



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:26 PM UTC

PDB ID : 3FFZ / pdb_00003ffz
Title : Domain organization in Clostridium butulinum neurotoxin type E is unique:
Its implication in faster translocation
Authors : Kumaran, D.; Eswaramoorthy, S.; Swaminathan, S.
Deposited on : 2008-12-04
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

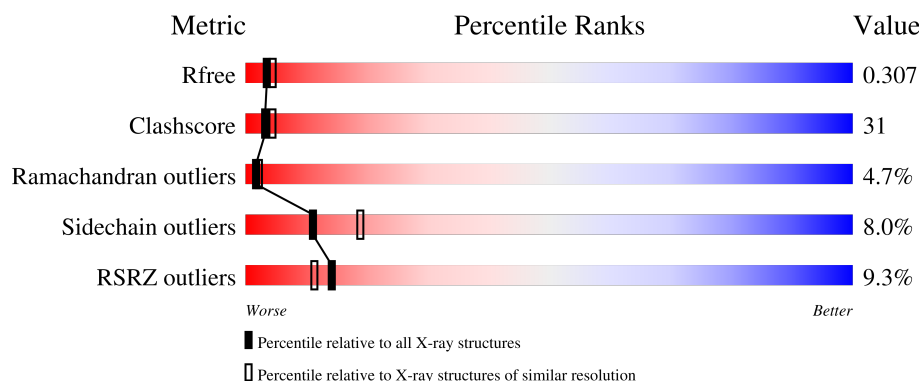
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

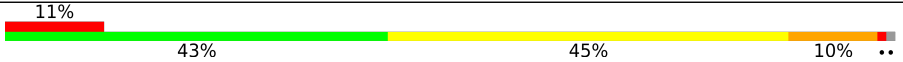
The reported resolution of this entry is 2.65 Å.

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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	1252	
1	B	1252	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	A	1301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20217 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 Botulinum neurotoxin type E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1246	Total	C	N	O	S	0	0	0
			10085	6414	1686	1961	24			
1	B	1238	Total	C	N	O	S	0	0	0
			10025	6375	1674	1952	24			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	177	GLY	ARG	SEE REMARK 999	UNP Q00496
A	340	ALA	ARG	SEE REMARK 999	UNP Q00496
A	963	LEU	PHE	SEE REMARK 999	UNP Q00496
A	964	GLN	GLU	SEE REMARK 999	UNP Q00496
A	967	ALA	ARG	SEE REMARK 999	UNP Q00496
A	1195	ASN	-	insertion	UNP Q00496
B	177	GLY	ARG	SEE REMARK 999	UNP Q00496
B	340	ALA	ARG	SEE REMARK 999	UNP Q00496
B	963	LEU	PHE	SEE REMARK 999	UNP Q00496
B	964	GLN	GLU	SEE REMARK 999	UNP Q00496
B	967	ALA	ARG	SEE REMARK 999	UNP Q00496
B	1195	ASN	-	insertion	UNP Q00496

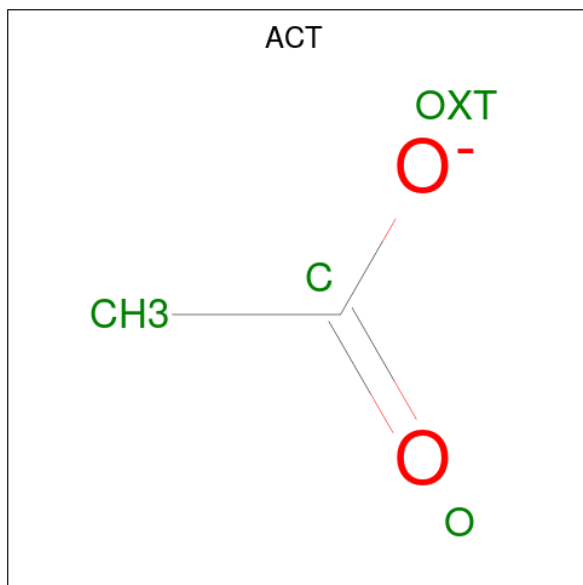
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

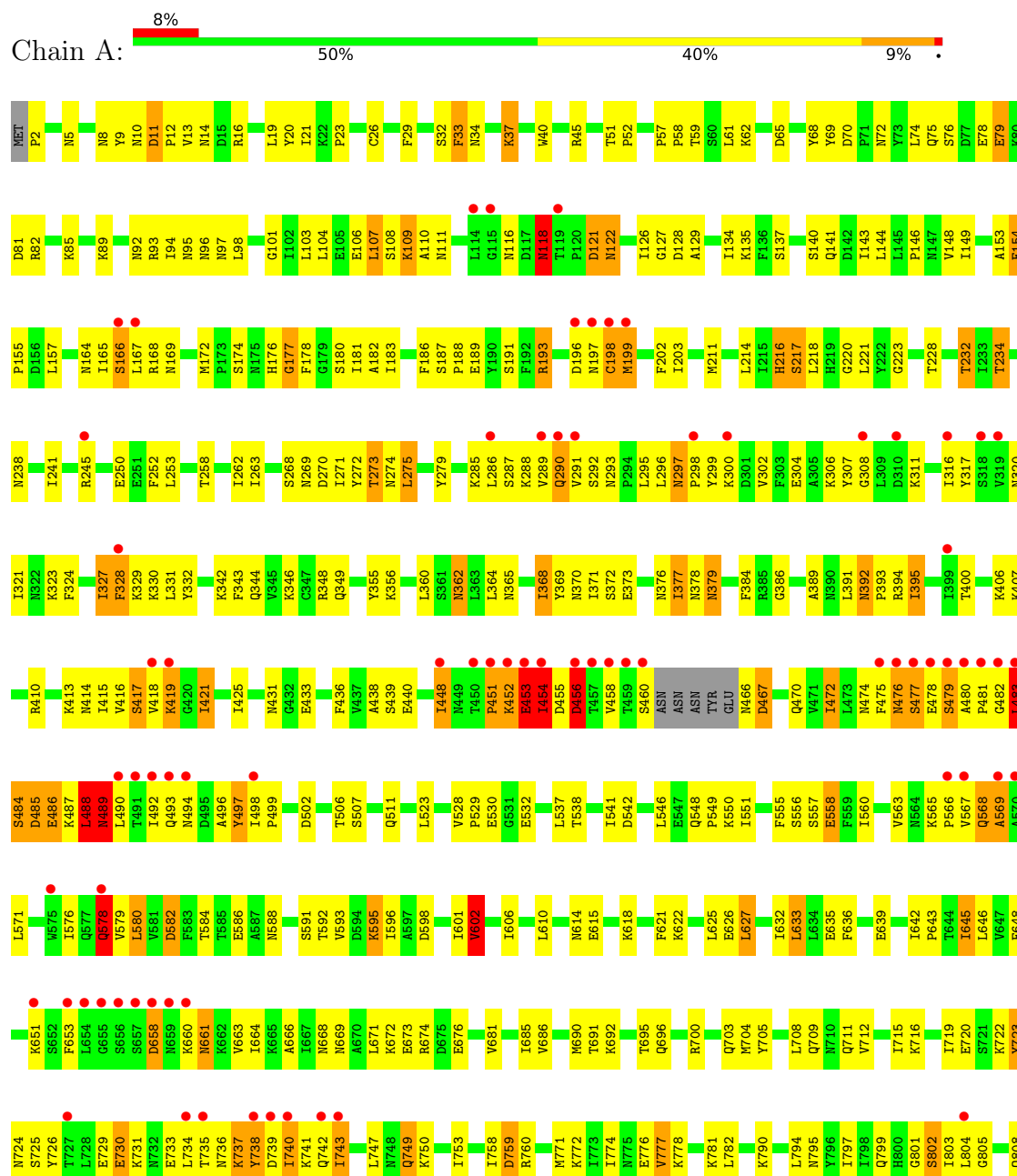
- Molecule 5 is water.

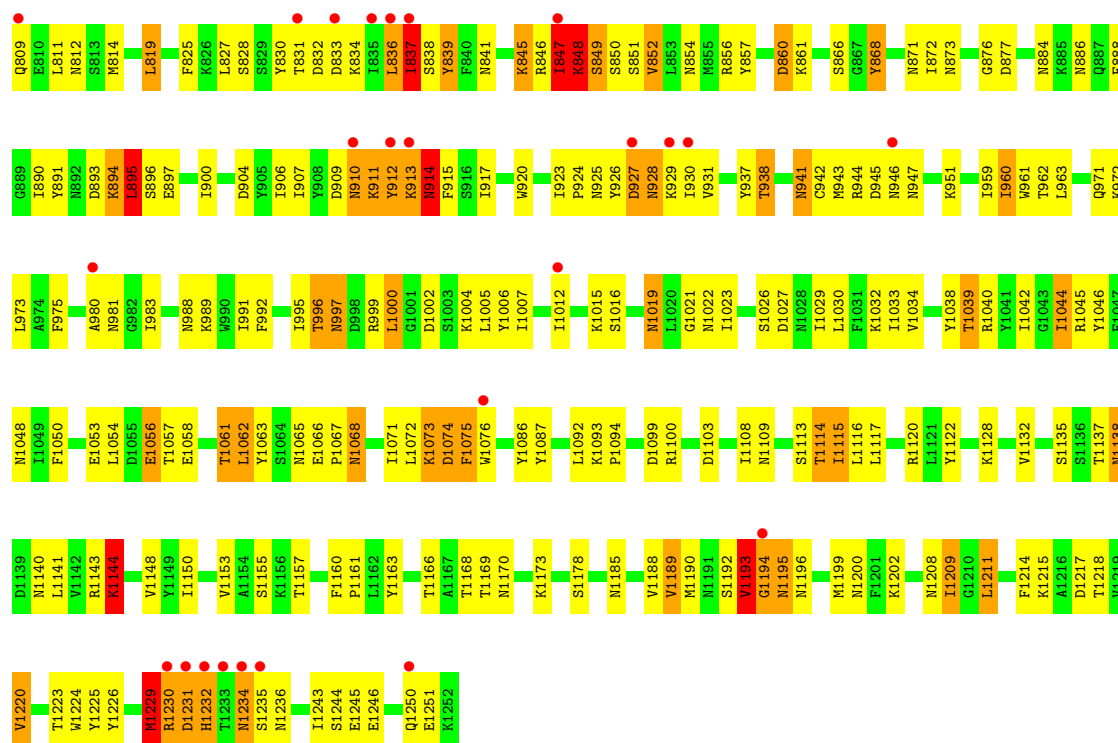
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	62	Total	O	0	0
			62	62		
5	B	32	Total	O	0	0
			32	32		

3 Residue-property plots

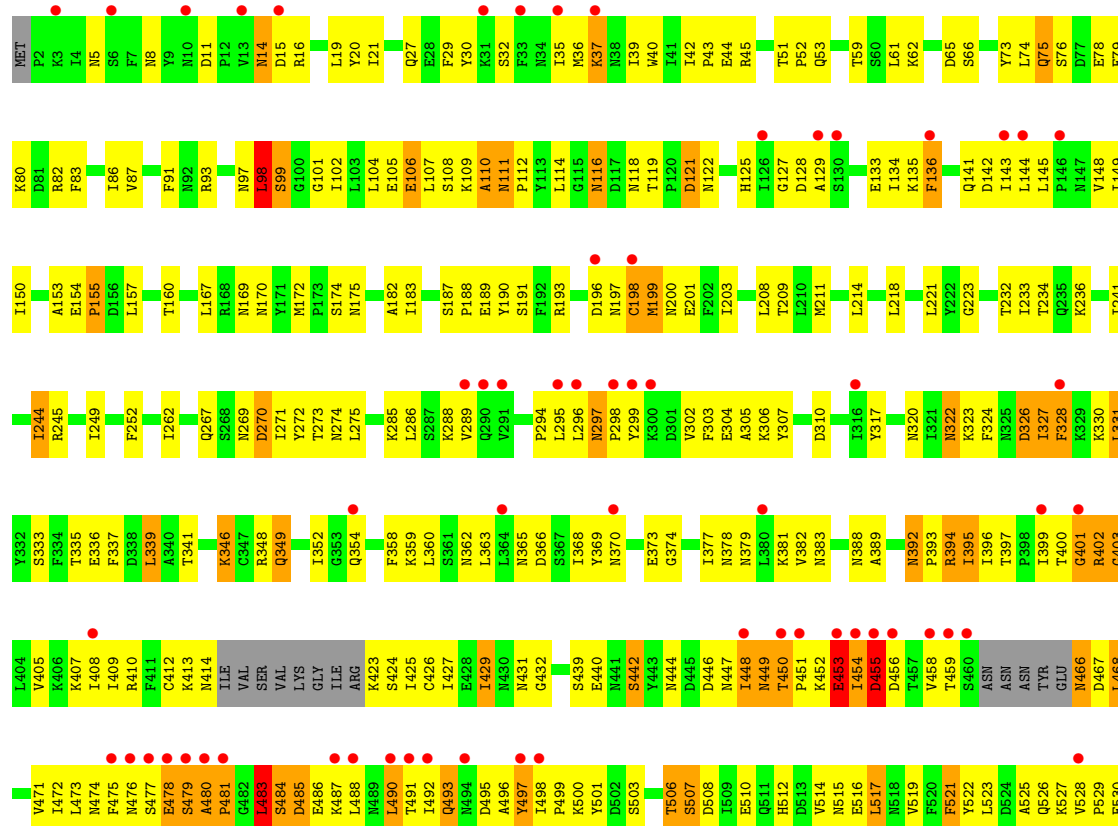
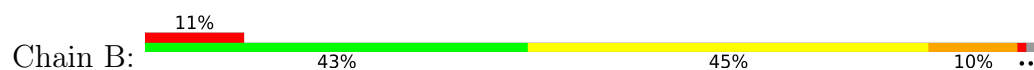
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

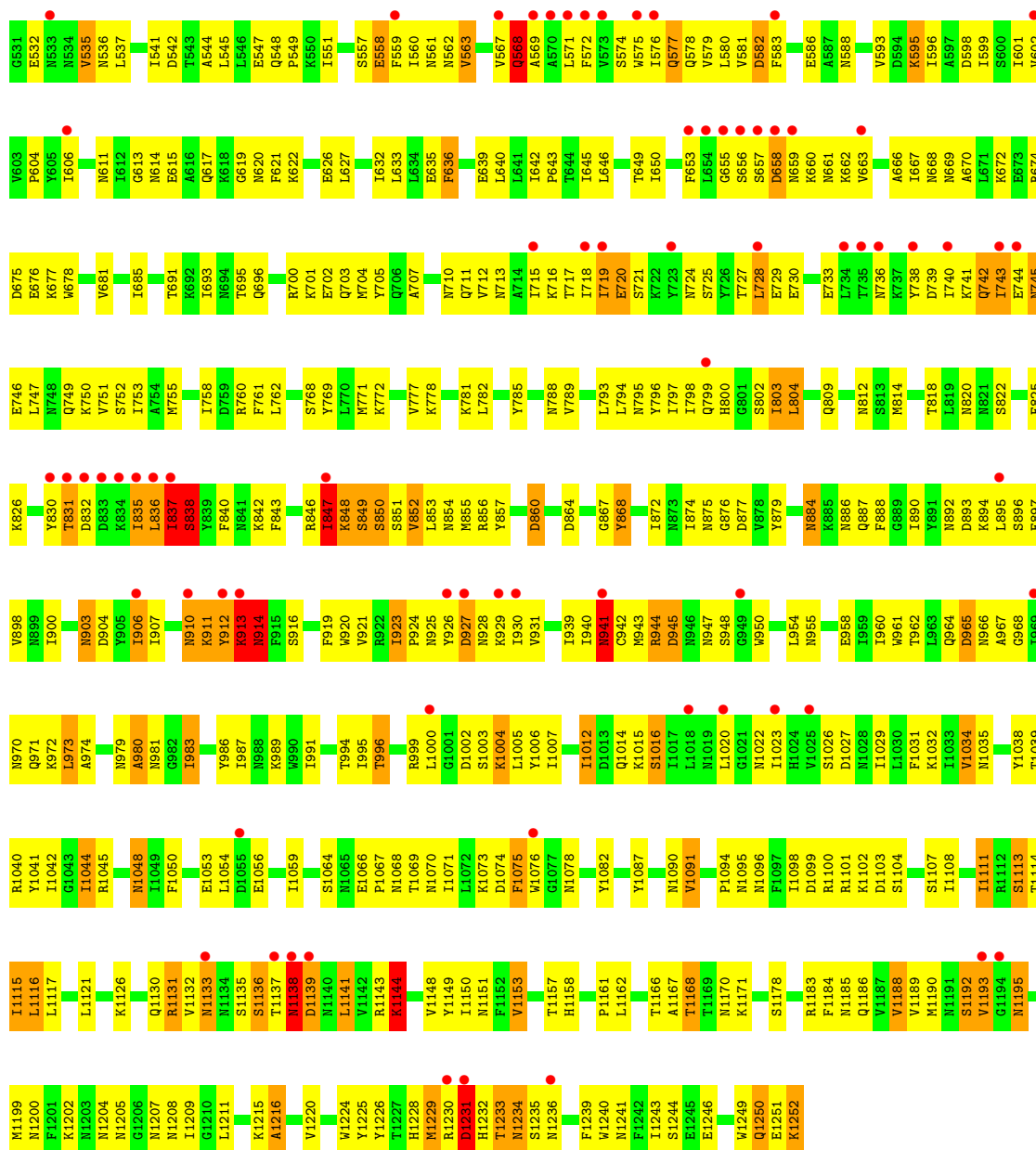
• Molecule 1: Botulinum neurotoxin type E





• Molecule 1: Botulinum neurotoxin type E





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.43Å 172.57Å 137.26Å 90.00° 99.84° 90.00°	Depositor
Resolution (Å)	29.49 – 2.65 29.49 – 2.65	Depositor EDS
% Data completeness (in resolution range)	86.5 (29.49-2.65) 86.5 (29.49-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.48Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.253 , 0.309 0.252 , 0.307	Depositor DCC
R_{free} test set	4751 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20217	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.24% 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: ACT, ZN, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.56	0/10285	1.11	80/13934 (0.6%)
1	B	0.51	4/10224 (0.0%)	1.07	70/13851 (0.5%)
All	All	0.54	4/20509 (0.0%)	1.09	150/27785 (0.5%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1136	SER	C-N	-7.99	1.22	1.33
1	B	1138	ASN	C-N	-6.81	1.24	1.33
1	B	1139	ASP	C-N	-6.79	1.22	1.33
1	B	449	ASN	C-N	5.12	1.49	1.33

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1138	ASN	CA-C-N	12.89	139.17	120.87
1	B	1138	ASN	C-N-CA	12.89	139.17	120.87
1	B	655	GLY	N-CA-C	-11.05	97.89	116.01
1	A	1229	MET	N-CA-C	-10.28	99.90	111.82
1	B	1232	HIS	N-CA-C	10.22	128.25	113.02
1	A	455	ASP	N-CA-C	-10.05	99.28	114.16
1	A	484	SER	N-CA-C	9.76	122.86	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1075	PHE	N-CA-C	-9.69	100.02	112.23
1	B	836	LEU	N-CA-C	-9.03	97.29	111.02
1	A	285	LYS	N-CA-C	-8.93	104.44	114.62
1	B	450	THR	C-N-CD	-8.92	88.41	125.00
1	B	187	SER	CA-C-N	8.65	128.80	119.28
1	B	187	SER	C-N-CA	8.65	128.80	119.28
1	A	868	TYR	N-CA-C	-8.56	97.85	110.52
1	A	860	ASP	N-CA-C	8.54	123.06	112.47
1	B	868	TYR	N-CA-C	-8.52	99.04	110.55
1	A	392	ASN	CA-C-N	8.46	128.59	119.28
1	A	392	ASN	C-N-CA	8.46	128.59	119.28
1	B	401	GLY	N-CA-C	8.46	123.84	111.24
1	A	1075	PHE	N-CA-C	-8.33	102.38	112.54
1	B	400	THR	N-CA-C	-8.28	102.21	111.07
1	A	477	SER	N-CA-C	-8.17	101.79	112.41
1	A	1236	ASN	N-CA-C	-8.17	101.48	112.26
1	B	1138	ASN	CA-C-O	-8.05	111.24	120.58
1	A	914	ASN	N-CA-C	7.90	127.63	110.80
1	A	1140	ASN	N-CA-C	-7.89	101.85	112.26
1	A	483	LEU	N-CA-C	7.87	127.56	110.80
1	B	1193	VAL	N-CA-C	-7.79	105.57	112.12
1	B	535	VAL	N-CA-C	7.77	119.15	108.89
1	A	395	ILE	N-CA-C	7.77	120.76	111.05
1	B	121	ASP	N-CA-C	7.75	121.84	112.38
1	B	1195	ASN	N-CA-C	-7.45	94.93	110.80
1	B	1091	VAL	N-CA-C	7.35	117.44	110.53
1	A	400	THR	N-CA-C	7.33	121.14	111.75
1	A	1138	ASN	N-CA-C	7.32	119.27	110.19
1	B	929	LYS	N-CA-C	-7.28	103.30	113.20
1	A	725	SER	N-CA-C	-7.22	104.03	112.92
1	B	742	GLN	N-CA-C	7.22	118.13	108.38
1	A	488	LEU	N-CA-C	7.14	126.02	110.80
1	A	232	THR	N-CA-C	7.11	120.92	108.75
1	A	187	SER	CA-C-N	7.09	127.69	119.47
1	A	187	SER	C-N-CA	7.09	127.69	119.47
1	B	720	GLU	N-CA-C	-7.01	103.72	112.90
1	B	1113	SER	N-CA-C	-7.00	101.30	110.33
1	A	121	ASP	N-CA-C	6.91	119.45	111.02
1	B	1250	GLN	N-CA-C	6.90	119.39	111.11
1	A	740	ILE	N-CA-C	6.87	123.63	109.34
1	B	645	ILE	N-CA-C	6.86	117.94	108.89
1	A	1073	LYS	N-CA-C	6.84	120.12	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	LYS	N-CA-C	-6.83	104.82	113.01
1	A	332	TYR	N-CA-C	6.82	121.68	112.88
1	B	1229	MET	N-CA-C	-6.80	104.60	113.17
1	A	929	LYS	N-CA-C	-6.74	105.46	113.21
1	B	583	PHE	N-CA-C	-6.72	103.57	111.03
1	B	577	GLN	N-CA-C	-6.68	105.42	113.97
1	A	551	ILE	N-CA-C	6.68	117.50	107.75
1	A	476	ASN	N-CA-C	6.60	120.64	112.59
1	B	468	LEU	N-CA-C	-6.56	104.21	111.36
1	B	1144	LYS	N-CA-C	6.53	124.72	110.80
1	B	1192	SER	CA-C-N	-6.53	115.91	122.77
1	B	1192	SER	C-N-CA	-6.53	115.91	122.77
1	B	477	SER	N-CA-C	-6.52	103.83	113.61
1	B	521	PHE	N-CA-C	-6.50	103.82	111.03
1	B	337	PHE	N-CA-C	6.49	118.15	111.14
1	B	450	THR	CA-C-N	6.46	127.92	119.84
1	B	450	THR	C-N-CA	6.46	127.92	119.84
1	A	327	ILE	N-CA-C	-6.45	104.04	110.62
1	B	272	TYR	N-CA-C	6.45	118.00	110.97
1	A	578	GLN	N-CA-C	-6.41	105.42	113.18
1	A	848	LYS	N-CA-C	-6.41	97.16	110.80
1	A	1195	ASN	N-CA-C	6.40	124.44	110.80
1	B	719	ILE	N-CA-C	-6.40	105.34	113.22
1	A	1220	VAL	N-CA-C	6.39	116.61	108.82
1	A	837	ILE	N-CA-C	6.35	122.54	109.34
1	B	501	TYR	N-CA-C	-6.18	102.21	110.24
1	A	467	ASP	N-CA-C	6.14	118.09	110.91
1	B	87	VAL	N-CA-C	-6.13	105.08	111.58
1	B	455	ASP	N-CA-C	-6.11	97.78	110.80
1	A	645	ILE	N-CA-C	6.10	117.57	108.54
1	B	1231	ASP	N-CA-C	6.09	123.78	110.80
1	B	188	PRO	N-CA-C	6.09	121.87	113.65
1	A	720	GLU	N-CA-C	-6.08	106.47	114.31
1	B	1220	VAL	N-CA-C	6.07	115.93	108.53
1	A	960	ILE	N-CA-C	6.05	116.83	108.12
1	B	960	ILE	N-CA-C	6.05	117.01	108.17
1	A	582	ASP	N-CA-C	-6.04	104.62	112.23
1	B	403	GLY	N-CA-C	-6.02	105.33	115.80
1	B	847	ILE	N-CA-C	6.01	121.84	109.34
1	A	621	PHE	N-CA-C	5.97	117.45	111.07
1	A	1160	PHE	CA-C-N	-5.97	114.48	120.21
1	A	1160	PHE	C-N-CA	-5.97	114.48	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	392	ASN	CA-C-N	5.96	127.28	119.84
1	B	392	ASN	C-N-CA	5.96	127.28	119.84
1	B	835	ILE	N-CA-C	-5.91	99.90	108.89
1	A	997	ASN	N-CA-C	5.91	118.84	107.44
1	A	453	GLU	CA-C-O	5.89	128.69	121.56
1	B	218	LEU	N-CA-C	-5.88	104.50	111.03
1	B	578	GLN	N-CA-C	-5.87	106.07	113.18
1	A	11	ASP	CA-C-N	5.86	126.16	119.83
1	A	11	ASP	C-N-CA	5.86	126.16	119.83
1	A	377	ILE	N-CA-C	5.84	116.27	107.80
1	A	421	ILE	N-CA-C	5.84	116.21	107.51
1	A	268	SER	N-CA-C	-5.83	104.83	111.07
1	A	1093	LYS	CA-C-N	5.81	126.21	119.47
1	A	1093	LYS	C-N-CA	5.81	126.21	119.47
1	B	75	GLN	N-CA-C	-5.79	106.38	113.50
1	B	1048	ASN	N-CA-C	5.73	117.81	108.76
1	B	333	SER	N-CA-C	-5.62	105.53	112.90
1	B	1004	LYS	N-CA-C	5.58	117.28	110.41
1	B	1236	ASN	N-CA-C	-5.58	105.13	112.72
1	B	1034	VAL	N-CA-C	5.57	115.91	108.11
1	A	598	ASP	N-CA-C	5.55	119.75	113.15
1	A	79	GLU	N-CA-C	-5.54	104.88	111.69
1	A	777	VAL	N-CA-C	5.49	117.95	111.09
1	A	781	LYS	N-CA-C	5.46	117.94	111.33
1	A	1223	THR	N-CA-C	-5.45	106.58	113.18
1	B	395	ILE	N-CA-C	5.45	117.86	111.05
1	A	216	HIS	N-CA-C	-5.44	104.75	111.33
1	A	904	ASP	N-CA-C	5.43	117.20	111.28
1	A	176	HIS	N-CA-C	5.41	116.17	108.54
1	B	507	SER	N-CA-C	-5.39	107.95	114.75
1	A	372	SER	N-CA-C	5.39	119.57	112.89
1	B	484	SER	N-CA-C	5.37	115.48	108.07
1	B	327	ILE	N-CA-C	-5.30	105.33	110.42
1	A	941	ASN	N-CA-C	5.30	117.60	109.07
1	B	974	ALA	N-CA-C	5.29	116.85	108.96
1	A	895	LEU	N-CA-C	-5.29	98.22	107.20
1	A	749	GLN	N-CA-C	-5.28	105.44	111.14
1	A	1074	ASP	N-CA-C	-5.28	103.92	110.41
1	A	5	ASN	N-CA-C	5.27	116.90	108.41
1	B	449	ASN	N-CA-C	-5.25	100.69	109.24
1	A	489	ASN	N-CA-C	5.23	121.94	110.80
1	A	1132	VAL	N-CA-C	-5.22	105.62	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	802	SER	N-CA-C	-5.21	106.44	114.16
1	A	1234	ASN	N-CA-C	5.20	121.87	110.80
1	B	636	PHE	N-CA-C	5.18	121.83	110.80
1	A	602	VAL	CB-CA-C	-5.17	102.43	110.69
1	B	568	GLN	CB-CA-C	-5.16	109.64	117.07
1	A	1209	ILE	N-CA-C	-5.12	105.71	110.53
1	A	913	LYS	CA-C-N	5.12	131.32	121.54
1	A	913	LYS	C-N-CA	5.12	131.32	121.54
1	A	913	LYS	N-CA-C	5.10	121.66	110.80
1	B	913	LYS	N-CA-C	5.09	121.63	110.80
1	B	721	SER	N-CA-C	-5.05	106.89	113.16
1	A	1144	LYS	N-CA-C	5.05	121.56	110.80
1	B	822	SER	N-CA-C	5.05	116.86	109.24
1	A	911	LYS	N-CA-C	-5.04	106.38	112.88
1	A	172	MET	CA-C-N	5.03	126.13	119.84
1	A	172	MET	C-N-CA	5.03	126.13	119.84
1	B	45	ARG	N-CA-C	-5.00	102.36	110.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1138	ASN	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10085	0	9924	567	0
1	B	10025	0	9851	665	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	2	0
3	B	1	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	62	0	0	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	32	0	0	1	0
All	All	20217	0	19781	1233	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

All (1233) 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:B:448:ILE:CG1	1:B:646:LEU:HG	1.80	1.10
1:B:1190:MET:HE1	1:B:1199:MET:HG2	1.22	1.10
1:A:914:ASN:H	1:A:914:ASN:ND2	1.42	1.09
1:A:852:VAL:HG13	1:A:906:ILE:HD12	1.35	1.08
1:A:568:GLN:HG3	1:A:571:LEU:HD22	1.36	1.06
1:B:448:ILE:HG13	1:B:646:LEU:HG	1.34	1.05
1:B:109:LYS:HE3	1:B:479:SER:HB2	1.39	1.03
1:B:606:ILE:HG12	1:B:704:MET:HE3	1.38	1.02
1:B:660:LYS:HG2	1:B:804:LEU:HB3	1.42	1.00
1:A:568:GLN:HB2	1:A:571:LEU:HD13	1.42	0.98
1:A:448:ILE:CG2	1:A:646:LEU:HG	1.93	0.98
1:A:297:ASN:H	1:A:298:PRO:HD2	1.27	0.97
3:A:1301:NA:NA	5:A:1317:HOH:O	1.34	0.97
1:B:448:ILE:HG12	1:B:646:LEU:CD1	1.96	0.95
1:A:448:ILE:HG23	1:A:646:LEU:H	1.32	0.94
1:A:238:ASN:HB3	1:A:241:ILE:HG12	1.50	0.93
1:A:1190:MET:HE1	1:A:1199:MET:HG2	1.50	0.93
1:A:856:ARG:HH21	1:A:1048:ASN:HD21	1.16	0.92
1:B:1190:MET:CE	1:B:1199:MET:HG2	2.00	0.92
1:A:944:ARG:HG2	1:A:1026:SER:HB2	1.51	0.92
1:B:996:THR:HG23	1:B:1053:GLU:HG2	1.52	0.91
1:B:1130:GLN:NE2	1:B:1151:ASN:HD21	1.69	0.91
1:A:914:ASN:HD22	1:A:914:ASN:N	1.59	0.90
1:A:1057:THR:O	1:A:1061:THR:HG22	1.71	0.90
1:A:836:LEU:HD12	1:A:837:ILE:H	1.37	0.90
1:B:197:ASN:HD21	1:B:346:LYS:HD3	1.34	0.89
1:B:884:ASN:HD21	1:B:886:ASN:HB2	1.37	0.89
1:A:417:SER:OG	1:A:421:ILE:HB	1.73	0.89
1:A:857:TYR:H	1:A:886:ASN:HD21	1.17	0.88
1:B:498:ILE:HG13	1:B:498:ILE:O	1.73	0.88
1:B:297:ASN:H	1:B:298:PRO:HD2	1.37	0.88
1:A:448:ILE:HD11	1:A:643:PRO:HG2	1.56	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:MET:HE1	1:B:898:VAL:HG11	1.57	0.86
1:B:742:GLN:HB3	1:B:743:ILE:HD12	1.57	0.86
1:A:635:GLU:H	1:A:696:GLN:NE2	1.74	0.85
1:B:295:LEU:HD23	1:B:488:LEU:HD13	1.58	0.85
1:B:295:LEU:H	1:B:295:LEU:HD12	1.40	0.85
1:B:981:ASN:HB3	1:B:1117:LEU:HB3	1.57	0.84
1:B:771:MET:HE1	1:B:825:PHE:HE2	1.40	0.84
1:A:615:GLU:CD	1:A:615:GLU:H	1.84	0.83
1:B:172:MET:HE3	1:B:175:ASN:HD21	1.43	0.83
1:B:448:ILE:CG1	1:B:646:LEU:CG	2.55	0.83
1:A:302:VAL:HG23	1:A:483:LEU:HD22	1.60	0.83
1:B:983:ILE:HD12	1:B:983:ILE:H	1.43	0.82
1:A:448:ILE:HD12	1:A:645:ILE:HA	1.61	0.82
1:A:857:TYR:H	1:A:886:ASN:ND2	1.76	0.82
1:B:1137:THR:HG22	1:B:1137:THR:O	1.77	0.82
1:A:197:ASN:O	1:A:198:CYS:HB2	1.79	0.82
1:B:448:ILE:HG12	1:B:646:LEU:HD12	1.62	0.82
1:A:925:ASN:C	1:A:927:ASP:H	1.82	0.82
1:A:660:LYS:HB2	1:A:803:ILE:HG22	1.59	0.81
1:A:1019:ASN:HD22	1:A:1019:ASN:N	1.76	0.81
1:A:297:ASN:H	1:A:298:PRO:CD	1.93	0.81
1:A:996:THR:HG22	1:A:1004:LYS:HB2	1.62	0.81
1:B:1130:GLN:HE21	1:B:1151:ASN:HD21	1.22	0.81
1:A:475:PHE:HB2	1:A:1143:ARG:HD3	1.61	0.81
1:B:536:ASN:C	1:B:537:LEU:HD12	2.07	0.80
1:A:292:SER:HB2	1:A:296:LEU:HD11	1.62	0.80
1:A:833:ASP:CB	1:A:836:LEU:HD23	2.10	0.80
1:A:636:PHE:H	1:A:696:GLN:HE22	1.30	0.80
1:A:914:ASN:H	1:A:914:ASN:HD22	0.80	0.80
1:B:642:ILE:HD11	1:B:685:ILE:HD11	1.63	0.80
1:B:275:LEU:HD23	1:B:328:PHE:CE1	2.16	0.79
1:B:448:ILE:CD1	1:B:646:LEU:HG	2.11	0.79
1:A:180:SER:O	1:A:221:LEU:HD23	1.82	0.79
1:A:454:ILE:HG13	1:A:666:ALA:HB1	1.62	0.79
1:B:453:GLU:HA	1:B:453:GLU:OE1	1.82	0.79
1:B:632:ILE:HG23	1:B:633:LEU:HD22	1.63	0.79
1:A:847:ILE:HD12	1:A:847:ILE:H	1.46	0.78
1:A:448:ILE:HG21	1:A:646:LEU:HG	1.65	0.78
1:B:294:PRO:HG2	1:B:295:LEU:HD12	1.65	0.78
1:B:410:ARG:HD2	1:B:426:CYS:SG	2.23	0.78
1:B:771:MET:HE1	1:B:825:PHE:CE2	2.19	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:LEU:C	1:A:393:PRO:HD3	2.09	0.78
1:A:1019:ASN:HD22	1:A:1019:ASN:H	1.27	0.78
1:B:579:VAL:HG23	1:B:580:LEU:HD23	1.64	0.78
1:A:451:PRO:HG2	1:A:648:PHE:HB3	1.65	0.77
1:B:999:ARG:HH11	1:B:999:ARG:HA	1.48	0.77
1:B:925:ASN:C	1:B:927:ASP:H	1.91	0.77
1:B:487:LYS:HD2	1:B:487:LYS:O	1.85	0.77
1:A:203:ILE:HD11	1:A:389:ALA:HB2	1.67	0.77
1:A:914:ASN:ND2	1:A:914:ASN:N	2.21	0.77
1:B:109:LYS:HA	1:B:483:LEU:HG	1.65	0.76
1:B:814:MET:O	1:B:818:THR:HG23	1.83	0.76
1:A:593:VAL:HG23	1:A:602:VAL:HG22	1.68	0.76
1:A:893:ASP:HB3	1:A:1039:THR:HG22	1.67	0.76
1:A:1211:LEU:HD13	1:A:1226:TYR:HE2	1.50	0.76
1:B:354:GLN:HG2	1:B:432:GLY:HA2	1.68	0.76
1:B:837:ILE:O	1:B:838:SER:HB3	1.86	0.76
1:A:961:TRP:CE3	1:A:995:ILE:HD13	2.20	0.76
1:B:116:ASN:HD22	1:B:118:ASN:H	1.34	0.75
1:A:981:ASN:HB3	1:A:1117:LEU:HD23	1.69	0.75
1:A:1190:MET:CE	1:A:1199:MET:HG2	2.16	0.75
1:B:148:VAL:HG22	1:B:182:ALA:HB3	1.69	0.75
1:B:875:ASN:HB2	1:B:897:GLU:HB2	1.69	0.75
1:A:836:LEU:CD1	1:A:837:ILE:H	1.98	0.75
1:A:972:LYS:O	1:A:1015:LYS:HE2	1.86	0.74
1:A:410:ARG:HB3	1:A:511:GLN:HG3	1.67	0.74
1:B:738:TYR:HA	1:B:743:ILE:HD13	1.69	0.74
1:A:109:LYS:HA	1:A:483:LEU:HD11	1.69	0.74
1:A:356:LYS:HD3	5:A:1283:HOH:O	1.87	0.74
1:A:910:ASN:CG	1:A:912:TYR:HB3	2.11	0.74
1:B:1251:GLU:HG2	1:B:1252:LYS:H	1.53	0.74
1:B:111:ASN:HD22	1:B:483:LEU:HD12	1.52	0.74
1:B:944:ARG:HD3	1:B:945:ASP:N	2.02	0.74
1:B:856:ARG:HH21	1:B:1048:ASN:HD22	1.35	0.74
1:A:484:SER:O	1:A:485:ASP:HB2	1.88	0.73
1:B:76:SER:HB3	1:B:79:GLU:HB2	1.70	0.73
1:A:1006:TYR:HE2	1:A:1056:GLU:HG2	1.54	0.73
1:B:448:ILE:HG13	1:B:646:LEU:CG	2.15	0.73
1:A:448:ILE:HG22	1:A:646:LEU:CG	2.18	0.73
1:B:857:TYR:CZ	1:B:860:ASP:HA	2.24	0.73
1:A:373:GLU:HB2	1:A:377:ILE:HG22	1.68	0.73
1:A:379:ASN:N	1:A:379:ASN:HD22	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ASN:OD1	1:A:912:TYR:HB3	1.88	0.73
1:B:93:ARG:HG3	1:B:93:ARG:HH11	1.51	0.73
1:A:379:ASN:HD22	1:A:379:ASN:H	1.35	0.73
1:B:1135:SER:O	1:B:1138:ASN:HB2	1.89	0.73
1:A:29:PHE:CE1	1:A:135:LYS:HG3	2.24	0.72
1:B:1116:LEU:HD12	5:B:1255:HOH:O	1.88	0.72
1:A:480:ALA:HB3	1:A:481:PRO:HD3	1.71	0.72
1:B:466:ASN:N	1:B:466:ASN:HD22	1.87	0.72
1:A:165:ILE:CD1	1:A:181:ILE:HB	2.20	0.72
1:A:851:SER:HB3	1:A:854:ASN:HD21	1.54	0.72
1:B:1188:VAL:HG21	1:B:1199:MET:HB3	1.71	0.72
1:B:715:ILE:O	1:B:718:ILE:HG22	1.89	0.72
1:A:203:ILE:CD1	1:A:389:ALA:HB2	2.20	0.72
1:A:856:ARG:NH2	1:A:1048:ASN:HD21	1.85	0.72
1:B:297:ASN:H	1:B:298:PRO:CD	2.02	0.72
1:B:529:PRO:HG3	1:B:548:GLN:O	1.89	0.72
1:A:448:ILE:HG22	1:A:646:LEU:HG	1.71	0.72
1:A:550:LYS:O	3:A:1301:NA:NA	1.61	0.72
1:A:537:LEU:HD22	1:A:563:VAL:HG11	1.71	0.72
1:A:467:ASP:HB3	1:A:470:GLN:HB3	1.73	0.71
1:B:208:LEU:HA	1:B:211:MET:HE3	1.71	0.71
1:B:448:ILE:CG1	1:B:646:LEU:CD1	2.68	0.71
1:B:1161:PRO:HG2	1:B:1178:SER:HB3	1.71	0.71
1:A:269:ASN:O	1:A:273:THR:HG22	1.90	0.71
1:A:1092:LEU:O	1:A:1094:PRO:HD3	1.90	0.71
1:B:98:LEU:HD12	1:B:472:ILE:HG23	1.73	0.71
1:B:1002:ASP:HA	1:B:1016:SER:HA	1.73	0.71
1:A:913:LYS:HB3	1:A:914:ASN:ND2	2.06	0.71
1:B:1190:MET:HE1	1:B:1199:MET:CG	2.12	0.70
1:A:1076:TRP:HZ3	1:A:1244:SER:O	1.73	0.70
1:B:962:THR:HG22	1:B:972:LYS:HG2	1.72	0.70
1:B:560:ILE:O	1:B:563:VAL:HG12	1.92	0.70
1:B:907:ILE:HD13	1:B:1027:ASP:HA	1.73	0.70
1:A:454:ILE:HG21	1:A:666:ALA:HB2	1.72	0.70
1:B:99:SER:HB3	1:B:472:ILE:HD11	1.74	0.70
1:A:20:TYR:HB3	1:A:29:PHE:HB3	1.74	0.70
1:B:109:LYS:CE	1:B:479:SER:HB2	2.19	0.69
1:B:1252:LYS:HE3	1:B:1252:LYS:HA	1.74	0.69
1:A:615:GLU:CD	1:A:615:GLU:N	2.50	0.69
1:A:941:ASN:HD22	1:A:942:CYS:N	1.90	0.69
1:B:299:TYR:HA	1:B:302:VAL:HG12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:ILE:HD13	1:B:545:LEU:HB3	1.74	0.69
1:B:944:ARG:HA	1:B:944:ARG:HH11	1.58	0.69
1:A:529:PRO:HG2	1:A:532:GLU:HG3	1.74	0.69
1:A:711:GLN:O	1:A:715:ILE:HG12	1.93	0.69
1:B:211:MET:HA	1:B:214:LEU:HD12	1.73	0.69
1:B:642:ILE:HD13	1:B:681:VAL:HG13	1.74	0.69
1:B:928:ASN:C	1:B:930:ILE:H	2.01	0.69
1:A:1148:VAL:O	1:A:1188:VAL:HG12	1.93	0.69
1:B:577:GLN:O	1:B:581:VAL:HG23	1.94	0.68
1:B:1095:ASN:C	1:B:1096:ASN:HD22	2.00	0.68
1:A:814:MET:HE1	1:A:913:LYS:HD3	1.75	0.68
1:A:1076:TRP:CZ3	1:A:1244:SER:O	2.46	0.68
1:B:199:MET:HG2	1:B:705:TYR:CE2	2.28	0.68
1:A:944:ARG:HG2	1:A:1026:SER:CB	2.22	0.68
1:B:835:ILE:CG2	1:B:837:ILE:HB	2.22	0.68
1:A:122:ASN:HA	1:A:289:VAL:HA	1.75	0.68
1:A:1092:LEU:C	1:A:1094:PRO:HD3	2.19	0.68
1:A:448:ILE:CG2	1:A:646:LEU:CG	2.70	0.68
1:A:925:ASN:C	1:A:927:ASP:N	2.49	0.68
1:B:110:ALA:HB3	1:B:221:LEU:HD13	1.75	0.68
1:B:1074:ASP:HB2	1:B:1078:ASN:H	1.59	0.68
1:B:877:ASP:O	1:B:896:SER:HB2	1.93	0.68
1:A:127:GLY:HA2	1:A:493:GLN:NE2	2.08	0.68
1:A:1225:TYR:O	1:A:1229:MET:HB3	1.94	0.68
1:B:925:ASN:C	1:B:927:ASP:N	2.52	0.68
1:B:20:TYR:HB3	1:B:29:PHE:HB3	1.76	0.67
1:B:111:ASN:HD21	1:B:484:SER:HB2	1.58	0.67
1:B:1202:LYS:HA	1:B:1209:ILE:HG12	1.75	0.67
1:B:622:LYS:O	1:B:626:GLU:HG2	1.93	0.67
1:A:365:ASN:O	1:A:368:ILE:HG22	1.94	0.67
1:B:466:ASN:N	1:B:466:ASN:ND2	2.40	0.67
1:A:141:GLN:HE21	1:A:490:LEU:HD23	1.59	0.67
1:A:297:ASN:N	1:A:298:PRO:HD2	2.07	0.67
1:A:568:GLN:CB	1:A:571:LEU:HD13	2.22	0.67
1:B:51:THR:HG22	1:B:52:PRO:HD2	1.76	0.67
1:B:672:LYS:O	1:B:675:ASP:HB2	1.95	0.67
1:B:21:ILE:HG12	1:B:134:ILE:HG22	1.77	0.66
1:A:57:PRO:HB3	1:A:69:TYR:HB2	1.76	0.66
1:A:451:PRO:HG2	1:A:648:PHE:CB	2.26	0.66
1:A:663:VAL:HG21	1:A:804:LEU:HD23	1.77	0.66
1:B:474:ASN:HD22	1:B:1070:ASN:HB2	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:ARG:HH11	1:B:999:ARG:CA	2.07	0.66
1:A:606:ILE:HG23	1:A:704:MET:CE	2.25	0.66
1:A:857:TYR:N	1:A:886:ASN:ND2	2.44	0.66
1:B:884:ASN:ND2	1:B:886:ASN:HB2	2.10	0.66
1:B:368:ILE:HG12	1:B:395:ILE:HG22	1.78	0.65
1:A:116:ASN:HD21	1:A:118:ASN:HB2	1.61	0.65
1:B:835:ILE:HG22	1:B:837:ILE:HB	1.77	0.65
1:B:955:ASN:HB3	1:B:958:GLU:CD	2.21	0.65
1:A:111:ASN:HD22	1:A:483:LEU:HD13	1.61	0.65
1:A:857:TYR:N	1:A:886:ASN:HD21	1.93	0.65
1:B:414:ASN:OD1	1:B:424:SER:HB3	1.96	0.65
1:A:94:ILE:HG22	1:A:104:LEU:HD11	1.79	0.65
1:B:964:GLN:HG3	1:B:970:ASN:HB3	1.79	0.65
1:A:296:LEU:O	1:A:296:LEU:HD12	1.96	0.65
1:B:429:ILE:HD13	1:B:429:ILE:H	1.62	0.65
1:B:981:ASN:HB3	1:B:1117:LEU:HD23	1.77	0.65
1:A:1230:ARG:O	1:A:1231:ASP:HB2	1.97	0.64
1:B:29:PHE:CE1	1:B:135:LYS:HG3	2.32	0.64
1:B:249:ILE:HA	1:B:252:PHE:HD1	1.62	0.64
1:B:448:ILE:HD11	1:B:646:LEU:HG	1.78	0.64
1:B:497:TYR:C	1:B:499:PRO:HD3	2.23	0.64
1:B:109:LYS:HD2	1:B:483:LEU:HD23	1.78	0.64
1:B:402:ARG:HE	1:B:402:ARG:HA	1.63	0.64
1:A:801:GLY:HA3	1:A:808:GLN:OE1	1.98	0.64
1:B:468:LEU:O	1:B:471:VAL:HG22	1.95	0.64
1:B:498:ILE:N	1:B:499:PRO:HD3	2.12	0.64
1:A:913:LYS:HA	1:A:999:ARG:CG	2.27	0.64
1:B:941:ASN:N	1:B:941:ASN:HD22	1.94	0.64
1:A:154:GLU:HB2	1:A:155:PRO:CD	2.28	0.64
1:B:659:ASN:HB3	1:B:662:LYS:HG2	1.79	0.64
1:B:275:LEU:HD23	1:B:328:PHE:HE1	1.60	0.64
1:B:1229:MET:HG2	1:B:1229:MET:O	1.95	0.64
1:A:700:ARG:HD3	1:A:703:GLN:NE2	2.13	0.64
1:A:989:LYS:HE2	1:A:1075:PHE:O	1.96	0.64
1:A:245:ARG:HH22	1:A:502:ASP:HB3	1.62	0.64
1:A:166:SER:HB3	1:A:498:ILE:HB	1.79	0.63
1:A:831:THR:HG23	1:A:831:THR:O	1.98	0.63
1:B:884:ASN:C	1:B:884:ASN:HD22	2.04	0.63
1:B:903:ASN:HD22	1:B:904:ASP:N	1.96	0.63
1:B:996:THR:HG22	1:B:996:THR:O	1.99	0.63
1:B:1167:ALA:O	1:B:1168:THR:HG23	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:931:VAL:HG13	1:B:1038:TYR:OH	1.98	0.63
1:A:1161:PRO:HG2	1:A:1178:SER:HB3	1.78	0.63
1:B:111:ASN:HD22	1:B:483:LEU:CD1	2.10	0.63
1:A:497:TYR:C	1:A:499:PRO:HD3	2.23	0.63
1:A:700:ARG:HD3	1:A:703:GLN:HE22	1.64	0.63
1:A:738:TYR:HA	1:A:743:ILE:HD13	1.81	0.63
1:A:778:LYS:HA	1:A:782:LEU:HB2	1.80	0.63
1:A:850:SER:O	1:A:1050:PHE:HA	1.99	0.63
1:A:1244:SER:O	1:A:1246:GLU:HG3	1.99	0.63
1:B:439:SER:O	1:B:442:SER:HB2	1.97	0.63
1:A:37:LYS:HE3	1:A:37:LYS:HA	1.80	0.63
1:A:1067:PRO:HA	5:A:1287:HOH:O	1.98	0.62
1:B:448:ILE:HG23	1:B:448:ILE:O	1.99	0.62
1:A:571:LEU:HD12	1:A:571:LEU:N	2.14	0.62
1:B:389:ALA:HA	1:B:396:ILE:HD11	1.81	0.62
1:B:749:GLN:O	1:B:753:ILE:HG12	1.98	0.62
1:B:197:ASN:ND2	1:B:346:LYS:HD3	2.12	0.62
1:B:1130:GLN:HE22	1:B:1183:ARG:HH22	1.46	0.62
1:A:642:ILE:HD13	1:A:681:VAL:HG13	1.81	0.62
1:B:746:GLU:O	1:B:750:LYS:HG2	1.99	0.62
1:A:109:LYS:HZ3	1:A:478:GLU:C	2.07	0.62
1:B:1225:TYR:O	1:B:1229:MET:HB3	2.00	0.62
1:A:660:LYS:HG3	1:A:804:LEU:HA	1.81	0.62
1:A:833:ASP:HB3	1:A:836:LEU:HD23	1.82	0.62
1:A:92:ASN:O	1:A:96:ASN:HB2	1.99	0.61
1:B:346:LYS:HE2	1:B:346:LYS:HA	1.81	0.61
1:B:401:GLY:C	1:B:403:GLY:H	2.07	0.61
1:A:847:ILE:HD12	1:A:847:ILE:N	2.14	0.61
1:B:606:ILE:HD12	1:B:761:PHE:HE2	1.64	0.61
1:B:831:THR:HG22	1:B:831:THR:O	2.00	0.61
1:B:615:GLU:CD	1:B:615:GLU:H	2.07	0.61
1:B:62:LYS:O	1:B:407:LYS:HE3	2.00	0.61
1:B:580:LEU:HD22	1:B:747:LEU:HD21	1.81	0.61
1:B:704:MET:HG3	1:B:758:ILE:HD13	1.81	0.61
1:B:106:GLU:CD	1:B:330:LYS:HD2	2.25	0.61
1:A:373:GLU:HB3	1:A:376:ASN:O	2.00	0.61
1:A:959:ILE:C	1:A:960:ILE:HD12	2.25	0.61
1:A:458:VAL:HG12	1:A:460:SER:H	1.66	0.61
1:A:719:ILE:HG22	1:A:719:ILE:O	2.01	0.61
1:A:238:ASN:HB3	1:A:241:ILE:CG1	2.29	0.61
1:B:378:ASN:N	1:B:378:ASN:HD22	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:ND2	1:A:118:ASN:HB2	2.15	0.61
1:A:895:LEU:N	1:A:895:LEU:HD12	2.16	0.60
1:B:857:TYR:H	1:B:886:ASN:ND2	1.98	0.60
1:B:872:ILE:HG12	1:B:900:ILE:HG12	1.83	0.60
1:B:1114:THR:CG2	1:B:1115:ILE:N	2.64	0.60
1:A:636:PHE:N	1:A:696:GLN:HE22	1.96	0.60
1:A:642:ILE:HD11	1:A:685:ILE:HD11	1.81	0.60
1:B:856:ARG:NH2	1:B:1048:ASN:HD22	1.99	0.60
1:A:668:ASN:ND2	1:A:913:LYS:NZ	2.48	0.60
1:A:833:ASP:CG	1:A:836:LEU:HD23	2.26	0.60
1:B:785:TYR:O	1:B:789:VAL:HG23	2.01	0.60
1:B:1171:LYS:NZ	1:B:1224:TRP:HB2	2.15	0.60
1:B:635:GLU:HB3	1:B:696:GLN:HE21	1.66	0.60
1:A:59:THR:HB	1:A:507:SER:HA	1.84	0.60
1:A:803:ILE:HD12	1:A:803:ILE:N	2.16	0.60
1:A:963:LEU:HD11	1:A:1023:ILE:HD13	1.82	0.60
1:A:1074:ASP:HB3	1:A:1076:TRP:H	1.67	0.60
1:A:593:VAL:HG23	1:A:602:VAL:CG2	2.32	0.60
1:A:742:GLN:CB	1:A:743:ILE:HD12	2.32	0.60
1:A:214:LEU:HA	1:A:217:SER:HB2	1.84	0.60
1:A:722:LYS:C	1:A:724:ASN:H	2.07	0.60
1:A:742:GLN:HB3	1:A:743:ILE:HD12	1.84	0.60
1:B:233:ILE:HD13	1:B:691:THR:HG21	1.84	0.60
1:B:848:LYS:O	1:B:848:LYS:HG3	2.01	0.60
1:A:454:ILE:HD12	1:A:666:ALA:HA	1.84	0.60
1:A:907:ILE:HD13	1:A:1027:ASP:HA	1.84	0.60
1:B:102:ILE:O	1:B:105:GLU:HB3	2.01	0.60
1:A:913:LYS:HA	1:A:999:ARG:HG3	1.83	0.60
1:B:174:SER:HA	1:B:223:GLY:HA2	1.84	0.60
1:B:795:ASN:O	1:B:799:GLN:HG2	2.02	0.60
1:B:847:ILE:O	1:B:848:LYS:HB3	2.02	0.60
1:A:854:ASN:HD22	1:A:866:SER:HA	1.66	0.59
1:A:1002:ASP:HB3	1:A:1016:SER:HA	1.83	0.59
1:B:1098:ILE:N	1:B:1098:ILE:HD12	2.17	0.59
1:B:1111:ILE:HD12	1:B:1111:ILE:C	2.27	0.59
1:A:216:HIS:CD2	5:A:1318:HOH:O	2.55	0.59
1:B:359:LYS:HB3	1:B:397:THR:HG23	1.83	0.59
1:B:668:ASN:HD21	1:B:913:LYS:HE2	1.67	0.59
1:B:928:ASN:CB	1:B:930:ILE:HD13	2.31	0.59
1:B:955:ASN:HB3	1:B:958:GLU:CG	2.33	0.59
1:A:228:THR:HB	1:A:250:GLU:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1109:ASN:HB3	1:A:1217:ASP:HB2	1.85	0.59
1:B:128:ASP:HB2	1:B:495:ASP:O	2.03	0.59
1:B:532:GLU:OE2	1:B:549:PRO:HB3	2.02	0.59
1:A:342:LYS:HE2	1:A:342:LYS:HA	1.85	0.59
1:B:269:ASN:O	1:B:273:THR:HG23	2.01	0.59
1:B:1132:VAL:HG23	1:B:1148:VAL:HA	1.83	0.59
1:B:244:ILE:HG12	1:B:245:ARG:O	2.01	0.59
1:B:1130:GLN:NE2	1:B:1183:ARG:HH22	2.01	0.59
1:B:169:ASN:O	1:B:170:ASN:HB2	2.01	0.59
1:B:487:LYS:HD2	1:B:487:LYS:C	2.28	0.59
1:B:642:ILE:CD1	1:B:685:ILE:HD11	2.32	0.59
1:B:728:LEU:HD23	1:B:728:LEU:C	2.28	0.59
1:B:966:ASN:ND2	1:B:1022:ASN:HD22	2.01	0.59
1:A:595:LYS:HB2	1:A:626:GLU:HB2	1.84	0.59
1:B:874:ILE:HD12	1:B:874:ILE:O	2.03	0.59
1:B:947:ASN:HB3	1:B:964:GLN:HE22	1.67	0.59
1:A:576:ILE:O	1:A:580:LEU:HB2	2.03	0.59
1:B:37:LYS:HA	1:B:37:LYS:HE3	1.84	0.59
1:B:480:ALA:N	1:B:481:PRO:HD3	2.18	0.58
1:B:707:ALA:O	1:B:711:GLN:HG2	2.03	0.58
1:A:668:ASN:HD21	1:A:913:LYS:NZ	2.01	0.58
1:A:836:LEU:HD12	1:A:837:ILE:HD13	1.84	0.58
1:B:606:ILE:HD12	1:B:761:PHE:CE2	2.37	0.58
1:B:620:ASN:N	1:B:620:ASN:HD22	2.00	0.58
1:B:1006:TYR:O	1:B:1007:ILE:HD13	2.03	0.58
1:A:438:ALA:HB3	1:A:692:LYS:HG2	1.85	0.58
1:A:1150:ILE:HG12	1:A:1188:VAL:HG11	1.86	0.58
1:B:172:MET:HE3	1:B:175:ASN:ND2	2.14	0.58
1:B:981:ASN:CB	1:B:1117:LEU:HB3	2.33	0.58
1:A:704:MET:HG3	1:A:758:ILE:HD13	1.85	0.58
1:B:852:VAL:HG13	1:B:906:ILE:CG1	2.34	0.58
1:B:892:ASN:OD1	1:B:1039:THR:HA	2.03	0.58
1:B:1230:ARG:O	1:B:1231:ASP:HB2	2.03	0.58
1:A:362:ASN:HD21	1:A:364:LEU:HB2	1.69	0.58
1:B:836:LEU:O	1:B:837:ILE:HG22	2.04	0.58
1:B:837:ILE:O	1:B:838:SER:CB	2.51	0.58
1:A:368:ILE:HD11	1:A:395:ILE:HG22	1.84	0.58
1:B:193:ARG:HD2	1:B:201:GLU:HB3	1.86	0.58
1:B:1171:LYS:HZ1	1:B:1224:TRP:HB2	1.68	0.58
1:A:498:ILE:HG12	1:A:498:ILE:O	2.04	0.58
1:B:660:LYS:O	1:B:660:LYS:HD3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:HD13	1:A:368:ILE:O	2.03	0.58
1:A:448:ILE:CG2	1:A:646:LEU:H	2.14	0.58
1:A:1211:LEU:HD13	1:A:1226:TYR:CE2	2.36	0.58
1:A:668:ASN:ND2	1:A:913:LYS:HZ1	2.02	0.57
1:B:21:ILE:HG23	1:B:134:ILE:HG22	1.86	0.57
1:B:285:LYS:NZ	1:B:285:LYS:HB3	2.20	0.57
1:B:961:TRP:HD1	1:B:973:LEU:HB2	1.70	0.57
1:B:1114:THR:HG21	1:B:1117:LEU:H	1.68	0.57
1:A:202:PHE:C	1:A:203:ILE:HD12	2.29	0.57
1:B:452:LYS:H	1:B:452:LYS:HD3	1.70	0.57
1:A:94:ILE:CG2	1:A:104:LEU:HD11	2.34	0.57
1:A:760:ARG:HE	1:A:830:TYR:HD2	1.50	0.57
1:B:755:MET:SD	1:B:758:ILE:HD12	2.44	0.57
1:B:913:LYS:HG3	1:B:914:ASN:H	1.69	0.57
1:B:914:ASN:HB3	1:B:1053:GLU:HB2	1.86	0.57
1:B:1132:VAL:HG22	1:B:1149:TYR:CZ	2.39	0.57
1:A:989:LYS:HG2	1:A:1076:TRP:HA	1.87	0.57
1:A:376:ASN:HD22	1:A:386:GLY:HA3	1.70	0.57
1:A:836:LEU:HB3	1:A:837:ILE:HG12	1.86	0.57
1:B:199:MET:SD	1:B:199:MET:C	2.87	0.57
1:B:480:ALA:N	1:B:481:PRO:CD	2.68	0.57
1:B:529:PRO:HG2	1:B:532:GLU:HB2	1.87	0.57
1:B:854:ASN:O	1:B:864:ASP:HA	2.03	0.57
1:B:947:ASN:HB3	1:B:964:GLN:NE2	2.18	0.57
1:B:1098:ILE:HA	1:B:1107:SER:O	2.04	0.57
1:A:760:ARG:HH21	1:A:831:THR:HG22	1.70	0.57
1:A:938:THR:HG23	1:A:1034:VAL:HB	1.85	0.57
1:A:1062:LEU:O	1:A:1066:GLU:HG3	2.05	0.57
1:A:1202:LYS:HG2	1:A:1208:ASN:HA	1.87	0.57
1:B:1132:VAL:HG22	1:B:1149:TYR:CE2	2.40	0.57
1:B:134:ILE:HD13	1:B:144:LEU:HB2	1.87	0.56
1:B:1200:ASN:HB2	1:B:1211:LEU:HD12	1.86	0.56
1:A:1071:ILE:O	1:A:1073:LYS:HE3	2.05	0.56
1:B:928:ASN:HB2	1:B:930:ILE:HD13	1.87	0.56
1:B:1114:THR:HG22	1:B:1115:ILE:N	2.20	0.56
1:A:165:ILE:HD11	1:A:181:ILE:HB	1.85	0.56
1:B:402:ARG:HA	1:B:402:ARG:NE	2.19	0.56
1:B:983:ILE:HD12	1:B:983:ILE:N	2.18	0.56
1:A:165:ILE:HB	1:A:180:SER:OG	2.06	0.56
1:A:329:LYS:HZ3	1:A:466:ASN:HD21	1.54	0.56
1:A:593:VAL:CG2	1:A:602:VAL:HG22	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:ASN:H	1:A:1019:ASN:ND2	1.96	0.56
1:B:635:GLU:HB3	1:B:696:GLN:NE2	2.20	0.56
1:B:1020:LEU:HD12	1:B:1020:LEU:H	1.70	0.56
1:A:62:LYS:HG2	1:A:506:THR:HG23	1.88	0.56
1:A:81:ASP:O	1:A:85:LYS:HG3	2.06	0.56
1:A:258:THR:HG22	1:A:690:MET:HE1	1.88	0.56
1:A:606:ILE:HG23	1:A:704:MET:HE1	1.87	0.56
1:A:857:TYR:CZ	1:A:860:ASP:HA	2.41	0.56
1:B:143:ILE:HG23	1:B:490:LEU:HD23	1.87	0.56
1:B:596:ILE:HG21	1:B:599:ILE:HD12	1.88	0.56
1:A:606:ILE:HG23	1:A:704:MET:HE3	1.88	0.56
1:A:635:GLU:H	1:A:696:GLN:HE21	1.53	0.56
1:A:981:ASN:HA	1:A:1117:LEU:O	2.05	0.56
1:B:111:ASN:ND2	1:B:484:SER:HB2	2.21	0.56
1:B:913:LYS:HG3	1:B:914:ASN:CG	2.30	0.56
1:B:1131:ARG:HG2	1:B:1133:ASN:ND2	2.21	0.56
1:A:13:VAL:HG13	1:A:19:LEU:HA	1.87	0.56
1:A:198:CYS:SG	1:A:759:ASP:OD2	2.64	0.56
1:B:42:ILE:HG22	1:B:44:GLU:HG2	1.86	0.56
1:B:82:ARG:O	1:B:82:ARG:HD3	2.06	0.56
1:B:454:ILE:HG21	1:B:666:ALA:HB2	1.88	0.56
1:B:898:VAL:HB	1:B:1031:PHE:HB2	1.88	0.56
1:B:910:ASN:C	1:B:912:TYR:H	2.13	0.56
1:A:453:GLU:HG2	1:A:454:ILE:HD13	1.88	0.56
1:A:578:GLN:O	1:A:578:GLN:HG3	2.04	0.56
1:A:960:ILE:HD12	1:A:960:ILE:N	2.20	0.56
1:B:127:GLY:HA2	1:B:493:GLN:NE2	2.21	0.56
1:B:627:LEU:HD13	1:B:627:LEU:O	2.05	0.55
1:B:86:ILE:HD11	1:B:363:LEU:HB2	1.87	0.55
1:B:459:THR:HG22	1:B:459:THR:O	2.06	0.55
1:B:636:PHE:N	1:B:696:GLN:HE22	2.04	0.55
1:B:995:ILE:HD12	1:B:995:ILE:N	2.21	0.55
1:B:116:ASN:ND2	1:B:118:ASN:H	2.01	0.55
1:B:191:SER:HB2	1:B:360:LEU:HD11	1.87	0.55
1:B:299:TYR:HD1	1:B:302:VAL:HG11	1.72	0.55
1:B:961:TRP:CE2	1:B:995:ILE:HG21	2.42	0.55
1:B:1096:ASN:HD22	1:B:1096:ASN:N	2.01	0.55
1:A:576:ILE:O	1:A:579:VAL:HG22	2.07	0.55
1:A:738:TYR:O	1:A:742:GLN:O	2.24	0.55
1:B:116:ASN:HD22	1:B:116:ASN:C	2.14	0.55
1:A:149:ILE:HB	1:A:183:ILE:HD13	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1168:THR:HG22	1:A:1169:THR:H	1.72	0.55
1:B:203:ILE:HD11	1:B:396:ILE:HD11	1.88	0.55
1:B:252:PHE:CD2	1:B:262:ILE:HD12	2.42	0.55
1:B:571:LEU:N	1:B:571:LEU:HD12	2.22	0.55
1:B:1091:VAL:O	1:B:1094:PRO:HD3	2.06	0.55
1:A:523:LEU:HD11	1:A:703:GLN:HG2	1.89	0.55
1:A:857:TYR:OH	1:A:860:ASP:HA	2.07	0.55
1:B:116:ASN:HD22	1:B:118:ASN:N	2.02	0.55
1:B:454:ILE:HG13	1:B:456:ASP:OD1	2.07	0.55
1:B:939:ILE:HG21	1:B:1042:ILE:HD13	1.87	0.55
1:A:295:LEU:HD12	1:A:295:LEU:H	1.72	0.55
1:B:73:TYR:CE2	1:B:74:LEU:HG	2.41	0.55
1:B:522:TYR:CD1	1:B:611:ASN:HB2	2.41	0.55
1:B:720:GLU:O	1:B:724:ASN:HB2	2.06	0.55
1:B:1071:ILE:O	1:B:1073:LYS:HE3	2.07	0.55
1:A:928:ASN:C	1:A:930:ILE:H	2.15	0.55
1:B:121:ASP:HB3	1:B:285:LYS:HE2	1.88	0.55
1:B:370:ASN:HD21	1:B:377:ILE:CG2	2.20	0.55
1:B:8:ASN:HB2	1:B:11:ASP:OD2	2.07	0.55
1:A:154:GLU:HB2	1:A:155:PRO:HD2	1.88	0.54
1:B:285:LYS:HB3	1:B:285:LYS:HZ2	1.73	0.54
1:A:651:LYS:HG2	1:A:653:PHE:H	1.72	0.54
1:B:354:GLN:HG2	1:B:432:GLY:CA	2.37	0.54
1:A:191:SER:HB2	1:A:360:LEU:HD11	1.89	0.54
1:B:196:ASP:CG	1:B:348:ARG:HA	2.32	0.54
1:B:943:MET:HG3	1:B:950:TRP:O	2.07	0.54
1:B:973:LEU:HD23	1:B:1005:LEU:HB2	1.88	0.54
1:B:1131:ARG:HG2	1:B:1133:ASN:HD21	1.72	0.54
1:A:988:ASN:HB2	5:A:1259:HOH:O	2.07	0.54
1:B:109:LYS:HE3	1:B:479:SER:CB	2.26	0.54
1:B:667:ILE:HG23	1:B:793:LEU:HD22	1.90	0.54
1:A:199:MET:HG2	1:A:705:TYR:OH	2.08	0.54
1:B:456:ASP:OD1	1:B:669:ASN:ND2	2.40	0.54
1:A:103:LEU:O	1:A:107:LEU:HD12	2.08	0.54
1:A:33:PHE:N	1:A:33:PHE:CD2	2.75	0.53
1:A:912:TYR:O	1:A:999:ARG:HG3	2.08	0.53
1:B:448:ILE:HD11	1:B:646:LEU:CG	2.37	0.53
1:B:559:PHE:CD1	1:B:582:ASP:HB3	2.43	0.53
1:A:271:ILE:O	1:A:275:LEU:HB2	2.08	0.53
1:A:362:ASN:ND2	1:A:364:LEU:H	2.05	0.53
1:A:907:ILE:CD1	1:A:1027:ASP:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:SER:OG	1:A:1120:ARG:HD2	2.07	0.53
1:A:81:ASP:OD2	1:A:85:LYS:HE3	2.07	0.53
1:A:1194:GLY:O	1:A:1196:ASN:N	2.40	0.53
1:B:874:ILE:HD12	1:B:874:ILE:C	2.33	0.53
1:A:295:LEU:HD12	1:A:295:LEU:N	2.24	0.53
1:A:723:TYR:CE2	1:A:731:LYS:HG3	2.44	0.53
1:A:920:TRP:HB2	1:A:1045:ARG:CG	2.38	0.53
1:B:409:ILE:HD12	1:B:409:ILE:N	2.23	0.53
1:B:109:LYS:NZ	1:B:478:GLU:HB2	2.23	0.53
1:B:447:ASN:C	1:B:449:ASN:H	2.17	0.53
1:B:632:ILE:CG2	1:B:633:LEU:HD22	2.36	0.53
1:B:965:ASP:HB2	1:B:1020:LEU:HB3	1.89	0.53
1:B:973:LEU:CD2	1:B:1005:LEU:HB2	2.38	0.53
1:A:93:ARG:HG3	1:A:371:ILE:O	2.08	0.53
1:A:448:ILE:CD1	1:A:643:PRO:HG2	2.35	0.53
1:A:877:ASP:O	1:A:896:SER:HB2	2.07	0.53
1:A:1050:PHE:CD2	1:A:1054:LEU:HD11	2.44	0.53
1:B:14:ASN:C	1:B:16:ARG:H	2.16	0.53
1:B:76:SER:O	1:B:80:LYS:HG3	2.09	0.53
1:B:1215:LYS:O	1:B:1216:ALA:HB3	2.08	0.53
1:A:148:VAL:HG22	1:A:182:ALA:HB3	1.89	0.53
1:A:279:TYR:HE2	1:A:327:ILE:HG21	1.74	0.53
1:A:299:TYR:HA	1:A:302:VAL:HG12	1.91	0.53
1:A:627:LEU:HD22	1:A:627:LEU:O	2.08	0.53
1:B:154:GLU:HB2	1:B:155:PRO:HD2	1.89	0.53
1:A:62:LYS:CG	1:A:506:THR:HG23	2.39	0.53
1:A:93:ARG:HG3	1:A:93:ARG:HH11	1.74	0.53
1:A:672:LYS:NZ	1:A:849:SER:OG	2.33	0.53
1:A:852:VAL:HG13	1:A:906:ILE:HG23	1.90	0.53
1:A:1190:MET:HE1	1:A:1199:MET:CG	2.32	0.53
1:B:197:ASN:O	1:B:199:MET:N	2.41	0.53
1:B:370:ASN:HD21	1:B:377:ILE:HG22	1.73	0.53
1:B:378:ASN:HD22	1:B:378:ASN:H	1.56	0.53
1:B:454:ILE:HD12	1:B:666:ALA:N	2.24	0.53
1:B:472:ILE:C	1:B:474:ASN:H	2.16	0.53
1:B:836:LEU:HD12	1:B:836:LEU:N	2.24	0.53
1:A:109:LYS:C	1:A:111:ASN:H	2.16	0.53
1:A:166:SER:CB	1:A:498:ILE:HB	2.39	0.53
1:A:289:VAL:O	1:A:289:VAL:HG13	2.09	0.53
1:B:492:ILE:C	1:B:492:ILE:HD12	2.34	0.53
1:B:778:LYS:HA	1:B:782:LEU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:903:ASN:HD22	1:B:903:ASN:C	2.16	0.53
1:B:910:ASN:O	1:B:912:TYR:N	2.39	0.53
1:A:771:MET:HE1	1:A:825:PHE:HE2	1.74	0.52
1:B:121:ASP:OD2	1:B:121:ASP:N	2.41	0.52
1:B:203:ILE:N	1:B:203:ILE:HD12	2.24	0.52
1:B:999:ARG:HB3	1:B:999:ARG:NH1	2.24	0.52
1:B:727:THR:O	1:B:729:GLU:N	2.42	0.52
1:B:1116:LEU:O	1:B:1117:LEU:HB2	2.09	0.52
1:B:1130:GLN:NE2	1:B:1151:ASN:ND2	2.49	0.52
1:A:94:ILE:HG22	1:A:104:LEU:CD1	2.39	0.52
1:A:827:LEU:HD12	1:A:828:SER:N	2.24	0.52
1:B:36:MET:SD	1:B:104:LEU:HB3	2.50	0.52
1:A:81:ASP:CG	1:A:85:LYS:HE3	2.35	0.52
1:A:548:GLN:HA	5:A:1313:HOH:O	2.08	0.52
1:A:924:PRO:O	1:A:1040:ARG:NH2	2.42	0.52
1:B:852:VAL:HG13	1:B:906:ILE:HG13	1.92	0.52
1:B:196:ASP:OD2	1:B:348:ARG:HA	2.10	0.52
1:B:270:ASP:O	1:B:274:ASN:HB2	2.10	0.52
1:A:555:PHE:CD1	1:A:586:GLU:HB3	2.44	0.52
1:A:888:PHE:CZ	1:A:1044:ILE:HG12	2.44	0.52
1:B:751:VAL:HG13	1:B:752:SER:N	2.24	0.52
1:B:912:TYR:O	1:B:999:ARG:HG3	2.10	0.52
1:B:1200:ASN:HB2	1:B:1211:LEU:CD1	2.39	0.52
1:B:429:ILE:HD13	1:B:429:ILE:N	2.24	0.52
1:B:973:LEU:HD21	1:B:1003:SER:O	2.09	0.52
1:B:800:HIS:O	1:B:803:ILE:HB	2.10	0.52
1:A:106:GLU:HG2	1:A:330:LYS:HD2	1.90	0.52
1:A:556:SER:O	1:A:560:ILE:HG13	2.10	0.52
1:A:888:PHE:CZ	1:A:1044:ILE:CG1	2.93	0.52
1:A:1214:PHE:HA	1:A:1220:VAL:HG22	1.92	0.52
1:B:154:GLU:HB2	1:B:155:PRO:CD	2.39	0.52
1:B:352:ILE:HD12	1:B:695:THR:HG22	1.91	0.52
1:B:944:ARG:HD3	1:B:945:ASP:H	1.73	0.52
1:B:994:THR:HG21	1:B:1059:ILE:HD12	1.91	0.52
1:A:287:SER:HB3	1:A:316:ILE:HA	1.92	0.52
1:B:36:MET:CE	1:B:39:ILE:HD12	2.40	0.52
1:B:297:ASN:N	1:B:298:PRO:CD	2.73	0.52
1:B:636:PHE:H	1:B:696:GLN:HE22	1.57	0.52
1:A:774:ILE:O	1:A:777:VAL:HG12	2.10	0.51
1:A:1006:TYR:CE2	1:A:1056:GLU:HG2	2.39	0.51
1:B:119:THR:HG21	1:B:125:HIS:CD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:TYR:OH	1:A:1040:ARG:NH1	2.43	0.51
1:B:110:ALA:HB1	1:B:221:LEU:HB3	1.92	0.51
1:B:693:ILE:HG21	1:B:769:TYR:CD2	2.46	0.51
1:B:868:TYR:HB3	1:B:903:ASN:OD1	2.09	0.51
1:A:368:ILE:HD13	1:A:368:ILE:C	2.36	0.51
1:B:1233:THR:O	1:B:1235:SER:N	2.43	0.51
1:A:68:TYR:CD2	1:A:157:LEU:HD22	2.45	0.51
1:B:561:ASN:C	1:B:562:ASN:HD22	2.18	0.51
1:A:214:LEU:O	1:A:217:SER:HB2	2.11	0.51
1:A:476:ASN:HD21	1:A:1144:LYS:HB3	1.75	0.51
1:A:712:VAL:HG13	1:A:747:LEU:HD13	1.91	0.51
1:B:267:GLN:O	1:B:271:ILE:HG13	2.11	0.51
1:B:728:LEU:HD23	1:B:728:LEU:O	2.10	0.51
1:B:777:VAL:HG13	1:B:778:LYS:N	2.26	0.51
1:B:1126:LYS:HB2	1:B:1153:VAL:CG2	2.40	0.51
1:A:263:ILE:HD12	1:A:263:ILE:N	2.26	0.51
1:A:614:ASN:O	1:A:618:LYS:HG3	2.11	0.51
1:A:635:GLU:H	1:A:696:GLN:HE22	1.57	0.51
1:A:1109:ASN:HB3	1:A:1217:ASP:CB	2.40	0.51
1:B:244:ILE:HG13	1:B:245:ARG:N	2.26	0.51
1:B:474:ASN:HD22	1:B:1070:ASN:HD22	1.59	0.51
1:B:593:VAL:CG2	1:B:602:VAL:HG23	2.40	0.51
1:B:924:PRO:HD2	1:B:1040:ARG:HH21	1.74	0.51
1:B:979:ASN:O	1:B:980:ALA:O	2.29	0.51
1:B:378:ASN:N	1:B:378:ASN:ND2	2.59	0.51
1:B:541:ILE:HG23	1:B:542:ASP:N	2.26	0.51
1:B:1139:ASP:OD2	1:B:1141:LEU:HG	2.10	0.51
1:B:660:LYS:HG2	1:B:804:LEU:CB	2.29	0.51
1:B:852:VAL:HG13	1:B:906:ILE:HG12	1.93	0.51
1:B:857:TYR:H	1:B:886:ASN:HD21	1.56	0.51
1:B:36:MET:HE1	1:B:104:LEU:O	2.11	0.51
1:B:299:TYR:CA	1:B:302:VAL:HG12	2.40	0.51
1:B:670:ALA:CB	1:B:793:LEU:HD21	2.41	0.51
1:A:122:ASN:HA	1:A:288:LYS:O	2.10	0.50
1:A:1251:GLU:O	1:A:1251:GLU:HG2	2.11	0.50
1:B:606:ILE:HB	1:B:621:PHE:CE1	2.46	0.50
1:B:712:VAL:HG22	1:B:747:LEU:HB3	1.94	0.50
1:B:943:MET:HG2	1:B:948:SER:O	2.10	0.50
1:B:1108:ILE:HG13	1:B:1108:ILE:O	2.10	0.50
1:A:567:VAL:HG11	1:A:722:LYS:CA	2.41	0.50
1:B:856:ARG:HH21	1:B:1048:ASN:ND2	2.07	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ASN:ND2	1:A:377:ILE:HG21	2.26	0.50
1:A:454:ILE:HG21	1:A:666:ALA:CB	2.40	0.50
1:A:852:VAL:CG1	1:A:906:ILE:HD12	2.24	0.50
1:A:1166:THR:HG21	1:A:1209:ILE:HD12	1.92	0.50
1:B:392:ASN:N	1:B:393:PRO:HD3	2.25	0.50
1:B:923:ILE:HD12	1:B:954:LEU:HD11	1.92	0.50
1:A:168:ARG:HG2	1:A:169:ASN:N	2.27	0.50
1:A:996:THR:CG2	1:A:1004:LYS:HB2	2.39	0.50
1:B:474:ASN:ND2	1:B:1070:ASN:HB2	2.25	0.50
1:B:942:CYS:HB2	1:B:1029:ILE:HG23	1.94	0.50
1:A:497:TYR:CE1	1:A:499:PRO:HD2	2.47	0.50
1:A:920:TRP:HB2	1:A:1045:ARG:HG2	1.92	0.50
1:B:519:VAL:O	1:B:523:LEU:HG	2.10	0.50
1:B:541:ILE:O	1:B:544:ALA:HB3	2.11	0.50
1:A:416:VAL:HA	1:A:421:ILE:O	2.11	0.50
1:A:635:GLU:N	1:A:696:GLN:NE2	2.52	0.50
1:A:890:ILE:HG22	1:A:891:TYR:N	2.26	0.50
1:A:1115:ILE:HG12	1:A:1115:ILE:O	2.10	0.50
1:B:576:ILE:HD12	1:B:576:ILE:O	2.12	0.50
1:B:713:ASN:C	1:B:715:ILE:H	2.17	0.50
1:A:795:ASN:O	1:A:799:GLN:HG2	2.12	0.50
1:A:453:GLU:OE2	1:A:673:GLU:HB2	2.11	0.50
1:A:716:LYS:HG2	1:A:738:TYR:OH	2.11	0.50
1:A:1193:VAL:HG22	1:A:1193:VAL:O	2.12	0.50
1:B:715:ILE:HA	1:B:718:ILE:HG22	1.94	0.49
1:B:981:ASN:HA	1:B:1117:LEU:O	2.12	0.49
1:B:1096:ASN:N	1:B:1096:ASN:ND2	2.58	0.49
1:B:1208:ASN:HB3	1:B:1226:TYR:OH	2.12	0.49
1:A:111:ASN:HD21	1:A:484:SER:CB	2.24	0.49
1:A:323:LYS:O	1:A:327:ILE:HG12	2.12	0.49
1:A:802:SER:C	1:A:803:ILE:HD12	2.37	0.49
1:A:1002:ASP:OD2	1:A:1002:ASP:N	2.44	0.49
1:B:40:TRP:CE2	1:B:144:LEU:HD21	2.47	0.49
1:B:297:ASN:N	1:B:298:PRO:HD2	2.17	0.49
1:B:1144:LYS:HE2	1:B:1192:SER:HB3	1.94	0.49
1:B:299:TYR:HA	1:B:302:VAL:CG1	2.41	0.49
1:B:525:ALA:HB2	1:B:545:LEU:CD2	2.43	0.49
1:B:924:PRO:O	1:B:1040:ARG:NH2	2.45	0.49
1:B:1150:ILE:HG12	1:B:1188:VAL:HG11	1.94	0.49
1:A:135:LYS:HA	1:A:140:SER:O	2.13	0.49
1:A:165:ILE:HD12	1:A:181:ILE:HB	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:876:GLY:HA3	1:A:895:LEU:O	2.11	0.49
1:A:961:TRP:CE2	1:A:995:ILE:HG21	2.48	0.49
1:B:897:GLU:CD	1:B:1032:LYS:HD2	2.37	0.49
1:B:926:TYR:O	1:B:1250:GLN:HB2	2.12	0.49
1:A:738:TYR:O	1:A:743:ILE:HB	2.11	0.49
1:A:894:LYS:C	1:A:895:LEU:HD12	2.37	0.49
1:B:719:ILE:CG2	1:B:738:TYR:HE1	2.25	0.49
1:B:893:ASP:CG	1:B:894:LYS:HG3	2.38	0.49
1:B:1184:PHE:O	1:B:1186:GLN:HG3	2.12	0.49
1:A:593:VAL:HG21	1:A:625:LEU:HD23	1.95	0.49
1:A:832:ASP:O	1:A:833:ASP:HB2	2.13	0.49
1:A:454:ILE:HD13	1:A:454:ILE:N	2.28	0.49
1:B:295:LEU:H	1:B:295:LEU:CD1	2.17	0.49
1:B:575:TRP:O	1:B:579:VAL:HG13	2.12	0.49
1:B:943:MET:HA	1:B:948:SER:O	2.12	0.49
1:B:1233:THR:C	1:B:1235:SER:N	2.69	0.49
1:A:34:ASN:HB2	1:A:40:TRP:CH2	2.47	0.49
1:A:568:GLN:HB2	1:A:571:LEU:CD1	2.30	0.49
1:A:983:ILE:CD1	1:A:1094:PRO:HB3	2.43	0.49
1:B:1103:ASP:O	1:B:1104:SER:OG	2.25	0.49
1:A:302:VAL:CG2	1:A:483:LEU:HD22	2.39	0.49
1:A:394:ARG:HG2	1:A:394:ARG:HH11	1.77	0.49
1:A:417:SER:O	1:A:419:LYS:N	2.46	0.49
1:B:21:ILE:HG12	1:B:134:ILE:CG2	2.42	0.49
1:B:160:THR:HG21	1:B:209:THR:HG22	1.95	0.49
1:B:233:ILE:HA	1:B:442:SER:OG	2.13	0.49
1:B:510:GLU:HG2	1:B:512:HIS:HE1	1.78	0.49
1:B:661:ASN:ND2	1:B:1000:LEU:HD21	2.27	0.49
1:B:920:TRP:O	1:B:1044:ILE:HA	2.12	0.49
1:B:576:ILE:O	1:B:579:VAL:HG22	2.12	0.48
1:B:1114:THR:CG2	1:B:1117:LEU:H	2.25	0.48
1:A:379:ASN:N	1:A:379:ASN:ND2	2.57	0.48
1:A:704:MET:CG	1:A:758:ILE:HD13	2.42	0.48
1:B:409:ILE:O	1:B:429:ILE:HD13	2.14	0.48
1:B:800:HIS:HA	1:B:803:ILE:HD12	1.95	0.48
1:B:1100:ARG:HH11	1:B:1100:ARG:HG2	1.79	0.48
1:A:453:GLU:C	1:A:454:ILE:HG12	2.38	0.48
1:A:467:ASP:HB3	1:A:470:GLN:CB	2.41	0.48
1:B:856:ARG:NH2	1:B:1048:ASN:ND2	2.61	0.48
1:B:1189:VAL:CG2	1:B:1200:ASN:HB3	2.43	0.48
1:A:106:GLU:OE2	1:A:477:SER:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ALA:HB2	1:A:167:LEU:HD11	1.94	0.48
1:A:497:TYR:CD1	1:A:498:ILE:N	2.82	0.48
1:A:941:ASN:HD22	1:A:942:CYS:H	1.61	0.48
1:A:1072:LEU:HG	1:A:1192:SER:OG	2.14	0.48
1:B:1064:SER:O	1:B:1069:THR:HG22	2.14	0.48
1:A:391:LEU:O	1:A:393:PRO:HD3	2.13	0.48
1:A:392:ASN:N	1:A:393:PRO:HD3	2.25	0.48
1:A:487:LYS:O	1:A:488:LEU:O	2.32	0.48
1:A:497:TYR:CD1	1:A:499:PRO:HD2	2.48	0.48
1:B:663:VAL:CG2	1:B:804:LEU:HD23	2.44	0.48
1:A:109:LYS:CG	1:A:483:LEU:HD21	2.43	0.48
1:A:407:LYS:HD2	1:A:431:ASN:HB2	1.95	0.48
1:A:686:VAL:O	1:A:690:MET:HG3	2.13	0.48
1:A:1006:TYR:O	1:A:1007:ILE:HD13	2.14	0.48
1:A:1033:ILE:HD11	1:A:1042:ILE:HG12	1.95	0.48
1:B:299:TYR:O	1:B:302:VAL:HG12	2.13	0.48
1:B:320:ASN:HB3	1:B:323:LYS:HG2	1.94	0.48
1:B:681:VAL:O	1:B:685:ILE:HG12	2.13	0.48
1:B:798:ILE:HG13	1:B:799:GLN:N	2.27	0.48
1:B:1251:GLU:CG	1:B:1252:LYS:H	2.21	0.48
1:A:415:ILE:HD12	1:A:425:ILE:HD12	1.96	0.48
1:A:733:GLU:O	1:A:734:LEU:HD23	2.13	0.48
1:A:854:ASN:HD22	1:A:866:SER:CA	2.26	0.48
1:B:83:PHE:O	1:B:86:ILE:HG22	2.14	0.48
1:B:197:ASN:O	1:B:198:CYS:C	2.56	0.48
1:B:249:ILE:HA	1:B:252:PHE:CD1	2.46	0.48
1:B:499:PRO:O	1:B:500:LYS:HB2	2.13	0.48
1:B:548:GLN:N	1:B:549:PRO:HD2	2.28	0.48
1:B:851:SER:OG	1:B:854:ASN:ND2	2.45	0.48
1:B:197:ASN:HD21	1:B:346:LYS:CD	2.17	0.48
1:B:916:SER:HB2	1:B:1054:LEU:HG	1.96	0.48
1:A:143:ILE:HG12	1:A:489:ASN:O	2.14	0.48
1:A:925:ASN:O	1:A:927:ASP:N	2.46	0.48
1:B:305:ALA:HB1	1:B:479:SER:OG	2.13	0.48
1:B:510:GLU:HG2	1:B:512:HIS:CE1	2.49	0.48
1:A:556:SER:HB2	1:A:558:GLU:HG2	1.96	0.48
1:B:359:LYS:O	1:B:397:THR:HG22	2.14	0.48
1:A:664:ILE:HD13	1:A:811:LEU:HD11	1.95	0.47
1:A:742:GLN:C	1:A:743:ILE:HD12	2.39	0.47
1:B:562:ASN:HD22	1:B:562:ASN:N	2.10	0.47
1:A:529:PRO:CG	1:A:532:GLU:HG3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1114:THR:HG21	1:B:1117:LEU:N	2.29	0.47
1:A:21:ILE:O	1:A:29:PHE:HA	2.14	0.47
1:A:146:PRO:O	1:A:181:ILE:HG12	2.14	0.47
1:A:252:PHE:CD2	1:A:262:ILE:HD12	2.49	0.47
1:B:1252:LYS:HA	1:B:1252:LYS:CE	2.44	0.47
1:A:111:ASN:HD21	1:A:484:SER:HB2	1.80	0.47
1:A:203:ILE:HD12	1:A:203:ILE:N	2.29	0.47
1:A:272:TYR:HA	1:A:328:PHE:CZ	2.48	0.47
1:A:467:ASP:O	1:A:470:GLN:HB3	2.13	0.47
1:A:971:GLN:HA	1:A:971:GLN:NE2	2.29	0.47
1:B:75:GLN:HA	1:B:75:GLN:HE21	1.80	0.47
1:B:602:VAL:O	1:B:604:PRO:HD3	2.14	0.47
1:B:1185:ASN:HA	1:B:1204:ASN:ND2	2.29	0.47
1:A:733:GLU:C	1:A:734:LEU:HD23	2.40	0.47
1:A:854:ASN:ND2	1:A:866:SER:HA	2.28	0.47
1:A:868:TYR:CD2	1:A:906:ILE:HD11	2.49	0.47
1:B:369:TYR:HA	1:B:374:GLY:O	2.15	0.47
1:B:836:LEU:C	1:B:838:SER:H	2.23	0.47
1:B:1137:THR:O	1:B:1137:THR:CG2	2.51	0.47
1:A:116:ASN:C	1:A:118:ASN:H	2.22	0.47
1:A:852:VAL:CG1	1:A:906:ILE:HG23	2.43	0.47
1:B:516:GLU:HA	1:B:516:GLU:OE2	2.14	0.47
1:B:1075:PHE:HD1	1:B:1241:ASN:HD22	1.62	0.47
1:A:144:LEU:C	1:A:146:PRO:HD3	2.40	0.47
1:A:316:ILE:HD12	1:A:316:ILE:C	2.40	0.47
1:B:396:ILE:HG22	1:B:397:THR:H	1.79	0.47
1:B:412:CYS:O	1:B:514:VAL:HG22	2.15	0.47
1:B:1126:LYS:HB2	1:B:1153:VAL:HG22	1.96	0.47
1:B:1193:VAL:CG2	1:B:1239:PHE:CE2	2.98	0.47
1:A:529:PRO:HG2	1:A:532:GLU:CG	2.44	0.47
1:B:306:LYS:HD3	1:B:307:TYR:CE1	2.49	0.47
1:B:484:SER:O	1:B:485:ASP:HB2	2.14	0.47
1:B:879:TYR:O	1:B:888:PHE:HA	2.15	0.47
1:B:939:ILE:HG13	1:B:940:ILE:N	2.29	0.47
1:B:1066:GLU:N	1:B:1067:PRO:CD	2.78	0.47
1:B:211:MET:SD	1:B:339:LEU:HD22	2.54	0.47
1:B:615:GLU:CD	1:B:615:GLU:N	2.72	0.47
1:B:971:GLN:NE2	1:B:1015:LYS:HB3	2.29	0.47
1:B:1114:THR:CG2	1:B:1117:LEU:N	2.78	0.47
1:A:89:LYS:HG3	1:A:371:ILE:HD11	1.97	0.47
1:A:286:LEU:HD11	1:A:300:LYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:GLN:N	1:A:549:PRO:HD2	2.29	0.47
1:B:122:ASN:HB3	1:B:288:LYS:HE2	1.97	0.47
1:B:497:TYR:HB3	1:B:498:ILE:H	1.41	0.47
1:B:558:GLU:CD	1:B:558:GLU:H	2.22	0.47
1:B:620:ASN:N	1:B:620:ASN:ND2	2.63	0.47
1:B:660:LYS:HE3	1:B:804:LEU:HB2	1.95	0.47
1:B:701:LYS:CG	1:B:762:LEU:HD12	2.45	0.47
1:B:955:ASN:HB3	1:B:958:GLU:HG2	1.96	0.47
1:B:1202:LYS:HB2	1:B:1207:ASN:O	2.15	0.47
1:A:476:ASN:ND2	1:A:1144:LYS:HB3	2.30	0.46
1:A:584:THR:OG1	1:A:750:LYS:HE2	2.15	0.46
1:A:610:LEU:CD1	1:A:704:MET:HE1	2.45	0.46
1:A:610:LEU:HG	1:A:704:MET:HE1	1.96	0.46
1:B:401:GLY:C	1:B:403:GLY:N	2.73	0.46
1:B:427:ILE:HD13	1:B:521:PHE:CD1	2.49	0.46
1:B:857:TYR:OH	1:B:860:ASP:HA	2.16	0.46
1:B:884:ASN:ND2	1:B:884:ASN:C	2.71	0.46
1:A:923:ILE:HG22	1:A:1040:ARG:NH2	2.30	0.46
1:A:1168:THR:HG22	1:A:1170:ASN:H	1.80	0.46
1:B:743:ILE:C	1:B:745:ASN:H	2.22	0.46
1:B:919:PHE:HE1	1:B:921:VAL:HB	1.81	0.46
1:A:392:ASN:O	1:A:395:ILE:HG12	2.14	0.46
1:A:448:ILE:HG22	1:A:646:LEU:CD1	2.46	0.46
1:A:1188:VAL:HA	1:A:1200:ASN:O	2.15	0.46
1:B:160:THR:HG21	1:B:209:THR:CG2	2.46	0.46
1:A:111:ASN:ND2	1:A:483:LEU:HD13	2.28	0.46
1:A:128:ASP:CB	1:A:496:ALA:HB2	2.45	0.46
1:A:1002:ASP:CB	1:A:1016:SER:HA	2.45	0.46
1:B:109:LYS:HZ2	1:B:478:GLU:HB2	1.80	0.46
1:B:941:ASN:N	1:B:941:ASN:ND2	2.61	0.46
1:A:299:TYR:O	1:A:302:VAL:HG12	2.15	0.46
1:A:592:THR:O	1:A:622:LYS:HE3	2.15	0.46
1:A:664:ILE:CD1	1:A:811:LEU:HD11	2.46	0.46
1:B:172:MET:HB2	1:B:175:ASN:ND2	2.30	0.46
1:B:677:LYS:HG2	1:B:785:TYR:CZ	2.51	0.46
1:B:999:ARG:HH11	1:B:999:ARG:CB	2.28	0.46
1:B:1185:ASN:HA	1:B:1204:ASN:HD21	1.80	0.46
1:A:1114:THR:HG22	5:A:1272:HOH:O	2.15	0.46
1:A:1189:VAL:HG13	1:A:1200:ASN:HB3	1.97	0.46
1:B:154:GLU:O	1:B:155:PRO:C	2.58	0.46
1:B:286:LEU:HG	1:B:317:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:965:ASP:OD1	1:B:967:ALA:HB3	2.15	0.46
1:A:108:SER:OG	1:A:109:LYS:HD3	2.15	0.46
1:B:20:TYR:HA	1:B:30:TYR:O	2.16	0.46
1:B:522:TYR:O	1:B:526:GLN:HG3	2.16	0.46
1:B:928:ASN:HB3	1:B:930:ILE:HD13	1.97	0.46
1:A:320:ASN:HB3	1:A:323:LYS:CG	2.45	0.46
1:A:413:LYS:HG3	1:A:414:ASN:N	2.31	0.46
1:A:593:VAL:HG11	1:A:596:ILE:HD12	1.98	0.46
1:B:110:ALA:O	1:B:111:ASN:C	2.58	0.46
1:B:236:LYS:HZ1	1:B:241:ILE:HD11	1.81	0.46
1:B:606:ILE:CG1	1:B:704:MET:HE3	2.28	0.46
1:B:1126:LYS:O	1:B:1153:VAL:HG13	2.16	0.46
1:A:797:ILE:HG21	1:A:812:ASN:HD21	1.80	0.46
1:B:32:SER:OG	1:B:42:ILE:HG12	2.15	0.46
1:B:323:LYS:O	1:B:326:ASP:HB2	2.15	0.46
1:B:925:ASN:O	1:B:927:ASP:N	2.49	0.46
1:A:19:LEU:HD12	1:A:19:LEU:C	2.41	0.46
1:A:128:ASP:O	1:A:165:ILE:HD13	2.16	0.46
1:A:1012:ILE:O	1:A:1012:ILE:HG13	2.16	0.46
1:B:581:VAL:HG12	1:B:581:VAL:O	2.16	0.46
1:B:586:GLU:C	1:B:588:ASN:H	2.23	0.46
1:B:1005:LEU:HD12	1:B:1012:ILE:HG22	1.98	0.46
1:B:1074:ASP:HB3	1:B:1076:TRP:H	1.81	0.46
1:B:1150:ILE:HG22	1:B:1162:LEU:HD12	1.97	0.46
1:A:197:ASN:HD21	1:A:346:LYS:NZ	2.14	0.45
1:A:272:TYR:HA	1:A:328:PHE:HZ	1.81	0.45
1:A:1224:TRP:CH2	1:A:1235:SER:HB2	2.52	0.45
1:B:453:GLU:HB2	1:B:649:THR:O	2.16	0.45
1:B:876:GLY:HA3	1:B:895:LEU:O	2.16	0.45
1:B:944:ARG:O	1:B:945:ASP:C	2.58	0.45
1:A:928:ASN:HB3	1:A:930:ILE:HG13	1.98	0.45
1:A:1157:THR:HG22	1:A:1157:THR:O	2.15	0.45
1:B:297:ASN:C	1:B:299:TYR:H	2.24	0.45
1:B:663:VAL:HG23	1:B:804:LEU:HD23	1.97	0.45
1:A:23:PRO:HD2	1:A:26:CYS:SG	2.56	0.45
1:A:320:ASN:HB3	1:A:323:LYS:HG2	1.98	0.45
1:A:448:ILE:N	1:A:448:ILE:HD13	2.31	0.45
1:A:584:THR:O	1:A:588:ASN:HB2	2.16	0.45
1:B:75:GLN:HA	1:B:75:GLN:NE2	2.31	0.45
1:B:396:ILE:HG22	1:B:397:THR:N	2.31	0.45
1:B:537:LEU:HA	1:B:551:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:TYR:HE1	1:B:1148:VAL:HG11	1.80	0.45
1:B:1193:VAL:HG21	1:B:1239:PHE:CE2	2.52	0.45
1:A:438:ALA:HB3	1:A:692:LYS:CG	2.46	0.45
1:A:941:ASN:ND2	1:A:942:CYS:N	2.62	0.45
1:A:1188:VAL:HG21	1:A:1199:MET:HB3	1.98	0.45
1:B:327:ILE:HG22	1:B:331:LEU:HD22	1.98	0.45
1:B:884:ASN:HD22	1:B:886:ASN:H	1.63	0.45
1:B:939:ILE:HG13	1:B:940:ILE:H	1.81	0.45
1:A:1046:TYR:HB3	1:A:1066:GLU:OE1	2.17	0.45
1:A:1116:LEU:O	1:A:1117:LEU:HB2	2.15	0.45
1:B:642:ILE:HD11	1:B:685:ILE:CD1	2.41	0.45
1:B:1121:LEU:HD12	1:B:1249:TRP:CE2	2.52	0.45
1:A:174:SER:O	1:A:223:GLY:HA2	2.16	0.45
1:A:308:GLY:HA3	1:A:323:LYS:HB3	1.99	0.45
1:A:593:VAL:CG2	1:A:602:VAL:CG2	2.94	0.45
1:B:382:VAL:HG23	1:B:382:VAL:O	2.15	0.45
1:B:484:SER:O	1:B:485:ASP:CB	2.64	0.45
1:B:498:ILE:O	1:B:498:ILE:CG1	2.52	0.45
1:B:719:ILE:O	1:B:719:ILE:HG22	2.17	0.45
1:A:1166:THR:HA	1:A:1173:LYS:HD2	1.98	0.45
1:A:293:ASN:HB3	1:A:295:LEU:HD13	1.99	0.45
1:A:729:GLU:O	1:A:730:GLU:HG3	2.16	0.45
1:A:897:GLU:OE1	1:A:1032:LYS:HD3	2.17	0.45
1:B:244:ILE:CG1	1:B:245:ARG:N	2.79	0.45
1:B:986:TYR:HB3	1:B:991:ILE:HD11	1.98	0.45
1:A:164:ASN:ND2	1:A:220:GLY:HA3	2.31	0.45
1:A:528:VAL:HG13	1:A:528:VAL:O	2.16	0.45
1:A:836:LEU:HD12	1:A:837:ILE:CD1	2.46	0.45
1:A:1135:SER:C	1:A:1137:THR:H	2.25	0.45
1:B:395:ILE:HG13	1:B:396:ILE:HG13	1.99	0.45
1:B:449:ASN:O	1:B:451:PRO:HD2	2.17	0.45
1:A:722:LYS:C	1:A:724:ASN:N	2.71	0.45
1:A:749:GLN:O	1:A:753:ILE:HG12	2.17	0.45
1:A:871:ASN:ND2	1:A:873:ASN:OD1	2.49	0.45
1:A:942:CYS:SG	1:A:1029:ILE:HG12	2.57	0.45
1:B:135:LYS:HG2	1:B:141:GLN:HA	1.98	0.45
1:B:541:ILE:HG23	1:B:542:ASP:H	1.81	0.45
1:B:567:VAL:HG11	1:B:572:PHE:HD1	1.82	0.45
1:B:568:GLN:HB3	1:B:569:ALA:H	1.61	0.45
1:B:65:ASP:CG	1:B:66:SER:H	2.25	0.44
1:B:105:GLU:O	1:B:108:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ASN:HB3	1:B:323:LYS:CG	2.47	0.44
1:A:306:LYS:O	1:A:327:ILE:HD12	2.17	0.44
1:A:872:ILE:HG12	1:A:900:ILE:HG12	1.99	0.44
1:B:141:GLN:HB3	1:B:490:LEU:HD11	1.99	0.44
1:B:335:THR:O	1:B:339:LEU:HB2	2.17	0.44
1:B:548:GLN:N	1:B:549:PRO:CD	2.80	0.44
1:B:742:GLN:O	1:B:744:GLU:N	2.50	0.44
1:B:1230:ARG:O	1:B:1231:ASP:CB	2.65	0.44
1:A:109:LYS:HZ3	1:A:479:SER:HB2	1.82	0.44
1:A:888:PHE:CE2	1:A:1044:ILE:HG13	2.52	0.44
1:A:1086:TYR:CE1	1:A:1244:SER:HB3	2.52	0.44
1:B:408:ILE:C	1:B:409:ILE:HD12	2.42	0.44
1:B:913:LYS:CG	1:B:914:ASN:H	2.31	0.44
1:A:1168:THR:HG22	1:A:1169:THR:N	2.31	0.44
1:A:1230:ARG:O	1:A:1231:ASP:CB	2.65	0.44
1:B:62:LYS:HG3	1:B:506:THR:OG1	2.18	0.44
1:B:97:ASN:O	1:B:101:GLY:N	2.42	0.44
1:B:522:TYR:CE1	1:B:611:ASN:HB2	2.53	0.44
1:B:595:LYS:HE3	1:B:626:GLU:OE2	2.16	0.44
1:B:601:ILE:CG2	1:B:760:ARG:HG2	2.47	0.44
1:A:126:ILE:N	1:A:126:ILE:HD12	2.33	0.44
1:A:456:ASP:OD1	1:A:456:ASP:N	2.50	0.44
1:A:1155:SER:C	1:A:1157:THR:H	2.25	0.44
1:B:136:PHE:CE2	1:B:142:ASP:OD2	2.70	0.44
1:B:352:ILE:HD12	1:B:695:THR:CG2	2.47	0.44
1:B:491:THR:HB	1:B:493:GLN:OE1	2.18	0.44
1:B:593:VAL:HB	1:B:599:ILE:O	2.17	0.44
1:B:593:VAL:HG22	1:B:602:VAL:CG2	2.47	0.44
1:B:613:GLY:HA3	1:B:617:GLN:HE21	1.83	0.44
1:A:214:LEU:C	1:A:217:SER:HB2	2.43	0.44
1:A:926:TYR:C	1:A:928:ASN:H	2.25	0.44
1:A:992:PHE:CD2	1:A:1063:TYR:HB2	2.53	0.44
1:A:1143:ARG:HD2	5:A:1279:HOH:O	2.17	0.44
1:B:43:PRO:HB2	1:B:80:LYS:HB3	1.99	0.44
1:B:109:LYS:C	1:B:111:ASN:H	2.25	0.44
1:B:559:PHE:HD1	1:B:582:ASP:HB3	1.83	0.44
1:B:966:ASN:HD22	1:B:1022:ASN:HD22	1.64	0.44
1:B:1005:LEU:C	1:B:1005:LEU:HD13	2.43	0.44
1:B:1233:THR:O	1:B:1234:ASN:C	2.61	0.44
1:A:674:ARG:HD3	1:A:674:ARG:C	2.42	0.44
1:B:359:LYS:HB3	1:B:397:THR:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:HD11	1:A:546:LEU:HD23	1.99	0.44
1:B:579:VAL:C	1:B:581:VAL:H	2.26	0.44
1:B:1188:VAL:CG2	1:B:1199:MET:HB3	2.46	0.44
1:A:595:LYS:HB2	1:A:626:GLU:OE1	2.18	0.44
1:A:709:GLN:HG2	5:A:1257:HOH:O	2.17	0.44
1:A:841:ASN:OD1	1:A:846:ARG:N	2.51	0.44
1:B:826:LYS:NZ	1:B:867:GLY:O	2.49	0.44
1:B:848:LYS:O	1:B:849:SER:C	2.61	0.44
1:B:887:GLN:HG2	1:B:1045:ARG:HD2	2.00	0.44
1:A:914:ASN:HA	1:A:997:ASN:O	2.18	0.43
1:A:920:TRP:HA	1:A:991:ILE:O	2.18	0.43
1:A:329:LYS:NZ	1:A:466:ASN:ND2	2.66	0.43
1:A:448:ILE:HG22	1:A:646:LEU:HD12	2.00	0.43
1:A:472:ILE:C	1:A:474:ASN:H	2.27	0.43
1:A:1087:TYR:HB2	1:A:1243:ILE:HB	1.99	0.43
1:B:454:ILE:HB	1:B:666:ALA:HA	2.00	0.43
1:B:526:GLN:O	1:B:710:ASN:HB3	2.18	0.43
1:B:614:ASN:O	1:B:615:GLU:C	2.61	0.43
1:B:617:GLN:C	1:B:619:GLY:H	2.26	0.43
1:A:81:ASP:OD1	1:A:85:LYS:HE3	2.18	0.43
1:A:217:SER:O	1:A:218:LEU:C	2.60	0.43
1:A:290:GLN:O	1:A:291:VAL:CG2	2.67	0.43
1:B:310:ASP:OD2	1:B:320:ASN:HB2	2.19	0.43
1:B:475:PHE:HD1	1:B:475:PHE:H	1.65	0.43
1:B:849:SER:O	1:B:850:SER:C	2.61	0.43
1:B:890:ILE:O	1:B:1041:TYR:HA	2.17	0.43
1:B:1100:ARG:NH1	1:B:1101:ARG:O	2.51	0.43
1:B:1130:GLN:HG2	1:B:1149:TYR:HB2	2.00	0.43
1:B:1244:SER:O	1:B:1246:GLU:HG3	2.18	0.43
1:A:8:ASN:HB2	1:A:11:ASP:OD2	2.18	0.43
1:A:9:TYR:HB2	1:A:81:ASP:HA	2.00	0.43
1:A:82:ARG:HH12	1:A:189:GLU:CD	2.25	0.43
1:A:365:ASN:HB3	1:A:368:ILE:HG22	1.99	0.43
1:A:492:ILE:HD12	1:A:493:GLN:N	2.32	0.43
1:A:737:LYS:HG2	1:A:741:LYS:HE3	1.99	0.43
1:B:497:TYR:C	1:B:499:PRO:CD	2.91	0.43
1:B:711:GLN:O	1:B:715:ILE:HG12	2.17	0.43
1:B:923:ILE:HD12	1:B:954:LEU:CD1	2.48	0.43
1:A:89:LYS:NZ	1:A:369:TYR:O	2.42	0.43
1:A:253:LEU:HD12	1:A:253:LEU:HA	1.84	0.43
1:B:51:THR:O	1:B:52:PRO:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:HD12	1:B:145:LEU:N	2.33	0.43
1:B:302:VAL:HG13	1:B:303:PHE:N	2.32	0.43
1:B:444:ASN:ND2	1:B:446:ASP:OD1	2.52	0.43
1:B:670:ALA:HB1	1:B:793:LEU:HD21	1.99	0.43
1:B:846:ARG:O	1:B:847:ILE:O	2.36	0.43
1:A:21:ILE:HG12	1:A:134:ILE:HG22	2.00	0.43
1:A:144:LEU:O	1:A:146:PRO:HD3	2.18	0.43
1:A:306:LYS:HD3	1:A:307:TYR:CE1	2.53	0.43
1:A:438:ALA:HB2	1:A:691:THR:HB	2.00	0.43
1:A:571:LEU:HD12	1:A:571:LEU:H	1.83	0.43
1:A:1122:TYR:CE1	1:A:1245:GLU:HA	2.54	0.43
1:B:286:LEU:HD12	1:B:289:VAL:HG21	2.00	0.43
1:A:197:ASN:HD21	1:A:346:LYS:CE	2.32	0.43
1:A:738:TYR:CA	1:A:743:ILE:HD13	2.48	0.43
1:B:193:ARG:NH1	1:B:358:PHE:HZ	2.17	0.43
1:B:551:ILE:HD12	1:B:551:ILE:N	2.34	0.43
1:B:769:TYR:O	1:B:772:LYS:HB3	2.18	0.43
1:B:1102:LYS:C	1:B:1104:SER:H	2.26	0.43
1:A:186:PHE:CE2	1:A:188:PRO:HB3	2.53	0.43
1:A:290:GLN:C	1:A:291:VAL:HG23	2.44	0.43
1:A:311:LYS:HB2	1:A:317:TYR:CE1	2.54	0.43
1:A:565:LYS:HB2	1:A:566:PRO:HD2	2.00	0.43
1:A:661:ASN:HD22	1:A:661:ASN:HA	1.69	0.43
1:A:797:ILE:HG21	1:A:812:ASN:ND2	2.33	0.43
1:A:830:TYR:O	1:A:831:THR:HG22	2.19	0.43
1:A:971:GLN:HE21	1:A:971:GLN:CA	2.31	0.43
1:B:409:ILE:HD13	1:B:431:ASN:HA	2.00	0.43
1:B:527:LYS:HE3	1:B:527:LYS:HB2	1.81	0.43
1:B:743:ILE:C	1:B:745:ASN:N	2.76	0.43
1:B:983:ILE:CG1	1:B:1094:PRO:HB2	2.48	0.43
1:A:82:ARG:NH2	1:A:362:ASN:ND2	2.67	0.43
1:A:121:ASP:HB2	1:A:288:LYS:HE2	2.01	0.43
1:A:214:LEU:CA	1:A:217:SER:HB2	2.48	0.43
1:A:234:THR:HG22	1:A:439:SER:HB3	2.01	0.43
1:A:304:GLU:OE1	1:A:317:TYR:HE1	2.02	0.43
1:A:920:TRP:O	1:A:1044:ILE:HA	2.18	0.43
1:B:493:GLN:C	1:B:493:GLN:CD	2.86	0.43
1:B:576:ILE:HD12	1:B:576:ILE:C	2.44	0.43
1:B:983:ILE:HG12	1:B:1094:PRO:HB2	2.00	0.43
1:A:376:ASN:ND2	1:A:386:GLY:CA	2.81	0.43
1:A:941:ASN:HD22	1:A:941:ASN:C	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1114:THR:OG1	1:A:1117:LEU:N	2.52	0.43
1:B:114:LEU:HD11	1:B:299:TYR:CD2	2.54	0.43
1:B:653:PHE:CE2	1:B:662:LYS:HB3	2.53	0.43
1:B:795:ASN:O	1:B:796:TYR:C	2.61	0.43
1:B:943:MET:C	1:B:1026:SER:HB3	2.44	0.43
1:A:324:PHE:HA	1:A:327:ILE:HG12	1.99	0.42
1:A:772:LYS:O	1:A:776:GLU:HB2	2.18	0.42
1:B:196:ASP:CG	1:B:349:GLN:H	2.25	0.42
1:B:393:PRO:O	1:B:394:ARG:C	2.61	0.42
1:B:528:VAL:O	1:B:528:VAL:HG13	2.19	0.42
1:B:536:ASN:O	1:B:537:LEU:HD12	2.17	0.42
1:B:727:THR:O	1:B:730:GLU:N	2.47	0.42
1:B:1020:LEU:HD12	1:B:1020:LEU:N	2.34	0.42
1:B:1143:ARG:HG3	1:B:1143:ARG:HH11	1.84	0.42
1:A:2:PRO:O	1:A:95:ASN:ND2	2.52	0.42
1:A:263:ILE:O	1:A:846:ARG:NH2	2.51	0.42
1:A:344:GLN:O	1:A:384:PHE:HE1	2.02	0.42
1:A:486:GLU:HB3	1:A:488:LEU:CD2	2.48	0.42
1:A:610:LEU:HD11	1:A:704:MET:CE	2.49	0.42
1:A:845:LYS:HZ2	1:A:848:LYS:HB3	1.83	0.42
1:A:971:GLN:HA	1:A:971:GLN:HE21	1.84	0.42
1:A:1103:ASP:OD1	1:A:1103:ASP:C	2.62	0.42
1:B:5:ASN:N	1:B:5:ASN:ND2	2.67	0.42
1:B:476:ASN:HD21	1:B:480:ALA:HB2	1.84	0.42
1:B:760:ARG:CZ	1:B:830:TYR:HD2	2.33	0.42
1:B:916:SER:CB	1:B:1054:LEU:HG	2.50	0.42
1:B:1004:LYS:HG2	1:B:1014:GLN:HB3	2.00	0.42
1:A:51:THR:O	1:A:52:PRO:C	2.62	0.42
1:A:295:LEU:O	1:A:298:PRO:HD2	2.19	0.42
1:A:557:SER:HA	1:A:560:ILE:HD12	2.01	0.42
1:A:909:ASP:O	1:A:910:ASN:O	2.37	0.42
1:B:76:SER:C	1:B:78:GLU:H	2.27	0.42
1:B:82:ARG:HH12	1:B:189:GLU:HG2	1.83	0.42
1:B:797:ILE:HG21	1:B:812:ASN:HD21	1.84	0.42
1:B:1157:THR:HG22	1:B:1158:HIS:N	2.34	0.42
1:B:1193:VAL:CG2	1:B:1239:PHE:HE2	2.32	0.42
1:A:234:THR:HG22	1:A:439:SER:CB	2.50	0.42
1:A:270:ASP:O	1:A:274:ASN:HB2	2.18	0.42
1:A:937:TYR:HB2	1:A:1034:VAL:O	2.19	0.42
1:A:1099:ASP:OD1	1:A:1100:ARG:N	2.52	0.42
1:B:606:ILE:HG23	1:B:704:MET:CE	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:855:MET:O	1:B:856:ARG:HD3	2.19	0.42
1:B:928:ASN:C	1:B:930:ILE:N	2.68	0.42
1:B:1087:TYR:HB2	1:B:1243:ILE:HB	2.01	0.42
1:A:68:TYR:HD2	1:A:157:LEU:HD22	1.83	0.42
1:A:76:SER:OG	1:A:79:GLU:HG3	2.18	0.42
1:A:164:ASN:HB3	1:A:180:SER:HB3	2.02	0.42
1:A:436:PHE:CD2	1:A:695:THR:HG21	2.55	0.42
1:A:452:LYS:H	1:A:452:LYS:HG3	1.65	0.42
1:A:672:LYS:HD2	1:A:672:LYS:HA	1.62	0.42
1:A:910:ASN:HA	1:A:1022:ASN:OD1	2.19	0.42
1:B:76:SER:HB3	1:B:79:GLU:OE2	2.19	0.42
1:B:111:ASN:HA	1:B:112:PRO:HD3	1.89	0.42
1:B:116:ASN:ND2	1:B:118:ASN:N	2.65	0.42
1:B:129:ALA:HB2	1:B:167:LEU:HD21	2.01	0.42
1:B:678:TRP:CE3	1:B:782:LEU:HD13	2.55	0.42
1:B:941:ASN:HD22	1:B:941:ASN:H	1.67	0.42
1:A:45:ARG:HD3	1:A:74:LEU:HB2	2.00	0.42
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.88	0.42
1:A:595:LYS:CB	1:A:626:GLU:HB2	2.48	0.42
1:A:708:LEU:HD23	1:A:708:LEU:HA	1.83	0.42
1:A:944:ARG:HD3	1:A:944:ARG:HA	1.70	0.42
1:B:413:LYS:HE3	1:B:515:ASN:O	2.20	0.42
1:A:379:ASN:H	1:A:379:ASN:ND2	2.09	0.42
1:A:632:ILE:HG23	1:A:633:LEU:HD13	2.02	0.42
1:B:27:GLN:N	1:B:27:GLN:CD	2.78	0.42
1:B:324:PHE:C	1:B:326:ASP:N	2.73	0.42
1:B:598:ASP:OD1	1:B:768:SER:HA	2.19	0.42
1:B:643:PRO:C	1:B:781:LYS:HZ3	2.27	0.42
1:B:1189:VAL:HG22	1:B:1200:ASN:HB3	2.01	0.42
1:A:70:ASP:OD1	1:A:70:ASP:C	2.62	0.42
1:A:234:THR:HG22	1:A:439:SER:OG	2.18	0.42
1:A:541:ILE:HG23	1:A:542:ASP:N	2.35	0.42
1:A:737:LYS:HG2	1:A:741:LYS:HG2	2.02	0.42
1:B:154:GLU:CB	1:B:155:PRO:CD	2.98	0.42
1:B:532:GLU:OE1	1:B:532:GLU:HA	2.20	0.42
1:B:715:ILE:O	1:B:716:LYS:C	2.63	0.42
1:B:1132:VAL:HG23	1:B:1148:VAL:CA	2.49	0.42
1:A:321:ILE:HD13	1:A:321:ILE:HA	1.84	0.42
1:A:567:VAL:HB	1:A:726:TYR:OH	2.19	0.42
1:B:661:ASN:HD22	1:B:661:ASN:HA	1.65	0.42
1:B:674:ARG:HD3	1:B:674:ARG:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:ARG:NH1	1:B:999:ARG:CB	2.82	0.42
1:A:293:ASN:C	1:A:295:LEU:N	2.78	0.42
1:A:837:ILE:HB	1:A:838:SER:H	1.76	0.42
1:A:847:ILE:N	1:A:847:ILE:CD1	2.81	0.42
1:A:1065:ASN:N	1:A:1065:ASN:HD22	2.17	0.42
1:B:111:ASN:ND2	1:B:483:LEU:HD12	2.29	0.42
1:B:1076:TRP:CZ3	1:B:1244:SER:O	2.72	0.42
1:B:1228:HIS:HB3	1:B:1233:THR:OG1	2.20	0.42
1:A:14:ASN:ND2	1:A:16:ARG:NH1	2.68	0.41
1:A:270:ASP:HA	1:A:273:THR:CG2	2.50	0.41
1:A:453:GLU:CG	1:A:454:ILE:HD13	2.49	0.41
1:A:529:PRO:O	1:A:530:GLU:C	2.62	0.41
1:A:1067:PRO:O	1:A:1068:ASN:C	2.62	0.41
1:A:32:SER:C	1:A:33:PHE:CD2	2.98	0.41
1:A:944:ARG:O	1:A:946:ASN:N	2.53	0.41
1:B:76:SER:C	1:B:78:GLU:N	2.77	0.41
1:B:93:ARG:HG3	1:B:93:ARG:NH1	2.25	0.41
1:B:379:ASN:C	1:B:381:LYS:H	2.28	0.41
1:B:476:ASN:OD1	1:B:480:ALA:HB2	2.20	0.41
1:B:657:SER:O	1:B:658:ASP:HB3	2.21	0.41
1:B:836:LEU:N	1:B:836:LEU:CD1	2.83	0.41
1:A:29:PHE:CD2	1:A:135:LYS:HE2	2.55	0.41
1:A:141:GLN:HE21	1:A:490:LEU:CD2	2.30	0.41
1:A:377:ILE:O	1:A:378:ASN:HB2	2.20	0.41
1:A:975:PHE:CE2	1:A:1007:ILE:HG21	2.56	0.41
1:B:35:ILE:HG23	1:B:36:MET:N	2.35	0.41
1:B:36:MET:HE2	1:B:39:ILE:HD12	2.01	0.41
1:B:91:PHE:HZ	1:B:150:ILE:HD11	1.85	0.41
1:B:453:GLU:HG2	1:B:650:ILE:HG12	2.02	0.41
1:B:617:GLN:C	1:B:619:GLY:N	2.77	0.41
1:B:639:GLU:O	1:B:640:LEU:HD23	2.21	0.41
1:B:720:GLU:HG2	1:B:738:TYR:OH	2.20	0.41
1:B:842:LYS:HE3	1:B:843:PHE:CZ	2.55	0.41
1:B:893:ASP:OD2	1:B:894:LYS:HG3	2.20	0.41
1:B:1136:SER:O	1:B:1137:THR:HB	2.20	0.41
1:A:72:ASN:O	1:A:75:GLN:HG2	2.20	0.41
1:A:193:ARG:HH11	1:A:193:ARG:CG	2.33	0.41
1:A:790:LYS:HB2	1:A:819:LEU:HD23	2.02	0.41
1:B:107:LEU:HD11	1:B:214:LEU:HB3	2.01	0.41
1:B:208:LEU:HG	1:B:336:GLU:HG3	2.03	0.41
1:B:286:LEU:HA	1:B:289:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:ASN:N	1:B:383:ASN:ND2	2.69	0.41
1:B:730:GLU:O	1:B:733:GLU:HG2	2.20	0.41
1:B:830:TYR:O	1:B:832:ASP:N	2.54	0.41
1:B:944:ARG:HD3	1:B:944:ARG:C	2.40	0.41
1:A:275:LEU:HB3	1:A:324:PHE:HZ	1.84	0.41
1:A:591:SER:O	1:A:601:ILE:HA	2.21	0.41
1:A:924:PRO:HB3	1:A:988:ASN:OD1	2.21	0.41
1:B:303:PHE:O	1:B:304:GLU:C	2.63	0.41
1:B:320:ASN:OD1	1:B:322:ASN:HB2	2.19	0.41
1:B:853:LEU:HD12	1:B:854:ASN:H	1.86	0.41
1:B:1166:THR:HG22	1:B:1209:ILE:HD12	2.03	0.41
1:A:57:PRO:HA	1:A:58:PRO:HD2	1.93	0.41
1:A:297:ASN:C	1:A:299:TYR:H	2.29	0.41
1:A:482:GLY:C	1:A:483:LEU:HG	2.45	0.41
1:B:200:ASN:ND2	1:B:388:ASN:ND2	2.69	0.41
1:B:362:ASN:HD22	1:B:365:ASN:HB2	1.84	0.41
1:B:413:LYS:HG2	1:B:517:LEU:CD2	2.50	0.41
1:B:557:SER:HA	1:B:560:ILE:HD12	2.01	0.41
1:B:788:ASN:HD22	1:B:788:ASN:HA	1.66	0.41
1:B:987:ILE:C	1:B:989:LYS:H	2.27	0.41
1:B:1067:PRO:O	1:B:1073:LYS:HE2	2.21	0.41
1:A:34:ASN:HB2	1:A:40:TRP:CZ2	2.56	0.41
1:A:454:ILE:HD12	1:A:669:ASN:HB2	2.03	0.41
1:A:915:PHE:O	1:A:997:ASN:HB2	2.20	0.41
1:A:1200:ASN:ND2	1:A:1202:LYS:HD2	2.35	0.41
1:B:370:ASN:ND2	1:B:377:ILE:CG2	2.83	0.41
1:B:701:LYS:HG3	1:B:762:LEU:HD12	2.02	0.41
1:A:11:ASP:HA	1:A:12:PRO:HD3	1.84	0.41
1:B:61:LEU:HD13	1:B:405:VAL:CG1	2.51	0.41
1:B:835:ILE:C	1:B:836:LEU:HD12	2.46	0.41
1:A:344:GLN:C	1:A:384:PHE:HE1	2.29	0.41
1:A:440:GLU:OE1	1:A:440:GLU:HA	2.20	0.41
1:A:578:GLN:O	1:A:582:ASP:HB2	2.21	0.41
1:A:1108:ILE:HG22	1:A:1217:ASP:HA	2.02	0.41
1:B:440:GLU:C	1:B:442:SER:H	2.29	0.41
1:B:453:GLU:OE1	1:B:453:GLU:CA	2.57	0.41
1:B:562:ASN:N	1:B:562:ASN:ND2	2.69	0.41
1:B:572:PHE:C	1:B:574:SER:N	2.78	0.41
1:B:713:ASN:C	1:B:715:ILE:N	2.76	0.41
1:B:1090:ASN:HB2	1:B:1240:TRP:CZ3	2.56	0.41
1:A:193:ARG:O	1:A:355:TYR:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLN:O	1:A:344:GLN:HG2	2.21	0.41
1:A:712:VAL:HG22	1:A:747:LEU:HB3	2.02	0.41
1:A:1058:GLU:HA	1:A:1061:THR:CG2	2.51	0.41
1:B:425:ILE:CD1	1:B:545:LEU:HD13	2.51	0.41
1:B:999:ARG:NH2	1:B:1023:ILE:HD11	2.36	0.41
1:A:193:ARG:HH11	1:A:193:ARG:HB3	1.86	0.40
1:A:348:ARG:HG2	5:A:1274:HOH:O	2.21	0.40
1:A:568:GLN:O	1:A:569:ALA:C	2.64	0.40
1:A:658:ASP:C	1:A:660:LYS:N	2.79	0.40
1:A:737:LYS:CB	1:A:741:LYS:HG2	2.50	0.40
1:A:1163:TYR:CD2	1:A:1178:SER:HB2	2.56	0.40
1:B:59:THR:HB	1:B:507:SER:HA	2.02	0.40
1:B:203:ILE:HD11	1:B:389:ALA:HA	2.04	0.40
1:B:716:LYS:HB2	1:B:744:GLU:OE2	2.20	0.40
1:B:994:THR:HB	1:B:1006:TYR:HB2	2.03	0.40
1:B:1050:PHE:CE2	1:B:1054:LEU:HD11	2.56	0.40
1:A:143:ILE:O	1:A:487:LYS:O	2.39	0.40
1:A:211:MET:HE1	1:A:343:PHE:CE2	2.57	0.40
1:A:342:LYS:HA	1:A:342:LYS:CE	2.49	0.40
1:A:448:ILE:HG22	1:A:646:LEU:CB	2.51	0.40
1:A:1000:LEU:HD12	1:A:1000:LEU:HA	1.87	0.40
1:A:1071:ILE:HD13	1:A:1141:LEU:HD13	2.03	0.40
1:B:157:LEU:HD23	1:B:190:TYR:CE1	2.55	0.40
1:B:700:ARG:HD3	1:B:703:GLN:HE22	1.86	0.40
1:B:1034:VAL:O	1:B:1035:ASN:HB2	2.21	0.40
1:A:196:ASP:CG	1:A:349:GLN:H	2.29	0.40
1:A:410:ARG:CB	1:A:511:GLN:HG3	2.46	0.40
1:A:453:GLU:HG2	1:A:454:ILE:CD1	2.51	0.40
1:A:827:LEU:HD12	1:A:828:SER:H	1.85	0.40
1:A:943:MET:HE2	1:A:951:LYS:HD3	2.03	0.40
1:B:149:ILE:HB	1:B:183:ILE:HD13	2.03	0.40
1:B:409:ILE:CD1	1:B:431:ASN:HA	2.51	0.40
1:B:535:VAL:HG11	1:B:717:THR:HG21	2.04	0.40
1:B:576:ILE:C	1:B:579:VAL:HG22	2.46	0.40
1:B:751:VAL:C	1:B:753:ILE:N	2.79	0.40
1:B:884:ASN:ND2	1:B:886:ASN:H	2.19	0.40
1:B:1150:ILE:O	1:B:1162:LEU:HB2	2.20	0.40
1:A:8:ASN:O	1:A:9:TYR:C	2.64	0.40
1:A:93:ARG:HG3	1:A:93:ARG:NH1	2.36	0.40
1:A:177:GLY:O	1:A:178:PHE:C	2.63	0.40
1:A:671:LEU:HD23	1:A:671:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:737:LYS:O	1:A:739:ASP:N	2.54	0.40
1:A:819:LEU:HD12	1:A:819:LEU:HA	1.93	0.40
1:A:941:ASN:ND2	1:A:941:ASN:C	2.79	0.40
1:B:346:LYS:HA	1:B:346:LYS:CE	2.48	0.40
1:B:802:SER:C	1:B:803:ILE:HG13	2.47	0.40
1:B:966:ASN:CB	1:B:1022:ASN:ND2	2.84	0.40
1:A:97:ASN:O	1:A:101:GLY:N	2.51	0.40
1:B:635:GLU:H	1:B:696:GLN:NE2	2.19	0.40
1:B:715:ILE:O	1:B:718:ILE:N	2.54	0.40
1:B:741:LYS:O	1:B:742:GLN:HG3	2.22	0.40
1:B:750:LYS:O	1:B:753:ILE:HB	2.21	0.40
1:B:910:ASN:C	1:B:912:TYR:N	2.77	0.40

There are no symmetry-related clashes.

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	1242/1252 (99%)	1056 (85%)	128 (10%)	58 (5%)	2	2
1	B	1232/1252 (98%)	1003 (81%)	171 (14%)	58 (5%)	2	2
All	All	2474/2504 (99%)	2059 (83%)	299 (12%)	116 (5%)	2	2

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ALA
1	A	198	CYS
1	A	290	GLN
1	A	418	VAL
1	A	419	LYS
1	A	485	ASP

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Mol	Chain	Res	Type
1	A	488	LEU
1	A	489	ASN
1	A	740	ILE
1	A	805	GLY
1	A	834	LYS
1	A	837	ILE
1	A	847	ILE
1	A	848	LYS
1	A	849	SER
1	A	910	ASN
1	A	914	ASN
1	A	927	ASP
1	A	928	ASN
1	A	945	ASP
1	A	980	ALA
1	A	1193	VAL
1	A	1195	ASN
1	A	1250	GLN
1	B	136	PHE
1	B	153	ALA
1	B	297	ASN
1	B	467	ASP
1	B	479	SER
1	B	485	ASP
1	B	497	TYR
1	B	728	LEU
1	B	743	ILE
1	B	831	THR
1	B	837	ILE
1	B	838	SER
1	B	847	ILE
1	B	848	LYS
1	B	849	SER
1	B	913	LYS
1	B	914	ASN
1	B	945	ASP
1	B	980	ALA
1	B	1144	LYS
1	B	1195	ASN
1	A	137	SER
1	A	297	ASN
1	A	417	SER

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Mol	Chain	Res	Type
1	A	456	ASP
1	A	569	ALA
1	A	658	ASP
1	A	738	TYR
1	A	1062	LEU
1	A	1068	ASN
1	A	1144	LYS
1	A	1231	ASP
1	A	1232	HIS
1	B	198	CYS
1	B	394	ARG
1	B	448	ILE
1	B	454	ILE
1	B	455	ASP
1	B	473	LEU
1	B	490	LEU
1	B	739	ASP
1	B	911	LYS
1	B	927	ASP
1	B	1016	SER
1	B	1231	ASP
1	B	1234	ASN
1	A	110	ALA
1	A	451	PRO
1	A	479	SER
1	A	723	TYR
1	A	730	GLU
1	A	839	TYR
1	B	98	LEU
1	B	486	GLU
1	B	656	SER
1	B	850	SER
1	B	884	ASN
1	B	1216	ALA
1	A	177	GLY
1	A	362	ASN
1	A	454	ILE
1	A	483	LEU
1	A	743	ILE
1	A	884	ASN
1	A	1194	GLY
1	B	15	ASP

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Mol	Chain	Res	Type
1	B	110	ALA
1	B	366	ASP
1	B	453	GLU
1	B	483	LEU
1	B	725	SER
1	B	910	ASN
1	B	1056	GLU
1	A	122	ASN
1	A	497	TYR
1	A	736	ASN
1	A	894	LYS
1	A	1021	GLY
1	A	1056	GLU
1	B	496	ALA
1	B	563	VAL
1	B	803	ILE
1	B	941	ASN
1	B	1068	ASN
1	A	118	ASN
1	A	737	LYS
1	B	658	ASP
1	B	1205	ASN
1	B	968	GLY
1	A	154	GLU
1	B	480	ALA
1	B	481	PRO

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	1146/1153 (99%)	1057 (92%)	89 (8%)	11	20
1	B	1139/1153 (99%)	1045 (92%)	94 (8%)	10	18
All	All	2285/2306 (99%)	2102 (92%)	183 (8%)	11	19

All (183) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	33	PHE
1	A	37	LYS
1	A	61	LEU
1	A	65	ASP
1	A	78	GLU
1	A	98	LEU
1	A	107	LEU
1	A	109	LYS
1	A	118	ASN
1	A	166	SER
1	A	193	ARG
1	A	199	MET
1	A	217	SER
1	A	232	THR
1	A	234	THR
1	A	273	THR
1	A	275	LEU
1	A	328	PHE
1	A	331	LEU
1	A	368	ILE
1	A	379	ASN
1	A	406	LYS
1	A	433	GLU
1	A	448	ILE
1	A	452	LYS
1	A	453	GLU
1	A	454	ILE
1	A	456	ASP
1	A	472	ILE
1	A	486	GLU
1	A	494	ASN
1	A	538	THR
1	A	558	GLU
1	A	568	GLN
1	A	578	GLN
1	A	580	LEU
1	A	602	VAL
1	A	627	LEU
1	A	633	LEU
1	A	639	GLU
1	A	661	ASN
1	A	676	GLU

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Mol	Chain	Res	Type
1	A	735	THR
1	A	759	ASP
1	A	794	LEU
1	A	809	GLN
1	A	819	LEU
1	A	836	LEU
1	A	837	ILE
1	A	839	TYR
1	A	845	LYS
1	A	847	ILE
1	A	852	VAL
1	A	861	LYS
1	A	895	LEU
1	A	911	LYS
1	A	912	TYR
1	A	914	ASN
1	A	917	ILE
1	A	931	VAL
1	A	938	THR
1	A	947	ASN
1	A	962	THR
1	A	973	LEU
1	A	996	THR
1	A	1000	LEU
1	A	1005	LEU
1	A	1019	ASN
1	A	1030	LEU
1	A	1039	THR
1	A	1044	ILE
1	A	1053	GLU
1	A	1061	THR
1	A	1114	THR
1	A	1115	ILE
1	A	1128	LYS
1	A	1138	ASN
1	A	1153	VAL
1	A	1185	ASN
1	A	1189	VAL
1	A	1193	VAL
1	A	1211	LEU
1	A	1215	LYS
1	A	1218	THR

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Mol	Chain	Res	Type
1	A	1229	MET
1	A	1230	ARG
1	A	1232	HIS
1	A	1234	ASN
1	B	14	ASN
1	B	19	LEU
1	B	37	LYS
1	B	53	GLN
1	B	98	LEU
1	B	99	SER
1	B	106	GLU
1	B	111	ASN
1	B	116	ASN
1	B	133	GLU
1	B	155	PRO
1	B	199	MET
1	B	232	THR
1	B	234	THR
1	B	244	ILE
1	B	270	ASP
1	B	296	LEU
1	B	322	ASN
1	B	326	ASP
1	B	328	PHE
1	B	331	LEU
1	B	339	LEU
1	B	341	THR
1	B	346	LYS
1	B	349	GLN
1	B	373	GLU
1	B	399	ILE
1	B	402	ARG
1	B	423	LYS
1	B	429	ILE
1	B	442	SER
1	B	450	THR
1	B	453	GLU
1	B	455	ASP
1	B	458	VAL
1	B	466	ASN
1	B	478	GLU
1	B	483	LEU

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Mol	Chain	Res	Type
1	B	493	GLN
1	B	503	SER
1	B	506	THR
1	B	508	ASP
1	B	517	LEU
1	B	530	GLU
1	B	547	GLU
1	B	558	GLU
1	B	568	GLN
1	B	582	ASP
1	B	595	LYS
1	B	676	GLU
1	B	702	GLU
1	B	736	ASN
1	B	740	ILE
1	B	745	ASN
1	B	794	LEU
1	B	804	LEU
1	B	809	GLN
1	B	820	ASN
1	B	837	ILE
1	B	838	SER
1	B	840	PHE
1	B	852	VAL
1	B	860	ASP
1	B	903	ASN
1	B	906	ILE
1	B	911	LYS
1	B	912	TYR
1	B	913	LYS
1	B	914	ASN
1	B	923	ILE
1	B	941	ASN
1	B	944	ARG
1	B	965	ASP
1	B	973	LEU
1	B	983	ILE
1	B	996	THR
1	B	1012	ILE
1	B	1044	ILE
1	B	1099	ASP
1	B	1111	ILE

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Mol	Chain	Res	Type
1	B	1113	SER
1	B	1115	ILE
1	B	1116	LEU
1	B	1131	ARG
1	B	1133	ASN
1	B	1138	ASN
1	B	1141	LEU
1	B	1144	LYS
1	B	1153	VAL
1	B	1168	THR
1	B	1170	ASN
1	B	1188	VAL
1	B	1233	THR
1	B	1252	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	53	GLN
1	A	72	ASN
1	A	95	ASN
1	A	111	ASN
1	A	118	ASN
1	A	141	GLN
1	A	164	ASN
1	A	169	ASN
1	A	176	HIS
1	A	197	ASN
1	A	325	ASN
1	A	344	GLN
1	A	354	GLN
1	A	362	ASN
1	A	376	ASN
1	A	378	ASN
1	A	379	ASN
1	A	383	ASN
1	A	466	ASN
1	A	470	GLN
1	A	494	ASN
1	A	512	HIS
1	A	526	GLN

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Mol	Chain	Res	Type
1	A	533	ASN
1	A	548	GLN
1	A	561	ASN
1	A	562	ASN
1	A	617	GLN
1	A	620	ASN
1	A	661	ASN
1	A	668	ASN
1	A	696	GLN
1	A	698	ASN
1	A	703	GLN
1	A	706	GLN
1	A	709	GLN
1	A	732	ASN
1	A	748	ASN
1	A	749	GLN
1	A	812	ASN
1	A	820	ASN
1	A	821	ASN
1	A	854	ASN
1	A	871	ASN
1	A	886	ASN
1	A	903	ASN
1	A	914	ASN
1	A	925	ASN
1	A	932	ASN
1	A	941	ASN
1	A	956	HIS
1	A	957	ASN
1	A	964	GLN
1	A	971	GLN
1	A	997	ASN
1	A	1019	ASN
1	A	1035	ASN
1	A	1048	ASN
1	A	1060	GLN
1	A	1065	ASN
1	A	1068	ASN
1	A	1109	ASN
1	A	1138	ASN
1	A	1147	GLN
1	A	1158	HIS

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Mol	Chain	Res	Type
1	A	1195	ASN
1	A	1196	ASN
1	A	1241	ASN
1	A	1250	GLN
1	B	5	ASN
1	B	27	GLN
1	B	46	ASN
1	B	75	GLN
1	B	111	ASN
1	B	116	ASN
1	B	125	HIS
1	B	175	ASN
1	B	197	ASN
1	B	200	ASN
1	B	290	GLN
1	B	293	ASN
1	B	349	GLN
1	B	370	ASN
1	B	378	ASN
1	B	383	ASN
1	B	444	ASN
1	B	470	GLN
1	B	512	HIS
1	B	536	ASN
1	B	561	ASN
1	B	562	ASN
1	B	568	GLN
1	B	617	GLN
1	B	620	ASN
1	B	661	ASN
1	B	668	ASN
1	B	696	GLN
1	B	698	ASN
1	B	703	GLN
1	B	706	GLN
1	B	709	GLN
1	B	748	ASN
1	B	788	ASN
1	B	799	GLN
1	B	812	ASN
1	B	821	ASN
1	B	854	ASN

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Mol	Chain	Res	Type
1	B	884	ASN
1	B	886	ASN
1	B	903	ASN
1	B	910	ASN
1	B	925	ASN
1	B	941	ASN
1	B	947	ASN
1	B	957	ASN
1	B	964	GLN
1	B	966	ASN
1	B	981	ASN
1	B	997	ASN
1	B	1022	ASN
1	B	1048	ASN
1	B	1065	ASN
1	B	1070	ASN
1	B	1096	ASN
1	B	1110	ASN
1	B	1130	GLN
1	B	1138	ASN
1	B	1170	ASN
1	B	1185	ASN
1	B	1196	ASN
1	B	1204	ASN
1	B	1241	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 5 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	$\# Z > 2$
4	ACT	B	1303	-	3,3,3	1.01	0	3,3,3	0.85	0
4	ACT	A	1303	-	3,3,3	0.98	0	3,3,3	0.78	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1246/1252 (99%)	0.39	100 (8%) 18 14	12, 45, 86, 109	0
1	B	1238/1252 (98%)	0.78	132 (10%) 11 9	24, 62, 96, 109	0
All	All	2484/2504 (99%)	0.58	232 (9%) 14 11	12, 53, 93, 109	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	453	GLU	6.9
1	A	498	ILE	5.8
1	A	492	ILE	5.6
1	A	567	VAL	5.6
1	B	912	TYR	5.6
1	B	1138	ASN	5.5
1	B	498	ILE	5.4
1	A	477	SER	5.3
1	B	492	ILE	5.1
1	A	837	ILE	5.0
1	B	831	THR	4.9
1	B	480	ALA	4.8
1	A	328	PHE	4.8
1	B	655	GLY	4.8
1	B	479	SER	4.7
1	B	740	ILE	4.7
1	B	654	LEU	4.6
1	A	738	TYR	4.5
1	B	328	PHE	4.5
1	A	476	ASN	4.5
1	B	567	VAL	4.4
1	A	451	PRO	4.4
1	A	198	CYS	4.3
1	A	654	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	490	LEU	4.3
1	A	740	ILE	4.3
1	B	847	ILE	4.2
1	B	569	ALA	4.2
1	B	475	PHE	4.2
1	A	483	LEU	4.1
1	A	418	VAL	4.1
1	A	310	ASP	4.1
1	B	476	ASN	4.1
1	B	477	SER	4.1
1	A	1233	THR	4.1
1	B	969	ILE	4.0
1	B	458	VAL	4.0
1	A	479	SER	3.9
1	B	1020	LEU	3.9
1	A	847	ILE	3.8
1	B	453	GLU	3.8
1	A	478	GLU	3.7
1	B	743	ILE	3.7
1	B	1137	THR	3.7
1	A	835	ILE	3.7
1	A	912	TYR	3.7
1	B	451	PRO	3.7
1	A	656	SER	3.6
1	A	119	THR	3.6
1	A	475	PHE	3.6
1	B	719	ILE	3.6
1	A	482	GLY	3.6
1	A	199	MET	3.6
1	B	448	ILE	3.6
1	A	930	ILE	3.5
1	A	655	GLY	3.5
1	B	1076	TRP	3.5
1	A	196	ASP	3.5
1	A	927	ASP	3.5
1	A	459	THR	3.5
1	B	570	ALA	3.5
1	B	573	VAL	3.5
1	B	735	THR	3.5
1	A	1232	HIS	3.5
1	B	656	SER	3.4
1	B	491	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	658	ASP	3.4
1	B	834	LYS	3.4
1	B	399	ILE	3.4
1	B	837	ILE	3.4
1	A	289	VAL	3.4
1	B	291	VAL	3.4
1	B	602	VAL	3.4
1	B	738	TYR	3.4
1	B	380	LEU	3.4
1	A	491	THR	3.3
1	B	734	LEU	3.3
1	B	1133	ASN	3.3
1	A	743	ILE	3.3
1	A	480	ALA	3.3
1	B	930	ILE	3.3
1	A	454	ILE	3.2
1	A	481	PRO	3.2
1	B	126	ILE	3.2
1	B	736	ASN	3.2
1	A	460	SER	3.1
1	B	653	PHE	3.1
1	B	571	LEU	3.1
1	B	576	ILE	3.1
1	A	734	LEU	3.1
1	B	478	GLU	3.1
1	A	458	VAL	3.1
1	B	833	ASP	3.0
1	B	6	SER	3.0
1	B	456	ASP	3.0
1	B	929	LYS	3.0
1	A	308	GLY	3.0
1	B	572	PHE	3.0
1	A	1230	ARG	3.0
1	B	1194	GLY	2.9
1	A	735	THR	2.9
1	A	1250	GLN	2.9
1	B	1236	ASN	2.9
1	B	926	TYR	2.9
1	B	295	LEU	2.9
1	B	728	LEU	2.9
1	A	298	PRO	2.9
1	B	1230	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	833	ASP	2.9
1	B	454	ILE	2.9
1	A	836	LEU	2.9
1	B	657	SER	2.8
1	B	658	ASP	2.8
1	B	13	VAL	2.8
1	B	575	TRP	2.8
1	B	836	LEU	2.8
1	B	481	PRO	2.8
1	A	570	ALA	2.8
1	A	197	ASN	2.7
1	B	488	LEU	2.7
1	B	459	THR	2.7
1	B	927	ASP	2.7
1	A	980	ALA	2.7
1	B	300	LYS	2.7
1	B	913	LYS	2.7
1	B	35	ILE	2.7
1	B	143	ILE	2.7
1	A	913	LYS	2.7
1	A	742	GLN	2.7
1	B	296	LEU	2.7
1	B	1018	LEU	2.7
1	B	460	SER	2.7
1	A	1012	ILE	2.6
1	B	663	VAL	2.6
1	B	1193	VAL	2.6
1	A	448	ILE	2.6
1	B	744	GLU	2.6
1	A	657	SER	2.6
1	A	316	ILE	2.6
1	B	364	LEU	2.6
1	A	245	ARG	2.6
1	B	198	CYS	2.6
1	A	319	VAL	2.6
1	B	10	ASN	2.6
1	B	832	ASP	2.5
1	B	299	TYR	2.5
1	A	566	PRO	2.5
1	A	493	GLN	2.5
1	A	300	LYS	2.5
1	B	723	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	830	TYR	2.5
1	A	318	SER	2.5
1	A	1235	SER	2.5
1	B	298	PRO	2.5
1	B	130	SER	2.4
1	B	37	LYS	2.4
1	A	286	LEU	2.4
1	A	659	ASN	2.4
1	B	455	ASP	2.4
1	A	115	GLY	2.4
1	B	559	PHE	2.4
1	B	490	LEU	2.4
1	B	196	ASP	2.4
1	B	497	TYR	2.4
1	A	739	ASP	2.4
1	B	487	LYS	2.4
1	A	167	LEU	2.3
1	A	450	THR	2.3
1	A	946	ASN	2.3
1	B	15	ASP	2.3
1	A	1076	TRP	2.3
1	B	354	GLN	2.3
1	B	401	GLY	2.3
1	A	831	THR	2.3
1	B	910	ASN	2.3
1	A	452	LYS	2.3
1	B	1055	ASP	2.3
1	B	290	GLN	2.3
1	B	528	VAL	2.3
1	A	660	LYS	2.3
1	A	809	GLN	2.3
1	A	399	ILE	2.3
1	B	606	ILE	2.3
1	A	457	THR	2.3
1	B	136	PHE	2.3
1	B	316	ILE	2.2
1	A	929	LYS	2.2
1	B	533	ASN	2.2
1	B	1231	ASP	2.2
1	B	1025	VAL	2.2
1	B	33	PHE	2.2
1	B	129	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	583	PHE	2.2
1	B	718	ILE	2.2
1	B	1023	ILE	2.2
1	B	659	ASN	2.2
1	A	456	ASP	2.2
1	B	895	LEU	2.2
1	A	494	ASN	2.2
1	B	31	LYS	2.2
1	A	114	LEU	2.2
1	B	949	GLY	2.2
1	B	408	ILE	2.2
1	A	419	LYS	2.1
1	B	941	ASN	2.1
1	A	804	LEU	2.1
1	B	144	LEU	2.1
1	A	1231	ASP	2.1
1	B	835	ILE	2.1
1	A	727	THR	2.1
1	A	651	LYS	2.1
1	B	3	LYS	2.1
1	B	146	PRO	2.1
1	A	910	ASN	2.1
1	B	494	ASN	2.1
1	B	1000	LEU	2.1
1	B	1139	ASP	2.1
1	A	569	ALA	2.1
1	A	575	TRP	2.1
1	A	578	GLN	2.1
1	A	1194	GLY	2.1
1	B	715	ILE	2.1
1	A	653	PHE	2.1
1	A	291	VAL	2.1
1	B	289	VAL	2.1
1	A	166	SER	2.0
1	B	450	THR	2.0
1	A	290	GLN	2.0
1	B	799	GLN	2.0
1	A	1234	ASN	2.0
1	B	370	ASN	2.0
1	B	906	ILE	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($\text{\AA}^2$)	Q<0.9
4	ACT	B	1303	4/4	0.57	0.24	65,65,66,66	0
4	ACT	A	1303	4/4	0.71	0.24	70,70,71,71	0
3	NA	A	1301	1/1	0.88	0.07	62,62,62,62	0
3	NA	A	1302	1/1	0.96	0.04	38,38,38,38	0
3	NA	B	1302	1/1	0.98	0.04	55,55,55,55	0
2	ZN	B	1300	1/1	0.99	0.06	47,47,47,47	0
2	ZN	A	1300	1/1	1.00	0.01	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.