.65	101.87	111.69
1	A	583	ASN	CA-C-N	5.64	125.55	119.85
1	A	583	ASN	C-N-CA	5.64	125.55	119.85
1	D	745	MET	N-CA-C	5.64	119.34	112.23
1	C	741	THR	CA-CB-CG2	-5.64	100.91	110.50
1	D	571	VAL	N-CA-C	5.64	116.86	108.46
1	C	730	LEU	CA-C-N	5.64	125.82	119.90
1	C	730	LEU	C-N-CA	5.64	125.82	119.90
1	B	161	TYR	N-CA-CB	-5.63	101.06	111.53
1	C	842	TRP	CE2-CD2-CE3	5.62	124.42	118.80
1	D	968	MET	N-CA-CB	-5.61	101.08	110.39
1	A	634	GLN	CA-C-N	-5.61	115.08	122.99
1	A	634	GLN	C-N-CA	-5.61	115.08	122.99
1	D	871	GLU	CA-C-N	-5.60	115.81	123.14
1	D	871	GLU	C-N-CA	-5.60	115.81	123.14
1	D	583	ASN	O-C-N	5.58	129.63	121.54
1	A	110	ASN	CA-C-N	5.58	126.13	120.38
1	A	110	ASN	C-N-CA	5.58	126.13	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	LEU	O-C-N	-5.58	116.43	122.79
1	A	373	VAL	CA-C-O	5.57	126.74	120.95
1	D	221	GLN	N-CA-C	5.56	117.43	109.14
1	C	776	LEU	N-CA-C	5.56	118.54	109.59
1	A	968	MET	CB-CA-C	-5.56	100.35	110.63
1	B	891	VAL	O-C-N	-5.56	117.31	123.20
1	A	612	THR	N-CA-C	-5.56	103.04	109.93
1	B	965	GLN	CA-C-O	5.55	127.17	121.07
1	D	949	HIS	N-CA-C	5.55	119.14	110.32
1	C	241	GLU	CB-CG-CD	-5.54	103.18	112.60
1	C	788	PRO	N-CA-CB	5.54	108.18	103.19
1	D	787	ALA	N-CA-C	-5.54	99.41	109.44
1	C	986	ILE	CA-CB-CG2	-5.54	101.08	110.50
1	C	147	ASN	N-CA-CB	-5.54	101.85	110.55
1	A	520	ILE	N-CA-C	5.54	116.27	110.62
1	D	320	GLY	CA-C-N	-5.53	114.39	122.19
1	D	320	GLY	C-N-CA	-5.53	114.39	122.19
1	B	336	ARG	CA-C-O	-5.53	115.36	121.33
1	C	599	ARG	N-CA-C	5.53	116.72	108.31
1	C	497	ASP	CA-CB-CG	-5.52	107.08	112.60
1	C	267	VAL	CA-CB-CG2	-5.52	101.02	110.40
1	B	14	ARG	N-CA-CB	5.51	119.50	111.62
1	C	79	PRO	N-CA-CB	5.51	108.80	103.51
1	C	682	LEU	N-CA-CB	5.51	117.47	110.04
1	C	601	PHE	CA-CB-CG	-5.51	108.29	113.80
1	B	345	ASN	CA-CB-CG	-5.50	107.10	112.60
1	C	823	LEU	N-CA-CB	5.50	118.49	110.47
1	B	1018	LEU	CB-CA-C	-5.49	97.91	109.38
1	C	138	GLN	N-CA-CB	-5.48	101.47	110.68
1	C	63	PHE	CA-C-O	5.47	125.54	120.50
1	B	553	TRP	CA-CB-CG	-5.47	103.20	113.60
1	A	98	PRO	N-CA-C	-5.47	102.54	111.68
1	D	44	THR	CA-C-N	-5.47	115.11	123.47
1	D	44	THR	C-N-CA	-5.47	115.11	123.47
1	A	185	ALA	N-CA-C	-5.46	99.19	108.26
1	B	777	LEU	N-CA-C	-5.46	107.16	113.88
1	A	382	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	113	PHE	CA-CB-CG	-5.46	108.34	113.80
1	A	177	LEU	N-CA-C	5.46	118.50	110.59
1	C	792	ASP	N-CA-C	-5.46	105.36	112.23
1	C	136	GLU	CB-CA-C	-5.45	98.08	110.07
1	D	499	ILE	CA-C-N	-5.44	116.79	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	499	ILE	C-N-CA	-5.44	116.79	122.89
1	C	868	VAL	N-CA-C	5.43	115.72	108.11
1	C	748	CYS	CA-CB-SG	-5.43	101.91	114.40
1	A	1018	LEU	CA-C-N	-5.43	116.03	123.14
1	A	1018	LEU	C-N-CA	-5.43	116.03	123.14
1	B	856	TYR	N-CA-C	-5.42	99.44	108.34
1	C	917	ARG	NE-CZ-NH2	5.42	124.08	119.20
1	D	931	PHE	CA-CB-CG	-5.42	108.38	113.80
1	B	434	PRO	N-CA-CB	5.42	109.03	103.23
1	B	504	ALA	N-CA-C	-5.42	102.26	110.28
1	C	889	ALA	CA-C-O	5.42	126.20	119.97
1	C	606	LEU	N-CA-C	-5.42	106.17	112.89
1	B	686	PRO	CB-CA-C	-5.41	102.63	111.56
1	B	1000	SER	N-CA-CB	5.41	116.78	111.10
1	C	1011	ALA	N-CA-C	5.41	119.14	112.54
1	B	907	PRO	N-CA-CB	5.41	109.04	103.15
1	D	635	THR	CA-CB-OG1	-5.40	101.50	109.60
1	A	949	HIS	N-CA-C	5.40	118.51	110.52
1	A	99	ILE	CA-C-N	-5.39	115.16	123.14
1	A	99	ILE	C-N-CA	-5.39	115.16	123.14
1	A	570	TRP	N-CA-C	5.39	117.01	111.03
1	C	653	HIS	N-CA-CB	5.39	119.21	110.43
1	B	747	PHE	N-CA-C	-5.39	98.59	108.02
1	C	355	ASN	CA-CB-CG	-5.38	107.22	112.60
1	B	989	PHE	CA-CB-CG	-5.38	108.42	113.80
1	C	938	ARG	CD-NE-CZ	-5.37	116.88	124.40
1	B	583	ASN	N-CA-CB	5.37	117.54	110.29
1	B	818	ALA	CA-C-N	-5.37	114.04	122.73
1	B	818	ALA	C-N-CA	-5.37	114.04	122.73
1	A	847	LYS	CA-C-N	-5.36	115.06	122.30
1	A	847	LYS	C-N-CA	-5.36	115.06	122.30
1	D	448	ARG	N-CA-C	5.36	118.92	112.38
1	C	731	PRO	CB-CA-C	-5.36	104.98	111.46
1	A	613	PRO	N-CA-CB	5.36	108.34	103.15
1	B	646	HIS	ND1-CE1-NE2	5.35	113.75	108.40
1	D	524	LEU	N-CA-C	5.35	117.80	111.33
1	D	164	ASP	N-CA-CB	5.35	119.52	110.49
1	A	808	GLU	N-CA-CB	-5.34	102.25	110.16
1	D	728	VAL	N-CA-C	-5.34	107.92	113.10
1	D	842	TRP	CA-C-N	-5.34	113.84	122.82
1	D	842	TRP	C-N-CA	-5.34	113.84	122.82
1	D	277	GLU	N-CA-CB	-5.34	102.73	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	519	SER	N-CA-C	-5.33	102.50	110.23
1	A	460	ASN	CA-CB-CG	5.33	117.93	112.60
1	B	886	CYS	CA-C-N	-5.33	115.54	123.11
1	B	886	CYS	C-N-CA	-5.33	115.54	123.11
1	D	14	ARG	N-CA-C	-5.33	102.19	109.71
1	A	601	PHE	CA-CB-CG	-5.33	108.47	113.80
1	D	136	GLU	N-CA-CB	-5.33	102.31	111.21
1	A	472	TYR	N-CA-C	-5.33	105.37	111.07
1	B	193	ASP	N-CA-C	-5.32	105.59	111.71
1	D	472	TYR	CA-C-O	5.32	126.59	120.90
1	A	93	HIS	CE1-NE2-CD2	-5.31	103.69	109.00
1	A	689	GLU	O-C-N	5.31	129.38	122.42
1	A	806	TRP	O-C-N	5.31	127.62	122.09
1	C	333	ARG	CG-CD-NE	5.31	123.69	112.00
1	C	997	ASP	CA-CB-CG	-5.29	107.31	112.60
1	D	50	GLN	OE1-CD-NE2	-5.29	117.31	122.60
1	D	646	HIS	ND1-CE1-NE2	5.29	113.69	108.40
1	A	815	HIS	CA-C-N	-5.29	111.27	121.58
1	A	815	HIS	C-N-CA	-5.29	111.27	121.58
1	A	1021	CYS	CA-CB-SG	-5.28	102.25	114.40
1	D	183	ARG	N-CA-C	5.28	116.99	108.34
1	B	986	ILE	CB-CG1-CD1	-5.27	102.73	113.80
1	D	683	PRO	CB-CA-C	-5.27	103.28	111.40
1	B	1020	TRP	CA-C-N	-5.27	113.73	122.11
1	B	1020	TRP	C-N-CA	-5.27	113.73	122.11
1	C	382	ASN	CA-C-N	-5.27	115.41	123.47
1	C	382	ASN	C-N-CA	-5.27	115.41	123.47
1	C	664	ALA	CB-CA-C	-5.27	100.97	110.03
1	A	315	LEU	CA-C-N	-5.26	113.75	122.11
1	A	315	LEU	C-N-CA	-5.26	113.75	122.11
1	A	958	ASN	N-CA-CB	5.26	121.31	111.53
1	B	823	LEU	N-CA-CB	5.26	117.58	110.59
1	B	917	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	D	338	GLU	CA-C-N	-5.26	114.77	122.40
1	D	338	GLU	C-N-CA	-5.26	114.77	122.40
1	C	555	ALA	CA-C-O	5.26	125.99	120.42
1	D	217	LYS	CB-CA-C	-5.26	100.87	108.91
1	D	996	ASP	N-CA-CB	5.25	117.94	110.06
1	B	252	ASP	CA-CB-CG	-5.24	107.36	112.60
1	B	396	PRO	N-CA-CB	5.24	109.05	103.39
1	C	987	ASP	N-CA-C	5.24	117.51	109.07
1	B	234	ASP	CA-CB-CG	-5.24	107.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1005	ALA	N-CA-C	5.24	117.67	111.33
1	D	442	ARG	CA-C-O	5.24	126.00	119.97
1	A	671	ASP	CA-C-N	-5.24	115.83	123.06
1	A	671	ASP	C-N-CA	-5.24	115.83	123.06
1	B	969	GLU	CA-CB-CG	-5.24	103.62	114.10
1	C	373	VAL	CA-CB-CG2	-5.24	101.50	110.40
1	D	139	THR	CA-C-N	-5.24	114.01	122.81
1	D	139	THR	C-N-CA	-5.24	114.01	122.81
1	A	577	LYS	N-CA-CB	5.23	119.67	111.20
1	A	434	PRO	CB-CA-C	-5.23	103.99	112.62
1	B	648	ASP	N-CA-C	5.23	119.37	113.15
1	D	593	GLY	CA-C-O	5.23	124.91	119.06
1	C	482	ARG	CB-CA-C	-5.22	101.36	109.20
1	B	235	PHE	CA-CB-CG	-5.22	108.58	113.80
1	B	875	ASP	CA-CB-CG	-5.22	107.38	112.60
1	D	997	ASP	N-CA-CB	5.22	119.81	111.56
1	A	15	ASP	CA-CB-CG	-5.22	107.38	112.60
1	A	772	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	640	SER	CB-CA-C	-5.22	101.25	109.80
1	D	855	THR	N-CA-CB	5.21	120.46	111.13
1	D	800	ARG	CB-CA-C	5.21	118.03	109.90
1	A	770	ILE	N-CA-C	-5.21	98.99	107.28
1	C	510	GLN	CA-C-O	5.21	126.89	121.00
1	C	704	ASN	CA-CB-CG	-5.21	107.39	112.60
1	D	987	ASP	N-CA-C	5.21	117.97	109.59
1	D	396	PRO	N-CA-CB	5.20	109.12	103.30
1	C	387	VAL	CA-C-N	-5.20	115.83	123.00
1	C	387	VAL	C-N-CA	-5.20	115.83	123.00
1	D	727	SER	CA-CB-OG	-5.20	100.70	111.10
1	A	368	ASP	CA-CB-CG	-5.19	107.41	112.60
1	C	650	GLU	CG-CD-OE2	-5.19	106.46	118.40
1	D	980	GLU	CA-C-N	-5.19	108.99	120.99
1	D	980	GLU	C-N-CA	-5.19	108.99	120.99
1	B	1007	PHE	CA-CB-CG	-5.19	108.61	113.80
1	A	513	PRO	CB-CA-C	-5.18	104.31	111.21
1	B	720	TRP	CA-C-N	-5.18	114.00	121.42
1	B	720	TRP	C-N-CA	-5.18	114.00	121.42
1	C	690	SER	CA-CB-OG	-5.18	100.74	111.10
1	B	988	GLY	N-CA-C	-5.18	106.14	112.77
1	C	178	ARG	N-CA-CB	5.18	120.79	111.37
1	A	362	LEU	CA-C-N	-5.17	114.01	122.54
1	A	362	LEU	C-N-CA	-5.17	114.01	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLN	N-CA-C	5.16	116.83	109.14
1	A	747	PHE	N-CA-CB	5.16	118.70	110.65
1	B	583	ASN	CA-C-O	5.16	124.53	120.19
1	C	83	THR	O-C-N	-5.16	117.34	123.22
1	C	685	LEU	O-C-N	5.16	127.69	121.60
1	C	940	GLY	O-C-N	5.16	126.69	122.51
1	D	377	LEU	CA-C-N	-5.16	112.97	120.29
1	D	377	LEU	C-N-CA	-5.16	112.97	120.29
1	B	747	PHE	N-CA-CB	5.16	118.80	110.65
1	C	825	CYS	O-C-N	-5.15	116.45	123.24
1	C	760	ARG	CA-C-N	-5.14	112.61	121.66
1	C	760	ARG	C-N-CA	-5.14	112.61	121.66
1	D	489	GLY	CA-C-N	-5.14	115.38	122.63
1	D	489	GLY	C-N-CA	-5.14	115.38	122.63
1	A	120	THR	N-CA-CB	-5.14	102.63	110.65
1	A	556	PHE	CA-CB-CG	5.14	118.94	113.80
1	D	251	ARG	CD-NE-CZ	5.14	131.59	124.40
1	A	484	VAL	CA-C-N	-5.13	114.19	122.82
1	A	484	VAL	C-N-CA	-5.13	114.19	122.82
1	C	529	GLU	N-CA-C	5.13	117.88	110.28
1	C	773	LYS	N-CA-C	5.13	117.12	108.96
1	B	613	PRO	CB-CA-C	-5.13	103.29	110.63
1	C	519	SER	N-CA-C	-5.13	102.79	110.23
1	D	412	GLU	N-CA-CB	-5.13	102.52	110.57
1	B	306	PRO	CB-CA-C	-5.13	106.17	112.89
1	D	80	GLU	O-C-N	-5.13	114.94	122.43
1	D	653	HIS	N-CA-CB	5.12	118.93	110.69
1	B	753	ASN	N-CA-CB	5.12	117.62	110.56
1	C	1005	ALA	N-CA-C	5.12	117.53	111.33
1	B	307	ASN	CA-C-N	-5.12	114.56	122.59
1	B	307	ASN	C-N-CA	-5.12	114.56	122.59
1	D	118	ASN	N-CA-CB	-5.12	102.02	111.03
1	D	263	GLY	O-C-N	-5.12	116.83	122.61
1	D	795	VAL	CA-CB-CG2	-5.12	101.70	110.40
1	A	832	ASP	CA-CB-CG	-5.12	107.48	112.60
1	C	735	HIS	N-CA-C	-5.11	107.33	113.21
1	A	239	VAL	N-CA-C	-5.11	100.76	108.12
1	D	98	PRO	N-CA-C	-5.11	102.59	111.32
1	C	75	GLU	N-CA-CB	-5.10	102.61	110.42
1	B	667	GLU	CA-C-N	5.10	128.87	121.68
1	B	667	GLU	C-N-CA	5.10	128.87	121.68
1	A	832	ASP	N-CA-CB	-5.10	103.03	111.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	616	ALA	CA-C-N	-5.10	112.94	120.28
1	B	616	ALA	C-N-CA	-5.10	112.94	120.28
1	C	567	VAL	CA-C-O	-5.10	116.48	121.58
1	A	93	HIS	N-CA-C	-5.09	106.65	112.92
1	B	335	VAL	CA-C-N	-5.09	112.94	121.75
1	B	335	VAL	C-N-CA	-5.09	112.94	121.75
1	B	819	GLU	O-C-N	5.09	129.49	123.27
1	C	469	ASP	N-CA-CB	-5.09	102.63	110.12
1	C	690	SER	CB-CA-C	-5.09	100.28	110.42
1	C	931	PHE	CA-CB-CG	-5.09	108.71	113.80
1	B	425	ARG	CA-CB-CG	-5.09	103.92	114.10
1	C	784	PHE	O-C-N	5.09	128.20	122.20
1	A	1015	HIS	CA-CB-CG	-5.09	108.71	113.80
1	B	395	HIS	CA-C-N	5.09	124.88	119.28
1	B	395	HIS	C-N-CA	5.09	124.88	119.28
1	D	504	ALA	N-CA-C	-5.09	102.75	110.28
1	D	536	CYS	N-CA-CB	5.08	118.16	110.28
1	A	179	ALA	N-CA-CB	5.08	117.50	109.83
1	A	384	PHE	CA-CB-CG	-5.08	108.72	113.80
1	A	347	LYS	CA-C-O	5.08	126.45	120.41
1	C	948	PRO	CB-CA-C	-5.08	103.72	110.88
1	A	155	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	729	THR	N-CA-CB	5.07	117.52	109.71
1	A	956	GLN	CA-C-N	-5.07	113.55	121.87
1	A	956	GLN	C-N-CA	-5.07	113.55	121.87
1	A	787	ALA	N-CA-C	-5.07	100.27	109.44
1	B	375	ASP	CA-CB-CG	-5.06	107.54	112.60
1	A	235	PHE	CA-CB-CG	-5.06	108.74	113.80
1	D	499	ILE	N-CA-C	-5.06	101.05	108.54
1	A	42	ALA	N-CA-C	-5.06	105.84	111.36
1	D	39	SER	N-CA-C	5.06	117.45	111.33
1	B	75	GLU	CA-C-N	-5.06	114.01	122.21
1	B	75	GLU	C-N-CA	-5.06	114.01	122.21
1	C	358	GLU	CA-CB-CG	-5.06	103.98	114.10
1	D	679	LEU	CB-CA-C	-5.06	101.40	109.75
1	B	323	ILE	CA-CB-CG1	-5.06	101.80	110.40
1	B	612	THR	CA-C-O	5.06	125.71	120.25
1	D	1006	GLU	CG-CD-OE2	-5.06	106.77	118.40
1	C	670	LEU	CA-C-N	-5.05	115.46	123.24
1	C	670	LEU	C-N-CA	-5.05	115.46	123.24
1	D	797	GLU	CA-C-N	5.05	128.69	120.60
1	D	797	GLU	C-N-CA	5.05	128.69	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	770	ILE	CA-CB-CG1	-5.05	101.81	110.40
1	C	683	PRO	CB-CA-C	-5.05	104.77	111.23
1	D	749	ILE	CB-CA-C	-5.05	102.96	110.33
1	B	735	HIS	N-CA-C	-5.05	105.87	112.23
1	B	816	TYR	CA-C-N	-5.05	114.31	122.23
1	B	816	TYR	C-N-CA	-5.05	114.31	122.23
1	C	395	HIS	ND1-CG-CD2	5.04	111.14	106.10
1	C	237	ARG	CA-CB-CG	-5.04	104.01	114.10
1	D	636	ILE	CB-CA-C	-5.04	103.98	110.84
1	A	140	ARG	CA-C-N	-5.04	116.11	123.06
1	A	140	ARG	C-N-CA	-5.04	116.11	123.06
1	A	224	ASP	O-C-N	5.04	127.94	123.41
1	D	562	LEU	N-CA-CB	5.04	117.86	110.35
1	C	221	GLN	N-CA-CB	-5.03	103.61	111.56
1	C	305	ILE	CB-CA-C	-5.03	102.20	111.36
1	D	45	ASP	N-CA-CB	5.03	120.73	112.63
1	D	115	PRO	N-CA-CB	5.03	107.72	103.35
1	B	833	ALA	N-CA-CB	-5.03	103.72	111.46
1	D	19	PRO	CB-CA-C	-5.03	103.85	111.44
1	A	987	ASP	N-CA-C	5.02	117.68	109.59
1	C	1017	GLN	CB-CG-CD	-5.02	104.07	112.60
1	B	165	SER	CB-CA-C	-5.02	100.53	110.27
1	B	809	ARG	CD-NE-CZ	5.02	131.42	124.40
1	B	453	VAL	O-C-N	5.02	128.15	122.68
1	C	336	ARG	O-C-N	-5.01	117.54	123.25
1	B	255	ARG	CA-C-N	-5.00	116.04	122.99
1	B	255	ARG	C-N-CA	-5.00	116.04	122.99
1	D	751	LEU	N-CA-CB	5.00	118.37	110.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	634	GLN	CA

There are no planarity outliers.

5.2 Too-close contacts

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	8205	0	7791	182	0
1	B	8205	0	7791	166	0
1	C	8205	0	7791	176	0
1	D	8125	0	7716	166	0
2	A	12	0	9	0	0
2	B	12	0	9	0	0
2	C	12	0	9	0	0
2	D	12	0	9	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	80	0	120	13	0
5	B	88	0	132	13	0
5	C	88	0	132	12	0
5	D	92	0	138	28	0
6	A	953	0	0	27	0
6	B	937	0	0	26	1
6	C	952	0	0	17	0
6	D	959	0	0	25	1
All	All	36964	0	31647	700	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (700) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:GLN:H	1:C:634:GLN:NE2	1.37	1.22
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.14	1.09
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.20	1.06
1:C:634:GLN:HE21	1:C:634:GLN:N	1.57	1.01
1:B:232:ASN:ND2	1:B:237:ARG:HG3	1.82	0.94
1:B:13:ARG:HG3	1:C:13:ARG:CZ	1.98	0.93
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.04	0.92
1:C:765:LEU:CD2	1:C:768:MET:HE2	2.00	0.92
1:A:128:ASN:HD21	1:A:180:GLY:HA2	1.36	0.91
1:D:237:ARG:HH11	1:D:237:ARG:HG2	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:PRO:HB2	5:D:8404:DMS:H13	1.54	0.88
1:D:804:ASN:CG	1:D:809:ARG:HH21	1.83	0.87
1:C:356:ARG:HH22	1:C:367:MET:HE2	1.40	0.86
1:C:816:TYR:CE2	1:C:968:MET:HE1	2.11	0.85
1:A:703:PRO:HG2	5:A:8425:DMS:H12	1.56	0.85
1:A:237:ARG:HH11	1:A:237:ARG:CB	1.90	0.84
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.60	0.83
1:A:1022:GLN:HG2	1:A:1023:LYS:N	1.92	0.82
1:D:622:HIS:O	1:D:625:GLN:HG3	1.79	0.82
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.62	0.81
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.16	0.81
1:B:878:HIS:HD2	6:B:8687:HOH:O	1.65	0.80
1:C:634:GLN:H	1:C:634:GLN:HE21	0.80	0.80
1:B:801[A]:ILE:HG22	1:B:802[A]:ASP:H	1.47	0.80
1:D:962:TYR:OH	5:D:8508:DMS:H11	1.80	0.80
1:B:13:ARG:HG3	1:C:13:ARG:NH1	1.97	0.80
1:A:653:HIS:CD2	1:A:667:GLU:HG3	2.17	0.79
1:B:473:ARG:NH2	1:B:477:SER:HB2	1.98	0.79
1:C:973:ARG:O	5:C:8423:DMS:H12	1.83	0.79
1:D:682:LEU:HB3	1:D:683:PRO:HD2	1.65	0.78
5:C:8417:DMS:H22	6:C:9205:HOH:O	1.82	0.78
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.82	0.78
1:C:653:HIS:ND1	1:C:667:GLU:HG2	1.98	0.78
1:D:651:LEU:O	1:D:651:LEU:HD12	1.84	0.77
1:C:634:GLN:NE2	1:C:634:GLN:N	2.21	0.77
1:C:781:ARG:HG2	1:C:781:ARG:HH11	1.48	0.77
1:A:262:GLN:HG3	6:A:9518:HOH:O	1.85	0.77
1:C:651:LEU:HD12	1:C:651:LEU:C	2.10	0.77
1:C:356:ARG:NH2	1:C:367:MET:HE2	1.99	0.77
1:B:93:HIS:NE2	5:B:8414:DMS:H23	1.99	0.76
1:B:651:LEU:O	1:B:651:LEU:HD23	1.84	0.76
1:B:1017:GLN:HB2	6:B:9454:HOH:O	1.86	0.76
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.18	0.76
1:A:887:GLN:NE2	1:A:980:GLU:O	2.17	0.76
1:B:668:VAL:HG12	1:B:669:PRO:O	1.85	0.76
1:C:508:GLU:OE2	5:C:8407:DMS:H11	1.87	0.75
1:B:737:ILE:HD11	6:B:9453:HOH:O	1.84	0.75
1:A:655:MET:HE2	1:A:656:VAL:N	2.02	0.75
1:D:847:LYS:HG3	1:D:848:THR:N	2.01	0.75
1:D:277:GLU:CD	1:D:277:GLU:H	1.95	0.75
1:C:748:CYS:C	1:C:749:ILE:HD12	2.12	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:SER:C	1:B:237:ARG:HG2	2.09	0.74
1:D:128:ASN:HB3	1:D:180:GLY:O	1.88	0.73
1:A:237:ARG:HB3	1:A:237:ARG:NH1	2.00	0.73
1:B:772:ASP:OD1	1:B:773:LYS:HD3	1.89	0.73
1:D:779:PRO:HG2	1:D:781:ARG:NH2	2.04	0.73
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.70	0.73
1:D:651:LEU:HD12	1:D:651:LEU:C	2.14	0.73
1:C:690:SER:HB2	6:C:9321:HOH:O	1.87	0.73
1:A:890:GLN:OE1	1:A:948:PRO:HD3	1.90	0.71
1:C:754:LYS:HE3	1:C:1022:GLN:OE1	1.90	0.71
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.26	0.71
1:A:878:HIS:HD2	6:A:8674:HOH:O	1.74	0.71
1:A:128:ASN:ND2	1:A:180:GLY:HA2	2.05	0.71
1:A:754:LYS:NZ	6:A:9425:HOH:O	2.23	0.71
1:D:292:ARG:HH12	5:D:8412:DMS:H23	1.54	0.71
1:B:600:GLN:H	1:B:600:GLN:HE21	1.36	0.71
1:C:44:THR:OG1	1:C:46:ARG:HD3	1.91	0.70
1:A:277:GLU:H	1:A:277:GLU:CD	1.98	0.70
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.25	0.70
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.55	0.70
1:C:724:GLU:O	1:D:847:LYS:NZ	2.24	0.70
1:C:230:ARG:CG	1:C:230:ARG:HH11	2.05	0.69
1:A:241:GLU:OE2	1:A:292:ARG:NE	2.25	0.69
1:D:237:ARG:HG2	1:D:237:ARG:NH1	2.03	0.69
1:A:635:THR:OG1	1:A:681:GLU:HG3	1.92	0.69
1:D:973:ARG:O	5:D:8423:DMS:H12	1.93	0.69
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.75	0.69
1:C:230:ARG:HB3	6:C:9470:HOH:O	1.92	0.69
5:D:8503:DMS:H22	6:D:9153:HOH:O	1.92	0.69
1:C:243:GLU:OE2	1:C:245:GLN:NE2	2.27	0.68
1:C:634:GLN:H	1:C:634:GLN:CD	1.97	0.68
1:D:962:TYR:CZ	5:D:8508:DMS:H11	2.28	0.68
1:D:1022:GLN:HG3	1:D:1023:LYS:N	2.05	0.68
1:C:794[B]:GLY:HA2	6:C:8944:HOH:O	1.94	0.68
1:C:800[A]:ARG:HA	1:C:800[A]:ARG:NE	2.09	0.68
1:D:480:PRO:HG2	6:D:9614:HOH:O	1.92	0.68
1:D:595:THR:HA	1:D:596:PRO:C	2.16	0.68
1:A:794[B]:GLY:HA2	6:A:8919:HOH:O	1.92	0.68
1:C:749:ILE:HD12	1:C:749:ILE:N	2.06	0.68
1:A:157:ARG:HD3	6:A:9380:HOH:O	1.93	0.68
1:D:890:GLN:HG3	1:D:891:VAL:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:637:GLU:OE2	1:C:677:LYS:NZ	2.26	0.68
1:D:653:HIS:NE2	1:D:667:GLU:OE2	2.27	0.68
1:A:737:ILE:O	1:A:737:ILE:HD13	1.95	0.67
1:A:651:LEU:C	1:A:651:LEU:HD12	2.19	0.67
1:A:770:ILE:HD12	1:A:775:GLN:NE2	2.09	0.67
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.76	0.67
1:B:233:ASP:HA	5:B:8417:DMS:H13	1.76	0.67
1:A:600:GLN:H	1:A:600:GLN:HE21	1.43	0.67
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.25	0.67
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.28	0.67
1:A:179:ALA:HB3	6:A:9338:HOH:O	1.94	0.67
1:D:320:GLY:HA2	5:D:8406:DMS:H23	1.77	0.67
1:C:651:LEU:HD12	1:C:651:LEU:O	1.95	0.66
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.06	0.66
1:D:237:ARG:NH1	6:D:9255:HOH:O	2.28	0.66
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.10	0.66
1:A:473:ARG:NH1	6:A:9253:HOH:O	2.22	0.66
1:C:625:GLN:NE2	6:C:8826:HOH:O	2.27	0.66
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.30	0.66
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.30	0.66
1:B:771:GLY:HA3	6:B:9446:HOH:O	1.95	0.66
1:D:682:LEU:CB	1:D:683:PRO:HD2	2.26	0.66
1:D:749:ILE:HD12	1:D:749:ILE:N	2.10	0.66
1:A:794[B]:GLY:O	6:A:8843:HOH:O	2.13	0.66
1:D:155:ASN:HB3	1:D:178:ARG:NH1	2.11	0.66
1:A:832:ASP:OD1	1:A:832:ASP:N	2.29	0.66
1:B:1022:GLN:HG3	1:B:1023:LYS:N	2.10	0.66
1:D:893:GLU:O	1:D:893:GLU:HG3	1.96	0.66
1:A:787:ALA:HA	1:A:968:MET:HG3	1.78	0.65
5:B:8508:DMS:H13	6:B:8724:HOH:O	1.95	0.65
1:D:634:GLN:NE2	1:D:682:LEU:O	2.28	0.65
1:B:671:ASP:N	1:B:678:GLN:OE1	2.19	0.65
1:B:651:LEU:HD23	1:B:651:LEU:C	2.22	0.65
1:A:581:ASN:HB2	1:A:583:ASN:ND2	2.11	0.65
1:A:804[B]:ASN:OD1	1:A:809:ARG:NH2	2.30	0.64
1:B:753:ASN:HB2	1:B:771:GLY:HA2	1.79	0.64
1:C:230:ARG:HH11	1:C:230:ARG:HG2	1.61	0.64
1:D:49:GLN:HB3	5:D:8703:DMS:O	1.98	0.64
1:B:801[A]:ILE:HG23	1:B:808:GLU:CD	2.22	0.64
1:C:671:ASP:N	1:C:678:GLN:OE1	2.22	0.64
1:A:949:HIS:O	1:A:1023:LYS:NZ	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:PRO:O	1:B:618:THR:HG22	1.98	0.64
1:A:615:PRO:O	1:A:618:THR:HG22	1.97	0.64
1:D:817:GLN:OE1	6:D:9154:HOH:O	2.14	0.64
1:A:595:THR:HA	1:A:596:PRO:C	2.23	0.64
1:A:781:ARG:HG2	1:A:781:ARG:NH1	2.13	0.64
1:A:686:PRO:HB2	1:A:688:PRO:HD3	1.80	0.63
1:A:1022:GLN:NE2	1:A:1023:LYS:O	2.26	0.63
1:B:183:ARG:HG2	1:B:183:ARG:HH11	1.64	0.63
1:D:135:GLN:C	1:D:136:GLU:HG2	2.22	0.63
1:A:770:ILE:HD12	1:A:775:GLN:CD	2.23	0.63
1:A:817:GLN:NE2	1:A:817:GLN:N	2.46	0.63
6:A:9350:HOH:O	5:C:8417:DMS:H11	1.99	0.63
1:B:893:GLU:HG3	6:B:9472:HOH:O	1.97	0.63
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.33	0.63
1:B:962:TYR:OH	5:B:8423:DMS:H21	1.98	0.63
1:B:13:ARG:HG3	1:C:13:ARG:NH2	2.14	0.63
1:A:367:MET:HB3	1:A:372:MET:HE3	1.81	0.62
1:C:781:ARG:HG2	1:C:781:ARG:NH1	2.13	0.62
1:D:804:ASN:OD1	1:D:809:ARG:NH2	2.31	0.62
1:D:859:ASP:OD1	1:D:861:SER:N	2.29	0.62
1:D:117:GLU:HB2	6:D:9142:HOH:O	1.99	0.62
1:C:730:LEU:N	1:C:730:LEU:HD23	2.15	0.62
1:B:595:THR:HA	1:B:596:PRO:C	2.24	0.62
1:C:890:GLN:HG3	1:C:891:VAL:N	2.13	0.62
1:D:250:LEU:O	1:D:251:ARG:HG2	2.00	0.62
1:A:873:ALA:O	1:A:876:THR:HG22	1.99	0.62
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.29	0.62
1:C:800[A]:ARG:HA	1:C:800[A]:ARG:CZ	2.29	0.62
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.65	0.62
1:C:878:HIS:HD2	6:C:8698:HOH:O	1.82	0.62
1:D:316:HIS:ND1	5:D:8406:DMS:H21	2.13	0.62
1:A:267:VAL:O	5:A:8602:DMS:H23	1.99	0.61
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.35	0.61
1:C:628:GLN:NE2	5:C:8402:DMS:O	2.27	0.61
1:A:703:PRO:HG2	5:A:8425:DMS:C1	2.26	0.61
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.82	0.61
1:C:615:PRO:O	1:C:618:THR:HG22	2.00	0.61
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.13	0.61
1:D:770:ILE:HD13	1:D:1022:GLN:OE1	1.99	0.61
5:D:8410:DMS:H22	6:D:9003:HOH:O	1.99	0.61
1:B:777:LEU:HG	1:B:889:ALA:HA	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:817:GLN:OE1	6:D:9079:HOH:O	2.16	0.61
1:D:878:HIS:HD2	6:D:8820:HOH:O	1.84	0.61
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.81	0.60
1:A:781:ARG:HG2	1:A:781:ARG:HH11	1.66	0.60
1:D:629:PHE:O	1:D:630:ARG:HD3	2.01	0.60
1:D:231:PHE:O	5:D:8417:DMS:H23	2.02	0.60
1:A:32:PRO:HB2	5:A:8404:DMS:H13	1.83	0.60
1:A:625:GLN:NE2	6:A:8801:HOH:O	2.24	0.60
1:A:804[B]:ASN:CG	1:A:809:ARG:NH2	2.59	0.60
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.37	0.60
1:C:797[A]:GLU:HB3	1:C:800[A]:ARG:H	1.67	0.60
1:D:651:LEU:HD11	1:D:701:VAL:HB	1.82	0.60
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.37	0.60
1:A:230:ARG:NH1	1:A:241:GLU:OE2	2.35	0.59
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.82	0.59
1:B:91:GLN:HG2	1:B:98:PRO:HA	1.83	0.59
1:B:1022:GLN:HG3	1:B:1023:LYS:O	2.02	0.59
1:C:796[A]:SER:OG	1:C:802[A]:ASP:N	2.29	0.59
1:C:251:ARG:HB3	1:C:251:ARG:HH11	1.67	0.59
1:D:106:PRO:C	5:D:8419:DMS:H23	2.28	0.59
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.38	0.59
1:D:818:ALA:HB1	1:D:842:TRP:HB3	1.84	0.59
1:B:381:GLN:O	1:B:621:LYS:HE3	2.03	0.59
1:B:49:GLN:HB3	6:B:9403:HOH:O	2.02	0.58
1:D:240:LEU:HD23	1:D:240:LEU:C	2.28	0.58
1:D:675:GLN:HG3	6:D:9517:HOH:O	2.01	0.58
5:B:8420:DMS:H11	6:C:9196:HOH:O	2.04	0.58
1:D:989:PHE:HA	6:D:9457:HOH:O	2.04	0.58
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.84	0.58
1:A:597:ASN:OD1	1:A:599:ARG:HD3	2.04	0.58
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.86	0.58
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.39	0.58
1:C:356:ARG:HD2	1:C:379:MET:CE	2.33	0.58
1:D:618:THR:HG21	6:D:9056:HOH:O	2.04	0.58
1:B:668:VAL:HG12	1:B:669:PRO:N	2.17	0.57
1:B:744:GLU:HB2	1:B:745:MET:HE3	1.86	0.57
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.19	0.57
1:A:830:LEU:HD12	1:A:833:ALA:HB3	1.84	0.57
1:A:521:LYS:HE2	6:A:9019:HOH:O	2.03	0.57
1:C:801[A]:ILE:HG23	1:C:808:GLU:CD	2.29	0.57
1:B:768:MET:SD	1:B:775:GLN:HG3	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:PRO:CB	5:D:8404:DMS:H13	2.30	0.57
1:B:634:GLN:HG3	1:B:682:LEU:O	2.04	0.57
1:B:369:GLU:HB2	1:B:397:LEU:CD2	2.35	0.57
1:A:593:GLY:O	1:A:595:THR:HG22	2.05	0.57
1:D:708:TRP:CZ2	5:D:8403:DMS:H13	2.40	0.57
1:D:754:LYS:NZ	6:D:9565:HOH:O	2.38	0.57
1:C:765:LEU:HD21	1:C:768:MET:CE	2.10	0.57
1:D:795:VAL:HG11	1:D:800:ARG:O	2.05	0.57
1:A:49:GLN:N	6:A:9254:HOH:O	2.26	0.56
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.74	0.56
1:C:802[A]:ASP:O	1:C:808:GLU:HG3	2.05	0.56
1:C:768:MET:HE1	1:C:1020:TRP:CZ3	2.40	0.56
1:B:577:LYS:O	1:B:584:PRO:HA	2.06	0.56
1:D:292:ARG:NH1	5:D:8412:DMS:H23	2.21	0.56
1:D:363:HIS:HD2	6:D:9297:HOH:O	1.88	0.56
1:B:157:ARG:HD3	6:B:9385:HOH:O	2.05	0.56
1:B:923:SER:HA	5:B:8508:DMS:H12	1.88	0.56
1:C:79:PRO:HD2	1:C:80:GLU:OE2	2.06	0.56
1:B:800[A]:ARG:O	1:B:801[A]:ILE:O	2.24	0.56
1:B:890:GLN:HG3	1:B:891:VAL:N	2.17	0.56
1:C:278:ILE:HD13	1:C:278:ILE:N	2.21	0.56
1:A:320:GLY:O	5:A:8406:DMS:H21	2.06	0.55
1:C:88:SER:HA	1:C:366:VAL:HG21	1.88	0.55
1:A:517:LYS:NZ	6:A:8748:HOH:O	2.37	0.55
1:A:655:MET:HE2	1:A:656:VAL:H	1.70	0.55
1:A:131:GLU:O	1:A:135:GLN:HG2	2.06	0.55
1:A:237:ARG:HH11	1:A:237:ARG:CG	2.18	0.55
1:A:737:ILE:HD13	1:A:737:ILE:C	2.32	0.55
1:A:127:PHE:N	1:A:127:PHE:CD2	2.74	0.55
1:C:240:LEU:C	1:C:240:LEU:HD23	2.31	0.55
1:D:646:HIS:ND1	6:D:9524:HOH:O	2.33	0.55
1:A:764:PHE:CD1	1:A:781:ARG:NH1	2.74	0.55
1:B:262:GLN:HE21	1:B:262:GLN:C	2.15	0.55
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.71	0.55
5:D:8508:DMS:H13	6:D:8857:HOH:O	2.07	0.55
1:D:893:GLU:HG2	1:D:894:ARG:CD	2.37	0.55
1:A:370:GLN:HB2	6:A:9087:HOH:O	2.06	0.55
1:A:750:GLU:HG3	1:A:755:ARG:HG2	1.88	0.55
1:A:804[B]:ASN:CG	1:A:809:ARG:HH21	2.15	0.55
1:D:887:GLN:NE2	1:D:980:GLU:O	2.36	0.55
1:B:669:PRO:HB3	6:B:9407:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:ASN:OD1	1:B:599:ARG:HD3	2.07	0.54
1:A:372:MET:HE1	1:A:395:HIS:HB3	1.88	0.54
1:A:817:GLN:N	1:A:817:GLN:HE21	2.04	0.54
1:A:249:GLU:OE2	1:A:251:ARG:NH2	2.40	0.54
1:A:601:PHE:CZ	1:A:796[B]:SER:HB2	2.43	0.54
1:B:654:TRP:O	1:B:665:SER:HB2	2.06	0.54
1:C:771:GLY:HA2	6:C:9478:HOH:O	2.06	0.54
1:B:78:LEU:HD23	6:B:9092:HOH:O	2.06	0.54
1:B:347:LYS:HE3	6:B:8873:HOH:O	2.07	0.54
1:D:748:CYS:C	1:D:749:ILE:HD12	2.32	0.54
1:A:658:LEU:O	1:A:659:ASP:C	2.50	0.54
1:B:759:ASN:OD1	1:B:761:GLN:N	2.37	0.54
1:A:363:HIS:HA	6:A:9154:HOH:O	2.07	0.54
1:D:584:PRO:HD2	6:D:9415:HOH:O	2.05	0.54
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.42	0.54
1:D:360:HIS:HE1	1:D:362:LEU:HG	1.73	0.54
1:D:911:THR:HA	6:D:9328:HOH:O	2.08	0.53
1:D:250:LEU:C	1:D:251:ARG:HG2	2.33	0.53
1:B:745:MET:SD	1:B:745:MET:N	2.77	0.53
1:B:809:ARG:HD2	6:B:9200:HOH:O	2.07	0.53
1:C:800[A]:ARG:NH1	1:C:800[A]:ARG:HB3	2.23	0.53
1:A:890:GLN:HG3	1:A:891:VAL:N	2.23	0.53
1:D:807:VAL:HG13	1:D:808:GLU:N	2.24	0.53
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.90	0.53
1:D:737:ILE:HD12	1:D:831:ALA:O	2.07	0.53
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.43	0.53
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.77	0.53
1:A:806:TRP:CD2	1:A:991:MET:HE1	2.44	0.53
5:A:8403:DMS:H12	6:A:8677:HOH:O	2.08	0.53
1:C:534:ILE:HB	6:C:9175:HOH:O	2.08	0.53
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.43	0.53
5:B:8410:DMS:H22	6:B:8875:HOH:O	2.09	0.53
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.91	0.53
1:C:595:THR:HA	1:C:596:PRO:C	2.34	0.53
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.72	0.53
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.44	0.52
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.90	0.52
1:A:637:GLU:OE2	1:A:677:LYS:HE3	2.10	0.52
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.40	0.52
1:A:372:MET:HE2	6:A:8791:HOH:O	2.10	0.52
1:D:107:ILE:HA	5:D:8419:DMS:H21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:893:GLU:HG2	1:D:894:ARG:HD2	1.91	0.52
1:B:521:LYS:HE2	6:B:9035:HOH:O	2.08	0.52
1:C:646:HIS:HB3	6:C:9414:HOH:O	2.08	0.52
1:C:687:GLN:CG	1:C:688:PRO:HD2	2.39	0.52
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.45	0.52
1:B:93:HIS:CD2	5:B:8414:DMS:H23	2.45	0.52
1:D:893:GLU:HG3	6:D:9241:HOH:O	2.08	0.52
1:C:251:ARG:NH1	1:C:253:TYR:CE2	2.78	0.52
1:A:655:MET:HE2	1:A:656:VAL:O	2.09	0.52
1:B:262:GLN:HE21	1:B:263:GLY:N	2.07	0.52
1:B:773:LYS:N	1:B:773:LYS:HD2	2.21	0.52
1:B:15:ASP:OD2	6:B:8788:HOH:O	2.19	0.51
1:B:246:MET:HE3	1:B:250:LEU:HD23	1.92	0.51
1:B:473:ARG:CZ	1:B:477:SER:HB2	2.40	0.51
1:C:687:GLN:CB	1:C:688:PRO:HD2	2.40	0.51
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.91	0.51
1:C:1020:TRP:HD1	1:C:1021:CYS:N	2.08	0.51
1:D:441:THR:O	1:D:445:GLN:HG3	2.09	0.51
1:A:508:GLU:OE2	5:A:8407:DMS:H11	2.10	0.51
1:A:891:VAL:HG23	1:A:981:GLY:HA2	1.93	0.51
5:A:8416:DMS:H12	6:A:9222:HOH:O	2.10	0.51
1:A:32:PRO:CB	5:A:8404:DMS:H13	2.41	0.51
1:B:135:GLN:HG3	1:B:136:GLU:HG2	1.93	0.51
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.54	0.51
1:B:655:MET:HG2	6:B:9494:HOH:O	2.11	0.51
1:B:363:HIS:HD2	6:B:9170:HOH:O	1.93	0.51
1:B:599:ARG:NH1	6:B:9488:HOH:O	2.44	0.51
1:C:794[A]:GLY:HA2	1:C:998:SER:O	2.11	0.51
1:B:533:LEU:HD23	1:B:533:LEU:C	2.36	0.51
1:C:930:VAL:O	1:C:932:PRO:HD3	2.11	0.51
1:D:778:THR:HG23	1:D:781:ARG:HH12	1.74	0.51
1:A:843:GLN:HG2	1:A:848:THR:HA	1.93	0.50
1:B:245:GLN:HG2	1:B:288:ARG:CG	2.37	0.50
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.45	0.50
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.47	0.50
1:C:651:LEU:C	1:C:651:LEU:CD1	2.83	0.50
1:B:625:GLN:HG2	1:B:716:ALA:CB	2.41	0.50
1:C:654:TRP:O	1:C:665:SER:HB2	2.12	0.50
1:B:822:LEU:HD21	1:B:825:CYS:HB2	1.93	0.50
1:B:890:GLN:OE1	1:B:948:PRO:HD2	2.12	0.50
1:C:816:TYR:CD2	1:C:968:MET:HE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:843:GLN:HB3	1:D:847:LYS:O	2.11	0.50
1:B:802[A]:ASP:OD1	1:B:802[A]:ASP:C	2.55	0.50
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.92	0.50
1:D:299:LYS:NZ	6:D:9389:HOH:O	2.43	0.50
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.46	0.50
1:C:654:TRP:CZ3	1:C:665:SER:HA	2.47	0.50
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.47	0.49
1:C:829:THR:HG22	1:C:830:LEU:O	2.12	0.49
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.28	0.49
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.11	0.49
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.95	0.49
1:D:651:LEU:CD1	1:D:653:HIS:CE1	2.95	0.49
1:D:962:TYR:CE1	5:D:8508:DMS:H11	2.48	0.49
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.42	0.49
1:C:251:ARG:NH1	1:C:253:TYR:HE2	2.10	0.49
1:D:793:ILE:HG22	1:D:795:VAL:HG22	1.94	0.49
1:B:146:VAL:O	1:B:165:SER:HA	2.13	0.49
1:A:347:LYS:HE3	6:A:9480:HOH:O	2.12	0.49
1:B:646:HIS:CE1	1:B:673:ALA:CA	2.96	0.49
1:B:687:GLN:CB	1:B:688:PRO:HD2	2.42	0.49
1:B:737:ILE:HD12	1:B:738:PRO:HD2	1.94	0.49
1:A:581:ASN:HB2	1:A:583:ASN:HD21	1.77	0.49
1:A:599:ARG:HB3	1:A:600:GLN:HE21	1.78	0.49
1:B:708:TRP:CZ2	5:B:8403:DMS:H13	2.47	0.49
1:C:728:VAL:O	1:C:730:LEU:HD23	2.13	0.49
1:D:316:HIS:CE1	5:D:8406:DMS:H21	2.47	0.49
1:D:653:HIS:ND1	1:D:701:VAL:CG2	2.75	0.49
1:D:804:ASN:HD21	1:D:809:ARG:NH2	2.11	0.49
1:A:646:HIS:ND1	6:A:9371:HOH:O	2.18	0.49
1:A:793:ILE:HG22	1:A:795[B]:VAL:HG22	1.94	0.49
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.94	0.49
1:B:824:GLN:HG2	1:B:825:CYS:N	2.27	0.49
1:D:340:GLY:O	1:D:561:ARG:HG2	2.13	0.49
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.94	0.48
1:A:128:ASN:ND2	1:A:180:GLY:CA	2.74	0.48
1:A:533:LEU:C	1:A:533:LEU:HD23	2.38	0.48
1:C:785:THR:O	1:C:881:ARG:HD2	2.11	0.48
1:C:55:ASN:O	5:C:8408:DMS:H11	2.13	0.48
1:C:431:ARG:HD2	6:C:9089:HOH:O	2.12	0.48
1:B:629:PHE:HA	1:B:637:GLU:O	2.14	0.48
1:D:367:MET:HB3	1:D:372:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ILE:HA	1:A:341:LEU:O	2.14	0.48
1:C:629:PHE:HA	1:C:637:GLU:O	2.14	0.48
1:D:933:SER:O	1:D:934:GLU:C	2.57	0.48
1:B:961:ARG:NE	1:B:981:GLY:O	2.44	0.48
1:C:114:VAL:HB	1:C:115:PRO:HD2	1.96	0.48
1:D:955:PHE:CD1	1:D:986:ILE:HD13	2.49	0.48
1:C:887:GLN:NE2	1:C:980:GLU:O	2.45	0.47
1:B:246:MET:CE	1:B:250:LEU:HD23	2.44	0.47
1:B:675:GLN:OE1	1:B:675:GLN:HA	2.14	0.47
1:C:757:GLN:NE2	6:C:9453:HOH:O	2.37	0.47
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.96	0.47
1:A:249:GLU:OE2	1:A:251:ARG:NE	2.42	0.47
1:A:687:GLN:N	1:A:688:PRO:CD	2.75	0.47
1:C:734:SER:CB	1:C:860:GLY:HA3	2.43	0.47
1:D:277:GLU:CD	1:D:277:GLU:N	2.69	0.47
1:D:651:LEU:C	1:D:651:LEU:CD1	2.87	0.47
1:B:622:HIS:CE1	5:B:8402:DMS:H12	2.49	0.47
1:B:738:PRO:HB3	1:B:751:LEU:HB2	1.96	0.47
1:C:13:ARG:O	1:C:14:ARG:C	2.57	0.47
1:C:811:LYS:HB3	1:C:811:LYS:HE2	1.82	0.47
1:C:824:GLN:CG	1:C:825:CYS:N	2.76	0.47
1:D:107:ILE:CA	5:D:8419:DMS:C2	2.93	0.47
1:D:147:ASN:HA	1:D:148:SER:HA	1.76	0.47
1:B:98:PRO:HB2	1:B:203:TRP:CE3	2.49	0.47
1:B:338:GLU:HG2	6:B:9297:HOH:O	2.14	0.47
1:B:748:CYS:C	1:B:749:ILE:HD12	2.40	0.47
1:C:622:HIS:CE1	5:C:8402:DMS:C1	2.97	0.47
1:C:833:ALA:HB1	1:C:858:ILE:O	2.15	0.47
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.44	0.47
1:A:696:LEU:HD23	1:A:720:TRP:CE3	2.50	0.47
1:A:718:GLN:CD	5:A:8503:DMS:H11	2.39	0.47
1:B:583:ASN:HA	1:B:584:PRO:HD3	1.67	0.47
1:B:773:LYS:N	1:B:773:LYS:CD	2.76	0.47
1:C:658:LEU:O	1:C:659:ASP:C	2.56	0.47
1:C:734:SER:C	1:C:736:ALA:H	2.23	0.47
1:C:986:ILE:HG23	1:C:986:ILE:HD13	1.35	0.47
1:D:962:TYR:OH	5:D:8423:DMS:H21	2.15	0.47
1:A:653:HIS:CD2	1:A:667:GLU:CG	2.96	0.47
1:B:872:VAL:O	1:B:873:ALA:C	2.57	0.47
1:B:74:LEU:HD22	1:B:153:TRP:CD2	2.51	0.46
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:GLU:HB2	6:B:9018:HOH:O	2.15	0.46
1:B:773:LYS:HD2	1:B:773:LYS:HA	1.59	0.46
1:B:93:HIS:CD2	5:B:8414:DMS:C2	2.99	0.46
1:C:230:ARG:HD3	6:C:9470:HOH:O	2.14	0.46
1:C:369:GLU:HB2	1:C:397:LEU:CD2	2.45	0.46
1:C:416:GLU:HA	1:C:460:ASN:O	2.14	0.46
1:C:610:ASP:O	1:C:611:ARG:HB2	2.15	0.46
1:A:320:GLY:C	5:A:8406:DMS:H21	2.40	0.46
1:C:822:LEU:HD11	1:C:824:GLN:O	2.14	0.46
1:A:780:LEU:C	1:A:781:ARG:HG3	2.41	0.46
1:B:768:MET:HG3	6:B:9511:HOH:O	2.15	0.46
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.51	0.46
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.46	0.46
1:D:92:MET:HA	1:D:92:MET:HE2	1.96	0.46
1:A:128:ASN:ND2	1:A:180:GLY:C	2.73	0.46
1:B:689:GLU:O	1:B:690:SER:OG	2.22	0.46
1:C:114:VAL:HB	1:C:115:PRO:CD	2.46	0.46
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.65	0.46
1:C:734:SER:HB3	1:C:860:GLY:C	2.40	0.46
1:C:788:PRO:HD3	1:C:968:MET:HE3	1.97	0.46
1:D:107:ILE:CA	5:D:8419:DMS:H21	2.45	0.46
1:A:246:MET:HE3	1:A:250:LEU:HD23	1.97	0.46
1:A:559:TYR:CE2	1:B:522:LYS:HA	2.51	0.46
1:B:801[A]:ILE:HG23	1:B:808:GLU:OE1	2.15	0.46
1:C:749:ILE:N	1:C:749:ILE:CD1	2.78	0.46
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.51	0.46
1:B:768:MET:O	1:B:775:GLN:HG2	2.16	0.46
1:C:835:LEU:C	1:C:836:ILE:HD13	2.41	0.46
1:D:800:ARG:NH2	6:D:9637:HOH:O	2.27	0.46
1:B:338:GLU:OE2	6:B:9297:HOH:O	2.20	0.46
1:C:689:GLU:O	1:C:690:SER:HB3	2.15	0.46
1:D:986:ILE:HD13	1:D:986:ILE:HG23	1.44	0.46
5:D:8423:DMS:H11	6:D:9269:HOH:O	2.16	0.46
1:A:125:LEU:O	1:A:183:ARG:HA	2.16	0.45
1:A:663:LEU:HB3	1:A:686:PRO:HG3	1.97	0.45
1:B:685:LEU:O	1:B:686:PRO:C	2.59	0.45
1:D:930:VAL:O	1:D:932:PRO:HD3	2.17	0.45
1:D:965:GLN:O	1:D:969:GLU:HG3	2.15	0.45
1:A:230:ARG:HH11	1:A:241:GLU:HG3	1.82	0.45
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.35	0.45
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:O	1:A:72:SER:C	2.58	0.45
1:B:416:GLU:HA	1:B:460:ASN:O	2.16	0.45
1:B:670:LEU:HA	1:B:670:LEU:HD23	1.35	0.45
1:D:654:TRP:CH2	1:D:685:LEU:HD21	2.51	0.45
1:A:127:PHE:O	1:A:182:ASN:N	2.39	0.45
1:A:686:PRO:C	1:A:688:PRO:HD3	2.41	0.45
1:C:990:HIS:HD2	1:C:991:MET:O	2.00	0.45
1:D:807:VAL:CG1	1:D:808:GLU:N	2.80	0.45
1:D:843:GLN:HA	1:D:847:LYS:O	2.17	0.45
1:D:1020:TRP:HD1	1:D:1021:CYS:N	2.13	0.45
1:A:94:GLY:O	1:A:95:TYR:C	2.59	0.45
1:C:230:ARG:HG2	1:C:230:ARG:NH1	2.30	0.45
1:C:278:ILE:N	1:C:278:ILE:CD1	2.80	0.45
1:D:55:ASN:O	5:D:8408:DMS:H21	2.17	0.45
1:A:822:LEU:HD11	1:A:824:GLN:O	2.17	0.45
1:A:906:TYR:CZ	1:A:937:LEU:HB2	2.52	0.45
1:B:655:MET:HE2	1:B:656:VAL:N	2.32	0.45
1:C:249:GLU:CD	1:C:251:ARG:HD3	2.41	0.45
1:D:688:PRO:C	1:D:690:SER:H	2.23	0.45
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.83	0.45
1:C:233:ASP:HA	5:C:8417:DMS:S	2.57	0.45
1:D:427:THR:HG21	1:D:462:SER:HB3	1.99	0.45
1:D:629:PHE:HA	1:D:637:GLU:O	2.17	0.45
1:D:962:TYR:CE1	5:D:8508:DMS:C1	3.00	0.45
1:A:49:GLN:HG2	6:A:9254:HOH:O	2.17	0.45
1:A:663:LEU:CD1	1:A:686:PRO:HG3	2.46	0.45
1:A:842:TRP:C	1:A:843:GLN:HG3	2.40	0.45
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.32	0.45
1:C:986:ILE:HG21	1:C:986:ILE:HD12	1.54	0.45
1:A:817:GLN:NE2	6:A:8937:HOH:O	2.49	0.45
1:C:633:GLY:HA3	1:C:634:GLN:HE21	1.81	0.45
1:D:802:ASP:OD1	1:D:803:PRO:HD2	2.16	0.45
1:C:805:ALA:O	1:C:806:TRP:C	2.58	0.44
1:C:824:GLN:HG2	1:C:825:CYS:N	2.31	0.44
1:D:93:HIS:HB3	1:D:95:TYR:CE1	2.51	0.44
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.98	0.44
1:A:178:ARG:HD2	6:A:9400:HOH:O	2.15	0.44
1:B:646:HIS:CE1	1:B:673:ALA:HB2	2.53	0.44
1:C:92:MET:HE3	1:C:205:MET:SD	2.57	0.44
1:C:579:ASP:OD1	1:C:583:ASN:N	2.32	0.44
1:A:781:ARG:NH1	6:A:9290:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:THR:O	1:A:829:THR:HG22	2.17	0.44
1:B:88:SER:HA	1:B:366:VAL:HG21	1.98	0.44
1:B:795[A]:VAL:HG13	1:B:999:TRP:CB	2.48	0.44
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.99	0.44
1:C:755:ARG:HG3	1:C:756:TRP:N	2.32	0.44
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.47	0.44
1:A:128:ASN:HD21	1:A:180:GLY:CA	2.17	0.44
1:A:804[B]:ASN:ND2	1:A:809:ARG:NH2	2.65	0.44
1:B:299:LYS:HE2	6:B:9258:HOH:O	2.17	0.44
1:C:734:SER:HB2	1:C:860:GLY:HA3	2.00	0.44
1:D:360:HIS:CE1	1:D:362:LEU:HG	2.52	0.44
1:D:738:PRO:HB3	1:D:751:LEU:HB2	1.99	0.44
1:D:749:ILE:N	1:D:749:ILE:CD1	2.80	0.44
1:A:651:LEU:HD13	1:A:667:GLU:HG2	1.99	0.44
1:B:183:ARG:HG2	1:B:183:ARG:NH1	2.31	0.44
1:D:88:SER:HA	1:D:366:VAL:HG21	2.00	0.44
1:D:262:GLN:O	1:D:263:GLY:C	2.60	0.44
1:A:576:ILE:HD13	1:A:576:ILE:HA	1.81	0.44
1:B:262:GLN:NE2	1:B:263:GLY:N	2.66	0.44
1:B:668:VAL:CG1	1:B:669:PRO:N	2.79	0.44
1:C:658:LEU:HB2	1:C:694:LEU:HD23	1.99	0.44
1:A:619:GLU:HA	1:A:912:ALA:HB2	2.00	0.44
1:A:850:PHE:HA	1:A:871:GLU:O	2.17	0.44
1:C:890:GLN:HG3	1:C:891:VAL:H	1.83	0.44
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.53	0.44
1:A:687:GLN:N	1:A:688:PRO:HD3	2.33	0.44
1:A:801[B]:ILE:HD12	1:A:801[B]:ILE:N	2.32	0.44
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.53	0.44
1:D:372:MET:HE2	6:D:8938:HOH:O	2.17	0.44
1:D:60:PHE:HA	1:D:122:CYS:O	2.17	0.44
1:D:80:GLU:O	1:D:81:ALA:C	2.55	0.44
1:D:804:ASN:HA	1:D:809:ARG:HE	1.83	0.44
1:A:557:ARG:HH11	1:A:557:ARG:HD2	1.65	0.43
1:A:416:GLU:OE2	1:A:418:HIS:HB2	2.18	0.43
1:A:577:LYS:O	1:A:584:PRO:HA	2.18	0.43
1:A:710:GLU:O	1:A:711:ALA:C	2.61	0.43
1:B:301:TRP:CH2	1:B:452:SER:HA	2.53	0.43
1:B:655:MET:HE2	1:B:664:ALA:O	2.17	0.43
1:B:687:GLN:CB	1:B:688:PRO:CD	2.95	0.43
1:B:755:ARG:O	1:B:768:MET:HG2	2.18	0.43
1:B:777:LEU:HD23	1:B:777:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1020:TRP:HD1	1:B:1021:CYS:N	2.15	0.43
1:C:80:GLU:CD	1:C:80:GLU:H	2.26	0.43
1:D:26:ARG:HD2	1:D:169:SER:HA	1.98	0.43
1:D:316:HIS:HA	1:D:323:ILE:HD12	1.99	0.43
1:A:390:SER:HA	1:A:391:HIS:HA	1.85	0.43
1:B:243:GLU:OE2	1:B:245:GLN:NE2	2.46	0.43
1:C:46:ARG:HG2	6:C:9454:HOH:O	2.18	0.43
1:C:995:GLY:O	1:C:996:ASP:C	2.60	0.43
1:D:370:GLN:HB2	6:D:9233:HOH:O	2.18	0.43
1:A:784:PHE:HA	1:A:881:ARG:O	2.19	0.43
1:C:730:LEU:CD2	1:C:730:LEU:H	2.19	0.43
1:D:56:GLY:HA3	5:D:8408:DMS:H11	2.01	0.43
1:D:58:TRP:CD1	1:D:86:VAL:HB	2.54	0.43
1:A:759:ASN:HB3	1:A:762:SER:OG	2.18	0.43
1:C:745:MET:HA	1:C:761:GLN:HE22	1.84	0.43
1:A:147:ASN:HA	1:A:148:SER:HA	1.66	0.43
1:A:687:GLN:O	1:A:688:PRO:C	2.62	0.43
1:B:651:LEU:HD21	1:B:701:VAL:HB	2.00	0.43
1:C:472:TYR:OH	1:C:476:LYS:HE2	2.19	0.43
1:C:513:PRO:O	1:C:514:ALA:HB3	2.19	0.43
1:A:575:LEU:HA	1:A:575:LEU:HD23	1.81	0.43
1:A:599:ARG:HG2	1:A:798[B]:ALA:HB2	2.00	0.43
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.18	0.43
1:C:835:LEU:O	1:C:836:ILE:HD13	2.18	0.43
1:A:126:THR:HA	1:A:182:ASN:O	2.19	0.43
1:B:595:THR:HG23	1:B:595:THR:O	2.18	0.43
1:C:847:LYS:NZ	6:C:9337:HOH:O	2.51	0.43
1:D:373:VAL:O	1:D:377:LEU:HG	2.18	0.43
1:B:225:PHE:HA	1:B:243:GLU:O	2.19	0.43
1:B:794[A]:GLY:HA2	1:B:998:SER:O	2.19	0.43
1:A:637:GLU:CD	1:A:677:LYS:HE3	2.44	0.43
1:B:36:TRP:CD2	1:B:42:ALA:HA	2.53	0.43
1:C:872:VAL:O	1:C:873:ALA:C	2.60	0.43
1:A:701:VAL:O	1:A:703:PRO:HD3	2.18	0.42
1:B:59:ARG:HB2	1:B:124:SER:OG	2.19	0.42
1:B:333:ARG:HG3	1:B:344:LEU:HD11	2.00	0.42
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.36	0.42
1:A:824:GLN:NE2	1:A:837:THR:HG22	2.34	0.42
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.54	0.42
1:C:334:GLU:OE1	1:C:336:ARG:HD3	2.19	0.42
1:C:653:HIS:CE1	1:C:667:GLU:CG	3.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:658:LEU:O	1:D:659:ASP:C	2.62	0.42
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.54	0.42
1:D:654:TRP:CZ3	1:D:685:LEU:HD21	2.54	0.42
1:B:859:ASP:OD1	1:B:861:SER:OG	2.23	0.42
1:D:588:TYR:O	1:D:591:ASP:HB2	2.19	0.42
1:D:765:LEU:HD21	1:D:768:MET:SD	2.60	0.42
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.20	0.42
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.54	0.42
1:A:663:LEU:CD1	1:A:686:PRO:CG	2.97	0.42
1:B:254:LEU:C	1:B:255:ARG:HG2	2.45	0.42
1:B:663:LEU:HD22	1:B:663:LEU:HA	1.68	0.42
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.00	0.42
1:C:749:ILE:O	1:C:755:ARG:HA	2.20	0.42
1:D:806:TRP:CD2	1:D:991:MET:HE1	2.55	0.42
1:D:859:ASP:OD1	1:D:861:SER:OG	2.24	0.42
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.55	0.42
1:C:333:ARG:HA	1:C:345:ASN:OD1	2.20	0.42
1:C:562:LEU:HD23	1:C:562:LEU:HA	1.78	0.42
5:C:8410:DMS:H13	6:C:9211:HOH:O	2.20	0.42
1:D:301:TRP:CH2	1:D:452:SER:HA	2.54	0.42
1:D:618:THR:HG23	6:D:9069:HOH:O	2.19	0.42
1:D:759:ASN:OD1	1:D:761:GLN:N	2.52	0.42
1:D:784:PHE:HA	1:D:881:ARG:O	2.20	0.42
1:C:956:GLN:CD	1:C:956:GLN:N	2.78	0.42
1:A:127:PHE:N	1:A:182:ASN:O	2.45	0.42
1:A:752:GLY:C	1:A:754:LYS:H	2.28	0.42
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.54	0.42
1:C:50:GLN:CD	1:C:50:GLN:N	2.77	0.42
1:C:86:VAL:HG13	1:C:87:PRO:HA	2.01	0.42
1:C:687:GLN:HG3	1:C:688:PRO:HD2	2.01	0.42
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.01	0.42
1:A:931:PHE:CD2	1:A:931:PHE:C	2.97	0.42
1:B:666:GLY:C	1:B:667:GLU:HG2	2.45	0.42
1:A:316:HIS:CB	5:A:8406:DMS:H23	2.49	0.42
1:B:962:TYR:OH	5:B:8508:DMS:H23	2.20	0.42
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.55	0.42
1:C:835:LEU:HD11	1:C:855:THR:HB	2.01	0.42
1:C:930:VAL:HA	1:C:973:ARG:HD3	2.02	0.42
1:D:952:ARG:HB2	1:D:952:ARG:NH1	2.35	0.42
1:A:915:PHE:C	1:A:915:PHE:CD2	2.97	0.41
1:C:388:ARG:HH11	1:C:388:ARG:HD3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:777:LEU:HA	1:C:777:LEU:HD23	1.74	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.66	0.41
1:B:599:ARG:HB3	1:B:600:GLN:HE21	1.85	0.41
1:C:800[A]:ARG:CZ	1:C:800[A]:ARG:CB	2.98	0.41
1:A:781:ARG:HH11	1:A:781:ARG:CG	2.29	0.41
1:A:59:ARG:HG3	1:A:77:ASP:OD1	2.20	0.41
1:B:646:HIS:CE1	1:B:673:ALA:CB	3.03	0.41
5:C:8402:DMS:H22	6:C:9405:HOH:O	2.20	0.41
1:D:359:HIS:CD2	1:D:573:GLN:HA	2.55	0.41
1:D:688:PRO:C	1:D:690:SER:N	2.77	0.41
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.47	0.41
1:C:796[A]:SER:OG	1:C:808:GLU:OE2	2.32	0.41
1:C:963:SER:HB3	1:C:983:TRP:CE2	2.55	0.41
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.21	0.41
1:A:651:LEU:C	1:A:651:LEU:CD1	2.92	0.41
1:C:808:GLU:OE1	1:C:811:LYS:NZ	2.49	0.41
1:D:106:PRO:O	5:D:8419:DMS:H23	2.21	0.41
1:A:88:SER:HA	1:A:366:VAL:HG21	2.02	0.41
1:A:431:ARG:HG3	6:A:9315:HOH:O	2.20	0.41
1:B:128:ASN:HA	1:B:180:GLY:O	2.21	0.41
1:C:890:GLN:CG	1:C:891:VAL:N	2.83	0.41
1:D:46:ARG:HB3	1:D:47:PRO:HD2	2.02	0.41
1:D:843:GLN:CA	1:D:847:LYS:O	2.68	0.41
1:A:143:PHE:O	1:A:168:PRO:HA	2.21	0.41
1:A:358:GLU:C	1:A:367:MET:HE3	2.45	0.41
1:B:183:ARG:HG2	6:B:8918:HOH:O	2.21	0.41
1:C:251:ARG:HH12	1:C:253:TYR:HE2	1.68	0.41
1:C:369:GLU:O	1:C:370:GLN:C	2.63	0.41
1:D:91:GLN:H	1:D:91:GLN:CD	2.28	0.41
1:A:774:LYS:HB2	1:A:774:LYS:HE2	1.81	0.41
1:A:843:GLN:HA	1:A:847:LYS:O	2.20	0.41
5:A:8405:DMS:O	6:A:9240:HOH:O	2.22	0.41
1:B:654:TRP:CE3	1:B:665:SER:HA	2.56	0.41
1:C:45:ASP:OD1	5:C:8501:DMS:H11	2.21	0.41
1:C:687:GLN:HG3	1:C:688:PRO:CD	2.51	0.41
1:A:226:HIS:O	1:A:242:ALA:HA	2.21	0.41
1:A:237:ARG:NH1	1:A:237:ARG:CG	2.82	0.41
1:A:262:GLN:NE2	1:A:299:LYS:CD	2.84	0.41
1:A:773:LYS:HE2	1:A:773:LYS:HB2	1.85	0.41
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.56	0.41
1:D:34:ALA:O	1:D:35:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ASP:HA	1:A:480:PRO:HD2	1.94	0.40
1:B:262:GLN:C	1:B:262:GLN:NE2	2.77	0.40
1:B:655:MET:O	1:B:655:MET:HG3	2.20	0.40
1:B:851:ILE:HB	1:B:871:GLU:HB2	2.03	0.40
1:C:789:LEU:O	1:C:790:ASP:C	2.63	0.40
1:D:635:THR:OG1	1:D:681:GLU:OE1	2.29	0.40
1:A:809:ARG:HD3	6:A:9187:HOH:O	2.21	0.40
1:C:110:ASN:O	1:C:113:PHE:HB2	2.22	0.40
1:C:746:ASP:HA	1:C:760:ARG:HG3	2.03	0.40
1:C:972:HIS:HB3	1:C:974:HIS:ND1	2.36	0.40
1:D:378:LEU:HG	6:D:9268:HOH:O	2.21	0.40
1:D:655:MET:HE1	1:D:699:ARG:HD2	2.03	0.40
1:D:844:HIS:O	1:D:845:GLN:C	2.63	0.40
1:A:816:TYR:C	1:A:817:GLN:HE21	2.29	0.40
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.57	0.40
1:C:800[A]:ARG:CZ	1:C:800[A]:ARG:CA	2.97	0.40
1:D:794:GLY:HA2	1:D:998:SER:O	2.21	0.40
1:D:808:GLU:OE2	1:D:811:LYS:NZ	2.46	0.40
1:A:594:ASP:C	1:A:595:THR:HG22	2.46	0.40
1:B:616:ALA:O	1:B:617:LEU:C	2.63	0.40
1:B:782:ASP:HA	1:B:884:LEU:HD23	2.03	0.40
6:B:9189:HOH:O	5:C:8420:DMS:H12	2.22	0.40
1:C:411:ASP:OD2	1:C:447:ASP:OD2	2.40	0.40
1:C:737:ILE:O	1:C:737:ILE:HG13	2.06	0.40
1:C:750:GLU:OE2	1:C:755:ARG:HD3	2.20	0.40
1:D:921:PRO:O	1:D:922:LEU:C	2.63	0.40
1:A:36:TRP:CD2	1:A:42:ALA:HA	2.57	0.40
1:B:91:GLN:HG2	1:B:98:PRO:CA	2.50	0.40
1:B:232:ASN:HD21	1:B:237:ARG:HG3	1.80	0.40
1:B:562:LEU:HD23	1:B:562:LEU:HA	1.83	0.40
1:B:655:MET:HB3	6:B:9494:HOH:O	2.21	0.40
1:B:749:ILE:HD12	1:B:749:ILE:N	2.37	0.40
1:C:802[A]:ASP:OD1	1:C:802[A]:ASP:C	2.63	0.40
1:D:577:LYS:O	1:D:584:PRO:HA	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:9538:HOH:O	6:D:9651:HOH:O[2_454]	2.09	0.11

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	1020/1023 (100%)	980 (96%)	35 (3%)	5 (0%)	24	14
1	B	1020/1023 (100%)	985 (97%)	34 (3%)	1 (0%)	48	34
1	C	1020/1023 (100%)	980 (96%)	38 (4%)	2 (0%)	43	31
1	D	1009/1023 (99%)	971 (96%)	35 (4%)	3 (0%)	36	25
All	All	4069/4092 (99%)	3916 (96%)	142 (4%)	11 (0%)	43	25

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	C	690	SER
1	D	688	PRO
1	A	688	PRO
1	A	164	ASP
1	D	164	ASP
1	D	201	ASP
1	A	798[A]	ALA
1	A	798[B]	ALA
1	C	164	ASP
1	A	687	GLN

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	873/875 (100%)	835 (96%)	38 (4%)	25	13
1	B	873/875 (100%)	833 (95%)	40 (5%)	24	12
1	C	873/875 (100%)	828 (95%)	45 (5%)	21	9
1	D	864/875 (99%)	823 (95%)	41 (5%)	23	11
All	All	3483/3500 (100%)	3319 (95%)	164 (5%)	24	11

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	GLU
1	A	128	ASN
1	A	131	GLU
1	A	237	ARG
1	A	344	LEU
1	A	431	ARG
1	A	478	VAL
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	595	THR
1	A	600	GLN
1	A	655	MET
1	A	671	ASP
1	A	675	GLN
1	A	684	GLU
1	A	687	GLN
1	A	689	GLU
1	A	729	THR
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	799[A]	THR
1	A	799[B]	THR
1	A	800[A]	ARG
1	A	800[B]	ARG
1	A	801[A]	ILE
1	A	801[B]	ILE
1	A	817	GLN
1	A	829	THR
1	A	885	ASN
1	A	890	GLN
1	A	917	ARG

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Mol	Chain	Res	Type
1	A	968	MET
1	A	984	LEU
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	13	ARG
1	B	80	GLU
1	B	117	GLU
1	B	136	GLU
1	B	230	ARG
1	B	237	ARG
1	B	264	GLU
1	B	344	LEU
1	B	362	LEU
1	B	370	GLN
1	B	477	SER
1	B	519	SER
1	B	546	LEU
1	B	580	GLU
1	B	581	ASN
1	B	600	GLN
1	B	634	GLN
1	B	635	THR
1	B	651	LEU
1	B	655	MET
1	B	663	LEU
1	B	667	GLU
1	B	672	VAL
1	B	687	GLN
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	770	ILE
1	B	773	LYS
1	B	799[A]	THR
1	B	799[B]	THR
1	B	801[A]	ILE
1	B	801[B]	ILE
1	B	819	GLU
1	B	845	GLN
1	B	847	LYS
1	B	885	ASN

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Mol	Chain	Res	Type
1	B	890	GLN
1	B	917	ARG
1	B	956	GLN
1	C	71	GLU
1	C	80	GLU
1	C	135	GLN
1	C	157	ARG
1	C	178	ARG
1	C	230	ARG
1	C	251	ARG
1	C	262	GLN
1	C	278	ILE
1	C	333	ARG
1	C	344	LEU
1	C	367	MET
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	581	ASN
1	C	634	GLN
1	C	655	MET
1	C	663	LEU
1	C	672	VAL
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	710	GLU
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	749	ILE
1	C	750	GLU
1	C	755	ARG
1	C	773	LYS
1	C	795[A]	VAL
1	C	795[B]	VAL
1	C	796[A]	SER
1	C	796[B]	SER
1	C	800[A]	ARG
1	C	800[B]	ARG

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Mol	Chain	Res	Type
1	C	819	GLU
1	C	917	ARG
1	C	923	SER
1	C	956	GLN
1	C	986	ILE
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	80	GLU
1	D	237	ARG
1	D	267	VAL
1	D	319	ASP
1	D	344	LEU
1	D	370	GLN
1	D	478	VAL
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	599	ARG
1	D	663	LEU
1	D	667	GLU
1	D	672	VAL
1	D	681	GLU
1	D	684	GLU
1	D	685	LEU
1	D	687	GLN
1	D	689	GLU
1	D	699	ARG
1	D	729	THR
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	801	ILE
1	D	804	ASN
1	D	824	GLN
1	D	829	THR
1	D	843	GLN
1	D	845	GLN
1	D	885	ASN
1	D	893	GLU

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Mol	Chain	Res	Type
1	D	956	GLN
1	D	986	ILE
1	D	1017	GLN
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	128	ASN
1	A	262	GLN
1	A	485	GLN
1	A	600	GLN
1	A	624	GLN
1	A	653	HIS
1	A	761	GLN
1	A	775	GLN
1	A	817	GLN
1	A	824	GLN
1	A	843	GLN
1	A	844	HIS
1	A	878	HIS
1	A	950	GLN
1	B	128	ASN
1	B	262	GLN
1	B	363	HIS
1	B	445	GLN
1	B	485	GLN
1	B	554	GLN
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	653	HIS
1	B	757	GLN
1	B	863	GLN
1	B	878	HIS
1	B	903	GLN
1	B	977	HIS
1	C	128	ASN

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Mol	Chain	Res	Type
1	C	163	GLN
1	C	221	GLN
1	C	363	HIS
1	C	485	GLN
1	C	624	GLN
1	C	634	GLN
1	C	704	ASN
1	C	761	GLN
1	C	783	GLN
1	C	824	GLN
1	C	878	HIS
1	C	977	HIS
1	D	135	GLN
1	D	266	GLN
1	D	363	HIS
1	D	394	ASN
1	D	583	ASN
1	D	624	GLN
1	D	878	HIS
1	D	903	GLN
1	D	977	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 118 ligands modelled in this entry, 27 are monoatomic - leaving 91 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8407	-	3,3,3	1.42	0	3,3,3	0.34	0
5	DMS	B	8408	-	3,3,3	0.28	0	3,3,3	0.49	0
5	DMS	D	8408	-	3,3,3	1.59	1 (33%)	3,3,3	0.39	0
2	149	B	2001	4	12,12,12	2.23	1 (8%)	15,17,17	1.06	0
5	DMS	B	8416	-	3,3,3	0.83	0	3,3,3	0.26	0
5	DMS	D	8404	-	3,3,3	1.05	0	3,3,3	0.18	0
5	DMS	A	8425	4	3,3,3	1.59	1 (33%)	3,3,3	0.17	0
5	DMS	A	8406	-	3,3,3	1.05	0	3,3,3	0.39	0
5	DMS	A	8404	-	3,3,3	1.91	1 (33%)	3,3,3	0.46	0
5	DMS	A	8401	-	3,3,3	0.81	0	3,3,3	0.49	0
5	DMS	D	8409	-	3,3,3	1.54	0	3,3,3	0.48	0
5	DMS	B	8417	-	3,3,3	1.24	0	3,3,3	0.60	0
5	DMS	C	8405	-	3,3,3	1.59	1 (33%)	3,3,3	0.51	0
5	DMS	D	8416	-	3,3,3	0.57	0	3,3,3	0.44	0
5	DMS	B	8401	-	3,3,3	0.90	0	3,3,3	0.55	0
5	DMS	C	8417	-	3,3,3	0.74	0	3,3,3	0.31	0
5	DMS	C	8404	-	3,3,3	1.74	1 (33%)	3,3,3	0.61	0
5	DMS	C	8420	-	3,3,3	1.25	1 (33%)	3,3,3	0.71	0
5	DMS	A	8421	-	3,3,3	0.93	0	3,3,3	0.83	0
5	DMS	A	8408	-	3,3,3	0.39	0	3,3,3	0.45	0
5	DMS	A	8419	-	3,3,3	1.14	0	3,3,3	0.19	0
5	DMS	C	8423	-	3,3,3	0.96	0	3,3,3	0.39	0
5	DMS	C	8425	4	3,3,3	1.00	0	3,3,3	0.52	0
5	DMS	A	8411	-	3,3,3	1.09	0	3,3,3	0.80	0
5	DMS	D	8402	-	3,3,3	0.72	0	3,3,3	0.68	0
5	DMS	B	8504	-	3,3,3	1.30	1 (33%)	3,3,3	0.33	0
5	DMS	C	8416	-	3,3,3	1.30	1 (33%)	3,3,3	0.35	0
2	149	A	2001	4	12,12,12	2.08	2 (16%)	15,17,17	3.77	4 (26%)
5	DMS	B	8402	-	3,3,3	1.40	1 (33%)	3,3,3	0.20	0
5	DMS	A	8405	-	3,3,3	0.61	0	3,3,3	0.63	0
5	DMS	B	8502	-	3,3,3	1.48	1 (33%)	3,3,3	0.87	0
5	DMS	A	8416	-	3,3,3	0.85	0	3,3,3	0.87	0
5	DMS	C	8408	-	3,3,3	0.99	0	3,3,3	0.42	0
5	DMS	C	8421	-	3,3,3	0.67	0	3,3,3	0.12	0
5	DMS	D	8503	-	3,3,3	0.52	0	3,3,3	0.29	0
5	DMS	B	8420	-	3,3,3	0.60	0	3,3,3	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8414	-	3,3,3	1.93	1 (33%)	3,3,3	0.66	0
5	DMS	A	8501	-	3,3,3	1.05	0	3,3,3	0.33	0
5	DMS	B	8412	-	3,3,3	1.28	1 (33%)	3,3,3	0.51	0
5	DMS	B	8409	-	3,3,3	1.79	1 (33%)	3,3,3	1.14	0
5	DMS	A	8414	-	3,3,3	1.35	0	3,3,3	0.30	0
5	DMS	D	8401	-	3,3,3	0.92	0	3,3,3	0.30	0
5	DMS	B	8410	-	3,3,3	1.26	0	3,3,3	0.32	0
5	DMS	B	8411	-	3,3,3	0.29	0	3,3,3	0.58	0
5	DMS	D	8705	-	3,3,3	0.92	0	3,3,3	0.19	0
5	DMS	C	8601	-	3,3,3	1.15	0	3,3,3	1.07	0
5	DMS	A	8503	-	3,3,3	1.39	1 (33%)	3,3,3	0.41	0
5	DMS	C	8402	-	3,3,3	2.22	1 (33%)	3,3,3	0.48	0
5	DMS	D	8419	-	3,3,3	1.83	1 (33%)	3,3,3	0.44	0
5	DMS	B	8414	-	3,3,3	0.66	0	3,3,3	0.30	0
5	DMS	C	8428	-	3,3,3	0.85	0	3,3,3	0.29	0
5	DMS	D	8423	-	3,3,3	0.65	0	3,3,3	0.26	0
5	DMS	C	8409	-	3,3,3	0.69	0	3,3,3	0.73	0
5	DMS	D	8501	-	3,3,3	0.66	0	3,3,3	0.38	0
5	DMS	A	8412	-	3,3,3	1.37	0	3,3,3	0.30	0
5	DMS	B	8403	-	3,3,3	1.73	1 (33%)	3,3,3	0.26	0
5	DMS	B	8406	-	3,3,3	0.81	0	3,3,3	0.32	0
5	DMS	C	8501	-	3,3,3	0.87	0	3,3,3	0.22	0
5	DMS	B	8425	4	3,3,3	2.82	1 (33%)	3,3,3	0.61	0
5	DMS	D	8412	-	3,3,3	1.03	0	3,3,3	0.43	0
2	149	D	2001	4	12,12,12	1.98	3 (25%)	15,17,17	2.61	5 (33%)
5	DMS	C	8410	-	3,3,3	0.95	0	3,3,3	0.40	0
5	DMS	A	8504	-	3,3,3	0.70	0	3,3,3	0.40	0
5	DMS	C	8411	-	3,3,3	1.16	0	3,3,3	0.10	0
5	DMS	D	8405	-	3,3,3	0.38	0	3,3,3	1.25	0
5	DMS	D	8410	-	3,3,3	1.75	0	3,3,3	0.52	0
5	DMS	A	8409	-	3,3,3	2.82	1 (33%)	3,3,3	0.23	0
5	DMS	D	8508	-	3,3,3	1.63	1 (33%)	3,3,3	0.11	0
5	DMS	D	8414	-	3,3,3	0.68	0	3,3,3	0.32	0
2	149	C	2001	4	12,12,12	1.56	2 (16%)	15,17,17	1.74	3 (20%)
5	DMS	B	8421	-	3,3,3	0.76	0	3,3,3	0.05	0
5	DMS	D	8406	-	3,3,3	0.70	0	3,3,3	0.72	0
5	DMS	A	8602	-	3,3,3	0.43	0	3,3,3	0.49	0
5	DMS	D	8417	-	3,3,3	0.83	0	3,3,3	0.15	0
5	DMS	A	8403	-	3,3,3	1.95	2 (66%)	3,3,3	1.02	0
5	DMS	D	8701	-	3,3,3	2.27	3 (100%)	3,3,3	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8415	-	3,3,3	1.86	1 (33%)	3,3,3	0.31	0
5	DMS	D	8403	-	3,3,3	1.80	1 (33%)	3,3,3	0.32	0
5	DMS	B	8601	-	3,3,3	0.88	0	3,3,3	0.61	0
5	DMS	A	8402	-	3,3,3	1.53	0	3,3,3	0.64	0
5	DMS	D	8703	-	3,3,3	1.84	1 (33%)	3,3,3	0.26	0
5	DMS	B	8423	-	3,3,3	0.83	0	3,3,3	0.32	0
5	DMS	D	8411	-	3,3,3	0.73	0	3,3,3	0.36	0
5	DMS	B	8404	-	3,3,3	0.79	0	3,3,3	0.07	0
5	DMS	B	8508	-	3,3,3	1.46	0	3,3,3	0.20	0
5	DMS	D	8421	-	3,3,3	0.81	0	3,3,3	0.42	0
5	DMS	C	8407	-	3,3,3	1.67	1 (33%)	3,3,3	0.54	0
5	DMS	B	8405	-	3,3,3	1.38	0	3,3,3	0.41	0
5	DMS	C	8412	-	3,3,3	0.93	0	3,3,3	0.51	0
5	DMS	C	8403	-	3,3,3	1.67	1 (33%)	3,3,3	0.57	0
5	DMS	C	8401	-	3,3,3	1.21	1 (33%)	3,3,3	0.05	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	149	D	2001	4	-	2/2/22/22	0/1/1/1
2	149	B	2001	4	-	1/2/22/22	0/1/1/1
2	149	A	2001	4	-	1/2/22/22	0/1/1/1
2	149	C	2001	4	-	1/2/22/22	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	149	O5-C1	6.69	1.44	1.34
2	D	2001	149	O5-C1	5.28	1.42	1.34
2	A	2001	149	O5-C1	5.04	1.42	1.34
5	B	8425	DMS	O-S	4.78	1.81	1.50
5	A	8409	DMS	O-S	4.43	1.79	1.50
2	A	2001	149	O2-C2	3.92	1.49	1.42
2	C	2001	149	O5-C1	3.41	1.39	1.34
5	C	8402	DMS	C2-S	3.21	1.99	1.76
5	D	8419	DMS	C2-S	-3.06	1.54	1.76
5	B	8409	DMS	O-S	3.04	1.70	1.50
5	D	8703	DMS	C1-S	2.98	1.97	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8414	DMS	O-S	-2.90	1.31	1.50
2	D	2001	149	O5-C5	-2.89	1.42	1.46
5	A	8404	DMS	C2-S	2.84	1.96	1.76
5	C	8404	DMS	C2-S	2.78	1.95	1.76
5	D	8408	DMS	C1-S	2.73	1.95	1.76
5	D	8508	DMS	O-S	2.70	1.68	1.50
5	B	8403	DMS	C2-S	2.68	1.95	1.76
5	C	8415	DMS	C1-S	2.61	1.94	1.76
5	D	8403	DMS	C2-S	2.60	1.94	1.76
5	A	8403	DMS	C2-S	2.52	1.94	1.76
5	D	8701	DMS	O-S	2.41	1.66	1.50
5	A	8425	DMS	O-S	2.38	1.66	1.50
5	B	8502	DMS	O-S	2.35	1.65	1.50
2	D	2001	149	C2-C1	-2.32	1.47	1.52
5	D	8701	DMS	C1-S	2.31	1.92	1.76
5	C	8407	DMS	C2-S	2.27	1.92	1.76
2	C	2001	149	C3-C2	2.27	1.56	1.53
5	A	8403	DMS	O-S	2.26	1.65	1.50
5	C	8405	DMS	O-S	2.23	1.65	1.50
5	B	8504	DMS	C2-S	-2.22	1.60	1.76
5	B	8402	DMS	C2-S	2.19	1.91	1.76
5	C	8416	DMS	C2-S	2.14	1.91	1.76
5	C	8420	DMS	O-S	2.11	1.64	1.50
5	D	8701	DMS	C2-S	2.09	1.90	1.76
5	B	8412	DMS	C1-S	2.05	1.90	1.76
5	C	8401	DMS	C2-S	2.05	1.90	1.76
5	C	8403	DMS	O-S	2.03	1.63	1.50
5	A	8503	DMS	O-S	-2.02	1.36	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	149	O5-C5-C6	-12.87	93.14	106.05
2	D	2001	149	O5-C5-C6	-7.40	98.63	106.05
2	A	2001	149	C3-C4-C5	-4.69	101.73	110.23
2	C	2001	149	O4-C4-C5	-4.14	99.14	109.32
2	D	2001	149	C3-C4-C5	-3.78	103.38	110.23
2	D	2001	149	O4-C4-C5	3.29	117.43	109.32
2	A	2001	149	O5-C1-O1	2.60	122.28	118.52
2	C	2001	149	O3-C3-C4	-2.58	104.30	110.38
2	D	2001	149	O3-C3-C4	-2.43	104.64	110.38
2	A	2001	149	O3-C3-C2	-2.38	104.93	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	149	O2-C2-C3	2.25	115.21	110.53
2	C	2001	149	O5-C5-C6	2.20	108.26	106.05

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2001	149	O5-C5-C6-O6
2	C	2001	149	O5-C5-C6-O6
2	A	2001	149	O5-C5-C6-O6
2	B	2001	149	O5-C5-C6-O6
2	D	2001	149	C4-C5-C6-O6

There are no ring outliers.

38 monomers are involved in 66 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8407	DMS	1	0
5	D	8408	DMS	2	0
5	D	8404	DMS	2	0
5	A	8425	DMS	2	0
5	A	8406	DMS	3	0
5	A	8404	DMS	2	0
5	B	8417	DMS	1	0
5	C	8417	DMS	3	0
5	C	8420	DMS	1	0
5	C	8423	DMS	1	0
5	B	8504	DMS	1	0
5	B	8402	DMS	1	0
5	A	8405	DMS	1	0
5	A	8416	DMS	1	0
5	C	8408	DMS	1	0
5	D	8503	DMS	1	0
5	B	8420	DMS	1	0
5	B	8410	DMS	1	0
5	A	8503	DMS	1	0
5	C	8402	DMS	3	0
5	D	8419	DMS	5	0
5	B	8414	DMS	3	0
5	D	8423	DMS	3	0
5	B	8403	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8501	DMS	1	0
5	D	8412	DMS	3	0
5	C	8410	DMS	1	0
5	D	8410	DMS	1	0
5	D	8508	DMS	5	0
5	D	8406	DMS	3	0
5	A	8602	DMS	1	0
5	D	8417	DMS	1	0
5	A	8403	DMS	1	0
5	D	8403	DMS	1	0
5	D	8703	DMS	1	0
5	B	8423	DMS	1	0
5	B	8508	DMS	3	0
5	C	8407	DMS	1	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1000/1023 (97%)	-0.65	8 (0%) 82 83	13, 23, 51, 90	0
1	B	1009/1023 (98%)	-0.60	13 (1%) 75 75	4, 23, 49, 90	9 (0%)
1	C	1011/1023 (98%)	-0.66	10 (0%) 79 80	4, 22, 52, 89	11 (1%)
1	D	1011/1023 (98%)	-0.65	9 (0%) 81 81	13, 23, 52, 94	0
All	All	4031/4092 (98%)	-0.64	40 (0%) 79 80	4, 23, 51, 94	20 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	801[A]	ILE	4.5
1	C	798[A]	ALA	4.0
1	C	801[A]	ILE	3.8
1	B	798[A]	ALA	3.7
1	D	801	ILE	3.7
1	C	803[A]	PRO	3.6
1	D	799	THR	3.1
1	B	799[A]	THR	3.1
1	D	735	HIS	3.1
1	D	634	GLN	3.0
1	A	686	PRO	3.0
1	B	730	LEU	2.8
1	D	686	PRO	2.8
1	C	802[A]	ASP	2.8
1	B	745	MET	2.7
1	C	761	GLN	2.6
1	A	772	ASP	2.6
1	D	685	LEU	2.6
1	B	795[A]	VAL	2.6
1	B	803[A]	PRO	2.6
1	C	799[A]	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	802[A]	ASP	2.5
1	D	734	SER	2.5
1	C	800[A]	ARG	2.5
1	C	795[A]	VAL	2.5
1	D	732	ALA	2.5
1	C	731	PRO	2.5
1	A	685	LEU	2.4
1	B	733	ALA	2.3
1	A	735	HIS	2.3
1	C	581	ASN	2.2
1	B	685	LEU	2.2
1	A	1023	LYS	2.1
1	A	688	PRO	2.1
1	B	804[A]	ASN	2.1
1	A	732	ALA	2.1
1	B	1023	LYS	2.1
1	A	634	GLN	2.1
1	D	802	ASP	2.1
1	B	686	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMS	A	8407	4/4	0.80	0.15	32,46,85,100	0
5	DMS	C	8416	4/4	0.82	0.15	47,66,73,96	0
5	DMS	B	8508	4/4	0.86	0.14	41,54,84,84	0
5	DMS	A	8503	4/4	0.86	0.16	35,51,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8421	4/4	0.87	0.16	61,66,87,100	0
5	DMS	D	8423	4/4	0.87	0.17	48,53,78,100	0
5	DMS	D	8417	4/4	0.88	0.11	30,32,35,100	0
5	DMS	B	8421	4/4	0.88	0.11	44,57,59,87	0
5	DMS	C	8420	4/4	0.89	0.14	48,49,57,96	0
5	DMS	C	8407	4/4	0.89	0.10	29,37,51,72	0
3	MG	B	3003	1/1	0.89	0.11	53,53,53,53	0
5	DMS	D	8503	4/4	0.89	0.13	36,66,84,90	0
5	DMS	D	8410	4/4	0.90	0.15	47,58,100,100	0
5	DMS	C	8417	4/4	0.90	0.12	33,36,57,63	0
5	DMS	B	8417	4/4	0.91	0.13	31,32,68,100	0
5	DMS	D	8416	4/4	0.91	0.12	32,42,47,79	0
5	DMS	B	8420	4/4	0.91	0.12	35,42,50,100	0
5	DMS	C	8421	4/4	0.91	0.12	41,65,100,100	0
5	DMS	C	8425	4/4	0.91	0.18	37,57,68,100	0
5	DMS	D	8703	4/4	0.91	0.13	28,62,66,100	0
5	DMS	B	8601	4/4	0.92	0.12	40,47,61,100	0
5	DMS	B	8414	4/4	0.92	0.14	39,55,61,100	0
5	DMS	C	8410	4/4	0.92	0.13	39,62,82,100	0
5	DMS	A	8414	4/4	0.92	0.12	35,40,65,100	0
5	DMS	A	8419	4/4	0.92	0.10	40,49,58,79	0
5	DMS	A	8602	4/4	0.92	0.15	50,51,100,100	0
5	DMS	B	8410	4/4	0.92	0.12	43,50,63,100	0
5	DMS	D	8419	4/4	0.93	0.12	42,45,63,78	0
5	DMS	D	8421	4/4	0.93	0.10	44,49,60,100	0
5	DMS	D	8414	4/4	0.93	0.14	36,58,70,100	0
5	DMS	A	8416	4/4	0.93	0.13	23,69,70,100	0
5	DMS	C	8414	4/4	0.93	0.10	28,31,53,70	0
5	DMS	D	8705	4/4	0.93	0.11	33,46,55,58	0
5	DMS	A	8425	4/4	0.94	0.12	34,43,49,89	0
5	DMS	B	8423	4/4	0.94	0.12	42,61,69,100	0
5	DMS	B	8425	4/4	0.94	0.09	24,31,42,49	0
5	DMS	B	8502	4/4	0.94	0.10	36,42,48,51	0
5	DMS	B	8409	4/4	0.94	0.09	29,33,37,43	0
5	DMS	A	8406	4/4	0.94	0.10	26,37,56,62	0
5	DMS	D	8404	4/4	0.95	0.10	39,39,54,63	0
5	DMS	D	8409	4/4	0.95	0.08	31,31,42,47	0
3	MG	A	3005	1/1	0.95	0.06	45,45,45,45	0
3	MG	D	3005	1/1	0.95	0.06	38,38,38,38	0
5	DMS	C	8415	4/4	0.95	0.09	27,32,55,59	0
5	DMS	A	8409	4/4	0.95	0.08	30,34,43,51	0
5	DMS	B	8504	4/4	0.95	0.09	26,46,64,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	D	3103	1/1	0.95	0.09	38,38,38,38	0
4	NA	D	3104	1/1	0.95	0.07	37,37,37,37	0
5	DMS	C	8423	4/4	0.95	0.12	35,64,64,100	0
5	DMS	B	8406	4/4	0.95	0.11	40,43,56,59	0
5	DMS	C	8601	4/4	0.95	0.09	37,45,50,57	0
5	DMS	A	8408	4/4	0.96	0.09	26,39,45,100	0
5	DMS	C	8501	4/4	0.96	0.08	26,39,40,53	0
5	DMS	D	8412	4/4	0.96	0.11	35,37,41,100	0
5	DMS	D	8501	4/4	0.96	0.08	40,45,46,55	0
5	DMS	B	8404	4/4	0.96	0.06	26,28,36,40	0
5	DMS	D	8508	4/4	0.96	0.11	47,58,68,100	0
5	DMS	A	8404	4/4	0.96	0.07	26,32,43,45	0
5	DMS	D	8406	4/4	0.96	0.11	29,34,37,57	0
5	DMS	A	8412	4/4	0.97	0.10	39,43,43,100	0
5	DMS	B	8408	4/4	0.97	0.08	35,38,40,45	0
5	DMS	A	8504	4/4	0.97	0.10	32,45,52,100	0
4	NA	C	3104	1/1	0.97	0.07	31,31,31,31	0
5	DMS	B	8412	4/4	0.97	0.06	29,30,35,38	0
5	DMS	B	8402	4/4	0.97	0.06	17,26,33,37	0
5	DMS	B	8416	4/4	0.97	0.07	38,42,47,50	0
5	DMS	A	8501	4/4	0.97	0.07	23,33,41,43	0
5	DMS	C	8428	4/4	0.97	0.14	10,19,20,29	4
5	DMS	C	8408	4/4	0.97	0.07	26,37,46,52	0
5	DMS	C	8409	4/4	0.97	0.09	30,40,52,64	0
5	DMS	B	8405	4/4	0.97	0.08	35,35,36,41	0
5	DMS	C	8412	4/4	0.97	0.09	31,35,41,100	0
5	DMS	D	8408	4/4	0.97	0.06	30,37,40,44	0
4	NA	C	3103	1/1	0.98	0.08	36,36,36,36	0
5	DMS	D	8405	4/4	0.98	0.07	26,30,41,43	0
3	MG	C	3002	1/1	0.98	0.05	18,18,18,18	0
5	DMS	C	8411	4/4	0.98	0.10	33,35,36,91	0
5	DMS	A	8411	4/4	0.98	0.07	25,34,38,59	0
3	MG	D	3001	1/1	0.98	0.03	23,23,23,23	0
5	DMS	D	8411	4/4	0.98	0.10	32,32,37,97	0
3	MG	B	3002	1/1	0.98	0.04	22,22,22,22	0
5	DMS	A	8402	4/4	0.98	0.08	22,36,36,52	0
5	DMS	A	8403	4/4	0.98	0.05	24,28,34,35	0
4	NA	A	3103	1/1	0.98	0.06	34,34,34,34	0
5	DMS	A	8405	4/4	0.98	0.07	26,30,34,46	0
5	DMS	B	8411	4/4	0.98	0.07	37,37,37,79	0
5	DMS	C	8402	4/4	0.98	0.07	17,30,34,43	0
5	DMS	C	8405	4/4	0.98	0.06	26,27,34,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	A	3104	1/1	0.98	0.07	30,30,30,30	0
4	NA	B	3104	1/1	0.98	0.07	33,33,33,33	0
5	DMS	D	8701	4/4	0.98	0.08	21,25,32,50	0
5	DMS	D	8402	4/4	0.98	0.07	18,37,39,40	0
5	DMS	D	8403	4/4	0.98	0.06	26,38,40,52	0
4	NA	B	3103	1/1	0.99	0.04	29,29,29,29	0
5	DMS	C	8403	4/4	0.99	0.05	25,26,27,33	0
5	DMS	C	8404	4/4	0.99	0.04	22,25,25,34	0
2	149	B	2001	12/12	0.99	0.04	16,20,24,33	0
4	NA	C	3101	1/1	0.99	0.02	19,19,19,19	0
4	NA	C	3102	1/1	0.99	0.02	19,19,19,19	0
2	149	C	2001	12/12	0.99	0.04	17,20,26,26	0
2	149	D	2001	12/12	0.99	0.04	12,16,21,25	0
4	NA	D	3101	1/1	0.99	0.02	21,21,21,21	0
4	NA	D	3102	1/1	0.99	0.02	19,19,19,19	0
3	MG	A	3001	1/1	0.99	0.02	23,23,23,23	0
3	MG	D	3002	1/1	0.99	0.06	20,20,20,20	0
5	DMS	A	8401	4/4	0.99	0.03	16,16,18,22	0
3	MG	A	3002	1/1	0.99	0.05	22,22,22,22	0
4	NA	A	3101	1/1	0.99	0.03	22,22,22,22	0
2	149	A	2001	12/12	0.99	0.04	16,19,26,28	0
5	DMS	B	8401	4/4	0.99	0.05	17,18,25,33	0
3	MG	B	3001	1/1	0.99	0.04	18,18,18,18	0
5	DMS	B	8403	4/4	0.99	0.05	25,29,35,37	0
4	NA	B	3101	1/1	0.99	0.02	21,21,21,21	0
5	DMS	C	8401	4/4	0.99	0.04	15,22,22,24	0
5	DMS	D	8401	4/4	0.99	0.04	15,21,22,23	0
3	MG	C	3001	1/1	1.00	0.03	18,18,18,18	0
4	NA	B	3102	1/1	1.00	0.03	20,20,20,20	0
4	NA	A	3102	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers ⓘ

There are no such residues in this entry.