Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:27 AM GMT

PDB ID	:	3II6
Title	:	Structure of human Xrcc4 in complex with the tandem BRCT domains of DNA LigaseIV.
Authors	:	Meesala, S.; Junop, M.
Deposited on	:	2009-07-31
Resolution	:	2.40 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:

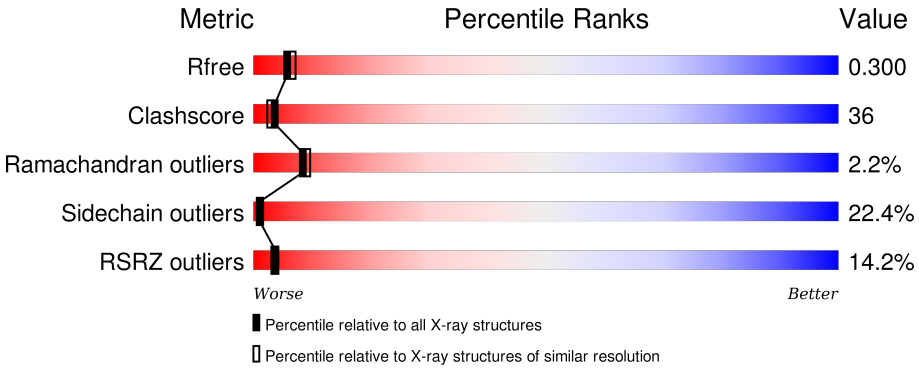
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	203	8% 39% 39% 15% 5%
1	B	203	36% 31% 41% 21%
1	C	203	6% 39% 37% 18%
1	D	203	35% 32% 40% 18% 6%
2	X	263	2% 29% 33% 25% 10%

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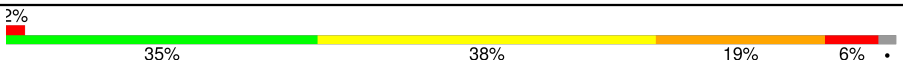
Mol	Chain	Length	Quality of chain
2	Y	263	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10925 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 DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1631	1031	278	315	7			
1	B	196	Total	C	N	O	S	0	0	0
			1606	1016	273	310	7			
1	C	201	Total	C	N	O	S	0	0	0
			1631	1031	278	315	7			
1	D	195	Total	C	N	O	S	0	0	0
			1598	1012	272	307	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	GLU	ALA	ENGINEERED	UNP Q13426
A	134	THR	ILE	ENGINEERED	UNP Q13426
B	60	GLU	ALA	ENGINEERED	UNP Q13426
B	134	THR	ILE	ENGINEERED	UNP Q13426
C	60	GLU	ALA	ENGINEERED	UNP Q13426
C	134	THR	ILE	ENGINEERED	UNP Q13426
D	60	GLU	ALA	ENGINEERED	UNP Q13426
D	134	THR	ILE	ENGINEERED	UNP Q13426

- Molecule 2 is a protein called DNA ligase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	256	Total	C	N	O	S	0	0	0
			2081	1326	351	391	13			
2	Y	258	Total	C	N	O	S	0	0	0
			2095	1333	353	396	13			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	649	GLY	-	EXPRESSION TAG	UNP P49917
X	650	ALA	-	EXPRESSION TAG	UNP P49917
X	651	MET	-	EXPRESSION TAG	UNP P49917
X	652	GLY	-	EXPRESSION TAG	UNP P49917
X	653	SER	-	EXPRESSION TAG	UNP P49917
Y	649	GLY	-	EXPRESSION TAG	UNP P49917
Y	650	ALA	-	EXPRESSION TAG	UNP P49917
Y	651	MET	-	EXPRESSION TAG	UNP P49917
Y	652	GLY	-	EXPRESSION TAG	UNP P49917
Y	653	SER	-	EXPRESSION TAG	UNP P49917

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Y	2	Total Cl 2 2	0	0

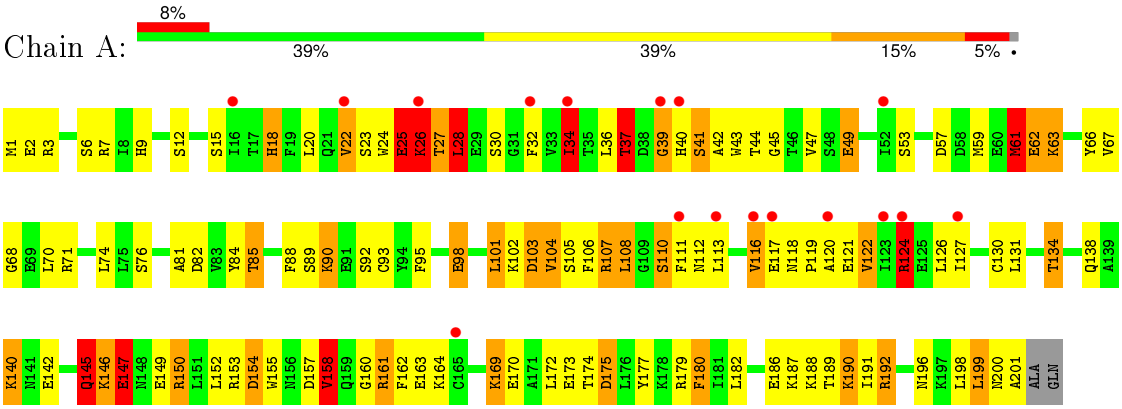
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	25	Total O 25 25	0	0
4	C	41	Total O 41 41	0	0
4	D	29	Total O 29 29	0	0
4	X	83	Total O 83 83	0	0
4	Y	59	Total O 59 59	0	0

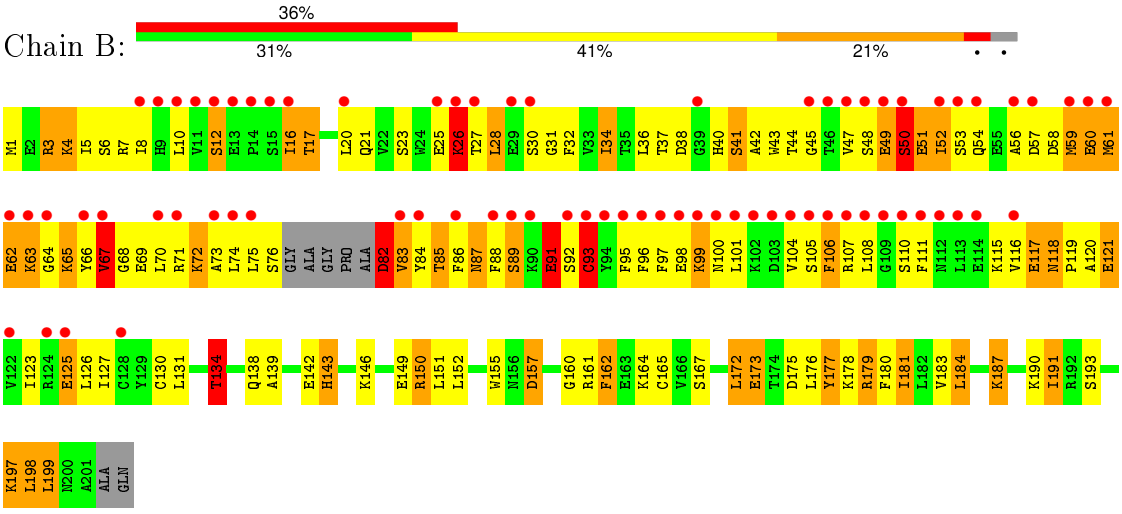
3 Residue-property plots (i)

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.

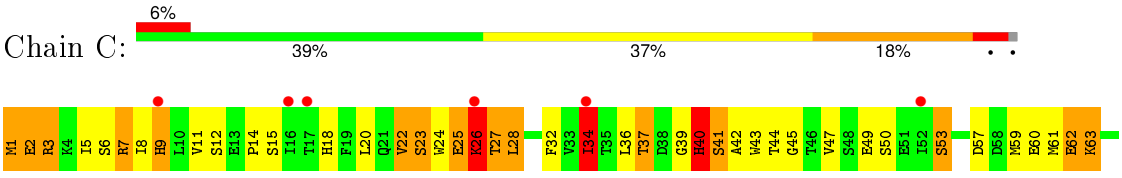
- Molecule 1: DNA repair protein XRCC4

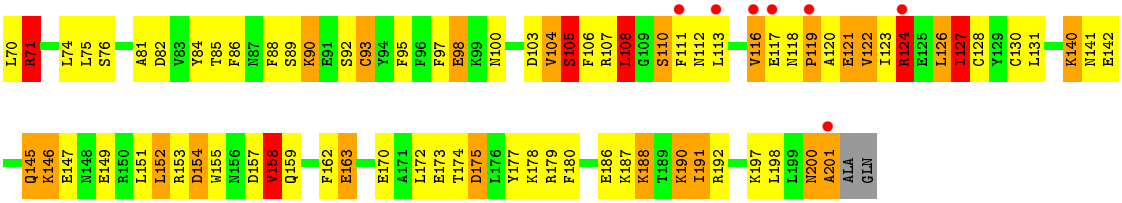


- Molecule 1: DNA repair protein XRCC4



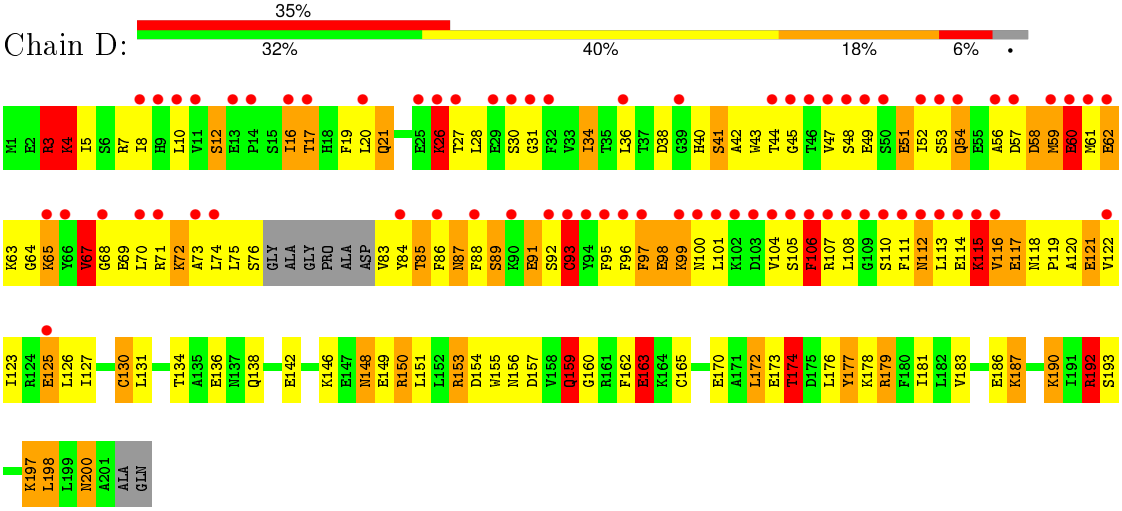
- Molecule 1: DNA repair protein XRCC4





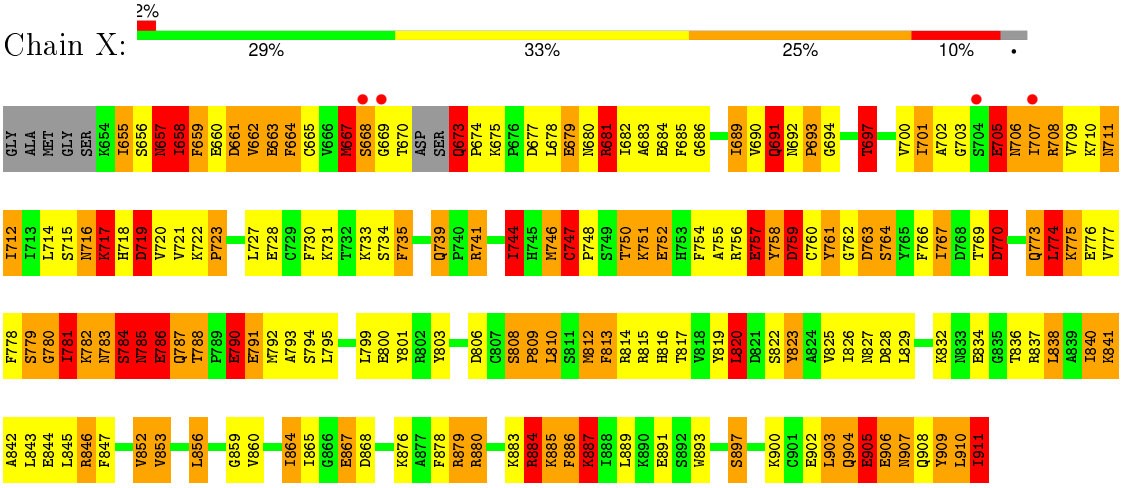
• Molecule 1: DNA repair protein XRCC4

Chain D:



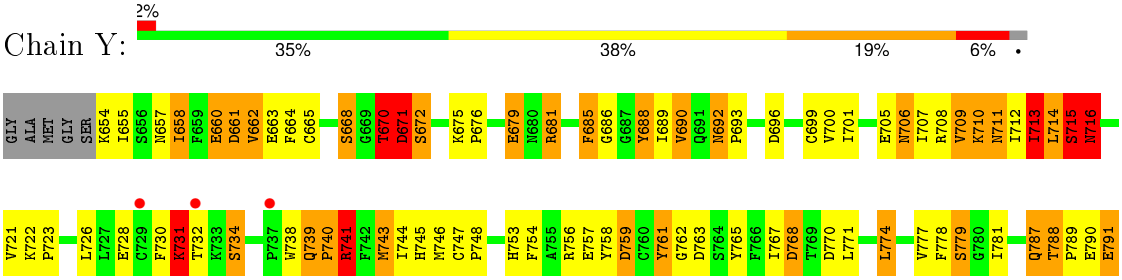
• Molecule 2: DNA ligase 4

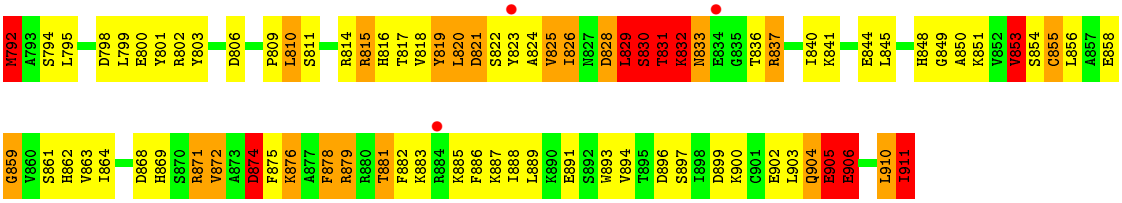
Chain X:



• Molecule 2: DNA ligase 4

Chain Y:




M792 A793 S794 L795 D798 L799 E800 Y801 R802 Y803 D806 P809 L810 S811 R814 R815 H816 T817 V818 Y819 L820 D821 S822 Y823 A824 V825 I826 N827 D828 L829 S830 T831 K832 N833 E834 G835 T836 R837 I840 K841 E844 L845 H848 G849 A850 K851 V852 Y853 S854 G855 L856 A857 E858
G859 V860 S861 H862 V863 I864 D868 H869 S870 R871 V872 A873 D874 F875 K876 A877 F878 R879 R880 T881 F882 K883 H884 K885 F886 K887 I888 L889 K890 E891 S892 W893 V894 T895 D896 S897 I898 D899 K900 C901 E902 L903 Q904 E905 E906 L910 I911

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.24Å 85.98Å 111.61Å 67.34° 82.86° 74.52°	Depositor
Resolution (Å)	20.00 – 2.40 45.26 – 2.28	Depositor EDS
% Data completeness (in resolution range)	86.9 (20.00-2.40) 83.6 (45.26-2.28)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.280 0.254 , 0.300	Depositor DCC
R_{free} test set	2972 reflections (3.55%)	DCC
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.8	EDS
Estimated twinning fraction	0.000 for -h,-k,-k+l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 96708 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10925	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: CL

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	1.93	44/1660 (2.7%)	1.68	38/2232 (1.7%)
1	B	1.81	36/1633 (2.2%)	1.41	23/2193 (1.0%)
1	C	1.91	44/1660 (2.7%)	1.63	39/2232 (1.7%)
1	D	1.84	29/1625 (1.8%)	1.54	27/2182 (1.2%)
2	X	2.20	84/2129 (3.9%)	1.95	73/2873 (2.5%)
2	Y	2.01	55/2144 (2.6%)	1.78	54/2895 (1.9%)
All	All	1.97	292/10851 (2.7%)	1.69	254/14607 (1.7%)

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	A	0	3
1	B	0	2
1	C	0	3
1	D	0	1
2	X	1	14
2	Y	0	12
All	All	1	35

All (292) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	GLU	CD-OE1	20.03	1.47	1.25
1	B	91	GLU	CD-OE1	15.02	1.42	1.25
2	X	909	TYR	CD1-CE1	13.72	1.59	1.39
1	A	179	ARG	CZ-NH1	-13.64	1.15	1.33
1	D	98	GLU	CD-OE1	13.47	1.40	1.25
1	D	117	GLU	CB-CG	-12.04	1.29	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	91	GLU	CD-OE2	11.58	1.38	1.25
1	B	162	PHE	CD1-CE1	11.50	1.62	1.39
1	A	22	VAL	CB-CG2	-11.35	1.29	1.52
1	C	15	SER	CB-OG	11.27	1.56	1.42
1	D	52	ILE	C-O	11.23	1.44	1.23
1	A	180	PHE	CE1-CZ	10.98	1.58	1.37
1	C	147	GLU	CD-OE2	-10.85	1.13	1.25
1	A	186	GLU	CG-CD	10.76	1.68	1.51
1	B	89	SER	CB-OG	10.32	1.55	1.42
1	C	22	VAL	CB-CG1	-10.30	1.31	1.52
1	A	173	GLU	CD-OE2	-10.06	1.14	1.25
1	A	186	GLU	CD-OE1	9.90	1.36	1.25
1	C	186	GLU	CD-OE1	9.52	1.36	1.25
1	C	179	ARG	CZ-NH1	-9.51	1.20	1.33
2	X	747	CYS	CB-SG	-9.50	1.66	1.82
1	A	22	VAL	CB-CG1	-9.45	1.33	1.52
1	C	186	GLU	CG-CD	9.38	1.66	1.51
1	A	15	SER	CB-OG	9.35	1.54	1.42
2	X	846	ARG	CG-CD	9.29	1.75	1.51
1	C	104	VAL	CB-CG2	-9.26	1.33	1.52
1	D	165	CYS	CB-SG	-9.26	1.66	1.82
2	X	757	GLU	CG-CD	9.23	1.65	1.51
1	A	180	PHE	CD2-CE2	9.12	1.57	1.39
1	B	177	TYR	CD2-CE2	-9.09	1.25	1.39
1	B	173	GLU	CB-CG	-9.07	1.34	1.52
1	B	50	SER	CB-OG	8.94	1.53	1.42
1	D	12	SER	CB-OG	8.80	1.53	1.42
1	C	180	PHE	CD1-CE1	8.71	1.56	1.39
1	D	173	GLU	CB-CG	-8.70	1.35	1.52
2	X	823	TYR	CD2-CE2	8.65	1.52	1.39
1	B	60	GLU	C-O	8.65	1.39	1.23
2	X	800	GLU	CB-CG	8.62	1.68	1.52
1	D	117	GLU	CD-OE1	8.58	1.35	1.25
2	X	730	PHE	CB-CG	8.55	1.65	1.51
1	C	173	GLU	CD-OE2	-8.44	1.16	1.25
1	B	177	TYR	CB-CG	8.41	1.64	1.51
1	C	170	GLU	CB-CG	8.34	1.68	1.52
2	Y	818	VAL	CA-CB	8.29	1.72	1.54
2	Y	902	GLU	CD-OE1	8.24	1.34	1.25
2	X	886	PHE	CE1-CZ	8.23	1.52	1.37
2	X	781	ILE	CA-CB	8.04	1.73	1.54
2	X	813	PHE	CE1-CZ	7.96	1.52	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	684	GLU	CB-CG	-7.95	1.37	1.52
2	X	790	GLU	CG-CD	7.94	1.63	1.51
1	C	92	SER	CB-OG	7.93	1.52	1.42
2	X	891	GLU	CD-OE2	7.93	1.34	1.25
1	A	92	SER	CB-OG	7.85	1.52	1.42
1	C	60	GLU	CD-OE1	7.84	1.34	1.25
2	Y	825	VAL	CB-CG2	7.82	1.69	1.52
1	A	169	LYS	CB-CG	-7.73	1.31	1.52
2	Y	765	TYR	CE2-CZ	7.73	1.48	1.38
2	X	659	PHE	CE1-CZ	7.72	1.52	1.37
2	Y	803	TYR	CD1-CE1	7.64	1.50	1.39
2	X	781	ILE	CA-C	7.62	1.72	1.52
1	B	125	GLU	CD-OE1	7.61	1.34	1.25
2	X	663	GLU	CD-OE2	7.51	1.33	1.25
2	Y	819	TYR	CD1-CE1	7.50	1.50	1.39
1	A	104	VAL	CB-CG2	-7.48	1.37	1.52
2	Y	762	GLY	N-CA	7.47	1.57	1.46
2	X	905	GLU	CD-OE2	7.44	1.33	1.25
2	X	741	ARG	CZ-NH1	7.42	1.42	1.33
2	Y	790	GLU	CG-CD	7.38	1.63	1.51
1	C	155	TRP	CG-CD1	7.29	1.47	1.36
1	D	136	GLU	CG-CD	7.29	1.62	1.51
2	Y	713	ILE	C-O	-7.24	1.09	1.23
1	A	162	PHE	CE2-CZ	7.22	1.51	1.37
2	X	773	GLN	CD-NE2	7.21	1.50	1.32
2	Y	779	SER	CB-OG	-7.18	1.32	1.42
2	Y	759	ASP	CB-CG	-7.16	1.36	1.51
1	A	175	ASP	CB-CG	-7.11	1.36	1.51
1	C	22	VAL	CB-CG2	-7.03	1.38	1.52
2	X	891	GLU	CG-CD	7.02	1.62	1.51
1	B	12	SER	CB-OG	7.00	1.51	1.42
2	Y	765	TYR	CD2-CE2	-6.99	1.28	1.39
2	X	777	VAL	CB-CG2	-6.98	1.38	1.52
2	Y	715	SER	C-O	6.96	1.36	1.23
2	X	770	ASP	CB-CG	-6.94	1.37	1.51
1	C	180	PHE	CE1-CZ	6.94	1.50	1.37
2	Y	905	GLU	CB-CG	6.94	1.65	1.52
2	Y	777	VAL	CB-CG1	-6.94	1.38	1.52
2	X	837	ARG	CZ-NH1	6.90	1.42	1.33
1	B	121	GLU	CG-CD	6.90	1.62	1.51
2	X	853	VAL	CB-CG2	-6.81	1.38	1.52
2	Y	685	PHE	CD1-CE1	6.80	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	154	ASP	CG-OD1	-6.79	1.09	1.25
2	Y	721	VAL	CA-CB	6.73	1.68	1.54
2	Y	744	ILE	CB-CG2	6.69	1.73	1.52
2	Y	660	GLU	CG-CD	6.66	1.61	1.51
1	C	201	ALA	CA-CB	6.65	1.66	1.52
1	D	125	GLU	CG-CD	6.63	1.61	1.51
1	B	164	LYS	CE-NZ	6.60	1.65	1.49
2	Y	859	GLY	N-CA	6.60	1.55	1.46
2	X	717	LYS	CD-CE	6.59	1.67	1.51
2	X	719	ASP	CB-CG	-6.58	1.38	1.51
1	C	175	ASP	CB-CG	-6.48	1.38	1.51
2	X	814	ARG	CB-CG	-6.45	1.35	1.52
2	X	780	GLY	C-O	-6.43	1.13	1.23
2	Y	741	ARG	CZ-NH1	6.41	1.41	1.33
1	D	8	ILE	CB-CG2	6.40	1.72	1.52
2	Y	731	LYS	CD-CE	6.38	1.67	1.51
1	B	177	TYR	CD1-CE1	6.38	1.49	1.39
2	X	819	TYR	CD1-CE1	6.36	1.48	1.39
2	Y	741	ARG	CB-CG	-6.35	1.35	1.52
1	D	54	GLN	CD-NE2	6.32	1.48	1.32
2	X	906	GLU	CD-OE2	6.31	1.32	1.25
1	D	183	VAL	CB-CG1	-6.30	1.39	1.52
2	X	879	ARG	CZ-NH2	6.29	1.41	1.33
1	D	136	GLU	CD-OE1	6.28	1.32	1.25
2	X	847	PHE	CD1-CE1	6.28	1.51	1.39
2	Y	730	PHE	CB-CG	6.27	1.62	1.51
2	X	760	CYS	CB-SG	-6.27	1.71	1.82
1	B	60	GLU	CD-OE1	6.25	1.32	1.25
1	C	158	VAL	CB-CG1	6.24	1.66	1.52
2	X	733	LYS	C-O	-6.24	1.11	1.23
1	A	180	PHE	CG-CD2	6.22	1.48	1.38
1	B	164	LYS	CD-CE	6.19	1.66	1.51
2	Y	761	TYR	CE2-CZ	6.18	1.46	1.38
1	C	53	SER	CB-OG	6.17	1.50	1.42
1	C	179	ARG	CG-CD	-6.15	1.36	1.51
2	X	909	TYR	CD2-CE2	6.10	1.48	1.39
1	D	174	THR	CB-CG2	-6.09	1.32	1.52
1	A	158	VAL	CB-CG2	-6.08	1.40	1.52
1	D	125	GLU	CD-OE1	6.07	1.32	1.25
1	B	60	GLU	CD-OE2	6.07	1.32	1.25
2	X	657	ASN	CB-CG	-6.07	1.37	1.51
1	C	170	GLU	CG-CD	6.04	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	663	GLU	CG-CD	-6.04	1.42	1.51
1	A	199	LEU	CG-CD1	-6.03	1.29	1.51
2	X	705	GLU	N-CA	6.02	1.58	1.46
1	A	158	VAL	CB-CG1	6.01	1.65	1.52
1	D	121	GLU	CG-CD	6.01	1.60	1.51
2	Y	859	GLY	CA-C	6.01	1.61	1.51
1	A	155	TRP	CG-CD1	6.00	1.45	1.36
1	A	199	LEU	CG-CD2	-6.00	1.29	1.51
2	X	717	LYS	CB-CG	5.99	1.68	1.52
2	Y	791	GLU	CD-OE1	5.98	1.32	1.25
2	Y	730	PHE	CE1-CZ	-5.96	1.26	1.37
1	C	153	ARG	CG-CD	5.95	1.66	1.51
1	B	91	GLU	CD-OE2	5.94	1.32	1.25
2	X	773	GLN	CG-CD	5.90	1.64	1.51
1	B	106	PHE	CD1-CE1	5.89	1.51	1.39
1	D	163	GLU	CB-CG	5.89	1.63	1.52
2	Y	757	GLU	CG-CD	5.89	1.60	1.51
2	X	759	ASP	CB-CG	-5.88	1.39	1.51
1	B	179	ARG	CB-CG	-5.86	1.36	1.52
2	Y	747	CYS	N-CA	-5.86	1.34	1.46
1	C	188	LYS	CD-CE	5.85	1.65	1.51
1	A	170	GLU	CB-CG	5.84	1.63	1.52
2	X	757	GLU	CD-OE2	5.84	1.32	1.25
1	C	187	LYS	CE-NZ	5.84	1.63	1.49
1	A	20	LEU	CG-CD1	5.84	1.73	1.51
2	Y	815	ARG	CZ-NH1	5.84	1.40	1.33
1	C	105	SER	CB-OG	-5.83	1.34	1.42
1	C	63	LYS	C-O	-5.81	1.12	1.23
2	X	664	PHE	CE2-CZ	5.81	1.48	1.37
2	Y	716	ASN	N-CA	-5.81	1.34	1.46
2	X	679	GLU	CG-CD	5.80	1.60	1.51
2	X	691	GLN	CB-CG	5.80	1.68	1.52
1	A	9	HIS	CE1-NE2	5.80	1.46	1.32
1	B	150	ARG	CZ-NH1	5.79	1.40	1.33
2	X	659	PHE	CB-CG	-5.76	1.41	1.51
2	X	905	GLU	CB-CG	5.76	1.63	1.52
1	A	142	GLU	CG-CD	5.74	1.60	1.51
2	Y	721	VAL	CB-CG2	-5.73	1.40	1.52
1	C	142	GLU	CG-CD	5.73	1.60	1.51
2	X	840	ILE	CG1-CD1	-5.73	1.10	1.50
2	X	842	ALA	N-CA	5.73	1.57	1.46
2	X	803	TYR	CG-CD1	5.72	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	LEU	CG-CD2	5.71	1.73	1.51
2	X	817	THR	N-CA	5.70	1.57	1.46
1	B	150	ARG	CZ-NH2	5.70	1.40	1.33
1	D	148	ASN	CB-CG	-5.68	1.38	1.51
1	B	49	GLU	CG-CD	5.66	1.60	1.51
1	A	180	PHE	C-O	-5.65	1.12	1.23
2	Y	757	GLU	CB-CG	5.64	1.62	1.52
1	C	191	ILE	N-CA	5.64	1.57	1.46
2	X	757	GLU	CB-CG	5.64	1.62	1.52
1	C	187	LYS	CD-CE	5.63	1.65	1.51
2	Y	902	GLU	CB-CG	-5.63	1.41	1.52
2	X	823	TYR	CB-CG	-5.61	1.43	1.51
1	B	177	TYR	CG-CD1	5.60	1.46	1.39
1	C	86	PHE	CE1-CZ	5.60	1.48	1.37
1	C	180	PHE	CG-CD2	5.60	1.47	1.38
2	X	864	ILE	N-CA	-5.58	1.35	1.46
1	B	191	ILE	C-O	-5.58	1.12	1.23
1	B	190	LYS	CG-CD	5.58	1.71	1.52
2	X	784	SER	C-O	5.56	1.33	1.23
2	Y	800	GLU	CB-CG	5.55	1.62	1.52
2	Y	662	VAL	CA-CB	5.55	1.66	1.54
1	C	104	VAL	CB-CG1	-5.54	1.41	1.52
2	Y	715	SER	CA-CB	-5.53	1.44	1.52
2	Y	794	SER	CB-OG	-5.53	1.35	1.42
2	X	777	VAL	CA-CB	5.53	1.66	1.54
2	X	859	GLY	C-O	-5.52	1.14	1.23
2	X	785	ASN	CB-CG	-5.50	1.38	1.51
1	D	4	LYS	CE-NZ	5.49	1.62	1.49
2	X	800	GLU	CD-OE1	5.49	1.31	1.25
1	B	117	GLU	CD-OE2	-5.49	1.19	1.25
2	X	909	TYR	CG-CD1	-5.48	1.32	1.39
2	Y	679	GLU	CB-CG	5.45	1.62	1.52
1	B	177	TYR	CE2-CZ	5.44	1.45	1.38
2	X	887	LYS	CD-CE	5.44	1.64	1.51
2	X	693	PRO	CA-C	-5.43	1.42	1.52
2	Y	739	GLN	CD-NE2	5.42	1.46	1.32
1	A	9	HIS	CG-CD2	5.42	1.45	1.35
1	A	162	PHE	CD1-CE1	5.42	1.50	1.39
2	X	819	TYR	CD2-CE2	5.40	1.47	1.39
1	C	146	LYS	CD-CE	5.39	1.64	1.51
1	A	146	LYS	CD-CE	5.39	1.64	1.51
1	A	201	ALA	CA-CB	5.39	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	153	ARG	CZ-NH1	-5.38	1.26	1.33
1	D	106	PHE	CE2-CZ	5.37	1.47	1.37
2	Y	837	ARG	CZ-NH2	5.37	1.40	1.33
2	Y	897	SER	CA-CB	-5.36	1.45	1.52
2	X	721	VAL	C-O	5.36	1.33	1.23
1	A	145	GLN	CB-CG	-5.36	1.38	1.52
2	X	844	GLU	CD-OE2	-5.34	1.19	1.25
2	Y	688	TYR	CD2-CE2	5.34	1.47	1.39
2	Y	906	GLU	CB-CG	-5.33	1.42	1.52
1	C	157	ASP	CB-CG	-5.32	1.40	1.51
1	A	179	ARG	CD-NE	-5.32	1.37	1.46
1	B	184	LEU	N-CA	5.31	1.56	1.46
2	Y	861	SER	C-O	-5.31	1.13	1.23
1	D	183	VAL	CA-CB	-5.30	1.43	1.54
1	C	191	ILE	CB-CG2	-5.30	1.36	1.52
2	Y	685	PHE	CE2-CZ	5.28	1.47	1.37
2	Y	688	TYR	CE2-CZ	5.28	1.45	1.38
2	X	909	TYR	CE1-CZ	-5.27	1.31	1.38
1	D	116	VAL	CA-CB	5.27	1.65	1.54
2	X	762	GLY	N-CA	-5.26	1.38	1.46
1	A	162	PHE	CE1-CZ	5.25	1.47	1.37
1	A	145	GLN	CG-CD	-5.25	1.39	1.51
2	Y	741	ARG	C-O	5.25	1.33	1.23
1	A	37	THR	CA-CB	5.24	1.67	1.53
1	A	174	THR	CB-CG2	-5.24	1.35	1.52
1	C	177	TYR	CG-CD2	5.23	1.46	1.39
1	A	160	GLY	N-CA	-5.23	1.38	1.46
1	A	196	ASN	CG-OD1	-5.22	1.12	1.24
1	A	28	LEU	CG-CD2	-5.21	1.32	1.51
2	X	820	LEU	N-CA	-5.21	1.35	1.46
1	B	165	CYS	N-CA	5.21	1.56	1.46
1	D	163	GLU	CD-OE1	-5.21	1.20	1.25
2	X	693	PRO	C-O	-5.20	1.12	1.23
1	A	177	TYR	CG-CD2	5.20	1.46	1.39
2	Y	731	LYS	C-O	-5.19	1.13	1.23
1	B	91	GLU	CG-CD	5.19	1.59	1.51
1	A	189	THR	N-CA	5.19	1.56	1.46
2	X	878	PHE	CE2-CZ	5.18	1.47	1.37
2	Y	810	LEU	CG-CD2	5.18	1.71	1.51
2	X	856	LEU	CG-CD1	-5.16	1.32	1.51
1	A	170	GLU	CD-OE2	5.16	1.31	1.25
1	B	176	LEU	CA-CB	-5.16	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	8	ILE	CB-CG1	5.16	1.68	1.54
1	B	184	LEU	CG-CD1	-5.16	1.32	1.51
1	B	160	GLY	C-O	-5.15	1.15	1.23
2	X	779	SER	C-O	-5.15	1.13	1.23
1	B	167	SER	CA-CB	-5.14	1.45	1.52
2	X	800	GLU	N-CA	5.13	1.56	1.46
1	B	49	GLU	CB-CG	5.13	1.61	1.52
1	A	164	LYS	CE-NZ	-5.13	1.36	1.49
1	D	177	TYR	CE2-CZ	-5.13	1.31	1.38
1	C	141	ASN	CG-OD1	-5.13	1.12	1.24
2	X	801	TYR	CE1-CZ	5.13	1.45	1.38
1	B	161	ARG	CG-CD	-5.12	1.39	1.51
1	C	9	HIS	CE1-NE2	5.12	1.44	1.32
2	X	662	VAL	CB-CG1	-5.12	1.42	1.52
2	X	667	MET	C-O	-5.10	1.13	1.23
1	C	97	PHE	CE2-CZ	5.09	1.47	1.37
2	X	844	GLU	CB-CG	5.08	1.61	1.52
2	Y	714	LEU	CG-CD1	5.08	1.70	1.51
1	C	20	LEU	CG-CD1	5.07	1.70	1.51
1	C	162	PHE	CG-CD1	5.07	1.46	1.38
2	X	697	THR	N-CA	-5.07	1.36	1.46
2	X	755	ALA	CA-CB	5.06	1.63	1.52
2	X	775	LYS	CD-CE	5.05	1.63	1.51
2	Y	765	TYR	CG-CD2	5.05	1.45	1.39
2	X	775	LYS	N-CA	-5.04	1.36	1.46
2	X	897	SER	C-O	5.04	1.32	1.23
1	C	178	LYS	C-O	-5.03	1.13	1.23
2	X	739	GLN	CG-CD	5.03	1.62	1.51
1	C	37	THR	CA-CB	5.03	1.66	1.53
2	Y	894	VAL	CA-CB	5.03	1.65	1.54
1	D	198	LEU	CG-CD2	-5.01	1.33	1.51
2	X	707	ILE	CA-CB	5.01	1.66	1.54
1	A	182	LEU	N-CA	5.00	1.56	1.46
2	X	907	ASN	CG-ND2	5.00	1.45	1.32

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	179	ARG	NE-CZ-NH2	17.97	129.28	120.30
1	D	179	ARG	NE-CZ-NH1	-16.36	112.12	120.30
1	C	147	GLU	OE1-CD-OE2	-13.46	107.15	123.30
1	A	154	ASP	CB-CG-OD1	13.08	130.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	837	ARG	NE-CZ-NH2	-13.07	113.77	120.30
1	C	154	ASP	CB-CG-OD2	12.96	129.97	118.30
2	X	879	ARG	NE-CZ-NH2	12.58	126.59	120.30
2	X	741	ARG	NE-CZ-NH1	12.29	126.44	120.30
1	C	179	ARG	NE-CZ-NH2	11.97	126.29	120.30
1	C	175	ASP	CB-CG-OD2	-11.90	107.59	118.30
1	A	163	GLU	OE1-CD-OE2	-11.20	109.86	123.30
1	A	103	ASP	CB-CG-OD1	11.02	128.21	118.30
2	X	806	ASP	CB-CG-OD2	10.67	127.91	118.30
2	X	741	ARG	NE-CZ-NH2	-10.62	114.99	120.30
1	B	175	ASP	CB-CG-OD1	10.22	127.50	118.30
1	C	22	VAL	CG1-CB-CG2	-10.16	94.64	110.90
2	X	812	MET	CG-SD-CE	-9.93	84.31	100.20
1	A	147	GLU	OE1-CD-OE2	-9.80	111.54	123.30
1	D	26	LYS	CB-CA-C	-9.77	90.85	110.40
2	Y	661	ASP	CB-CG-OD2	-9.76	109.51	118.30
2	X	763	ASP	CB-CG-OD1	9.68	127.02	118.30
2	X	784	SER	CB-CA-C	9.67	128.48	110.10
1	B	179	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	A	124	ARG	NE-CZ-NH1	9.62	125.11	120.30
2	Y	792	MET	CG-SD-CE	9.59	115.54	100.20
2	X	719	ASP	N-CA-CB	-9.52	93.46	110.60
2	Y	661	ASP	CB-CG-OD1	9.48	126.84	118.30
2	X	759	ASP	CB-CA-C	-9.38	91.63	110.40
1	B	177	TYR	CD1-CE1-CZ	-9.38	111.36	119.80
1	A	150	ARG	NE-CZ-NH2	9.04	124.82	120.30
2	X	719	ASP	CB-CA-C	8.89	128.17	110.40
2	X	719	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	D	117	GLU	N-CA-CB	-8.75	94.85	110.60
2	Y	696	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	192	ARG	NE-CZ-NH2	-8.67	115.96	120.30
2	X	814	ARG	CB-CA-C	-8.65	93.11	110.40
1	D	148	ASN	CB-CA-C	8.51	127.42	110.40
2	X	667	MET	CG-SD-CE	-8.48	86.63	100.20
2	Y	726	LEU	CB-CG-CD2	8.45	125.36	111.00
1	C	163	GLU	OE1-CD-OE2	-8.43	113.19	123.30
1	C	157	ASP	CB-CG-OD2	-8.43	110.72	118.30
1	C	158	VAL	CA-CB-CG2	-8.38	98.33	110.90
1	D	190	LYS	CD-CE-NZ	8.34	130.88	111.70
2	X	837	ARG	NE-CZ-NH1	8.27	124.44	120.30
2	X	853	VAL	CA-CB-CG1	8.22	123.23	110.90
1	C	153	ARG	NE-CZ-NH1	8.18	124.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	741	ARG	CG-CD-NE	8.16	128.93	111.80
1	D	174	THR	OG1-CB-CG2	-8.14	91.28	110.00
1	C	124	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	179	ARG	NH1-CZ-NH2	-8.06	110.53	119.40
2	Y	792	MET	CA-CB-CG	-8.04	99.64	113.30
1	B	26	LYS	CB-CA-C	-7.96	94.47	110.40
2	Y	774	LEU	CB-CG-CD2	7.91	124.45	111.00
2	X	841	LYS	CD-CE-NZ	-7.89	93.56	111.70
1	D	179	ARG	NE-CZ-NH2	7.79	124.19	120.30
2	X	661	ASP	CB-CG-OD1	-7.71	111.36	118.30
1	B	184	LEU	CB-CG-CD2	7.71	124.10	111.00
1	A	22	VAL	CG1-CB-CG2	-7.69	98.59	110.90
2	X	880	ARG	NE-CZ-NH1	7.69	124.15	120.30
2	Y	806	ASP	CB-CG-OD1	7.65	125.18	118.30
1	C	179	ARG	NH1-CZ-NH2	-7.64	111.00	119.40
2	Y	716	ASN	N-CA-CB	-7.63	96.87	110.60
1	C	175	ASP	CB-CG-OD1	7.60	125.14	118.30
1	D	59	MET	CG-SD-CE	7.60	112.36	100.20
2	Y	902	GLU	OE1-CD-OE2	7.54	132.35	123.30
1	A	175	ASP	CB-CG-OD2	-7.54	111.51	118.30
2	X	911	ILE	CB-CA-C	7.54	126.68	111.60
1	A	61	MET	CG-SD-CE	7.53	112.25	100.20
2	Y	829	LEU	CA-CB-CG	-7.51	98.02	115.30
1	A	107	ARG	NE-CZ-NH1	-7.43	116.58	120.30
2	X	681	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	169	LYS	CD-CE-NZ	7.40	128.73	111.70
1	C	63	LYS	O-C-N	-7.33	110.74	123.20
1	A	153	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	153	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	B	157	ASP	CB-CG-OD2	7.27	124.85	118.30
1	D	4	LYS	CD-CE-NZ	-7.23	95.07	111.70
1	B	157	ASP	CB-CG-OD1	-7.21	111.81	118.30
2	X	784	SER	C-N-CA	-7.20	103.69	121.70
2	X	764	SER	CA-CB-OG	-7.13	91.95	111.20
1	C	174	THR	OG1-CB-CG2	-7.12	93.62	110.00
2	X	843	LEU	CB-CG-CD1	7.10	123.07	111.00
2	X	911	ILE	CB-CG1-CD1	-7.10	94.02	113.90
2	X	845	LEU	CB-CG-CD2	7.07	123.02	111.00
2	X	905	GLU	OE1-CD-OE2	7.06	131.77	123.30
1	A	157	ASP	CB-CG-OD2	-7.03	111.97	118.30
2	Y	681	ARG	NE-CZ-NH2	-7.02	116.79	120.30
2	Y	743	MET	CG-SD-CE	-7.01	88.98	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	62	GLU	CA-CB-CG	6.99	128.77	113.40
1	D	148	ASN	CB-CG-OD1	-6.96	107.67	121.60
1	A	154	ASP	OD1-CG-OD2	-6.96	110.08	123.30
2	X	782	LYS	N-CA-C	6.94	129.73	111.00
2	Y	761	TYR	C-N-CA	-6.93	107.74	122.30
2	X	814	ARG	N-CA-CB	6.92	123.06	110.60
2	X	744	ILE	CG1-CB-CG2	-6.88	96.26	111.40
1	B	172	LEU	CA-CB-CG	6.81	130.97	115.30
1	D	150	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	C	192	ARG	NE-CZ-NH2	-6.79	116.91	120.30
2	X	891	GLU	CA-CB-CG	6.78	128.32	113.40
2	X	814	ARG	NE-CZ-NH1	-6.74	116.93	120.30
2	X	829	LEU	CB-CG-CD2	6.69	122.38	111.00
2	Y	896	ASP	CB-CG-OD2	-6.68	112.29	118.30
2	Y	761	TYR	N-CA-C	-6.66	93.02	111.00
1	D	163	GLU	CG-CD-OE2	6.65	131.60	118.30
2	X	911	ILE	CA-CB-CG1	6.64	123.62	111.00
1	C	34	ILE	CG1-CB-CG2	-6.63	96.81	111.40
1	C	108	LEU	CA-CB-CG	6.62	130.53	115.30
2	Y	711	ASN	CB-CA-C	6.62	123.64	110.40
2	Y	891	GLU	CA-CB-CG	6.61	127.93	113.40
2	Y	771	LEU	CB-CG-CD2	-6.59	99.80	111.00
2	Y	759	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	B	190	LYS	CD-CE-NZ	6.58	126.83	111.70
1	C	3	ARG	NE-CZ-NH1	6.55	123.58	120.30
2	Y	831	THR	CA-CB-CG2	-6.54	103.25	112.40
2	X	784	SER	CA-C-N	-6.52	102.85	117.20
2	Y	853	VAL	N-CA-CB	-6.50	97.21	111.50
2	Y	829	LEU	CB-CG-CD1	6.48	122.01	111.00
2	X	708	ARG	NE-CZ-NH2	6.45	123.52	120.30
2	X	658	ILE	CB-CA-C	-6.43	98.74	111.60
1	C	62	GLU	CB-CA-C	6.43	123.26	110.40
2	X	879	ARG	NE-CZ-NH1	-6.42	117.09	120.30
2	Y	759	ASP	CB-CA-C	-6.40	97.59	110.40
1	C	71	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	A	101	LEU	O-C-N	-6.39	112.47	122.70
1	C	62	GLU	CA-CB-CG	6.39	127.46	113.40
2	X	814	ARG	CA-CB-CG	6.33	127.34	113.40
2	Y	902	GLU	N-CA-CB	-6.33	99.20	110.60
2	Y	767	ILE	CG1-CB-CG2	-6.33	97.47	111.40
2	Y	741	ARG	CD-NE-CZ	-6.32	114.75	123.60
2	X	844	GLU	OE1-CD-OE2	-6.29	115.75	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	153	ARG	NE-CZ-NH2	6.27	123.44	120.30
1	C	104	VAL	CG1-CB-CG2	-6.27	100.87	110.90
2	X	681	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	C	153	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	Y	759	ASP	N-CA-CB	-6.22	99.40	110.60
2	X	812	MET	CA-CB-CG	6.21	123.86	113.30
1	A	175	ASP	N-CA-CB	-6.11	99.60	110.60
2	X	868	ASP	CB-CG-OD1	6.09	123.78	118.30
2	Y	828	ASP	CB-CG-OD2	6.08	123.77	118.30
2	Y	658	ILE	CG1-CB-CG2	-6.07	98.05	111.40
2	X	785	ASN	N-CA-C	-6.06	94.65	111.00
2	X	904	GLN	N-CA-C	-6.04	94.69	111.00
1	B	193	SER	CB-CA-C	-6.04	98.63	110.10
2	Y	696	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	149	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	D	130	CYS	CA-CB-SG	-5.98	103.24	114.00
1	D	179	ARG	CG-CD-NE	-5.98	99.24	111.80
1	C	63	LYS	CA-C-N	5.97	128.15	116.20
2	X	774	LEU	CB-CG-CD2	5.97	121.16	111.00
2	X	828	ASP	CB-CG-OD1	5.96	123.67	118.30
1	A	34	ILE	CG1-CB-CG2	-5.95	98.31	111.40
2	X	838	LEU	CA-CB-CG	5.93	128.94	115.30
1	A	173	GLU	CG-CD-OE1	5.92	130.14	118.30
2	Y	741	ARG	CB-CA-C	-5.89	98.63	110.40
2	Y	739	GLN	N-CA-C	-5.88	95.12	111.00
2	X	810	LEU	CB-CG-CD1	5.86	120.97	111.00
1	D	154	ASP	CB-CG-OD2	5.85	123.57	118.30
2	X	840	ILE	CA-CB-CG1	-5.84	99.91	111.00
2	Y	770	ASP	CB-CG-OD2	5.83	123.55	118.30
1	C	152	LEU	CB-CG-CD2	-5.81	101.12	111.00
2	Y	759	ASP	N-CA-C	-5.81	95.31	111.00
1	A	158	VAL	CA-CB-CG2	-5.79	102.22	110.90
2	Y	758	TYR	C-N-CA	5.79	136.17	121.70
2	X	770	ASP	CB-CA-C	-5.78	98.83	110.40
1	B	177	TYR	CZ-CE2-CD2	5.78	125.00	119.80
2	Y	868	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	150	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	172	LEU	CB-CG-CD2	5.71	120.71	111.00
1	D	149	GLU	OE1-CD-OE2	-5.71	116.45	123.30
2	X	719	ASP	N-CA-C	-5.70	95.61	111.00
1	A	28	LEU	CD1-CG-CD2	-5.69	93.42	110.50
2	X	773	GLN	CB-CA-C	5.69	121.78	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	199	LEU	CD1-CG-CD2	-5.68	93.46	110.50
2	Y	768	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	C	154	ASP	OD1-CG-OD2	-5.67	112.52	123.30
2	X	814	ARG	CG-CD-NE	-5.66	99.91	111.80
1	A	124	ARG	CD-NE-CZ	5.65	131.51	123.60
1	B	180	PHE	N-CA-C	5.65	126.24	111.00
1	A	104	VAL	CG1-CB-CG2	-5.63	101.88	110.90
2	Y	696	ASP	CB-CA-C	-5.62	99.15	110.40
2	X	767	ILE	CG1-CB-CG2	-5.62	99.03	111.40
1	D	136	GLU	CA-CB-CG	5.61	125.74	113.40
1	B	161	ARG	CB-CG-CD	-5.60	97.04	111.60
1	A	192	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	39	GLY	C-N-CA	5.57	135.63	121.70
2	X	787	GLN	N-CA-C	5.57	126.05	111.00
1	D	8	ILE	CB-CG1-CD1	-5.56	98.34	113.90
1	D	91	GLU	CG-CD-OE2	-5.55	107.20	118.30
1	A	63	LYS	CA-C-N	5.54	127.29	116.20
1	A	190	LYS	N-CA-CB	-5.54	100.62	110.60
2	Y	798	ASP	CB-CG-OD1	5.54	123.29	118.30
2	Y	714	LEU	N-CA-C	-5.52	96.09	111.00
1	A	200	ASN	CB-CA-C	5.52	121.44	110.40
2	Y	821	ASP	CB-CG-OD2	5.51	123.26	118.30
2	Y	891	GLU	CB-CA-C	-5.51	99.39	110.40
1	D	3	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	108	LEU	CA-CB-CG	5.50	127.94	115.30
1	C	147	GLU	CG-CD-OE1	5.49	129.28	118.30
1	C	15	SER	CB-CA-C	5.47	120.50	110.10
1	B	199	LEU	CB-CG-CD1	5.43	120.22	111.00
1	C	200	ASN	C-N-CA	-5.43	108.13	121.70
1	C	200	ASN	O-C-N	-5.42	114.03	122.70
1	D	159	GLN	CG-CD-OE1	-5.40	110.80	121.60
2	X	661	ASP	CB-CG-OD2	5.39	123.16	118.30
2	Y	911	ILE	N-CA-C	5.37	125.49	111.00
1	A	124	ARG	CG-CD-NE	5.34	123.02	111.80
2	X	820	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	A	161	ARG	NE-CZ-NH1	-5.31	117.65	120.30
2	X	764	SER	CB-CA-C	-5.28	100.07	110.10
2	Y	871	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	D	136	GLU	CB-CA-C	-5.27	99.87	110.40
1	C	63	LYS	C-N-CA	-5.27	111.24	122.30
1	D	157	ASP	CB-CG-OD1	-5.26	113.56	118.30
1	B	161	ARG	NE-CZ-NH1	-5.25	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	192	ARG	CG-CD-NE	5.25	122.83	111.80
2	X	744	ILE	CB-CA-C	5.23	122.06	111.60
1	B	82	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	161	ARG	CG-CD-NE	5.23	122.78	111.80
2	X	761	TYR	N-CA-C	-5.22	96.90	111.00
2	X	785	ASN	CA-C-N	-5.21	105.73	117.20
2	X	812	MET	N-CA-CB	-5.21	101.21	110.60
2	X	739	GLN	N-CA-C	-5.21	96.93	111.00
2	X	904	GLN	C-N-CA	-5.20	108.69	121.70
2	Y	759	ASP	CB-CG-OD1	5.19	122.97	118.30
2	Y	709	VAL	CG1-CB-CG2	5.18	119.19	110.90
1	C	192	ARG	NE-CZ-NH1	5.18	122.89	120.30
2	Y	671	ASP	CB-CG-OD2	5.17	122.95	118.30
2	X	808	SER	CA-CB-OG	-5.17	97.24	111.20
1	C	103	ASP	CB-CG-OD2	5.16	122.95	118.30
2	X	781	ILE	CB-CA-C	5.16	121.93	111.60
2	Y	904	GLN	C-N-CA	-5.16	108.80	121.70
1	C	126	LEU	CA-CB-CG	5.16	127.16	115.30
1	C	61	MET	CG-SD-CE	5.15	108.44	100.20
1	D	159	GLN	CA-CB-CG	5.15	124.73	113.40
1	C	197	LYS	CD-CE-NZ	5.14	123.52	111.70
1	B	152	LEU	CB-CG-CD2	-5.13	102.28	111.00
1	B	177	TYR	OH-CZ-CE2	-5.12	106.27	120.10
2	X	758	TYR	C-N-CA	5.12	134.50	121.70
2	X	727	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	174	THR	OG1-CB-CG2	-5.10	98.26	110.00
2	X	903	LEU	CB-CG-CD1	-5.10	102.33	111.00
2	Y	779	SER	CB-CA-C	5.09	119.77	110.10
1	C	71	ARG	NE-CZ-NH2	5.07	122.83	120.30
2	X	714	LEU	CA-CB-CG	5.05	126.91	115.30
2	Y	871	ARG	NE-CZ-NH2	5.05	122.82	120.30
2	X	799	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	B	199	LEU	CB-CG-CD2	-5.04	102.43	111.00
1	C	1	MET	CA-CB-CG	-5.04	104.73	113.30
1	A	59	MET	CG-SD-CE	5.04	108.26	100.20
2	Y	874	ASP	N-CA-CB	-5.02	101.56	110.60
1	B	134	THR	OG1-CB-CG2	-5.01	98.47	110.00
1	C	200	ASN	CA-C-N	5.01	128.22	117.20
2	X	852	VAL	CG1-CB-CG2	5.00	118.91	110.90
2	Y	830	SER	N-CA-CB	5.00	118.00	110.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	X	911	ILE	CA

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	GLU	Peptide
1	A	26	LYS	Peptide
1	A	39	GLY	Peptide
1	B	82	ASP	Peptide
1	B	83	VAL	Peptide
1	C	127	ILE	Peptide
1	C	25	GLU	Peptide
1	C	26	LYS	Peptide
1	D	60	GLU	Peptide
2	X	668	SER	Peptide
2	X	669	GLY	Peptide
2	X	673	GLN	Peptide
2	X	701	ILE	Peptide
2	X	746	MET	Peptide
2	X	759	ASP	Mainchain
2	X	781	ILE	Peptide
2	X	783	ASN	Peptide
2	X	784	SER	Peptide
2	X	785	ASN	Peptide
2	X	813	PHE	Sidechain
2	X	884	ARG	Peptide
2	X	905	GLU	Peptide
2	X	910	LEU	Peptide
2	Y	668	SER	Peptide
2	Y	670	THR	Peptide
2	Y	671	ASP	Peptide
2	Y	713	ILE	Peptide
2	Y	714	LEU	Peptide
2	Y	817	THR	Peptide
2	Y	830	SER	Peptide
2	Y	833	ASN	Peptide
2	Y	859	GLY	Peptide
2	Y	881	THR	Peptide
2	Y	903	LEU	Peptide
2	Y	905	GLU	Peptide

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	1631	0	1617	89	0
1	B	1606	0	1593	147	0
1	C	1631	0	1617	94	0
1	D	1598	0	1589	140	0
2	X	2081	0	2036	192	0
2	Y	2095	0	2046	146	0
3	Y	2	0	0	0	0
4	A	44	0	0	3	0
4	B	25	0	0	2	0
4	C	41	0	0	4	0
4	D	29	0	0	5	0
4	X	83	0	0	3	0
4	Y	59	0	0	3	0
All	All	10925	0	10498	756	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 36.

All (756) 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)
2:X:846:ARG:CD	2:X:846:ARG:CG	1.75	1.61
1:B:82:ASP:N	1:B:83:VAL:HG23	1.09	1.36
1:A:127:ILE:HD11	1:B:127:ILE:CD1	1.65	1.27
1:B:82:ASP:N	1:B:83:VAL:CG2	1.95	1.26
1:C:40:HIS:CD2	1:D:120:ALA:HB2	1.73	1.22
1:B:119:PRO:O	1:B:123:ILE:HD12	1.37	1.22
1:D:49:GLU:HG3	1:D:49:GLU:O	1.39	1.18
1:A:127:ILE:CD1	1:B:127:ILE:HD11	1.76	1.15
2:X:673:GLN:N	2:X:674:PRO:HD3	1.47	1.13
2:X:717:LYS:HG2	2:X:718:HIS:CE1	1.84	1.12
1:C:44:THR:HG22	1:C:45:GLY:H	0.96	1.12
2:X:719:ASP:HB2	2:X:747:CYS:HB3	1.30	1.12
2:Y:671:ASP:HB2	2:Y:672:SER:HB2	1.30	1.12
1:D:192:ARG:HH11	1:D:192:ARG:HB2	1.12	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:673:GLN:O	2:X:673:GLN:HG2	1.52	1.10
1:C:40:HIS:HD2	1:D:120:ALA:HB2	0.96	1.09
1:A:44:THR:HG22	1:A:45:GLY:H	0.95	1.08
1:C:140:LYS:HE2	4:C:209:HOH:O	1.49	1.08
1:B:65:LYS:HG2	1:B:65:LYS:O	1.51	1.07
1:D:119:PRO:O	1:D:123:ILE:HD12	1.54	1.06
1:A:44:THR:HG22	1:A:45:GLY:N	1.71	1.04
1:A:104:VAL:HG23	1:A:106:PHE:CE1	1.92	1.04
1:A:44:THR:CG2	1:A:45:GLY:H	1.69	1.03
1:C:123:ILE:O	1:C:127:ILE:HG23	1.56	1.03
2:X:663:GLU:OE1	2:X:697:THR:HG22	1.58	1.03
1:C:40:HIS:HD2	1:D:120:ALA:CB	1.72	1.02
2:Y:878:PHE:CE1	2:Y:882:PHE:HE2	1.78	1.02
2:X:719:ASP:OD1	2:X:750:THR:HG21	1.58	1.02
1:A:127:ILE:HG12	1:B:127:ILE:HG12	1.41	1.02
1:D:192:ARG:HH11	1:D:192:ARG:CB	1.73	1.02
2:Y:905:GLU:HB3	4:Y:117:HOH:O	1.57	1.02
2:Y:732:THR:CG2	2:Y:734:SER:HB3	1.90	1.01
2:Y:732:THR:HG22	2:Y:734:SER:HB3	1.41	1.01
1:D:197:LYS:HE3	4:D:269:HOH:O	1.60	1.01
1:C:44:THR:HG22	1:C:45:GLY:N	1.75	1.01
1:C:44:THR:CG2	1:C:45:GLY:H	1.73	1.00
1:D:107:ARG:HD3	1:D:108:LEU:H	1.26	1.00
2:X:702:ALA:HB3	2:X:744:ILE:HD11	1.44	1.00
1:B:86:PHE:C	1:B:87:ASN:HD22	1.64	1.00
1:D:92:SER:O	1:D:93:CYS:HB2	1.61	0.99
2:X:711:ASN:HD22	2:X:711:ASN:C	1.65	0.99
2:X:836:THR:HG22	2:X:838:LEU:H	1.28	0.98
2:X:785:ASN:C	2:X:787:GLN:H	1.64	0.97
2:Y:660:GLU:HA	2:Y:686:GLY:O	1.65	0.97
2:X:679:GLU:HB3	2:X:689:ILE:HD13	1.48	0.95
2:X:759:ASP:HB3	2:X:761:TYR:H	1.32	0.95
2:X:667:MET:HE3	2:X:709:VAL:HG22	1.47	0.94
2:X:673:GLN:N	2:X:674:PRO:CD	2.30	0.94
2:Y:759:ASP:HB3	2:Y:761:TYR:O	1.67	0.94
1:B:130:CYS:O	1:B:134:THR:HG22	1.68	0.93
1:D:86:PHE:C	1:D:87:ASN:HD22	1.72	0.93
2:X:812:MET:CE	2:X:897:SER:HB3	1.98	0.93
1:B:83:VAL:HG11	1:B:100:ASN:O	1.67	0.92
1:B:107:ARG:HD3	1:B:108:LEU:H	1.35	0.92
2:X:739:GLN:HE22	2:X:741:ARG:HH21	1.07	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:660:GLU:HA	2:X:686:GLY:O	1.69	0.91
1:D:59:MET:O	1:D:60:GLU:HB2	1.69	0.90
1:C:120:ALA:HB2	1:D:40:HIS:HB2	1.54	0.90
1:B:20:LEU:HD11	1:B:34:ILE:HD11	1.54	0.89
1:B:83:VAL:CG1	1:B:100:ASN:O	2.21	0.89
2:X:910:LEU:C	2:X:911:ILE:HG23	1.90	0.89
2:X:658:ILE:CG2	2:X:735:PHE:HB2	2.04	0.88
1:B:16:ILE:CG2	1:B:17:THR:N	2.37	0.87
1:B:16:ILE:HG23	1:B:17:THR:H	1.40	0.86
1:D:20:LEU:HD11	1:D:34:ILE:HD11	1.57	0.86
2:Y:878:PHE:CE1	2:Y:882:PHE:CE2	2.64	0.85
2:Y:728:GLU:O	2:Y:732:THR:HB	1.77	0.85
2:Y:732:THR:CG2	2:Y:734:SER:CB	2.55	0.85
2:X:711:ASN:ND2	2:X:711:ASN:C	2.28	0.85
1:D:88:PHE:HB2	1:D:95:PHE:HD2	1.40	0.85
2:Y:654:LYS:HG3	2:Y:655:ILE:H	1.40	0.85
1:D:16:ILE:HG23	1:D:17:THR:N	1.92	0.85
2:Y:878:PHE:HE1	2:Y:882:PHE:HE2	1.21	0.84
1:C:124:ARG:HH11	1:C:124:ARG:HG3	1.41	0.84
2:Y:819:TYR:O	2:Y:863:VAL:HA	1.77	0.84
2:X:785:ASN:C	2:X:787:GLN:N	2.30	0.84
1:C:131:LEU:HD21	1:D:5:ILE:HG22	1.57	0.84
1:A:24:TRP:CD1	1:A:27:THR:O	2.31	0.84
2:Y:732:THR:HG22	2:Y:734:SER:CB	2.06	0.83
2:Y:904:GLN:O	2:Y:905:GLU:HG3	1.79	0.83
1:A:118:ASN:O	1:A:118:ASN:ND2	2.10	0.83
2:X:739:GLN:NE2	2:X:741:ARG:HH21	1.75	0.83
1:D:192:ARG:NH1	1:D:192:ARG:HB2	1.93	0.83
1:C:118:ASN:O	1:C:118:ASN:ND2	2.10	0.83
2:X:846:ARG:HG3	2:X:852:VAL:HG13	1.60	0.83
2:X:670:THR:HA	2:X:675:LYS:H	1.44	0.82
1:B:92:SER:O	1:B:93:CYS:HB2	1.78	0.82
1:D:63:LYS:O	1:D:67:VAL:HB	1.80	0.82
1:B:89:SER:HB3	1:B:91:GLU:OE1	1.78	0.82
2:X:792:MET:HE2	2:X:795:LEU:HD12	1.60	0.82
2:X:706:ASN:ND2	2:X:709:VAL:HG23	1.95	0.82
2:Y:820:LEU:HD13	2:Y:864:ILE:HB	1.61	0.82
1:A:22:VAL:HG12	1:A:34:ILE:HG12	1.62	0.81
2:X:910:LEU:C	2:X:911:ILE:CG2	2.47	0.81
1:A:24:TRP:HD1	1:A:27:THR:O	1.63	0.81
1:D:170:GLU:O	1:D:174:THR:HG22	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:GLU:CG	1:D:49:GLU:O	2.24	0.81
2:X:722:LYS:HE2	2:X:741:ARG:O	1.80	0.81
2:X:780:GLY:O	2:X:781:ILE:CG1	2.29	0.81
1:D:116:VAL:HG12	1:D:117:GLU:H	1.44	0.80
1:D:65:LYS:O	1:D:69:GLU:CG	2.29	0.80
1:C:104:VAL:HG23	1:C:106:PHE:CE1	2.16	0.80
2:X:910:LEU:HB3	2:X:911:ILE:HG23	1.61	0.80
2:Y:889:LEU:HD21	2:Y:906:GLU:HB2	1.63	0.80
1:A:88:PHE:CE1	1:A:113:LEU:HD12	2.17	0.80
1:B:116:VAL:HG12	1:B:117:GLU:H	1.47	0.79
1:C:120:ALA:CB	1:D:40:HIS:HB2	2.12	0.79
1:D:186:GLU:HG3	2:Y:759:ASP:OD2	1.81	0.79
1:C:128:CYS:SG	1:D:19:PHE:HZ	2.05	0.79
1:C:26:LYS:O	1:C:26:LYS:HG2	1.81	0.79
2:X:910:LEU:HB3	2:X:911:ILE:CG2	2.12	0.79
1:C:28:LEU:HD13	1:C:75:LEU:HD11	1.65	0.79
2:Y:706:ASN:O	2:Y:710:LYS:HD3	1.83	0.78
2:Y:710:LYS:HD2	2:Y:710:LYS:N	1.99	0.78
2:X:786:GLU:O	2:X:787:GLN:HG3	1.84	0.78
1:B:83:VAL:HG12	1:B:83:VAL:O	1.82	0.78
2:X:660:GLU:O	2:X:661:ASP:HB2	1.82	0.78
2:X:846:ARG:HG3	2:X:852:VAL:CG1	2.14	0.77
1:B:83:VAL:HG13	1:B:100:ASN:HB2	1.66	0.77
2:Y:787:GLN:HB3	2:Y:792:MET:HG3	1.66	0.77
2:Y:878:PHE:HE1	2:Y:882:PHE:CE2	1.99	0.77
1:B:4:LYS:HD2	1:B:75:LEU:HB3	1.67	0.77
1:C:127:ILE:CG1	1:C:127:ILE:O	2.30	0.76
1:D:89:SER:HB3	1:D:91:GLU:OE1	1.86	0.76
2:X:846:ARG:CD	2:X:846:ARG:CB	2.63	0.76
2:Y:705:GLU:HG3	2:Y:710:LYS:HE2	1.68	0.76
1:B:88:PHE:HB2	1:B:95:PHE:HD2	1.50	0.76
2:Y:706:ASN:ND2	2:Y:709:VAL:HG23	2.01	0.76
1:A:44:THR:O	1:A:113:LEU:HA	1.86	0.75
1:D:16:ILE:CG2	1:D:17:THR:N	2.49	0.75
1:B:16:ILE:CG2	1:B:17:THR:H	1.97	0.75
1:A:104:VAL:HG23	1:A:106:PHE:CZ	2.22	0.75
2:X:667:MET:CE	2:X:709:VAL:HG22	2.16	0.75
2:X:823:TYR:CE2	2:X:832:LYS:HG2	2.22	0.75
1:A:34:ILE:O	1:A:34:ILE:CG2	2.34	0.75
2:X:658:ILE:HG22	2:X:735:PHE:HB2	1.66	0.74
2:Y:654:LYS:HG3	2:Y:655:ILE:N	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:862:HIS:HD2	2:Y:889:LEU:CD1	2.00	0.74
2:X:782:LYS:HG3	2:X:783:ASN:H	1.52	0.74
1:D:65:LYS:O	1:D:69:GLU:HB2	1.88	0.74
2:X:706:ASN:C	2:X:706:ASN:HD22	1.90	0.74
2:X:792:MET:HA	2:X:792:MET:HE2	1.69	0.74
1:C:44:THR:O	1:C:113:LEU:HA	1.88	0.73
2:Y:819:TYR:HH	2:Y:823:TYR:HD2	1.36	0.73
1:D:107:ARG:HD3	1:D:108:LEU:N	2.02	0.73
2:X:673:GLN:O	2:X:673:GLN:CG	2.30	0.73
1:D:87:ASN:HB2	1:D:96:PHE:CZ	2.23	0.73
2:Y:823:TYR:OH	2:Y:832:LYS:NZ	2.22	0.73
2:Y:887:LYS:HE2	2:Y:906:GLU:HG3	1.70	0.73
1:B:53:SER:HB3	1:B:63:LYS:NZ	2.04	0.73
1:D:3:ARG:HG2	1:D:4:LYS:N	2.04	0.72
1:A:198:LEU:HD21	1:B:197:LYS:HG2	1.71	0.72
1:B:87:ASN:HB2	1:B:96:PHE:CZ	2.24	0.72
1:B:16:ILE:HG22	1:B:17:THR:N	2.03	0.72
1:A:131:LEU:HD21	1:B:5:ILE:HG22	1.71	0.72
1:A:127:ILE:CG1	1:B:127:ILE:HG12	2.18	0.72
2:X:780:GLY:O	2:X:781:ILE:HG12	1.87	0.72
2:Y:671:ASP:HB2	2:Y:672:SER:CB	2.14	0.72
1:B:138:GLN:O	1:B:142:GLU:HG3	1.90	0.72
2:Y:862:HIS:HD2	2:Y:889:LEU:HD12	1.54	0.71
2:Y:876:LYS:NZ	2:Y:911:ILE:HG12	2.05	0.71
1:A:110:SER:O	1:A:111:PHE:CD2	2.43	0.71
1:B:52:ILE:CG2	1:B:53:SER:N	2.54	0.71
1:A:147:GLU:OE1	1:A:150:ARG:NH2	2.23	0.71
1:A:127:ILE:HD11	1:B:127:ILE:HD11	0.80	0.71
2:X:706:ASN:ND2	2:X:709:VAL:H	1.88	0.71
1:A:127:ILE:O	1:A:127:ILE:HG22	1.89	0.71
1:B:86:PHE:C	1:B:87:ASN:ND2	2.43	0.70
1:B:69:GLU:OE2	1:B:72:LYS:NZ	2.25	0.70
1:D:65:LYS:O	1:D:69:GLU:CB	2.39	0.70
2:Y:823:TYR:CE1	2:Y:832:LYS:NZ	2.59	0.70
2:Y:887:LYS:HD3	2:Y:910:LEU:HD21	1.73	0.70
2:X:792:MET:CE	2:X:795:LEU:HD12	2.22	0.70
2:X:667:MET:HE3	2:X:709:VAL:CG2	2.22	0.70
2:Y:828:ASP:O	2:Y:830:SER:N	2.25	0.70
2:X:879:ARG:HB2	2:X:886:PHE:CZ	2.27	0.70
1:C:124:ARG:NH1	1:D:38:ASP:O	2.25	0.69
2:Y:716:ASN:OD1	2:Y:745:HIS:HE1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:706:ASN:O	2:Y:710:LYS:CD	2.40	0.69
1:C:59:MET:HE1	1:C:108:LEU:HA	1.73	0.69
1:D:16:ILE:HG23	1:D:17:THR:H	1.55	0.69
1:B:8:ILE:HD13	1:B:20:LEU:HB2	1.75	0.69
1:D:192:ARG:NH2	4:D:212:HOH:O	2.24	0.69
1:C:131:LEU:HD21	1:D:5:ILE:CG2	2.22	0.69
1:B:134:THR:O	1:B:138:GLN:HG3	1.93	0.69
1:A:18:HIS:HD2	1:A:36:LEU:HD11	1.57	0.69
1:B:3:ARG:HG2	1:B:4:LYS:N	2.08	0.69
2:X:904:GLN:O	2:X:905:GLU:HG3	1.92	0.68
1:B:131:LEU:HA	1:B:134:THR:CG2	2.23	0.68
1:A:127:ILE:CD1	1:B:127:ILE:CG1	2.71	0.68
1:D:68:GLY:HA2	1:D:71:ARG:HG2	1.74	0.68
2:X:702:ALA:CB	2:X:744:ILE:HD11	2.22	0.68
2:Y:713:ILE:CG2	2:Y:713:ILE:O	2.41	0.68
1:A:34:ILE:O	1:A:34:ILE:HG22	1.94	0.68
1:D:177:TYR:O	1:D:181:ILE:HG12	1.93	0.68
1:B:177:TYR:O	1:B:181:ILE:HG13	1.93	0.68
2:X:711:ASN:ND2	2:X:711:ASN:O	2.27	0.68
1:C:89:SER:O	1:C:93:CYS:HA	1.93	0.68
1:C:128:CYS:SG	1:D:19:PHE:CZ	2.85	0.67
1:B:63:LYS:O	1:B:67:VAL:HB	1.95	0.67
2:X:657:ASN:HB2	2:X:660:GLU:HB2	1.75	0.67
1:D:181:ILE:HD13	2:Y:799:LEU:HD11	1.76	0.67
1:D:85:THR:HB	1:D:100:ASN:HD21	1.59	0.67
1:C:34:ILE:O	1:C:34:ILE:HG23	1.95	0.67
1:A:127:ILE:CD1	1:B:127:ILE:CD1	2.53	0.67
1:D:10:LEU:HA	1:D:86:PHE:O	1.95	0.67
1:B:107:ARG:HD3	1:B:108:LEU:N	2.08	0.66
1:D:51:GLU:HA	1:D:54:GLN:HB3	1.77	0.66
1:A:124:ARG:HH11	1:A:124:ARG:HG3	1.59	0.66
2:X:812:MET:HE1	2:X:897:SER:HB3	1.75	0.66
1:A:18:HIS:CD2	1:A:36:LEU:HD11	2.30	0.66
1:A:104:VAL:CG2	1:A:106:PHE:CZ	2.79	0.66
2:Y:707:ILE:HA	2:Y:710:LYS:HG2	1.78	0.66
1:A:44:THR:CG2	1:A:45:GLY:N	2.39	0.66
2:Y:671:ASP:CB	2:Y:672:SER:HB2	2.18	0.66
1:B:48:SER:O	1:B:52:ILE:HB	1.95	0.66
1:B:49:GLU:O	1:B:50:SER:HB2	1.96	0.66
2:X:739:GLN:HE21	2:X:741:ARG:HE	1.43	0.66
2:X:657:ASN:HA	2:X:685:PHE:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ILE:HG12	1:C:127:ILE:O	1.95	0.65
1:B:51:GLU:HA	1:B:54:GLN:HB3	1.77	0.65
1:D:73:ALA:HA	1:D:84:TYR:CD2	2.32	0.65
1:D:36:LEU:O	1:D:43:TRP:HE3	1.78	0.65
2:X:722:LYS:HB3	2:X:744:ILE:HD13	1.79	0.65
2:X:739:GLN:HE22	2:X:741:ARG:NH2	1.89	0.65
1:B:41:SER:HA	1:B:119:PRO:HB3	1.78	0.65
2:X:905:GLU:HG2	2:X:906:GLU:HG3	1.79	0.65
2:X:783:ASN:HA	2:X:784:SER:OG	1.95	0.65
2:Y:657:ASN:ND2	4:Y:92:HOH:O	2.30	0.65
2:Y:661:ASP:H	2:Y:688:TYR:HE1	1.44	0.65
1:A:127:ILE:HD11	1:B:127:ILE:CG1	2.27	0.65
1:B:52:ILE:HG23	1:B:53:SER:N	2.12	0.65
1:B:31:GLY:HA3	1:B:48:SER:HA	1.79	0.65
1:B:30:SER:O	1:B:49:GLU:HB2	1.96	0.65
1:A:34:ILE:HD12	1:A:111:PHE:CE1	2.33	0.64
1:D:192:ARG:NH1	1:D:192:ARG:CB	2.54	0.64
2:Y:732:THR:HG21	2:Y:734:SER:OG	1.97	0.64
1:A:1:MET:HA	1:A:25:GLU:HG3	1.80	0.64
1:D:56:ALA:O	1:D:61:MET:N	2.31	0.64
2:Y:878:PHE:CD1	2:Y:882:PHE:HE2	2.14	0.64
1:A:42:ALA:O	1:A:116:VAL:HB	1.98	0.64
1:D:88:PHE:HB2	1:D:95:PHE:CD2	2.29	0.64
2:X:719:ASP:HB2	2:X:747:CYS:CB	2.19	0.64
1:C:18:HIS:HD2	1:C:36:LEU:HD11	1.63	0.64
1:D:65:LYS:O	1:D:69:GLU:HG2	1.97	0.63
2:Y:904:GLN:O	2:Y:905:GLU:CG	2.47	0.63
1:D:159:GLN:O	1:D:163:GLU:HG2	1.98	0.63
1:D:92:SER:O	1:D:93:CYS:CB	2.42	0.63
2:X:706:ASN:C	2:X:706:ASN:ND2	2.51	0.63
1:C:18:HIS:CD2	1:C:36:LEU:HD11	2.33	0.63
2:X:887:LYS:NZ	2:X:906:GLU:OE1	2.24	0.63
1:D:41:SER:HA	1:D:119:PRO:HB3	1.81	0.62
1:C:119:PRO:O	1:C:123:ILE:HG13	1.97	0.62
1:D:86:PHE:C	1:D:87:ASN:ND2	2.48	0.62
2:Y:876:LYS:HZ2	2:Y:911:ILE:HG12	1.64	0.62
2:X:832:LYS:HD2	2:X:834:GLU:HG3	1.81	0.62
1:C:200:ASN:O	1:C:201:ALA:HB3	1.99	0.62
2:Y:889:LEU:HD21	2:Y:906:GLU:CB	2.29	0.62
2:Y:706:ASN:ND2	2:Y:709:VAL:H	1.98	0.62
2:Y:823:TYR:CZ	2:Y:832:LYS:NZ	2.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:ASP:O	1:D:58:ASP:OD1	2.18	0.62
2:X:679:GLU:CB	2:X:689:ILE:HD13	2.26	0.62
1:D:87:ASN:HD22	1:D:87:ASN:N	1.96	0.62
2:X:782:LYS:CG	2:X:783:ASN:N	2.62	0.62
1:B:98:GLU:HB2	1:B:106:PHE:O	1.98	0.62
2:X:846:ARG:CG	2:X:852:VAL:HG13	2.30	0.61
2:X:681:ARG:HG2	2:X:681:ARG:HH11	1.65	0.61
2:X:900:LYS:O	2:X:902:GLU:N	2.33	0.61
2:Y:713:ILE:HG22	2:Y:713:ILE:O	1.99	0.61
1:D:73:ALA:HB2	1:D:84:TYR:CE1	2.36	0.61
1:A:98:GLU:HB3	1:A:107:ARG:HA	1.82	0.61
2:X:665:CYS:SG	2:X:693:PRO:HD3	2.40	0.61
2:X:780:GLY:O	2:X:781:ILE:HG13	2.00	0.61
1:D:71:ARG:HB2	1:D:75:LEU:HD12	1.82	0.61
2:Y:690:VAL:HG13	2:Y:692:ASN:O	2.00	0.61
1:D:30:SER:O	1:D:49:GLU:HB2	2.00	0.61
1:D:62:GLU:C	1:D:64:GLY:H	2.01	0.61
1:A:127:ILE:HG12	1:B:127:ILE:CG1	2.23	0.61
1:C:40:HIS:NE2	1:D:119:PRO:HD2	2.16	0.61
2:X:905:GLU:HB3	4:X:88:HOH:O	2.01	0.61
1:D:138:GLN:O	1:D:142:GLU:HG3	2.01	0.61
2:X:711:ASN:HD22	2:X:712:ILE:N	1.99	0.60
1:C:42:ALA:O	1:C:116:VAL:HB	2.02	0.60
2:Y:738:TRP:HB3	2:Y:743:MET:HE3	1.83	0.60
1:A:130:CYS:O	1:A:134:THR:HG22	2.00	0.60
1:D:59:MET:O	1:D:60:GLU:CB	2.48	0.60
2:X:659:PHE:O	2:X:662:VAL:HB	2.01	0.60
1:B:62:GLU:C	1:B:64:GLY:H	2.05	0.60
2:X:717:LYS:CG	2:X:718:HIS:CE1	2.74	0.60
2:Y:670:THR:HB	2:Y:671:ASP:CB	2.31	0.60
2:X:792:MET:HA	2:X:792:MET:CE	2.31	0.60
2:Y:716:ASN:OD1	2:Y:745:HIS:CE1	2.55	0.59
1:C:172:LEU:O	1:C:175:ASP:HB2	2.02	0.59
1:D:153:ARG:HD2	4:D:204:HOH:O	2.02	0.59
1:D:200:ASN:N	1:D:200:ASN:HD22	2.00	0.59
1:B:70:LEU:CD2	1:B:97:PHE:HE2	2.15	0.59
2:X:846:ARG:CG	2:X:846:ARG:NE	2.64	0.59
2:X:706:ASN:O	2:X:710:LYS:CG	2.51	0.59
2:Y:874:ASP:O	2:Y:875:PHE:C	2.37	0.59
1:B:40:HIS:O	1:B:119:PRO:HB2	2.01	0.59
1:D:73:ALA:HB2	1:D:84:TYR:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:790:GLU:CD	2:X:790:GLU:H	2.05	0.59
1:C:50:SER:HB3	4:C:261:HOH:O	2.02	0.59
1:B:42:ALA:O	1:B:115:LYS:HB2	2.02	0.58
1:D:118:ASN:HB3	1:D:121:GLU:HB3	1.85	0.58
2:X:663:GLU:OE1	2:X:697:THR:CG2	2.41	0.58
1:A:120:ALA:HB2	1:B:40:HIS:HB2	1.86	0.58
2:X:706:ASN:HD22	2:X:709:VAL:H	1.48	0.58
1:B:59:MET:CE	1:B:59:MET:HA	2.32	0.58
2:Y:829:LEU:O	2:Y:830:SER:CB	2.47	0.58
1:D:62:GLU:C	1:D:64:GLY:N	2.56	0.58
1:A:120:ALA:CB	1:B:40:HIS:HB2	2.33	0.58
1:D:53:SER:HB3	1:D:63:LYS:NZ	2.19	0.58
1:B:150:ARG:HG3	4:B:211:HOH:O	2.03	0.58
2:X:746:MET:SD	2:X:754:PHE:HD1	2.26	0.58
2:Y:844:GLU:O	2:Y:848:HIS:HD2	1.86	0.58
2:X:719:ASP:OD1	2:X:750:THR:CG2	2.42	0.58
1:D:131:LEU:HA	1:D:134:THR:CG2	2.34	0.58
2:Y:705:GLU:CG	2:Y:710:LYS:HE2	2.34	0.58
1:B:4:LYS:HG3	1:B:5:ILE:N	2.15	0.58
2:X:693:PRO:HA	2:X:697:THR:HG21	1.86	0.58
1:A:88:PHE:CZ	1:A:113:LEU:HD12	2.38	0.58
1:B:87:ASN:HD22	1:B:87:ASN:N	2.01	0.58
2:X:782:LYS:HG3	2:X:783:ASN:N	2.18	0.58
1:D:70:LEU:HD22	1:D:97:PHE:HE2	1.69	0.58
1:A:145:GLN:O	1:A:149:GLU:HG3	2.04	0.58
1:B:86:PHE:O	1:B:87:ASN:ND2	2.37	0.57
1:B:73:ALA:HB2	1:B:84:TYR:CE1	2.39	0.57
1:B:31:GLY:HA2	1:B:52:ILE:HD13	1.85	0.57
1:C:104:VAL:HG23	1:C:106:PHE:CZ	2.38	0.57
2:Y:872:VAL:O	2:Y:876:LYS:HG3	2.03	0.57
1:A:7:ARG:HG3	1:A:7:ARG:O	2.05	0.57
2:X:812:MET:HE1	2:X:897:SER:CB	2.35	0.57
1:D:181:ILE:HD13	2:Y:799:LEU:CD1	2.35	0.57
1:C:70:LEU:HD22	1:C:74:LEU:HD12	1.86	0.57
2:Y:819:TYR:OH	2:Y:823:TYR:HD2	1.88	0.57
1:C:34:ILE:O	1:C:34:ILE:CG2	2.52	0.57
2:Y:706:ASN:HD22	2:Y:706:ASN:C	2.07	0.57
1:C:36:LEU:HG	1:C:37:THR:N	2.19	0.57
1:B:68:GLY:HA2	1:B:71:ARG:HG2	1.87	0.57
1:C:7:ARG:O	1:C:7:ARG:HG3	2.05	0.57
1:C:88:PHE:CE1	1:C:113:LEU:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:732:THR:CG2	2:Y:734:SER:OG	2.54	0.56
1:B:179:ARG:NH1	2:X:781:ILE:HB	2.20	0.56
2:Y:816:HIS:CD2	2:Y:893:TRP:HH2	2.23	0.56
2:X:675:LYS:O	2:X:679:GLU:HG3	2.05	0.56
2:X:910:LEU:CB	2:X:911:ILE:HG23	2.33	0.56
1:B:53:SER:HB3	1:B:63:LYS:HZ3	1.68	0.56
1:B:85:THR:HB	1:B:100:ASN:HD21	1.71	0.56
1:A:127:ILE:O	1:A:127:ILE:CG2	2.54	0.56
2:X:812:MET:HE3	2:X:897:SER:C	2.26	0.56
1:D:70:LEU:CD2	1:D:97:PHE:HE2	2.18	0.56
1:B:25:GLU:O	1:B:26:LYS:HB2	2.06	0.56
2:X:717:LYS:HG2	2:X:718:HIS:NE2	2.18	0.56
1:C:151:LEU:CD1	1:D:148:ASN:HB2	2.35	0.56
1:A:101:LEU:O	1:A:103:ASP:N	2.38	0.56
1:D:190:LYS:NZ	4:D:237:HOH:O	2.32	0.56
1:D:131:LEU:HA	1:D:134:THR:HG22	1.88	0.56
1:D:187:LYS:NZ	2:Y:759:ASP:OD1	2.34	0.56
2:X:908:GLN:HB2	2:X:909:TYR:CD1	2.40	0.56
2:Y:670:THR:HB	2:Y:671:ASP:HB2	1.88	0.55
2:X:812:MET:CE	2:X:897:SER:CB	2.78	0.55
2:X:903:LEU:C	2:X:904:GLN:O	2.41	0.55
1:D:31:GLY:HA3	1:D:48:SER:HA	1.87	0.55
1:B:118:ASN:HD22	1:B:118:ASN:H	1.53	0.55
1:C:70:LEU:HD22	1:C:74:LEU:CD1	2.36	0.55
2:Y:657:ASN:OD1	2:Y:657:ASN:N	2.36	0.55
1:C:1:MET:HG3	1:C:24:TRP:O	2.07	0.55
1:C:24:TRP:HD1	1:C:27:THR:O	1.89	0.55
1:C:127:ILE:HG13	1:C:127:ILE:O	2.05	0.55
2:X:783:ASN:CA	2:X:784:SER:OG	2.54	0.55
1:B:36:LEU:O	1:B:43:TRP:HE3	1.90	0.55
2:Y:821:ASP:OD1	2:Y:871:ARG:NH1	2.38	0.55
1:A:70:LEU:HD22	1:A:74:LEU:HD12	1.89	0.55
1:D:179:ARG:NH1	2:Y:781:ILE:O	2.35	0.55
1:D:98:GLU:HB2	1:D:106:PHE:O	2.06	0.55
1:A:172:LEU:O	1:A:175:ASP:HB3	2.07	0.55
1:B:62:GLU:C	1:B:64:GLY:N	2.57	0.55
1:D:4:LYS:HG2	1:D:75:LEU:HB3	1.89	0.55
2:X:716:ASN:HD22	2:X:748:PRO:HD3	1.72	0.55
1:B:119:PRO:O	1:B:123:ILE:CD1	2.32	0.54
1:B:71:ARG:HB2	1:B:75:LEU:HD12	1.90	0.54
1:A:70:LEU:HD22	1:A:74:LEU:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:675:LYS:N	2:Y:676:PRO:CD	2.70	0.54
1:B:56:ALA:CB	1:B:63:LYS:HG3	2.37	0.54
1:C:32:PHE:CE1	1:C:34:ILE:HD12	2.42	0.54
1:C:100:ASN:OD1	1:C:105:SER:HB2	2.08	0.54
2:X:694:GLY:H	2:X:697:THR:HG23	1.71	0.54
1:A:131:LEU:HD21	1:B:5:ILE:CG2	2.38	0.54
2:X:681:ARG:CG	2:X:681:ARG:HH11	2.20	0.54
1:B:85:THR:HB	1:B:100:ASN:ND2	2.23	0.54
2:Y:710:LYS:HD2	2:Y:710:LYS:H	1.69	0.54
1:B:95:PHE:O	1:B:110:SER:HA	2.08	0.54
1:C:34:ILE:HD13	1:C:111:PHE:CE1	2.43	0.54
2:X:823:TYR:CD2	2:X:832:LYS:HA	2.42	0.54
1:A:36:LEU:HG	1:A:37:THR:N	2.23	0.54
1:C:154:ASP:O	1:C:158:VAL:HG23	2.08	0.54
1:C:39:GLY:O	1:D:120:ALA:HA	2.08	0.54
2:X:705:GLU:HG3	2:X:710:LYS:NZ	2.22	0.54
1:C:44:THR:CG2	1:C:45:GLY:N	2.44	0.53
2:X:706:ASN:ND2	2:X:707:ILE:N	2.56	0.53
2:X:706:ASN:H	2:X:710:LYS:HG2	1.73	0.53
2:X:812:MET:HE2	2:X:903:LEU:HD23	1.88	0.53
2:X:665:CYS:O	2:X:700:VAL:HA	2.07	0.53
1:D:69:GLU:OE1	1:D:99:LYS:HD2	2.06	0.53
1:C:2:GLU:OE2	1:C:26:LYS:HB2	2.08	0.53
1:B:88:PHE:HB2	1:B:95:PHE:CD2	2.39	0.53
1:C:190:LYS:NZ	4:C:219:HOH:O	2.41	0.53
1:A:117:GLU:HG3	1:A:118:ASN:N	2.22	0.53
1:D:69:GLU:OE2	1:D:72:LYS:NZ	2.40	0.53
2:Y:658:ILE:HD11	2:Y:685:PHE:HD2	1.73	0.53
1:D:172:LEU:HD11	1:D:176:LEU:HD11	1.91	0.53
1:D:85:THR:O	1:D:97:PHE:HA	2.08	0.53
2:X:752:GLU:O	2:X:756:ARG:HG3	2.09	0.53
1:C:121:GLU:O	1:C:124:ARG:HB2	2.08	0.53
1:D:192:ARG:CG	1:D:192:ARG:HH11	2.20	0.53
1:D:70:LEU:O	1:D:74:LEU:N	2.42	0.53
2:X:691:GLN:HA	2:X:691:GLN:NE2	2.24	0.53
2:X:876:LYS:HE2	2:X:911:ILE:CD1	2.38	0.53
2:X:680:ASN:O	2:X:683:ALA:HB3	2.09	0.53
2:X:658:ILE:HG21	2:X:735:PHE:HB2	1.90	0.53
1:B:56:ALA:HB3	1:B:63:LYS:HG3	1.91	0.53
2:X:710:LYS:HA	2:X:710:LYS:CE	2.39	0.53
1:B:70:LEU:O	1:B:74:LEU:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:TYR:O	1:B:181:ILE:CG1	2.57	0.52
1:B:21:GLN:OE1	1:B:126:LEU:HD12	2.09	0.52
2:X:825:VAL:O	2:X:826:ILE:C	2.47	0.52
1:A:127:ILE:CG1	1:B:127:ILE:CG1	2.85	0.52
1:B:53:SER:HB3	1:B:63:LYS:HZ2	1.71	0.52
1:C:59:MET:CE	1:C:108:LEU:HA	2.38	0.52
1:A:118:ASN:ND2	1:A:122:VAL:HG22	2.24	0.52
1:D:130:CYS:O	1:D:134:THR:HG22	2.09	0.52
2:X:706:ASN:O	2:X:710:LYS:HB2	2.10	0.52
1:C:117:GLU:HG3	1:C:118:ASN:N	2.24	0.52
2:X:906:GLU:O	2:X:909:TYR:N	2.40	0.52
2:Y:825:VAL:HG23	2:Y:831:THR:HG21	1.90	0.52
2:Y:710:LYS:N	2:Y:710:LYS:CD	2.72	0.52
2:X:787:GLN:NE2	2:X:792:MET:HE1	2.24	0.52
1:D:85:THR:HB	1:D:100:ASN:ND2	2.23	0.52
1:D:97:PHE:CD1	1:D:97:PHE:N	2.76	0.52
1:B:40:HIS:O	1:B:119:PRO:CB	2.58	0.52
1:B:131:LEU:HA	1:B:134:THR:HG22	1.91	0.52
2:X:780:GLY:C	2:X:781:ILE:HG13	2.30	0.52
2:X:693:PRO:HB2	2:X:718:HIS:CE1	2.45	0.52
2:Y:710:LYS:CD	2:Y:710:LYS:H	2.23	0.52
1:C:32:PHE:HE1	1:C:34:ILE:HD12	1.74	0.52
1:D:56:ALA:HB1	1:D:61:MET:O	2.10	0.52
1:D:159:GLN:HG2	2:Y:840:ILE:HD11	1.90	0.52
1:B:179:ARG:O	1:B:183:VAL:HG23	2.10	0.51
1:D:155:TRP:CZ3	1:D:159:GLN:HG3	2.46	0.51
1:B:118:ASN:N	1:B:118:ASN:ND2	2.57	0.51
1:B:31:GLY:HA2	1:B:52:ILE:CD1	2.40	0.51
1:C:104:VAL:CG2	1:C:106:PHE:CZ	2.93	0.51
2:Y:828:ASP:C	2:Y:828:ASP:OD2	2.48	0.51
1:A:53:SER:HA	1:A:63:LYS:HE3	1.91	0.51
1:A:154:ASP:O	1:A:158:VAL:HG23	2.10	0.51
2:X:907:ASN:HA	2:X:910:LEU:HG	1.92	0.51
1:B:178:LYS:NZ	2:X:784:SER:O	2.29	0.51
2:Y:829:LEU:HD21	2:Y:854:SER:HB2	1.91	0.51
1:A:121:GLU:O	1:A:124:ARG:HB2	2.11	0.51
1:C:47:VAL:HG21	1:C:111:PHE:CE2	2.45	0.51
2:Y:825:VAL:O	2:Y:826:ILE:C	2.49	0.51
1:C:28:LEU:CD1	1:C:75:LEU:HD11	2.38	0.51
1:B:73:ALA:HA	1:B:84:TYR:CD2	2.45	0.51
2:Y:824:ALA:N	2:Y:833:ASN:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:667:MET:HG2	2:X:708:ARG:HD3	1.92	0.51
2:Y:862:HIS:HD2	2:Y:889:LEU:HD11	1.75	0.51
1:C:1:MET:HA	1:C:25:GLU:HG3	1.92	0.51
2:X:691:GLN:HE21	2:X:691:GLN:CA	2.23	0.51
1:D:116:VAL:CG1	1:D:117:GLU:H	2.18	0.51
1:D:42:ALA:O	1:D:115:LYS:HB2	2.11	0.51
1:C:26:LYS:O	1:C:26:LYS:CG	2.52	0.51
2:Y:879:ARG:HG3	2:Y:886:PHE:CZ	2.46	0.51
1:B:117:GLU:HB3	1:D:117:GLU:OE2	2.10	0.50
2:Y:823:TYR:HE1	2:Y:832:LYS:HZ2	1.49	0.50
1:A:104:VAL:HG23	1:A:106:PHE:HE1	1.64	0.50
1:B:87:ASN:CB	1:B:96:PHE:CZ	2.92	0.50
1:B:91:GLU:H	1:B:91:GLU:CD	2.15	0.50
2:X:826:ILE:O	2:X:827:ASN:HB2	2.11	0.50
1:A:180:PHE:CD2	1:A:180:PHE:N	2.79	0.50
2:X:770:ASP:O	2:X:774:LEU:HB2	2.12	0.50
2:X:785:ASN:O	2:X:787:GLN:N	2.45	0.50
2:Y:664:PHE:HD1	2:Y:699:CYS:HG	1.59	0.50
2:X:739:GLN:NE2	2:X:741:ARG:NH2	2.54	0.50
2:Y:878:PHE:CD1	2:Y:882:PHE:CE2	2.97	0.50
2:X:910:LEU:CB	2:X:911:ILE:CG2	2.87	0.50
2:Y:828:ASP:O	2:Y:828:ASP:OD2	2.30	0.50
1:A:82:ASP:HB3	1:A:84:TYR:CE1	2.47	0.50
2:X:784:SER:HB2	2:X:786:GLU:OE1	2.11	0.49
2:Y:732:THR:HG23	2:Y:734:SER:HB3	1.89	0.49
1:B:56:ALA:O	1:B:61:MET:N	2.44	0.49
1:A:140:LYS:NZ	4:A:258:HOH:O	2.44	0.49
1:A:118:ASN:O	1:A:122:VAL:HG22	2.11	0.49
1:A:124:ARG:NH1	1:B:38:ASP:O	2.45	0.49
1:C:118:ASN:O	1:C:122:VAL:HG22	2.12	0.49
1:B:89:SER:HA	4:B:206:HOH:O	2.12	0.49
2:Y:675:LYS:N	2:Y:676:PRO:HD3	2.28	0.49
1:A:28:LEU:HD23	1:A:32:PHE:CD2	2.48	0.49
2:X:884:ARG:O	2:X:885:LYS:C	2.50	0.49
1:B:30:SER:O	1:B:49:GLU:CB	2.61	0.49
1:B:118:ASN:HD22	1:B:118:ASN:N	2.11	0.49
1:C:1:MET:CE	1:C:23:SER:HB3	2.42	0.49
1:D:112:ASN:H	1:D:112:ASN:ND2	2.11	0.49
1:B:65:LYS:O	1:B:69:GLU:CG	2.61	0.49
2:Y:826:ILE:HD11	2:Y:871:ARG:HB3	1.95	0.49
2:Y:876:LYS:HZ1	2:Y:911:ILE:HG12	1.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:664:PHE:HD1	2:Y:699:CYS:SG	2.36	0.49
2:X:668:SER:C	2:X:703:GLY:H	2.15	0.49
2:X:706:ASN:O	2:X:710:LYS:CB	2.61	0.49
1:A:1:MET:CA	1:A:25:GLU:HG3	2.42	0.49
2:Y:882:PHE:O	2:Y:885:LYS:NZ	2.46	0.48
1:C:151:LEU:HD12	1:D:148:ASN:HB2	1.93	0.48
2:X:876:LYS:HE2	2:X:911:ILE:HD11	1.94	0.48
2:Y:706:ASN:HD22	2:Y:709:VAL:H	1.59	0.48
1:B:52:ILE:HG22	1:B:53:SER:H	1.77	0.48
1:B:69:GLU:OE1	1:B:99:LYS:HD2	2.13	0.48
2:Y:787:GLN:HA	2:Y:791:GLU:OE1	2.13	0.48
1:B:44:THR:OG1	1:B:116:VAL:HG23	2.13	0.48
2:X:702:ALA:HB2	2:X:720:VAL:HG12	1.95	0.48
2:Y:788:THR:HG22	2:Y:789:PRO:HD2	1.95	0.48
1:D:26:LYS:O	1:D:27:THR:HG23	2.14	0.48
2:X:759:ASP:HB2	2:X:763:ASP:H	1.78	0.48
2:Y:862:HIS:CD2	2:Y:889:LEU:HD12	2.42	0.48
2:X:746:MET:HB2	2:X:751:LYS:HG2	1.95	0.48
1:A:30:SER:HA	1:A:49:GLU:OE1	2.13	0.48
1:B:52:ILE:CG2	1:B:53:SER:H	2.26	0.48
1:B:59:MET:HE2	1:B:59:MET:HA	1.95	0.48
1:A:41:SER:HB2	1:A:43:TRP:CH2	2.49	0.48
1:A:61:MET:HG2	1:A:66:TYR:HB2	1.95	0.48
2:X:910:LEU:CA	2:X:911:ILE:CG2	2.92	0.48
1:D:160:GLY:HA2	1:D:163:GLU:HG3	1.96	0.48
2:X:780:GLY:C	2:X:781:ILE:CG1	2.82	0.48
1:C:24:TRP:CD1	1:C:27:THR:O	2.67	0.48
1:B:73:ALA:HB2	1:B:84:TYR:CZ	2.49	0.48
1:B:23:SER:O	1:B:32:PHE:HB2	2.14	0.48
1:D:193:SER:O	1:D:197:LYS:HB2	2.13	0.47
1:D:179:ARG:NH1	2:Y:778:PHE:O	2.47	0.47
2:X:812:MET:HE2	2:X:897:SER:HB3	1.91	0.47
1:C:130:CYS:HB3	1:D:130:CYS:HB3	1.96	0.47
2:Y:746:MET:SD	2:Y:754:PHE:CD1	3.07	0.47
2:X:786:GLU:C	2:X:787:GLN:HG3	2.34	0.47
2:X:757:GLU:HG3	2:X:757:GLU:O	2.06	0.47
1:C:53:SER:HA	1:C:63:LYS:HE3	1.95	0.47
1:B:70:LEU:HD22	1:B:97:PHE:HE2	1.79	0.47
1:A:188:LYS:NZ	2:X:763:ASP:OD1	2.37	0.47
1:B:49:GLU:O	1:B:49:GLU:HG3	2.14	0.47
2:Y:662:VAL:HG12	2:Y:664:PHE:CZ	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLU:OE2	1:A:105:SER:OG	2.32	0.47
1:B:83:VAL:CG1	1:B:83:VAL:O	2.55	0.47
1:D:40:HIS:O	1:D:119:PRO:HB2	2.14	0.47
1:D:89:SER:CB	1:D:91:GLU:OE1	2.61	0.47
1:D:73:ALA:HA	1:D:84:TYR:CE2	2.50	0.47
1:D:44:THR:HG22	1:D:45:GLY:H	1.80	0.47
2:X:681:ARG:O	2:X:682:ILE:C	2.51	0.47
2:Y:738:TRP:CG	2:Y:743:MET:HE1	2.50	0.47
1:B:74:LEU:C	1:B:76:SER:H	2.18	0.47
1:B:187:LYS:O	1:B:191:ILE:HG13	2.15	0.47
1:C:118:ASN:ND2	1:C:122:VAL:HG22	2.30	0.47
2:Y:679:GLU:O	2:Y:689:ILE:CD1	2.63	0.47
2:X:757:GLU:HG2	2:X:758:TYR:CE1	2.50	0.47
1:C:26:LYS:HB3	1:C:26:LYS:HE2	1.78	0.46
2:X:691:GLN:NE2	2:X:691:GLN:CA	2.78	0.46
1:C:200:ASN:O	1:C:201:ALA:CB	2.51	0.46
2:X:790:GLU:N	2:X:790:GLU:CD	2.69	0.46
1:A:161:ARG:NH2	4:A:220:HOH:O	2.41	0.46
2:X:908:GLN:O	4:X:137:HOH:O	2.21	0.46
2:X:885:LYS:HE3	4:X:146:HOH:O	2.15	0.46
2:X:706:ASN:O	2:X:710:LYS:HG2	2.15	0.46
2:Y:845:LEU:HB3	2:Y:850:ALA:HB3	1.97	0.46
1:D:95:PHE:O	1:D:110:SER:HA	2.14	0.46
1:B:121:GLU:OE1	1:D:121:GLU:OE1	2.33	0.46
2:X:769:THR:OG1	2:X:770:ASP:N	2.48	0.46
2:Y:665:CYS:SG	2:Y:693:PRO:HD3	2.56	0.46
1:B:131:LEU:CA	1:B:134:THR:HG22	2.45	0.46
2:Y:759:ASP:OD1	2:Y:763:ASP:HB3	2.15	0.46
1:A:40:HIS:HB2	1:B:120:ALA:HB2	1.98	0.46
1:D:113:LEU:O	1:D:114:GLU:HG3	2.16	0.46
1:D:30:SER:O	1:D:49:GLU:CB	2.64	0.46
1:A:161:ARG:HA	1:A:161:ARG:HD3	1.70	0.46
1:B:69:GLU:OE2	1:B:99:LYS:NZ	2.49	0.45
2:Y:670:THR:HB	2:Y:671:ASP:CG	2.37	0.45
2:X:900:LYS:O	2:X:902:GLU:HG2	2.16	0.45
1:C:158:VAL:H	1:C:158:VAL:HG23	1.19	0.45
1:C:159:GLN:NE2	1:C:163:GLU:OE1	2.42	0.45
2:X:705:GLU:HG3	2:X:710:LYS:HZ2	1.81	0.45
2:X:677:ASP:O	2:X:680:ASN:HB2	2.17	0.45
2:Y:712:ILE:O	2:Y:715:SER:O	2.35	0.45
2:Y:809:PRO:HD2	4:Y:228:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HA	1:A:187:LYS:HD3	1.77	0.45
2:Y:738:TRP:HB3	2:Y:743:MET:CE	2.46	0.45
1:D:131:LEU:CA	1:D:134:THR:HG22	2.47	0.45
2:Y:731:LYS:HG3	2:Y:732:THR:N	2.31	0.45
2:Y:862:HIS:CD2	2:Y:889:LEU:CD1	2.90	0.45
1:C:98:GLU:HB3	1:C:107:ARG:HA	1.98	0.45
2:Y:675:LYS:O	2:Y:679:GLU:HG3	2.17	0.45
2:X:655:ILE:HD13	2:X:655:ILE:HG23	1.60	0.45
1:D:43:TRP:HA	1:D:115:LYS:HB2	1.97	0.45
1:C:89:SER:O	1:C:93:CYS:CA	2.62	0.45
2:X:784:SER:HB2	2:X:786:GLU:CD	2.36	0.45
1:A:118:ASN:HB2	1:A:121:GLU:OE1	2.17	0.45
2:Y:829:LEU:O	2:Y:830:SER:HB2	2.17	0.45
2:X:655:ILE:O	2:X:656:SER:HB2	2.16	0.45
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.82	0.45
1:C:26:LYS:HB3	1:C:26:LYS:NZ	2.28	0.45
1:A:85:THR:HG22	1:A:98:GLU:HG3	1.99	0.45
2:X:662:VAL:HG12	2:X:664:PHE:CE1	2.52	0.45
1:A:140:LYS:HG3	1:A:140:LYS:O	2.17	0.45
1:B:20:LEU:HD12	1:B:36:LEU:HB2	1.97	0.45
2:Y:658:ILE:HD11	2:Y:685:PHE:CD2	2.51	0.45
2:Y:879:ARG:HH12	2:Y:888:ILE:HG13	1.82	0.45
1:A:1:MET:N	1:A:26:LYS:HE3	2.32	0.44
1:D:118:ASN:O	1:D:122:VAL:HG23	2.17	0.44
1:D:131:LEU:O	1:D:134:THR:HG22	2.18	0.44
2:Y:821:ASP:CG	2:Y:871:ARG:HH11	2.20	0.44
1:D:51:GLU:HG3	1:D:51:GLU:H	1.74	0.44
2:Y:706:ASN:HD21	2:Y:708:ARG:HB2	1.83	0.44
1:C:95:PHE:O	1:C:111:PHE:N	2.39	0.44
1:B:85:THR:O	1:B:97:PHE:HA	2.16	0.44
1:A:34:ILE:O	1:A:34:ILE:HG23	2.14	0.44
2:X:816:HIS:CD2	2:X:893:TRP:HH2	2.34	0.44
2:X:865:ILE:H	2:X:865:ILE:HG12	1.48	0.44
1:B:82:ASP:CA	1:B:83:VAL:HG23	2.25	0.44
2:X:910:LEU:CA	2:X:911:ILE:HG22	2.47	0.44
2:Y:753:HIS:O	2:Y:756:ARG:HG2	2.18	0.44
2:X:717:LYS:CG	2:X:718:HIS:NE2	2.80	0.44
1:A:104:VAL:HG21	1:A:106:PHE:CZ	2.52	0.44
1:D:87:ASN:N	1:D:87:ASN:ND2	2.66	0.44
2:Y:679:GLU:HB3	2:Y:689:ILE:HD13	1.99	0.44
2:X:788:THR:HG22	2:X:791:GLU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:853:VAL:HG13	2:Y:855:CYS:H	1.83	0.44
2:X:701:ILE:HG22	2:X:723:PRO:HG3	2.00	0.44
2:X:864:ILE:HD13	2:X:889:LEU:HB2	2.00	0.44
2:Y:706:ASN:O	2:Y:710:LYS:HG2	2.17	0.43
1:B:44:THR:HG22	1:B:45:GLY:H	1.83	0.43
2:Y:831:THR:O	2:Y:832:LYS:C	2.56	0.43
1:D:61:MET:O	1:D:62:GLU:C	2.56	0.43
1:A:90:LYS:HE3	1:A:90:LYS:HB2	1.28	0.43
1:B:117:GLU:O	1:B:119:PRO:HD3	2.18	0.43
2:X:702:ALA:HB2	2:X:720:VAL:CG1	2.47	0.43
2:X:674:PRO:O	2:X:675:LYS:C	2.56	0.43
2:Y:759:ASP:HB2	2:Y:763:ASP:O	2.18	0.43
2:X:812:MET:CE	2:X:897:SER:C	2.86	0.43
2:Y:819:TYR:O	2:Y:863:VAL:CA	2.60	0.43
2:Y:706:ASN:N	2:Y:710:LYS:HD3	2.32	0.43
1:B:66:TYR:O	1:B:67:VAL:C	2.57	0.43
2:X:739:GLN:NE2	2:X:741:ARG:HE	2.11	0.43
2:Y:706:ASN:ND2	2:Y:706:ASN:C	2.72	0.43
2:Y:869:HIS:O	2:Y:872:VAL:HG13	2.19	0.43
1:C:110:SER:O	1:C:111:PHE:CD2	2.71	0.43
1:D:131:LEU:C	1:D:134:THR:HG22	2.39	0.43
1:C:41:SER:HB2	1:C:43:TRP:CH2	2.53	0.43
1:D:197:LYS:CE	4:D:269:HOH:O	2.39	0.43
1:B:36:LEU:HG	1:B:37:THR:N	2.34	0.43
2:Y:665:CYS:O	2:Y:700:VAL:HA	2.18	0.43
1:B:10:LEU:HB3	1:B:12:SER:OG	2.17	0.43
1:C:90:LYS:HG3	1:C:90:LYS:H	1.48	0.43
2:X:767:ILE:HD12	2:X:767:ILE:HG23	1.67	0.43
1:D:101:LEU:HB2	1:D:104:VAL:HG23	2.01	0.43
1:D:117:GLU:O	1:D:119:PRO:HD3	2.17	0.43
2:X:744:ILE:HD12	2:X:744:ILE:HG21	1.44	0.43
1:B:116:VAL:HG12	1:B:117:GLU:N	2.25	0.43
2:X:783:ASN:HB3	2:X:784:SER:OG	2.18	0.43
1:B:187:LYS:NZ	2:X:759:ASP:OD1	2.42	0.43
2:Y:799:LEU:HA	2:Y:799:LEU:HD23	1.90	0.43
1:C:159:GLN:HA	1:C:159:GLN:OE1	2.17	0.43
2:X:867:GLU:HG3	2:X:867:GLU:H	1.57	0.43
1:B:85:THR:CB	1:B:100:ASN:HD21	2.31	0.43
1:C:120:ALA:O	1:C:124:ARG:NH1	2.52	0.43
2:X:904:GLN:O	2:X:905:GLU:CG	2.63	0.43
2:X:655:ILE:HG21	2:X:655:ILE:HD12	1.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:722:LYS:HA	2:Y:723:PRO:HD2	1.15	0.43
1:D:53:SER:HB3	1:D:63:LYS:HZ2	1.82	0.42
1:A:102:LYS:HE2	4:A:211:HOH:O	2.18	0.42
1:B:83:VAL:CG1	1:B:100:ASN:HB2	2.44	0.42
1:B:87:ASN:HB2	1:B:96:PHE:CE2	2.53	0.42
2:X:705:GLU:O	2:X:706:ASN:CB	2.68	0.42
1:A:192:ARG:HD3	2:X:766:PHE:O	2.19	0.42
2:X:790:GLU:O	2:X:793:ALA:HB3	2.19	0.42
1:C:82:ASP:HB3	1:C:84:TYR:CE1	2.54	0.42
1:B:43:TRP:HD1	1:B:115:LYS:HB3	1.84	0.42
1:C:11:VAL:O	1:C:14:PRO:HD3	2.19	0.42
1:C:8:ILE:HG13	1:C:9:HIS:N	2.34	0.42
2:X:707:ILE:HD13	2:X:707:ILE:HA	1.95	0.42
2:Y:788:THR:OG1	2:Y:791:GLU:OE1	2.38	0.42
2:X:900:LYS:O	2:X:902:GLU:CG	2.67	0.42
1:B:118:ASN:HB2	1:B:121:GLU:HB3	2.01	0.42
1:A:67:VAL:O	1:A:68:GLY:C	2.57	0.42
1:B:65:LYS:O	1:B:65:LYS:CG	2.38	0.42
2:X:659:PHE:HD2	2:X:659:PHE:HA	1.68	0.42
1:A:47:VAL:HG21	1:A:111:PHE:CE2	2.54	0.42
1:C:151:LEU:HD13	1:D:148:ASN:HB2	2.00	0.42
1:B:151:LEU:HA	1:B:151:LEU:HD23	1.82	0.42
1:C:119:PRO:HD2	4:C:229:HOH:O	2.19	0.42
1:A:110:SER:O	1:A:111:PHE:HD2	2.01	0.42
1:C:59:MET:HE2	1:C:107:ARG:O	2.20	0.42
1:B:26:LYS:O	1:B:27:THR:HG23	2.20	0.42
2:Y:706:ASN:O	2:Y:710:LYS:CG	2.68	0.42
1:D:115:LYS:CG	1:D:116:VAL:N	2.83	0.41
2:X:820:LEU:O	2:X:822:SER:N	2.50	0.41
2:Y:706:ASN:H	2:Y:710:LYS:HD3	1.83	0.41
1:B:72:LYS:O	1:B:76:SER:C	2.58	0.41
2:X:658:ILE:HG21	2:X:658:ILE:HD13	1.82	0.41
1:C:5:ILE:HD13	1:C:130:CYS:SG	2.61	0.41
1:D:87:ASN:HB2	1:D:96:PHE:CE1	2.54	0.41
2:Y:801:TYR:O	2:Y:802:ARG:C	2.58	0.41
2:Y:814:ARG:HA	2:Y:849:GLY:O	2.20	0.41
1:B:61:MET:CE	1:B:62:GLU:HG2	2.50	0.41
1:D:68:GLY:HA2	1:D:71:ARG:CG	2.47	0.41
1:C:188:LYS:HD2	2:Y:768:ASP:HA	2.03	0.41
1:D:21:GLN:OE1	1:D:126:LEU:HD12	2.20	0.41
2:Y:900:LYS:CB	2:Y:904:GLN:NE2	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PHE:O	1:A:111:PHE:N	2.49	0.41
2:X:808:SER:HA	2:X:809:PRO:HD3	1.83	0.41
2:X:783:ASN:CB	2:X:784:SER:OG	2.69	0.41
2:X:657:ASN:HB3	2:X:686:GLY:HA3	2.03	0.41
2:Y:705:GLU:O	2:Y:706:ASN:HB3	2.20	0.41
1:B:198:LEU:HD23	1:B:198:LEU:HA	1.86	0.41
1:A:2:GLU:HB2	1:A:24:TRP:CZ2	2.56	0.41
2:X:884:ARG:CD	2:X:884:ARG:O	2.69	0.41
2:Y:701:ILE:HG23	2:Y:701:ILE:HD12	1.71	0.41
1:B:101:LEU:HB2	1:B:104:VAL:HG23	2.02	0.41
2:Y:878:PHE:O	2:Y:881:THR:HB	2.20	0.41
1:D:110:SER:O	1:D:110:SER:OG	2.36	0.41
1:C:71:ARG:HB3	1:C:75:LEU:HD12	2.01	0.41
1:D:123:ILE:HG22	1:D:127:ILE:HD12	2.03	0.41
2:X:820:LEU:HD23	2:X:838:LEU:HD22	2.02	0.41
2:Y:705:GLU:HG3	2:Y:710:LYS:CE	2.46	0.41
2:Y:792:MET:HA	2:Y:795:LEU:HD12	2.03	0.41
1:D:74:LEU:C	1:D:76:SER:H	2.24	0.41
2:X:678:LEU:O	2:X:682:ILE:HG13	2.20	0.41
2:Y:879:ARG:HG2	2:Y:886:PHE:CE1	2.56	0.41
1:C:145:GLN:O	1:C:149:GLU:HG3	2.20	0.41
1:B:155:TRP:CZ2	2:X:840:ILE:CD1	3.04	0.41
1:C:43:TRP:HB3	1:C:113:LEU:HB3	2.03	0.41
1:A:118:ASN:HD22	1:A:122:VAL:HG22	1.86	0.41
1:D:151:LEU:HD23	1:D:151:LEU:HA	1.94	0.41
1:D:115:LYS:HG3	1:D:116:VAL:N	2.36	0.40
1:D:40:HIS:O	1:D:119:PRO:CB	2.68	0.40
2:X:700:VAL:HG22	2:X:720:VAL:HG13	2.02	0.40
2:Y:660:GLU:O	2:Y:661:ASP:HB2	2.21	0.40
2:X:776:GLU:O	2:X:779:SER:HB3	2.21	0.40
2:X:679:GLU:HA	2:X:689:ILE:HD11	2.03	0.40
2:X:744:ILE:HD13	2:X:744:ILE:HG23	1.45	0.40
1:D:107:ARG:CD	1:D:108:LEU:N	2.80	0.40
2:X:836:THR:HG22	2:X:838:LEU:N	2.13	0.40
1:D:186:GLU:CG	2:Y:759:ASP:OD2	2.62	0.40
1:D:87:ASN:CB	1:D:96:PHE:CZ	3.01	0.40
1:B:49:GLU:O	1:B:49:GLU:CG	2.69	0.40
2:Y:739:GLN:HA	2:Y:740:PRO:HD3	1.87	0.40
1:A:89:SER:O	1:A:93:CYS:HA	2.21	0.40
1:B:87:ASN:HB2	1:B:96:PHE:CE1	2.56	0.40
1:B:28:LEU:HB2	1:B:71:ARG:NH2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:HD21	1:D:197:LYS:HD2	2.03	0.40
1:B:139:ALA:O	1:B:143:HIS:ND1	2.55	0.40
1:D:174:THR:O	1:D:178:LYS:HG3	2.21	0.40
1:B:179:ARG:NH1	2:X:778:PHE:O	2.54	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	199/203 (98%)	170 (85%)	26 (13%)	3 (2%)	13 17
1	B	192/203 (95%)	168 (88%)	19 (10%)	5 (3%)	7 6
1	C	199/203 (98%)	172 (86%)	22 (11%)	5 (2%)	7 7
1	D	191/203 (94%)	167 (87%)	19 (10%)	5 (3%)	7 6
2	X	252/263 (96%)	217 (86%)	32 (13%)	3 (1%)	16 23
2	Y	256/263 (97%)	221 (86%)	27 (10%)	8 (3%)	5 4
All	All	1289/1338 (96%)	1115 (86%)	145 (11%)	29 (2%)	8 9

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	50	SER
2	X	747	CYS
2	X	786	GLU
2	Y	829	LEU
1	A	34	ILE
1	B	67	VAL
1	C	34	ILE
1	D	115	LYS

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Mol	Chain	Res	Type
2	Y	741	ARG
1	B	26	LYS
1	B	63	LYS
1	D	26	LYS
1	D	60	GLU
1	D	67	VAL
2	Y	716	ASN
2	Y	832	LYS
1	A	81	ALA
1	C	40	HIS
1	C	93	CYS
2	Y	899	ASP
1	A	119	PRO
1	B	93	CYS
1	C	119	PRO
1	D	93	CYS
2	Y	858	GLU
1	C	81	ALA
2	X	781	ILE
2	Y	810	LEU
2	Y	826	ILE

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	181/182 (100%)	142 (78%)	39 (22%)	1	1
1	B	180/182 (99%)	134 (74%)	46 (26%)	0	0
1	C	181/182 (100%)	144 (80%)	37 (20%)	1	1
1	D	179/182 (98%)	135 (75%)	44 (25%)	1	1
2	X	232/236 (98%)	175 (75%)	57 (25%)	1	1
2	Y	234/236 (99%)	191 (82%)	43 (18%)	2	2
All	All	1187/1200 (99%)	921 (78%)	266 (22%)	1	1

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	6	SER
1	A	12	SER
1	A	18	HIS
1	A	23	SER
1	A	25	GLU
1	A	26	LYS
1	A	27	THR
1	A	28	LEU
1	A	34	ILE
1	A	37	THR
1	A	41	SER
1	A	49	GLU
1	A	57	ASP
1	A	61	MET
1	A	62	GLU
1	A	71	ARG
1	A	76	SER
1	A	85	THR
1	A	90	LYS
1	A	98	GLU
1	A	108	LEU
1	A	110	SER
1	A	112	ASN
1	A	116	VAL
1	A	122	VAL
1	A	124	ARG
1	A	126	LEU
1	A	134	THR
1	A	138	GLN
1	A	140	LYS
1	A	145	GLN
1	A	146	LYS
1	A	147	GLU
1	A	152	LEU
1	A	158	VAL
1	A	169	LYS
1	A	190	LYS
1	A	191	ILE
1	B	1	MET
1	B	3	ARG
1	B	4	LYS

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Mol	Chain	Res	Type
1	B	6	SER
1	B	7	ARG
1	B	16	ILE
1	B	17	THR
1	B	26	LYS
1	B	28	LEU
1	B	34	ILE
1	B	41	SER
1	B	47	VAL
1	B	51	GLU
1	B	52	ILE
1	B	57	ASP
1	B	58	ASP
1	B	59	MET
1	B	60	GLU
1	B	61	MET
1	B	62	GLU
1	B	65	LYS
1	B	67	VAL
1	B	72	LYS
1	B	82	ASP
1	B	85	THR
1	B	87	ASN
1	B	91	GLU
1	B	93	CYS
1	B	99	LYS
1	B	105	SER
1	B	111	PHE
1	B	118	ASN
1	B	125	GLU
1	B	134	THR
1	B	143	HIS
1	B	146	LYS
1	B	157	ASP
1	B	162	PHE
1	B	172	LEU
1	B	173	GLU
1	B	181	ILE
1	B	184	LEU
1	B	187	LYS
1	B	197	LYS
1	B	198	LEU

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Mol	Chain	Res	Type
1	B	199	LEU
1	C	2	GLU
1	C	3	ARG
1	C	6	SER
1	C	7	ARG
1	C	12	SER
1	C	22	VAL
1	C	23	SER
1	C	26	LYS
1	C	27	THR
1	C	28	LEU
1	C	40	HIS
1	C	41	SER
1	C	49	GLU
1	C	57	ASP
1	C	62	GLU
1	C	71	ARG
1	C	76	SER
1	C	85	THR
1	C	90	LYS
1	C	98	GLU
1	C	105	SER
1	C	108	LEU
1	C	110	SER
1	C	112	ASN
1	C	116	VAL
1	C	121	GLU
1	C	122	VAL
1	C	124	ARG
1	C	126	LEU
1	C	127	ILE
1	C	140	LYS
1	C	145	GLN
1	C	146	LYS
1	C	152	LEU
1	C	158	VAL
1	C	190	LYS
1	C	191	ILE
1	D	3	ARG
1	D	4	LYS
1	D	7	ARG
1	D	12	SER

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Mol	Chain	Res	Type
1	D	16	ILE
1	D	17	THR
1	D	21	GLN
1	D	28	LEU
1	D	34	ILE
1	D	41	SER
1	D	47	VAL
1	D	51	GLU
1	D	57	ASP
1	D	58	ASP
1	D	60	GLU
1	D	62	GLU
1	D	65	LYS
1	D	67	VAL
1	D	72	LYS
1	D	83	VAL
1	D	85	THR
1	D	87	ASN
1	D	89	SER
1	D	93	CYS
1	D	97	PHE
1	D	99	LYS
1	D	105	SER
1	D	106	PHE
1	D	111	PHE
1	D	112	ASN
1	D	115	LYS
1	D	125	GLU
1	D	146	LYS
1	D	150	ARG
1	D	156	ASN
1	D	159	GLN
1	D	162	PHE
1	D	163	GLU
1	D	174	THR
1	D	187	LYS
1	D	192	ARG
1	D	197	LYS
1	D	198	LEU
1	D	200	ASN
2	X	655	ILE
2	X	657	ASN

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Mol	Chain	Res	Type
2	X	658	ILE
2	X	667	MET
2	X	673	GLN
2	X	681	ARG
2	X	689	ILE
2	X	690	VAL
2	X	691	GLN
2	X	692	ASN
2	X	697	THR
2	X	705	GLU
2	X	706	ASN
2	X	711	ASN
2	X	712	ILE
2	X	715	SER
2	X	716	ASN
2	X	717	LYS
2	X	719	ASP
2	X	723	PRO
2	X	728	GLU
2	X	731	LYS
2	X	734	SER
2	X	735	PHE
2	X	744	ILE
2	X	747	CYS
2	X	750	THR
2	X	751	LYS
2	X	752	GLU
2	X	757	GLU
2	X	759	ASP
2	X	764	SER
2	X	770	ASP
2	X	773	GLN
2	X	774	LEU
2	X	775	LYS
2	X	785	ASN
2	X	786	GLU
2	X	788	THR
2	X	790	GLU
2	X	791	GLU
2	X	794	SER
2	X	809	PRO
2	X	810	LEU

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Mol	Chain	Res	Type
2	X	815	ARG
2	X	820	LEU
2	X	841	LYS
2	X	853	VAL
2	X	856	LEU
2	X	860	VAL
2	X	867	GLU
2	X	880	ARG
2	X	883	LYS
2	X	884	ARG
2	X	885	LYS
2	X	887	LYS
2	X	911	ILE
2	Y	668	SER
2	Y	670	THR
2	Y	672	SER
2	Y	681	ARG
2	Y	690	VAL
2	Y	692	ASN
2	Y	706	ASN
2	Y	710	LYS
2	Y	711	ASN
2	Y	715	SER
2	Y	731	LYS
2	Y	734	SER
2	Y	740	PRO
2	Y	741	ARG
2	Y	748	PRO
2	Y	774	LEU
2	Y	779	SER
2	Y	787	GLN
2	Y	788	THR
2	Y	792	MET
2	Y	811	SER
2	Y	815	ARG
2	Y	820	LEU
2	Y	822	SER
2	Y	830	SER
2	Y	831	THR
2	Y	832	LYS
2	Y	836	THR
2	Y	837	ARG

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Mol	Chain	Res	Type
2	Y	841	LYS
2	Y	851	LYS
2	Y	853	VAL
2	Y	855	CYS
2	Y	856	LEU
2	Y	872	VAL
2	Y	874	ASP
2	Y	876	LYS
2	Y	878	PHE
2	Y	879	ARG
2	Y	883	LYS
2	Y	906	GLU
2	Y	910	LEU
2	Y	911	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	118	ASN
1	A	141	ASN
1	B	54	GLN
1	B	87	ASN
1	B	100	ASN
1	B	118	ASN
1	B	200	ASN
1	C	40	HIS
1	C	118	ASN
1	D	54	GLN
1	D	87	ASN
1	D	100	ASN
1	D	112	ASN
1	D	156	ASN
1	D	196	ASN
1	D	200	ASN
2	X	673	GLN
2	X	706	ASN
2	X	711	ASN
2	X	716	ASN
2	X	718	HIS
2	X	739	GLN
2	X	787	GLN

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Mol	Chain	Res	Type
2	X	816	HIS
2	X	848	HIS
2	X	907	ASN
2	Y	706	ASN
2	Y	745	HIS
2	Y	787	GLN
2	Y	848	HIS
2	Y	904	GLN
2	Y	908	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	201/203 (99%)	0.60	17 (8%) 13 13	35, 71, 104, 125	0
1	B	196/203 (96%)	1.86	74 (37%) 0 0	33, 99, 134, 147	0
1	C	201/203 (99%)	0.42	13 (6%) 22 22	32, 72, 103, 132	0
1	D	195/203 (96%)	1.88	71 (36%) 0 0	29, 94, 134, 148	0
2	X	256/263 (97%)	0.07	4 (1%) 74 74	31, 50, 83, 96	0
2	Y	258/263 (98%)	0.07	6 (2%) 64 63	33, 49, 79, 112	0
All	All	1307/1338 (97%)	0.75	185 (14%) 4 3	29, 63, 125, 148	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	56	ALA	12.4
1	D	103	ASP	11.5
1	B	56	ALA	11.4
1	D	106	PHE	9.5
1	D	74	LEU	8.7
1	B	101	LEU	8.3
1	B	107	ARG	8.2
1	D	61	MET	8.1
1	B	74	LEU	8.0
1	D	52	ILE	7.9
1	B	103	ASP	7.6
1	B	49	GLU	7.4
1	D	66	TYR	7.4
1	D	53	SER	7.0
1	D	9	HIS	6.9
1	B	16	ILE	6.9
1	B	61	MET	6.8
1	B	104	VAL	6.8
1	D	112	ASN	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	53	SER	6.8
1	D	84	TYR	6.5
1	D	50	SER	6.5
1	D	49	GLU	6.4
1	D	48	SER	6.3
1	D	54	GLN	6.2
1	D	47	VAL	6.1
1	B	99	LYS	6.1
1	D	100	ASN	6.1
1	B	54	GLN	6.0
1	D	70	LEU	5.9
1	A	116	VAL	5.9
1	B	29	GLU	5.8
1	B	94	TYR	5.8
1	B	100	ASN	5.8
1	D	92	SER	5.8
1	B	60	GLU	5.8
1	D	113	LEU	5.7
1	D	26	LYS	5.7
1	D	86	PHE	5.6
1	D	60	GLU	5.6
1	B	92	SER	5.6
1	D	102	LYS	5.6
1	B	106	PHE	5.5
1	B	52	ILE	5.5
1	D	108	LEU	5.5
1	D	99	LYS	5.4
1	B	11	VAL	5.4
1	B	108	LEU	5.4
1	B	64	GLY	5.2
1	D	25	GLU	5.2
1	B	97	PHE	5.1
1	B	102	LYS	5.0
1	B	66	TYR	5.0
1	D	8	ILE	5.0
1	D	11	VAL	5.0
1	B	26	LYS	5.0
1	D	104	VAL	5.0
1	A	113	LEU	4.9
1	D	94	TYR	4.9
1	B	111	PHE	4.9
1	B	86	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	105	SER	4.7
1	B	83	VAL	4.7
1	D	107	ARG	4.6
1	B	95	PHE	4.5
1	B	48	SER	4.5
1	D	111	PHE	4.5
1	D	16	ILE	4.4
1	D	57	ASP	4.4
1	B	62	GLU	4.3
1	B	88	PHE	4.3
1	D	62	GLU	4.3
1	B	12	SER	4.2
1	B	70	LEU	4.2
1	C	116	VAL	4.2
1	D	29	GLU	4.2
1	D	95	PHE	4.1
1	D	101	LEU	4.0
1	B	96	PHE	4.0
1	B	109	GLY	4.0
1	C	124	ARG	3.9
1	B	63	LYS	3.9
1	D	114	GLU	3.9
1	D	32	PHE	3.9
1	D	116	VAL	3.9
1	D	45	GLY	3.8
1	B	20	LEU	3.8
1	A	124	ARG	3.8
1	D	20	LEU	3.8
1	A	120	ALA	3.7
1	B	39	GLY	3.7
2	X	669	GLY	3.7
1	B	9	HIS	3.6
1	C	16	ILE	3.6
1	B	13	GLU	3.6
1	B	50	SER	3.6
1	B	84	TYR	3.6
1	B	27	THR	3.6
1	B	73	ALA	3.6
1	B	90	LYS	3.5
1	D	96	PHE	3.4
1	C	113	LEU	3.4
1	B	112	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	123	ILE	3.3
1	B	113	LEU	3.3
1	C	119	PRO	3.3
1	C	26	LYS	3.2
1	B	116	VAL	3.2
1	C	117	GLU	3.2
1	D	59	MET	3.2
1	D	13	GLU	3.2
1	D	10	LEU	3.2
1	B	45	GLY	3.2
1	D	90	LYS	3.2
1	D	71	ARG	3.1
1	B	98	GLU	3.1
1	B	110	SER	3.1
1	B	46	THR	3.1
1	B	57	ASP	3.0
1	D	27	THR	3.0
1	D	73	ALA	3.0
1	B	30	SER	3.0
1	A	117	GLU	3.0
1	D	46	THR	3.0
2	X	707	ILE	3.0
1	A	34	ILE	2.9
1	B	114	GLU	2.9
1	A	39	GLY	2.9
1	A	26	LYS	2.9
1	C	17	THR	2.8
1	B	71	ARG	2.8
1	B	47	VAL	2.8
1	B	25	GLU	2.8
1	D	68	GLY	2.7
1	D	115	LYS	2.7
1	A	111	PHE	2.7
1	D	36	LEU	2.6
1	D	44	THR	2.6
2	X	704	SER	2.6
1	D	17	THR	2.6
1	B	125	GLU	2.6
1	B	93	CYS	2.6
1	D	97	PHE	2.5
1	D	88	PHE	2.5
2	Y	884	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	89	SER	2.5
1	D	122	VAL	2.4
1	B	14	PRO	2.4
1	B	8	ILE	2.4
1	B	59	MET	2.4
1	A	127	ILE	2.4
1	D	30	SER	2.3
1	D	110	SER	2.3
1	B	67	VAL	2.3
1	D	105	SER	2.3
1	D	109	GLY	2.3
1	D	31	GLY	2.2
1	D	93	CYS	2.2
1	A	22	VAL	2.2
1	C	52	ILE	2.2
1	D	65	LYS	2.2
1	D	39	GLY	2.2
1	D	125	GLU	2.1
1	B	15	SER	2.1
2	Y	729	CYS	2.1
2	Y	834	GLU	2.1
1	C	111	PHE	2.1
1	B	122	VAL	2.1
1	C	9	HIS	2.1
2	Y	732	THR	2.1
1	B	128	CYS	2.1
1	A	32	PHE	2.1
1	A	52	ILE	2.0
1	A	165	CYS	2.0
1	B	10	LEU	2.0
1	A	40	HIS	2.0
1	A	16	ILE	2.0
1	C	34	ILE	2.0
1	D	14	PRO	2.0
2	Y	823	TYR	2.0
1	B	124	ARG	2.0
1	C	201	ALA	2.0
2	Y	737	PRO	2.0
1	B	75	LEU	2.0
2	X	668	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	CL	Y	302	1/1	0.83	0.27	-	65,65,65,65	0
3	CL	Y	301	1/1	0.95	0.08	-	65,65,65,65	0

6.5 Other polymers (i)

There are no such residues in this entry.