



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:43 PM UTC

PDB ID : 5HXB / pdb_00005hxb
Title : Cereblon in complex with DDB1, CC-885, and GSPT1
Authors : Chamberlain, P.P.; Matyskiela, M.; Pagarigan, B.
Deposited on : 2016-01-30
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

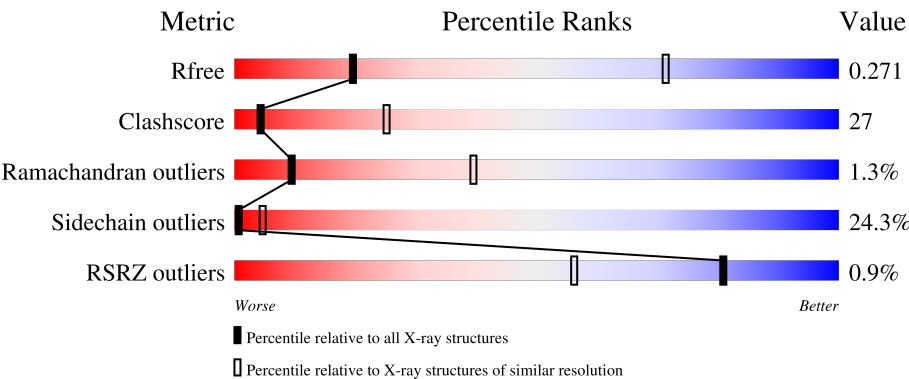
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	199	% 33%39%23%. .
1	X	199	% 28%41%21%9%. .
2	B	1140	% 49%36%9%. 6%
2	Y	1140	% 49%36%9%. 5%
3	C	406	% 47%35%9%. 9%

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Mol	Chain	Length	Quality of chain
3	Z	406	

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
4	ZN	C	501	-	-	X	-
5	85C	Z	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 25089 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 Eukaryotic peptide chain release factor GTP-binding subunit ERF3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	195	Total	C	N	O	S	0	0	0
			1481	941	254	275	11			
1	A	196	Total	C	N	O	S	0	0	0
			1441	919	245	267	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	436	GLY	-	expression tag	UNP P15170
X	437	SER	-	expression tag	UNP P15170
A	436	GLY	-	expression tag	UNP P15170
A	437	SER	-	expression tag	UNP P15170

- Molecule 2 is a protein called DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	1080	Total	C	N	O	S	0	0	0
			8178	5215	1369	1550	44			
2	B	1075	Total	C	N	O	S	0	0	0
			8096	5164	1351	1536	45			

- Molecule 3 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	380	Total	C	N	O	S	0	0	0
			2960	1891	502	544	23			
3	C	370	Total	C	N	O	S	0	0	0
			2869	1835	485	526	23			

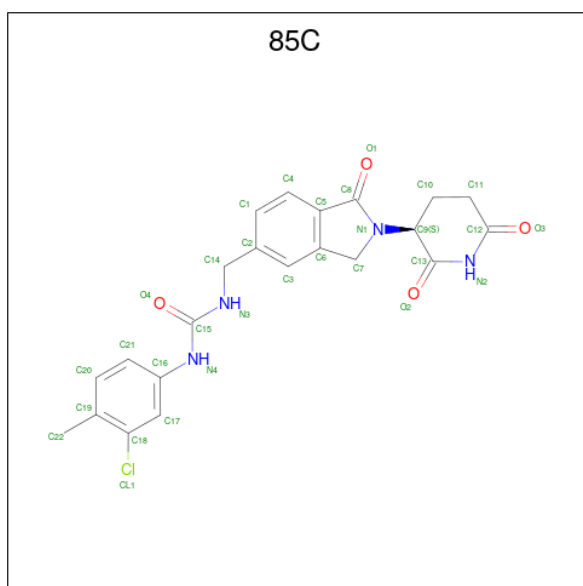
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	37	GLY	-	expression tag	UNP Q96SW2
Z	38	SER	-	expression tag	UNP Q96SW2
Z	39	MET	-	expression tag	UNP Q96SW2
C	37	GLY	-	expression tag	UNP Q96SW2
C	38	SER	-	expression tag	UNP Q96SW2
C	39	MET	-	expression tag	UNP Q96SW2

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Z	1	Total Zn 1 1	0	0
4	C	1	Total Zn 1 1	0	0

- Molecule 5 is 1-(3-chloro-4-methylphenyl)-3-({2-[(3S)-2,6-dioxopiperidin-3-yl]-1-oxo-2,3-dihydro-1H-isoindol-5-yl}methyl)urea (CCD ID: 85C) (formula: C₂₂H₂₁ClN₄O₄).

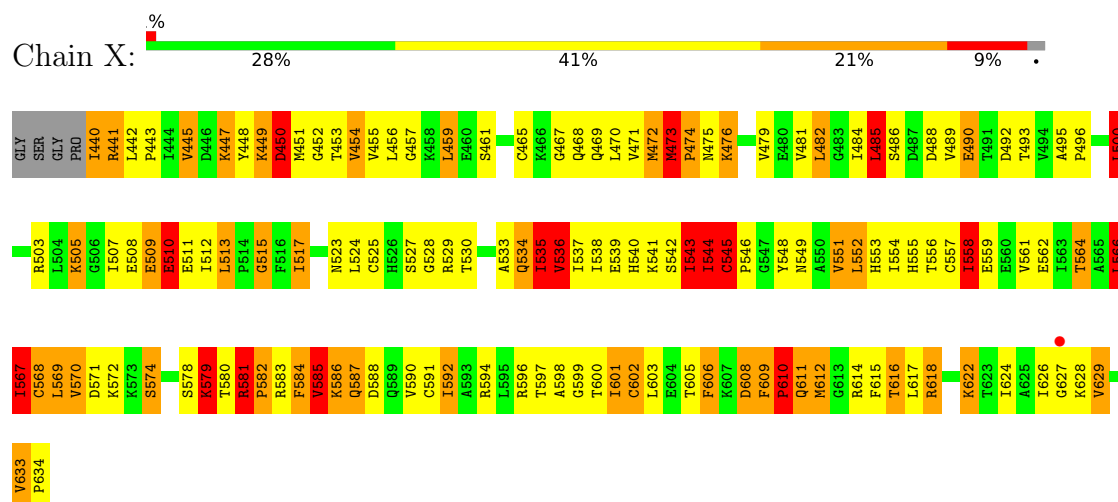


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Z	1	Total C Cl N O 31 22 1 4 4	0	0
5	C	1	Total C Cl N O 31 22 1 4 4	0	0

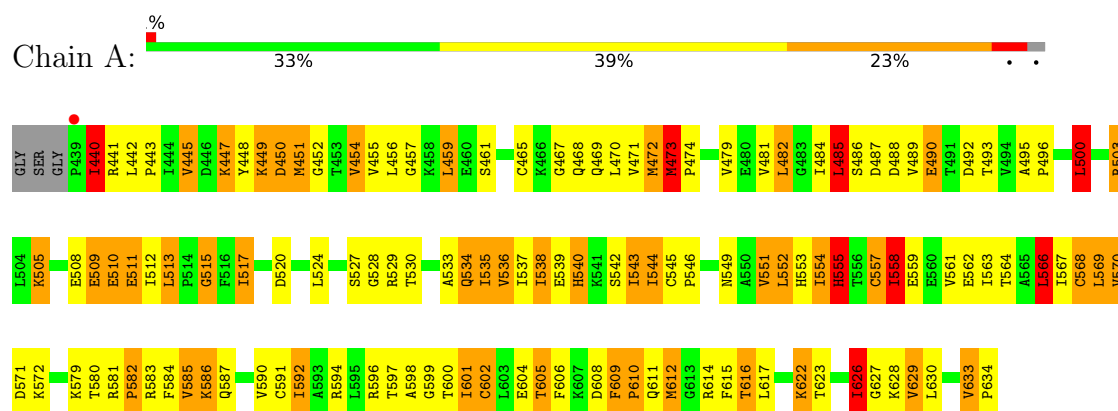
3 Residue-property plots

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

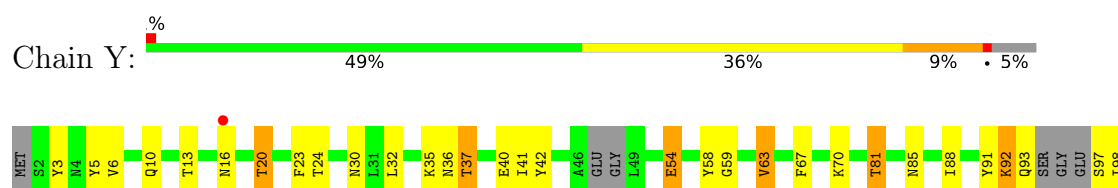
- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A

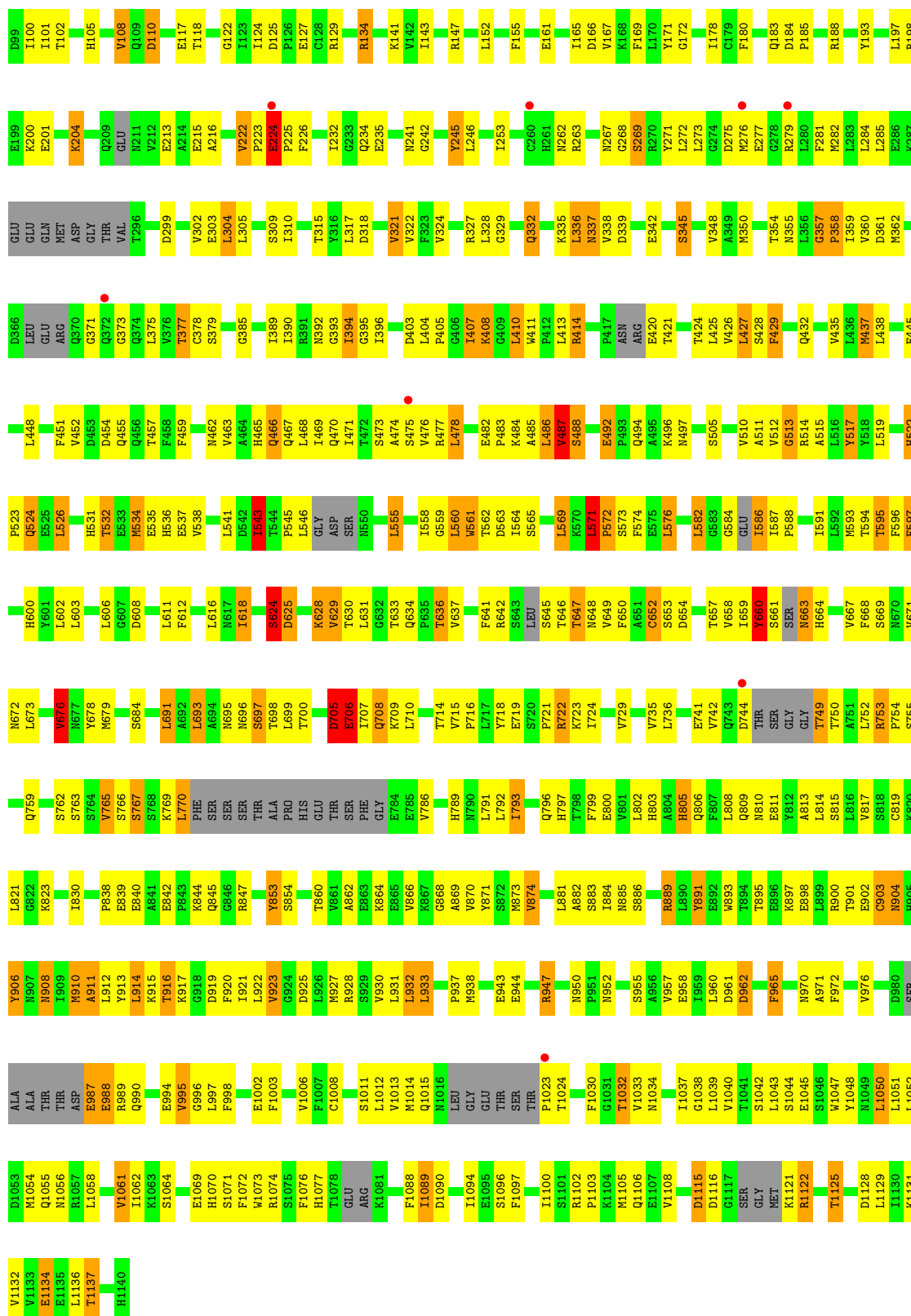


- Molecule 1: Eukaryotic peptide chain release factor GTP-binding subunit ERF3A



- Molecule 2: DNA damage-binding protein 1



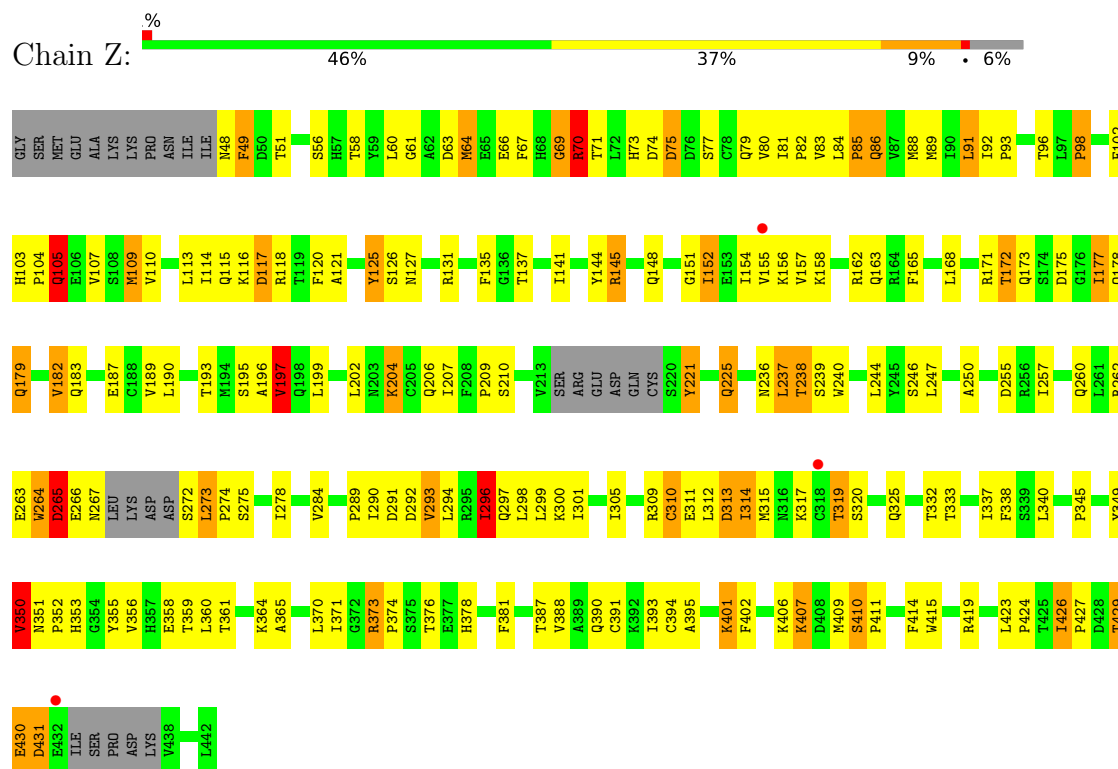


• Molecule 2: DNA damage-binding protein 1

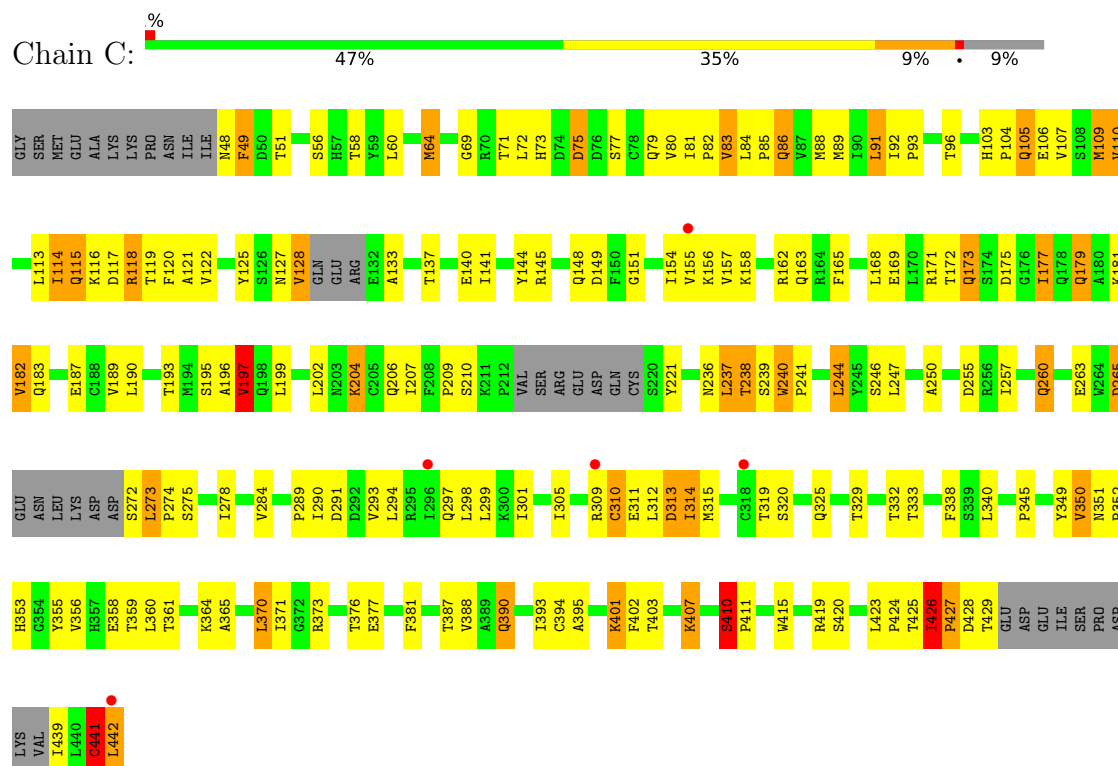




- Molecule 3: Protein cereblon



- Molecule 3: Protein cereblon



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.75Å 111.52Å 175.06Å 90.00° 95.81° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.00-3.60) 94.4 (50.00-3.60)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.224 , 0.273 0.225 , 0.271	Depositor DCC
R_{free} test set	3289 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.467	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 103.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25089	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.76% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 85C, ZN

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	1.28	6/1463 (0.4%)	1.24	16/1987 (0.8%)
1	X	1.35	7/1502 (0.5%)	1.37	19/2032 (0.9%)
2	B	1.14	21/8235 (0.3%)	1.13	28/11187 (0.3%)
2	Y	1.15	17/8319 (0.2%)	1.14	29/11295 (0.3%)
3	C	1.08	5/2937 (0.2%)	1.16	15/4003 (0.4%)
3	Z	1.12	6/3030 (0.2%)	1.20	15/4125 (0.4%)
All	All	1.16	62/25486 (0.2%)	1.17	122/34629 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	13
1	X	0	16
2	B	0	17
2	Y	0	19
3	C	0	5
3	Z	0	5
All	All	0	75

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	676	VAL	C-O	-8.93	1.14	1.24
2	Y	624	SER	C-O	8.64	1.30	1.24
2	B	676	VAL	C-O	-8.11	1.15	1.24
2	Y	769	LYS	CA-C	7.75	1.62	1.53
2	B	669	SER	CA-C	-7.55	1.44	1.52
2	Y	1024	THR	N-CA	7.38	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	441	CYS	CA-C	7.17	1.60	1.53
3	Z	114	ILE	CA-CB	-6.85	1.46	1.54
2	B	475	SER	C-O	-6.73	1.15	1.23
2	B	833	THR	CA-CB	6.70	1.63	1.53
2	Y	882	ALA	CA-C	-6.60	1.44	1.52
2	B	629	VAL	CA-CB	-6.58	1.48	1.55
1	A	614	ARG	CA-C	-6.58	1.44	1.52
2	B	853	TYR	CA-CB	-6.40	1.44	1.53
2	Y	394	ILE	CA-C	-6.30	1.44	1.52
2	Y	853	TYR	CA-CB	-6.23	1.45	1.53
1	A	583	ARG	CA-C	6.22	1.61	1.52
2	Y	487	VAL	CA-CB	-6.14	1.46	1.54
2	B	882	ALA	CA-C	-6.14	1.45	1.52
2	B	583	GLY	N-CA	6.11	1.51	1.44
3	C	173	GLN	CA-C	6.10	1.60	1.52
1	A	586	LYS	N-CA	6.04	1.52	1.45
1	X	586	LYS	N-CA	6.04	1.52	1.46
1	X	583	ARG	CA-C	6.03	1.61	1.52
2	B	345	SER	CA-C	6.00	1.59	1.52
2	Y	475	SER	C-O	-5.92	1.16	1.23
2	B	1013	VAL	CA-C	-5.85	1.45	1.52
2	Y	345	SER	CA-C	5.84	1.61	1.53
2	B	394	ILE	CA-C	-5.80	1.45	1.52
3	Z	431	ASP	N-CA	5.75	1.53	1.46
2	B	975	PHE	CA-C	-5.74	1.45	1.52
1	X	485	LEU	CA-CB	5.62	1.61	1.53
2	Y	976	VAL	C-O	-5.56	1.18	1.24
2	Y	793	ILE	C-O	-5.50	1.17	1.24
3	C	122	VAL	CA-CB	-5.46	1.47	1.54
1	X	568	CYS	N-CA	-5.40	1.39	1.46
1	A	441	ARG	CA-C	5.39	1.59	1.52
2	B	210	GLU	CA-C	5.39	1.59	1.52
2	B	921	ILE	N-CA	-5.39	1.39	1.46
2	B	811	GLU	CA-CB	5.37	1.61	1.53
1	A	622	LYS	CA-C	-5.32	1.46	1.52
3	Z	178	GLN	C-O	-5.29	1.17	1.23
2	Y	789	HIS	C-O	-5.28	1.17	1.23
2	B	976	VAL	C-O	-5.26	1.18	1.24
1	X	545	CYS	CA-C	5.23	1.59	1.52
2	B	965	PHE	C-O	-5.23	1.18	1.24
2	Y	478	LEU	C-O	-5.21	1.17	1.24
1	X	581	ARG	CA-C	-5.19	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1015	GLN	CA-C	5.19	1.59	1.52
3	C	151	GLY	CA-C	-5.18	1.44	1.51
3	C	329	THR	CA-CB	5.16	1.61	1.53
1	A	543	ILE	C-O	-5.16	1.18	1.24
2	B	1134	GLU	CA-CB	5.16	1.61	1.53
2	Y	862	ALA	N-CA	5.15	1.52	1.46
3	Z	429	THR	CA-CB	5.15	1.60	1.53
2	Y	629	VAL	CA-CB	-5.14	1.50	1.55
2	B	649	VAL	C-O	-5.14	1.18	1.24
1	X	579	LYS	CA-C	-5.09	1.47	1.53
3	Z	430	GLU	CA-C	5.07	1.58	1.52
2	B	527	ARG	C-O	-5.06	1.17	1.24
2	Y	1032	THR	CA-CB	-5.03	1.44	1.54
3	Z	85	PRO	C-O	5.01	1.29	1.23

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	606	PHE	N-CA-C	-12.43	95.12	110.41
1	X	510	GLU	N-CA-C	-11.94	92.26	108.74
2	Y	576	LEU	N-CA-C	10.62	122.44	111.07
2	Y	767	SER	N-CA-C	9.79	123.95	109.07
1	A	555	HIS	CB-CA-C	-9.67	103.12	115.89
2	Y	597	GLU	N-CA-C	-9.46	92.09	108.08
2	B	623	LEU	N-CA-C	-8.86	94.29	108.73
2	Y	394	ILE	N-CA-C	-8.71	94.88	107.77
3	Z	70	ARG	N-CA-C	8.68	123.60	112.92
2	B	1015	GLN	N-CA-C	8.59	122.22	109.24
1	X	473	MET	CA-C-N	8.53	130.51	119.84
1	X	473	MET	C-N-CA	8.53	130.51	119.84
3	C	426	ILE	CA-C-N	8.47	130.43	119.84
3	C	426	ILE	C-N-CA	8.47	130.43	119.84
1	A	485	LEU	N-CA-C	-8.40	95.03	108.73
3	Z	265	ASP	N-CA-C	8.31	128.51	110.80
2	Y	1013	VAL	N-CA-C	-8.23	96.52	107.88
2	B	210	GLU	N-CA-C	8.20	120.30	111.36
3	Z	296	ILE	CB-CA-C	-7.97	99.35	112.26
2	B	224	GLU	CA-C-N	-7.83	110.05	119.84
2	B	224	GLU	C-N-CA	-7.83	110.05	119.84
2	Y	224	GLU	CA-C-N	-7.71	110.20	119.84
2	Y	224	GLU	C-N-CA	-7.71	110.20	119.84
2	Y	357	GLY	CA-C-N	7.57	129.30	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	357	GLY	C-N-CA	7.57	129.30	119.84
2	B	209	GLN	N-CA-C	7.44	119.66	107.23
2	B	626	ARG	N-CA-C	-7.43	97.02	108.76
2	B	394	ILE	N-CA-C	-7.36	97.01	107.75
2	B	357	GLY	CA-C-N	7.34	129.01	119.84
2	B	357	GLY	C-N-CA	7.34	129.01	119.84
1	A	489	VAL	N-CA-C	7.28	119.22	108.45
1	A	440	ILE	N-CA-C	7.18	119.80	108.89
1	X	545	CYS	CA-C-N	7.16	127.14	119.76
1	X	545	CYS	C-N-CA	7.16	127.14	119.76
1	X	452	GLY	N-CA-C	-7.11	103.89	112.49
3	Z	117	ASP	N-CA-C	7.06	118.98	111.28
2	Y	910	MET	N-CA-C	-7.02	99.89	110.28
1	A	473	MET	CA-C-N	7.01	126.83	119.05
1	A	473	MET	C-N-CA	7.01	126.83	119.05
2	B	98	ILE	CB-CA-C	-6.92	100.39	110.63
2	Y	98	ILE	CB-CA-C	-6.86	100.47	110.63
2	B	627	LYS	N-CA-C	-6.83	97.97	108.76
1	X	445	VAL	CB-CA-C	-6.57	103.31	111.92
2	Y	102	THR	CB-CA-C	6.54	122.30	111.31
3	Z	350	VAL	CB-CA-C	-6.53	102.26	111.21
2	B	102	THR	CB-CA-C	6.51	122.25	111.31
3	C	350	VAL	CB-CA-C	-6.50	102.31	111.21
3	C	110	VAL	CB-CA-C	-6.49	103.54	112.04
2	B	1013	VAL	N-CA-C	-6.47	98.33	108.81
3	Z	152	ILE	N-CA-C	-6.30	98.58	108.86
1	A	551	VAL	CB-CA-C	-6.30	104.66	111.59
2	Y	1032	THR	N-CA-CB	-6.29	100.75	111.69
1	X	450	ASP	N-CA-C	-6.28	99.19	108.79
2	Y	1061	VAL	CB-CA-C	-6.26	104.35	111.55
3	Z	350	VAL	N-CA-CB	6.17	119.07	110.56
2	Y	819	CYS	N-CA-C	6.13	117.45	108.14
3	C	350	VAL	N-CA-CB	6.12	119.00	110.56
1	A	490	GLU	N-CA-C	6.10	119.10	110.50
3	C	105	GLN	N-CA-CB	6.07	119.04	109.82
1	X	543	ILE	CB-CA-C	-6.01	101.44	111.29
2	B	819	CYS	N-CA-C	5.96	117.20	108.14
2	B	625	ASP	N-CA-C	-5.95	98.13	110.80
3	C	86	GLN	CB-CA-C	-5.93	101.52	110.06
3	Z	86	GLN	CB-CA-C	-5.85	101.63	110.06
2	B	1032	THR	N-CA-CB	-5.85	101.51	111.69
3	Z	110	VAL	CB-CA-C	-5.84	104.39	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	608	ASP	N-CA-C	-5.83	104.92	111.28
2	B	909	ILE	N-CA-C	5.82	116.39	110.05
2	B	522	HIS	CA-C-N	-5.78	113.58	119.83
2	B	522	HIS	C-N-CA	-5.78	113.58	119.83
1	X	488	ASP	N-CA-C	-5.78	105.06	111.36
2	B	910	MET	N-CA-C	-5.76	99.89	109.46
1	A	445	VAL	CB-CA-C	-5.74	104.40	111.92
2	B	373	GLY	N-CA-C	5.73	120.72	112.82
2	B	909	ILE	CB-CA-C	-5.71	105.31	111.59
2	Y	469	ILE	N-CA-C	5.67	116.03	108.27
2	B	970	ASN	N-CA-C	5.67	118.23	110.24
3	C	83	VAL	CB-CA-C	-5.67	102.73	110.77
2	Y	1023	PRO	CA-C-N	5.66	131.48	122.59
2	Y	1023	PRO	C-N-CA	5.66	131.48	122.59
2	Y	970	ASN	N-CA-C	5.63	118.17	110.24
2	B	1013	VAL	CA-C-O	-5.63	115.31	121.28
1	A	538	ILE	N-CA-C	5.58	116.36	111.56
2	Y	1013	VAL	CA-C-O	-5.55	116.30	120.96
1	X	570	VAL	N-CA-C	5.51	115.81	108.27
3	Z	105	GLN	N-CA-CB	5.49	118.17	109.82
3	Z	264	TRP	N-CA-C	-5.40	105.50	111.71
1	X	551	VAL	CB-CA-C	-5.40	104.04	111.49
2	Y	706	GLU	N-CA-C	-5.38	101.11	109.72
3	Z	197	VAL	N-CA-CB	-5.37	105.33	112.26
2	B	469	ILE	N-CA-C	5.37	115.62	108.27
3	Z	426	ILE	CA-C-N	5.36	125.36	119.89
3	Z	426	ILE	C-N-CA	5.36	125.36	119.89
3	C	197	VAL	N-CA-CB	-5.34	105.37	112.26
1	X	585	VAL	CA-CB-CG2	5.30	119.41	110.40
1	A	570	VAL	N-CA-C	5.30	115.53	108.27
2	Y	373	GLY	N-CA-C	5.29	118.96	112.14
1	A	543	ILE	N-CA-C	5.27	117.05	109.51
1	A	581	ARG	N-CA-C	-5.25	102.40	110.01
1	A	609	PHE	CA-C-N	-5.24	113.28	119.84
1	A	609	PHE	C-N-CA	-5.24	113.28	119.84
3	C	410	SER	CA-C-N	5.24	126.39	119.84
3	C	410	SER	C-N-CA	5.24	126.39	119.84
1	A	511	GLU	N-CA-C	-5.22	106.86	113.18
2	Y	597	GLU	CB-CA-C	-5.21	110.58	116.63
3	C	114	ILE	CB-CA-C	-5.21	105.10	112.14
2	Y	522	HIS	CA-C-N	-5.21	114.20	119.83
2	Y	522	HIS	C-N-CA	-5.21	114.20	119.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Z	263	GLU	N-CA-C	-5.19	105.63	111.28
3	C	390	GLN	N-CA-C	5.19	117.07	109.24
2	Y	765	VAL	CB-CA-C	5.18	119.98	110.71
2	Y	911	ALA	N-CA-C	5.15	117.84	110.68
2	Y	923	VAL	CB-CA-C	-5.14	103.00	110.81
1	X	536	VAL	CG1-CB-CG2	5.13	122.08	110.80
2	B	6	VAL	CB-CA-C	-5.12	103.88	110.84
2	Y	705	ASP	N-CA-CB	5.11	117.81	109.69
1	X	610	PRO	CA-N-CD	-5.10	104.86	112.00
3	C	426	ILE	C-N-CD	-5.10	104.10	125.00
1	X	567	ILE	CB-CA-C	-5.08	102.96	111.29
2	B	877	ASN	CB-CA-C	-5.08	104.52	111.73
3	C	240	TRP	N-CA-C	5.02	116.39	108.55
1	X	535	ILE	N-CA-CB	-5.01	107.64	112.65

There are no chirality outliers.

All (75) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	449	LYS	Peptide
1	A	451	MET	Peptide
1	A	472	MET	Peptide
1	A	500	LEU	Peptide
1	A	509	GLU	Peptide
1	A	515	GLY	Peptide
1	A	534	GLN	Peptide
1	A	555	HIS	Peptide
1	A	564	THR	Peptide
1	A	566	LEU	Peptide
1	A	601	ILE	Peptide
1	A	626	ILE	Peptide
1	A	633	VAL	Peptide
2	B	1015	GLN	Peptide
2	B	1116	ASP	Peptide
2	B	209	GLN	Peptide
2	B	224	GLU	Peptide
2	B	332	GLN	Peptide
2	B	345	SER	Peptide
2	B	357	GLY	Peptide
2	B	465	HIS	Sidechain
2	B	476	VAL	Peptide
2	B	482	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	571	LEU	Peptide
2	B	660	TYR	Mainchain,Peptide
2	B	664	HIS	Peptide
2	B	805	HIS	Sidechain
2	B	853	TYR	Sidechain
2	B	965	PHE	Sidechain
3	C	103	HIS	Sidechain
3	C	181	LYS	Peptide
3	C	410	SER	Peptide
3	C	426	ILE	Peptide
3	C	441	CYS	Peptide
1	X	472	MET	Peptide
1	X	473	MET	Peptide
1	X	500	LEU	Peptide
1	X	509	GLU	Peptide
1	X	515	GLY	Peptide
1	X	534	GLN	Peptide
1	X	543	ILE	Mainchain
1	X	544	ILE	Peptide
1	X	545	CYS	Peptide
1	X	564	THR	Peptide
1	X	566	LEU	Peptide
1	X	574	SER	Peptide
1	X	587	GLN	Peptide
1	X	601	ILE	Peptide
1	X	603	LEU	Peptide
1	X	633	VAL	Peptide
2	Y	1014	MET	Peptide
2	Y	224	GLU	Peptide
2	Y	332	GLN	Peptide
2	Y	337	ASN	Mainchain
2	Y	338	VAL	Peptide
2	Y	342	GLU	Peptide
2	Y	345	SER	Peptide
2	Y	357	GLY	Peptide
2	Y	392	ASN	Peptide
2	Y	482	GLU	Peptide
2	Y	571	LEU	Peptide
2	Y	660	TYR	Mainchain,Peptide
2	Y	664	HIS	Peptide
2	Y	706	GLU	Peptide
2	Y	805	HIS	Sidechain

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Mol	Chain	Res	Type	Group
2	Y	891	TYR	Sidechain
2	Y	950	ASN	Peptide
2	Y	965	PHE	Sidechain
3	Z	125	TYR	Peptide
3	Z	151	GLY	Peptide
3	Z	410	SER	Peptide
3	Z	430	GLU	Peptide
3	Z	69	GLY	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1441	0	1439	160	2
1	X	1481	0	1519	216	0
2	B	8096	0	7807	358	0
2	Y	8178	0	7930	358	0
3	C	2869	0	2758	131	0
3	Z	2960	0	2851	151	2
4	C	1	0	0	2	0
4	Z	1	0	0	0	0
5	C	31	0	0	4	0
5	Z	31	0	0	10	0
All	All	25089	0	24304	1326	2

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 27.

All (1326) 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:X:606:PHE:CD2	1:X:628:LYS:HG2	1.44	1.49
1:A:606:PHE:CE2	1:A:628:LYS:HG2	1.50	1.47
1:A:606:PHE:CD2	1:A:628:LYS:HG2	1.48	1.45
1:X:606:PHE:CE2	1:X:628:LYS:HG2	1.64	1.30
3:Z:352:PRO:HG3	3:Z:378:HIS:ND1	1.44	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:606:PHE:CD2	1:X:628:LYS:CG	2.15	1.28
1:X:628:LYS:HG3	5:Z:502:85C:CL1	1.73	1.25
1:A:606:PHE:CD2	1:A:628:LYS:CG	2.19	1.23
1:X:606:PHE:HD2	1:X:628:LYS:CG	1.49	1.20
1:X:540:HIS:CE1	1:X:542:SER:H	1.66	1.13
1:X:554:ILE:HG22	1:X:555:HIS:HD2	1.13	1.11
1:A:606:PHE:HD2	1:A:628:LYS:CB	1.62	1.11
2:Y:35:LYS:HE3	2:Y:40:GLU:OE1	1.50	1.11
1:X:453:THR:O	1:X:503:ARG:HG3	1.52	1.08
3:Z:352:PRO:CG	3:Z:378:HIS:ND1	2.17	1.07
1:A:606:PHE:CE2	1:A:628:LYS:CG	2.37	1.05
1:X:441:ARG:HG2	1:X:612:MET:SD	1.98	1.03
1:A:606:PHE:HD2	1:A:628:LYS:CG	1.61	1.02
1:X:449:LYS:NZ	1:X:510:GLU:OE2	1.96	0.99
1:A:606:PHE:HD2	1:A:628:LYS:HB3	1.27	0.99
1:A:540:HIS:CD2	1:A:544:ILE:HG22	1.98	0.98
3:C:199:LEU:HD21	3:C:237:LEU:HD11	1.42	0.98
1:X:554:ILE:HG22	1:X:555:HIS:CD2	1.99	0.96
3:Z:265:ASP:OD1	3:Z:266:GLU:N	1.97	0.96
2:Y:595:THR:OG1	2:Y:600:HIS:CE1	2.19	0.95
1:X:606:PHE:HD2	1:X:628:LYS:CB	1.78	0.95
2:Y:595:THR:OG1	2:Y:600:HIS:ND1	1.98	0.95
1:X:628:LYS:CG	5:Z:502:85C:CL1	2.53	0.93
2:Y:741:GLU:OE1	2:Y:749:THR:HG23	1.68	0.92
1:X:606:PHE:CE2	1:X:628:LYS:CG	2.47	0.92
1:A:485:LEU:HA	1:A:490:GLU:CB	2.01	0.91
2:B:808:LEU:HD12	2:B:808:LEU:H	1.34	0.91
1:A:606:PHE:HE2	1:A:628:LYS:HG2	1.28	0.91
1:X:552:LEU:HD11	1:X:554:ILE:CG1	2.01	0.91
2:Y:660:TYR:O	2:Y:667:VAL:N	2.04	0.90
3:Z:173:GLN:CB	3:Z:179:GLN:NE2	2.35	0.90
3:C:125:TYR:CE1	3:C:133:ALA:HB2	2.06	0.90
1:A:540:HIS:CD2	1:A:544:ILE:CG2	2.55	0.90
1:X:467:GLY:HA2	1:X:481:VAL:O	1.72	0.89
3:Z:401:LYS:HG3	3:Z:415:TRP:CE2	2.08	0.89
2:B:660:TYR:O	2:B:667:VAL:N	2.06	0.88
3:C:115:GLN:HE21	3:C:115:GLN:HA	1.38	0.88
1:A:467:GLY:HA2	1:A:481:VAL:O	1.72	0.88
2:Y:988:GLU:OE1	2:Y:988:GLU:HA	1.73	0.88
1:A:606:PHE:CD2	1:A:628:LYS:CB	2.55	0.87
2:Y:908:ASN:OD1	2:Y:908:ASN:N	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:PHE:CD2	1:A:628:LYS:HB3	2.09	0.87
1:X:540:HIS:CE1	1:X:542:SER:N	2.43	0.86
3:Z:352:PRO:CD	3:Z:378:HIS:ND1	2.37	0.86
1:X:486:SER:O	1:X:489:VAL:O	1.93	0.86
2:B:988:GLU:HA	2:B:988:GLU:OE1	1.76	0.85
1:X:605:THR:OG1	1:X:608:ASP:HB2	1.75	0.85
1:X:451:MET:CB	1:X:503:ARG:HD3	2.06	0.85
3:C:125:TYR:HE1	3:C:133:ALA:HB2	1.41	0.84
2:Y:629:VAL:HG11	2:Y:668:PHE:CE2	2.12	0.84
3:C:394:CYS:HG	4:C:501:ZN:ZN	0.54	0.84
1:A:558:ILE:HG22	1:A:558:ILE:O	1.76	0.84
1:X:540:HIS:ND1	1:X:542:SER:N	2.26	0.83
2:Y:997:LEU:HB3	2:Y:1076:PHE:HD2	1.42	0.83
1:A:512:ILE:C	1:A:513:LEU:HD12	2.04	0.83
1:A:605:THR:HG22	1:A:630:LEU:O	1.77	0.83
3:C:425:THR:HG22	3:C:426:ILE:H	1.44	0.82
1:A:538:ILE:HD11	1:A:623:THR:HG22	1.60	0.82
1:X:515:GLY:HA2	1:X:556:THR:OG1	1.80	0.82
1:A:472:MET:HE1	1:A:512:ILE:HG22	1.62	0.82
1:A:515:GLY:HA3	1:A:557:CYS:HB2	1.61	0.82
3:Z:352:PRO:N	3:Z:378:HIS:HE1	1.79	0.81
1:X:510:GLU:O	1:X:511:GLU:HB3	1.81	0.80
2:Y:327:ARG:HD3	3:Z:199:LEU:HD22	1.63	0.80
3:C:394:CYS:SG	4:C:501:ZN:ZN	1.69	0.80
3:Z:352:PRO:N	3:Z:378:HIS:CE1	2.48	0.80
2:Y:204:LYS:HA	2:Y:204:LYS:HE2	1.63	0.80
3:Z:199:LEU:HD21	3:Z:237:LEU:HD11	1.62	0.80
1:X:489:VAL:HG22	1:X:490:GLU:O	1.82	0.79
3:Z:70:ARG:H	3:Z:70:ARG:HD2	1.47	0.79
3:C:401:LYS:HG3	3:C:415:TRP:CE2	2.18	0.79
2:Y:451:PHE:CE2	2:Y:470:GLN:HB2	2.18	0.79
1:X:558:ILE:O	1:X:558:ILE:HG22	1.81	0.78
1:X:533:ALA:HB1	1:X:628:LYS:O	1.83	0.78
2:B:889:ARG:HD3	2:B:901:THR:HG23	1.66	0.78
3:Z:401:LYS:HG3	3:Z:415:TRP:NE1	1.98	0.78
2:Y:118:THR:HG21	2:Y:165:ILE:O	1.84	0.78
1:X:548:TYR:OH	1:X:624:ILE:CD1	2.32	0.77
2:B:900:ARG:HG3	2:B:900:ARG:O	1.80	0.77
2:B:546:LEU:O	2:B:549:SER:N	2.17	0.77
3:C:426:ILE:HG12	3:C:427:PRO:HA	1.65	0.77
1:X:606:PHE:HD2	1:X:628:LYS:HB3	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:THR:HG21	2:B:165:ILE:O	1.85	0.77
1:X:540:HIS:HE1	1:X:542:SER:OG	1.68	0.77
1:X:605:THR:HA	1:X:629:VAL:HG22	1.65	0.77
2:Y:889:ARG:HD3	2:Y:901:THR:HG23	1.66	0.77
3:Z:165:PHE:CD1	3:Z:182:VAL:CG2	2.67	0.76
2:Y:35:LYS:HE3	2:Y:40:GLU:CD	2.10	0.76
3:C:127:ASN:ND2	3:C:128:VAL:H	1.83	0.76
1:A:557:CYS:SG	1:A:558:ILE:N	2.57	0.76
2:Y:753:ARG:HB2	2:Y:754:PRO:HD2	1.65	0.76
3:Z:273:LEU:HB2	3:Z:274:PRO:CD	2.15	0.76
3:C:48:ASN:HA	3:C:410:SER:HB3	1.66	0.76
2:Y:118:THR:HG22	2:Y:118:THR:O	1.84	0.76
3:C:273:LEU:HB2	3:C:274:PRO:CD	2.16	0.76
1:X:485:LEU:HD11	1:X:503:ARG:NH2	2.00	0.76
3:Z:125:TYR:HE2	3:Z:131:ARG:HA	1.49	0.76
1:A:552:LEU:HD11	1:A:554:ILE:HG12	1.66	0.76
1:X:449:LYS:HZ1	1:X:510:GLU:CD	1.93	0.75
1:A:543:ILE:HG22	1:A:586:LYS:HG2	1.68	0.75
2:Y:997:LEU:HB3	2:Y:1076:PHE:CD2	2.22	0.75
2:Y:35:LYS:CE	2:Y:40:GLU:OE1	2.33	0.75
2:Y:928:ARG:HD2	2:Y:928:ARG:O	1.86	0.75
1:X:441:ARG:CZ	1:X:525:CYS:SG	2.74	0.75
2:B:118:THR:O	2:B:118:THR:HG22	1.86	0.75
1:A:633:VAL:HG12	1:A:634:PRO:CD	2.16	0.75
2:Y:927:MET:O	2:Y:928:ARG:HB3	1.85	0.75
2:Y:900:ARG:O	2:Y:900:ARG:HG3	1.84	0.75
1:X:474:PRO:O	1:X:476:LYS:HE2	1.87	0.74
3:Z:48:ASN:HA	3:Z:410:SER:HB3	1.69	0.74
1:X:554:ILE:CG2	1:X:555:HIS:HD2	1.98	0.74
2:B:883:SER:HB2	2:B:911:ALA:HB3	1.68	0.74
3:C:313:ASP:OD2	3:C:441:CYS:O	2.06	0.74
2:B:304:LEU:HG	2:B:304:LEU:O	1.86	0.74
2:B:753:ARG:HB2	2:B:754:PRO:HD2	1.68	0.74
2:B:972:PHE:CZ	3:C:196:ALA:O	2.40	0.74
1:A:540:HIS:NE2	1:A:544:ILE:HG22	2.01	0.74
3:C:175:ASP:OD1	3:C:177:ILE:HB	1.88	0.74
3:Z:351:ASN:C	3:Z:378:HIS:HE1	1.96	0.73
2:Y:928:ARG:NH2	2:Y:994:GLU:OE2	2.21	0.73
2:Y:987:GLU:OE1	2:Y:989:ARG:NH2	2.21	0.73
2:B:327:ARG:HD3	3:C:199:LEU:HD22	1.68	0.73
2:B:997:LEU:HB3	2:B:1076:PHE:HD2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:59:GLY:HA2	2:Y:1073:TRP:CZ3	2.23	0.73
3:Z:352:PRO:HD3	3:Z:378:HIS:ND1	2.03	0.73
1:X:633:VAL:HG12	1:X:634:PRO:HD2	1.70	0.73
1:X:512:ILE:C	1:X:513:LEU:HD12	2.14	0.73
2:Y:304:LEU:O	2:Y:304:LEU:HG	1.87	0.73
3:Z:165:PHE:CD1	3:Z:182:VAL:HG22	2.22	0.73
1:A:604:GLU:HG3	1:A:612:MET:HE2	1.70	0.73
1:X:548:TYR:OH	1:X:624:ILE:HD13	1.88	0.73
1:X:606:PHE:CE2	1:X:628:LYS:HD2	2.24	0.73
3:Z:352:PRO:CD	3:Z:378:HIS:CE1	2.72	0.73
1:A:508:GLU:HG3	1:A:511:GLU:HB3	1.70	0.73
1:A:533:ALA:HB1	1:A:628:LYS:O	1.88	0.73
1:A:535:ILE:HG22	1:A:535:ILE:O	1.89	0.72
3:Z:69:GLY:O	3:Z:118:ARG:NH2	2.21	0.72
2:B:928:ARG:HD2	2:B:928:ARG:O	1.89	0.72
2:Y:660:TYR:HB2	2:Y:661:SER:HB3	1.70	0.72
2:B:3:TYR:CE2	2:B:1045:GLU:HG3	2.25	0.72
2:B:808:LEU:CD1	2:B:847:ARG:HH21	2.03	0.72
1:A:447:LYS:H	1:A:447:LYS:HD3	1.55	0.72
2:Y:118:THR:HB	2:Y:134:ARG:NH2	2.05	0.71
2:B:596:PHE:HD2	2:B:601:TYR:HD2	1.38	0.71
1:X:606:PHE:CD2	1:X:628:LYS:CD	2.73	0.71
1:A:472:MET:HE1	1:A:512:ILE:CG2	2.19	0.71
2:B:928:ARG:NH2	2:B:994:GLU:OE2	2.23	0.71
3:Z:144:TYR:HE1	3:Z:155:VAL:HG13	1.55	0.71
1:A:450:ASP:O	1:A:452:GLY:N	2.24	0.71
3:C:114:ILE:HG13	3:C:144:TYR:CE2	2.25	0.71
2:B:927:MET:O	2:B:928:ARG:HB3	1.89	0.71
1:X:606:PHE:CD2	1:X:628:LYS:HB3	2.25	0.71
2:Y:3:TYR:CE2	2:Y:1045:GLU:HG3	2.26	0.71
2:B:59:GLY:HA2	2:B:1073:TRP:CZ3	2.26	0.71
2:B:660:TYR:HB2	2:B:661:SER:HB3	1.72	0.71
1:X:453:THR:O	1:X:454:VAL:HG22	1.91	0.71
2:Y:118:THR:HB	2:Y:134:ARG:HH22	1.56	0.71
2:B:629:VAL:HG11	2:B:668:PHE:CE2	2.26	0.70
2:B:661:SER:OG	2:B:663:ASN:ND2	2.23	0.70
2:B:808:LEU:HD12	2:B:808:LEU:N	2.06	0.70
2:Y:471:ILE:HG23	2:Y:476:VAL:HG22	1.73	0.70
2:B:808:LEU:HD11	2:B:847:ARG:NH2	2.06	0.70
1:X:535:ILE:HG22	1:X:535:ILE:O	1.90	0.70
1:X:618:ARG:HG3	1:X:622:LYS:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:537:ILE:HG22	1:X:587:GLN:HA	1.74	0.70
1:X:447:LYS:H	1:X:447:LYS:HD3	1.56	0.70
2:B:997:LEU:HB3	2:B:1076:PHE:CD2	2.27	0.70
2:B:471:ILE:HG23	2:B:476:VAL:HG22	1.73	0.70
1:X:515:GLY:CA	1:X:556:THR:OG1	2.39	0.70
2:Y:906:TYR:CD1	2:Y:906:TYR:N	2.58	0.70
1:A:445:VAL:HG23	1:A:457:GLY:HA2	1.74	0.70
2:Y:714:THR:HG22	2:Y:716:PRO:HD3	1.73	0.69
2:Y:716:PRO:HB3	2:Y:718:TYR:CE1	2.27	0.69
5:C:502:85C:C20	1:A:628:LYS:HD3	2.22	0.69
1:A:605:THR:CG2	1:A:630:LEU:O	2.40	0.69
2:B:118:THR:HB	2:B:134:ARG:HH22	1.58	0.69
2:B:118:THR:HB	2:B:134:ARG:NH2	2.07	0.69
2:Y:913:TYR:HH	3:Z:240:TRP:HZ3	1.40	0.69
1:A:484:ILE:O	1:A:490:GLU:CB	2.41	0.69
1:X:453:THR:HG22	1:X:454:VAL:N	2.08	0.69
2:Y:629:VAL:HG11	2:Y:668:PHE:HE2	1.56	0.69
3:Z:273:LEU:HB2	3:Z:274:PRO:HD2	1.75	0.69
1:X:610:PRO:HD2	1:X:611:GLN:H	1.58	0.68
2:B:987:GLU:OE1	2:B:989:ARG:NH2	2.26	0.68
1:X:535:ILE:O	1:X:535:ILE:CG2	2.42	0.68
3:C:75:ASP:OD1	3:C:75:ASP:N	2.26	0.68
1:A:535:ILE:O	1:A:535:ILE:CG2	2.41	0.68
3:C:127:ASN:HD22	3:C:128:VAL:H	1.39	0.68
2:B:5:TYR:CE2	2:B:1136:LEU:HD22	2.28	0.68
3:C:273:LEU:HB2	3:C:274:PRO:HD2	1.74	0.68
2:B:914:LEU:HD21	2:B:921:ILE:HG23	1.75	0.68
3:C:427:PRO:O	3:C:428:ASP:HB2	1.93	0.68
2:Y:914:LEU:HD21	2:Y:921:ILE:HG23	1.76	0.68
2:B:715:VAL:HG12	2:B:715:VAL:O	1.92	0.68
1:X:606:PHE:CE2	1:X:628:LYS:CD	2.77	0.68
2:Y:563:ASP:OD1	2:Y:565:SER:HB3	1.93	0.68
3:Z:173:GLN:CB	3:Z:179:GLN:HE21	2.04	0.68
1:A:534:GLN:O	1:A:627:GLY:HA2	1.94	0.68
3:C:144:TYR:HE1	3:C:155:VAL:HG13	1.60	0.67
3:Z:262:ARG:O	3:Z:265:ASP:HA	1.93	0.67
3:Z:264:TRP:CD1	3:Z:337:ILE:HG22	2.30	0.67
3:C:353:HIS:NE2	5:C:502:85C:O4	2.25	0.67
2:Y:715:VAL:HG12	2:Y:715:VAL:O	1.93	0.67
2:B:20:THR:HG23	2:B:315:THR:HG21	1.77	0.67
2:B:714:THR:HG22	2:B:716:PRO:HD3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:716:PRO:HB3	2:B:718:TYR:CE1	2.30	0.67
1:A:605:THR:OG1	1:A:608:ASP:HB2	1.95	0.67
1:X:473:MET:HE1	1:X:476:LYS:CD	2.25	0.67
2:B:414:ARG:N	2:B:462:ASN:HD21	1.92	0.67
1:A:558:ILE:O	1:A:558:ILE:CG2	2.42	0.66
2:Y:537:GLU:HG3	2:Y:561:TRP:CG	2.31	0.66
2:B:914:LEU:HD21	2:B:921:ILE:CG2	2.25	0.66
3:Z:70:ARG:H	3:Z:70:ARG:CD	2.08	0.66
2:B:913:TYR:CE1	3:C:240:TRP:HH2	2.13	0.66
1:A:510:GLU:HG2	1:A:510:GLU:O	1.96	0.66
1:X:606:PHE:CD2	1:X:628:LYS:CB	2.66	0.66
2:Y:404:LEU:HD22	2:Y:407:ILE:HD11	1.77	0.66
1:A:606:PHE:HD1	1:A:606:PHE:O	1.79	0.66
1:X:473:MET:HE1	1:X:476:LYS:HD3	1.77	0.66
2:B:166:ASP:OD2	3:C:204:LYS:HD3	1.95	0.66
1:X:552:LEU:HD11	1:X:554:ILE:HG12	1.77	0.66
2:B:744:ASP:CB	2:B:749:THR:N	2.59	0.66
1:X:552:LEU:HD11	1:X:554:ILE:HG13	1.78	0.65
1:X:606:PHE:HA	1:X:609:PHE:O	1.96	0.65
3:Z:264:TRP:NE1	3:Z:337:ILE:HG22	2.11	0.65
2:B:541:LEU:HD23	2:B:558:ILE:CD1	2.26	0.65
3:Z:75:ASP:OD1	3:Z:75:ASP:N	2.29	0.65
1:X:445:VAL:HG23	1:X:457:GLY:HA2	1.77	0.65
2:Y:20:THR:HG23	2:Y:315:THR:HG21	1.76	0.65
1:A:537:ILE:HG22	1:A:587:GLN:HA	1.79	0.65
1:A:633:VAL:HG12	1:A:634:PRO:HD2	1.78	0.65
3:C:165:PHE:CD1	3:C:182:VAL:CG2	2.80	0.65
2:Y:569:LEU:HD13	2:Y:576:LEU:CB	2.27	0.65
2:Y:913:TYR:CE1	3:Z:240:TRP:HH2	2.15	0.65
1:A:552:LEU:HD11	1:A:554:ILE:CG1	2.27	0.65
2:B:928:ARG:HB3	2:B:952:ASN:O	1.97	0.64
2:Y:275:ASP:OD2	2:Y:279:ARG:HB2	1.96	0.64
3:C:117:ASP:O	3:C:119:THR:N	2.31	0.64
1:A:566:LEU:CD2	1:A:585:VAL:HG12	2.28	0.64
1:X:615:PHE:HE1	1:X:617:LEU:CD1	2.10	0.64
2:B:245:TYR:CD1	2:B:245:TYR:C	2.76	0.64
2:Y:914:LEU:HD21	2:Y:921:ILE:CG2	2.28	0.64
1:A:606:PHE:CE2	1:A:628:LYS:CD	2.80	0.64
3:Z:63:ASP:O	3:Z:145:ARG:NH2	2.31	0.64
2:Y:805:HIS:CD2	2:Y:806:GLN:N	2.66	0.64
2:B:394:ILE:HD11	2:B:669:SER:CB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:LEU:HD22	2:B:407:ILE:HD11	1.78	0.64
3:Z:310:CYS:O	3:Z:314:ILE:HD12	1.98	0.64
2:B:451:PHE:CE2	2:B:470:GLN:HB2	2.32	0.64
3:C:60:LEU:HB3	3:C:64:MET:HE1	1.78	0.64
3:C:265:ASP:OD1	3:C:265:ASP:C	2.40	0.63
2:Y:394:ILE:HD12	2:Y:658:VAL:HB	1.80	0.63
2:Y:913:TYR:CE1	3:Z:240:TRP:CH2	2.87	0.63
1:A:545:CYS:HB3	1:A:546:PRO:HD2	1.79	0.63
2:Y:541:LEU:HD23	2:Y:558:ILE:CD1	2.27	0.63
2:B:511:ALA:HB1	2:B:538:VAL:HG11	1.80	0.63
3:Z:266:GLU:HA	3:Z:266:GLU:OE1	1.96	0.63
2:B:394:ILE:HD12	2:B:658:VAL:HB	1.80	0.63
3:C:401:LYS:HG3	3:C:415:TRP:NE1	2.12	0.63
1:X:633:VAL:HG12	1:X:634:PRO:CD	2.28	0.63
2:B:913:TYR:CE1	3:C:240:TRP:CH2	2.86	0.63
1:X:601:ILE:HG22	1:X:602:CYS:N	2.12	0.63
3:C:353:HIS:ND1	1:A:572:LYS:HD3	2.14	0.63
1:X:441:ARG:HB2	1:X:461:SER:HB3	1.81	0.63
1:X:558:ILE:O	1:X:558:ILE:CG2	2.46	0.63
2:Y:413:LEU:HB3	2:Y:424:THR:HB	1.80	0.63
2:B:903:CYS:SG	2:B:904:ASN:N	2.72	0.63
3:Z:135:PHE:CE1	3:Z:300:LYS:HD3	2.33	0.63
1:A:486:SER:H	1:A:490:GLU:HA	1.63	0.63
2:Y:558:ILE:HG22	2:Y:559:GLY:N	2.13	0.63
3:C:165:PHE:CD1	3:C:182:VAL:HG22	2.34	0.63
3:C:310:CYS:O	3:C:314:ILE:HD12	1.99	0.63
3:C:425:THR:CG2	3:C:426:ILE:H	2.12	0.63
2:Y:928:ARG:HB3	2:Y:952:ASN:O	1.99	0.62
3:C:49:PHE:CE1	3:C:340:LEU:HD22	2.33	0.62
2:B:482:GLU:HA	2:B:482:GLU:OE2	1.99	0.62
1:X:628:LYS:HD3	5:Z:502:85C:C17	2.29	0.62
2:Y:1054:MET:HE1	2:Y:1129:LEU:HG	1.82	0.62
2:Y:245:TYR:CD1	2:Y:245:TYR:C	2.77	0.62
3:Z:257:ILE:HG23	3:Z:315:MET:HE1	1.80	0.62
2:Y:361:ASP:OD1	2:Y:362:MET:N	2.32	0.62
2:Y:634:GLN:CB	2:Y:654:ASP:OD1	2.46	0.62
2:B:596:PHE:HD2	2:B:601:TYR:CD2	2.17	0.62
3:Z:60:LEU:HB3	3:Z:64:MET:HE1	1.82	0.62
1:X:515:GLY:HA3	1:X:557:CYS:HB2	1.81	0.62
1:X:537:ILE:CG2	1:X:587:GLN:HA	2.30	0.62
1:X:606:PHE:HE2	1:X:628:LYS:HG2	1.57	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:802:LEU:HD23	2:Y:802:LEU:N	2.13	0.62
1:A:606:PHE:CE2	1:A:628:LYS:HD2	2.34	0.62
3:Z:144:TYR:CE1	3:Z:155:VAL:HG13	2.35	0.62
2:Y:403:ASP:O	2:B:768:SER:OG	2.09	0.61
3:Z:265:ASP:CG	3:Z:266:GLU:HG2	2.25	0.61
3:Z:352:PRO:CG	3:Z:378:HIS:CE1	2.84	0.61
2:B:361:ASP:OD1	2:B:362:MET:N	2.32	0.61
1:A:487:ASP:CG	1:A:488:ASP:H	2.08	0.61
3:C:257:ILE:HG23	3:C:315:MET:HE1	1.80	0.61
3:Z:264:TRP:NE1	3:Z:337:ILE:CG2	2.64	0.61
1:A:510:GLU:O	1:A:510:GLU:CG	2.47	0.61
1:X:441:ARG:CB	1:X:461:SER:HB3	2.30	0.61
3:C:115:GLN:HA	3:C:115:GLN:NE2	2.14	0.61
1:X:610:PRO:CD	1:X:611:GLN:H	2.13	0.61
2:Y:642:ARG:NH2	2:Y:645:SER:O	2.34	0.61
2:Y:511:ALA:HB1	2:Y:538:VAL:HG11	1.82	0.61
2:B:558:ILE:HG22	2:B:559:GLY:N	2.16	0.61
2:B:275:ASP:OD2	2:B:279:ARG:HB2	2.01	0.61
2:B:1054:MET:HE1	2:B:1129:LEU:HG	1.83	0.61
2:Y:691:LEU:HD23	2:Y:693:LEU:HD11	1.83	0.61
3:Z:49:PHE:CE1	3:Z:340:LEU:HD22	2.35	0.61
2:Y:13:THR:OG1	2:Y:355:ASN:OD1	2.19	0.60
2:Y:394:ILE:HD11	2:Y:669:SER:CB	2.30	0.60
1:X:451:MET:CB	1:X:503:ARG:CD	2.78	0.60
2:B:537:GLU:HG3	2:B:561:TRP:CG	2.36	0.60
1:A:601:ILE:HG22	1:A:602:CYS:N	2.16	0.60
1:A:543:ILE:HD12	1:A:545:CYS:SG	2.41	0.60
2:B:413:LEU:HB3	2:B:424:THR:HB	1.82	0.60
1:X:597:THR:HG21	1:X:601:ILE:HG13	1.83	0.60
2:Y:445:GLU:OE2	2:B:770:LEU:C	2.44	0.60
2:Y:903:CYS:SG	2:Y:904:ASN:N	2.74	0.60
2:B:466:GLN:OE1	2:B:466:GLN:HA	2.01	0.60
1:A:508:GLU:O	1:A:509:GLU:OE2	2.20	0.60
2:Y:404:LEU:C	2:Y:404:LEU:HD23	2.27	0.60
2:Y:910:MET:HG2	2:Y:912:LEU:HD21	1.84	0.60
1:A:540:HIS:N	1:A:587:GLN:OE1	2.32	0.60
2:Y:59:GLY:CA	2:Y:1073:TRP:CZ3	2.84	0.59
3:Z:172:THR:O	3:Z:173:GLN:C	2.44	0.59
2:B:884:ILE:HD12	2:B:884:ILE:N	2.17	0.59
1:X:540:HIS:CD2	1:X:544:ILE:HG22	2.37	0.59
2:B:222:VAL:HG12	2:B:223:PRO:HD2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:691:LEU:HD23	2:B:693:LEU:HD11	1.83	0.59
1:X:540:HIS:CE1	1:X:542:SER:C	2.79	0.59
2:Y:661:SER:OG	2:Y:663:ASN:ND2	2.35	0.59
2:Y:883:SER:HB2	2:Y:911:ALA:HB3	1.82	0.59
2:B:802:LEU:N	2:B:802:LEU:HD23	2.16	0.59
1:A:543:ILE:CD1	1:A:545:CYS:SG	2.91	0.59
2:Y:913:TYR:OH	3:Z:240:TRP:HZ3	1.86	0.59
3:Z:173:GLN:CB	3:Z:179:GLN:HE22	2.15	0.59
2:B:913:TYR:OH	3:C:240:TRP:HZ3	1.85	0.59
2:B:914:LEU:CD2	2:B:921:ILE:HG23	2.32	0.59
2:B:1008:CYS:O	2:B:1008:CYS:SG	2.61	0.59
2:B:1097:PHE:CE2	2:B:1129:LEU:HB3	2.37	0.59
1:X:534:GLN:O	1:X:627:GLY:HA2	2.02	0.59
2:B:735:VAL:HB	2:B:792:LEU:HB2	1.84	0.59
2:B:868:GLY:HA3	2:B:885:ASN:ND2	2.17	0.59
2:B:167:VAL:HG23	2:B:180:PHE:HB3	1.84	0.59
1:X:628:LYS:HD3	5:Z:502:85C:CL1	2.40	0.59
2:Y:414:ARG:N	2:Y:462:ASN:HD21	2.00	0.59
2:B:13:THR:OG1	2:B:355:ASN:OD1	2.20	0.59
1:A:471:VAL:HG12	1:A:472:MET:N	2.18	0.59
1:X:517:ILE:HD11	1:X:602:CYS:HB2	1.85	0.59
2:Y:36:ASN:ND2	2:Y:37:THR:HG23	2.18	0.59
2:Y:972:PHE:CZ	3:Z:196:ALA:O	2.56	0.59
1:A:468:GLN:O	1:A:470:LEU:HG	2.03	0.59
3:C:427:PRO:O	3:C:428:ASP:CB	2.49	0.58
2:Y:466:GLN:OE1	2:Y:466:GLN:HA	2.01	0.58
2:Y:1032:THR:HG22	2:Y:1034:ASN:N	2.17	0.58
1:X:449:LYS:HZ2	1:X:510:GLU:HB3	1.67	0.58
2:Y:884:ILE:N	2:Y:884:ILE:HD12	2.18	0.58
3:Z:264:TRP:CD1	3:Z:337:ILE:O	2.56	0.58
2:B:23:PHE:H	2:B:30:ASN:ND2	2.01	0.58
2:B:465:HIS:O	2:B:467:GLN:HG3	2.03	0.58
2:B:1076:PHE:CD1	2:B:1076:PHE:C	2.81	0.58
2:B:1097:PHE:CZ	2:B:1129:LEU:HB3	2.39	0.58
1:A:539:GLU:O	1:A:540:HIS:HB2	2.03	0.58
1:X:448:TYR:O	1:X:449:LYS:C	2.47	0.58
1:X:510:GLU:O	1:X:511:GLU:CB	2.50	0.58
2:Y:23:PHE:H	2:Y:30:ASN:ND2	2.00	0.58
3:Z:352:PRO:HG3	3:Z:378:HIS:CE1	2.32	0.58
2:B:695:ASN:OD1	2:B:696:ASN:N	2.36	0.58
2:B:1050:LEU:HD12	2:B:1050:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:500:LEU:CD1	1:X:500:LEU:N	2.66	0.58
3:C:425:THR:HG22	3:C:426:ILE:N	2.16	0.58
2:Y:1076:PHE:CD1	2:Y:1076:PHE:C	2.82	0.58
2:B:972:PHE:CE1	3:C:196:ALA:O	2.56	0.58
3:C:104:PRO:HA	3:C:107:VAL:HB	1.86	0.58
1:X:557:CYS:SG	1:X:558:ILE:N	2.77	0.58
2:Y:628:LYS:HG2	2:Y:629:VAL:N	2.18	0.57
1:A:615:PHE:CD1	1:A:615:PHE:C	2.82	0.57
2:Y:167:VAL:HG23	2:Y:180:PHE:HB3	1.86	0.57
2:Y:537:GLU:O	2:Y:561:TRP:HB2	2.04	0.57
3:Z:61:GLY:HA3	3:Z:145:ARG:NH1	2.19	0.57
3:Z:144:TYR:CD1	3:Z:145:ARG:N	2.72	0.57
2:Y:868:GLY:HA3	2:Y:885:ASN:ND2	2.19	0.57
1:X:515:GLY:N	1:X:556:THR:OG1	2.37	0.57
2:Y:596:PHE:O	2:Y:597:GLU:C	2.46	0.57
1:A:448:TYR:CE1	1:A:454:VAL:HB	2.40	0.57
1:A:606:PHE:HE2	1:A:628:LYS:CG	1.99	0.57
1:X:453:THR:O	1:X:454:VAL:CG2	2.52	0.57
1:X:473:MET:C	1:X:475:ASN:H	2.11	0.57
2:Y:1050:LEU:HD12	2:Y:1050:LEU:O	2.04	0.57
2:B:32:LEU:HD11	2:B:41:ILE:HG12	1.86	0.57
1:A:510:GLU:OE1	1:A:510:GLU:C	2.47	0.57
1:X:597:THR:HG21	1:X:601:ILE:CG1	2.35	0.57
1:X:605:THR:C	1:X:606:PHE:O	2.38	0.57
2:Y:222:VAL:HG12	2:Y:223:PRO:HD2	1.84	0.57
2:Y:695:ASN:OD1	2:Y:696:ASN:N	2.37	0.57
2:Y:1032:THR:HG22	2:Y:1034:ASN:H	1.68	0.57
2:Y:805:HIS:HD2	2:Y:806:GLN:C	2.13	0.57
2:Y:998:PHE:HB2	2:Y:1088:PHE:CD2	2.40	0.57
3:Z:175:ASP:OD1	3:Z:177:ILE:HB	2.04	0.57
1:A:537:ILE:CG2	1:A:587:GLN:HA	2.35	0.57
2:Y:394:ILE:CD1	2:Y:658:VAL:HB	2.35	0.57
2:B:642:ARG:NH2	2:B:645:SER:O	2.38	0.57
2:B:1058:LEU:HD22	2:B:1062:ILE:HD11	1.86	0.57
1:A:568:CYS:HB3	1:A:592:ILE:HD11	1.87	0.57
3:Z:293:VAL:O	3:Z:296:ILE:HG13	2.04	0.57
2:B:414:ARG:H	2:B:462:ASN:HD21	1.51	0.57
3:C:117:ASP:C	3:C:119:THR:H	2.13	0.57
2:Y:914:LEU:CD2	2:Y:921:ILE:HG23	2.35	0.56
3:Z:70:ARG:HD2	3:Z:70:ARG:N	2.19	0.56
3:Z:115:GLN:HA	3:Z:115:GLN:NE2	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:559:GLU:OE2	1:X:599:GLY:CA	2.53	0.56
1:X:605:THR:OG1	1:X:608:ASP:CB	2.49	0.56
2:Y:395:GLY:N	2:Y:705:ASP:OD1	2.39	0.56
2:Y:560:LEU:N	2:Y:560:LEU:HD23	2.21	0.56
2:Y:646:THR:OG1	2:Y:647:THR:N	2.37	0.56
2:Y:735:VAL:HB	2:Y:792:LEU:HB2	1.87	0.56
2:Y:1058:LEU:HD22	2:Y:1062:ILE:HD11	1.86	0.56
2:B:59:GLY:CA	2:B:1073:TRP:CZ3	2.87	0.56
2:B:465:HIS:CG	2:B:523:PRO:HD3	2.40	0.56
2:B:573:SER:O	2:B:574:PHE:HB2	2.05	0.56
3:C:56:SER:O	3:C:158:LYS:NZ	2.38	0.56
1:A:440:ILE:HA	1:A:461:SER:O	2.06	0.56
2:Y:534:MET:HE3	2:Y:534:MET:HA	1.87	0.56
2:B:971:ALA:HB3	2:B:1077:HIS:O	2.06	0.56
1:X:508:GLU:O	1:X:509:GLU:OE2	2.23	0.56
2:B:16:ASN:HD21	2:B:36:ASN:HA	1.70	0.56
2:B:1032:THR:HG22	2:B:1034:ASN:H	1.71	0.56
1:A:543:ILE:HG22	1:A:586:LYS:CG	2.34	0.56
1:X:515:GLY:HA2	1:X:556:THR:HG1	1.70	0.56
2:B:578:HIS:O	2:B:579:LYS:HB2	2.05	0.56
2:B:913:TYR:HH	3:C:240:TRP:HZ3	1.53	0.56
2:B:1072:PHE:CD1	2:B:1072:PHE:C	2.83	0.56
2:Y:515:ALA:HB1	2:Y:532:THR:O	2.05	0.56
2:Y:1097:PHE:CE2	2:Y:1129:LEU:HB3	2.40	0.56
1:X:566:LEU:HD21	1:X:584:PHE:HA	1.88	0.56
1:X:552:LEU:HB2	1:X:561:VAL:HG11	1.88	0.56
2:Y:465:HIS:O	2:Y:467:GLN:HG3	2.06	0.56
2:B:408:LYS:HA	2:B:678:TYR:CE2	2.41	0.56
2:B:634:GLN:CB	2:B:654:ASP:OD1	2.53	0.56
2:B:646:THR:OG1	2:B:647:THR:N	2.39	0.56
1:A:517:ILE:HD11	1:A:602:CYS:HB2	1.87	0.56
2:Y:108:VAL:O	2:Y:108:VAL:HG23	2.05	0.55
1:A:495:ALA:HB1	1:A:496:PRO:CD	2.37	0.55
1:A:572:LYS:HE2	1:A:590:VAL:HG23	1.89	0.55
1:X:459:LEU:HD13	1:X:496:PRO:HA	1.87	0.55
2:B:394:ILE:CD1	2:B:658:VAL:HB	2.36	0.55
2:B:515:ALA:HB1	2:B:532:THR:O	2.06	0.55
2:B:967:GLY:HA3	2:B:975:PHE:CE2	2.41	0.55
2:Y:928:ARG:CB	2:Y:952:ASN:O	2.54	0.55
2:B:108:VAL:HG23	2:B:108:VAL:O	2.06	0.55
2:B:448:LEU:HD23	2:B:451:PHE:CD1	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:765:VAL:HG23	2:B:806:GLN:HB3	1.89	0.55
3:C:349:TYR:HD2	3:C:359:THR:HG22	1.72	0.55
1:A:615:PHE:HE1	1:A:617:LEU:CD1	2.20	0.55
1:X:566:LEU:CD2	1:X:585:VAL:HG12	2.37	0.55
2:Y:618:ILE:HD12	2:Y:618:ILE:N	2.21	0.55
2:Y:928:ARG:O	2:Y:928:ARG:CD	2.54	0.55
3:Z:85:PRO:O	3:Z:86:GLN:HB2	2.06	0.55
2:B:1032:THR:HG22	2:B:1034:ASN:N	2.20	0.55
1:X:572:LYS:HE2	1:X:590:VAL:HG23	1.88	0.55
2:Y:32:LEU:HD11	2:Y:41:ILE:HG12	1.88	0.55
2:Y:869:ALA:O	2:Y:884:ILE:HA	2.06	0.55
3:Z:85:PRO:O	3:Z:86:GLN:CB	2.54	0.55
3:Z:351:ASN:HB2	3:Z:352:PRO:CD	2.37	0.55
2:B:608:ASP:O	2:B:633:THR:HA	2.07	0.55
2:B:1003:PHE:CD2	3:C:197:VAL:HG23	2.42	0.55
1:A:606:PHE:CE1	1:A:610:PRO:HB3	2.42	0.55
1:X:537:ILE:HG12	1:X:585:VAL:HG21	1.88	0.55
1:X:553:HIS:HB2	1:X:616:THR:HG23	1.88	0.55
1:X:554:ILE:C	1:X:555:HIS:CD2	2.85	0.55
1:X:568:CYS:HB3	1:X:592:ILE:HD11	1.89	0.55
2:Y:944:GLU:OE1	2:Y:947:ARG:NH2	2.37	0.55
2:Y:1097:PHE:CZ	2:Y:1129:LEU:HB3	2.42	0.55
2:B:534:MET:HE3	2:B:534:MET:HA	1.88	0.55
2:B:920:PHE:HE2	2:B:962:ASP:HB3	1.72	0.55
2:Y:608:ASP:O	2:Y:633:THR:HA	2.07	0.55
1:A:597:THR:HG21	1:A:601:ILE:HG13	1.87	0.55
2:Y:118:THR:O	2:Y:118:THR:CG2	2.54	0.55
2:Y:817:VAL:HG13	2:Y:830:ILE:HB	1.89	0.55
2:B:513:GLY:O	2:B:538:VAL:HG12	2.07	0.55
3:C:426:ILE:H	3:C:426:ILE:HD13	1.72	0.55
1:A:529:ARG:HD2	1:A:599:GLY:O	2.07	0.55
1:X:559:GLU:OE2	1:X:599:GLY:N	2.40	0.55
3:C:351:ASN:HB2	3:C:352:PRO:CD	2.37	0.55
1:A:472:MET:O	1:A:473:MET:CB	2.55	0.55
1:A:552:LEU:HB2	1:A:561:VAL:HG11	1.89	0.55
1:X:615:PHE:HE1	1:X:617:LEU:HD13	1.71	0.54
2:B:245:TYR:C	2:B:245:TYR:HD1	2.15	0.54
1:A:569:LEU:H	1:A:582:PRO:HG3	1.72	0.54
1:X:440:ILE:HA	1:X:461:SER:O	2.08	0.54
1:X:443:PRO:HA	1:X:517:ILE:HG22	1.88	0.54
2:Y:765:VAL:HG23	2:Y:806:GLN:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:VAL:HG11	2:B:122:GLY:HA3	1.89	0.54
2:B:628:LYS:HG2	2:B:629:VAL:N	2.20	0.54
1:X:552:LEU:C	1:X:552:LEU:HD12	2.32	0.54
2:Y:513:GLY:O	2:Y:538:VAL:HG12	2.07	0.54
2:Y:754:PRO:HB2	2:Y:759:GLN:NE2	2.22	0.54
2:B:652:CYS:HB3	2:B:676:VAL:O	2.07	0.54
2:B:808:LEU:CD1	2:B:847:ARG:NH2	2.66	0.54
3:C:69:GLY:HA2	3:C:118:ARG:NH2	2.21	0.54
1:A:527:SER:HB2	1:A:602:CYS:HA	1.89	0.54
1:X:476:LYS:HE3	1:X:476:LYS:N	2.22	0.54
2:Y:913:TYR:CZ	3:Z:240:TRP:CH2	2.95	0.54
3:Z:352:PRO:CA	3:Z:378:HIS:CE1	2.91	0.54
1:A:597:THR:HG21	1:A:601:ILE:CG1	2.38	0.54
1:X:601:ILE:CG2	1:X:602:CYS:N	2.70	0.54
2:Y:427:LEU:HD12	2:Y:427:LEU:N	2.23	0.54
3:Z:352:PRO:HG3	3:Z:378:HIS:CG	2.36	0.54
2:B:537:GLU:O	2:B:561:TRP:HB2	2.08	0.54
2:B:928:ARG:O	2:B:928:ARG:CG	2.56	0.54
2:B:389:ILE:N	2:B:389:ILE:HD12	2.23	0.54
2:B:427:LEU:N	2:B:427:LEU:HD12	2.22	0.54
2:B:817:VAL:HG13	2:B:830:ILE:HB	1.90	0.54
2:B:1030:PHE:CZ	2:B:1038:GLY:HA3	2.43	0.54
1:A:540:HIS:ND1	1:A:542:SER:O	2.41	0.54
1:A:615:PHE:HE1	1:A:617:LEU:HD13	1.72	0.54
3:Z:104:PRO:HA	3:Z:107:VAL:HB	1.90	0.54
5:C:502:85C:C21	1:A:628:LYS:HD3	2.37	0.54
1:A:559:GLU:OE2	1:A:599:GLY:CA	2.55	0.54
1:X:471:VAL:HG12	1:X:472:MET:N	2.21	0.54
2:Y:63:VAL:HG11	2:Y:122:GLY:HA3	1.89	0.54
3:C:85:PRO:O	3:C:86:GLN:CB	2.56	0.54
2:B:404:LEU:C	2:B:404:LEU:HD23	2.33	0.54
3:C:353:HIS:CG	1:A:572:LYS:HD3	2.43	0.54
1:A:566:LEU:HD23	1:A:585:VAL:HG12	1.89	0.54
1:X:628:LYS:CD	5:Z:502:85C:CL1	2.92	0.53
2:Y:541:LEU:HD23	2:Y:558:ILE:HD13	1.89	0.53
2:Y:1058:LEU:O	2:Y:1062:ILE:HD12	2.08	0.53
2:B:928:ARG:CB	2:B:952:ASN:O	2.55	0.53
3:Z:56:SER:O	3:Z:158:LYS:NZ	2.42	0.53
2:B:541:LEU:HD23	2:B:558:ILE:HD13	1.89	0.53
2:B:928:ARG:O	2:B:928:ARG:CD	2.55	0.53
1:A:443:PRO:HA	1:A:517:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:453:THR:CG2	1:X:454:VAL:N	2.71	0.53
1:X:574:SER:O	5:Z:502:85C:C8	2.56	0.53
3:Z:264:TRP:HD1	3:Z:337:ILE:O	1.91	0.53
2:B:908:ASN:OD1	2:B:908:ASN:N	2.41	0.53
3:C:85:PRO:O	3:C:86:GLN:HB2	2.08	0.53
1:A:606:PHE:CD1	1:A:606:PHE:C	2.86	0.53
2:B:118:THR:O	2:B:118:THR:CG2	2.56	0.53
2:B:414:ARG:HB2	2:B:462:ASN:ND2	2.23	0.53
2:B:538:VAL:HG23	2:B:558:ILE:HG23	1.88	0.53
2:B:1102:ARG:N	2:B:1103:PRO:HD2	2.23	0.53
1:X:552:LEU:CD1	1:X:554:ILE:HG13	2.37	0.53
3:Z:351:ASN:C	3:Z:378:HIS:CE1	2.83	0.53
2:B:433:THR:O	2:B:434:ARG:CD	2.57	0.53
1:A:538:ILE:HD11	1:A:623:THR:CG2	2.36	0.53
1:X:448:TYR:O	1:X:448:TYR:CG	2.61	0.53
2:B:660:TYR:O	2:B:667:VAL:HB	2.09	0.53
1:X:552:LEU:CD1	1:X:554:ILE:CG1	2.83	0.53
2:Y:317:LEU:HB2	2:Y:321:VAL:HG12	1.91	0.53
2:Y:538:VAL:HG23	2:Y:558:ILE:HG23	1.90	0.53
2:B:807:PHE:CZ	2:B:831:VAL:HG11	2.44	0.53
2:B:808:LEU:H	2:B:808:LEU:CD1	2.16	0.53
2:B:869:ALA:O	2:B:884:ILE:HA	2.08	0.53
1:X:495:ALA:HB1	1:X:496:PRO:CD	2.39	0.53
1:X:511:GLU:OE1	1:X:511:GLU:HA	2.09	0.53
1:X:544:ILE:HG12	1:X:544:ILE:O	2.08	0.53
2:Y:910:MET:HG2	2:Y:912:LEU:CD2	2.38	0.53
2:Y:913:TYR:OH	2:Y:955:SER:C	2.52	0.53
2:B:584:GLY:O	2:B:586:ILE:N	2.42	0.53
1:X:495:ALA:HB1	1:X:496:PRO:HD2	1.91	0.53
2:Y:736:LEU:HD13	2:Y:813:ALA:HB1	1.90	0.53
2:Y:971:ALA:HB3	2:Y:1077:HIS:O	2.08	0.53
2:B:950:ASN:C	2:B:950:ASN:HD22	2.17	0.53
1:A:508:GLU:C	1:A:509:GLU:OE2	2.51	0.53
1:X:513:LEU:CD1	1:X:513:LEU:N	2.72	0.52
2:Y:276:MET:HE2	3:Z:202:LEU:HD22	1.91	0.52
2:Y:389:ILE:HD12	2:Y:389:ILE:N	2.24	0.52
2:Y:663:ASN:HB2	2:Y:1134:GLU:OE2	2.09	0.52
2:B:995:VAL:O	2:B:995:VAL:HG23	2.09	0.52
1:A:495:ALA:HB1	1:A:496:PRO:HD2	1.91	0.52
1:X:453:THR:C	1:X:454:VAL:CG2	2.82	0.52
2:Y:20:THR:HG23	2:Y:315:THR:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1072:PHE:CD1	2:Y:1072:PHE:C	2.87	0.52
1:A:515:GLY:HA3	1:A:557:CYS:CB	2.37	0.52
1:A:597:THR:O	1:A:599:GLY:N	2.41	0.52
2:B:317:LEU:HB2	2:B:321:VAL:HG12	1.92	0.52
1:A:513:LEU:N	1:A:513:LEU:CD1	2.73	0.52
1:X:448:TYR:CE1	1:X:454:VAL:HB	2.44	0.52
2:Y:88:ILE:HD12	2:Y:152:LEU:HD21	1.90	0.52
3:Z:83:VAL:HG22	3:Z:121:ALA:HB3	1.91	0.52
2:B:88:ILE:HD12	2:B:152:LEU:HD21	1.92	0.52
1:X:450:ASP:OD1	1:X:451:MET:N	2.43	0.52
1:X:537:ILE:HG21	1:X:586:LYS:O	2.09	0.52
2:Y:805:HIS:CD2	2:Y:805:HIS:C	2.86	0.52
3:Z:91:LEU:HD22	3:Z:92:ILE:H	1.75	0.52
2:B:560:LEU:HD23	2:B:560:LEU:N	2.24	0.52
1:A:485:LEU:CD1	1:A:485:LEU:N	2.73	0.52
2:Y:912:LEU:HB3	3:Z:240:TRP:CZ2	2.45	0.52
2:B:486:LEU:HD11	2:B:488:SER:C	2.35	0.52
2:B:972:PHE:HZ	3:C:196:ALA:O	1.91	0.52
1:X:615:PHE:CD1	1:X:615:PHE:C	2.88	0.52
2:Y:618:ILE:HD12	2:Y:618:ILE:H	1.74	0.52
2:Y:618:ILE:CD1	2:Y:618:ILE:H	2.23	0.52
2:Y:995:VAL:O	2:Y:995:VAL:HG23	2.09	0.52
3:Z:135:PHE:CZ	3:Z:300:LYS:HD3	2.44	0.52
3:Z:237:LEU:N	3:Z:237:LEU:HD23	2.24	0.52
2:B:812:TYR:CZ	3:C:241:PRO:HB3	2.45	0.52
2:B:868:GLY:HA3	2:B:885:ASN:HD21	1.75	0.52
3:C:173:GLN:CB	3:C:179:GLN:NE2	2.73	0.52
2:Y:928:ARG:O	2:Y:928:ARG:CG	2.58	0.52
3:Z:407:LYS:HD2	3:Z:407:LYS:N	2.24	0.52
2:B:459:PHE:CD1	2:B:459:PHE:C	2.88	0.52
3:C:79:GLN:HE21	3:C:79:GLN:HA	1.75	0.52
3:C:407:LYS:HD2	3:C:407:LYS:N	2.25	0.52
1:A:606:PHE:HD1	1:A:606:PHE:C	2.17	0.52
1:A:606:PHE:HA	1:A:609:PHE:O	2.10	0.52
1:X:443:PRO:HB3	1:X:556:THR:HG23	1.92	0.51
2:Y:36:ASN:ND2	2:Y:37:THR:CG2	2.73	0.51
2:Y:408:LYS:HA	2:Y:678:TYR:CE2	2.45	0.51
1:A:555:HIS:HB3	1:A:557:CYS:H	1.75	0.51
1:A:566:LEU:HD21	1:A:584:PHE:HA	1.91	0.51
1:X:537:ILE:HG12	1:X:585:VAL:CG2	2.39	0.51
2:Y:660:TYR:O	2:Y:667:VAL:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:265:ASP:OD1	3:Z:266:GLU:HG2	2.09	0.51
2:B:535:GLU:CB	2:B:536:HIS:CE1	2.93	0.51
1:X:468:GLN:O	1:X:470:LEU:HG	2.09	0.51
3:Z:364:LYS:O	3:Z:365:ALA:HB2	2.10	0.51
2:B:998:PHE:HB2	2:B:1088:PHE:CD2	2.45	0.51
3:C:310:CYS:HA	3:C:442:LEU:HA	1.90	0.51
1:A:568:CYS:O	1:A:592:ILE:CG1	2.58	0.51
1:X:610:PRO:CD	1:X:611:GLN:N	2.73	0.51
2:Y:996:GLY:O	2:Y:997:LEU:HD23	2.11	0.51
2:B:736:LEU:HD13	2:B:813:ALA:HB1	1.91	0.51
1:A:513:LEU:HD12	1:A:513:LEU:N	2.24	0.51
1:A:604:GLU:CG	1:A:612:MET:HE2	2.38	0.51
1:X:474:PRO:O	1:X:476:LYS:CE	2.56	0.51
2:Y:245:TYR:C	2:Y:245:TYR:HD1	2.17	0.51
3:C:237:LEU:HD23	3:C:237:LEU:N	2.24	0.51
2:Y:652:CYS:HB3	2:Y:676:VAL:O	2.11	0.51
2:B:429:PHE:CD1	2:B:429:PHE:N	2.77	0.51
2:B:596:PHE:HB3	2:B:661:SER:C	2.35	0.51
1:A:553:HIS:HB2	1:A:616:THR:HG23	1.93	0.51
1:X:552:LEU:HD11	1:X:554:ILE:CD1	2.40	0.51
2:Y:486:LEU:O	2:Y:486:LEU:HG	2.10	0.51
3:Z:250:ALA:HB2	3:Z:305:ILE:HD13	1.93	0.51
2:Y:166:ASP:OD2	3:Z:204:LYS:HD3	2.11	0.51
2:Y:426:VAL:C	2:Y:427:LEU:HD12	2.35	0.51
2:B:276:MET:HE2	3:C:202:LEU:HD22	1.92	0.51
2:B:426:VAL:C	2:B:427:LEU:HD12	2.35	0.51
2:B:484:LYS:O	2:B:485:ALA:HB2	2.11	0.51
3:C:83:VAL:HG22	3:C:121:ALA:HB3	1.92	0.51
3:C:91:LEU:HD22	3:C:92:ILE:H	1.75	0.51
1:A:610:PRO:O	1:A:612:MET:N	2.44	0.51
1:X:597:THR:O	1:X:599:GLY:N	2.44	0.51
3:Z:349:TYR:HD2	3:Z:359:THR:HG22	1.76	0.51
2:B:535:GLU:C	2:B:536:HIS:CG	2.89	0.51
1:X:540:HIS:CE1	1:X:542:SER:CA	2.94	0.50
2:Y:10:GLN:HB3	2:Y:1037:ILE:HB	1.93	0.50
2:Y:596:PHE:HB3	2:Y:661:SER:C	2.35	0.50
2:B:944:GLU:OE1	2:B:947:ARG:NH2	2.41	0.50
2:Y:273:LEU:HB2	2:Y:281:PHE:HB2	1.93	0.50
2:Y:868:GLY:HA3	2:Y:885:ASN:HD21	1.77	0.50
3:Z:64:MET:HE3	3:Z:158:LYS:HE3	1.93	0.50
3:Z:338:PHE:CE2	3:Z:340:LEU:HG	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:513:LEU:HD12	1:X:513:LEU:N	2.25	0.50
2:Y:920:PHE:HE2	2:Y:962:ASP:HB3	1.77	0.50
2:Y:1030:PHE:CZ	2:Y:1038:GLY:HA3	2.46	0.50
2:B:517:TYR:N	2:B:517:TYR:CD1	2.80	0.50
2:Y:276:MET:CE	3:Z:202:LEU:HD22	2.41	0.50
3:Z:77:SER:O	3:Z:183:GLN:HA	2.12	0.50
2:B:596:PHE:CD2	2:B:601:TYR:HD2	2.24	0.50
2:B:618:ILE:HD12	2:B:618:ILE:N	2.26	0.50
1:A:601:ILE:CG2	1:A:602:CYS:N	2.74	0.50
2:Y:16:ASN:HD21	2:Y:36:ASN:HA	1.76	0.50
2:Y:337:ASN:HB2	2:Y:339:ASP:O	2.11	0.50
2:B:913:TYR:OH	2:B:955:SER:C	2.54	0.50
3:C:236:ASN:OD1	3:C:237:LEU:HD23	2.11	0.50
1:X:533:ALA:HB2	1:X:629:VAL:HA	1.93	0.50
1:X:559:GLU:OE2	1:X:599:GLY:HA3	2.11	0.50
2:Y:1102:ARG:N	2:Y:1103:PRO:HD2	2.25	0.50
2:B:649:VAL:HB	2:B:659:ILE:HB	1.94	0.50
2:B:889:ARG:HD3	2:B:901:THR:CG2	2.39	0.50
1:A:585:VAL:HG11	1:A:591:CYS:SG	2.51	0.50
1:A:606:PHE:HE1	1:A:610:PRO:HB3	1.76	0.50
1:X:443:PRO:CA	1:X:517:ILE:HG22	2.41	0.50
1:X:449:LYS:NZ	1:X:510:GLU:CG	2.75	0.50
1:A:552:LEU:HD12	1:A:552:LEU:C	2.37	0.50
1:X:568:CYS:O	1:X:592:ILE:CG1	2.60	0.50
2:Y:535:GLU:C	2:Y:536:HIS:CG	2.89	0.50
3:Z:247:LEU:O	3:Z:309:ARG:HD2	2.12	0.50
1:A:448:TYR:CG	1:A:448:TYR:O	2.65	0.50
1:A:459:LEU:HD13	1:A:496:PRO:HA	1.92	0.50
1:X:527:SER:HB2	1:X:602:CYS:HA	1.92	0.50
1:X:527:SER:OG	1:X:528:GLY:N	2.45	0.50
2:Y:1048:TYR:HD1	2:Y:1089:ILE:HD12	1.77	0.50
2:B:10:GLN:HB3	2:B:1037:ILE:HB	1.94	0.50
2:B:805:HIS:CD2	2:B:806:GLN:N	2.80	0.50
2:B:913:TYR:CZ	3:C:240:TRP:CH2	2.99	0.50
3:C:77:SER:O	3:C:183:GLN:HA	2.12	0.50
2:Y:913:TYR:CZ	3:Z:240:TRP:HH2	2.30	0.49
2:Y:1039:LEU:C	2:Y:1039:LEU:HD23	2.37	0.49
2:Y:1039:LEU:HD23	2:Y:1040:VAL:N	2.27	0.49
2:B:20:THR:HG23	2:B:315:THR:CG2	2.40	0.49
2:B:241:ASN:O	2:B:242:GLY:C	2.55	0.49
1:X:554:ILE:HG12	1:X:615:PHE:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:393:GLY:O	2:Y:708:GLN:CB	2.60	0.49
2:B:582:LEU:HD23	2:B:612:PHE:CG	2.47	0.49
3:C:426:ILE:HG12	3:C:427:PRO:CA	2.38	0.49
2:B:172:GLY:HA2	2:B:224:GLU:CD	2.37	0.49
3:C:64:MET:HE3	3:C:158:LYS:HE3	1.94	0.49
2:Y:1003:PHE:CD2	3:Z:197:VAL:HG23	2.48	0.49
3:C:238:THR:OG1	3:C:239:SER:N	2.40	0.49
2:Y:81:THR:HG23	2:Y:85:ASN:HB2	1.94	0.49
2:Y:513:GLY:O	2:Y:537:GLU:HA	2.12	0.49
2:Y:582:LEU:HD23	2:Y:612:PHE:CG	2.48	0.49
2:Y:649:VAL:HB	2:Y:659:ILE:HB	1.95	0.49
2:Y:762:SER:O	2:Y:803:HIS:HA	2.12	0.49
2:B:1058:LEU:O	2:B:1062:ILE:HD12	2.13	0.49
3:C:199:LEU:CD2	3:C:237:LEU:HD11	2.30	0.49
1:A:559:GLU:OE2	1:A:599:GLY:HA3	2.11	0.49
1:X:545:CYS:HB2	1:X:584:PHE:HB3	1.93	0.49
1:X:569:LEU:H	1:X:582:PRO:HG3	1.77	0.49
2:Y:377:THR:OG1	2:Y:379:SER:OG	2.22	0.49
2:Y:1008:CYS:O	2:Y:1008:CYS:SG	2.71	0.49
3:Z:48:ASN:CA	3:Z:410:SER:HB3	2.42	0.49
2:B:455:GLN:OE1	2:B:455:GLN:HA	2.12	0.49
5:C:502:85C:C4	1:A:572:LYS:O	2.60	0.49
1:X:440:ILE:HD11	1:X:470:LEU:HD22	1.94	0.49
2:Y:838:PRO:HB2	3:Z:225:GLN:OE1	2.12	0.49
2:B:555:LEU:HD13	2:B:593:MET:SD	2.52	0.49
1:A:559:GLU:OE2	1:A:599:GLY:N	2.45	0.49
2:Y:871:TYR:HE2	2:Y:885:ASN:HA	1.77	0.49
3:Z:64:MET:O	3:Z:66:GLU:OE2	2.30	0.49
2:B:127:GLU:HB2	2:B:129:ARG:HG2	1.95	0.49
2:B:275:ASP:HB2	2:B:279:ARG:HB2	1.95	0.49
2:B:762:SER:O	2:B:803:HIS:HA	2.13	0.49
3:C:247:LEU:O	3:C:309:ARG:HD2	2.13	0.49
2:Y:241:ASN:O	2:Y:242:GLY:C	2.55	0.49
2:Y:263:ARG:HA	2:Y:271:TYR:CD1	2.48	0.49
2:Y:322:VAL:HG23	2:Y:336:LEU:HD21	1.95	0.49
2:Y:537:GLU:HG3	2:Y:561:TRP:CD1	2.47	0.49
2:Y:596:PHE:O	2:Y:597:GLU:CB	2.61	0.49
3:Z:236:ASN:OD1	3:Z:237:LEU:HD23	2.12	0.49
2:B:427:LEU:N	2:B:427:LEU:CD1	2.75	0.49
2:B:513:GLY:O	2:B:537:GLU:HA	2.13	0.49
2:B:996:GLY:O	2:B:997:LEU:HD23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:473:MET:CE	1:X:476:LYS:HD3	2.40	0.49
2:Y:805:HIS:HD2	2:Y:806:GLN:N	2.09	0.49
2:B:40:GLU:HG2	2:B:54:GLU:HG3	1.95	0.49
2:B:390:ILE:CG2	2:B:710:LEU:HD13	2.43	0.49
3:Z:317:LYS:O	3:Z:426:ILE:HD13	2.13	0.48
2:Y:92:LYS:HE2	2:Y:101:ILE:HD13	1.94	0.48
2:B:805:HIS:HD2	2:B:806:GLN:C	2.20	0.48
2:B:1039:LEU:HD23	2:B:1040:VAL:N	2.28	0.48
1:X:581:ARG:HH11	1:X:581:ARG:CG	2.25	0.48
2:Y:427:LEU:N	2:Y:427:LEU:CD1	2.76	0.48
2:Y:817:VAL:CG1	2:Y:830:ILE:HB	2.43	0.48
3:Z:407:LYS:N	3:Z:407:LYS:CD	2.75	0.48
3:C:73:HIS:CG	3:C:79:GLN:OE1	2.66	0.48
1:X:449:LYS:NZ	1:X:510:GLU:CD	2.65	0.48
2:Y:796:GLN:OE1	2:Y:797:HIS:CE1	2.67	0.48
3:Z:165:PHE:CD1	3:Z:182:VAL:HG21	2.48	0.48
2:B:171:TYR:CG	2:B:223:PRO:HA	2.49	0.48
2:B:663:ASN:HB2	2:B:1134:GLU:OE2	2.14	0.48
2:B:715:VAL:HG21	2:B:799:PHE:CG	2.49	0.48
3:C:364:LYS:O	3:C:365:ALA:HB2	2.13	0.48
2:Y:172:GLY:HA2	2:Y:224:GLU:CD	2.38	0.48
2:Y:484:LYS:O	2:Y:485:ALA:HB2	2.12	0.48
2:Y:517:TYR:N	2:Y:517:TYR:CD1	2.81	0.48
2:B:263:ARG:HA	2:B:271:TYR:CD1	2.48	0.48
2:B:967:GLY:HA3	2:B:975:PHE:CZ	2.48	0.48
3:C:110:VAL:O	3:C:114:ILE:HG12	2.12	0.48
3:C:407:LYS:N	3:C:407:LYS:CD	2.76	0.48
2:Y:24:THR:HG22	2:Y:91:TYR:CE2	2.49	0.48
2:Y:385:GLY:HA3	2:Y:719:GLU:O	2.14	0.48
2:Y:429:PHE:CD1	2:Y:429:PHE:N	2.81	0.48
2:Y:492:GLU:OE1	2:Y:494:GLN:N	2.37	0.48
2:Y:1055:GLN:HE22	2:Y:1090:ASP:H	1.60	0.48
3:Z:105:GLN:H	3:Z:105:GLN:CD	2.22	0.48
3:Z:401:LYS:CG	3:Z:415:TRP:CE2	2.90	0.48
2:B:385:GLY:HA3	2:B:719:GLU:O	2.13	0.48
2:B:874:VAL:HG12	2:B:881:LEU:HB3	1.95	0.48
1:A:471:VAL:CG1	1:A:472:MET:N	2.76	0.48
1:A:536:VAL:HG13	1:A:626:ILE:HD12	1.96	0.48
2:Y:183:GLN:HE22	3:Z:209:PRO:HA	1.78	0.48
2:Y:1051:LEU:HB2	2:Y:1089:ILE:HD13	1.94	0.48
2:B:5:TYR:HE1	2:B:7:VAL:HB	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1051:LEU:HD22	2:B:1094:ILE:HD12	1.96	0.48
1:A:443:PRO:CA	1:A:517:ILE:HG22	2.43	0.48
2:Y:275:ASP:HB2	2:Y:279:ARG:HB2	1.95	0.48
2:Y:378:CYS:SG	2:Y:721:PRO:HB2	2.54	0.48
2:Y:390:ILE:CG2	2:Y:710:LEU:HD13	2.44	0.48
2:B:58:TYR:CE1	2:B:1070:HIS:HD2	2.32	0.48
2:B:377:THR:OG1	2:B:379:SER:OG	2.23	0.48
2:B:511:ALA:CB	2:B:538:VAL:HG11	2.43	0.48
3:C:144:TYR:CE1	3:C:155:VAL:HG13	2.44	0.48
3:C:425:THR:HG23	3:C:426:ILE:HD13	1.96	0.48
1:A:500:LEU:N	1:A:500:LEU:CD1	2.76	0.48
1:X:500:LEU:N	1:X:500:LEU:HD13	2.29	0.48
1:X:540:HIS:CE1	1:X:543:ILE:N	2.82	0.48
2:Y:537:GLU:HG3	2:Y:561:TRP:CB	2.44	0.48
2:Y:972:PHE:CE1	3:Z:196:ALA:O	2.66	0.48
3:Z:73:HIS:CG	3:Z:79:GLN:OE1	2.67	0.48
2:B:624:SER:O	2:B:625:ASP:HB2	2.14	0.48
3:C:250:ALA:HB2	3:C:305:ILE:HD13	1.95	0.48
2:Y:40:GLU:HG2	2:Y:54:GLU:HG3	1.96	0.48
2:Y:414:ARG:H	2:Y:462:ASN:HD21	1.59	0.48
2:B:537:GLU:HG3	2:B:561:TRP:HB2	1.96	0.48
2:B:871:TYR:HE2	2:B:885:ASN:HA	1.78	0.48
2:B:900:ARG:O	2:B:900:ARG:CG	2.56	0.48
3:C:82:PRO:HB3	3:C:109:MET:HE1	1.96	0.48
1:A:606:PHE:CD2	1:A:628:LYS:CD	2.93	0.48
1:X:568:CYS:O	1:X:592:ILE:HG13	2.14	0.47
1:X:581:ARG:HH11	1:X:581:ARG:HG2	1.79	0.47
2:Y:5:TYR:HB2	2:Y:1043:LEU:HD11	1.96	0.47
2:Y:537:GLU:HG3	2:Y:561:TRP:HB2	1.95	0.47
2:Y:558:ILE:CG2	2:Y:559:GLY:N	2.78	0.47
2:Y:931:LEU:HD11	2:Y:947:ARG:NH2	2.29	0.47
3:Z:351:ASN:OD1	3:Z:355:TYR:HB2	2.14	0.47
2:B:663:ASN:O	2:B:1134:GLU:OE1	2.32	0.47
1:X:540:HIS:ND1	1:X:540:HIS:C	2.72	0.47
2:Y:188:ARG:NH1	2:Y:216:ALA:O	2.46	0.47
2:Y:663:ASN:O	2:Y:1134:GLU:OE1	2.31	0.47
2:Y:809:GLN:O	2:Y:810:ASN:HB2	2.14	0.47
3:Z:70:ARG:CD	3:Z:70:ARG:N	2.70	0.47
2:B:5:TYR:HB2	2:B:1043:LEU:HD11	1.96	0.47
3:C:168:LEU:HD11	3:C:183:GLN:HB2	1.96	0.47
1:A:482:LEU:HD21	1:A:505:LYS:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:508:GLU:C	1:X:509:GLU:OE2	2.57	0.47
2:Y:889:ARG:HD3	2:Y:901:THR:CG2	2.39	0.47
3:Z:109:MET:HE3	3:Z:109:MET:HB2	1.79	0.47
2:B:81:THR:HG23	2:B:85:ASN:HB2	1.96	0.47
2:B:650:PHE:CD2	2:B:679:MET:HE3	2.49	0.47
1:A:552:LEU:CD1	1:A:554:ILE:HG12	2.41	0.47
2:Y:127:GLU:HB2	2:Y:129:ARG:HG2	1.96	0.47
2:Y:267:ASN:ND2	2:Y:269:SER:OG	2.47	0.47
2:B:618:ILE:HD12	2:B:618:ILE:H	1.80	0.47
2:B:676:VAL:O	2:B:676:VAL:HG12	2.13	0.47
3:C:49:PHE:CD1	3:C:49:PHE:C	2.92	0.47
3:C:114:ILE:CD1	3:C:144:TYR:CD2	2.97	0.47
3:C:338:PHE:CE2	3:C:340:LEU:HG	2.49	0.47
3:C:349:TYR:HD2	3:C:359:THR:CG2	2.28	0.47
1:X:474:PRO:HD3	1:X:602:CYS:SG	2.55	0.47
1:X:561:VAL:HG22	1:X:562:GLU:N	2.28	0.47
1:X:606:PHE:HE2	1:X:628:LYS:HD2	1.75	0.47
3:Z:120:PHE:N	3:Z:120:PHE:CD1	2.82	0.47
2:B:807:PHE:CE1	2:B:831:VAL:HG11	2.50	0.47
3:C:127:ASN:HD22	3:C:128:VAL:CG1	2.27	0.47
3:C:313:ASP:OD1	3:C:313:ASP:C	2.58	0.47
3:Z:381:PHE:HD2	3:Z:402:PHE:CE2	2.33	0.47
2:B:172:GLY:HA3	2:B:224:GLU:HG3	1.97	0.47
2:B:322:VAL:HG23	2:B:336:LEU:HD21	1.96	0.47
3:C:109:MET:HE3	3:C:109:MET:HB2	1.82	0.47
1:X:465:CYS:HA	1:X:493:THR:HG22	1.97	0.47
2:Y:805:HIS:CD2	2:Y:806:GLN:C	2.92	0.47
2:B:708:GLN:O	2:B:709:LYS:HB3	2.15	0.47
2:B:716:PRO:HB3	2:B:718:TYR:HE1	1.75	0.47
2:B:766:SER:O	2:B:767:SER:HB3	2.14	0.47
2:B:970:ASN:O	2:B:973:ASN:ND2	2.47	0.47
2:B:1048:TYR:HD1	2:B:1089:ILE:HD12	1.80	0.47
3:C:381:PHE:HD2	3:C:402:PHE:CE2	2.33	0.47
1:A:485:LEU:HA	1:A:490:GLU:CA	2.44	0.47
2:Y:455:GLN:HA	2:Y:455:GLN:OE1	2.15	0.47
3:Z:238:THR:OG1	3:Z:239:SER:N	2.40	0.47
2:B:792:LEU:O	2:B:793:ILE:HD13	2.15	0.47
1:A:447:LYS:HD3	1:A:447:LYS:N	2.28	0.47
1:A:465:CYS:HA	1:A:493:THR:HG22	1.96	0.47
1:A:527:SER:OG	1:A:528:GLY:N	2.48	0.47
1:X:540:HIS:ND1	1:X:541:LYS:N	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:815:SER:OG	2:Y:873:MET:HE2	2.15	0.47
2:Y:1055:GLN:NE2	2:Y:1090:ASP:H	2.12	0.47
3:Z:265:ASP:CG	3:Z:266:GLU:N	2.73	0.47
2:B:926:LEU:HA	2:B:926:LEU:HD12	1.53	0.47
2:B:1051:LEU:HB2	2:B:1089:ILE:HD13	1.96	0.47
2:Y:282:MET:HE3	2:Y:284:LEU:HD11	1.97	0.47
3:Z:165:PHE:CG	3:Z:182:VAL:HG22	2.50	0.47
1:X:628:LYS:N	5:Z:502:85C:CL1	2.85	0.46
2:Y:171:TYR:CG	2:Y:223:PRO:HA	2.50	0.46
2:Y:874:VAL:HG12	2:Y:881:LEU:HB3	1.97	0.46
2:B:282:MET:HE3	2:B:284:LEU:HD11	1.97	0.46
2:B:432:GLN:OE1	2:B:434:ARG:NH2	2.45	0.46
2:B:933:LEU:HD22	2:B:944:GLU:HA	1.97	0.46
3:C:310:CYS:HB2	3:C:442:LEU:HB3	1.97	0.46
1:A:487:ASP:CG	1:A:488:ASP:N	2.73	0.46
1:A:540:HIS:HD2	1:A:544:ILE:CG2	2.24	0.46
1:X:475:ASN:C	1:X:476:LYS:HE3	2.40	0.46
1:X:572:LYS:HD3	3:Z:353:HIS:ND1	2.29	0.46
2:B:155:PHE:C	2:B:155:PHE:CD1	2.94	0.46
2:B:817:VAL:CG1	2:B:830:ILE:HB	2.44	0.46
3:C:120:PHE:N	3:C:120:PHE:CD1	2.83	0.46
1:X:473:MET:HE1	1:X:476:LYS:HD2	1.96	0.46
1:X:585:VAL:HG11	1:X:591:CYS:SG	2.56	0.46
2:Y:486:LEU:HD11	2:Y:488:SER:C	2.40	0.46
3:Z:168:LEU:HD11	3:Z:183:GLN:HB2	1.98	0.46
2:B:16:ASN:ND2	2:B:36:ASN:H	2.13	0.46
2:B:726:TYR:CD1	2:B:733:PHE:CE1	3.03	0.46
2:Y:663:ASN:C	2:Y:663:ASN:HD22	2.23	0.46
2:B:390:ILE:HG21	2:B:710:LEU:HD13	1.96	0.46
2:B:925:ASP:OD1	2:B:925:ASP:C	2.58	0.46
2:Y:676:VAL:O	2:Y:676:VAL:HG12	2.14	0.46
3:Z:79:GLN:HE21	3:Z:79:GLN:HA	1.81	0.46
3:Z:266:GLU:O	3:Z:267:ASN:C	2.54	0.46
3:Z:394:CYS:O	3:Z:395:ALA:HB3	2.16	0.46
2:B:575:GLU:O	2:B:576:LEU:C	2.59	0.46
2:B:948:ASP:HB2	2:B:992:LEU:HB2	1.97	0.46
1:X:584:PHE:C	1:X:584:PHE:CD1	2.93	0.46
2:Y:459:PHE:CD1	2:Y:459:PHE:C	2.93	0.46
2:Y:555:LEU:HD13	2:Y:593:MET:SD	2.55	0.46
3:Z:115:GLN:NE2	3:Z:115:GLN:CA	2.78	0.46
2:B:815:SER:OG	2:B:873:MET:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:36:ASN:ND2	2:Y:1002:GLU:OE2	2.48	0.46
2:Y:272:LEU:HD11	2:Y:322:VAL:HG21	1.98	0.46
2:B:267:ASN:ND2	2:B:269:SER:OG	2.49	0.46
2:B:652:CYS:HB3	2:B:676:VAL:HG12	1.96	0.46
1:X:441:ARG:N	1:X:461:SER:HB3	2.30	0.46
1:X:540:HIS:CE1	1:X:542:SER:OG	2.57	0.46
3:Z:345:PRO:O	3:Z:360:LEU:HD12	2.16	0.46
2:Y:722:ARG:C	2:Y:723:LYS:HG2	2.41	0.46
3:Z:313:ASP:OD1	3:Z:313:ASP:C	2.59	0.46
2:B:930:VAL:HG12	2:B:931:LEU:N	2.31	0.46
3:C:351:ASN:OD1	3:C:355:TYR:HB2	2.16	0.46
1:X:471:VAL:CG1	1:X:472:MET:N	2.78	0.45
2:Y:715:VAL:HG21	2:Y:799:PHE:CG	2.51	0.45
2:Y:916:THR:OG1	2:Y:917:LYS:N	2.47	0.45
2:B:24:THR:HG22	2:B:91:TYR:CE2	2.52	0.45
2:B:328:LEU:HD23	2:B:328:LEU:N	2.32	0.45
2:B:808:LEU:HD11	2:B:847:ARG:CZ	2.46	0.45
2:B:913:TYR:CZ	3:C:240:TRP:CZ3	3.04	0.45
2:B:914:LEU:O	2:B:915:LYS:HG2	2.16	0.45
2:B:932:LEU:C	2:B:933:LEU:HD23	2.41	0.45
3:C:91:LEU:HD22	3:C:92:ILE:N	2.31	0.45
2:Y:511:ALA:HB1	2:Y:538:VAL:CG1	2.46	0.45
1:A:459:LEU:HB2	1:A:500:LEU:HD22	1.98	0.45
1:A:561:VAL:HG22	1:A:562:GLU:N	2.31	0.45
2:Y:390:ILE:HG21	2:Y:710:LEU:HD13	1.98	0.45
2:Y:511:ALA:CB	2:Y:538:VAL:HG11	2.45	0.45
2:Y:958:GLU:OE1	2:Y:958:GLU:HA	2.16	0.45
2:Y:1051:LEU:HD22	2:Y:1094:ILE:HD12	1.99	0.45
3:Z:91:LEU:HD22	3:Z:92:ILE:N	2.29	0.45
2:B:564:ILE:CD1	2:B:584:GLY:N	2.79	0.45
1:A:568:CYS:O	1:A:592:ILE:HG13	2.15	0.45
1:X:449:LYS:HZ2	1:X:510:GLU:CB	2.30	0.45
1:X:554:ILE:O	1:X:555:HIS:CD2	2.70	0.45
2:Y:881:LEU:HD12	2:Y:889:ARG:O	2.17	0.45
2:Y:914:LEU:O	2:Y:915:LYS:HG2	2.17	0.45
3:Z:49:PHE:CD1	3:Z:49:PHE:C	2.94	0.45
3:Z:402:PHE:CD1	3:Z:402:PHE:N	2.84	0.45
2:B:537:GLU:HG3	2:B:561:TRP:CB	2.46	0.45
2:B:617:ASN:CB	2:B:620:THR:CB	2.95	0.45
1:X:447:LYS:HD3	1:X:447:LYS:N	2.29	0.45
2:Y:105:HIS:HA	2:Y:152:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:576:LEU:O	2:B:578:HIS:N	2.49	0.45
2:B:591:ILE:HG13	2:B:603:LEU:O	2.17	0.45
2:B:912:LEU:HD11	3:C:244:LEU:HD21	1.99	0.45
2:B:1122:ARG:NH1	2:B:1128:ASP:OD2	2.49	0.45
2:Y:155:PHE:CD1	2:Y:155:PHE:C	2.94	0.45
2:Y:161:GLU:OE2	2:Y:193:TYR:OH	2.29	0.45
3:Z:82:PRO:HB3	3:Z:109:MET:HE1	1.99	0.45
3:C:48:ASN:CA	3:C:410:SER:HB3	2.40	0.45
3:C:351:ASN:CB	3:C:352:PRO:CD	2.95	0.45
1:A:533:ALA:HB2	1:A:629:VAL:HA	1.97	0.45
1:A:540:HIS:CE1	1:A:542:SER:O	2.70	0.45
1:X:449:LYS:HZ2	1:X:510:GLU:CG	2.30	0.45
1:X:459:LEU:HB2	1:X:500:LEU:HD22	1.97	0.45
1:X:482:LEU:HD21	1:X:505:LYS:HB3	1.98	0.45
1:X:610:PRO:HD2	1:X:611:GLN:HG2	1.98	0.45
2:Y:410:LEU:C	2:Y:411:TRP:CD2	2.95	0.45
2:Y:706:GLU:HA	2:Y:707:ILE:HA	1.86	0.45
2:Y:910:MET:HE3	2:Y:910:MET:HB2	1.77	0.45
3:Z:145:ARG:NH2	3:Z:145:ARG:HG3	2.31	0.45
2:B:119:GLY:O	2:B:134:ARG:NH1	2.50	0.45
2:B:618:ILE:H	2:B:618:ILE:CD1	2.28	0.45
1:X:605:THR:HG1	1:X:608:ASP:HB2	1.78	0.45
1:X:610:PRO:CG	1:X:611:GLN:H	2.29	0.45
2:Y:268:GLY:O	2:Y:285:LEU:HD12	2.17	0.45
2:Y:998:PHE:HD2	2:Y:1088:PHE:CB	2.30	0.45
2:B:172:GLY:CA	2:B:224:GLU:CD	2.90	0.45
2:B:883:SER:HB2	2:B:911:ALA:CB	2.43	0.45
2:B:1115:ASP:O	2:B:1115:ASP:CG	2.60	0.45
3:C:114:ILE:HG13	3:C:144:TYR:HE2	1.80	0.45
3:C:394:CYS:O	3:C:395:ALA:HB3	2.16	0.45
1:X:581:ARG:CG	1:X:581:ARG:NH1	2.80	0.45
1:X:610:PRO:HD2	1:X:611:GLN:N	2.28	0.45
2:B:324:VAL:HB	2:B:332:GLN:HB2	1.98	0.45
2:B:486:LEU:HG	2:B:486:LEU:O	2.16	0.45
2:B:805:HIS:CD2	2:B:805:HIS:C	2.95	0.45
1:X:482:LEU:HD21	1:X:505:LYS:CB	2.47	0.45
2:Y:118:THR:CG2	2:Y:165:ILE:O	2.62	0.45
2:Y:172:GLY:HA3	2:Y:224:GLU:HG3	1.99	0.45
2:Y:324:VAL:HB	2:Y:332:GLN:HB2	1.99	0.45
2:Y:414:ARG:HB2	2:Y:462:ASN:ND2	2.31	0.45
1:A:508:GLU:OE2	1:A:511:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:913:TYR:CZ	3:Z:240:TRP:CZ3	3.05	0.44
2:B:405:PRO:HA	2:B:697:SER:HA	1.99	0.44
2:B:558:ILE:CG2	2:B:559:GLY:N	2.80	0.44
1:X:443:PRO:CB	1:X:556:THR:HG23	2.48	0.44
1:X:606:PHE:HB2	1:X:628:LYS:HB3	1.99	0.44
2:Y:410:LEU:HD12	2:Y:410:LEU:HA	1.80	0.44
2:Y:545:PRO:C	2:Y:546:LEU:HG	2.41	0.44
2:Y:571:LEU:O	2:Y:573:SER:N	2.44	0.44
2:Y:584:GLY:O	2:Y:586:ILE:N	2.50	0.44
2:Y:808:LEU:HB2	2:Y:811:GLU:HB2	1.99	0.44
2:Y:821:LEU:HD11	2:Y:830:ILE:HD11	1.99	0.44
2:Y:925:ASP:OD1	2:Y:925:ASP:C	2.60	0.44
3:Z:104:PRO:HD2	3:Z:105:GLN:OE1	2.18	0.44
3:Z:351:ASN:CB	3:Z:352:PRO:CD	2.94	0.44
3:Z:391:CYS:HB3	3:Z:394:CYS:SG	2.57	0.44
2:B:273:LEU:HB2	2:B:281:PHE:HB2	1.97	0.44
2:B:378:CYS:SG	2:B:721:PRO:HB2	2.57	0.44
2:B:459:PHE:CD1	2:B:460:CYS:N	2.85	0.44
2:B:881:LEU:HD12	2:B:889:ARG:O	2.17	0.44
2:B:1072:PHE:C	2:B:1072:PHE:HD1	2.24	0.44
2:B:1125:THR:HG23	2:B:1128:ASP:OD2	2.18	0.44
3:C:284:VAL:HG23	3:C:311:GLU:CD	2.43	0.44
1:X:553:HIS:CE1	1:X:558:ILE:HG12	2.52	0.44
1:X:606:PHE:O	1:X:608:ASP:N	2.48	0.44
2:Y:183:GLN:HB2	2:Y:188:ARG:HG2	1.99	0.44
2:Y:792:LEU:O	2:Y:793:ILE:HD13	2.18	0.44
2:B:571:LEU:O	2:B:573:SER:N	2.45	0.44
3:C:351:ASN:ND2	1:A:572:LYS:O	2.50	0.44
1:A:485:LEU:N	1:A:485:LEU:HD12	2.33	0.44
1:A:503:ARG:CZ	1:A:503:ARG:HB2	2.46	0.44
1:X:536:VAL:HG11	5:Z:502:85C:C20	2.47	0.44
1:X:552:LEU:HD11	1:X:554:ILE:HD11	1.98	0.44
2:Y:569:LEU:N	2:Y:569:LEU:HD22	2.33	0.44
2:Y:914:LEU:C	2:Y:915:LYS:HG2	2.42	0.44
2:B:183:GLN:NE2	3:C:209:PRO:HA	2.32	0.44
3:C:93:PRO:HD3	3:C:137:THR:HG21	2.00	0.44
1:X:537:ILE:CG1	1:X:585:VAL:HG22	2.48	0.44
2:Y:184:ASP:HB2	2:Y:185:PRO:HD2	2.00	0.44
2:Y:930:VAL:HG12	2:Y:931:LEU:N	2.32	0.44
2:B:437:MET:C	2:B:438:LEU:HD12	2.41	0.44
2:B:931:LEU:HD23	2:B:933:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:522:HIS:O	2:Y:523:PRO:C	2.59	0.44
2:Y:998:PHE:HD2	2:Y:1088:PHE:HB2	1.82	0.44
3:Z:187:GLU:HG2	3:Z:278:ILE:HG12	1.98	0.44
2:B:1039:LEU:HD23	2:B:1039:LEU:C	2.43	0.44
1:A:530:THR:HG23	1:A:596:ARG:HG2	2.00	0.44
2:Y:67:PHE:CG	2:Y:124:ILE:HD13	2.53	0.44
2:Y:110:ASP:OD1	2:Y:110:ASP:N	2.50	0.44
2:Y:404:LEU:C	2:Y:404:LEU:CD2	2.90	0.44
2:Y:889:ARG:HG2	2:Y:891:TYR:CE2	2.53	0.44
2:Y:937:PRO:HD2	2:Y:938:MET:CE	2.47	0.44
2:B:118:THR:CG2	2:B:165:ILE:O	2.63	0.44
2:B:914:LEU:C	2:B:915:LYS:HG2	2.43	0.44
3:C:117:ASP:C	3:C:119:THR:N	2.70	0.44
1:X:472:MET:HE2	1:X:472:MET:HB3	1.92	0.44
2:Y:405:PRO:HA	2:Y:697:SER:HA	1.99	0.44
2:Y:933:LEU:HD22	2:Y:944:GLU:HA	1.99	0.44
2:Y:1122:ARG:NH1	2:Y:1128:ASP:OD2	2.50	0.44
2:Y:1125:THR:HG23	2:Y:1128:ASP:OD2	2.18	0.44
3:Z:338:PHE:HE2	3:Z:340:LEU:HG	1.83	0.44
2:B:217:SER:HB2	3:C:204:LYS:HB3	1.98	0.44
2:B:478:LEU:HD22	2:B:526:LEU:HG	1.99	0.44
2:B:511:ALA:HB1	2:B:538:VAL:CG1	2.45	0.44
2:B:545:PRO:C	2:B:546:LEU:HG	2.42	0.44
2:B:578:HIS:O	2:B:579:LYS:CB	2.66	0.44
1:X:443:PRO:HA	1:X:517:ILE:CG2	2.47	0.44
1:X:538:ILE:HG13	1:X:539:GLU:N	2.33	0.44
1:X:545:CYS:SG	1:X:546:PRO:HD2	2.58	0.44
2:Y:591:ILE:HG13	2:Y:603:LEU:O	2.18	0.44
2:Y:932:LEU:HD12	2:Y:932:LEU:HA	1.79	0.44
1:X:453:THR:C	1:X:454:VAL:HG23	2.43	0.43
2:Y:853:TYR:CD1	2:Y:853:TYR:C	2.95	0.43
3:Z:292:ASP:O	3:Z:296:ILE:HG12	2.18	0.43
2:B:110:ASP:OD1	2:B:110:ASP:N	2.50	0.43
2:B:718:TYR:CD1	2:B:718:TYR:N	2.85	0.43
2:B:821:LEU:HD11	2:B:830:ILE:HD11	2.00	0.43
3:C:173:GLN:CB	3:C:179:GLN:HE21	2.31	0.43
3:C:425:THR:CG2	3:C:426:ILE:HD13	2.47	0.43
2:Y:723:LYS:O	2:Y:735:VAL:HA	2.18	0.43
2:Y:900:ARG:O	2:Y:900:ARG:CG	2.59	0.43
2:Y:1030:PHE:CE2	2:Y:1040:VAL:HG23	2.53	0.43
2:B:796:GLN:OE1	2:B:797:HIS:CE1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:847:ARG:NH1	2:B:849:VAL:HG22	2.33	0.43
1:X:524:LEU:HD12	1:X:524:LEU:C	2.44	0.43
1:X:545:CYS:HB2	1:X:584:PHE:CB	2.48	0.43
1:X:553:HIS:ND1	1:X:558:ILE:HD11	2.33	0.43
2:Y:110:ASP:OD1	2:Y:141:LYS:NZ	2.51	0.43
2:Y:328:LEU:N	2:Y:328:LEU:HD23	2.32	0.43
2:Y:329:GLY:O	2:Y:355:ASN:ND2	2.50	0.43
2:Y:448:LEU:HD23	2:Y:451:PHE:CD1	2.53	0.43
2:Y:478:LEU:HD22	2:Y:526:LEU:HG	2.00	0.43
2:Y:564:ILE:O	2:Y:582:LEU:HD12	2.19	0.43
2:Y:663:ASN:HB2	2:Y:1134:GLU:CD	2.43	0.43
2:Y:932:LEU:C	2:Y:933:LEU:HD23	2.44	0.43
2:Y:1115:ASP:O	2:Y:1115:ASP:CG	2.61	0.43
2:B:58:TYR:HE1	2:B:1070:HIS:HD2	1.65	0.43
2:B:110:ASP:OD1	2:B:141:LYS:NZ	2.51	0.43
2:B:268:GLY:O	2:B:285:LEU:HD12	2.18	0.43
2:B:998:PHE:CZ	2:B:1074:ARG:HD2	2.53	0.43
1:A:605:THR:HA	1:A:629:VAL:HG22	2.00	0.43
2:Y:40:GLU:HB3	2:Y:42:TYR:CE1	2.54	0.43
2:Y:616:LEU:HD12	2:Y:616:LEU:HA	1.92	0.43
2:Y:652:CYS:HB3	2:Y:676:VAL:HG12	2.01	0.43
2:Y:718:TYR:CD1	2:Y:718:TYR:N	2.86	0.43
3:Z:340:LEU:HD23	3:Z:340:LEU:HA	1.79	0.43
2:B:576:LEU:C	2:B:578:HIS:N	2.76	0.43
2:B:869:ALA:HB3	2:B:871:TYR:CZ	2.53	0.43
3:Z:250:ALA:HB2	3:Z:305:ILE:CD1	2.48	0.43
3:Z:284:VAL:HG23	3:Z:311:GLU:CD	2.43	0.43
2:B:359:ILE:HB	2:B:1032:THR:H	1.84	0.43
2:B:958:GLU:HA	2:B:958:GLU:OE1	2.18	0.43
2:B:1030:PHE:CE2	2:B:1040:VAL:HG23	2.54	0.43
3:C:82:PRO:CB	3:C:109:MET:HE1	2.48	0.43
1:A:482:LEU:HD21	1:A:505:LYS:CB	2.48	0.43
1:X:441:ARG:NE	1:X:525:CYS:SG	2.92	0.43
2:Y:457:THR:HG23	2:Y:470:GLN:HG3	2.00	0.43
2:Y:631:LEU:HD12	2:Y:636:THR:HG21	2.01	0.43
2:B:433:THR:C	2:B:434:ARG:HG2	2.44	0.43
2:B:492:GLU:OE1	2:B:494:GLN:N	2.39	0.43
2:B:916:THR:OG1	2:B:917:LYS:N	2.50	0.43
2:Y:204:LYS:HE2	2:Y:204:LYS:CA	2.42	0.43
2:Y:245:TYR:C	2:Y:246:LEU:HD12	2.43	0.43
2:Y:573:SER:O	2:Y:574:PHE:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:571:LEU:HB3	2:B:572:PRO:CD	2.49	0.43
2:B:723:LYS:O	2:B:735:VAL:HA	2.18	0.43
3:C:260:GLN:O	3:C:263:GLU:HG2	2.18	0.43
1:X:572:LYS:O	5:Z:502:85C:C4	2.66	0.43
2:Y:172:GLY:CA	2:Y:224:GLU:CD	2.92	0.43
2:Y:487:VAL:CG2	2:Y:524:GLN:HA	2.49	0.43
2:Y:883:SER:O	2:Y:883:SER:OG	2.37	0.43
2:B:809:GLN:O	2:B:810:ASN:HB2	2.19	0.43
3:C:199:LEU:HD21	3:C:237:LEU:CD1	2.31	0.43
1:A:524:LEU:C	1:A:524:LEU:HD12	2.44	0.43
1:X:572:LYS:O	3:Z:351:ASN:ND2	2.51	0.42
2:Y:650:PHE:CD2	2:Y:679:MET:HE3	2.54	0.42
2:Y:1121:LYS:O	2:Y:1122:ARG:HB3	2.19	0.42
2:B:410:LEU:HD12	2:B:410:LEU:HA	1.78	0.42
2:B:487:VAL:CG2	2:B:524:GLN:HA	2.48	0.42
2:B:538:VAL:HG23	2:B:558:ILE:CG2	2.49	0.42
2:B:1032:THR:CG2	2:B:1033:VAL:N	2.81	0.42
1:A:554:ILE:O	1:A:557:CYS:O	2.37	0.42
1:X:628:LYS:HD3	5:Z:502:85C:C18	2.49	0.42
2:Y:58:TYR:CE1	2:Y:1070:HIS:HD2	2.37	0.42
2:Y:624:SER:O	2:Y:625:ASP:C	2.61	0.42
2:Y:1061:VAL:HG21	2:Y:1108:VAL:CG2	2.49	0.42
3:Z:289:PRO:O	3:Z:424:PRO:HG3	2.19	0.42
2:B:161:GLU:OE2	2:B:193:TYR:OH	2.31	0.42
2:B:245:TYR:C	2:B:246:LEU:HD12	2.44	0.42
2:B:932:LEU:HB3	2:B:945:ILE:HB	2.00	0.42
2:B:960:LEU:HD23	2:B:960:LEU:HA	1.80	0.42
1:A:563:ILE:O	1:A:563:ILE:CG1	2.67	0.42
3:Z:113:LEU:HD12	3:Z:113:LEU:HA	1.82	0.42
3:Z:345:PRO:O	3:Z:360:LEU:HA	2.18	0.42
1:X:537:ILE:HG13	1:X:585:VAL:HG22	2.00	0.42
2:Y:6:VAL:HG22	2:Y:1040:VAL:HG22	2.01	0.42
2:Y:998:PHE:CD2	2:Y:1088:PHE:HB3	2.54	0.42
3:Z:67:PHE:CD2	3:Z:118:ARG:HD3	2.54	0.42
2:B:5:TYR:CE1	2:B:7:VAL:HB	2.54	0.42
2:B:281:PHE:HD1	2:B:304:LEU:HA	1.84	0.42
2:B:537:GLU:HG3	2:B:561:TRP:CD1	2.53	0.42
2:B:913:TYR:CZ	3:C:240:TRP:HH2	2.36	0.42
3:C:426:ILE:N	3:C:426:ILE:HD13	2.34	0.42
1:A:440:ILE:HG13	1:A:520:ASP:H	1.84	0.42
1:A:553:HIS:CE1	1:A:558:ILE:HG12	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:492:GLU:HB3	2:Y:496:LYS:H	1.84	0.42
3:Z:70:ARG:HD3	3:Z:70:ARG:C	2.44	0.42
3:Z:221:TYR:O	3:Z:225:GLN:NE2	2.51	0.42
2:B:522:HIS:O	2:B:523:PRO:C	2.59	0.42
2:B:722:ARG:C	2:B:723:LYS:HG2	2.45	0.42
2:B:937:PRO:HD2	2:B:938:MET:CE	2.49	0.42
3:C:113:LEU:HD12	3:C:113:LEU:HA	1.82	0.42
3:C:119:THR:HG22	3:C:140:GLU:HA	2.01	0.42
1:X:468:GLN:O	1:X:469:GLN:C	2.61	0.42
2:Y:535:GLU:CB	2:Y:536:HIS:CE1	3.03	0.42
2:Y:537:GLU:O	2:Y:561:TRP:CD1	2.73	0.42
2:Y:541:LEU:HD23	2:Y:558:ILE:HD12	2.00	0.42
2:B:40:GLU:CG	2:B:54:GLU:HG3	2.49	0.42
2:B:282:MET:HE2	2:B:282:MET:HB3	1.91	0.42
3:C:187:GLU:HG2	3:C:278:ILE:HG12	2.01	0.42
1:A:474:PRO:HD3	1:A:602:CYS:SG	2.60	0.42
2:Y:437:MET:C	2:Y:438:LEU:HD12	2.45	0.42
2:Y:913:TYR:OH	3:Z:240:TRP:CZ3	2.70	0.42
2:Y:1032:THR:CG2	2:Y:1033:VAL:N	2.82	0.42
3:Z:319:THR:OG1	3:Z:427:PRO:HG3	2.19	0.42
2:B:912:LEU:HD23	2:B:912:LEU:HA	1.72	0.42
2:B:932:LEU:HD12	2:B:932:LEU:HA	1.77	0.42
2:B:955:SER:OG	2:B:1004:VAL:O	2.23	0.42
1:A:442:LEU:HB2	1:A:459:LEU:HD23	2.01	0.42
1:A:510:GLU:C	1:A:510:GLU:CD	2.87	0.42
1:A:610:PRO:HD2	1:A:611:GLN:NE2	2.35	0.42
1:X:473:MET:C	1:X:475:ASN:N	2.77	0.42
1:X:554:ILE:CG2	1:X:555:HIS:CD2	2.85	0.42
3:Z:93:PRO:HD3	3:Z:137:THR:HG21	2.02	0.42
2:B:821:LEU:HB3	2:B:893:TRP:CB	2.49	0.42
2:Y:5:TYR:CE2	2:Y:1136:LEU:HD22	2.55	0.42
2:Y:1056:ASN:N	2:Y:1056:ASN:HD22	2.18	0.42
3:Z:81:ILE:HB	3:Z:121:ALA:HB2	2.01	0.42
3:Z:117:ASP:O	3:Z:118:ARG:HB2	2.20	0.42
2:B:283:LEU:HD12	2:B:302:VAL:HG22	2.02	0.42
3:C:349:TYR:CD2	3:C:359:THR:CG2	3.03	0.42
1:X:610:PRO:CG	1:X:611:GLN:N	2.82	0.42
2:Y:40:GLU:CG	2:Y:54:GLU:HG3	2.49	0.42
2:Y:571:LEU:HB3	2:Y:572:PRO:CD	2.50	0.42
2:Y:998:PHE:CZ	2:Y:1074:ARG:HD2	2.55	0.42
3:Z:145:ARG:HG3	3:Z:145:ARG:HH21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:PRO:O	2:B:379:SER:HA	2.20	0.42
2:B:492:GLU:HB3	2:B:496:LYS:H	1.85	0.42
2:B:541:LEU:HD23	2:B:558:ILE:HD12	1.99	0.42
2:B:543:ILE:HG23	2:B:543:ILE:O	2.20	0.42
2:B:1051:LEU:CD2	2:B:1094:ILE:HD12	2.49	0.42
2:B:1070:HIS:CE1	2:B:1093:LEU:CD2	3.02	0.42
1:X:442:LEU:HB2	1:X:459:LEU:HD23	2.01	0.41
2:Y:404:LEU:HD22	2:Y:407:ILE:CD1	2.47	0.41
2:Y:455:GLN:HE21	2:Y:474:ALA:HB2	1.85	0.41
2:Y:716:PRO:HB3	2:Y:718:TYR:HE1	1.80	0.41
2:B:169:PHE:CD1	2:B:178:ILE:HG22	2.55	0.41
2:B:588:PRO:HA	2:B:606:LEU:HD23	2.01	0.41
2:B:805:HIS:CD2	2:B:806:GLN:C	2.98	0.41
3:C:85:PRO:HD2	3:C:106:GLU:HG2	2.02	0.41
1:A:511:GLU:HA	1:A:511:GLU:OE1	2.19	0.41
1:A:538:ILE:HG13	1:A:539:GLU:N	2.34	0.41
1:X:530:THR:HG23	1:X:596:ARG:HG2	2.00	0.41
1:X:540:HIS:HE1	1:X:542:SER:CA	2.32	0.41
2:Y:930:VAL:CG1	2:Y:931:LEU:N	2.83	0.41
2:Y:965:PHE:CD2	2:Y:965:PHE:N	2.88	0.41
2:B:234:GLN:OE1	2:B:257:THR:HG23	2.21	0.41
2:B:661:SER:H	2:B:666:LEU:HA	1.85	0.41
2:B:661:SER:HG	2:B:663:ASN:ND2	2.16	0.41
3:C:93:PRO:HD3	3:C:137:THR:CG2	2.51	0.41
1:X:447:LYS:O	1:X:447:LYS:HG2	2.20	0.41
1:X:551:VAL:HG12	1:X:552:LEU:N	2.35	0.41
1:X:572:LYS:HD3	3:Z:353:HIS:CG	2.55	0.41
2:Y:485:ALA:O	2:Y:487:VAL:HG13	2.20	0.41
2:Y:641:PHE:CE1	2:Y:648:ASN:HB2	2.56	0.41
3:Z:406:LYS:HE2	3:Z:409:MET:CE	2.51	0.41
2:B:631:LEU:HD12	2:B:636:THR:HG21	2.02	0.41
2:B:893:TRP:CZ2	2:B:897:LYS:HG3	2.56	0.41
3:C:81:ILE:HB	3:C:121:ALA:HB2	2.01	0.41
1:A:450:ASP:C	1:A:452:GLY:N	2.79	0.41
1:X:447:LYS:HD2	1:X:512:ILE:O	2.20	0.41
2:Y:359:ILE:HB	2:Y:1032:THR:H	1.85	0.41
2:Y:543:ILE:HG23	2:Y:543:ILE:O	2.21	0.41
3:Z:137:THR:HA	3:Z:163:GLN:O	2.21	0.41
2:B:928:ARG:HB2	2:B:954:MET:HB2	2.02	0.41
3:C:250:ALA:HB2	3:C:305:ILE:CD1	2.50	0.41
2:Y:23:PHE:H	2:Y:30:ASN:HD22	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:358:PRO:O	2:Y:379:SER:HA	2.21	0.41
2:Y:538:VAL:HG23	2:Y:558:ILE:CG2	2.51	0.41
2:B:272:LEU:HD11	2:B:322:VAL:HG21	2.02	0.41
2:B:451:PHE:HA	2:B:470:GLN:NE2	2.36	0.41
2:B:558:ILE:HG22	2:B:560:LEU:HD23	2.01	0.41
2:B:569:LEU:N	2:B:569:LEU:HD22	2.35	0.41
1:X:564:THR:HG21	1:X:596:ARG:HG3	2.03	0.41
2:Y:744:ASP:CB	2:Y:749:THR:N	2.83	0.41
2:Y:770:LEU:HD23	2:B:445:GLU:HG3	2.03	0.41
2:Y:931:LEU:HD23	2:Y:933:LEU:HD21	2.01	0.41
2:Y:961:ASP:C	2:Y:961:ASP:OD1	2.63	0.41
2:B:1055:GLN:HE22	2:B:1090:ASP:H	1.69	0.41
2:B:1121:LYS:O	2:B:1122:ARG:HB3	2.19	0.41
3:C:165:PHE:CG	3:C:182:VAL:HG22	2.55	0.41
1:A:597:THR:C	1:A:599:GLY:N	2.78	0.41
1:X:481:VAL:HG11	1:X:484:ILE:HD11	2.03	0.41
1:X:540:HIS:HE1	1:X:542:SER:N	2.12	0.41
1:X:567:ILE:HA	1:X:581:ARG:HH12	1.85	0.41
2:Y:467:GLN:HE22	2:Y:524:GLN:H	1.67	0.41
2:Y:811:GLU:OE1	2:Y:847:ARG:NH2	2.47	0.41
2:Y:906:TYR:H	2:Y:906:TYR:HD1	1.64	0.41
3:Z:126:SER:O	3:Z:127:ASN:C	2.63	0.41
2:B:183:GLN:HE22	3:C:209:PRO:HA	1.84	0.41
2:B:1072:PHE:CD1	2:B:1072:PHE:O	2.74	0.41
3:C:257:ILE:CG1	3:C:312:LEU:HG	2.51	0.41
1:X:578:SER:OG	1:X:579:LYS:N	2.53	0.41
2:Y:411:TRP:O	2:Y:425:LEU:HD12	2.21	0.41
2:Y:497:ASN:O	2:Y:512:VAL:HG13	2.21	0.41
2:Y:658:VAL:HG23	2:Y:671:VAL:HG22	2.03	0.41
2:Y:821:LEU:HB3	2:Y:893:TRP:CB	2.51	0.41
2:Y:960:LEU:HD23	2:Y:960:LEU:HA	1.76	0.41
2:Y:1134:GLU:HA	2:Y:1137:THR:OG1	2.21	0.41
3:Z:102:PHE:N	3:Z:102:PHE:CD1	2.89	0.41
2:B:216:ALA:HA	2:B:233:GLY:HA2	2.03	0.41
2:B:378:CYS:SG	2:B:724:ILE:HB	2.60	0.41
2:B:1003:PHE:CG	3:C:197:VAL:HG23	2.56	0.41
2:B:1007:PHE:CD1	2:B:1030:PHE:HB3	2.56	0.41
3:C:72:LEU:HD23	3:C:163:GLN:HE21	1.86	0.41
3:C:370:LEU:HD21	3:C:401:LYS:HD3	2.02	0.41
1:A:568:CYS:O	1:A:592:ILE:HG12	2.20	0.41
3:Z:98:PRO:HB2	3:Z:350:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:257:ILE:CG1	3:Z:312:LEU:HG	2.51	0.41
2:B:184:ASP:HB2	2:B:185:PRO:HD2	2.02	0.41
2:B:479:VAL:HG12	2:B:480:SER:O	2.21	0.41
2:B:564:ILE:HD12	2:B:583:GLY:C	2.45	0.41
2:B:658:VAL:HG23	2:B:671:VAL:HG22	2.03	0.41
3:C:289:PRO:O	3:C:424:PRO:HG3	2.21	0.41
1:A:486:SER:O	1:A:487:ASP:HB3	2.20	0.41
1:X:503:ARG:HB2	1:X:503:ARG:CZ	2.51	0.40
3:Z:373:ARG:HB3	3:Z:374:PRO:CD	2.50	0.40
2:B:40:GLU:HB3	2:B:42:TYR:CE1	2.56	0.40
2:B:624:SER:O	2:B:625:ASP:CB	2.69	0.40
2:B:930:VAL:CG1	2:B:931:LEU:N	2.83	0.40
3:C:426:ILE:HG13	3:C:429:THR:HB	2.03	0.40
1:A:512:ILE:O	1:A:513:LEU:HD12	2.19	0.40
2:Y:588:PRO:HA	2:Y:606:LEU:HD23	2.03	0.40
2:Y:922:LEU:HD13	2:Y:965:PHE:CD1	2.56	0.40
2:Y:1003:PHE:CG	3:Z:197:VAL:HG23	2.57	0.40
2:Y:1044:SER:OG	2:Y:1047:TRP:HD1	2.04	0.40
3:Z:82:PRO:CB	3:Z:109:MET:HE1	2.50	0.40
1:A:447:LYS:O	1:A:447:LYS:HG2	2.20	0.40
1:A:469:GLN:O	1:A:470:LEU:HD23	2.22	0.40
1:A:551:VAL:HG12	1:A:552:LEU:N	2.36	0.40
2:Y:452:VAL:HG12	2:Y:470:GLN:NE2	2.37	0.40
2:Y:791:LEU:HD12	2:Y:792:LEU:N	2.36	0.40
3:Z:414:PHE:CD1	3:Z:414:PHE:C	2.99	0.40
2:B:457:THR:HG23	2:B:470:GLN:HG3	2.04	0.40
2:B:616:LEU:HD12	2:B:616:LEU:HA	1.91	0.40
1:A:443:PRO:HA	1:A:517:ILE:CG2	2.49	0.40
2:Y:282:MET:HE2	2:Y:282:MET:HB3	1.93	0.40
2:Y:594:THR:OG1	2:Y:595:THR:N	2.55	0.40
2:B:322:VAL:CG2	2:B:336:LEU:HD21	2.51	0.40
2:B:663:ASN:HB2	2:B:1134:GLU:CD	2.47	0.40
2:B:928:ARG:O	2:B:928:ARG:HG3	2.20	0.40
3:C:345:PRO:O	3:C:360:LEU:HA	2.20	0.40
1:X:606:PHE:HE2	1:X:628:LYS:CG	2.17	0.40
2:Y:59:GLY:HA2	2:Y:1073:TRP:CE3	2.54	0.40
2:Y:169:PHE:CD1	2:Y:178:ILE:HG22	2.57	0.40
2:Y:171:TYR:CD2	2:Y:223:PRO:HA	2.56	0.40
2:Y:215:GLU:HB3	2:Y:234:GLN:HG2	2.04	0.40
2:Y:322:VAL:CG2	2:Y:336:LEU:HD21	2.51	0.40
2:Y:378:CYS:SG	2:Y:724:ILE:HB	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1048:TYR:HD1	2:Y:1089:ILE:CD1	2.33	0.40
2:B:410:LEU:C	2:B:411:TRP:CD2	3.00	0.40
2:B:430:VAL:HA	2:B:456:GLN:NE2	2.36	0.40
2:B:502:SER:HB3	2:B:541:LEU:HB2	2.04	0.40
2:B:872:SER:OG	2:B:914:LEU:HB2	2.22	0.40
2:B:931:LEU:HD11	2:B:947:ARG:NH2	2.36	0.40
3:C:338:PHE:HE2	3:C:340:LEU:HG	1.87	0.40
3:C:351:ASN:HB2	3:C:352:PRO:HD2	2.03	0.40
1:A:472:MET:HE2	1:A:472:MET:HB3	1.93	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:103:HIS:CD2	1:A:542:SER:OG[2_546]	2.05	0.15
3:Z:116:LYS:CB	1:A:448:TYR:CB[1_544]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	194/199 (98%)	155 (80%)	30 (16%)	9 (5%)	2	17
1	X	193/199 (97%)	152 (79%)	33 (17%)	8 (4%)	2	19
2	B	1039/1140 (91%)	955 (92%)	76 (7%)	8 (1%)	16	49
2	Y	1046/1140 (92%)	959 (92%)	78 (8%)	9 (1%)	14	46
3	C	360/406 (89%)	322 (89%)	32 (9%)	6 (2%)	7	35
3	Z	372/406 (92%)	332 (89%)	37 (10%)	3 (1%)	16	49
All	All	3204/3490 (92%)	2875 (90%)	286 (9%)	43 (1%)	9	39

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	474	PRO
1	X	610	PRO
2	Y	224	GLU
2	Y	358	PRO
2	Y	483	PRO
2	Y	572	PRO
3	Z	411	PRO
2	B	224	GLU
2	B	358	PRO
2	B	483	PRO
2	B	572	PRO
3	C	116	LYS
3	C	118	ARG
3	C	411	PRO
3	C	427	PRO
1	A	473	MET
1	A	610	PRO
1	X	473	MET
2	Y	225	PRO
2	Y	513	GLY
2	B	225	PRO
2	B	513	GLY
3	Z	195	SER
3	Z	265	ASP
3	C	195	SER
1	A	450	ASP
1	X	582	PRO
1	X	598	ALA
2	Y	371	GLY
2	B	579	LYS
1	A	451	MET
1	A	540	HIS
1	A	582	PRO
2	Y	543	ILE
2	Y	1015	GLN
1	A	598	ALA
1	X	584	PHE
3	C	377	GLU
1	A	558	ILE
2	B	543	ILE
1	X	558	ILE
1	X	479	VAL
1	A	479	VAL

5.3.2 Protein sidechains ⓘ

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	153/175 (87%)	110 (72%)	43 (28%)	0	3
1	X	165/175 (94%)	111 (67%)	54 (33%)	0	2
2	B	855/999 (86%)	670 (78%)	185 (22%)	1	7
2	Y	868/999 (87%)	674 (78%)	194 (22%)	1	6
3	C	306/368 (83%)	220 (72%)	86 (28%)	0	3
3	Z	316/368 (86%)	232 (73%)	84 (27%)	0	3
All	All	2663/3084 (86%)	2017 (76%)	646 (24%)	1	5

All (646) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	440	ILE
1	X	441	ARG
1	X	447	LYS
1	X	449	LYS
1	X	450	ASP
1	X	454	VAL
1	X	455	VAL
1	X	456	LEU
1	X	459	LEU
1	X	473	MET
1	X	476	LYS
1	X	482	LEU
1	X	485	LEU
1	X	490	GLU
1	X	492	ASP
1	X	500	LEU
1	X	505	LYS
1	X	507	ILE
1	X	510	GLU
1	X	513	LEU
1	X	517	ILE
1	X	523	ASN

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Mol	Chain	Res	Type
1	X	529	ARG
1	X	535	ILE
1	X	536	VAL
1	X	543	ILE
1	X	544	ILE
1	X	545	CYS
1	X	549	ASN
1	X	552	LEU
1	X	558	ILE
1	X	566	LEU
1	X	567	ILE
1	X	569	LEU
1	X	570	VAL
1	X	571	ASP
1	X	579	LYS
1	X	580	THR
1	X	581	ARG
1	X	585	VAL
1	X	588	ASP
1	X	592	ILE
1	X	594	ARG
1	X	600	THR
1	X	602	CYS
1	X	609	PHE
1	X	611	GLN
1	X	612	MET
1	X	614	ARG
1	X	616	THR
1	X	618	ARG
1	X	622	LYS
1	X	626	ILE
1	X	629	VAL
2	Y	20	THR
2	Y	37	THR
2	Y	54	GLU
2	Y	63	VAL
2	Y	70	LYS
2	Y	81	THR
2	Y	92	LYS
2	Y	93	GLN
2	Y	97	SER
2	Y	100	ILE

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Mol	Chain	Res	Type
2	Y	108	VAL
2	Y	110	ASP
2	Y	117	GLU
2	Y	125	ASP
2	Y	134	ARG
2	Y	143	ILE
2	Y	147	ARG
2	Y	197	LEU
2	Y	198	ARG
2	Y	200	LYS
2	Y	201	GLU
2	Y	204	LYS
2	Y	213	GLU
2	Y	222	VAL
2	Y	226	PHE
2	Y	232	ILE
2	Y	235	GLU
2	Y	245	TYR
2	Y	253	ILE
2	Y	262	ASN
2	Y	269	SER
2	Y	277	GLU
2	Y	299	ASP
2	Y	302	VAL
2	Y	303	GLU
2	Y	304	LEU
2	Y	305	LEU
2	Y	309	SER
2	Y	310	ILE
2	Y	318	ASP
2	Y	321	VAL
2	Y	335	LYS
2	Y	336	LEU
2	Y	348	VAL
2	Y	350	MET
2	Y	354	THR
2	Y	360	VAL
2	Y	375	LEU
2	Y	377	THR
2	Y	396	ILE
2	Y	407	ILE
2	Y	408	LYS

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Mol	Chain	Res	Type
2	Y	410	LEU
2	Y	414	ARG
2	Y	420	GLU
2	Y	421	THR
2	Y	427	LEU
2	Y	428	SER
2	Y	429	PHE
2	Y	432	GLN
2	Y	435	VAL
2	Y	437	MET
2	Y	454	ASP
2	Y	463	VAL
2	Y	466	GLN
2	Y	468	LEU
2	Y	473	SER
2	Y	477	ARG
2	Y	486	LEU
2	Y	487	VAL
2	Y	488	SER
2	Y	492	GLU
2	Y	505	SER
2	Y	510	VAL
2	Y	514	ARG
2	Y	517	TYR
2	Y	519	LEU
2	Y	524	GLN
2	Y	526	LEU
2	Y	531	HIS
2	Y	532	THR
2	Y	534	MET
2	Y	543	ILE
2	Y	555	LEU
2	Y	560	LEU
2	Y	561	TRP
2	Y	562	THR
2	Y	569	LEU
2	Y	571	LEU
2	Y	582	LEU
2	Y	586	ILE
2	Y	587	ILE
2	Y	595	THR
2	Y	602	LEU

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Mol	Chain	Res	Type
2	Y	611	LEU
2	Y	618	ILE
2	Y	624	SER
2	Y	625	ASP
2	Y	628	LYS
2	Y	630	THR
2	Y	636	THR
2	Y	637	VAL
2	Y	647	THR
2	Y	652	CYS
2	Y	653	SER
2	Y	657	THR
2	Y	660	TYR
2	Y	663	ASN
2	Y	672	ASN
2	Y	673	LEU
2	Y	676	VAL
2	Y	684	SER
2	Y	691	LEU
2	Y	693	LEU
2	Y	697	SER
2	Y	698	THR
2	Y	699	LEU
2	Y	700	THR
2	Y	705	ASP
2	Y	708	GLN
2	Y	709	LYS
2	Y	722	ARG
2	Y	729	VAL
2	Y	742	VAL
2	Y	749	THR
2	Y	750	THR
2	Y	752	LEU
2	Y	753	ARG
2	Y	755	SER
2	Y	763	SER
2	Y	766	SER
2	Y	767	SER
2	Y	770	LEU
2	Y	786	VAL
2	Y	800	GLU
2	Y	814	LEU

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Mol	Chain	Res	Type
2	Y	823	LYS
2	Y	839	GLU
2	Y	840	GLU
2	Y	842	GLU
2	Y	844	LYS
2	Y	845	GLN
2	Y	854	SER
2	Y	860	THR
2	Y	864	LYS
2	Y	866	VAL
2	Y	870	VAL
2	Y	874	VAL
2	Y	886	SER
2	Y	889	ARG
2	Y	895	THR
2	Y	897	LYS
2	Y	898	GLU
2	Y	902	GLU
2	Y	903	CYS
2	Y	904	ASN
2	Y	906	TYR
2	Y	908	ASN
2	Y	914	LEU
2	Y	916	THR
2	Y	919	ASP
2	Y	923	VAL
2	Y	932	LEU
2	Y	933	LEU
2	Y	943	GLU
2	Y	947	ARG
2	Y	957	VAL
2	Y	962	ASP
2	Y	987	GLU
2	Y	988	GLU
2	Y	990	GLN
2	Y	995	VAL
2	Y	1006	VAL
2	Y	1011	SER
2	Y	1012	LEU
2	Y	1042	SER
2	Y	1050	LEU
2	Y	1052	LEU

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Mol	Chain	Res	Type
2	Y	1064	SER
2	Y	1069	GLU
2	Y	1071	SER
2	Y	1089	ILE
2	Y	1096	SER
2	Y	1100	ILE
2	Y	1105	MET
2	Y	1106	GLN
2	Y	1115	ASP
2	Y	1116	ASP
2	Y	1122	ARG
2	Y	1125	THR
2	Y	1131	LYS
2	Y	1132	VAL
2	Y	1134	GLU
2	Y	1137	THR
3	Z	49	PHE
3	Z	51	THR
3	Z	58	THR
3	Z	64	MET
3	Z	70	ARG
3	Z	71	THR
3	Z	74	ASP
3	Z	75	ASP
3	Z	80	VAL
3	Z	84	LEU
3	Z	88	MET
3	Z	89	MET
3	Z	91	LEU
3	Z	96	THR
3	Z	98	PRO
3	Z	105	GLN
3	Z	109	MET
3	Z	141	ILE
3	Z	145	ARG
3	Z	148	GLN
3	Z	152	ILE
3	Z	154	ILE
3	Z	156	LYS
3	Z	157	VAL
3	Z	162	ARG
3	Z	171	ARG

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Mol	Chain	Res	Type
3	Z	172	THR
3	Z	177	ILE
3	Z	179	GLN
3	Z	182	VAL
3	Z	189	VAL
3	Z	190	LEU
3	Z	193	THR
3	Z	197	VAL
3	Z	204	LYS
3	Z	206	GLN
3	Z	207	ILE
3	Z	210	SER
3	Z	221	TYR
3	Z	225	GLN
3	Z	237	LEU
3	Z	238	THR
3	Z	244	LEU
3	Z	246	SER
3	Z	255	ASP
3	Z	260	GLN
3	Z	272	SER
3	Z	273	LEU
3	Z	275	SER
3	Z	290	ILE
3	Z	291	ASP
3	Z	293	VAL
3	Z	294	LEU
3	Z	296	ILE
3	Z	297	GLN
3	Z	298	LEU
3	Z	299	LEU
3	Z	301	ILE
3	Z	310	CYS
3	Z	313	ASP
3	Z	314	ILE
3	Z	319	THR
3	Z	320	SER
3	Z	325	GLN
3	Z	332	THR
3	Z	333	THR
3	Z	350	VAL
3	Z	356	VAL

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Mol	Chain	Res	Type
3	Z	358	GLU
3	Z	361	THR
3	Z	370	LEU
3	Z	371	ILE
3	Z	373	ARG
3	Z	376	THR
3	Z	387	THR
3	Z	388	VAL
3	Z	390	GLN
3	Z	393	ILE
3	Z	401	LYS
3	Z	407	LYS
3	Z	419	ARG
3	Z	423	LEU
3	Z	429	THR
3	Z	431	ASP
2	B	20	THR
2	B	37	THR
2	B	54	GLU
2	B	63	VAL
2	B	70	LYS
2	B	81	THR
2	B	93	GLN
2	B	97	SER
2	B	100	ILE
2	B	108	VAL
2	B	110	ASP
2	B	117	GLU
2	B	125	ASP
2	B	134	ARG
2	B	143	ILE
2	B	197	LEU
2	B	200	LYS
2	B	201	GLU
2	B	222	VAL
2	B	226	PHE
2	B	232	ILE
2	B	245	TYR
2	B	253	ILE
2	B	262	ASN
2	B	269	SER
2	B	299	ASP

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Mol	Chain	Res	Type
2	B	302	VAL
2	B	303	GLU
2	B	304	LEU
2	B	305	LEU
2	B	309	SER
2	B	310	ILE
2	B	318	ASP
2	B	321	VAL
2	B	335	LYS
2	B	336	LEU
2	B	348	VAL
2	B	350	MET
2	B	354	THR
2	B	360	VAL
2	B	375	LEU
2	B	377	THR
2	B	396	ILE
2	B	407	ILE
2	B	408	LYS
2	B	410	LEU
2	B	414	ARG
2	B	420	GLU
2	B	421	THR
2	B	427	LEU
2	B	428	SER
2	B	429	PHE
2	B	432	GLN
2	B	435	VAL
2	B	437	MET
2	B	454	ASP
2	B	463	VAL
2	B	466	GLN
2	B	468	LEU
2	B	473	SER
2	B	477	ARG
2	B	482	GLU
2	B	486	LEU
2	B	487	VAL
2	B	488	SER
2	B	492	GLU
2	B	505	SER
2	B	510	VAL

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Mol	Chain	Res	Type
2	B	514	ARG
2	B	517	TYR
2	B	519	LEU
2	B	524	GLN
2	B	526	LEU
2	B	527	ARG
2	B	531	HIS
2	B	532	THR
2	B	534	MET
2	B	543	ILE
2	B	555	LEU
2	B	560	LEU
2	B	561	TRP
2	B	562	THR
2	B	569	LEU
2	B	571	LEU
2	B	579	LYS
2	B	582	LEU
2	B	586	ILE
2	B	587	ILE
2	B	595	THR
2	B	598	SER
2	B	602	LEU
2	B	611	LEU
2	B	618	ILE
2	B	628	LYS
2	B	630	THR
2	B	636	THR
2	B	637	VAL
2	B	647	THR
2	B	653	SER
2	B	657	THR
2	B	660	TYR
2	B	663	ASN
2	B	672	ASN
2	B	673	LEU
2	B	676	VAL
2	B	684	SER
2	B	691	LEU
2	B	693	LEU
2	B	697	SER
2	B	698	THR

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Mol	Chain	Res	Type
2	B	700	THR
2	B	709	LYS
2	B	722	ARG
2	B	729	VAL
2	B	742	VAL
2	B	750	THR
2	B	752	LEU
2	B	755	SER
2	B	763	SER
2	B	768	SER
2	B	786	VAL
2	B	800	GLU
2	B	808	LEU
2	B	814	LEU
2	B	818	SER
2	B	823	LYS
2	B	839	GLU
2	B	840	GLU
2	B	842	GLU
2	B	844	LYS
2	B	845	GLN
2	B	854	SER
2	B	860	THR
2	B	864	LYS
2	B	866	VAL
2	B	870	VAL
2	B	874	VAL
2	B	886	SER
2	B	889	ARG
2	B	895	THR
2	B	897	LYS
2	B	898	GLU
2	B	902	GLU
2	B	903	CYS
2	B	904	ASN
2	B	907	ASN
2	B	908	ASN
2	B	909	ILE
2	B	914	LEU
2	B	916	THR
2	B	919	ASP
2	B	923	VAL

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Mol	Chain	Res	Type
2	B	927	MET
2	B	929	SER
2	B	932	LEU
2	B	933	LEU
2	B	943	GLU
2	B	947	ARG
2	B	957	VAL
2	B	962	ASP
2	B	987	GLU
2	B	988	GLU
2	B	990	GLN
2	B	995	VAL
2	B	1006	VAL
2	B	1011	SER
2	B	1012	LEU
2	B	1013	VAL
2	B	1050	LEU
2	B	1052	LEU
2	B	1064	SER
2	B	1069	GLU
2	B	1071	SER
2	B	1096	SER
2	B	1100	ILE
2	B	1105	MET
2	B	1106	GLN
2	B	1115	ASP
2	B	1116	ASP
2	B	1122	ARG
2	B	1125	THR
2	B	1131	LYS
2	B	1132	VAL
2	B	1134	GLU
2	B	1137	THR
3	C	49	PHE
3	C	51	THR
3	C	58	THR
3	C	64	MET
3	C	71	THR
3	C	75	ASP
3	C	80	VAL
3	C	84	LEU
3	C	88	MET

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Mol	Chain	Res	Type
3	C	89	MET
3	C	91	LEU
3	C	96	THR
3	C	105	GLN
3	C	109	MET
3	C	115	GLN
3	C	128	VAL
3	C	141	ILE
3	C	145	ARG
3	C	148	GLN
3	C	149	ASP
3	C	154	ILE
3	C	156	LYS
3	C	157	VAL
3	C	162	ARG
3	C	169	GLU
3	C	171	ARG
3	C	172	THR
3	C	177	ILE
3	C	179	GLN
3	C	182	VAL
3	C	189	VAL
3	C	190	LEU
3	C	193	THR
3	C	197	VAL
3	C	204	LYS
3	C	206	GLN
3	C	207	ILE
3	C	210	SER
3	C	221	TYR
3	C	237	LEU
3	C	238	THR
3	C	244	LEU
3	C	246	SER
3	C	255	ASP
3	C	260	GLN
3	C	265	ASP
3	C	272	SER
3	C	273	LEU
3	C	275	SER
3	C	290	ILE
3	C	291	ASP

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Mol	Chain	Res	Type
3	C	293	VAL
3	C	294	LEU
3	C	297	GLN
3	C	298	LEU
3	C	299	LEU
3	C	301	ILE
3	C	310	CYS
3	C	313	ASP
3	C	314	ILE
3	C	319	THR
3	C	320	SER
3	C	325	GLN
3	C	332	THR
3	C	333	THR
3	C	350	VAL
3	C	356	VAL
3	C	358	GLU
3	C	361	THR
3	C	370	LEU
3	C	371	ILE
3	C	373	ARG
3	C	376	THR
3	C	387	THR
3	C	388	VAL
3	C	390	GLN
3	C	393	ILE
3	C	401	LYS
3	C	403	THR
3	C	407	LYS
3	C	419	ARG
3	C	420	SER
3	C	423	LEU
3	C	426	ILE
3	C	439	ILE
3	C	442	LEU
1	A	440	ILE
1	A	447	LYS
1	A	449	LYS
1	A	454	VAL
1	A	455	VAL
1	A	456	LEU
1	A	459	LEU

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Mol	Chain	Res	Type
1	A	482	LEU
1	A	485	LEU
1	A	492	ASP
1	A	500	LEU
1	A	503	ARG
1	A	505	LYS
1	A	510	GLU
1	A	513	LEU
1	A	517	ILE
1	A	535	ILE
1	A	536	VAL
1	A	544	ILE
1	A	549	ASN
1	A	552	LEU
1	A	554	ILE
1	A	557	CYS
1	A	558	ILE
1	A	566	LEU
1	A	567	ILE
1	A	568	CYS
1	A	569	LEU
1	A	570	VAL
1	A	571	ASP
1	A	579	LYS
1	A	580	THR
1	A	585	VAL
1	A	592	ILE
1	A	594	ARG
1	A	600	THR
1	A	602	CYS
1	A	605	THR
1	A	612	MET
1	A	616	THR
1	A	622	LYS
1	A	626	ILE
1	A	629	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	469	GLN
1	X	540	HIS

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Mol	Chain	Res	Type
1	X	555	HIS
2	Y	16	ASN
2	Y	30	ASN
2	Y	36	ASN
2	Y	156	ASN
2	Y	255	GLN
2	Y	267	ASN
2	Y	439	ASN
2	Y	456	GLN
2	Y	462	ASN
2	Y	467	GLN
2	Y	470	GLN
2	Y	536	HIS
2	Y	663	ASN
2	Y	672	ASN
2	Y	796	GLN
2	Y	803	HIS
2	Y	805	HIS
2	Y	810	ASN
2	Y	852	GLN
2	Y	885	ASN
2	Y	950	ASN
2	Y	990	GLN
2	Y	999	HIS
2	Y	1034	ASN
2	Y	1055	GLN
2	Y	1056	ASN
2	Y	1070	HIS
2	Y	1111	ASN
3	Z	86	GLN
3	Z	115	GLN
3	Z	163	GLN
3	Z	179	GLN
3	Z	206	GLN
3	Z	260	GLN
3	Z	335	ASN
3	Z	367	ASN
2	B	16	ASN
2	B	22	HIS
2	B	30	ASN
2	B	36	ASN
2	B	105	HIS

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Mol	Chain	Res	Type
2	B	156	ASN
2	B	255	GLN
2	B	267	ASN
2	B	397	HIS
2	B	439	ASN
2	B	456	GLN
2	B	462	ASN
2	B	467	GLN
2	B	470	GLN
2	B	536	HIS
2	B	663	ASN
2	B	711	HIS
2	B	796	GLN
2	B	803	HIS
2	B	805	HIS
2	B	852	GLN
2	B	859	GLN
2	B	885	ASN
2	B	950	ASN
2	B	999	HIS
2	B	1034	ASN
2	B	1055	GLN
2	B	1056	ASN
2	B	1070	HIS
2	B	1111	ASN
3	C	48	ASN
3	C	86	GLN
3	C	95	GLN
3	C	115	GLN
3	C	127	ASN
3	C	163	GLN
3	C	206	GLN
3	C	260	GLN
3	C	335	ASN
3	C	367	ASN
1	A	611	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	85C	Z	502	-	34,34,34	1.51	3 (8%)	49,49,49	2.34	11 (22%)
5	85C	C	502	-	34,34,34	1.54	3 (8%)	49,49,49	2.32	12 (24%)

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
5	85C	Z	502	-	-	2/13/38/38	0/4/4/4
5	85C	C	502	-	-	1/13/38/38	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502	85C	C5-C8	-5.86	1.39	1.48
5	Z	502	85C	C5-C8	-5.42	1.40	1.48
5	Z	502	85C	C16-N4	-4.24	1.33	1.41
5	C	502	85C	C16-N4	-3.95	1.33	1.41
5	C	502	85C	C8-N1	-3.37	1.32	1.36
5	Z	502	85C	C8-N1	-3.05	1.33	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Z	502	85C	C5-C8-N1	8.19	111.63	106.42
5	C	502	85C	C7-N1-C8	-8.05	109.76	113.15
5	Z	502	85C	C7-N1-C8	-7.25	110.09	113.15
5	C	502	85C	C5-C8-N1	7.09	110.93	106.42
5	C	502	85C	C10-C9-N1	-4.53	109.07	114.03
5	Z	502	85C	C10-C9-N1	-4.45	109.16	114.03
5	C	502	85C	C7-C6-C5	-4.30	107.03	109.73
5	Z	502	85C	C12-N2-C13	-4.29	121.03	126.69
5	C	502	85C	C12-N2-C13	-4.23	121.11	126.69
5	Z	502	85C	C9-C13-N2	3.99	122.06	116.24
5	Z	502	85C	C13-C9-N1	-3.58	107.01	110.32
5	C	502	85C	C9-C13-N2	3.58	121.46	116.24
5	Z	502	85C	C7-C6-C5	-3.50	107.53	109.73
5	Z	502	85C	C16-N4-C15	-3.21	120.07	126.61
5	Z	502	85C	C11-C12-N2	3.19	120.08	116.69
5	C	502	85C	C16-N4-C15	-3.06	120.36	126.61
5	C	502	85C	C13-C9-N1	-2.90	107.64	110.32
5	C	502	85C	O1-C8-C5	-2.85	123.14	128.66
5	C	502	85C	C11-C12-N2	2.77	119.63	116.69
5	Z	502	85C	C2-C14-N3	-2.29	108.25	113.07
5	Z	502	85C	O1-C8-C5	-2.24	124.33	128.66
5	C	502	85C	O1-C8-N1	-2.23	123.57	125.34
5	C	502	85C	C17-C18-C19	-2.15	119.61	122.72

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Z	502	85C	C17-C16-N4-C15
5	Z	502	85C	C21-C16-N4-C15
5	C	502	85C	C21-C16-N4-C15

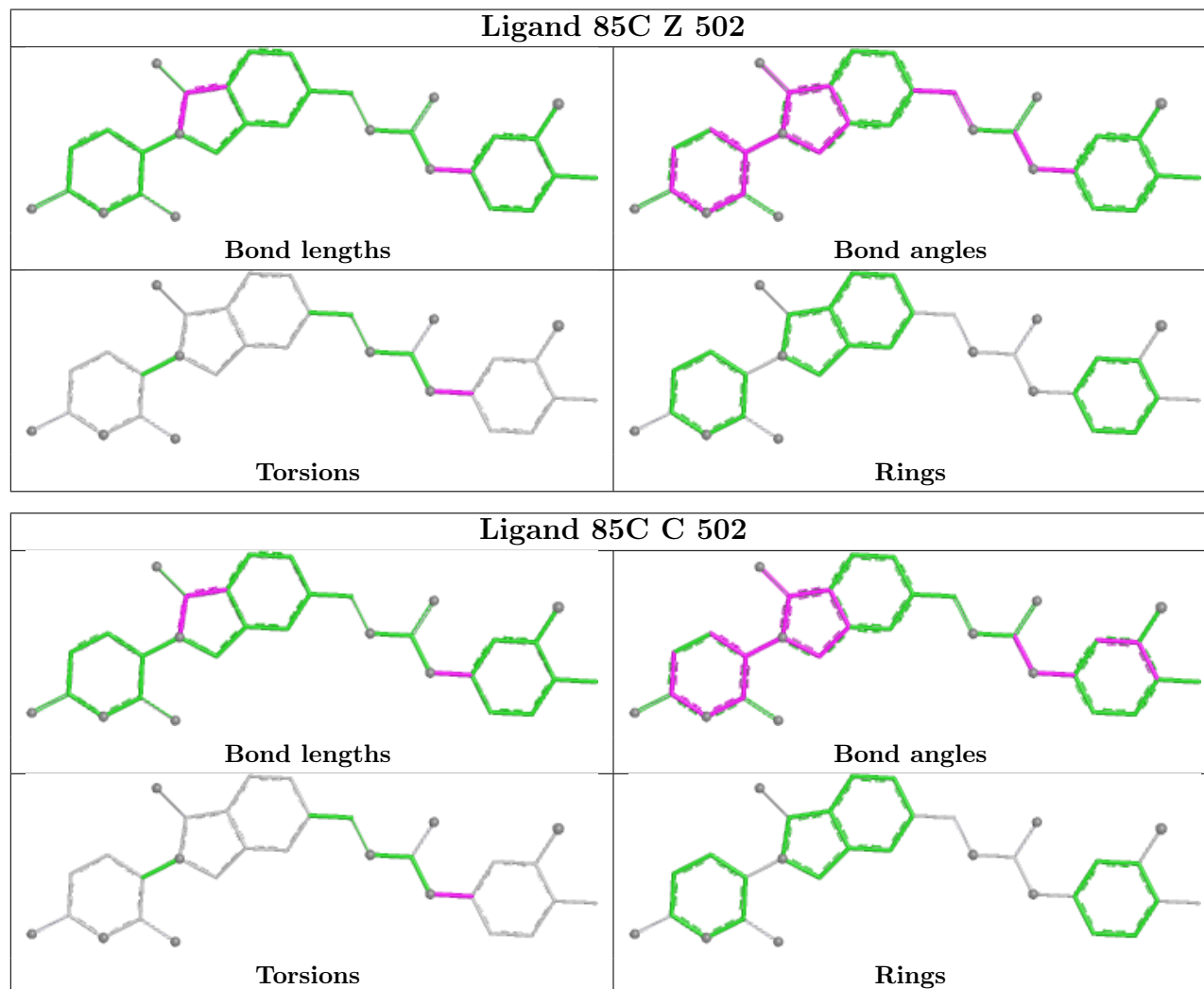
There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Z	502	85C	10	0
5	C	502	85C	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	196/199 (98%)	-0.31	1 (0%) 87 66	56, 112, 160, 183	0
1	X	195/199 (97%)	-0.26	1 (0%) 87 66	66, 109, 160, 185	0
2	B	1075/1140 (94%)	-0.17	10 (0%) 81 56	39, 114, 185, 240	5 (0%)
2	Y	1080/1140 (94%)	-0.21	9 (0%) 82 58	38, 113, 174, 221	5 (0%)
3	C	370/406 (91%)	-0.10	5 (1%) 73 46	62, 111, 165, 225	0
3	Z	380/406 (93%)	-0.10	3 (0%) 82 58	64, 109, 169, 213	0
All	All	3296/3490 (94%)	-0.18	29 (0%) 81 56	38, 112, 174, 240	10 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	475	SER	5.0
2	B	16	ASN	4.8
2	B	276	MET	4.3
2	B	260	CYS	4.2
3	C	318	CYS	4.2
1	X	627	GLY	3.9
2	Y	276	MET	3.4
3	C	442	LEU	3.3
2	Y	16	ASN	3.2
2	Y	744	ASP	2.9
2	Y	224	GLU	2.7
2	Y	1023	PRO	2.6
2	B	863	GLU	2.6
2	Y	260	CYS	2.5
3	C	296	ILE	2.4
1	A	439	PRO	2.4
2	B	343	GLN	2.4
2	B	501	ALA	2.2
2	Y	372	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	Y	475	SER	2.2
3	Z	318	CYS	2.2
2	Y	279	ARG	2.2
2	B	744	ASP	2.2
3	C	155	VAL	2.1
3	C	309	ARG	2.1
2	B	1103	PRO	2.1
2	B	179	CYS	2.1
3	Z	155	VAL	2.0
3	Z	432	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

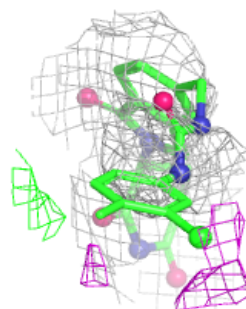
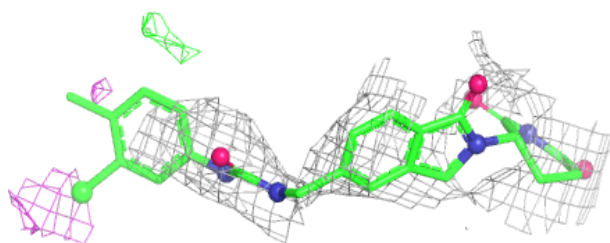
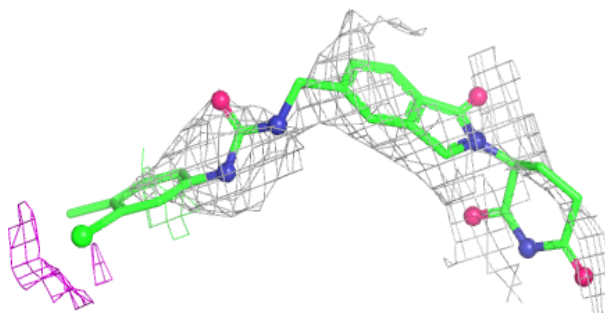
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	85C	Z	502	31/31	0.95	0.12	70,95,210,235	0
5	85C	C	502	31/31	0.96	0.10	61,90,177,227	0
4	ZN	C	501	1/1	0.97	0.07	187,187,187,187	0
4	ZN	Z	501	1/1	0.98	0.07	191,191,191,191	0

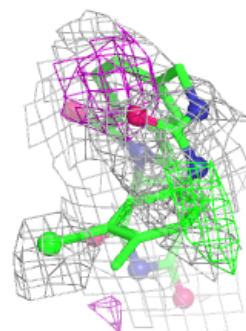
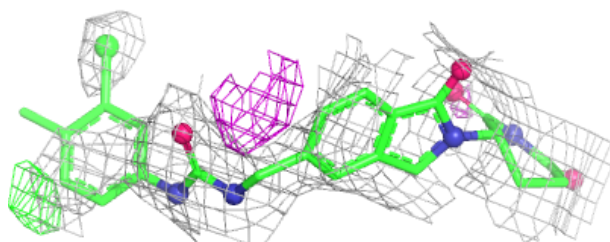
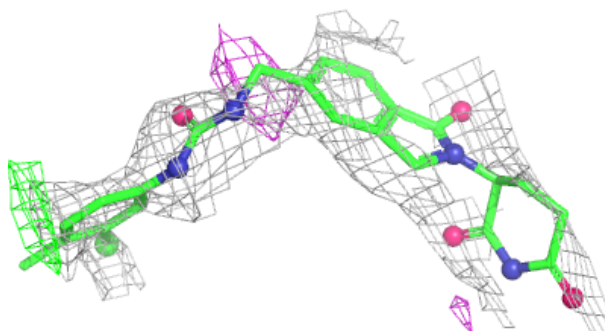
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 85C Z 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 85C C 502:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.