Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:23 PM GMT

PDB ID	:	1JZ6
Title	:	E. COLI (lacZ) BETA-GALACTOSIDASE IN COMPLEX WITH GALACTO-TETRAZOLE
Authors	:	Juers, D.H.; Heightman, T.D.; Vasella, A.; Matthews, B.W.
Deposited on	:	2001-09-13
Resolution	:	2.10 Å(reported)

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

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

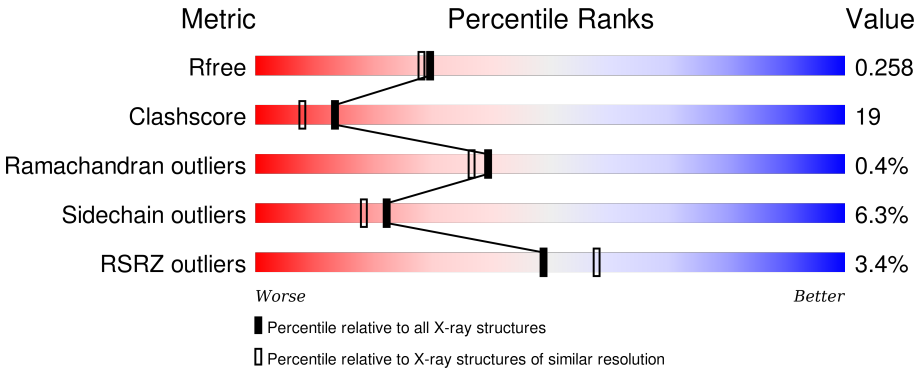
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	1023	3% 61% 31% 7% ••
1	B	1023	4% 54% 35% 9% ••
1	C	1023	3% 60% 31% 7% ••
1	D	1023	3% 59% 33% 6% ••

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
3	MG	C	3105	-	-	-	X
5	DMS	A	8404	-	-	X	-
5	DMS	A	8406	-	-	-	X
5	DMS	A	8417	-	-	-	X
5	DMS	A	8504	-	-	-	X
5	DMS	B	8408	-	-	-	X
5	DMS	B	8416	-	-	X	-
5	DMS	B	8425	-	-	-	X
5	DMS	C	8403	-	-	-	X
5	DMS	C	8407	-	-	-	X
5	DMS	C	8423	-	-	X	-
5	DMS	C	8425	-	-	-	X
5	DMS	C	8504	-	-	X	-
5	DMS	D	8403	-	-	X	-
5	DMS	D	8404	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 35881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Beta-Galactosidase.

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

There are 32 discrepancies between the modelled and reference sequences:

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

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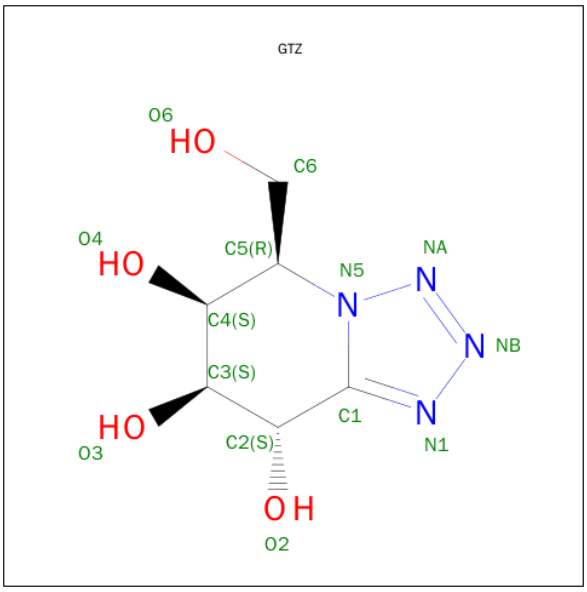
Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLU	SER	CLONING ARTIFACT	? P00722
C	7	ASP	LEU	CLONING ARTIFACT	? P00722
C	8	PRO	ALA	CLONING ARTIFACT	? P00722
D	1	GLY	THR	CLONING ARTIFACT	? P00722
D	2	SER	MET	CLONING ARTIFACT	? P00722
D	3	HIS	ILE	CLONING ARTIFACT	? P00722
D	4	MET	THR	CLONING ARTIFACT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

- Molecule 2 is SUGAR (5-HYDROXYMETHYL-5,6,7,8-TETRAHYDRO-TETRAZOLO[1,5-A]PYRIDINE-6,7,8-TRIOL) (three-letter code: GTZ) (formula: $C_6H_{10}N_4O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 6 4 4	0	0
2	B	1	Total C N O 14 6 4 4	0	0
2	C	1	Total C N O 14 6 4 4	0	0
2	D	1	Total C N O 14 6 4 4	0	0

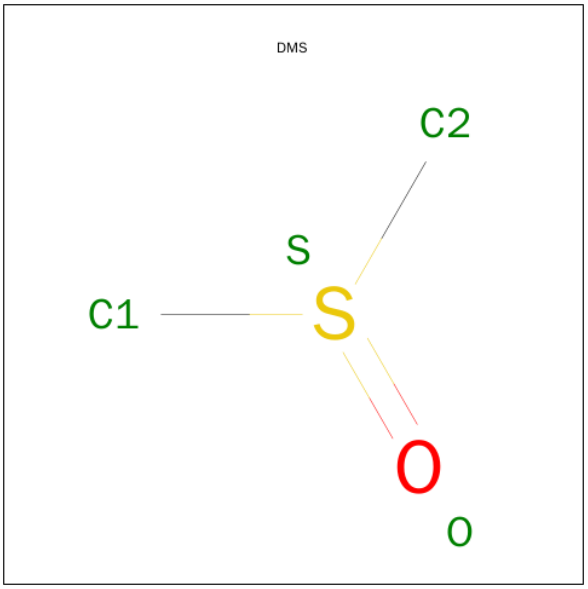
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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



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

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

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

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

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

- Molecule 6 is water.

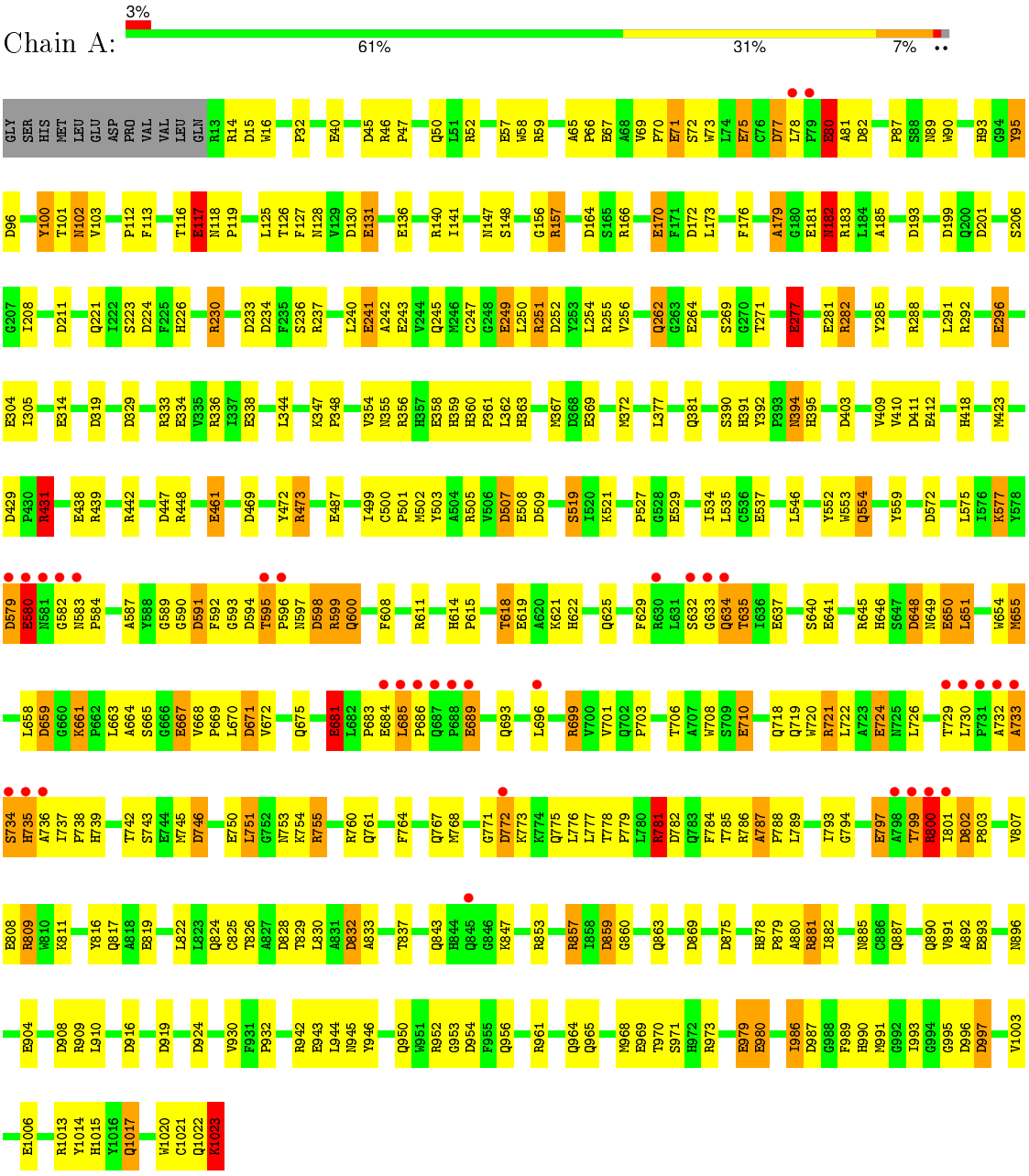
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	775	Total O 775 775	0	0
6	B	747	Total O 747 747	0	0
6	C	719	Total O 719 719	0	0
6	D	764	Total O 764 764	0	0

3 Residue-property plots (i)

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

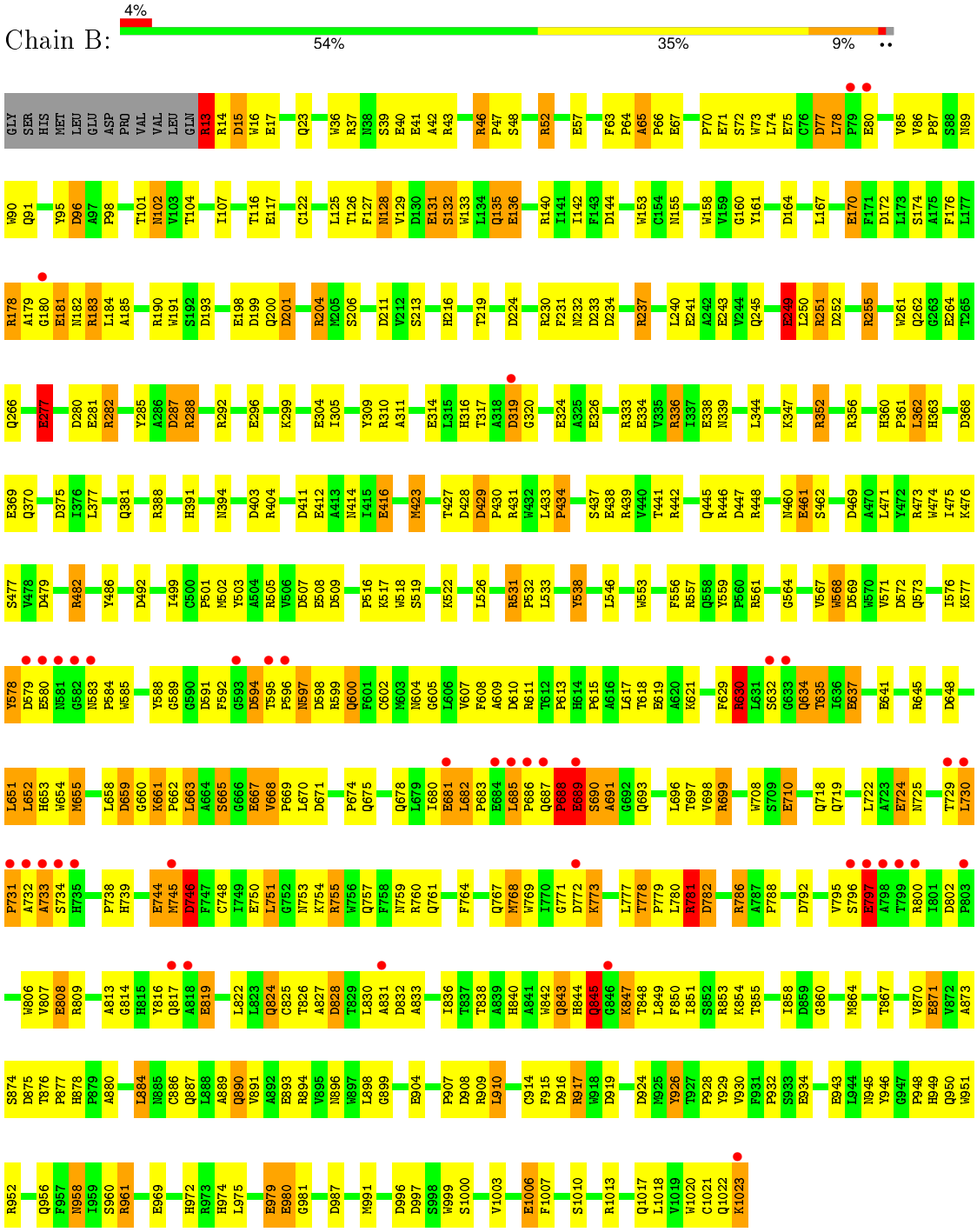
- Molecule 1: Beta-Galactosidase

Chain A:



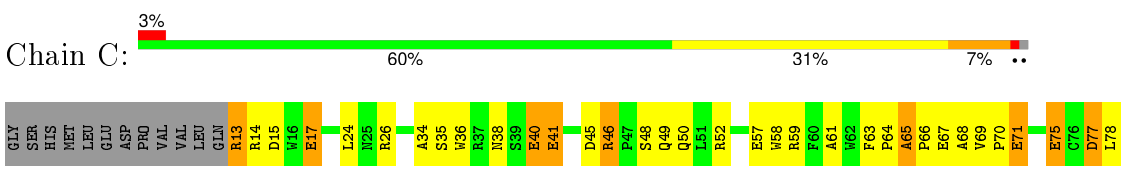
• Molecule 1: Beta-Galactosidase

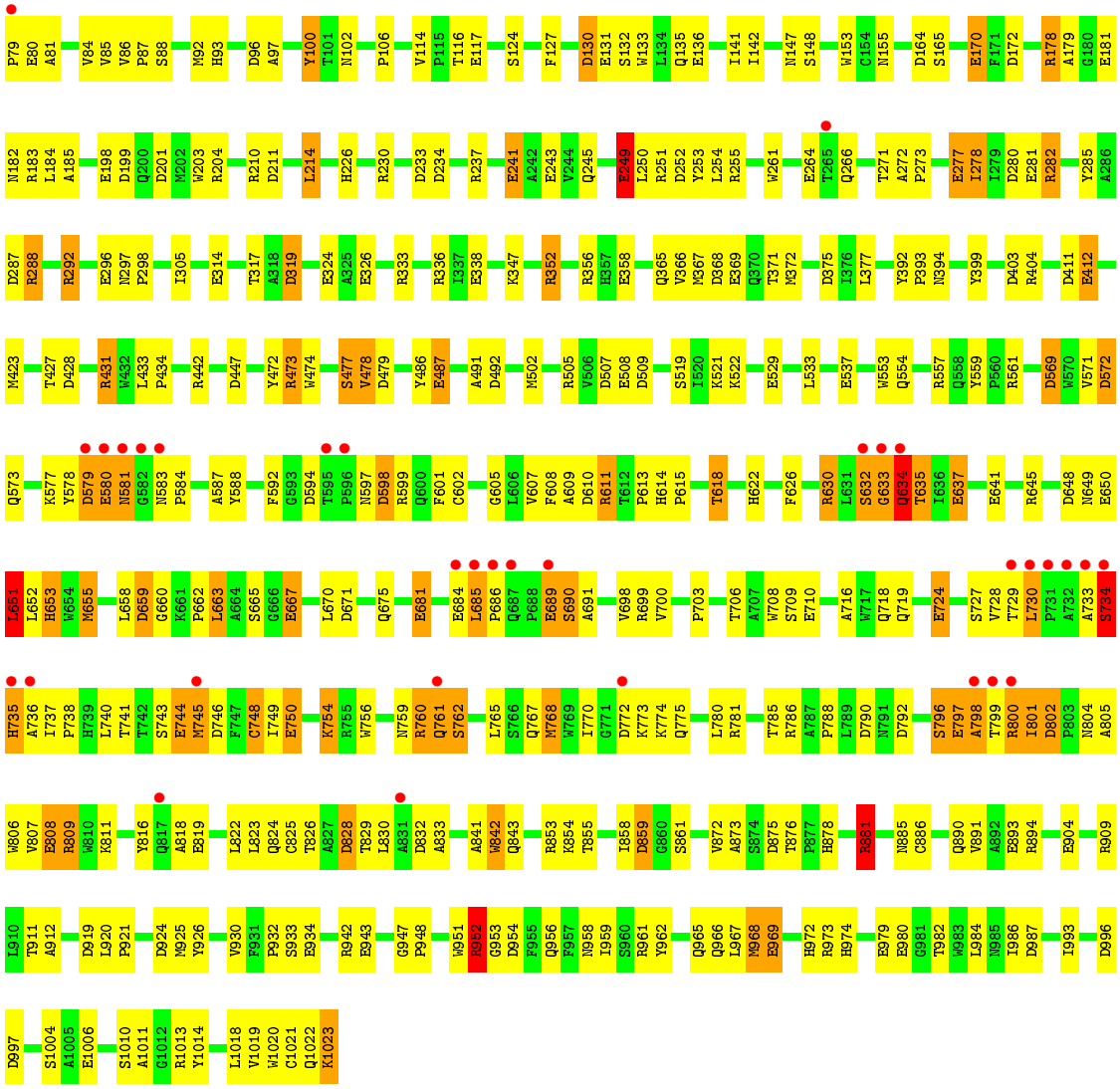
Chain B:



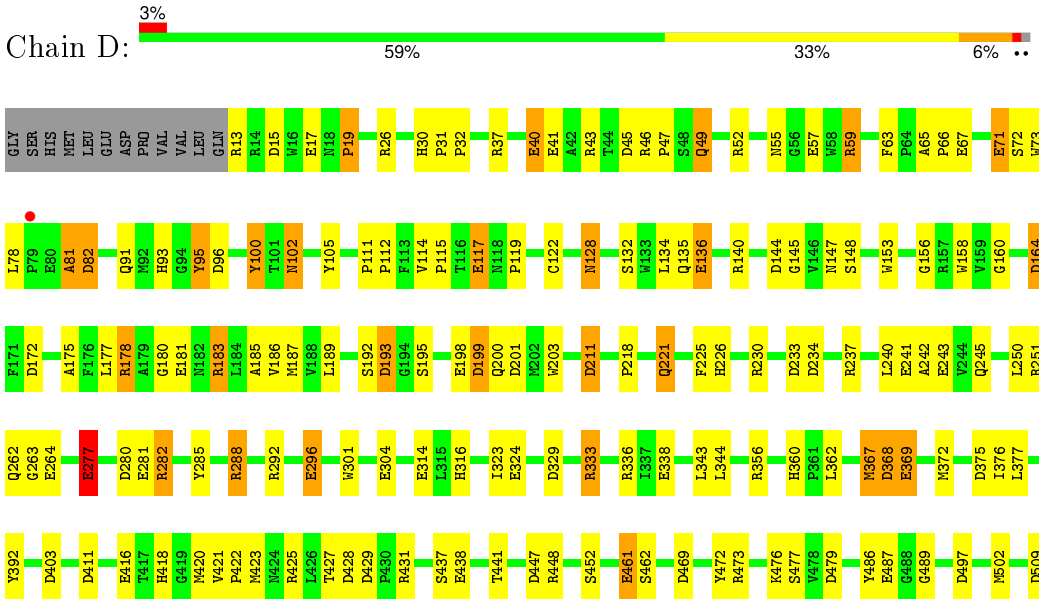
• Molecule 1: Beta-Galactosidase

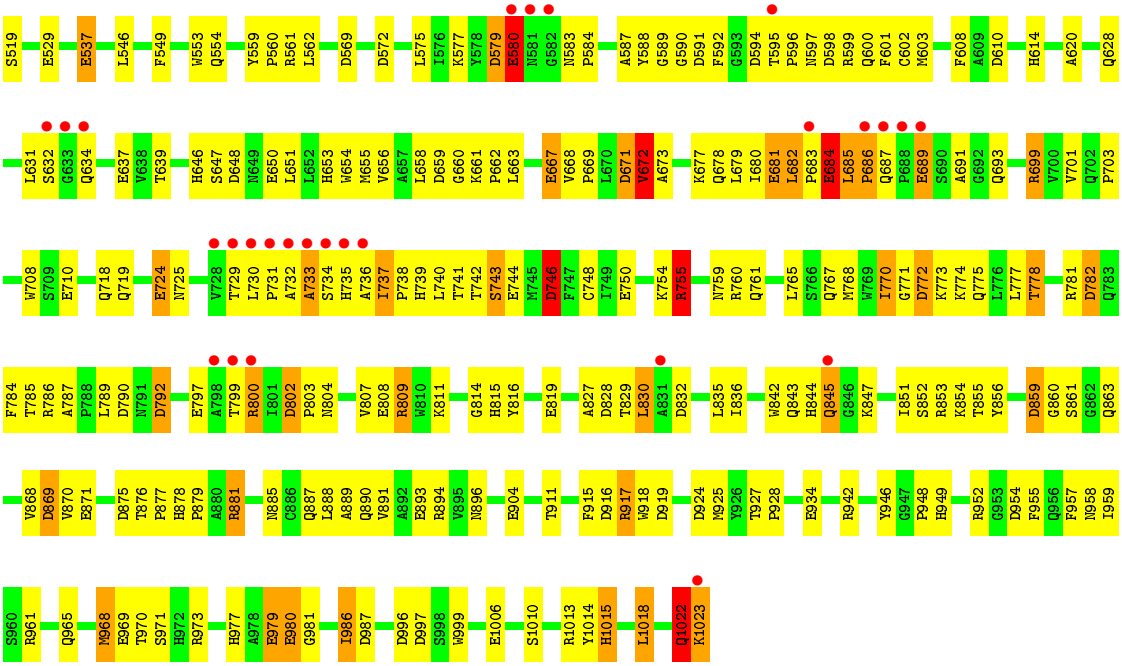
Chain C:





• Molecule 1: Beta-Galactosidase




S519 E529 E537 L546 F549 W553 Q554 Y559 P560 R561 L562 D569 D572 L575 I576 K577 Y578 D579 E580 N581 G582 N583 P584 A587 Y588 G589 G590 D591 F592 G593 D594 T595 P596 N597 D598 R599 Q600 F601 C602 N603 F608 A609 D610 H614 A620 Q628
L631 S632 G633 Q634 E637 V638 T639 H646 S647 D648 N649 E650 L651 L652 H653 W654 M655 V656 A657 L658 D659 G660 K661 P662 L663 E667 V668 P669 L670 D671 V672 A673 K677 Q678 L679 I680 E681 L682 P683 E684 L685 P686 Q687 P688 E689 S690 A691 G692 Q693 R699 V700 V701 Q702 P703
W708 S709 E710 Q718 Q719 E724 N725 V728 T729 L730 P731 A732 A733 S734 H735 A736 I737 P738 H739 L740 T741 T742 S743 E744 M745 D746 F747 C748 I749 E750 K754 R755 N759 R760 Q761 L765 S766 Q767 M768 W769 I770 G771 D772 K773 K774 Q775 L776 L777 T778 R781 D782 Q783
F784 T785 R786 A787 P788 L789 D790 N791 D792 E797 A798 T799 R800 I801 D802 P803 N804 V807 E808 R809 W810 K811 G814 H815 Y816 E819 A827 D828 T829 L830 A831 D832 L835 I836 W842 Q843 H844 Q845 G846 K847 I851 S852 R853 K854 T855 Y856 D859 G860 S861 G862 Q863
V868 D869 V870 E871 D875 T876 P877 H878 P879 A880 R881 N885 C886 Q887 L888 A889 Q890 V891 A892 E893 R894 V895 N896 E904 T911 F915 D916 R917 W918 D919 D924 M925 Y926 T927 P928 E934 R942 Y946 G947 P948 H949 R952 G953 D954 F955 Q956 F957 N958 I959
S960 R961 Q965 N968 E969 T970 S971 H972 R973 H977 A978 E979 E980 G981 I986 D987 D996 D997 S998 W999 E1006 S1010 R1013 Y1014 H1015 L1018 Q1022 K1023

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	149.69Å 168.40Å 200.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 2.10 17.07 – 2.10	Depositor EDS
% Data completeness (in resolution range)	86.2 (17.00-2.10) 84.6 (17.07-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.37 (at 2.11Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.163 , 0.270 0.162 , 0.258	Depositor DCC
R_{free} test set	3546 reflections (1.45%)	DCC
Wilson B-factor (Å^2)	21.9	Xtriage
Anisotropy	0.743	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 118.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 248269 reflections (0.000%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	35881	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 38.93 % 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 3.4238e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GTZ, DMS, 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	1.15	49/8367 (0.6%)	1.60	139/11415 (1.2%)
1	B	1.14	48/8367 (0.6%)	1.66	169/11415 (1.5%)
1	C	1.15	56/8367 (0.7%)	1.60	144/11415 (1.3%)
1	D	1.15	48/8367 (0.6%)	1.62	150/11415 (1.3%)
All	All	1.15	201/33468 (0.6%)	1.62	602/45660 (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	B	1	0
1	D	1	0
All	All	2	0

All (201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	GLU	CD-OE2	10.20	1.36	1.25
1	B	461	GLU	CD-OE2	9.77	1.36	1.25
1	A	136	GLU	CD-OE2	9.02	1.35	1.25
1	A	249	GLU	CD-OE2	8.92	1.35	1.25
1	C	1006	GLU	CD-OE2	8.85	1.35	1.25
1	A	80	GLU	CD-OE2	8.76	1.35	1.25
1	D	136	GLU	CD-OE2	8.34	1.34	1.25
1	A	508	GLU	CD-OE2	8.31	1.34	1.25
1	D	487	GLU	CD-OE2	8.30	1.34	1.25
1	B	667	GLU	CD-OE2	8.26	1.34	1.25
1	D	461	GLU	CD-OE2	8.24	1.34	1.25
1	B	689	GLU	CD-OE2	8.19	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	980	GLU	CD-OE2	8.18	1.34	1.25
1	A	529	GLU	CD-OE2	8.14	1.34	1.25
1	D	71	GLU	CD-OE2	8.04	1.34	1.25
1	C	57	GLU	CD-OE2	7.99	1.34	1.25
1	C	724	GLU	CD-OE2	7.88	1.34	1.25
1	C	750	GLU	CD-OE2	7.84	1.34	1.25
1	A	181	GLU	CD-OE2	7.81	1.34	1.25
1	D	689	GLU	CD-OE2	7.76	1.34	1.25
1	B	724	GLU	CD-OE2	7.75	1.34	1.25
1	A	461	GLU	CD-OE2	7.75	1.34	1.25
1	C	650	GLU	CD-OE2	7.73	1.34	1.25
1	C	41	GLU	CD-OE2	7.70	1.34	1.25
1	C	198	GLU	CD-OE2	7.69	1.34	1.25
1	D	684	GLU	CD-OE2	7.67	1.34	1.25
1	D	281	GLU	CD-OE2	7.60	1.34	1.25
1	A	281	GLU	CD-OE2	7.55	1.33	1.25
1	A	710	GLU	CD-OE2	7.54	1.33	1.25
1	C	281	GLU	CD-OE2	7.50	1.33	1.25
1	C	324	GLU	CD-OE2	7.45	1.33	1.25
1	A	650	GLU	CD-OE2	7.42	1.33	1.25
1	A	684	GLU	CD-OE2	7.40	1.33	1.25
1	B	281	GLU	CD-OE2	7.36	1.33	1.25
1	B	264	GLU	CD-OE2	7.35	1.33	1.25
1	C	80	GLU	CD-OE2	7.32	1.33	1.25
1	D	40	GLU	CD-OE2	7.28	1.33	1.25
1	D	1006	GLU	CD-OE1	-7.24	1.17	1.25
1	A	580	GLU	CD-OE2	7.24	1.33	1.25
1	D	893	GLU	CD-OE2	7.22	1.33	1.25
1	C	296	GLU	CD-OE2	7.14	1.33	1.25
1	C	338	GLU	CD-OE2	7.10	1.33	1.25
1	A	75	GLU	CD-OE2	7.09	1.33	1.25
1	C	684	GLU	CD-OE2	7.04	1.33	1.25
1	D	819	GLU	CD-OE2	7.03	1.33	1.25
1	D	369	GLU	CD-OE2	6.99	1.33	1.25
1	A	969	GLU	CD-OE2	6.97	1.33	1.25
1	A	1006	GLU	CD-OE2	6.97	1.33	1.25
1	B	181	GLU	CD-OE2	6.96	1.33	1.25
1	A	893	GLU	CD-OE2	6.93	1.33	1.25
1	C	689	GLU	CD-OE2	6.93	1.33	1.25
1	D	750	GLU	CD-OE2	6.93	1.33	1.25
1	B	744	GLU	CD-OE2	6.90	1.33	1.25
1	D	580	GLU	CD-OE2	6.90	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	40	GLU	CD-OE1	-6.88	1.18	1.25
1	B	893	GLU	CD-OE2	6.88	1.33	1.25
1	C	71	GLU	CD-OE2	6.84	1.33	1.25
1	D	667	GLU	CD-OE2	6.83	1.33	1.25
1	A	797	GLU	CD-OE2	6.82	1.33	1.25
1	C	904	GLU	CD-OE1	-6.82	1.18	1.25
1	A	487	GLU	CD-OE2	6.82	1.33	1.25
1	B	710	GLU	CD-OE2	6.80	1.33	1.25
1	C	580	GLU	CD-OE2	6.78	1.33	1.25
1	C	529	GLU	CD-OE2	6.76	1.33	1.25
1	C	117	GLU	CD-OE2	6.73	1.33	1.25
1	D	338	GLU	CD-OE2	6.73	1.33	1.25
1	C	744	GLU	CD-OE2	6.69	1.33	1.25
1	D	117	GLU	CD-OE2	6.66	1.32	1.25
1	A	117	GLU	CD-OE2	6.65	1.32	1.25
1	B	979	GLU	CD-OE2	6.60	1.32	1.25
1	B	508	GLU	CD-OE2	6.59	1.32	1.25
1	A	40	GLU	CD-OE2	6.58	1.32	1.25
1	C	681	GLU	CD-OE2	6.58	1.32	1.25
1	C	980	GLU	CD-OE2	6.57	1.32	1.25
1	C	249	GLU	CD-OE2	6.56	1.32	1.25
1	B	170	GLU	CD-OE2	6.54	1.32	1.25
1	A	641	GLU	CD-OE2	6.53	1.32	1.25
1	D	637	GLU	CD-OE2	6.49	1.32	1.25
1	D	724	GLU	CD-OE2	6.47	1.32	1.25
1	B	619	GLU	CD-OE2	6.47	1.32	1.25
1	C	819	GLU	CD-OE2	6.46	1.32	1.25
1	B	67	GLU	CD-OE2	6.45	1.32	1.25
1	A	689	GLU	CD-OE2	6.43	1.32	1.25
1	A	619	GLU	CD-OE2	6.42	1.32	1.25
1	A	943	GLU	CD-OE2	6.42	1.32	1.25
1	C	979	GLU	CD-OE2	6.42	1.32	1.25
1	D	75	GLU	CD-OE2	6.42	1.32	1.25
1	D	529	GLU	CD-OE2	6.41	1.32	1.25
1	C	710	GLU	CD-OE2	6.39	1.32	1.25
1	C	40	GLU	CD-OE2	6.37	1.32	1.25
1	D	710	GLU	CD-OE2	6.36	1.32	1.25
1	D	934	GLU	CD-OE2	6.36	1.32	1.25
1	B	249	GLU	CD-OE2	6.33	1.32	1.25
1	D	198	GLU	CD-OE2	6.32	1.32	1.25
1	C	136	GLU	CD-OE2	6.32	1.32	1.25
1	B	681	GLU	CD-OE2	6.30	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	980	GLU	CD-OE2	6.30	1.32	1.25
1	B	277	GLU	CD-OE2	6.29	1.32	1.25
1	A	667	GLU	CD-OE2	6.28	1.32	1.25
1	D	264	GLU	CD-OE2	6.27	1.32	1.25
1	B	41	GLU	CD-OE2	6.25	1.32	1.25
1	D	650	GLU	CD-OE2	6.25	1.32	1.25
1	B	819	GLU	CD-OE2	6.25	1.32	1.25
1	B	969	GLU	CD-OE2	6.24	1.32	1.25
1	A	264	GLU	CD-OE2	6.24	1.32	1.25
1	D	904	GLU	CD-OE2	6.23	1.32	1.25
1	C	934	GLU	CD-OE2	6.21	1.32	1.25
1	D	438	GLU	CD-OE2	6.20	1.32	1.25
1	A	131	GLU	CD-OE2	6.19	1.32	1.25
1	C	314	GLU	CD-OE2	6.17	1.32	1.25
1	B	797	GLU	CD-OE2	6.15	1.32	1.25
1	B	1006	GLU	CD-OE2	6.14	1.32	1.25
1	D	57	GLU	CD-OE2	6.13	1.32	1.25
1	D	537	GLU	CD-OE2	6.13	1.32	1.25
1	C	487	GLU	CD-OE2	6.13	1.32	1.25
1	D	904	GLU	CD-OE1	-6.11	1.19	1.25
1	A	979	GLU	CD-OE2	6.10	1.32	1.25
1	B	412	GLU	CD-OE1	-6.08	1.19	1.25
1	A	724	GLU	CD-OE2	6.05	1.32	1.25
1	C	508	GLU	CD-OE2	6.05	1.32	1.25
1	D	487	GLU	CD-OE1	-6.04	1.19	1.25
1	B	934	GLU	CD-OE2	6.03	1.32	1.25
1	D	41	GLU	CD-OE2	6.03	1.32	1.25
1	C	893	GLU	CD-OE2	5.99	1.32	1.25
1	B	296	GLU	CD-OE2	5.99	1.32	1.25
1	A	819	GLU	CD-OE2	5.98	1.32	1.25
1	D	17	GLU	CD-OE2	5.95	1.32	1.25
1	B	131	GLU	CD-OE2	5.91	1.32	1.25
1	A	650	GLU	CD-OE1	-5.91	1.19	1.25
1	C	369	GLU	CD-OE2	5.88	1.32	1.25
1	B	80	GLU	CD-OE2	5.86	1.32	1.25
1	C	969	GLU	CD-OE2	5.86	1.32	1.25
1	A	57	GLU	CD-OE2	5.86	1.32	1.25
1	B	136	GLU	CD-OE2	5.86	1.32	1.25
1	B	198	GLU	CD-OE2	5.83	1.32	1.25
1	B	95	TYR	CB-CG	-5.83	1.43	1.51
1	C	67	GLU	CD-OE2	5.82	1.32	1.25
1	C	264	GLU	CD-OE2	5.82	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	277	GLU	CD-OE2	5.81	1.32	1.25
1	C	641	GLU	CD-OE2	5.80	1.32	1.25
1	B	580	GLU	CD-OE2	5.79	1.32	1.25
1	D	979	GLU	CD-OE2	5.78	1.32	1.25
1	A	170	GLU	CD-OE2	5.76	1.31	1.25
1	D	170	GLU	CD-OE2	5.76	1.31	1.25
1	B	904	GLU	CD-OE2	5.75	1.31	1.25
1	C	808	GLU	CD-OE2	5.74	1.31	1.25
1	D	934	GLU	CD-OE1	-5.74	1.19	1.25
1	A	681	GLU	CD-OE2	5.73	1.31	1.25
1	D	314	GLU	CD-OE2	5.72	1.31	1.25
1	A	277	GLU	CD-OE2	5.71	1.31	1.25
1	D	67	GLU	CD-OE2	5.71	1.31	1.25
1	C	131	GLU	CD-OE2	5.70	1.31	1.25
1	A	412	GLU	CD-OE2	5.70	1.31	1.25
1	C	75	GLU	CD-OE2	5.69	1.31	1.25
1	A	438	GLU	CD-OE2	5.69	1.31	1.25
1	C	412	GLU	CD-OE2	5.69	1.31	1.25
1	B	241	GLU	CD-OE2	5.68	1.31	1.25
1	B	75	GLU	CD-OE2	5.68	1.31	1.25
1	B	71	GLU	CD-OE2	5.68	1.31	1.25
1	B	369	GLU	CD-OE2	5.67	1.31	1.25
1	A	304	GLU	CD-OE2	5.63	1.31	1.25
1	C	637	GLU	CD-OE2	5.63	1.31	1.25
1	A	980	GLU	CD-OE2	5.61	1.31	1.25
1	D	681	GLU	CD-OE2	5.61	1.31	1.25
1	A	369	GLU	CD-OE2	5.59	1.31	1.25
1	C	797	GLU	CD-OE2	5.59	1.31	1.25
1	A	904	GLU	CD-OE1	-5.58	1.19	1.25
1	D	296	GLU	CD-OE2	5.58	1.31	1.25
1	A	334	GLU	CD-OE2	5.58	1.31	1.25
1	D	181	GLU	CD-OE2	5.58	1.31	1.25
1	C	277	GLU	CD-OE2	5.55	1.31	1.25
1	C	314	GLU	CD-OE1	-5.54	1.19	1.25
1	D	198	GLU	CB-CG	5.54	1.62	1.52
1	D	1006	GLU	CD-OE2	5.53	1.31	1.25
1	B	637	GLU	CD-OE2	5.52	1.31	1.25
1	A	71	GLU	CD-OE2	5.52	1.31	1.25
1	B	17	GLU	CD-OE2	5.51	1.31	1.25
1	B	808	GLU	CD-OE2	5.51	1.31	1.25
1	A	750	GLU	CD-OE2	5.45	1.31	1.25
1	C	943	GLU	CD-OE2	5.44	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	GLU	CD-OE2	5.42	1.31	1.25
1	C	667	GLU	CD-OE2	5.39	1.31	1.25
1	C	358	GLU	CD-OE2	5.39	1.31	1.25
1	B	641	GLU	CD-OE2	5.37	1.31	1.25
1	C	650	GLU	CD-OE1	-5.35	1.19	1.25
1	A	338	GLU	CD-OE2	5.34	1.31	1.25
1	A	904	GLU	CD-OE2	5.34	1.31	1.25
1	B	871	GLU	CD-OE1	-5.29	1.19	1.25
1	B	57	GLU	CD-OE2	5.27	1.31	1.25
1	D	324	GLU	CD-OE2	5.25	1.31	1.25
1	C	326	GLU	CD-OE2	5.23	1.31	1.25
1	B	637	GLU	CD-OE1	-5.18	1.20	1.25
1	A	358	GLU	CD-OE2	5.16	1.31	1.25
1	A	241	GLU	CD-OE2	5.11	1.31	1.25
1	C	243	GLU	CD-OE2	5.10	1.31	1.25
1	B	324	GLU	CD-OE2	5.10	1.31	1.25
1	C	241	GLU	CD-OE2	5.08	1.31	1.25
1	C	17	GLU	CD-OE2	5.05	1.31	1.25
1	A	314	GLU	CD-OE2	5.04	1.31	1.25
1	D	304	GLU	CD-OE2	5.02	1.31	1.25
1	B	314	GLU	CD-OE2	5.00	1.31	1.25

All (602) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	687	GLN	C-N-CD	-17.57	81.95	120.60
1	D	336	ARG	NE-CZ-NH1	14.18	127.39	120.30
1	B	95	TYR	CB-CG-CD2	-12.66	113.41	121.00
1	C	961	ARG	NE-CZ-NH1	11.97	126.29	120.30
1	B	144	ASP	CB-CG-OD2	-11.94	107.56	118.30
1	B	356	ARG	NE-CZ-NH1	11.93	126.27	120.30
1	C	790	ASP	CB-CG-OD1	11.81	128.93	118.30
1	B	336	ARG	NE-CZ-NH1	11.50	126.05	120.30
1	D	282	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	A	853	ARG	NE-CZ-NH1	11.27	125.93	120.30
1	A	251	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	B	356	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	C	505	ARG	NE-CZ-NH1	10.85	125.73	120.30
1	B	172	ASP	CB-CG-OD2	-10.84	108.54	118.30
1	B	310	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	D	282	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	A	987	ASP	CB-CG-OD1	10.30	127.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	671	ASP	CB-CG-OD2	-10.26	109.07	118.30
1	C	204	ARG	NE-CZ-NH1	10.24	125.42	120.30
1	D	172	ASP	CB-CG-OD2	-10.21	109.11	118.30
1	B	172	ASP	CB-CG-OD1	10.16	127.45	118.30
1	C	611	ARG	NE-CZ-NH1	10.12	125.36	120.30
1	A	828	ASP	CB-CG-OD2	-9.97	109.33	118.30
1	A	255	ARG	NE-CZ-NH2	-9.97	115.32	120.30
1	B	448	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	D	411	ASP	CB-CG-OD1	9.96	127.26	118.30
1	B	611	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	A	164	ASP	CB-CG-OD1	9.91	127.22	118.30
1	B	144	ASP	CB-CG-OD1	9.79	127.11	118.30
1	D	792	ASP	CB-CG-OD1	9.74	127.07	118.30
1	B	46	ARG	NE-CZ-NH2	-9.71	115.45	120.30
1	B	648	ASP	CB-CG-OD2	-9.62	109.65	118.30
1	A	952	ARG	NE-CZ-NH1	9.61	125.11	120.30
1	C	233	ASP	CB-CG-OD2	-9.59	109.67	118.30
1	A	853	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	A	164	ASP	CB-CG-OD2	-9.44	109.80	118.30
1	D	233	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	A	157	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	D	172	ASP	CB-CG-OD1	9.36	126.73	118.30
1	D	594	ASP	CB-CG-OD2	-9.36	109.88	118.30
1	B	952	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	C	961	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	B	282	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	857	ARG	NE-CZ-NH1	9.22	124.91	120.30
1	D	255	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	336	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	D	288	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	C	507	ASP	CB-CG-OD2	-9.14	110.08	118.30
1	B	557	ARG	NE-CZ-NH1	9.09	124.84	120.30
1	B	442	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	B	557	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	A	411	ASP	CB-CG-OD2	-8.91	110.28	118.30
1	A	172	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	A	201	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	A	234	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	A	282	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	D	952	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	A	100	TYR	N-CA-CB	8.78	126.40	110.60
1	D	144	ASP	CB-CG-OD1	8.75	126.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	442	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	B	671	ASP	CB-CG-OD1	8.71	126.14	118.30
1	B	572	ASP	CB-CG-OD2	-8.70	110.47	118.30
1	A	507	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	A	403	ASP	CB-CG-OD2	-8.67	110.50	118.30
1	D	211	ASP	CB-CG-OD1	8.63	126.07	118.30
1	B	448	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	D	786	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	B	96	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	C	130	ASP	CB-CG-OD1	8.56	126.00	118.30
1	B	352	ARG	NE-CZ-NH1	-8.55	116.02	120.30
1	D	746	ASP	CB-CG-OD2	-8.53	110.62	118.30
1	A	594	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	A	505	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	D	233	ASP	CB-CG-OD1	8.47	125.92	118.30
1	B	832	ASP	CB-CG-OD2	-8.43	110.72	118.30
1	B	310	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	447	ASP	CB-CG-OD1	8.39	125.86	118.30
1	C	809	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	D	199	ASP	CB-CG-OD2	-8.37	110.76	118.30
1	B	611	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	B	482	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	A	403	ASP	CB-CG-OD1	8.32	125.79	118.30
1	C	594	ASP	CB-CG-OD2	-8.31	110.83	118.30
1	B	561	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	D	77	ASP	CB-CG-OD2	-8.27	110.85	118.30
1	B	77	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	B	909	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	C	881	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	B	403	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	411	ASP	CB-CG-OD1	8.19	125.67	118.30
1	A	553	TRP	CA-CB-CG	-8.19	98.15	113.70
1	C	473	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	D	329	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	B	531	ARG	NE-CZ-NH1	-8.17	116.22	120.30
1	D	333	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	C	336	ARG	NE-CZ-NH1	8.14	124.37	120.30
1	A	659	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	B	388	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	164	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	D	987	ASP	CB-CG-OD1	8.02	125.52	118.30
1	D	802	ASP	CB-CG-OD2	-8.02	111.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	832	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	A	77	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	B	961	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	C	572	ASP	CB-CG-OD2	-7.99	111.11	118.30
1	D	853	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	D	792	ASP	CB-CG-OD2	-7.96	111.14	118.30
1	C	252	ASP	CB-CG-OD2	-7.94	111.15	118.30
1	D	1015	HIS	CA-CB-CG	-7.94	100.11	113.60
1	B	997	ASP	N-CA-CB	7.91	124.84	110.60
1	C	233	ASP	CB-CG-OD1	7.91	125.42	118.30
1	B	572	ASP	CB-CG-OD1	7.90	125.41	118.30
1	C	352	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	507	ASP	CB-CG-OD1	7.89	125.40	118.30
1	D	875	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	D	648	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	C	172	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	C	958	ASN	N-CA-CB	7.84	124.71	110.60
1	D	594	ASP	CB-CG-OD1	7.82	125.34	118.30
1	D	987	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	C	760	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	C	579	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	C	336	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	B	224	ASP	CB-CG-OD1	7.76	125.28	118.30
1	A	721	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	B	447	ASP	CB-CG-OD1	7.74	125.27	118.30
1	D	368	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	A	442	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	C	632	SER	N-CA-CB	7.66	121.99	110.50
1	D	859	ASP	CB-CG-OD1	7.64	125.18	118.30
1	B	594	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	D	59	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	C	875	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	C	368	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	D	329	ASP	CB-CG-OD1	7.61	125.15	118.30
1	D	853	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	D	919	ASP	CB-CG-OD2	-7.57	111.48	118.30
1	C	853	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	D	875	ASP	CB-CG-OD1	7.56	125.11	118.30
1	B	442	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	688	PRO	N-CA-CB	7.55	112.36	103.30
1	D	790	ASP	CB-CG-OD1	7.54	125.09	118.30
1	A	755	ARG	NE-CZ-NH2	-7.51	116.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	790	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	C	46	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	C	648	ASP	CB-CG-OD1	7.49	125.04	118.30
1	C	832	ASP	CB-CG-OD1	7.48	125.03	118.30
1	D	772	ASP	CB-CG-OD1	7.46	125.01	118.30
1	A	140	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	45	ASP	CB-CG-OD1	7.43	124.98	118.30
1	A	954	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	D	659	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	D	489	GLY	C-N-CA	-7.36	106.84	122.30
1	A	509	ASP	CB-CG-OD2	-7.35	111.69	118.30
1	A	431	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	599	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	B	772	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	B	336	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	579	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	509	ASP	CB-CG-OD2	-7.30	111.72	118.30
1	A	996	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	509	ASP	CB-CG-OD1	7.29	124.86	118.30
1	C	611	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	280	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	739	HIS	CA-CB-CG	7.28	125.97	113.60
1	D	881	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	881	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	A	185	ALA	N-CA-CB	7.22	120.21	110.10
1	B	15	ASP	CB-CG-OD1	7.22	124.80	118.30
1	A	916	ASP	CB-CG-OD1	7.21	124.79	118.30
1	A	598	ASP	CB-CG-OD1	7.19	124.77	118.30
1	B	52	ARG	CB-CA-C	-7.19	96.03	110.40
1	D	201	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	A	857	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	C	996	ASP	CB-CG-OD1	7.15	124.73	118.30
1	C	509	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	D	221	GLN	N-CA-CB	-7.14	97.75	110.60
1	A	319	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	C	288	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	C	234	ASP	CB-CG-OD1	7.13	124.72	118.30
1	C	492	ASP	CB-CG-OD1	7.12	124.71	118.30
1	D	95	TYR	CB-CG-CD2	-7.11	116.73	121.00
1	C	411	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	D	828	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	588	TYR	CB-CG-CD2	-7.09	116.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	204	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	D	292	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	D	447	ASP	CB-CG-OD1	7.05	124.64	118.30
1	D	673	ALA	N-CA-CB	-7.05	100.23	110.10
1	D	572	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	C	648	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	C	924	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	B	786	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	C	569	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	832	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	B	594	ASP	CB-CG-OD1	7.02	124.62	118.30
1	C	505	ARG	NE-CZ-NH2	-7.02	116.79	120.30
1	D	671	ASP	CB-CG-OD1	7.02	124.62	118.30
1	C	762	SER	N-CA-CB	-6.99	100.01	110.50
1	B	507	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	B	507	ASP	CB-CG-OD1	6.99	124.59	118.30
1	C	875	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	869	ASP	CB-CG-OD2	-6.98	112.01	118.30
1	D	428	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	832	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	96	ASP	CB-CG-OD1	6.97	124.58	118.30
1	C	802	ASP	CB-CG-OD2	-6.97	112.02	118.30
1	B	772	ASP	CB-CG-OD1	6.97	124.57	118.30
1	C	492	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	A	82	ASP	CB-CG-OD2	-6.95	112.05	118.30
1	C	234	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	B	368	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	A	447	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	B	688	PRO	CA-C-N	-6.91	102.00	117.20
1	A	140	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	C	287	ASP	CB-CG-OD1	6.90	124.51	118.30
1	D	579	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	C	77	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	505	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	469	ASP	CB-CG-OD1	6.88	124.49	118.30
1	C	428	ASP	CB-CG-OD1	6.88	124.49	118.30
1	C	859	ASP	CB-CG-OD1	6.87	124.48	118.30
1	D	164	ASP	CB-CG-OD1	6.87	124.48	118.30
1	D	610	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	D	659	ASP	CB-CG-OD1	6.86	124.48	118.30
1	D	211	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	C	553	TRP	CA-CB-CG	-6.84	100.71	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	280	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	C	442	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	234	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	B	140	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	A	594	ASP	CB-CG-OD1	6.81	124.42	118.30
1	C	130	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	A	919	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	D	469	ASP	CB-CG-OD1	6.79	124.41	118.30
1	D	572	ASP	CB-CG-OD1	6.79	124.41	118.30
1	C	579	ASP	CB-CG-OD1	6.78	124.40	118.30
1	B	255	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	B	598	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	D	403	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	C	172	ASP	CB-CG-OD1	6.74	124.37	118.30
1	C	52	ARG	NE-CZ-NH2	-6.74	116.93	120.30
1	D	996	ASP	CB-CG-OD1	6.74	124.37	118.30
1	A	52	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	D	52	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	954	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	96	ASP	CB-CG-OD1	6.74	124.36	118.30
1	B	95	TYR	CA-CB-CG	-6.73	100.62	113.40
1	D	288	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	C	13	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	233	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	559	TYR	CB-CG-CD2	-6.70	116.98	121.00
1	D	425	ARG	NE-CZ-NH1	6.69	123.65	120.30
1	B	746	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	C	594	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	572	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	630	ARG	NE-CZ-NH1	6.67	123.63	120.30
1	D	952	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	77	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	A	671	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	B	479	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	A	881	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	D	802	ASP	CB-CG-OD1	6.62	124.26	118.30
1	C	598	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	77	ASP	CB-CG-OD1	6.61	124.25	118.30
1	B	919	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	787	ALA	C-N-CD	-6.60	106.08	120.60
1	C	319	ASP	CB-CG-OD1	6.58	124.23	118.30
1	C	65	ALA	N-CA-CB	6.57	119.30	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	659	ASP	CB-CG-OD2	-6.56	112.39	118.30
1	A	875	ASP	CB-CG-OD1	6.55	124.20	118.30
1	B	919	ASP	CB-CG-OD1	6.55	124.19	118.30
1	B	958	ASN	N-CA-CB	6.55	122.39	110.60
1	B	71	GLU	CB-CA-C	6.55	123.50	110.40
1	A	952	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	B	287	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	B	234	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	B	908	ASP	CB-CG-OD1	6.51	124.16	118.30
1	C	802	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	659	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	997	ASP	N-CA-CB	6.48	122.27	110.60
1	A	179	ALA	N-CA-CB	6.46	119.14	110.10
1	B	15	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	C	199	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	C	211	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	D	748	CYS	N-CA-CB	6.38	122.09	110.60
1	A	15	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	809	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	446	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	A	987	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	A	591	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	859	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	B	13	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	439	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	45	ASP	CB-CG-OD1	6.34	124.01	118.30
1	B	1013	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	D	82	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	A	648	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	172	ASP	CB-CG-OD1	6.32	123.99	118.30
1	D	166	ARG	NE-CZ-NH1	6.31	123.46	120.30
1	D	100	TYR	N-CA-CB	6.31	121.96	110.60
1	C	997	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	161	TYR	N-CA-CB	-6.30	99.25	110.60
1	C	210	ARG	NE-CZ-NH2	6.30	123.45	120.30
1	C	15	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	356	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	D	924	ASP	CB-CG-OD1	6.29	123.96	118.30
1	B	43	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	954	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	B	792	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	929	TYR	CB-CG-CD2	-6.24	117.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	699	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	746	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	B	288	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	633	GLY	N-CA-C	-6.23	97.52	113.10
1	B	875	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	519	SER	N-CA-CB	-6.22	101.17	110.50
1	D	193	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	280	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	D	497	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	579	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	B	908	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	C	842	TRP	N-CA-CB	6.21	121.77	110.60
1	A	96	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	D	809	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	A	800	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	760	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	252	ASP	CA-CB-CG	-6.18	99.81	113.40
1	B	884	LEU	CB-CA-C	-6.17	98.48	110.20
1	D	672	VAL	CB-CA-C	-6.17	99.68	111.40
1	D	185	ALA	N-CA-CB	6.17	118.73	110.10
1	A	130	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	A	632	SER	N-CA-CB	6.16	119.74	110.50
1	D	388	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	802	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	C	183	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	875	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	D	469	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	37	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	411	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	B	961	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	199	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	252	ASP	CB-CG-OD1	6.13	123.82	118.30
1	C	282	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	C	561	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	C	578	TYR	CB-CG-CD1	-6.11	117.34	121.00
1	C	909	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	B	211	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	599	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	952	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	D	800	ARG	NE-CZ-NH1	6.09	123.34	120.30
1	A	746	ASP	CB-CA-C	-6.08	98.23	110.40
1	D	479	ASP	CB-CG-OD2	-6.08	112.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	611	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	375	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	B	65	ALA	CB-CA-C	6.07	119.20	110.10
1	A	598	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	C	96	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	D	946	TYR	CB-CG-CD1	-6.05	117.37	121.00
1	D	832	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	996	ASP	CB-CG-OD1	6.03	123.73	118.30
1	D	164	ASP	N-CA-CB	6.03	121.45	110.60
1	C	734	SER	N-CA-CB	6.01	119.52	110.50
1	A	95	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	B	473	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	128	ASN	N-CA-CB	6.00	121.39	110.60
1	D	19	PRO	N-CA-CB	5.99	110.49	103.30
1	D	610	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	336	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	A	116	THR	CA-CB-CG2	-5.98	104.03	112.40
1	D	553	TRP	CA-CB-CG	-5.97	102.36	113.70
1	B	201	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	280	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	285	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	A	429	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	651	LEU	N-CA-CB	5.94	122.28	110.40
1	C	292	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	B	952	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	601	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	A	77	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	509	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	77	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	469	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	D	49	GLN	N-CA-CB	5.91	121.24	110.60
1	D	411	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	C	832	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	B	251	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	59	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	569	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	204	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	D	448	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	427	THR	CA-CB-CG2	-5.87	104.18	112.40
1	C	199	ASP	CB-CG-OD1	5.87	123.58	118.30
1	A	282	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	C	431	ARG	NE-CZ-NH1	5.87	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	828	ASP	N-CA-CB	5.84	121.11	110.60
1	C	479	ASP	CB-CG-OD1	5.84	123.55	118.30
1	C	735	HIS	CB-CA-C	5.84	122.07	110.40
1	A	659	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	828	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	C	630	ARG	N-CA-CB	5.82	121.07	110.60
1	B	230	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	343	LEU	CB-CG-CD2	-5.80	101.14	111.00
1	D	134	LEU	CB-CA-C	-5.79	99.19	110.20
1	B	319	ASP	CB-CG-OD1	5.79	123.51	118.30
1	C	772	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	252	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	D	1013	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	434	PRO	N-CA-CB	5.77	110.22	103.30
1	D	772	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	D	679	LEU	CB-CA-C	-5.77	99.24	110.20
1	C	786	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	233	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	D	782	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	909	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	A	234	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	93	HIS	CA-CB-CG	5.75	123.38	113.60
1	B	855	THR	CA-CB-CG2	5.74	120.44	112.40
1	C	507	ASP	CB-CG-OD1	5.74	123.46	118.30
1	D	1018	LEU	CB-CA-C	-5.74	99.30	110.20
1	B	996	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	1013	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	C	842	TRP	CG-CD2-CE3	-5.73	128.74	133.90
1	C	855	THR	N-CA-CB	5.71	121.16	110.30
1	A	251	ARG	CD-NE-CZ	5.71	131.60	123.60
1	C	61	ALA	CB-CA-C	5.70	118.65	110.10
1	C	287	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	199	ASP	CB-CG-OD1	5.70	123.43	118.30
1	D	486	TYR	CB-CG-CD2	-5.70	117.58	121.00
1	A	908	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	411	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	610	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	987	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	45	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	503	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	B	546	LEU	N-CA-CB	5.67	121.74	110.40
1	C	375	ASP	CB-CG-OD1	5.66	123.40	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	746	ASP	CB-CG-OD1	5.65	123.39	118.30
1	D	598	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	A	329	ASP	CB-CG-OD1	5.63	123.37	118.30
1	D	509	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	C	403	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	B	509	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	46	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	771	GLY	N-CA-C	-5.62	99.06	113.10
1	A	211	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	1022	GLN	N-CA-CB	5.61	120.69	110.60
1	B	926	TYR	CB-CG-CD1	5.60	124.36	121.00
1	C	288	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	404	ARG	NE-CZ-NH2	5.59	123.10	120.30
1	B	429	ASP	CB-CG-OD1	5.59	123.34	118.30
1	A	572	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	C	472	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	B	319	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	C	651	LEU	CB-CA-C	5.58	120.80	110.20
1	A	130	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	15	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	869	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	648	ASP	CB-CG-OD1	5.56	123.30	118.30
1	D	175	ALA	CB-CA-C	-5.56	101.77	110.10
1	D	919	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	781	ARG	CG-CD-NE	-5.54	100.16	111.80
1	A	472	TYR	CB-CG-CD2	-5.54	117.68	121.00
1	D	685	LEU	C-N-CD	-5.54	108.42	120.60
1	D	26	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	116	THR	N-CA-CB	5.53	120.81	110.30
1	D	15	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	D	968	MET	CB-CA-C	-5.52	99.36	110.40
1	D	117	GLU	N-CA-CB	-5.52	100.66	110.60
1	C	809	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	97	ALA	N-CA-CB	-5.51	102.39	110.10
1	A	429	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	598	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	859	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	193	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	569	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	755	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	509	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	233	ASP	CB-CG-OD1	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	338	GLU	CG-CD-OE2	-5.48	107.34	118.30
1	C	828	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	C	100	TYR	N-CA-CB	5.47	120.44	110.60
1	D	225	PHE	N-CA-CB	5.46	120.43	110.60
1	A	117	GLU	N-CA-CB	5.46	120.43	110.60
1	B	140	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	894	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	D	392	TYR	CB-CG-CD2	5.45	124.27	121.00
1	D	894	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	D	977	HIS	CA-CB-CG	5.45	122.86	113.60
1	B	193	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	469	ASP	CB-CG-OD1	5.45	123.20	118.30
1	B	578	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	D	996	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	781	ARG	N-CA-CB	-5.43	100.83	110.60
1	C	375	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	B	688	PRO	O-C-N	5.42	131.38	122.70
1	A	77	ASP	CB-CA-C	-5.42	99.56	110.40
1	C	147	ASN	N-CA-CB	-5.41	100.86	110.60
1	D	140	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	252	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	403	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	201	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	15	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	B	311	ALA	N-CA-CB	5.39	117.65	110.10
1	B	782	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	782	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	362	LEU	CB-CA-C	-5.38	99.97	110.20
1	B	326	GLU	CG-CD-OE1	5.38	129.06	118.30
1	C	699	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	70	PRO	N-CA-CB	5.38	109.75	103.30
1	D	770	ILE	N-CA-C	-5.36	96.52	111.00
1	B	287	ASP	CB-CG-OD1	5.36	123.13	118.30
1	B	473	ARG	CD-NE-CZ	5.36	131.10	123.60
1	C	792	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	D	367	MET	CG-SD-CE	5.36	108.78	100.20
1	A	182	ASN	N-CA-CB	5.35	120.23	110.60
1	B	262	GLN	N-CA-CB	5.35	120.23	110.60
1	C	919	ASP	CB-CG-OD1	5.35	123.11	118.30
1	B	492	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	178	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	447	ASP	CB-CG-OD1	5.34	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	842	TRP	CB-CG-CD2	-5.33	119.67	126.60
1	B	199	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	C	987	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	D	561	ARG	NE-CZ-NH2	-5.31	117.65	120.30
1	B	579	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	234	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	786	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	880	ALA	N-CA-CB	5.29	117.51	110.10
1	B	233	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	486	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	618	THR	CA-CB-CG2	-5.28	105.01	112.40
1	C	371	THR	CA-CB-CG2	-5.27	105.02	112.40
1	C	842	TRP	CE2-CD2-CE3	5.27	125.02	118.70
1	B	363	HIS	CA-CB-CG	-5.27	104.65	113.60
1	B	568	TRP	CA-CB-CG	-5.26	103.70	113.70
1	A	802	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	309	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	C	486	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	157	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	924	ASP	CB-CG-OD1	5.25	123.02	118.30
1	C	659	ASP	CB-CG-OD1	5.23	123.00	118.30
1	D	729	THR	CA-CB-CG2	-5.22	105.10	112.40
1	B	423	MET	CG-SD-CE	-5.21	91.87	100.20
1	C	136	GLU	CB-CA-C	-5.21	99.99	110.40
1	D	869	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	221	GLN	N-CA-CB	-5.19	101.26	110.60
1	D	958	ASN	N-CA-CB	5.18	119.93	110.60
1	D	598	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	781	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	755	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	438	GLU	CB-CA-C	-5.17	100.06	110.40
1	B	832	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	907	PRO	N-CA-CB	5.16	109.49	103.30
1	B	219	THR	CA-CB-CG2	-5.15	105.19	112.40
1	C	399	TYR	CB-CG-CD2	5.15	124.09	121.00
1	B	538	TYR	CB-CG-CD1	-5.15	117.91	121.00
1	B	802	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	24	LEU	N-CA-CB	5.13	120.67	110.40
1	B	610	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	552	TYR	CB-CG-CD1	5.13	124.08	121.00
1	D	790	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	A	269	SER	N-CA-CB	-5.12	102.81	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	96	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	375	ASP	CB-CG-OD1	5.11	122.90	118.30
1	B	578	TYR	CB-CA-C	-5.11	100.18	110.40
1	C	404	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	C	792	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	828	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	144	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	D	1014	TYR	CB-CG-CD2	-5.11	117.94	121.00
1	D	770	ILE	C-N-CA	-5.10	111.59	122.30
1	C	671	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	428	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	356	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	319	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	214	LEU	CB-CG-CD1	5.09	119.65	111.00
1	A	131	GLU	CB-CA-C	-5.09	100.23	110.40
1	D	45	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	618	THR	CA-CB-CG2	-5.08	105.29	112.40
1	A	82	ASP	CB-CG-OD1	5.08	122.87	118.30
1	D	927	THR	CA-CB-CG2	-5.08	105.29	112.40
1	A	101	THR	N-CA-CB	5.07	119.94	110.30
1	B	668	VAL	CB-CA-C	-5.07	101.76	111.40
1	A	924	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	1013	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	43	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	128	ASN	CB-CA-C	5.05	120.50	110.40
1	A	201	ASP	CB-CG-OD1	5.05	122.84	118.30
1	A	362	LEU	CB-CA-C	-5.05	100.61	110.20
1	D	671	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	B	665	SER	N-CA-CB	-5.04	102.93	110.50
1	D	479	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	262	GLN	C-N-CA	-5.04	111.73	122.30
1	B	894	ARG	CD-NE-CZ	-5.03	116.56	123.60
1	B	416	GLU	N-CA-CB	5.02	119.64	110.60
1	D	648	ASP	N-CA-C	5.01	124.54	111.00
1	C	557	ARG	NE-CZ-NH2	-5.01	117.80	120.30
1	A	394	ASN	N-CA-CB	-5.00	101.59	110.60
1	D	924	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	A	1023	LYS	N-CA-CB	5.00	119.60	110.60
1	D	916	ASP	CB-CG-OD2	-5.00	113.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	855	THR	CB
1	D	128	ASN	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8125	0	7716	279	0
1	B	8125	0	7716	350	0
1	C	8125	0	7716	311	0
1	D	8125	0	7716	282	0
2	A	14	0	10	2	0
2	B	14	0	9	1	0
2	C	14	0	9	0	0
2	D	14	0	9	3	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	2	0	0	0	0
4	D	3	0	0	0	0
5	A	76	0	114	11	0
5	B	68	0	102	13	0
5	C	80	0	120	15	0
5	D	72	0	108	10	0
6	A	775	0	0	30	0
6	B	747	0	0	29	0
6	C	719	0	0	26	0
6	D	764	0	0	28	0
All	All	35881	0	31345	1198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1198) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.40	1.17
1:B:685:LEU:HD23	1:B:686:PRO:HD2	1.17	1.16
1:C:800:ARG:HA	1:C:800:ARG:HE	1.08	1.12
1:C:761:GLN:HE21	1:C:761:GLN:N	1.48	1.11
1:B:251:ARG:HD2	5:B:8416:DMS:H22	1.36	1.07
1:B:718:GLN:NE2	1:B:719:GLN:H	1.56	1.04
1:B:237:ARG:HB3	1:B:237:ARG:HH11	1.21	1.02
1:B:786:ARG:HG2	1:B:880:ALA:HB1	1.42	1.00
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.42	0.99
1:B:718:GLN:HE21	1:B:719:GLN:N	1.61	0.97
1:B:261:TRP:CH2	1:B:266:GLN:HB2	2.01	0.96
1:B:251:ARG:HD2	5:B:8416:DMS:C2	1.98	0.94
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.50	0.94
1:C:761:GLN:HE21	1:C:761:GLN:H	1.08	0.93
1:D:797:GLU:HB2	1:D:800:ARG:HB2	1.50	0.93
1:D:718:GLN:HE21	1:D:719:GLN:H	1.17	0.92
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.19	0.91
1:B:600:GLN:H	1:B:600:GLN:HE21	1.16	0.91
1:B:78:LEU:HD23	6:B:9054:HOH:O	1.70	0.90
1:C:38:ASN:HB3	1:C:41:GLU:HG3	1.54	0.90
1:A:634:GLN:NE2	1:A:634:GLN:H	1.69	0.90
1:B:597:ASN:ND2	1:B:599:ARG:H	1.70	0.90
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.51	0.90
1:B:786:ARG:HG2	1:B:880:ALA:CB	2.02	0.89
1:B:282:ARG:HG2	1:C:423:MET:HE2	1.55	0.89
1:A:655:MET:HB3	1:A:699:ARG:HH22	1.39	0.88
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.72	0.88
1:D:577:LYS:HG3	1:D:587:ALA:HB2	1.56	0.87
1:B:597:ASN:HD22	1:B:599:ARG:H	1.23	0.87
1:B:685:LEU:HD23	1:B:686:PRO:CD	2.02	0.87
1:C:800:ARG:NE	1:C:800:ARG:HA	1.85	0.86
1:B:773:LYS:HD2	1:B:773:LYS:N	1.87	0.86
1:B:423:MET:HE2	1:C:282:ARG:HG2	1.54	0.86
1:A:423:MET:HE2	1:D:282:ARG:HG2	1.57	0.85
1:D:634:GLN:HG2	1:D:681:GLU:HG3	1.58	0.85
1:B:830:LEU:HD12	1:B:833:ALA:HB3	1.55	0.85
1:C:760:ARG:N	1:C:761:GLN:NE2	2.23	0.85
1:C:597:ASN:HD22	1:C:599:ARG:H	1.23	0.85
1:D:804:ASN:HD22	1:D:809:ARG:HH21	0.86	0.84
1:C:634:GLN:N	1:C:634:GLN:NE2	2.26	0.84
1:B:251:ARG:HH11	5:B:8416:DMS:C2	1.90	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:GLN:HG2	1:B:682:LEU:O	1.77	0.84
1:D:356:ARG:HH22	1:D:367:MET:HE2	1.43	0.84
1:B:615:PRO:O	1:B:618:THR:HG22	1.79	0.83
1:D:473:ARG:NH1	1:D:476:LYS:HB2	1.94	0.83
1:A:597:ASN:HD22	1:A:599:ARG:H	1.25	0.83
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.61	0.83
1:C:761:GLN:NE2	1:C:761:GLN:H	1.74	0.83
1:D:588:TYR:O	1:D:591:ASP:HB2	1.79	0.82
1:B:237:ARG:CB	1:B:237:ARG:HH11	1.91	0.82
1:C:737:ILE:HG23	1:C:738:PRO:HD2	1.59	0.82
1:C:178:ARG:HD3	6:C:9258:HOH:O	1.79	0.82
1:A:117:GLU:HG3	6:A:8889:HOH:O	1.78	0.82
1:D:183:ARG:HH11	1:D:183:ARG:HG2	1.44	0.82
1:C:634:GLN:N	1:C:634:GLN:HE21	1.78	0.81
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.62	0.81
1:C:926:TYR:CE2	5:C:8423:DMS:H22	2.16	0.81
1:B:251:ARG:HH11	5:B:8416:DMS:H21	1.45	0.81
1:C:761:GLN:NE2	1:C:761:GLN:N	2.28	0.81
1:D:631:LEU:HD12	1:D:632:SER:N	1.97	0.80
1:A:634:GLN:HE21	1:A:634:GLN:H	1.25	0.80
1:A:658:LEU:O	1:A:661:LYS:HG3	1.81	0.80
1:B:827:ALA:HA	1:B:836:ILE:HD13	1.63	0.80
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.46	0.80
1:C:718:GLN:HE21	1:C:719:GLN:H	1.30	0.80
1:D:691:ALA:HA	1:D:725:ASN:HB2	1.64	0.80
1:D:683:PRO:O	1:D:685:LEU:HG	1.80	0.80
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.64	0.79
1:B:1022:GLN:HG2	1:B:1023:LYS:N	1.96	0.79
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.64	0.79
1:B:738:PRO:HD3	1:B:751:LEU:HD13	1.63	0.79
1:B:781:ARG:HG2	1:B:781:ARG:HH11	1.47	0.79
1:B:930:VAL:O	1:B:932:PRO:HD3	1.82	0.79
1:C:88:SER:HA	1:C:366:VAL:HG21	1.62	0.79
1:D:32:PRO:HB2	5:D:8404:DMS:C1	2.12	0.79
1:D:634:GLN:CG	1:D:681:GLU:HG3	2.13	0.78
1:A:69:VAL:CG1	1:A:70:PRO:HD2	2.13	0.78
1:B:730:LEU:HD12	1:B:730:LEU:H	1.47	0.78
1:A:367:MET:HB3	1:A:372:MET:HE3	1.66	0.78
1:D:699:ARG:NH2	6:D:9381:HOH:O	2.15	0.78
1:A:755:ARG:NH2	1:A:771:GLY:O	2.17	0.77
1:B:890:GLN:HG3	1:B:891:VAL:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:NH1	1:C:13:ARG:HG2	1.98	0.77
1:D:718:GLN:NE2	1:D:719:GLN:H	1.82	0.77
1:B:261:TRP:CZ3	1:B:266:GLN:HB2	2.19	0.77
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.49	0.77
1:C:85:VAL:N	5:C:8414:DMS:O	2.17	0.77
1:A:615:PRO:O	1:A:618:THR:HG22	1.85	0.77
1:C:746:ASP:CA	1:C:760:ARG:HG3	2.14	0.76
1:A:243:GLU:OE1	1:A:245:GLN:NE2	2.17	0.76
1:B:613:PRO:HB3	1:B:617:LEU:HD23	1.66	0.76
1:C:50:GLN:HG3	5:C:8504:DMS:C2	2.16	0.76
1:C:730:LEU:HD23	1:C:730:LEU:H	1.47	0.76
1:B:132:SER:O	1:B:135:GLN:NE2	2.19	0.75
1:D:887:GLN:NE2	1:D:980:GLU:O	2.19	0.75
1:C:797:GLU:HB2	1:C:800:ARG:HB2	1.67	0.75
1:C:890:GLN:HG3	1:C:891:VAL:N	2.02	0.75
1:D:277:GLU:H	1:D:277:GLU:CD	1.87	0.75
1:C:649:ASN:OD1	1:C:703:PRO:HD2	1.87	0.75
1:B:945:ASN:OD1	1:B:950:GLN:HG3	1.86	0.75
1:A:887:GLN:NE2	1:A:980:GLU:O	2.19	0.75
1:A:699:ARG:HH11	1:A:699:ARG:HG2	1.51	0.74
1:D:597:ASN:HD22	1:D:599:ARG:H	1.33	0.74
1:C:816:TYR:HB2	6:C:9004:HOH:O	1.86	0.74
1:A:830:LEU:HD12	1:A:833:ALA:HB3	1.69	0.74
1:B:360:HIS:CG	1:B:361:PRO:HD2	2.22	0.74
1:A:738:PRO:HD3	1:A:751:LEU:HD13	1.68	0.74
1:C:952:ARG:HH11	1:C:952:ARG:HG3	1.52	0.74
1:C:745:MET:O	1:C:761:GLN:NE2	2.20	0.74
1:C:809:ARG:NE	6:C:9303:HOH:O	2.20	0.74
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.70	0.74
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.19	0.73
1:B:878:HIS:HD2	6:B:8687:HOH:O	1.70	0.73
1:D:797:GLU:HB2	1:D:800:ARG:CB	2.18	0.73
1:C:767:GLN:HG3	1:C:768:MET:N	2.04	0.73
1:D:787:ALA:HA	1:D:968:MET:HG3	1.71	0.73
1:C:730:LEU:HD23	1:C:730:LEU:N	2.03	0.73
1:A:277:GLU:CD	1:A:277:GLU:H	1.92	0.73
1:C:241:GLU:HG3	1:C:292:ARG:HG2	1.70	0.72
1:D:802:ASP:OD1	1:D:803:PRO:HD2	1.88	0.72
1:A:655:MET:CB	1:A:699:ARG:HH22	2.01	0.72
1:D:135:GLN:C	1:D:136:GLU:HG2	2.09	0.72
1:B:822:LEU:HD21	1:B:825:CYS:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:HIS:ND1	6:C:9074:HOH:O	2.21	0.72
1:B:797:GLU:HB3	1:B:800:ARG:H	1.54	0.72
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.24	0.72
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.20	0.72
1:D:770:ILE:HD12	1:D:775:GLN:CD	2.10	0.72
1:A:579:ASP:OD1	1:A:583:ASN:N	2.19	0.72
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.70	0.72
1:A:890:GLN:HG3	1:A:891:VAL:N	2.04	0.72
1:B:682:LEU:HB3	1:B:683:PRO:HD2	1.71	0.72
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.87	0.72
1:A:646:HIS:ND1	6:A:9166:HOH:O	2.23	0.71
1:B:718:GLN:HE21	1:B:719:GLN:H	0.79	0.71
1:B:13:ARG:HG3	1:C:13:ARG:HH12	1.54	0.71
1:C:942:ARG:HG3	1:C:942:ARG:NH1	2.05	0.71
1:B:853:ARG:NH1	6:B:8957:HOH:O	2.21	0.71
1:A:787:ALA:HA	1:A:968:MET:HG3	1.72	0.71
1:C:155:ASN:CG	1:C:178:ARG:HH12	1.92	0.71
1:B:670:LEU:N	6:B:9274:HOH:O	2.23	0.71
1:D:117:GLU:HB2	6:D:9108:HOH:O	1.89	0.71
1:B:630:ARG:NH1	1:B:637:GLU:OE1	2.24	0.71
1:C:767:GLN:HE21	1:C:774:LYS:HE2	1.54	0.70
1:C:797:GLU:O	1:C:801:ILE:HD13	1.91	0.70
1:B:887:GLN:NE2	1:B:980:GLU:O	2.24	0.70
1:D:634:GLN:HG3	1:D:682:LEU:O	1.91	0.70
1:A:1022:GLN:NE2	1:A:1023:LYS:O	2.25	0.70
1:C:942:ARG:HG3	1:C:942:ARG:HH11	1.57	0.70
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.00	0.70
1:B:822:LEU:HA	1:B:840:HIS:HD2	1.55	0.70
1:D:32:PRO:HB2	5:D:8404:DMS:H12	1.71	0.70
1:B:678:GLN:HG2	1:B:680:ILE:HD11	1.74	0.69
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.89	0.69
1:A:577:LYS:HD2	1:A:592:PHE:CE2	2.27	0.69
1:B:360:HIS:CE1	1:B:362:LEU:H	2.10	0.69
1:D:646:HIS:ND1	6:D:9377:HOH:O	2.25	0.69
1:D:631:LEU:HD12	1:D:632:SER:H	1.57	0.69
1:C:724:GLU:O	1:D:847:LYS:NZ	2.26	0.69
1:A:724:GLU:O	1:B:847:LYS:NZ	2.24	0.69
1:D:183:ARG:NH1	1:D:183:ARG:HG2	2.03	0.69
5:A:8420:DMS:H21	6:A:9277:HOH:O	1.92	0.69
1:B:899:GLY:HA2	1:B:915:PHE:CE1	2.28	0.69
1:D:718:GLN:HE21	1:D:719:GLN:N	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:774:LYS:HE2	6:D:9203:HOH:O	1.93	0.68
1:B:63:PHE:HB3	1:B:64:PRO:HD2	1.74	0.68
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.62	0.68
1:C:655:MET:HG3	1:C:655:MET:O	1.90	0.68
1:B:595:THR:HA	1:B:596:PRO:C	2.14	0.68
1:C:633:GLY:O	1:C:635:THR:N	2.26	0.68
1:C:155:ASN:CG	1:C:178:ARG:HH22	1.96	0.68
1:B:753:ASN:OD1	1:B:754:LYS:HE2	1.94	0.67
1:A:249:GLU:OE2	1:A:251:ARG:NH2	2.21	0.67
1:A:32:PRO:HB2	5:A:8404:DMS:C1	2.24	0.67
1:B:733:ALA:O	1:B:734:SER:C	2.33	0.67
1:B:722:LEU:HB3	6:B:8865:HOH:O	1.94	0.67
1:C:785:THR:O	1:C:881:ARG:HD2	1.94	0.67
1:D:595:THR:HA	1:D:596:PRO:C	2.13	0.67
1:A:654:TRP:CZ3	1:A:665:SER:HA	2.29	0.67
1:B:423:MET:CE	1:C:282:ARG:HG2	2.25	0.67
1:C:634:GLN:HE21	1:C:634:GLN:H	1.43	0.67
1:C:261:TRP:CH2	1:C:266:GLN:HB2	2.30	0.67
1:A:423:MET:HB2	1:D:282:ARG:CG	2.25	0.67
1:D:681:GLU:HA	1:D:681:GLU:OE1	1.93	0.67
1:A:753:ASN:OD1	1:A:754:LYS:HG3	1.95	0.67
1:A:668:VAL:HG12	1:A:669:PRO:O	1.95	0.67
1:B:730:LEU:HD12	1:B:730:LEU:N	2.09	0.67
1:C:737:ILE:CG2	1:C:738:PRO:HD2	2.25	0.66
1:A:809:ARG:HD3	6:A:9250:HOH:O	1.94	0.66
1:C:830:LEU:HD12	1:C:833:ALA:HB3	1.77	0.66
1:C:579:ASP:OD1	1:C:583:ASN:HB2	1.94	0.66
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.76	0.66
1:B:423:MET:HE2	1:C:282:ARG:CG	2.26	0.66
1:C:178:ARG:NH1	1:C:182:ASN:OD1	2.28	0.66
1:D:356:ARG:HH22	1:D:367:MET:CE	2.07	0.66
1:D:243:GLU:OE1	1:D:245:GLN:NE2	2.27	0.66
1:B:1000:SER:O	6:B:8868:HOH:O	2.14	0.66
1:B:237:ARG:HB3	1:B:237:ARG:NH1	2.05	0.66
1:C:261:TRP:CZ3	1:C:266:GLN:HB2	2.30	0.66
1:A:863:GLN:HG2	1:A:1021:CYS:HB3	1.76	0.66
1:B:946:TYR:O	1:B:949:HIS:HB2	1.95	0.66
1:D:861:SER:OG	1:D:863:GLN:HG3	1.96	0.66
1:C:317:THR:OG1	1:C:319:ASP:OD2	2.12	0.66
1:C:127:PHE:HE1	1:C:214:LEU:HD21	1.61	0.66
1:B:767:GLN:HG3	1:B:768:MET:N	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:9279:HOH:O	1:D:473:ARG:HD3	1.96	0.66
1:A:971:SER:N	6:A:9067:HOH:O	2.28	0.66
1:A:775:GLN:O	1:A:776:LEU:HD23	1.96	0.66
1:B:674:PRO:O	1:B:675:GLN:HB2	1.96	0.66
1:D:577:LYS:HG3	1:D:587:ALA:CB	2.24	0.66
1:B:830:LEU:HD12	1:B:833:ALA:CB	2.25	0.66
1:C:760:ARG:N	1:C:761:GLN:HE21	1.94	0.66
1:C:804:ASN:OD1	1:C:809:ARG:NH2	2.28	0.66
1:D:777:LEU:HD11	1:D:889:ALA:HA	1.78	0.65
1:B:251:ARG:NH1	5:B:8416:DMS:O	2.29	0.65
1:B:651:LEU:C	1:B:651:LEU:HD23	2.17	0.65
1:A:69:VAL:HG12	1:A:70:PRO:HD2	1.76	0.65
1:B:231:PHE:O	5:B:8417:DMS:H22	1.97	0.65
1:C:155:ASN:HD21	1:C:178:ARG:NH1	1.94	0.65
1:C:155:ASN:ND2	1:C:178:ARG:NH1	2.44	0.65
1:A:964:GLN:O	1:A:968:MET:HB2	1.97	0.65
1:A:600:GLN:H	1:A:600:GLN:HE21	1.45	0.65
1:B:482:ARG:O	6:B:8808:HOH:O	2.14	0.65
1:B:613:PRO:HB3	1:B:617:LEU:CD2	2.26	0.65
1:B:577:LYS:HE2	1:B:591:ASP:O	1.97	0.65
1:C:92:MET:HA	1:C:92:MET:HE2	1.77	0.65
1:A:579:ASP:OD1	1:A:582:GLY:N	2.29	0.65
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.27	0.64
1:A:721:ARG:NH2	6:A:8983:HOH:O	2.30	0.64
1:B:817:GLN:HA	1:B:817:GLN:NE2	2.12	0.64
1:C:577:LYS:HG3	1:C:587:ALA:HB2	1.80	0.64
1:B:655:MET:HE2	1:B:697:THR:HB	1.78	0.64
1:C:632:SER:C	1:C:633:GLY:O	2.32	0.64
5:A:8425:DMS:H21	6:A:9144:HOH:O	1.97	0.64
1:A:878:HIS:HD2	6:A:8576:HOH:O	1.81	0.64
1:C:41:GLU:OE2	1:C:46:ARG:NH1	2.29	0.64
1:C:155:ASN:ND2	1:C:178:ARG:HH12	1.96	0.64
1:B:1022:GLN:HG2	1:B:1023:LYS:H	1.63	0.64
1:B:77:ASP:HA	1:B:183:ARG:NH2	2.13	0.64
1:A:772:ASP:HB2	6:A:9270:HOH:O	1.98	0.64
1:C:237:ARG:HB3	1:C:237:ARG:NH1	2.13	0.64
1:C:767:GLN:NE2	1:C:774:LYS:HE2	2.13	0.64
1:A:423:MET:HB2	1:D:282:ARG:HG2	1.80	0.64
1:B:651:LEU:O	1:B:651:LEU:HD23	1.98	0.64
1:D:285:TYR:CG	1:D:288:ARG:HD2	2.32	0.64
1:B:655:MET:HE1	6:B:9263:HOH:O	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.33	0.63
1:D:250:LEU:C	1:D:251:ARG:HG2	2.17	0.63
1:A:75:GLU:OE2	1:A:156:GLY:HA3	1.98	0.63
1:C:808:GLU:OE1	1:C:811:LYS:NZ	2.32	0.63
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.80	0.63
1:C:878:HIS:HD2	6:C:8687:HOH:O	1.81	0.63
1:C:573:GLN:HB2	1:C:602:CYS:O	1.98	0.63
1:D:1022:GLN:O	1:D:1022:GLN:HG3	1.97	0.63
1:A:634:GLN:NE2	1:A:634:GLN:N	2.45	0.62
1:B:830:LEU:HB2	1:B:833:ALA:HB3	1.79	0.62
1:B:678:GLN:HG2	1:B:680:ILE:CD1	2.29	0.62
1:B:759:ASN:OD1	1:B:761:GLN:N	2.29	0.62
1:C:633:GLY:C	1:C:635:THR:H	2.02	0.62
1:B:104:THR:HG22	6:B:9037:HOH:O	1.98	0.62
1:C:277:GLU:N	1:C:277:GLU:OE2	2.27	0.62
1:B:730:LEU:H	1:B:730:LEU:CD1	2.12	0.62
1:D:513:PRO:HD2	6:D:9420:HOH:O	1.98	0.62
1:C:760:ARG:C	1:C:761:GLN:HE21	2.02	0.62
1:B:739:HIS:O	1:B:750:GLU:OE2	2.18	0.62
1:D:75:GLU:OE1	1:D:156:GLY:HA3	2.00	0.62
1:C:92:MET:HA	1:C:92:MET:CE	2.30	0.62
1:D:49:GLN:HB3	6:D:9424:HOH:O	1.98	0.62
1:A:800:ARG:NH1	1:A:800:ARG:HB2	2.15	0.62
1:A:112:PRO:HD2	1:A:113:PHE:CE1	2.34	0.62
1:C:1023:LYS:HB3	1:C:1023:LYS:HZ2	1.63	0.62
1:C:718:GLN:NE2	1:C:719:GLN:H	1.97	0.62
1:C:760:ARG:N	1:C:761:GLN:HE22	1.96	0.62
1:B:39:SER:O	1:B:42:ALA:HB3	1.99	0.62
1:D:240:LEU:C	1:D:240:LEU:HD23	2.20	0.62
1:C:155:ASN:ND2	1:C:178:ARG:NH2	2.48	0.61
5:B:8601:DMS:H11	6:B:9266:HOH:O	1.99	0.61
1:D:145:GLY:HA2	6:D:8796:HOH:O	2.00	0.61
1:C:658:LEU:O	1:C:659:ASP:C	2.34	0.61
1:D:634:GLN:CD	1:D:681:GLU:HG3	2.20	0.61
1:A:1015:HIS:NE2	1:A:1017:GLN:HG2	2.15	0.61
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.82	0.61
1:A:285:TYR:HB3	1:A:288:ARG:HG3	1.83	0.61
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.34	0.61
1:D:1022:GLN:O	1:D:1023:LYS:HB2	1.99	0.61
1:C:965:GLN:O	1:C:969:GLU:HG3	2.00	0.61
1:D:634:GLN:HG2	1:D:681:GLU:CG	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:LEU:CB	1:B:683:PRO:HD2	2.29	0.61
1:C:365:GLN:HG2	6:C:8730:HOH:O	2.01	0.61
1:C:736:ALA:C	1:C:737:ILE:HG13	2.21	0.60
1:C:277:GLU:H	1:C:277:GLU:CD	2.05	0.60
1:B:788:PRO:HD3	1:B:816:TYR:OH	2.01	0.60
1:B:65:ALA:HB1	1:B:66:PRO:HD2	1.83	0.60
1:C:38:ASN:CB	1:C:41:GLU:HG3	2.30	0.60
1:D:693:GLN:HE22	1:D:724:GLU:HB2	1.65	0.60
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.82	0.60
1:D:192:SER:O	1:D:195:SER:HB2	2.01	0.60
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.83	0.60
1:A:655:MET:SD	1:A:699:ARG:NH2	2.74	0.60
1:A:32:PRO:HB2	5:A:8404:DMS:H13	1.82	0.60
1:A:801:ILE:O	1:A:803:PRO:HD3	2.01	0.60
1:A:663:LEU:HB3	1:A:686:PRO:HG3	1.82	0.60
1:B:77:ASP:HA	1:B:183:ARG:HH21	1.65	0.60
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.82	0.60
1:D:429:ASP:OD1	1:D:431:ARG:HG3	2.02	0.60
1:B:360:HIS:ND1	1:B:362:LEU:N	2.47	0.60
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.14	0.60
1:C:660:GLY:O	1:C:662:PRO:HD3	2.01	0.60
1:B:128:ASN:HB2	1:B:181:GLU:OE2	2.02	0.60
1:C:278:ILE:N	1:C:278:ILE:CD1	2.65	0.60
1:C:746:ASP:N	1:C:760:ARG:HG3	2.16	0.60
1:B:843:GLN:HG2	1:B:848:THR:HA	1.83	0.60
1:B:46:ARG:HB3	1:B:47:PRO:HD2	1.84	0.60
1:C:155:ASN:ND2	1:C:178:ARG:HH22	2.00	0.59
1:A:431:ARG:NH2	6:A:8899:HOH:O	2.16	0.59
1:A:773:LYS:HD2	1:A:773:LYS:N	2.17	0.59
1:D:742:THR:HG22	1:D:743:SER:N	2.17	0.59
1:C:272:ALA:HB1	1:C:273:PRO:HD2	1.84	0.59
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.18	0.59
1:A:90:TRP:CD1	1:A:95:TYR:HB2	2.37	0.59
1:A:90:TRP:HD1	1:A:95:TYR:HB2	1.68	0.59
1:D:658:LEU:O	1:D:661:LYS:HG3	2.02	0.59
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.37	0.59
1:D:890:GLN:HB2	6:D:9359:HOH:O	2.02	0.59
1:B:13:ARG:HG2	1:C:13:ARG:CZ	2.33	0.59
1:A:808:GLU:OE1	1:A:811:LYS:HE2	2.02	0.59
1:B:718:GLN:NE2	1:B:719:GLN:N	2.35	0.59
1:D:835:LEU:HD11	1:D:855:THR:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:GLN:HE21	1:A:719:GLN:H	1.50	0.59
1:D:683:PRO:O	1:D:684:GLU:C	2.41	0.59
1:B:827:ALA:HA	1:B:836:ILE:CD1	2.31	0.59
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.84	0.59
1:D:32:PRO:CB	5:D:8404:DMS:H12	2.32	0.59
1:C:571:VAL:CG2	1:C:609:ALA:HA	2.33	0.59
1:C:760:ARG:H	1:C:761:GLN:HE22	1.51	0.59
1:B:13:ARG:HG3	1:C:13:ARG:NH1	2.18	0.59
1:B:652:LEU:HG	1:B:653:HIS:N	2.17	0.59
1:A:587:ALA:HB1	1:A:591:ASP:HB2	1.84	0.59
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.70	0.58
1:B:822:LEU:HA	1:B:840:HIS:CD2	2.37	0.58
1:A:507:ASP:OD1	1:A:521:LYS:NZ	2.29	0.58
1:B:652:LEU:HD11	1:B:698:VAL:HB	1.83	0.58
1:C:59:ARG:NH2	1:C:81:ALA:HB3	2.18	0.58
1:D:734:SER:HB3	1:D:860:GLY:HA3	1.85	0.58
1:D:356:ARG:NH2	1:D:367:MET:CE	2.66	0.58
1:C:890:GLN:OE1	1:C:947:GLY:HA3	2.03	0.58
1:B:63:PHE:HB3	1:B:64:PRO:CD	2.33	0.58
1:B:14:ARG:HA	1:B:16:TRP:CZ3	2.38	0.58
5:A:8410:DMS:H21	6:A:8758:HOH:O	2.02	0.58
1:A:423:MET:CE	1:D:282:ARG:HG2	2.31	0.58
1:C:59:ARG:O	1:C:124:SER:N	2.35	0.58
1:B:813:ALA:O	6:B:8880:HOH:O	2.17	0.58
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.71	0.58
1:A:173:LEU:O	1:A:176:PHE:N	2.28	0.58
1:B:660:GLY:O	1:B:662:PRO:HD3	2.04	0.58
1:B:237:ARG:HH11	1:B:237:ARG:CG	2.17	0.58
1:B:288:ARG:NH1	6:B:9018:HOH:O	2.26	0.58
1:A:296:GLU:HA	1:A:296:GLU:OE2	2.04	0.58
1:A:593:GLY:O	1:A:595:THR:HG22	2.02	0.58
1:B:85:VAL:HG12	1:B:86:VAL:N	2.18	0.58
1:C:133:TRP:CD1	5:C:8504:DMS:H11	2.39	0.58
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.39	0.58
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.84	0.58
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.38	0.58
1:A:80:GLU:O	1:A:81:ALA:C	2.41	0.58
1:A:634:GLN:HE21	1:A:634:GLN:N	1.99	0.58
1:D:815:HIS:HE1	1:D:877:PRO:O	1.87	0.58
1:B:849:LEU:N	1:B:849:LEU:HD23	2.19	0.58
1:B:738:PRO:CD	1:B:751:LEU:HD13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:GLN:HA	1:A:847:LYS:O	2.04	0.58
1:B:381:GLN:O	1:B:621:LYS:HE3	2.02	0.58
1:A:580:GLU:O	1:A:580:GLU:OE2	2.21	0.58
1:B:890:GLN:OE1	1:B:948:PRO:HD3	2.03	0.57
1:B:13:ARG:CG	1:C:13:ARG:NH1	2.67	0.57
1:A:696:LEU:HB2	1:A:722:LEU:HD11	1.86	0.57
1:A:832:ASP:OD1	1:A:857:ARG:NH2	2.38	0.57
1:A:651:LEU:HD13	1:A:667:GLU:HG2	1.86	0.57
1:D:842:TRP:NE1	6:D:9468:HOH:O	2.27	0.57
1:D:277:GLU:N	1:D:277:GLU:OE2	2.31	0.57
1:A:738:PRO:CD	1:A:751:LEU:HD13	2.35	0.57
1:C:768:MET:HE3	1:C:1020:TRP:CZ2	2.38	0.57
1:B:243:GLU:OE1	1:B:245:GLN:NE2	2.36	0.57
1:C:748:CYS:C	1:C:749:ILE:HD12	2.25	0.57
1:D:928:PRO:HB2	1:D:973:ARG:HH11	1.70	0.57
1:B:132:SER:O	1:B:135:GLN:HG3	2.05	0.57
1:A:930:VAL:O	1:A:932:PRO:HD3	2.04	0.57
1:B:347:LYS:HE3	6:B:8862:HOH:O	2.04	0.57
1:D:128:ASN:HB3	1:D:180:GLY:O	2.05	0.57
1:C:474:TRP:O	1:C:478:VAL:HG13	2.05	0.57
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.87	0.57
1:A:125:LEU:O	1:A:183:ARG:HA	2.04	0.56
5:A:8406:DMS:H22	6:A:9070:HOH:O	2.04	0.56
1:D:685:LEU:O	1:D:686:PRO:O	2.23	0.56
1:C:807:VAL:O	1:C:811:LYS:HG3	2.04	0.56
1:B:183:ARG:HG2	1:B:183:ARG:HH11	1.71	0.56
1:B:128:ASN:HA	1:B:180:GLY:O	2.06	0.56
1:D:461:GLU:OE1	2:D:2001:GTZ:H2	2.06	0.56
1:B:592:PHE:HB2	1:B:594:ASP:OD1	2.06	0.56
1:D:742:THR:CG2	1:D:743:SER:N	2.69	0.56
1:B:571:VAL:CG2	1:B:609:ALA:HA	2.36	0.56
1:A:742:THR:HG22	1:A:743:SER:N	2.20	0.56
1:B:778:THR:HG22	1:B:779:PRO:HD2	1.88	0.56
1:B:858:ILE:HG13	1:B:864:MET:HG3	1.87	0.56
1:D:634:GLN:NE2	1:D:681:GLU:CG	2.69	0.56
1:A:554:GLN:NE2	6:A:8659:HOH:O	2.38	0.56
1:A:126:THR:HA	1:A:182:ASN:O	2.06	0.56
1:D:102:ASN:C	1:D:102:ASN:ND2	2.58	0.56
1:D:736:ALA:O	1:D:737:ILE:HG22	2.05	0.56
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.06	0.56
1:B:777:LEU:HG	1:B:889:ALA:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:TYR:CD1	1:C:317:THR:HG22	2.41	0.55
1:A:742:THR:CG2	1:A:743:SER:N	2.69	0.55
1:D:102:ASN:C	1:D:102:ASN:HD22	2.08	0.55
1:A:625:GLN:NE2	6:A:8701:HOH:O	2.36	0.55
1:A:179:ALA:HB3	6:A:9146:HOH:O	2.05	0.55
1:C:730:LEU:CD2	1:C:730:LEU:H	2.11	0.55
1:B:822:LEU:HD13	1:B:840:HIS:NE2	2.21	0.55
1:C:1023:LYS:CB	1:C:1023:LYS:HZ2	2.19	0.55
1:B:844:HIS:CE1	1:B:845:GLN:HG2	2.42	0.55
1:B:961:ARG:N	6:B:8724:HOH:O	2.32	0.55
1:A:635:THR:HG23	1:A:681:GLU:OE2	2.07	0.55
1:C:797:GLU:O	1:C:799:THR:N	2.39	0.55
1:A:237:ARG:HD2	1:A:296:GLU:OE2	2.06	0.55
1:A:59:ARG:NH2	1:A:81:ALA:HB3	2.21	0.55
1:B:658:LEU:O	1:B:661:LYS:HG2	2.07	0.55
1:D:634:GLN:NE2	1:D:681:GLU:HG3	2.21	0.55
1:D:367:MET:HB3	1:D:372:MET:CE	2.37	0.55
1:A:230:ARG:NH1	1:A:241:GLU:HG3	2.21	0.55
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.88	0.55
1:D:100:TYR:HB3	1:D:589:GLY:HA2	1.88	0.55
1:D:693:GLN:NE2	1:D:724:GLU:HB2	2.22	0.55
1:C:754:LYS:HE3	1:C:1022:GLN:OE1	2.07	0.55
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.71	0.55
1:A:521:LYS:HE2	6:A:8908:HOH:O	2.06	0.55
1:D:732:ALA:O	1:D:733:ALA:O	2.26	0.55
1:B:781:ARG:HG2	1:B:781:ARG:NH1	2.20	0.54
1:C:930:VAL:O	1:C:932:PRO:HD3	2.06	0.54
1:D:808:GLU:OE1	1:D:811:LYS:NZ	2.37	0.54
1:C:760:ARG:CA	1:C:761:GLN:HE21	2.21	0.54
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.35	0.54
1:A:910:LEU:N	6:A:8599:HOH:O	2.23	0.54
1:A:461:GLU:OE2	2:A:2001:GTZ:N1	2.40	0.54
1:B:668:VAL:HG12	1:B:669:PRO:O	2.08	0.54
1:D:639:THR:OG1	1:D:677:LYS:HG2	2.08	0.54
1:B:655:MET:HE1	1:B:699:ARG:NH1	2.23	0.54
1:D:961:ARG:NH2	1:D:979:GLU:O	2.41	0.54
1:B:685:LEU:CD2	1:B:686:PRO:HD2	2.11	0.54
1:D:356:ARG:NH2	1:D:367:MET:HE2	2.18	0.54
1:B:764:PHE:CD2	1:B:781:ARG:HG3	2.42	0.54
1:A:473:ARG:NH1	6:A:9241:HOH:O	2.25	0.54
1:A:89:ASN:HA	1:A:206:SER:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:827:ALA:CB	1:B:836:ILE:CD1	2.86	0.54
1:B:654:TRP:CE3	1:B:665:SER:HA	2.43	0.54
1:B:680:ILE:HG22	1:B:682:LEU:HD21	1.90	0.54
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.07	0.54
1:B:845:GLN:OE1	1:B:845:GLN:HA	2.08	0.54
1:B:102:ASN:ND2	1:B:201:ASP:HB2	2.22	0.54
1:A:816:TYR:N	6:A:8830:HOH:O	2.37	0.54
1:A:822:LEU:HD11	1:A:824:GLN:O	2.07	0.54
1:B:155:ASN:CG	1:B:178:ARG:HH12	2.11	0.54
1:D:701:VAL:O	1:D:703:PRO:HD3	2.08	0.54
1:A:683:PRO:O	1:A:685:LEU:HD23	2.08	0.54
1:D:32:PRO:HB2	5:D:8404:DMS:H13	1.90	0.54
1:C:49:GLN:HB2	1:C:50:GLN:OE1	2.08	0.54
1:D:770:ILE:HD12	1:D:775:GLN:OE1	2.08	0.54
1:B:655:MET:CE	1:B:699:ARG:NH1	2.71	0.54
1:D:736:ALA:C	1:D:737:ILE:HG22	2.28	0.54
1:B:814:GLY:HA3	1:B:844:HIS:CG	2.43	0.54
1:C:554:GLN:NE2	6:C:8771:HOH:O	2.22	0.54
1:C:972:HIS:HB3	1:C:974:HIS:ND1	2.23	0.54
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.89	0.54
1:C:962:TYR:OH	5:C:8423:DMS:H21	2.07	0.54
1:D:770:ILE:O	1:D:771:GLY:C	2.42	0.54
1:B:738:PRO:HD3	1:B:860:GLY:HA2	1.90	0.53
1:C:890:GLN:CG	1:C:891:VAL:N	2.71	0.53
1:C:942:ARG:HD2	1:C:954:ASP:HA	1.90	0.53
1:D:777:LEU:CD1	1:D:889:ALA:HA	2.37	0.53
1:C:788:PRO:HD2	1:C:968:MET:HB2	1.89	0.53
1:A:734:SER:CB	1:A:860:GLY:HA3	2.38	0.53
1:D:73:TRP:CZ3	1:D:187:MET:HB2	2.44	0.53
1:C:797:GLU:C	1:C:799:THR:H	2.12	0.53
1:A:655:MET:HB3	1:A:699:ARG:NH2	2.16	0.53
1:A:577:LYS:O	1:A:584:PRO:HA	2.09	0.53
1:B:960:SER:CA	6:B:8724:HOH:O	2.55	0.53
1:D:971:SER:HB3	6:D:9451:HOH:O	2.08	0.53
1:C:615:PRO:O	1:C:618:THR:HG22	2.08	0.53
1:C:569:ASP:O	1:C:605:GLY:HA2	2.08	0.53
1:B:64:PRO:O	1:B:117:GLU:HG2	2.08	0.53
1:B:788:PRO:HG2	6:B:9090:HOH:O	2.07	0.53
1:B:568:TRP:CG	1:B:569:ASP:HB3	2.43	0.53
1:C:770:ILE:HD12	1:C:775:GLN:CD	2.29	0.53
1:C:689:GLU:O	1:C:690:SER:HB3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:LEU:C	1:C:533:LEU:HD23	2.28	0.53
1:B:251:ARG:HD2	5:B:8416:DMS:H21	1.90	0.53
1:C:249:GLU:OE1	1:C:251:ARG:NE	2.39	0.53
1:C:885:ASN:HB2	1:C:984:LEU:O	2.08	0.53
1:A:381:GLN:O	1:A:621:LYS:HE3	2.08	0.53
1:C:942:ARG:HA	1:C:953:GLY:O	2.09	0.53
1:D:579:ASP:OD2	1:D:583:ASN:HB2	2.09	0.53
1:B:632:SER:N	1:B:635:THR:O	2.35	0.53
1:C:155:ASN:ND2	1:C:178:ARG:CZ	2.72	0.53
1:B:896:ASN:HB3	1:B:945:ASN:HB2	1.90	0.53
1:D:55:ASN:ND2	1:D:211:ASP:OD1	2.37	0.53
1:C:802:ASP:OD1	1:C:804:ASN:N	2.39	0.53
1:B:655:MET:HE1	1:B:699:ARG:HH11	1.74	0.53
1:A:781:ARG:HB3	1:A:781:ARG:CZ	2.33	0.53
1:A:696:LEU:HD23	1:A:720:TRP:CE3	2.43	0.53
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.73	0.52
1:D:878:HIS:HD2	6:D:8799:HOH:O	1.90	0.52
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.91	0.52
1:A:658:LEU:O	1:A:659:ASP:C	2.46	0.52
1:C:253:TYR:CE1	1:C:317:THR:HG22	2.45	0.52
1:B:991:MET:HE2	1:B:1003:VAL:HG21	1.91	0.52
1:B:754:LYS:NZ	1:B:1022:GLN:OE1	2.43	0.52
1:D:252:ASP:OD1	1:D:252:ASP:N	2.42	0.52
1:A:599:ARG:HD2	1:A:600:GLN:NE2	2.25	0.52
1:C:952:ARG:HH11	1:C:952:ARG:CG	2.20	0.52
1:B:577:LYS:O	1:B:585:TRP:N	2.38	0.52
1:A:734:SER:HB2	1:A:860:GLY:HA3	1.91	0.52
1:C:933:SER:O	1:C:967:LEU:HD13	2.09	0.52
1:D:740:LEU:HD12	1:D:741:THR:N	2.23	0.52
1:B:474:TRP:O	1:B:477:SER:HB3	2.08	0.52
1:A:608:PHE:CD1	1:A:614:HIS:HD2	2.28	0.52
1:A:824:GLN:NE2	1:A:837:THR:HG22	2.25	0.52
1:D:651:LEU:HG	1:D:653:HIS:CE1	2.45	0.52
1:B:680:ILE:HG22	1:B:682:LEU:CD2	2.39	0.52
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.44	0.52
1:B:960:SER:HA	6:B:8724:HOH:O	2.10	0.52
1:C:347:LYS:HE3	6:C:8868:HOH:O	2.09	0.52
1:D:896:ASN:HD21	1:D:917:ARG:HD2	1.73	0.52
1:B:183:ARG:HG2	1:B:183:ARG:NH1	2.25	0.52
1:A:797:GLU:N	1:A:800:ARG:O	2.36	0.52
1:D:203:TRP:CH2	1:D:592:PHE:CE1	2.98	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.91	0.52
1:C:920:LEU:HD12	1:C:925:MET:SD	2.50	0.52
1:A:718:GLN:NE2	1:A:719:GLN:H	2.07	0.52
1:B:178:ARG:CG	1:B:179:ALA:N	2.70	0.52
1:D:744:GLU:O	1:D:760:ARG:HD3	2.10	0.52
1:D:37:ARG:NH2	1:D:218:PRO:HD3	2.24	0.52
1:A:863:GLN:HG2	1:A:1021:CYS:CB	2.39	0.51
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.45	0.51
1:B:516:PRO:HG3	1:B:518:TRP:CZ2	2.46	0.51
1:C:254:LEU:C	1:C:255:ARG:HG2	2.30	0.51
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.92	0.51
1:B:250:LEU:HD22	6:B:9148:HOH:O	2.10	0.51
1:D:859:ASP:OD1	1:D:861:SER:N	2.42	0.51
1:D:73:TRP:HH2	1:D:186:VAL:C	2.12	0.51
1:B:796:SER:OG	1:B:808:GLU:OE2	2.22	0.51
1:A:896:ASN:HB3	1:A:945:ASN:HB2	1.92	0.51
1:A:751:LEU:O	1:A:754:LYS:HB2	2.10	0.51
1:B:250:LEU:O	1:B:251:ARG:HG2	2.11	0.51
1:B:597:ASN:HD22	1:B:599:ARG:N	2.01	0.51
1:C:926:TYR:HE2	5:C:8423:DMS:H22	1.68	0.51
1:B:658:LEU:O	1:B:659:ASP:C	2.47	0.51
1:D:59:ARG:HD3	6:D:9327:HOH:O	2.09	0.51
1:D:367:MET:HE2	1:D:372:MET:HG2	1.93	0.51
1:A:32:PRO:CB	5:A:8404:DMS:C1	2.89	0.51
1:C:1023:LYS:NZ	1:C:1023:LYS:CB	2.73	0.51
1:D:842:TRP:CH2	1:D:852:SER:HB3	2.46	0.51
1:A:58:TRP:CZ2	1:A:125:LEU:HD22	2.45	0.51
1:B:427:THR:HG21	1:B:462:SER:HB3	1.93	0.51
1:D:789:LEU:O	1:D:792:ASP:N	2.43	0.51
1:D:158:TRP:CZ2	1:D:160:GLY:HA2	2.46	0.51
1:A:655:MET:CG	1:A:699:ARG:NH2	2.74	0.51
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.93	0.51
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.45	0.51
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.46	0.51
1:A:826:THR:OG1	1:A:837:THR:HB	2.11	0.51
1:B:319:ASP:OD1	1:B:320:GLY:N	2.43	0.51
1:B:824:GLN:O	1:B:838:THR:HA	2.11	0.51
1:A:970:THR:HA	6:A:9067:HOH:O	2.10	0.51
1:A:595:THR:HA	1:A:596:PRO:C	2.31	0.51
1:B:13:ARG:HH12	1:C:13:ARG:HG2	1.71	0.51
1:C:250:LEU:O	1:C:251:ARG:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLU:OE1	1:B:179:ALA:HB2	2.11	0.51
1:C:610:ASP:O	1:C:611:ARG:HB2	2.11	0.51
1:A:699:ARG:HH11	1:A:699:ARG:CG	2.17	0.51
1:B:155:ASN:CG	1:B:178:ARG:HH22	2.14	0.51
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.22	0.51
1:B:731:PRO:O	1:B:732:ALA:HB2	2.11	0.51
1:A:944:LEU:O	1:A:950:GLN:HA	2.11	0.51
1:D:367:MET:HB3	1:D:372:MET:HE3	1.93	0.50
1:C:178:ARG:HG2	1:C:179:ALA:O	2.12	0.50
1:C:581:ASN:HB2	1:C:583:ASN:ND2	2.26	0.50
1:A:718:GLN:HG3	1:A:719:GLN:N	2.25	0.50
1:D:797:GLU:CB	1:D:800:ARG:HB2	2.33	0.50
1:A:127:PHE:N	1:A:182:ASN:O	2.41	0.50
1:D:237:ARG:HD3	1:D:296:GLU:OE2	2.11	0.50
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.93	0.50
1:D:804:ASN:HA	1:D:809:ARG:HE	1.76	0.50
1:B:13:ARG:HG3	1:B:15:ASP:OD1	2.12	0.50
1:B:654:TRP:CZ3	1:B:665:SER:CA	2.94	0.50
1:D:843:GLN:HB3	1:D:847:LYS:O	2.10	0.50
1:D:316:HIS:HA	1:D:323:ILE:CD1	2.41	0.50
1:B:573:GLN:HG3	1:B:602:CYS:O	2.11	0.50
1:D:915:PHE:CD2	1:D:915:PHE:C	2.85	0.50
1:A:778:THR:HG23	1:A:887:GLN:HB3	1.94	0.50
1:A:32:PRO:CB	5:A:8404:DMS:H12	2.42	0.50
1:C:614:HIS:HB3	1:C:615:PRO:HD2	1.94	0.50
1:D:153:TRP:CD1	1:D:158:TRP:HA	2.47	0.50
1:B:585:TRP:HZ3	1:B:972:HIS:CD2	2.29	0.50
1:A:73:TRP:O	1:A:183:ARG:NH2	2.38	0.50
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.93	0.50
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.93	0.50
1:A:634:GLN:CD	1:A:634:GLN:H	2.04	0.50
1:B:46:ARG:HB3	1:B:47:PRO:CD	2.41	0.50
1:D:754:LYS:NZ	6:D:9399:HOH:O	2.45	0.50
1:C:607:VAL:HG12	1:C:613:PRO:HA	1.94	0.50
1:B:578:TYR:HA	1:B:583:ASN:O	2.12	0.50
1:D:32:PRO:CB	5:D:8404:DMS:C1	2.88	0.50
1:D:965:GLN:O	1:D:969:GLU:HG3	2.12	0.50
1:B:1006:GLU:HG2	1:B:1007:PHE:CD1	2.47	0.50
1:C:759:ASN:OD1	1:C:761:GLN:N	2.42	0.49
1:C:473:ARG:O	1:C:477:SER:HB3	2.12	0.49
1:C:741:THR:O	6:C:9163:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:VAL:HG22	1:A:355:ASN:N	2.27	0.49
1:B:745:MET:SD	1:B:745:MET:N	2.85	0.49
1:A:372:MET:HE2	1:A:395:HIS:HB3	1.93	0.49
1:A:701:VAL:O	1:A:703:PRO:HD3	2.11	0.49
1:D:784:PHE:HA	1:D:881:ARG:O	2.11	0.49
1:C:759:ASN:OD1	1:C:761:GLN:NE2	2.45	0.49
1:D:513:PRO:O	1:D:514:ALA:HB3	2.12	0.49
1:D:827:ALA:HB2	1:D:836:ILE:CD1	2.42	0.49
1:D:369:GLU:HB3	6:D:9147:HOH:O	2.12	0.49
1:D:691:ALA:HB1	1:D:725:ASN:O	2.12	0.49
1:A:779:PRO:O	1:A:781:ARG:HG3	2.12	0.49
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.94	0.49
1:A:288:ARG:HD2	6:A:8916:HOH:O	2.12	0.49
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.27	0.49
1:D:844:HIS:O	1:D:845:GLN:HB2	2.13	0.49
1:C:278:ILE:N	1:C:278:ILE:HD13	2.28	0.49
1:B:128:ASN:ND2	1:B:129:VAL:N	2.60	0.49
1:A:100:TYR:HB3	1:A:589:GLY:HA2	1.93	0.49
1:B:600:GLN:N	1:B:600:GLN:HE21	1.96	0.49
1:B:826:THR:O	1:B:836:ILE:HA	2.13	0.49
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.47	0.49
1:D:759:ASN:OD1	1:D:761:GLN:HB3	2.13	0.49
1:C:352:ARG:HD2	1:C:626:PHE:CZ	2.48	0.49
1:C:141:ILE:CD1	1:C:184:LEU:HD11	2.43	0.49
1:A:730:LEU:HD12	1:A:730:LEU:H	1.78	0.49
1:A:633:GLY:HA3	1:A:634:GLN:HE21	1.78	0.49
1:D:708:TRP:CZ2	5:D:8403:DMS:H12	2.48	0.49
1:B:533:LEU:HD23	1:B:533:LEU:C	2.33	0.49
1:A:359:HIS:N	1:A:367:MET:HE1	2.28	0.49
1:D:656:VAL:HG21	1:D:685:LEU:HD22	1.95	0.48
1:D:844:HIS:N	1:D:847:LYS:O	2.45	0.48
1:A:282:ARG:HG2	1:D:423:MET:HB2	1.94	0.48
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.47	0.48
1:C:521:LYS:HG2	1:C:559:TYR:CZ	2.48	0.48
1:A:991:MET:HE2	1:A:1003:VAL:HG21	1.95	0.48
1:B:190:ARG:HG2	1:B:191:TRP:CE2	2.48	0.48
1:C:630:ARG:NE	1:C:637:GLU:OE1	2.32	0.48
1:A:699:ARG:NH1	1:A:699:ARG:CG	2.76	0.48
1:B:830:LEU:O	1:B:831:ALA:C	2.52	0.48
1:B:778:THR:OG1	1:B:887:GLN:HB3	2.14	0.48
1:B:13:ARG:HG2	1:C:13:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:911:THR:HA	6:D:9246:HOH:O	2.13	0.48
1:C:133:TRP:HD1	5:C:8504:DMS:H11	1.78	0.48
1:D:30:HIS:ND1	1:D:31:PRO:O	2.41	0.48
1:B:86:VAL:HG12	1:B:87:PRO:N	2.27	0.48
1:A:965:GLN:HA	1:A:968:MET:HE3	1.95	0.48
1:B:910:LEU:C	1:B:910:LEU:HD12	2.34	0.48
1:A:305:ILE:O	1:A:305:ILE:HG22	2.14	0.48
1:B:531:ARG:HB3	1:B:532:PRO:HD2	1.95	0.48
1:D:628:GLN:HG3	6:D:9128:HOH:O	2.14	0.48
1:C:781:ARG:HG2	1:C:781:ARG:HH11	1.79	0.48
1:A:655:MET:CG	1:A:699:ARG:HH22	2.26	0.48
1:A:746:ASP:CA	1:A:760:ARG:HG3	2.43	0.48
1:B:36:TRP:NE1	1:B:46:ARG:O	2.42	0.48
1:C:271:THR:HG22	1:C:272:ALA:N	2.29	0.48
1:B:102:ASN:HD22	1:B:201:ASP:HB2	1.79	0.48
1:B:688:PRO:C	1:B:690:SER:H	2.17	0.48
5:C:8417:DMS:C2	6:C:9123:HOH:O	2.61	0.48
1:A:102:ASN:HD22	1:A:102:ASN:C	2.16	0.48
1:A:699:ARG:HG2	1:A:699:ARG:NH1	2.25	0.48
1:A:431:ARG:NH1	6:A:8899:HOH:O	2.44	0.48
1:D:778:THR:HB	1:D:887:GLN:HB3	1.96	0.47
1:B:360:HIS:ND1	1:B:361:PRO:CD	2.76	0.47
1:B:538:TYR:O	1:B:567:VAL:HA	2.14	0.47
1:C:13:ARG:O	1:C:14:ARG:C	2.52	0.47
1:B:178:ARG:HG2	1:B:179:ALA:N	2.09	0.47
1:B:502:MET:O	1:B:517:LYS:HE3	2.14	0.47
1:D:390:SER:HA	1:D:391:HIS:HA	1.65	0.47
1:D:942:ARG:HB3	6:D:9366:HOH:O	2.13	0.47
1:A:66:PRO:HD2	1:A:67:GLU:OE1	2.14	0.47
1:A:764:PHE:HE1	1:A:781:ARG:NH1	2.11	0.47
1:B:232:ASN:C	5:B:8417:DMS:H22	2.33	0.47
1:D:580:GLU:N	1:D:580:GLU:OE1	2.47	0.47
1:B:635:THR:HG23	1:B:681:GLU:OE2	2.14	0.47
1:C:178:ARG:HG2	1:C:179:ALA:N	2.11	0.47
1:C:433:LEU:N	1:C:434:PRO:CD	2.77	0.47
1:C:433:LEU:N	1:C:434:PRO:HD2	2.30	0.47
1:D:890:GLN:HG3	1:D:891:VAL:N	2.28	0.47
1:C:651:LEU:CD1	1:C:651:LEU:C	2.82	0.47
1:A:832:ASP:CG	1:A:857:ARG:HH22	2.18	0.47
1:A:651:LEU:CD1	1:A:667:GLU:HG2	2.43	0.47
1:B:681:GLU:C	1:B:682:LEU:HD23	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:781:ARG:CG	1:B:781:ARG:HH11	2.21	0.47
1:A:32:PRO:HB2	5:A:8404:DMS:H12	1.96	0.47
1:B:843:GLN:CG	1:B:848:THR:HA	2.43	0.47
1:A:423:MET:HB2	1:D:282:ARG:HG3	1.94	0.47
1:A:664:ALA:O	1:A:665:SER:HB3	2.14	0.47
1:D:744:GLU:HB3	6:D:9371:HOH:O	2.14	0.47
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.97	0.47
1:B:261:TRP:CZ2	1:B:266:GLN:HB2	2.46	0.47
1:B:680:ILE:N	1:B:680:ILE:HD12	2.29	0.47
1:A:608:PHE:CE1	1:A:614:HIS:HD2	2.32	0.47
1:A:773:LYS:HD2	6:A:9270:HOH:O	2.15	0.47
1:B:126:THR:HG22	1:B:181:GLU:OE1	2.14	0.47
1:D:740:LEU:HD12	1:D:741:THR:H	1.80	0.47
1:D:427:THR:HG21	1:D:462:SER:HB3	1.96	0.47
1:D:925:MET:HB3	6:D:8753:HOH:O	2.14	0.47
1:C:622:HIS:NE2	6:C:8872:HOH:O	2.36	0.47
1:B:416:GLU:HA	1:B:460:ASN:O	2.15	0.47
1:D:854:LYS:HG2	1:D:868:VAL:HG22	1.95	0.47
1:D:575:LEU:HB2	1:D:592:PHE:HZ	1.80	0.47
1:C:842:TRP:N	1:C:842:TRP:CE3	2.83	0.47
1:D:78:LEU:O	1:D:81:ALA:HB3	2.15	0.47
1:B:807:VAL:CG1	1:B:808:GLU:N	2.77	0.47
1:A:166:ARG:HD2	1:A:392:TYR:CD1	2.50	0.47
1:D:870:VAL:HG12	1:D:871:GLU:N	2.29	0.47
1:A:784:PHE:HA	1:A:881:ARG:O	2.15	0.47
1:C:890:GLN:HG3	1:C:891:VAL:H	1.79	0.47
1:D:132:SER:HA	1:D:135:GLN:HB2	1.95	0.47
1:A:773:LYS:CD	1:A:773:LYS:N	2.76	0.47
1:D:226:HIS:O	1:D:242:ALA:HA	2.14	0.47
1:B:822:LEU:HD12	1:B:840:HIS:CD2	2.50	0.46
1:A:965:GLN:HA	1:A:968:MET:CE	2.45	0.46
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.97	0.46
1:D:647:SER:OG	1:D:672:VAL:HG23	2.15	0.46
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.15	0.46
1:B:240:LEU:C	1:B:240:LEU:HD23	2.36	0.46
1:C:571:VAL:HG22	1:C:572:ASP:O	2.15	0.46
1:D:226:HIS:ND1	6:D:9192:HOH:O	2.36	0.46
1:A:995:GLY:C	1:A:997:ASP:N	2.67	0.46
1:B:158:TRP:CZ2	1:B:160:GLY:HA2	2.49	0.46
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.51	0.46
1:C:728:VAL:O	1:C:730:LEU:HD23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:GLN:CG	1:B:768:MET:N	2.77	0.46
1:C:278:ILE:HD13	1:C:278:ILE:H	1.79	0.46
1:A:100:TYR:CE2	1:A:598:ASP:HB2	2.50	0.46
1:B:958:ASN:HA	6:B:8640:HOH:O	2.15	0.46
1:D:660:GLY:HA3	6:D:9216:HOH:O	2.14	0.46
1:B:693:GLN:HE22	1:B:724:GLU:HB2	1.81	0.46
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.80	0.46
1:C:663:LEU:HD22	1:C:663:LEU:HA	1.75	0.46
1:A:367:MET:HB3	1:A:372:MET:CE	2.43	0.46
1:A:654:TRP:O	1:A:665:SER:HB2	2.15	0.46
1:B:255:ARG:CB	1:B:316:HIS:CE1	2.99	0.46
1:D:781:ARG:CZ	6:D:9320:HOH:O	2.63	0.46
1:B:899:GLY:HA2	1:B:915:PHE:CD1	2.50	0.46
1:D:288:ARG:NH1	6:D:9133:HOH:O	2.19	0.46
1:D:869:ASP:OD2	1:D:1015:HIS:ND1	2.41	0.46
1:A:390:SER:HB2	1:A:391:HIS:CE1	2.50	0.46
1:A:65:ALA:HA	1:A:118:ASN:O	2.16	0.46
1:A:802:ASP:OD1	1:A:802:ASP:C	2.50	0.46
1:B:251:ARG:NH1	5:B:8416:DMS:S	2.89	0.46
1:C:633:GLY:C	1:C:634:GLN:NE2	2.69	0.46
1:D:135:GLN:O	1:D:136:GLU:HG2	2.16	0.46
1:B:822:LEU:HD21	1:B:825:CYS:CB	2.42	0.46
1:B:629:PHE:HA	1:B:637:GLU:O	2.16	0.46
1:B:183:ARG:HB3	6:B:9260:HOH:O	2.15	0.46
1:B:807:VAL:HG13	1:B:808:GLU:N	2.31	0.46
1:A:503:TYR:CZ	1:A:537:GLU:HB3	2.51	0.46
1:B:1017:GLN:HB2	6:B:9296:HOH:O	2.15	0.46
1:B:607:VAL:HG23	1:B:608:PHE:O	2.15	0.46
1:B:287:ASP:OD1	1:B:287:ASP:N	2.40	0.46
1:A:990:HIS:HD2	1:A:991:MET:O	1.99	0.46
1:B:204:ARG:HB3	6:B:8802:HOH:O	2.16	0.46
1:B:576:ILE:O	1:B:576:ILE:HG22	2.16	0.46
1:A:670:LEU:HA	1:A:670:LEU:HD23	1.57	0.46
1:C:760:ARG:H	1:C:761:GLN:NE2	2.05	0.46
1:B:63:PHE:HA	1:B:64:PRO:HD3	1.58	0.46
1:B:814:GLY:HA3	1:B:844:HIS:CD2	2.51	0.46
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.97	0.46
1:C:597:ASN:ND2	1:C:599:ARG:H	2.03	0.46
1:B:86:VAL:CG1	1:B:87:PRO:HA	2.39	0.46
1:D:250:LEU:O	1:D:251:ARG:HG2	2.16	0.46
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.76	0.46
1:A:103:VAL:HG22	1:A:418:HIS:CE1	2.51	0.46
1:B:782:ASP:HA	1:B:884:LEU:HD23	1.98	0.46
1:D:768:MET:HB2	1:D:768:MET:HE3	1.90	0.46
1:D:95:TYR:O	1:D:96:ASP:HB3	2.16	0.46
1:D:785:THR:HB	1:D:816:TYR:CE2	2.51	0.46
1:D:816:TYR:HB2	6:D:9117:HOH:O	2.16	0.46
1:A:409:VAL:CG1	1:A:410:VAL:N	2.79	0.46
1:B:696:LEU:HB2	1:B:722:LEU:HD11	1.98	0.46
1:A:800:ARG:CB	1:A:800:ARG:NH1	2.79	0.46
1:A:14:ARG:HG2	1:A:16:TRP:CZ2	2.51	0.46
1:A:614:HIS:HB3	1:A:615:PRO:HD2	1.99	0.45
1:B:360:HIS:C	1:B:360:HIS:ND1	2.69	0.45
1:A:800:ARG:CB	1:A:800:ARG:HH11	2.29	0.45
1:D:808:GLU:HA	1:D:811:LYS:HE3	1.97	0.45
1:D:316:HIS:HA	1:D:323:ILE:HD12	1.98	0.45
1:C:872:VAL:O	1:C:873:ALA:C	2.52	0.45
1:B:691:ALA:HA	1:B:725:ASN:HB2	1.98	0.45
1:D:421:VAL:HA	1:D:422:PRO:HA	1.84	0.45
1:C:798:ALA:C	1:C:799:THR:HG23	2.37	0.45
1:D:32:PRO:C	5:D:8404:DMS:H11	2.37	0.45
1:D:100:TYR:O	1:D:597:ASN:HA	2.16	0.45
1:A:102:ASN:ND2	1:A:102:ASN:C	2.69	0.45
1:C:805:ALA:O	1:C:806:TRP:C	2.53	0.45
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.69	0.45
1:B:433:LEU:HD12	1:B:433:LEU:O	2.17	0.45
1:A:1022:GLN:O	1:A:1023:LYS:CG	2.64	0.45
1:A:773:LYS:HD2	1:A:773:LYS:H	1.80	0.45
1:B:858:ILE:CG1	1:B:864:MET:HG3	2.46	0.45
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.52	0.45
1:B:755:ARG:NH2	6:B:9283:HOH:O	2.35	0.45
1:B:475:ILE:O	1:B:476:LYS:C	2.52	0.45
1:B:781:ARG:NH1	1:B:781:ARG:CG	2.78	0.45
1:A:772:ASP:CB	6:A:9270:HOH:O	2.62	0.45
1:A:799:THR:OG1	1:A:800:ARG:N	2.49	0.45
1:B:128:ASN:HD22	1:B:128:ASN:C	2.20	0.45
1:D:601:PHE:CE2	2:D:2001:GTZ:H62	2.50	0.45
1:C:972:HIS:CB	1:C:974:HIS:CE1	3.00	0.45
1:D:827:ALA:HB2	1:D:836:ILE:HD13	1.99	0.45
1:C:203:TRP:CH2	1:C:592:PHE:CE1	3.05	0.45
1:A:706:THR:HB	6:A:8936:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ARG:HD3	6:C:9279:HOH:O	2.16	0.45
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.23	0.45
1:D:654:TRP:CZ3	1:D:685:LEU:CD2	2.99	0.45
1:A:461:GLU:OE1	2:A:2001:GTZ:H2	2.16	0.45
1:D:203:TRP:CH2	1:D:592:PHE:CD1	3.05	0.45
1:D:323:ILE:HD12	1:D:323:ILE:N	2.31	0.45
1:A:282:ARG:HG3	1:D:420:MET:O	2.17	0.45
1:C:781:ARG:HG2	1:C:781:ARG:NH1	2.31	0.45
1:A:788:PRO:HB2	1:A:793:ILE:HG13	1.99	0.45
1:B:216:HIS:HE1	6:B:9228:HOH:O	1.97	0.45
1:C:959:ILE:HG13	1:C:982:THR:HG22	1.98	0.45
1:A:141:ILE:O	1:A:170:GLU:HA	2.16	0.45
1:B:174:SER:HB2	6:B:9232:HOH:O	2.14	0.45
1:B:914:CYS:HB2	6:B:8959:HOH:O	2.16	0.45
1:B:107:ILE:O	1:B:107:ILE:HG13	2.17	0.45
1:B:786:ARG:CG	1:B:880:ALA:HB1	2.30	0.45
1:D:577:LYS:HE2	1:D:577:LYS:HB3	1.77	0.45
1:A:685:LEU:HG	1:A:685:LEU:H	1.40	0.45
1:D:63:PHE:CE1	1:D:122:CYS:SG	3.09	0.45
1:D:63:PHE:HE1	1:D:122:CYS:SG	2.39	0.45
1:C:823:LEU:HD11	1:C:841:ALA:HB2	1.99	0.45
1:D:986:ILE:HD13	1:D:986:ILE:HG23	1.64	0.45
1:B:282:ARG:HG2	1:C:423:MET:CE	2.36	0.45
1:C:633:GLY:C	1:C:635:THR:N	2.68	0.45
1:B:797:GLU:N	1:B:800:ARG:O	2.39	0.45
1:C:942:ARG:NE	1:C:953:GLY:O	2.50	0.45
1:A:787:ALA:CA	1:A:968:MET:HG3	2.44	0.45
1:C:250:LEU:C	1:C:251:ARG:HG2	2.37	0.45
1:C:577:LYS:HG3	1:C:587:ALA:CB	2.45	0.45
1:C:106:PRO:O	5:C:8419:DMS:H22	2.16	0.45
1:C:733:ALA:O	1:C:734:SER:O	2.35	0.45
1:D:577:LYS:O	1:D:584:PRO:HA	2.16	0.45
1:C:804:ASN:HB3	6:C:8774:HOH:O	2.16	0.45
1:B:569:ASP:O	1:B:605:GLY:HA2	2.17	0.45
1:C:741:THR:HG22	1:C:741:THR:O	2.16	0.45
1:B:661:LYS:HG2	1:B:661:LYS:H	1.57	0.45
1:C:675:GLN:HG3	6:C:8868:HOH:O	2.17	0.45
1:D:360:HIS:HE1	1:D:362:LEU:HD12	1.82	0.45
1:B:693:GLN:NE2	1:B:724:GLU:HB2	2.32	0.45
1:D:82:ASP:OD2	1:D:95:TYR:OH	2.31	0.45
1:C:77:ASP:O	1:C:79:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:PRO:HB3	1:B:339:ASN:O	2.17	0.45
1:C:706:THR:OG1	1:C:709:SER:N	2.50	0.45
1:C:40:GLU:O	1:C:40:GLU:HG3	2.16	0.45
1:A:785:THR:HG22	6:A:8507:HOH:O	2.17	0.45
1:D:730:LEU:HA	1:D:731:PRO:HD3	1.86	0.45
1:A:93:HIS:HB3	1:A:95:TYR:CE1	2.52	0.45
1:C:818:ALA:HB1	1:C:842:TRP:HB3	1.97	0.45
1:A:500:CYS:HA	1:A:534:ILE:O	2.17	0.45
1:D:668:VAL:HG11	1:D:680:ILE:HG12	1.99	0.45
1:D:502:MET:HA	1:D:537:GLU:O	2.17	0.45
1:C:822:LEU:HD21	1:C:825:CYS:HB2	1.99	0.45
1:B:74:LEU:HD23	1:B:74:LEU:HA	1.60	0.45
1:B:89:ASN:HA	1:B:206:SER:O	2.17	0.45
1:C:100:TYR:CE2	1:C:598:ASP:HB2	2.52	0.45
1:C:65:ALA:CB	1:C:66:PRO:HD2	2.36	0.45
1:C:84:VAL:HA	5:C:8414:DMS:O	2.17	0.45
1:C:253:TYR:CD1	1:C:317:THR:CG2	3.00	0.45
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.52	0.45
1:B:853:ARG:HH11	1:B:853:ARG:HG3	1.83	0.44
1:D:811:LYS:HE3	1:D:811:LYS:HB2	1.88	0.44
1:C:854:LYS:HG3	6:C:8617:HOH:O	2.17	0.44
1:D:200:GLN:N	1:D:200:GLN:OE1	2.44	0.44
1:B:634:GLN:HG2	1:B:682:LEU:C	2.36	0.44
1:C:155:ASN:OD1	1:C:178:ARG:NH1	2.41	0.44
1:D:847:LYS:HD2	6:D:9174:HOH:O	2.16	0.44
1:A:878:HIS:HA	1:A:879:PRO:HD3	1.85	0.44
1:A:730:LEU:HD12	1:A:730:LEU:N	2.32	0.44
1:D:105:TYR:CE2	1:D:199:ASP:HB2	2.52	0.44
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.99	0.44
1:A:622:HIS:CE1	5:A:8402:DMS:C1	3.00	0.44
1:A:777:LEU:HA	1:A:777:LEU:HD23	1.74	0.44
1:B:132:SER:HA	1:B:135:GLN:CG	2.47	0.44
1:C:241:GLU:OE1	1:C:292:ARG:NE	2.44	0.44
1:B:155:ASN:CB	1:B:178:ARG:HH22	2.30	0.44
1:A:745:MET:HE3	1:A:761:GLN:CB	2.48	0.44
1:A:87:PRO:HA	1:A:208:ILE:O	2.17	0.44
1:D:708:TRP:CZ3	5:D:8403:DMS:H13	2.52	0.44
1:B:125:LEU:HD11	5:B:8408:DMS:H21	1.99	0.44
1:D:437:SER:O	1:D:441:THR:HG23	2.17	0.44
5:C:8601:DMS:H13	6:C:9254:HOH:O	2.18	0.44
1:C:608:PHE:CD1	1:C:614:HIS:HD2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:842:TRP:N	1:C:842:TRP:HE3	2.15	0.44
1:D:851:ILE:HB	1:D:871:GLU:HB2	1.99	0.44
1:B:101:THR:HG23	1:B:204:ARG:NH2	2.32	0.44
1:C:367:MET:HB3	1:C:372:MET:HE2	1.99	0.44
1:B:974:HIS:CE1	1:B:975:LEU:HD21	2.53	0.44
1:D:230:ARG:NH1	1:D:241:GLU:OE2	2.50	0.44
1:D:608:PHE:CD1	1:D:614:HIS:CD2	3.05	0.44
1:C:802:ASP:O	1:C:808:GLU:HG3	2.17	0.44
1:B:585:TRP:CZ3	1:B:972:HIS:CD2	3.05	0.44
1:D:93:HIS:HB2	1:D:95:TYR:CD1	2.52	0.44
1:C:367:MET:HB3	1:C:372:MET:CE	2.48	0.44
1:A:347:LYS:HA	1:A:348:PRO:HD3	1.81	0.44
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.52	0.44
1:D:368:ASP:O	1:D:372:MET:HG3	2.16	0.44
1:C:736:ALA:O	1:C:737:ILE:HG13	2.17	0.44
1:A:787:ALA:CB	1:A:968:MET:HG3	2.47	0.44
1:C:741:THR:HG22	6:C:9163:HOH:O	2.18	0.44
1:D:737:ILE:HA	1:D:738:PRO:HD3	1.74	0.44
1:B:961:ARG:NH2	1:B:979:GLU:O	2.51	0.44
1:B:961:ARG:NE	1:B:981:GLY:O	2.48	0.44
1:D:73:TRP:HH2	1:D:187:MET:N	2.16	0.44
1:D:896:ASN:HA	1:D:918:TRP:O	2.18	0.44
1:B:583:ASN:HA	1:B:584:PRO:HD3	1.74	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.85	0.44
1:D:948:PRO:HD2	1:D:949:HIS:CD2	2.52	0.44
1:B:251:ARG:NH1	5:B:8416:DMS:H21	2.23	0.44
1:C:285:TYR:CG	1:C:288:ARG:HD2	2.53	0.44
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.76	0.44
1:D:811:LYS:O	1:D:814:GLY:N	2.40	0.44
1:A:793:ILE:O	1:A:794:GLY:C	2.54	0.44
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.34	0.44
1:B:237:ARG:NH1	1:B:237:ARG:CG	2.79	0.44
1:D:685:LEU:O	1:D:686:PRO:C	2.56	0.44
1:B:13:ARG:HG2	1:C:13:ARG:NH2	2.33	0.44
1:C:767:GLN:CG	1:C:768:MET:N	2.76	0.44
1:D:559:TYR:HB2	1:D:562:LEU:HB2	2.00	0.44
1:D:955:PHE:CD2	1:D:1018:LEU:CD2	3.00	0.44
1:B:780:LEU:HD12	1:B:886:CYS:HB3	1.99	0.44
1:B:898:LEU:HD12	1:B:916:ASP:O	2.18	0.44
1:A:240:LEU:HD23	1:A:240:LEU:C	2.38	0.44
1:D:262:GLN:O	1:D:263:GLY:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLU:HG3	1:B:250:LEU:O	2.17	0.43
1:C:765:LEU:HD21	1:C:768:MET:SD	2.58	0.43
1:D:111:PRO:HA	1:D:112:PRO:HA	1.69	0.43
1:B:461:GLU:OE2	2:B:2001:GTZ:N1	2.51	0.43
1:C:729:THR:HG23	6:C:9121:HOH:O	2.18	0.43
1:B:282:ARG:HB2	1:C:423:MET:H	1.82	0.43
1:A:809:ARG:NH1	6:A:9238:HOH:O	2.29	0.43
1:A:650:GLU:N	5:A:8425:DMS:O	2.48	0.43
1:A:807:VAL:CG1	1:A:808:GLU:N	2.82	0.43
1:D:147:ASN:HA	1:D:148:SER:HA	1.66	0.43
1:D:40:GLU:O	1:D:40:GLU:HG3	2.16	0.43
1:C:759:ASN:OD1	1:C:761:GLN:HB2	2.18	0.43
1:B:830:LEU:CD1	1:B:833:ALA:HB3	2.35	0.43
1:B:779:PRO:HB2	1:B:781:ARG:HD2	2.00	0.43
1:C:130:ASP:OD1	1:C:132:SER:OG	2.32	0.43
1:B:135:GLN:HG3	1:B:135:GLN:H	1.49	0.43
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.59	0.43
1:D:285:TYR:CB	1:D:288:ARG:HD2	2.48	0.43
1:D:928:PRO:HB2	1:D:973:ARG:NH1	2.32	0.43
1:D:870:VAL:CG1	1:D:871:GLU:N	2.81	0.43
1:B:133:TRP:CE3	1:B:216:HIS:HB2	2.52	0.43
1:B:441:THR:O	1:B:445:GLN:HG3	2.18	0.43
1:C:760:ARG:CA	1:C:761:GLN:NE2	2.80	0.43
1:A:608:PHE:CE1	1:A:614:HIS:CD2	3.06	0.43
1:D:836:ILE:HD12	1:D:836:ILE:HG23	1.69	0.43
1:B:688:PRO:O	1:B:690:SER:N	2.48	0.43
1:B:917:ARG:NH1	1:B:943:GLU:OE1	2.37	0.43
1:C:297:ASN:N	1:C:298:PRO:CD	2.81	0.43
1:A:615:PRO:HD2	6:A:8671:HOH:O	2.18	0.43
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.48	0.43
1:C:251:ARG:NH1	1:C:253:TYR:HE2	2.17	0.43
1:B:231:PHE:N	1:B:231:PHE:CD1	2.85	0.43
1:C:622:HIS:HB3	1:C:912:ALA:HB2	2.00	0.43
1:D:668:VAL:HG12	1:D:669:PRO:O	2.19	0.43
1:A:629:PHE:HA	1:A:637:GLU:O	2.18	0.43
1:A:360:HIS:CE1	1:A:363:HIS:CD2	3.06	0.43
1:C:745:MET:C	1:C:760:ARG:HG3	2.38	0.43
1:A:1022:GLN:C	1:A:1023:LYS:HG3	2.38	0.43
1:D:599:ARG:HB2	1:D:600:GLN:OE1	2.19	0.43
1:D:777:LEU:CG	1:D:889:ALA:HA	2.48	0.43
1:A:807:VAL:HG13	1:A:808:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PHE:N	1:A:127:PHE:CD2	2.86	0.43
1:D:829:THR:C	1:D:830:LEU:HD23	2.38	0.43
1:A:693:GLN:NE2	1:B:874:SER:OG	2.41	0.43
1:A:226:HIS:O	1:A:242:ALA:HA	2.18	0.43
1:D:970:THR:HA	6:D:9287:HOH:O	2.17	0.43
1:A:251:ARG:H	1:A:254:LEU:HD12	1.82	0.43
1:B:126:THR:HA	1:B:182:ASN:O	2.19	0.43
1:A:587:ALA:HB1	1:A:591:ASP:CB	2.48	0.43
1:A:726:LEU:HD11	1:B:873:ALA:N	2.33	0.43
1:D:685:LEU:HA	1:D:686:PRO:HD2	1.61	0.43
1:B:655:MET:CE	1:B:697:THR:HB	2.46	0.43
1:B:128:ASN:HD22	1:B:129:VAL:N	2.17	0.43
1:C:740:LEU:HG	1:C:741:THR:N	2.33	0.43
1:D:360:HIS:ND1	1:D:362:LEU:N	2.64	0.43
1:A:409:VAL:HG12	1:A:410:VAL:N	2.34	0.43
1:C:522:LYS:HE3	1:D:560:PRO:HD3	2.01	0.43
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.53	0.43
1:D:177:LEU:HA	1:D:177:LEU:HD23	1.77	0.43
1:B:526:LEU:HD23	1:B:526:LEU:HA	1.78	0.43
1:A:69:VAL:HG13	1:A:70:PRO:HD2	1.94	0.43
1:C:133:TRP:CD1	5:C:8504:DMS:C1	3.01	0.43
1:C:583:ASN:HA	1:C:584:PRO:HD3	1.95	0.43
1:B:52:ARG:O	1:B:213:SER:HB2	2.18	0.43
1:C:393:PRO:HD3	1:C:412:GLU:O	2.19	0.43
1:B:414:ASN:O	1:B:439:ARG:HD3	2.19	0.43
1:C:652:LEU:HD11	1:C:698:VAL:HB	2.00	0.43
1:A:423:MET:HB2	1:A:423:MET:HE2	1.86	0.43
1:D:472:TYR:OH	1:D:476:LYS:HE2	2.19	0.43
1:B:779:PRO:HB2	1:B:781:ARG:CD	2.49	0.43
1:D:100:TYR:CZ	1:D:602:CYS:HB3	2.54	0.43
1:B:870:VAL:HG12	1:B:871:GLU:N	2.33	0.43
1:B:577:LYS:O	1:B:585:TRP:CD1	2.72	0.43
1:A:93:HIS:CB	1:A:95:TYR:CE1	3.02	0.43
1:D:19:PRO:HA	1:D:193:ASP:OD1	2.19	0.43
1:C:68:ALA:O	1:C:70:PRO:HD3	2.19	0.43
1:D:416:GLU:OE2	1:D:418:HIS:HB2	2.18	0.43
1:C:132:SER:OG	5:C:8504:DMS:H11	2.18	0.42
1:B:499:ILE:O	1:B:533:LEU:HA	2.19	0.42
1:C:36:TRP:CD1	1:C:48:SER:HB2	2.53	0.42
1:B:86:VAL:CG1	1:B:87:PRO:N	2.78	0.42
1:C:253:TYR:CE1	1:C:317:THR:CG2	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:767:GLN:HG3	1:D:768:MET:N	2.34	0.42
1:B:917:ARG:HD3	1:B:917:ARG:HH11	1.65	0.42
1:C:63:PHE:HB3	1:C:64:PRO:HD2	2.01	0.42
1:C:859:ASP:OD1	1:C:861:SER:OG	2.25	0.42
1:B:588:TYR:HB2	1:B:589:GLY:H	1.61	0.42
1:C:634:GLN:OE1	1:C:681:GLU:HG3	2.19	0.42
1:D:708:TRP:CH2	5:D:8403:DMS:C1	3.02	0.42
1:D:461:GLU:OE2	2:D:2001:GTZ:N1	2.51	0.42
1:D:737:ILE:HG21	1:D:737:ILE:HD13	1.77	0.42
1:C:690:SER:HB2	1:C:691:ALA:H	1.54	0.42
1:A:502:MET:HB2	1:A:537:GLU:HB2	2.00	0.42
1:C:911:THR:CG2	6:C:9027:HOH:O	2.67	0.42
1:B:176:PHE:N	1:B:176:PHE:CD1	2.88	0.42
1:C:951:TRP:HA	1:C:1019:VAL:O	2.19	0.42
1:C:756:TRP:CD2	1:C:858:ILE:HD13	2.54	0.42
1:B:795:VAL:HG13	1:B:999:TRP:HB2	2.02	0.42
1:C:148:SER:HA	1:C:165:SER:OG	2.20	0.42
1:B:23:GLN:NE2	6:B:8981:HOH:O	2.52	0.42
1:A:291:LEU:C	1:A:292:ARG:HG3	2.39	0.42
1:D:959:ILE:HD13	1:D:959:ILE:HG21	1.77	0.42
1:C:796:SER:OG	1:C:801:ILE:HA	2.20	0.42
1:D:800:ARG:HG3	1:D:800:ARG:HH11	1.84	0.42
1:C:926:TYR:CE2	5:C:8423:DMS:C2	2.96	0.42
1:C:890:GLN:OE1	1:C:948:PRO:HD3	2.20	0.42
1:C:966:GLN:O	1:C:969:GLU:N	2.45	0.42
1:D:807:VAL:O	1:D:811:LYS:HG3	2.19	0.42
1:A:735:HIS:O	1:A:736:ALA:HB2	2.20	0.42
1:B:91:GLN:HG2	1:B:98:PRO:HA	2.01	0.42
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.02	0.42
1:A:961:ARG:NH2	1:A:979:GLU:O	2.46	0.42
1:A:640:SER:O	1:A:675:GLN:HA	2.18	0.42
1:A:882:ILE:HD12	1:A:1014:TYR:CD1	2.55	0.42
1:C:797:GLU:HB2	1:C:800:ARG:CB	2.45	0.42
1:B:13:ARG:HD3	1:B:13:ARG:HA	1.76	0.42
1:D:896:ASN:OD1	1:D:917:ARG:NH1	2.36	0.42
1:D:502:MET:HE2	1:D:537:GLU:CD	2.39	0.42
1:A:575:LEU:HD12	1:A:592:PHE:CE1	2.55	0.42
1:A:800:ARG:CZ	1:A:800:ARG:HB2	2.50	0.42
1:A:93:HIS:HB2	1:A:95:TYR:CD1	2.54	0.42
1:D:842:TRP:CZ2	6:D:9468:HOH:O	2.72	0.42
1:B:155:ASN:HB3	1:B:178:ARG:HH22	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:HA	1:C:70:PRO:HD2	1.70	0.42
1:C:17:GLU:OE2	1:C:114:VAL:N	2.34	0.42
1:B:437:SER:CB	1:B:471:LEU:HD21	2.50	0.42
1:B:200:GLN:HG2	1:B:391:HIS:HB2	2.01	0.42
1:B:597:ASN:ND2	1:B:599:ARG:N	2.53	0.42
1:C:622:HIS:CB	1:C:912:ALA:HB2	2.49	0.42
1:B:663:LEU:HA	1:B:663:LEU:HD22	1.63	0.42
1:C:251:ARG:HH11	1:C:253:TYR:HE2	1.68	0.42
1:A:58:TRP:CE2	1:A:125:LEU:HD22	2.54	0.42
1:D:782:ASP:OD1	1:D:854:LYS:NZ	2.45	0.42
1:A:118:ASN:HA	1:A:119:PRO:HD2	1.61	0.42
1:B:854:LYS:HA	1:B:867:THR:O	2.20	0.42
1:C:700:VAL:HB	1:C:716:ALA:HB3	2.01	0.42
1:D:957:PHE:CD1	1:D:957:PHE:C	2.93	0.42
1:B:231:PHE:O	5:B:8417:DMS:C2	2.68	0.42
1:C:920:LEU:HB3	1:C:921:PRO:HD2	2.00	0.42
1:B:277:GLU:H	1:B:277:GLU:HG3	1.27	0.42
1:D:367:MET:HB3	1:D:372:MET:HE2	2.01	0.41
1:C:155:ASN:CG	1:C:178:ARG:NH2	2.69	0.41
1:C:740:LEU:HD12	1:C:748:CYS:O	2.19	0.41
1:A:360:HIS:ND1	1:A:361:PRO:HD2	2.35	0.41
1:C:502:MET:HB2	1:C:537:GLU:HB2	2.01	0.41
1:D:218:PRO:O	1:D:221:GLN:HB3	2.20	0.41
1:B:689:GLU:O	1:B:690:SER:HB3	2.20	0.41
1:A:256:VAL:O	1:A:271:THR:HA	2.20	0.41
1:B:592:PHE:CD1	1:B:592:PHE:N	2.88	0.41
1:B:430:PRO:HB2	6:C:9213:HOH:O	2.21	0.41
1:A:732:ALA:O	1:A:733:ALA:O	2.38	0.41
1:C:993:ILE:HD13	1:C:993:ILE:HG21	1.83	0.41
1:A:577:LYS:HE3	1:A:577:LYS:HB3	1.62	0.41
1:A:775:GLN:C	1:A:776:LEU:HD23	2.41	0.41
1:A:78:LEU:O	1:A:81:ALA:HB3	2.20	0.41
1:D:767:GLN:CG	1:D:768:MET:N	2.84	0.41
1:D:986:ILE:HD12	1:D:986:ILE:HG21	1.82	0.41
6:B:8981:HOH:O	1:C:431:ARG:NH2	2.53	0.41
1:D:888:LEU:O	1:D:981:GLY:HA3	2.20	0.41
1:B:431:ARG:NH2	1:C:26:ARG:O	2.52	0.41
1:D:91:GLN:H	1:D:91:GLN:CD	2.24	0.41
1:A:50:GLN:N	1:A:50:GLN:CD	2.73	0.41
1:B:746:ASP:OD1	1:B:746:ASP:N	2.51	0.41
1:B:304:GLU:C	1:B:305:ILE:HG13	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:942:ARG:CG	1:C:942:ARG:HH11	2.23	0.41
1:A:575:LEU:HB2	1:A:592:PHE:HZ	1.85	0.41
1:A:767:GLN:HG3	1:A:768:MET:N	2.35	0.41
1:B:568:TRP:C	1:B:568:TRP:CD1	2.94	0.41
1:D:651:LEU:HD12	1:D:651:LEU:HA	1.52	0.41
1:D:878:HIS:HA	1:D:879:PRO:HD2	1.94	0.41
1:A:236:SER:C	1:A:237:ARG:HG2	2.41	0.41
1:A:230:ARG:HH12	1:A:241:GLU:HG3	1.83	0.41
1:C:780:LEU:HA	1:C:886:CYS:HB3	2.01	0.41
1:C:798:ALA:C	1:C:799:THR:CG2	2.89	0.41
1:A:777:LEU:CD1	1:A:980:GLU:CG	2.96	0.41
1:C:942:ARG:CD	1:C:954:ASP:HA	2.50	0.41
1:B:851:ILE:HB	1:B:871:GLU:HB2	2.01	0.41
1:A:991:MET:CE	1:A:1003:VAL:HG21	2.51	0.41
1:A:226:HIS:CD2	1:A:448:ARG:HD3	2.56	0.41
1:A:77:ASP:CB	6:A:8811:HOH:O	2.68	0.41
1:A:942:ARG:HA	1:A:953:GLY:O	2.20	0.41
1:C:34:ALA:O	1:C:35:SER:C	2.58	0.41
1:A:223:SER:O	1:A:224:ASP:HB2	2.20	0.41
1:D:682:LEU:HA	1:D:682:LEU:HD22	1.74	0.41
1:C:767:GLN:HG3	1:C:768:MET:H	1.80	0.41
1:D:746:ASP:HA	1:D:760:ARG:HG3	2.03	0.41
1:A:732:ALA:O	1:A:733:ALA:C	2.58	0.41
1:B:926:TYR:CZ	1:B:928:PRO:HA	2.56	0.41
1:A:986:ILE:HG23	1:A:986:ILE:HD13	1.80	0.41
1:D:473:ARG:NH1	1:D:476:LYS:CB	2.76	0.41
1:C:178:ARG:HD2	1:C:181:GLU:O	2.21	0.41
1:B:1022:GLN:HG2	1:B:1023:LYS:O	2.20	0.41
1:C:84:VAL:CA	5:C:8414:DMS:O	2.69	0.41
1:C:730:LEU:CD2	1:C:730:LEU:N	2.72	0.41
1:C:811:LYS:HB3	1:C:811:LYS:HE2	1.74	0.41
1:C:768:MET:CE	1:C:1020:TRP:CZ2	3.04	0.41
1:C:92:MET:CE	1:C:92:MET:CA	2.98	0.41
1:C:271:THR:CG2	1:C:272:ALA:N	2.84	0.41
1:D:708:TRP:CH2	5:D:8403:DMS:H13	2.55	0.41
1:C:959:ILE:HG13	1:C:982:THR:CG2	2.51	0.41
1:D:63:PHE:O	1:D:119:PRO:HA	2.21	0.41
1:C:1013:ARG:NE	6:C:9315:HOH:O	2.37	0.41
1:B:806:TRP:HA	1:B:809:ARG:HG3	2.03	0.41
1:D:301:TRP:CH2	1:D:452:SER:HA	2.55	0.41
1:B:282:ARG:HD2	1:B:282:ARG:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:GLY:C	1:A:592:PHE:H	2.24	0.41
1:A:773:LYS:CD	1:A:773:LYS:H	2.34	0.41
1:B:352:ARG:CG	1:B:553:TRP:CH2	3.02	0.41
1:B:782:ASP:HA	1:B:884:LEU:HA	2.03	0.41
1:B:73:TRP:NE1	1:B:122:CYS:HB3	2.36	0.41
1:A:645:ARG:NH2	1:A:648:ASP:OD1	2.50	0.40
1:C:65:ALA:HB1	1:C:66:PRO:CD	2.42	0.40
1:D:671:ASP:N	1:D:678:GLN:OE1	2.40	0.40
1:B:853:ARG:HH12	1:B:871:GLU:HG3	1.86	0.40
1:A:654:TRP:CE3	1:A:665:SER:HA	2.56	0.40
1:A:824:GLN:HG2	1:A:825:CYS:N	2.35	0.40
1:D:896:ASN:OD1	1:D:917:ARG:HD3	2.22	0.40
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.21	0.40
1:D:765:LEU:HD21	1:D:768:MET:SD	2.60	0.40
1:B:755:ARG:NH1	6:B:9283:HOH:O	2.42	0.40
1:C:733:ALA:O	1:C:734:SER:C	2.58	0.40
1:B:588:TYR:O	1:B:589:GLY:C	2.59	0.40
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.20	0.40
1:C:762:SER:CB	6:C:8988:HOH:O	2.68	0.40
1:C:759:ASN:CG	1:C:761:GLN:NE2	2.75	0.40
1:C:100:TYR:CD1	1:C:602:CYS:HB3	2.57	0.40
1:C:100:TYR:O	1:C:597:ASN:HA	2.22	0.40
1:A:734:SER:C	1:A:736:ALA:H	2.23	0.40
1:C:347:LYS:HD2	6:C:8868:HOH:O	2.20	0.40
1:C:230:ARG:HB3	6:C:9279:HOH:O	2.21	0.40
1:C:733:ALA:C	1:C:734:SER:O	2.59	0.40
1:A:745:MET:HE3	1:A:761:GLN:HB3	2.04	0.40
1:D:614:HIS:HB3	6:D:8896:HOH:O	2.21	0.40
1:B:556:PHE:CD1	1:B:564:GLY:HA2	2.56	0.40
1:D:376:ILE:HG21	1:D:376:ILE:HD13	1.89	0.40
1:A:789:LEU:HD11	1:A:993:ILE:HG22	2.03	0.40
1:C:58:TRP:CD1	1:C:86:VAL:HB	2.56	0.40
1:D:754:LYS:C	1:D:755:ARG:HG2	2.38	0.40
1:D:660:GLY:O	1:D:662:PRO:HD3	2.21	0.40
1:A:989:PHE:CD1	1:A:989:PHE:N	2.90	0.40
1:D:597:ASN:C	1:D:597:ASN:ND2	2.75	0.40
1:B:870:VAL:CG1	1:B:871:GLU:N	2.84	0.40
1:B:63:PHE:CB	1:B:64:PRO:CD	2.86	0.40
1:D:842:TRP:HH2	1:D:852:SER:HB3	1.86	0.40
1:C:828:ASP:HB3	1:D:830:LEU:HD13	2.02	0.40
1:C:487:GLU:HG2	1:C:491:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:TYR:CE2	1:B:522:LYS:HA	2.57	0.40
1:D:356:ARG:NH2	1:D:367:MET:HE1	2.34	0.40
1:D:600:GLN:HB2	1:D:603:MET:CE	2.52	0.40
1:B:949:HIS:CE1	1:B:1020:TRP:HZ2	2.40	0.40
1:B:817:GLN:HA	1:B:817:GLN:HE21	1.83	0.40
1:C:965:GLN:HB2	6:C:8995:HOH:O	2.21	0.40
1:D:590:GLY:C	1:D:592:PHE:H	2.25	0.40
1:C:431:ARG:HD2	6:C:9045:HOH:O	2.20	0.40
1:B:167:LEU:HD23	1:B:167:LEU:HA	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	956 (95%)	52 (5%)	1 (0%)	56	58
1	B	1009/1023 (99%)	947 (94%)	55 (6%)	7 (1%)	26	21
1	C	1009/1023 (99%)	954 (94%)	50 (5%)	5 (0%)	34	30
1	D	1009/1023 (99%)	963 (95%)	42 (4%)	4 (0%)	39	37
All	All	4036/4092 (99%)	3820 (95%)	199 (5%)	17 (0%)	39	37

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	733	ALA
1	B	688	PRO
1	B	689	GLU
1	B	731	PRO
1	B	733	ALA
1	C	634	GLN

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Mol	Chain	Res	Type
1	C	798	ALA
1	D	686	PRO
1	D	733	ALA
1	B	845	GLN
1	C	690	SER
1	B	690	SER
1	C	734	SER
1	B	691	ALA
1	D	81	ALA
1	D	164	ASP
1	C	164	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	808 (94%)	56 (6%)	21	17
1	B	864/875 (99%)	797 (92%)	67 (8%)	16	11
1	C	864/875 (99%)	812 (94%)	52 (6%)	24	20
1	D	864/875 (99%)	821 (95%)	43 (5%)	30	27
All	All	3456/3500 (99%)	3238 (94%)	218 (6%)	22	18

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	72	SER
1	A	80	GLU
1	A	102	ASN
1	A	117	GLU
1	A	128	ASN
1	A	131	GLU
1	A	157	ARG
1	A	182	ASN
1	A	230	ARG

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Mol	Chain	Res	Type
1	A	247	CYS
1	A	250	LEU
1	A	262	GLN
1	A	277	GLU
1	A	296	GLU
1	A	333	ARG
1	A	344	LEU
1	A	394	ASN
1	A	431	ARG
1	A	473	ARG
1	A	519	SER
1	A	535	LEU
1	A	546	LEU
1	A	554	GLN
1	A	577	LYS
1	A	580	GLU
1	A	595	THR
1	A	600	GLN
1	A	634	GLN
1	A	635	THR
1	A	655	MET
1	A	661	LYS
1	A	671	ASP
1	A	672	VAL
1	A	681	GLU
1	A	685	LEU
1	A	689	GLU
1	A	699	ARG
1	A	710	GLU
1	A	729	THR
1	A	734	SER
1	A	735	HIS
1	A	737	ILE
1	A	751	LEU
1	A	772	ASP
1	A	781	ARG
1	A	799	THR
1	A	800	ARG
1	A	817	GLN
1	A	829	THR
1	A	859	ASP
1	A	885	ASN

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Mol	Chain	Res	Type
1	A	956	GLN
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	13	ARG
1	B	48	SER
1	B	72	SER
1	B	78	LEU
1	B	90	TRP
1	B	102	ASN
1	B	128	ASN
1	B	132	SER
1	B	135	GLN
1	B	136	GLU
1	B	178	ARG
1	B	183	ARG
1	B	237	ARG
1	B	249	GLU
1	B	277	GLU
1	B	292	ARG
1	B	299	LYS
1	B	333	ARG
1	B	344	LEU
1	B	370	GLN
1	B	394	ASN
1	B	519	SER
1	B	597	ASN
1	B	600	GLN
1	B	604	ASN
1	B	630	ARG
1	B	634	GLN
1	B	635	THR
1	B	651	LEU
1	B	652	LEU
1	B	655	MET
1	B	661	LYS
1	B	663	LEU
1	B	667	GLU
1	B	682	LEU
1	B	685	LEU
1	B	699	ARG
1	B	710	GLU

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Mol	Chain	Res	Type
1	B	729	THR
1	B	730	LEU
1	B	744	GLU
1	B	745	MET
1	B	746	ASP
1	B	748	CYS
1	B	751	LEU
1	B	757	GLN
1	B	768	MET
1	B	769	TRP
1	B	773	LYS
1	B	778	THR
1	B	781	ARG
1	B	797	GLU
1	B	819	GLU
1	B	824	GLN
1	B	828	ASP
1	B	842	TRP
1	B	843	GLN
1	B	845	GLN
1	B	847	LYS
1	B	850	PHE
1	B	890	GLN
1	B	910	LEU
1	B	917	ARG
1	B	951	TRP
1	B	956	GLN
1	B	1018	LEU
1	B	1023	LYS
1	C	71	GLU
1	C	75	GLU
1	C	102	ASN
1	C	116	THR
1	C	135	GLN
1	C	178	ARG
1	C	249	GLU
1	C	278	ILE
1	C	333	ARG
1	C	392	TYR
1	C	394	ASN
1	C	477	SER
1	C	478	VAL

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Mol	Chain	Res	Type
1	C	519	SER
1	C	580	GLU
1	C	581	ASN
1	C	634	GLN
1	C	635	THR
1	C	651	LEU
1	C	653	HIS
1	C	655	MET
1	C	663	LEU
1	C	665	SER
1	C	685	LEU
1	C	727	SER
1	C	730	LEU
1	C	735	HIS
1	C	743	SER
1	C	744	GLU
1	C	745	MET
1	C	748	CYS
1	C	750	GLU
1	C	754	LYS
1	C	761	GLN
1	C	768	MET
1	C	773	LYS
1	C	796	SER
1	C	800	ARG
1	C	801	ILE
1	C	824	GLN
1	C	826	THR
1	C	829	THR
1	C	843	GLN
1	C	876	THR
1	C	881	ARG
1	C	952	ARG
1	C	956	GLN
1	C	968	MET
1	C	986	ILE
1	C	1004	SER
1	C	1018	LEU
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	72	SER

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Mol	Chain	Res	Type
1	D	76	CYS
1	D	102	ASN
1	D	178	ARG
1	D	183	ARG
1	D	189	LEU
1	D	277	GLU
1	D	333	ARG
1	D	344	LEU
1	D	477	SER
1	D	519	SER
1	D	546	LEU
1	D	554	GLN
1	D	580	GLU
1	D	655	MET
1	D	663	LEU
1	D	667	GLU
1	D	672	VAL
1	D	682	LEU
1	D	684	GLU
1	D	687	GLN
1	D	689	GLU
1	D	699	ARG
1	D	735	HIS
1	D	737	ILE
1	D	739	HIS
1	D	743	SER
1	D	746	ASP
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	778	THR
1	D	799	THR
1	D	830	LEU
1	D	845	GLN
1	D	856	TYR
1	D	885	ASN
1	D	917	ARG
1	D	986	ILE
1	D	1022	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	363	HIS
1	A	554	GLN
1	A	558	GLN
1	A	597	ASN
1	A	600	GLN
1	A	624	GLN
1	A	628	GLN
1	A	634	GLN
1	A	646	HIS
1	A	693	GLN
1	A	718	GLN
1	A	761	GLN
1	A	824	GLN
1	A	878	HIS
1	A	885	ASN
1	A	887	GLN
1	A	890	GLN
1	B	102	ASN
1	B	128	ASN
1	B	262	GLN
1	B	294	ASN
1	B	485	GLN
1	B	554	GLN
1	B	597	ASN
1	B	600	GLN
1	B	624	GLN
1	B	653	HIS
1	B	675	GLN
1	B	693	GLN
1	B	718	GLN
1	B	757	GLN
1	B	817	GLN
1	B	843	GLN
1	B	844	HIS
1	B	878	HIS
1	B	974	HIS
1	B	977	HIS
1	C	102	ASN
1	C	262	GLN
1	C	266	GLN
1	C	294	ASN
1	C	583	ASN

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Mol	Chain	Res	Type
1	C	597	ASN
1	C	624	GLN
1	C	628	GLN
1	C	653	HIS
1	C	693	GLN
1	C	718	GLN
1	C	761	GLN
1	C	878	HIS
1	D	102	ASN
1	D	363	HIS
1	D	394	ASN
1	D	597	ASN
1	D	624	GLN
1	D	634	GLN
1	D	653	HIS
1	D	675	GLN
1	D	693	GLN
1	D	702	GLN
1	D	718	GLN
1	D	761	GLN
1	D	804	ASN
1	D	824	GLN
1	D	863	GLN
1	D	878	HIS
1	D	903	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 102 ligands modelled in this entry, 24 are monoatomic - leaving 78 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	$\#\|Z\| > 2$
2	GTZ	A	2001	4	12,15,15	0.81	0	12,22,22	2.04	4 (33%)
5	DMS	A	8401	-	3,3,3	0.89	0	3,3,3	0.43	0
5	DMS	A	8402	-	3,3,3	0.88	0	3,3,3	0.92	0
5	DMS	A	8403	-	3,3,3	1.64	1 (33%)	3,3,3	1.11	0
5	DMS	A	8404	-	3,3,3	1.32	0	3,3,3	0.30	0
5	DMS	A	8405	-	3,3,3	2.07	1 (33%)	3,3,3	0.17	0
5	DMS	A	8406	-	3,3,3	0.78	0	3,3,3	0.25	0
5	DMS	A	8407	-	3,3,3	1.18	1 (33%)	3,3,3	0.26	0
5	DMS	A	8408	-	3,3,3	1.03	0	3,3,3	0.13	0
5	DMS	A	8409	-	3,3,3	2.91	1 (33%)	3,3,3	0.35	0
5	DMS	A	8410	-	3,3,3	0.44	0	3,3,3	0.51	0
5	DMS	A	8411	-	3,3,3	0.60	0	3,3,3	0.22	0
5	DMS	A	8412	-	3,3,3	0.92	0	3,3,3	0.69	0
5	DMS	A	8414	-	3,3,3	1.09	0	3,3,3	0.55	0
5	DMS	A	8417	-	3,3,3	0.97	0	3,3,3	0.27	0
5	DMS	A	8420	-	3,3,3	0.76	0	3,3,3	0.66	0
5	DMS	A	8421	-	3,3,3	0.95	0	3,3,3	0.44	0
5	DMS	A	8425	3	3,3,3	1.59	1 (33%)	3,3,3	0.09	0
5	DMS	A	8501	-	3,3,3	1.29	1 (33%)	3,3,3	0.43	0
5	DMS	A	8504	-	3,3,3	0.41	0	3,3,3	0.23	0
2	GTZ	B	2001	4	12,15,15	0.56	0	12,22,22	2.05	5 (41%)
5	DMS	B	8401	-	3,3,3	0.55	0	3,3,3	0.96	0
5	DMS	B	8402	-	3,3,3	1.02	0	3,3,3	0.08	0
5	DMS	B	8403	-	3,3,3	1.52	0	3,3,3	0.60	0
5	DMS	B	8404	-	3,3,3	0.35	0	3,3,3	0.73	0
5	DMS	B	8405	-	3,3,3	1.74	1 (33%)	3,3,3	0.21	0
5	DMS	B	8407	-	3,3,3	1.39	1 (33%)	3,3,3	0.67	0
5	DMS	B	8408	-	3,3,3	0.96	0	3,3,3	0.65	0
5	DMS	B	8409	-	3,3,3	0.78	0	3,3,3	1.08	0
5	DMS	B	8411	-	3,3,3	1.31	0	3,3,3	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	B	8412	-	3,3,3	1.01	0	3,3,3	0.69	0
5	DMS	B	8414	-	3,3,3	0.57	0	3,3,3	0.53	0
5	DMS	B	8416	-	3,3,3	0.76	0	3,3,3	0.36	0
5	DMS	B	8417	-	3,3,3	1.46	1 (33%)	3,3,3	0.11	0
5	DMS	B	8421	-	3,3,3	0.77	0	3,3,3	0.34	0
5	DMS	B	8423	-	3,3,3	0.80	0	3,3,3	0.16	0
5	DMS	B	8425	3	3,3,3	1.06	0	3,3,3	0.32	0
5	DMS	B	8601	-	3,3,3	0.80	0	3,3,3	0.45	0
2	GTZ	C	2001	4	12,15,15	0.95	1 (8%)	12,22,22	1.43	2 (16%)
5	DMS	C	8401	-	3,3,3	1.61	1 (33%)	3,3,3	0.98	0
5	DMS	C	8402	-	3,3,3	1.43	0	3,3,3	0.30	0
5	DMS	C	8403	-	3,3,3	1.25	0	3,3,3	1.02	0
5	DMS	C	8404	-	3,3,3	2.07	2 (66%)	3,3,3	0.46	0
5	DMS	C	8405	-	3,3,3	1.98	1 (33%)	3,3,3	0.35	0
5	DMS	C	8407	-	3,3,3	0.93	0	3,3,3	0.31	0
5	DMS	C	8409	-	3,3,3	0.62	0	3,3,3	0.41	0
5	DMS	C	8411	-	3,3,3	1.56	0	3,3,3	0.95	0
5	DMS	C	8412	-	3,3,3	1.16	0	3,3,3	0.66	0
5	DMS	C	8414	-	3,3,3	1.06	0	3,3,3	0.88	0
5	DMS	C	8415	-	3,3,3	2.11	2 (66%)	3,3,3	0.39	0
5	DMS	C	8417	-	3,3,3	0.70	0	3,3,3	0.14	0
5	DMS	C	8419	-	3,3,3	0.41	0	3,3,3	0.13	0
5	DMS	C	8421	-	3,3,3	0.60	0	3,3,3	0.53	0
5	DMS	C	8423	-	3,3,3	0.65	0	3,3,3	0.19	0
5	DMS	C	8425	3	3,3,3	0.80	0	3,3,3	0.05	0
5	DMS	C	8501	-	3,3,3	0.99	0	3,3,3	0.50	0
5	DMS	C	8504	-	3,3,3	0.43	0	3,3,3	0.22	0
5	DMS	C	8601	-	3,3,3	1.14	0	3,3,3	0.83	0
5	DMS	C	8602	-	3,3,3	0.73	0	3,3,3	0.44	0
2	GTZ	D	2001	4	12,15,15	1.44	2 (16%)	12,22,22	2.10	4 (33%)
5	DMS	D	8401	-	3,3,3	1.04	0	3,3,3	0.28	0
5	DMS	D	8402	-	3,3,3	1.06	0	3,3,3	1.17	0
5	DMS	D	8403	-	3,3,3	1.61	1 (33%)	3,3,3	0.22	0
5	DMS	D	8404	-	3,3,3	0.54	0	3,3,3	0.21	0
5	DMS	D	8405	-	3,3,3	1.33	1 (33%)	3,3,3	0.78	0
5	DMS	D	8406	-	3,3,3	0.77	0	3,3,3	0.35	0
5	DMS	D	8407	-	3,3,3	0.81	0	3,3,3	0.07	0
5	DMS	D	8408	-	3,3,3	1.39	1 (33%)	3,3,3	0.59	0
5	DMS	D	8409	-	3,3,3	1.14	0	3,3,3	0.58	0
5	DMS	D	8411	-	3,3,3	1.24	0	3,3,3	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	D	8412	-	3,3,3	1.41	0	3,3,3	1.27	1 (33%)
5	DMS	D	8413	-	3,3,3	0.96	0	3,3,3	0.19	0
5	DMS	D	8414	-	3,3,3	0.31	0	3,3,3	0.71	0
5	DMS	D	8501	-	3,3,3	1.03	0	3,3,3	0.26	0
5	DMS	D	8506	-	3,3,3	1.99	1 (33%)	3,3,3	0.42	0
5	DMS	D	8701	-	3,3,3	0.70	0	3,3,3	0.68	0
5	DMS	D	8703	-	3,3,3	1.47	0	3,3,3	0.30	0
5	DMS	D	8705	-	3,3,3	0.99	0	3,3,3	0.23	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	GTZ	A	2001	4	-	0/2/22/22	0/1/2/2
5	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8420	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8425	3	-	0/0/0/0	0/0/0/0
5	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
2	GTZ	B	2001	4	-	0/2/22/22	0/1/2/2
5	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8407	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8425	3	-	0/0/0/0	0/0/0/0
5	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
2	GTZ	C	2001	4	-	0/2/22/22	0/1/2/2
5	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8425	3	-	0/0/0/0	0/0/0/0
5	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
2	GTZ	D	2001	4	-	0/2/22/22	0/1/2/2
5	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8409	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8413	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8506	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8705	-	-	0/0/0/0	0/0/0/0

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8405	DMS	C2-S	-2.56	1.56	1.75
5	A	8407	DMS	C2-S	2.02	1.91	1.75
2	D	2001	GTZ	C4-C3	2.12	1.58	1.52
5	D	8405	DMS	O-S	2.17	1.65	1.50
5	A	8501	DMS	O-S	2.22	1.65	1.50
5	A	8425	DMS	C1-S	2.27	1.93	1.75
5	B	8407	DMS	C2-S	2.27	1.93	1.75
5	D	8408	DMS	C1-S	2.34	1.93	1.75
5	C	8415	DMS	O-S	2.38	1.66	1.50
5	B	8417	DMS	O-S	2.44	1.66	1.50
5	C	8404	DMS	O-S	2.50	1.67	1.50
5	B	8405	DMS	O-S	2.51	1.67	1.50
5	A	8403	DMS	C2-S	2.54	1.95	1.75
5	C	8404	DMS	C2-S	2.54	1.95	1.75
2	C	2001	GTZ	N1-NB	2.65	1.39	1.34
5	D	8403	DMS	C2-S	2.76	1.97	1.75
5	C	8415	DMS	C1-S	2.76	1.97	1.75
5	C	8401	DMS	C2-S	2.76	1.97	1.75
5	D	8506	DMS	C2-S	2.94	1.98	1.75
5	A	8405	DMS	O-S	3.36	1.73	1.50
2	D	2001	GTZ	N1-NB	3.62	1.40	1.34
5	A	8409	DMS	O-S	4.87	1.83	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	GTZ	C1-C2-C3	-4.58	104.08	113.17
2	D	2001	GTZ	O3-C3-C2	-3.99	99.63	108.90
2	B	2001	GTZ	O2-C2-C1	-3.58	104.78	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2001	GTZ	C3-C4-C5	-3.37	106.84	111.39
2	A	2001	GTZ	C3-C4-C5	-3.22	107.04	111.39
2	C	2001	GTZ	NB-NA-N5	-3.16	104.57	106.20
2	B	2001	GTZ	NB-NA-N5	-3.03	104.64	106.20
2	B	2001	GTZ	O4-C4-C3	-2.70	104.26	110.34
2	A	2001	GTZ	NB-NA-N5	-2.50	104.91	106.20
2	B	2001	GTZ	C1-C2-C3	-2.39	108.43	113.17
2	C	2001	GTZ	C3-C4-C5	-2.37	108.19	111.39
2	B	2001	GTZ	C3-C4-C5	-2.34	108.23	111.39
2	A	2001	GTZ	O2-C2-C1	-2.33	106.59	109.97
2	D	2001	GTZ	C1-C2-C3	-2.31	108.59	113.17
5	D	8412	DMS	C2-S-C1	-2.20	87.10	98.46
2	D	2001	GTZ	O2-C2-C3	3.39	115.69	108.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	GTZ	2	0
5	A	8402	DMS	1	0
5	A	8404	DMS	5	0
5	A	8406	DMS	1	0
5	A	8410	DMS	1	0
5	A	8420	DMS	1	0
5	A	8425	DMS	2	0
2	B	2001	GTZ	1	0
5	B	8408	DMS	1	0
5	B	8416	DMS	8	0
5	B	8417	DMS	3	0
5	B	8601	DMS	1	0
5	C	8414	DMS	3	0
5	C	8417	DMS	1	0
5	C	8419	DMS	1	0
5	C	8423	DMS	4	0
5	C	8504	DMS	5	0
5	C	8601	DMS	1	0
2	D	2001	GTZ	3	0
5	D	8403	DMS	4	0
5	D	8404	DMS	6	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1011/1023 (98%)	-0.31	34 (3%)	49	58	16, 29, 58, 100	0
1	B	1011/1023 (98%)	-0.19	40 (3%)	42	51	18, 32, 62, 100	0
1	C	1011/1023 (98%)	-0.23	33 (3%)	50	59	16, 31, 62, 100	0
1	D	1011/1023 (98%)	-0.29	29 (2%)	55	63	16, 29, 60, 100	0
All	All	4044/4092 (98%)	-0.26	136 (3%)	49	58	16, 30, 61, 100	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	732	ALA	10.5
1	A	799	THR	8.1
1	C	732	ALA	7.8
1	C	731	PRO	7.5
1	B	733	ALA	7.3
1	D	735	HIS	6.9
1	A	735	HIS	6.8
1	D	733	ALA	6.7
1	B	731	PRO	6.4
1	B	730	LEU	6.3
1	D	730	LEU	6.0
1	C	730	LEU	6.0
1	A	732	ALA	5.7
1	A	686	PRO	5.6
1	C	800	ARG	5.4
1	D	800	ARG	5.2
1	D	734	SER	5.1
1	C	633	GLY	5.1
1	A	733	ALA	5.0
1	C	799	THR	5.0
1	A	734	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	731	PRO	4.9
1	A	580	GLU	4.9
1	D	798	ALA	4.9
1	D	686	PRO	4.4
1	A	729	THR	4.3
1	C	735	HIS	4.3
1	B	689	GLU	4.3
1	B	581	ASN	4.2
1	C	761	GLN	4.2
1	D	799	THR	4.1
1	D	689	GLU	4.1
1	B	799	THR	4.0
1	A	687	GLN	3.9
1	A	79	PRO	3.8
1	C	745	MET	3.8
1	A	689	GLU	3.8
1	C	734	SER	3.7
1	B	732	ALA	3.7
1	B	595	THR	3.6
1	D	729	THR	3.6
1	C	772	ASP	3.5
1	D	581	ASN	3.5
1	C	581	ASN	3.5
1	D	79	PRO	3.5
1	B	687	GLN	3.4
1	D	632	SER	3.4
1	C	831	ALA	3.4
1	D	731	PRO	3.3
1	A	736	ALA	3.3
1	A	595	THR	3.3
1	A	634	GLN	3.3
1	A	582	GLY	3.3
1	D	687	GLN	3.3
1	B	686	PRO	3.2
1	A	800	ARG	3.2
1	C	733	ALA	3.2
1	B	818	ALA	3.2
1	B	798	ALA	3.1
1	B	734	SER	3.1
1	C	689	GLU	3.1
1	A	730	LEU	3.0
1	D	1023	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	687	GLN	3.0
1	A	798	ALA	2.9
1	A	688	PRO	2.9
1	B	79	PRO	2.9
1	D	580	GLU	2.9
1	D	728	VAL	2.9
1	C	634	GLN	2.8
1	A	685	LEU	2.8
1	B	797	GLU	2.8
1	D	688	PRO	2.8
1	C	684	GLU	2.8
1	D	633	GLY	2.8
1	D	634	GLN	2.8
1	B	800	ARG	2.8
1	D	76	CYS	2.8
1	D	582	GLY	2.7
1	C	729	THR	2.7
1	B	580	GLU	2.7
1	D	736	ALA	2.7
1	C	579	ASP	2.7
1	C	580	GLU	2.7
1	A	772	ASP	2.7
1	A	684	GLU	2.7
1	B	796	SER	2.7
1	D	845	GLN	2.6
1	C	736	ALA	2.6
1	B	582	GLY	2.6
1	B	593	GLY	2.6
1	C	798	ALA	2.6
1	D	683	PRO	2.5
1	A	581	ASN	2.5
1	C	685	LEU	2.5
1	B	684	GLU	2.5
1	B	831	ALA	2.5
1	B	596	PRO	2.5
1	B	745	MET	2.5
1	A	696	LEU	2.5
1	D	595	THR	2.5
1	D	831	ALA	2.4
1	A	632	SER	2.4
1	A	633	GLY	2.4
1	B	846	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	583	ASN	2.4
1	A	845	GLN	2.4
1	A	78	LEU	2.3
1	C	632	SER	2.3
1	B	583	ASN	2.3
1	B	817	GLN	2.3
1	C	817	GLN	2.3
1	A	801	ILE	2.3
1	C	79	PRO	2.3
1	A	579	ASP	2.3
1	B	772	ASP	2.2
1	C	265	THR	2.2
1	B	579	ASP	2.2
1	B	681	GLU	2.2
1	B	729	THR	2.2
1	B	319	ASP	2.2
1	B	735	HIS	2.1
1	A	596	PRO	2.1
1	B	80	GLU	2.1
1	B	803	PRO	2.1
1	B	633	GLY	2.1
1	C	686	PRO	2.1
1	C	582	GLY	2.1
1	B	685	LEU	2.1
1	A	630	ARG	2.1
1	B	1023	LYS	2.1
1	C	595	THR	2.0
1	A	583	ASN	2.0
1	B	180	GLY	2.0
1	B	632	SER	2.0
1	C	596	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	A	8417	4/4	0.90	0.34	7.82	34,100,100,100	0
5	DMS	A	8504	4/4	0.99	0.13	6.90	23,50,53,92	0
3	MG	C	3105	1/1	0.99	0.21	3.93	41,41,41,41	0
5	DMS	C	8407	4/4	0.96	0.13	3.29	42,64,100,100	0
5	DMS	A	8406	4/4	0.97	0.12	3.08	28,55,72,77	0
5	DMS	C	8403	4/4	0.98	0.19	2.70	25,28,38,39	0
5	DMS	B	8408	4/4	0.96	0.20	2.54	22,43,53,84	0
5	DMS	C	8425	4/4	0.95	0.15	2.18	38,40,45,55	0
5	DMS	B	8425	4/4	0.98	0.15	2.11	49,53,54,100	0
5	DMS	A	8401	4/4	0.99	0.14	1.79	16,22,28,29	0
5	DMS	B	8401	4/4	0.99	0.12	1.75	29,31,38,46	0
5	DMS	C	8419	4/4	0.95	0.22	1.55	51,90,100,100	0
5	DMS	D	8403	4/4	0.98	0.11	1.37	20,40,42,48	0
5	DMS	A	8420	4/4	0.97	0.09	1.36	45,54,56,58	0
3	MG	A	3105	1/1	0.98	0.11	1.33	33,33,33,33	0
5	DMS	B	8407	4/4	0.95	0.10	1.31	28,31,59,100	0
5	DMS	A	8404	4/4	0.97	0.09	1.27	28,36,46,57	0
5	DMS	D	8407	4/4	0.95	0.11	1.16	45,65,73,80	0
5	DMS	D	8408	4/4	0.98	0.15	1.11	34,39,50,58	0
5	DMS	A	8407	4/4	0.96	0.12	0.93	32,53,72,100	0
5	DMS	C	8411	4/4	0.98	0.14	0.68	31,44,51,100	0
5	DMS	D	8412	4/4	0.96	0.10	0.58	20,40,45,59	0
5	DMS	C	8501	4/4	0.98	0.10	0.52	31,35,42,75	0
2	GTZ	B	2001	14/14	0.94	0.10	0.48	18,30,37,38	0
5	DMS	D	8404	4/4	0.97	0.09	0.47	32,62,64,77	0
3	MG	D	3002	1/1	0.99	0.09	0.47	27,27,27,27	0
5	DMS	A	8425	4/4	0.96	0.11	0.41	34,36,51,55	0
5	DMS	A	8403	4/4	0.99	0.10	0.39	29,35,42,56	0
5	DMS	C	8602	4/4	0.98	0.10	0.32	55,63,64,100	0
5	DMS	D	8406	4/4	0.98	0.09	0.31	29,29,34,34	0
5	DMS	C	8405	4/4	0.98	0.09	0.30	30,37,39,40	0
5	DMS	D	8401	4/4	0.99	0.09	0.29	21,25,27,28	0
5	DMS	C	8402	4/4	0.98	0.09	0.20	19,33,40,45	0
5	DMS	A	8501	4/4	0.97	0.10	0.18	31,40,43,51	0
5	DMS	C	8423	4/4	0.97	0.11	0.15	65,71,86,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GTZ	A	2001	14/14	0.95	0.09	0.08	21,30,50,56	0
5	DMS	A	8411	4/4	0.97	0.11	0.06	45,50,77,100	0
5	DMS	B	8423	4/4	0.97	0.10	-0.07	50,60,68,100	0
5	DMS	D	8701	4/4	0.98	0.08	-0.08	22,26,33,100	0
2	GTZ	C	2001	14/14	0.95	0.09	-0.09	18,27,32,41	0
5	DMS	B	8405	4/4	0.98	0.09	-0.15	31,38,44,64	0
5	DMS	D	8405	4/4	0.99	0.08	-0.19	29,37,39,67	0
5	DMS	D	8705	4/4	0.98	0.11	-0.22	43,50,68,69	0
5	DMS	C	8412	4/4	0.98	0.09	-0.26	35,44,48,66	0
5	DMS	A	8412	4/4	0.99	0.08	-0.30	30,45,46,100	0
5	DMS	A	8410	4/4	0.94	0.11	-0.49	51,59,81,100	0
5	DMS	C	8401	4/4	0.99	0.07	-0.51	25,27,29,31	0
4	NA	D	3101	1/1	0.99	0.08	-0.53	28,28,28,28	0
5	DMS	A	8405	4/4	0.98	0.07	-0.61	25,39,43,49	0
3	MG	B	3001	1/1	0.97	0.08	-0.63	31,31,31,31	0
5	DMS	C	8404	4/4	0.99	0.07	-0.66	31,31,34,41	0
5	DMS	B	8417	4/4	0.98	0.09	-0.71	40,42,65,92	0
5	DMS	D	8501	4/4	0.99	0.07	-0.76	37,38,47,52	0
5	DMS	B	8403	4/4	0.99	0.08	-0.77	28,35,38,42	0
4	NA	D	3103	1/1	0.98	0.08	-0.79	45,45,45,45	0
3	MG	B	3002	1/1	0.97	0.09	-0.90	27,27,27,27	0
5	DMS	A	8402	4/4	0.99	0.06	-0.94	21,35,46,52	0
5	DMS	B	8412	4/4	0.98	0.07	-0.95	37,41,45,55	0
2	GTZ	D	2001	14/14	0.97	0.07	-0.95	13,23,36,46	0
5	DMS	B	8404	4/4	0.98	0.07	-1.05	33,35,51,63	0
5	DMS	C	8417	4/4	0.97	0.08	-1.14	29,51,57,58	0
5	DMS	D	8402	4/4	0.99	0.07	-1.15	21,30,39,39	0
5	DMS	D	8411	4/4	0.99	0.07	-1.16	29,41,62,100	0
4	NA	A	3102	1/1	0.99	0.07	-1.19	24,24,24,24	0
4	NA	A	3103	1/1	0.99	0.09	-1.34	37,37,37,37	0
4	NA	B	3103	1/1	0.98	0.06	-1.46	41,41,41,41	0
5	DMS	B	8402	4/4	0.99	0.07	-1.56	21,27,35,38	0
4	NA	C	3101	1/1	0.97	0.05	-1.63	28,28,28,28	0
3	MG	B	3105	1/1	0.98	0.06	-1.64	36,36,36,36	0
4	NA	A	3101	1/1	0.98	0.05	-1.76	29,29,29,29	0
5	DMS	B	8411	4/4	0.99	0.07	-1.81	36,38,42,100	0
5	DMS	A	8408	4/4	0.98	0.06	-1.83	27,56,63,80	0
3	MG	C	3002	1/1	0.98	0.06	-1.87	27,27,27,27	0
4	NA	D	3102	1/1	0.97	0.05	-1.93	25,25,25,25	0
4	NA	B	3102	1/1	0.99	0.05	-2.14	24,24,24,24	0
4	NA	B	3101	1/1	0.98	0.05	-2.30	35,35,35,35	0
3	MG	A	3001	1/1	0.99	0.05	-2.53	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	C	3001	1/1	0.99	0.04	-2.84	25,25,25,25	0
3	MG	D	3001	1/1	0.99	0.04	-2.91	27,27,27,27	0
3	MG	A	3002	1/1	0.98	0.03	-3.42	28,28,28,28	0
4	NA	C	3102	1/1	0.99	0.05	-3.74	22,22,22,22	0
5	DMS	D	8703	4/4	0.94	0.16	-	32,58,79,100	0
5	DMS	C	8421	4/4	0.97	0.18	-	48,49,61,61	0
5	DMS	C	8601	4/4	0.96	0.12	-	43,48,53,54	0
5	DMS	B	8421	4/4	0.89	0.19	-	30,50,73,100	0
5	DMS	B	8414	4/4	0.95	0.13	-	54,57,64,83	0
5	DMS	A	8421	4/4	0.96	0.30	-	60,63,93,100	0
5	DMS	A	8409	4/4	0.92	0.15	-	38,43,63,69	0
5	DMS	B	8409	4/4	0.97	0.13	-	35,37,43,66	0
5	DMS	D	8409	4/4	0.98	0.11	-	33,33,42,43	0
5	DMS	C	8415	4/4	0.94	0.10	-	35,39,40,90	0
3	MG	D	3005	1/1	0.98	0.02	-	39,39,39,39	0
5	DMS	A	8414	4/4	0.97	0.11	-	56,58,63,100	0
5	DMS	D	8506	4/4	0.96	0.10	-	47,60,62,100	0
5	DMS	C	8414	4/4	0.95	0.14	-	26,70,72,100	0
5	DMS	C	8504	4/4	0.96	0.12	-	43,73,100,100	0
5	DMS	B	8601	4/4	0.94	0.14	-	39,46,100,100	0
5	DMS	D	8414	4/4	0.96	0.15	-	31,44,67,100	0
3	MG	A	3005	1/1	0.94	0.10	-	49,49,49,49	0
5	DMS	D	8413	4/4	0.91	0.30	-	82,100,100,100	0
5	DMS	C	8409	4/4	0.95	0.13	-	34,42,66,66	0
5	DMS	B	8416	4/4	0.91	0.25	-	55,62,100,100	0

6.5 Other polymers (i)

There are no such residues in this entry.