



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:10 AM UTC

PDB ID : 3EGX / pdb_00003egx
Title : Crystal structure of the mammalian COPII-coat protein Sec23a/24a complexed with the SNARE protein Sec22b and bound to the transport signal sequence of the SNARE protein Bet1
Authors : Goldberg, J.; Mancias, J.D.
Deposited on : 2008-09-11
Resolution : 3.30 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
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

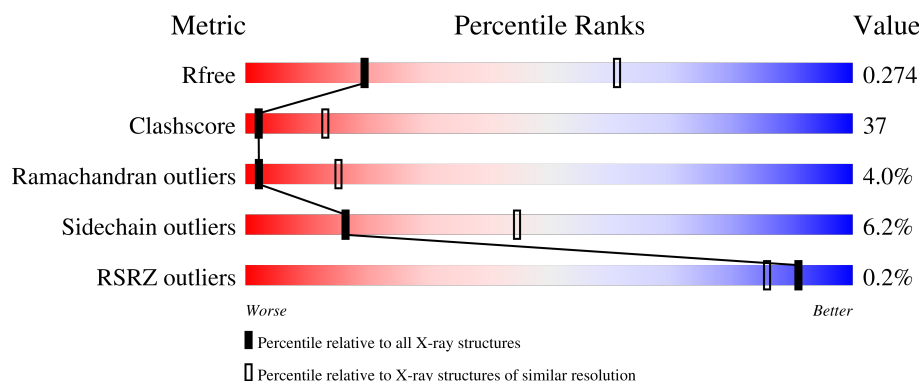
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	764	11% 40% 43% 10% 7%
2	B	748	41% 48% 7% ..
3	C	157	% 36% 42% 6% 14%
4	D	9	11% 22% 22% 11% 11% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12523 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	0	0
			5627	3585	968	1034	40			

- Molecule 2 is a protein called Protein transport protein Sec24A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	729	Total	C	N	O	S	0	0	0
			5761	3675	981	1071	34			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1056	ALA	ARG	conflict	UNP O95486

- Molecule 3 is a protein called Vesicle-trafficking protein SEC22b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	135	Total	C	N	O	S	0	0	0
			1088	699	177	204	8			

- Molecule 4 is a protein called 9-residue synthetic peptide from SNARE protein Bet1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	6	Total	C	N	O	S	0	0	0
			45	25	6	13	1			

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

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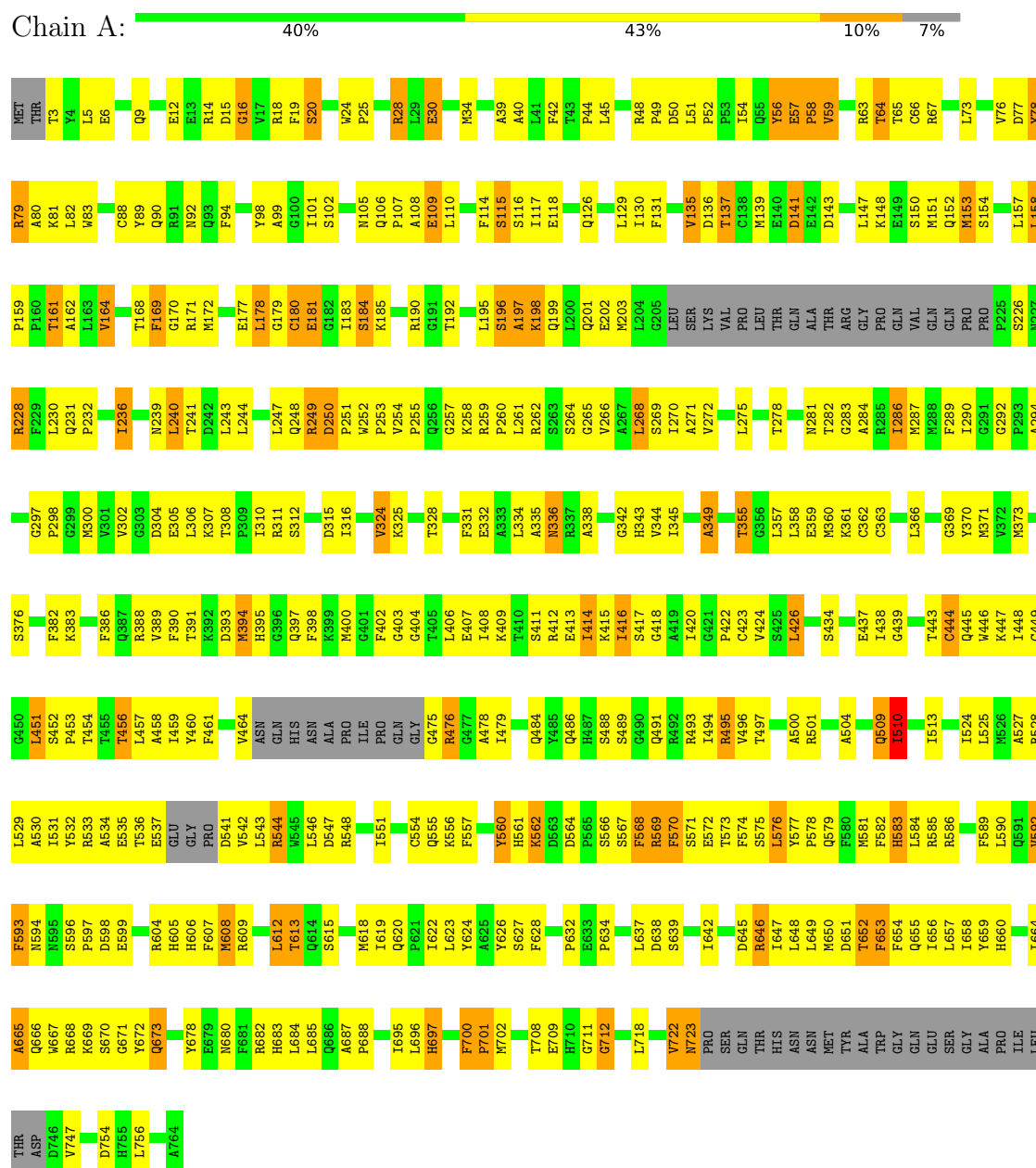
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		

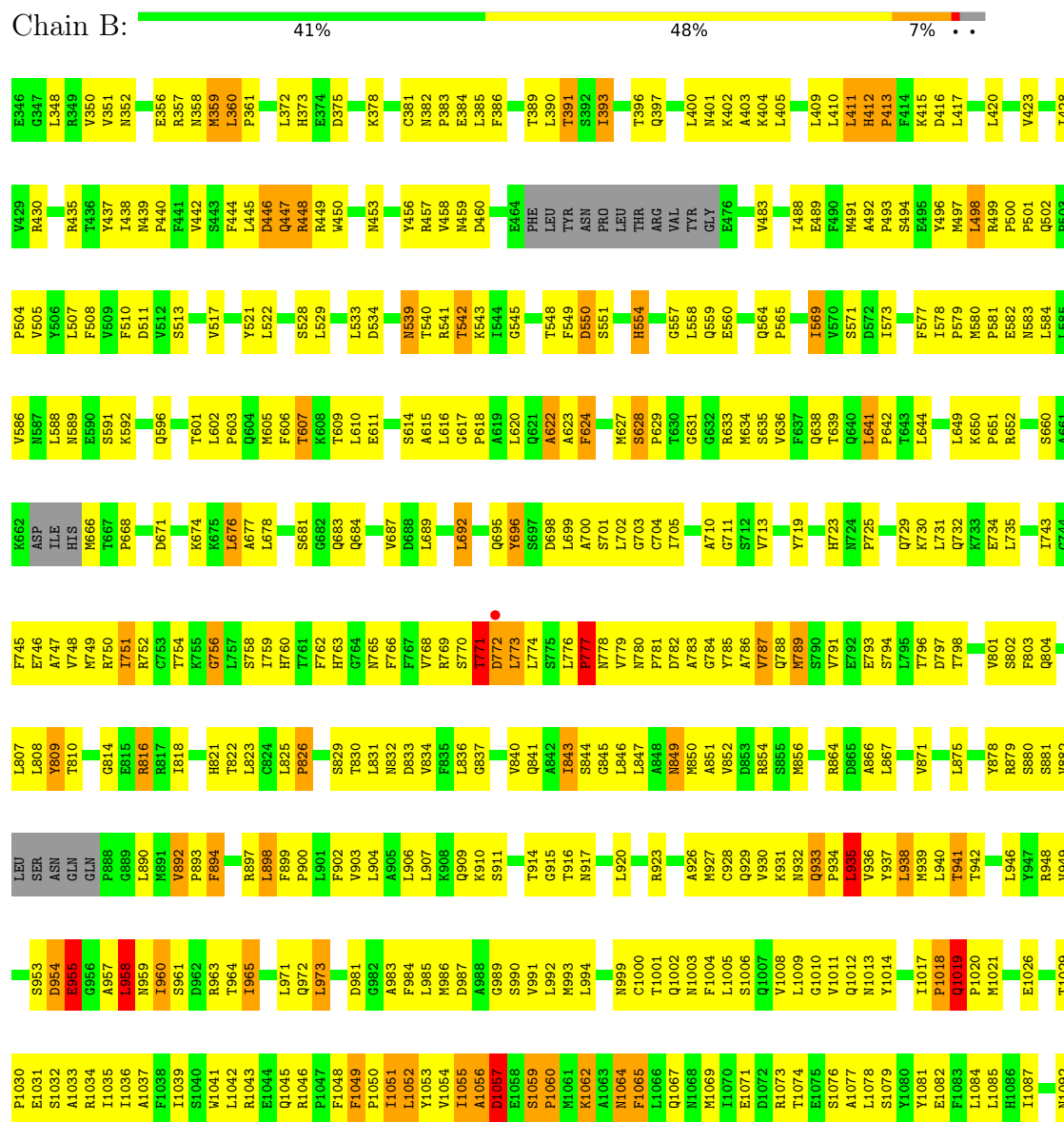
3 Residue-property plots

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.

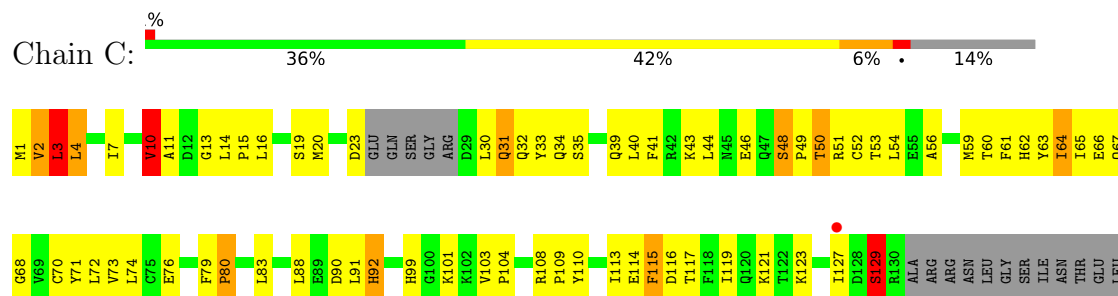
• Molecule 1: Protein transport protein Sec23A

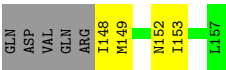


• Molecule 2: Protein transport protein Sec24A

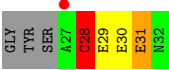


• Molecule 3: Vesicle-trafficking protein SEC22b





● Molecule 4: 9-residue synthetic peptide from SNARE protein Bet1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.15Å 97.23Å 129.51Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	25.00 – 3.30 25.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-3.30) 86.4 (25.00-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 3.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.292 0.199 , 0.274	Depositor DCC
R_{free} test set	1290 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12523	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.53	0/5758	1.08	44/7795 (0.6%)
2	B	0.59	2/5884 (0.0%)	1.12	52/7997 (0.7%)
3	C	0.44	0/1107	1.04	7/1489 (0.5%)
4	D	0.95	0/44	1.77	1/56 (1.8%)
All	All	0.55	2/12793 (0.0%)	1.09	104/17337 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	771	THR	CA-CB	10.00	1.70	1.53
2	B	773	LEU	CA-C	-6.42	1.44	1.53

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	N-CA-C	-12.88	89.84	110.20
4	D	28	CYS	N-CA-C	-10.18	100.99	113.41
2	B	772	ASP	N-CA-C	10.12	125.26	111.90
1	A	198	LYS	N-CA-C	-9.97	100.37	111.14
1	A	135	VAL	N-CA-C	9.82	122.40	108.36
3	C	10	VAL	N-CA-C	9.74	120.56	110.62
1	A	57	GLU	N-CA-C	-9.62	89.17	108.12
2	B	412	HIS	CA-C-N	9.27	129.89	119.32
2	B	412	HIS	C-N-CA	9.27	129.89	119.32
2	B	949	VAL	N-CA-C	9.06	121.59	112.90
2	B	711	GLY	N-CA-C	-8.76	102.28	112.79
2	B	1064	ASN	N-CA-C	-8.53	102.58	113.16
1	A	572	GLU	N-CA-C	-8.45	102.72	112.87
1	A	652	THR	N-CA-C	-8.43	99.17	110.55
2	B	569	ILE	N-CA-C	8.43	120.02	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1057	ASP	N-CA-C	-8.41	97.47	110.17
3	C	3	LEU	N-CA-C	8.36	120.81	108.60
2	B	954	ASP	N-CA-C	8.12	121.97	112.72
3	C	115	PHE	N-CA-C	-8.03	103.46	113.18
1	A	228	ARG	N-CA-C	-7.22	103.13	112.23
1	A	426	LEU	N-CA-C	-7.21	104.22	113.16
2	B	955	GLU	N-CA-C	-7.20	104.38	113.02
1	A	12	GLU	N-CA-C	-6.94	103.65	111.14
2	B	809	TYR	N-CA-C	6.87	117.10	108.45
2	B	393	ILE	N-CA-C	6.82	115.63	108.95
2	B	631	GLY	N-CA-C	-6.63	102.00	112.61
2	B	551	SER	N-CA-C	-6.47	105.42	113.38
2	B	1019	GLN	CA-C-N	-6.29	111.22	120.46
2	B	1019	GLN	C-N-CA	-6.29	111.22	120.46
1	A	250	ASP	N-CA-C	-6.27	102.39	109.60
1	A	178	LEU	N-CA-C	6.20	119.46	110.28
2	B	359	MET	N-CA-C	6.16	117.99	111.28
1	A	458	ALA	N-CA-C	-6.12	98.92	108.90
2	B	931	LYS	N-CA-C	6.12	117.95	111.28
2	B	591	SER	N-CA-C	6.11	120.23	113.21
1	A	349	ALA	N-CA-C	6.10	119.18	109.24
1	A	655	GLN	N-CA-C	6.09	117.97	107.93
2	B	413	PRO	N-CA-C	5.97	122.65	113.75
1	A	56	TYR	CA-C-N	5.95	128.80	122.26
1	A	56	TYR	C-N-CA	5.95	128.80	122.26
2	B	360	LEU	CA-C-N	5.92	125.83	119.85
2	B	360	LEU	C-N-CA	5.92	125.83	119.85
2	B	933	GLN	CA-C-N	5.92	126.84	119.98
2	B	933	GLN	C-N-CA	5.92	126.84	119.98
2	B	843	ILE	CB-CA-C	-5.90	104.18	112.14
1	A	576	LEU	N-CA-C	5.88	118.47	111.71
2	B	821	HIS	N-CA-C	-5.83	100.29	109.50
1	A	271	ALA	N-CA-C	-5.83	104.85	111.14
2	B	723	HIS	N-CA-C	5.80	120.22	113.20
2	B	393	ILE	CA-C-N	5.72	126.62	119.98
2	B	393	ILE	C-N-CA	5.72	126.62	119.98
1	A	158	LEU	CA-C-N	5.71	123.77	119.66
1	A	158	LEU	C-N-CA	5.71	123.77	119.66
1	A	99	ALA	N-CA-C	-5.70	105.21	111.82
2	B	1065	PHE	N-CA-C	-5.70	104.97	111.07
1	A	560	TYR	N-CA-C	5.61	116.76	107.73
1	A	642	ILE	CB-CA-C	-5.61	105.86	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	930	VAL	N-CA-C	-5.61	105.04	110.42
1	A	665	ALA	N-CA-C	-5.57	105.21	111.28
1	A	444	CYS	N-CA-C	-5.49	105.37	113.61
2	B	938	LEU	N-CA-C	-5.49	105.31	112.23
1	A	241	THR	N-CA-C	-5.46	105.02	110.97
1	A	456	THR	N-CA-C	5.46	117.32	108.26
2	B	843	ILE	N-CA-C	-5.45	105.06	110.62
1	A	414	ILE	N-CA-C	5.44	116.42	108.53
2	B	622	ALA	N-CA-C	-5.43	105.02	111.69
2	B	798	THR	N-CA-C	5.43	117.53	110.53
1	A	20	SER	N-CA-C	-5.36	105.51	111.36
1	A	583	HIS	N-CA-C	5.35	117.11	111.28
2	B	773	LEU	N-CA-C	-5.35	95.93	107.49
1	A	568	PHE	N-CA-C	5.35	117.78	110.24
2	B	1062	LYS	N-CA-C	-5.35	104.46	112.54
1	A	42	PHE	N-CA-C	5.31	117.62	109.07
1	A	416	ILE	N-CA-C	5.31	115.50	107.80
3	C	48	SER	CA-C-N	5.31	126.14	119.98
3	C	48	SER	C-N-CA	5.31	126.14	119.98
1	A	159	PRO	CA-C-N	5.25	125.31	119.32
1	A	159	PRO	C-N-CA	5.25	125.31	119.32
2	B	756	GLY	N-CA-C	-5.23	107.67	113.79
2	B	641	LEU	CA-C-N	5.22	126.66	120.23
2	B	641	LEU	C-N-CA	5.22	126.66	120.23
1	A	391	THR	N-CA-C	-5.22	103.14	110.50
2	B	953	SER	N-CA-C	5.22	121.92	110.80
1	A	646	ARG	N-CA-C	5.21	117.94	109.24
2	B	973	LEU	N-CA-C	5.20	117.57	108.52
1	A	653	PHE	N-CA-C	-5.17	105.82	111.82
2	B	448	ARG	N-CA-C	-5.17	104.97	113.50
1	A	181	GLU	N-CA-C	5.16	121.80	110.80
2	B	1006	SER	N-CA-C	5.16	116.72	111.14
3	C	43	LYS	N-CA-C	5.15	116.98	111.36
1	A	281	ASN	N-CA-C	5.13	118.67	111.74
2	B	542	THR	N-CA-C	5.13	117.65	109.96
1	A	478	ALA	N-CA-C	5.12	117.59	109.50
2	B	391	THR	N-CA-C	-5.12	106.14	112.38
2	B	578	ILE	CA-C-N	5.12	124.81	119.64
2	B	578	ILE	C-N-CA	5.12	124.81	119.64
2	B	607	THR	N-CA-C	5.11	117.58	111.71
1	A	79	ARG	N-CA-C	-5.10	105.90	112.68
2	B	624	PHE	N-CA-C	5.04	116.47	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	169	PHE	N-CA-C	5.02	114.95	107.88
1	A	388	ARG	N-CA-C	-5.02	106.67	112.89
3	C	13	GLY	N-CA-C	-5.01	106.23	114.76
2	B	892	VAL	N-CA-C	5.01	113.30	109.19
2	B	735	LEU	N-CA-C	-5.01	105.73	111.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5627	0	5575	399	0
2	B	5761	0	5815	471	0
3	C	1088	0	1091	70	0
4	D	45	0	31	18	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	12523	0	12512	930	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 37.

All (930) 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:A:510:ILE:HD12	1:A:510:ILE:H	1.05	1.11
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.33	1.06
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.38	1.01
2:B:666:MET:HE1	2:B:927:MET:HE1	1.44	0.99
2:B:437:TYR:HB2	2:B:804:GLN:NE2	1.77	0.99
1:A:283:GLY:H	1:A:486:GLN:HE22	1.06	0.98
1:A:28:ARG:HH11	1:A:28:ARG:HB3	1.26	0.98
1:A:417:SER:HB3	1:A:438:ILE:HD13	1.42	0.98
2:B:437:TYR:HB2	2:B:804:GLN:HE22	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ILE:H	1:A:510:ILE:CD1	1.76	0.96
1:A:722:VAL:HG22	1:A:723:ASN:H	1.30	0.96
3:C:3:LEU:HB2	3:C:123:LYS:HZ3	1.32	0.94
2:B:411:LEU:N	2:B:411:LEU:HD23	1.85	0.91
2:B:397:GLN:HE22	2:B:400:LEU:HD23	1.35	0.91
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.53	0.90
1:A:510:ILE:HD12	1:A:510:ILE:N	1.86	0.90
2:B:430:ARG:HH21	2:B:435:ARG:HB3	1.36	0.89
2:B:642:PRO:HD2	2:B:649:LEU:HD12	1.52	0.89
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.53	0.88
2:B:382:ASN:HD22	2:B:383:PRO:CD	1.85	0.88
2:B:397:GLN:NE2	2:B:400:LEU:HD23	1.88	0.88
2:B:1074:THR:HG23	2:B:1076:SER:H	1.36	0.87
1:A:592:VAL:HG23	1:A:593:PHE:H	1.42	0.85
2:B:504:PRO:HG2	2:B:542:THR:HA	1.56	0.85
1:A:183:ILE:HG23	1:A:184:SER:H	1.41	0.85
1:A:357:LEU:HD12	1:A:373:MET:HE3	1.59	0.85
2:B:958:LEU:HA	2:B:964:THR:HA	1.58	0.85
2:B:760:HIS:CE1	2:B:788:GLN:HG2	2.12	0.85
1:A:575:SER:O	1:A:578:PRO:HD2	1.75	0.85
2:B:752:ARG:HH21	4:D:30:GLU:HG2	1.41	0.84
2:B:958:LEU:HB3	2:B:964:THR:HG23	1.60	0.84
2:B:770:SER:O	2:B:771:THR:O	1.96	0.83
1:A:622:ILE:C	1:A:622:ILE:HD12	2.03	0.83
2:B:382:ASN:HD22	2:B:383:PRO:HD2	1.43	0.82
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.61	0.82
2:B:358:ASN:HA	2:B:972:GLN:HE22	1.46	0.81
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.64	0.80
3:C:113:ILE:O	3:C:116:ASP:HB2	1.81	0.80
1:A:80:ALA:O	1:A:82:LEU:HG	1.82	0.80
2:B:494:SER:HA	2:B:497:MET:HE3	1.62	0.79
1:A:48:ARG:HB2	1:A:49:PRO:CD	2.12	0.79
2:B:430:ARG:NH2	4:D:29:GLU:O	2.16	0.78
2:B:1019:GLN:HB3	2:B:1020:PRO:CD	2.14	0.78
3:C:62:HIS:HB2	3:C:73:VAL:CG1	2.14	0.78
2:B:1014:TYR:O	2:B:1017:ILE:HG12	1.83	0.78
1:A:528:ARG:HA	1:A:608:MET:HE1	1.63	0.78
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.49	0.77
1:A:426:LEU:HD21	1:A:447:LYS:HB2	1.67	0.77
1:A:24:TRP:HB3	1:A:25:PRO:HD2	1.66	0.77
2:B:752:ARG:NH2	4:D:30:GLU:HG2	1.98	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:915:GLY:HA3	2:B:1076:SER:HB2	1.66	0.77
1:A:407:GLU:HG3	1:A:445:GLN:HG2	1.65	0.76
1:A:183:ILE:HG23	1:A:184:SER:N	1.98	0.76
1:A:647:ILE:HD12	1:A:660:HIS:ND1	2.00	0.76
2:B:430:ARG:NH1	4:D:29:GLU:O	2.19	0.76
1:A:310:ILE:HD12	1:A:310:ILE:H	1.49	0.76
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.51	0.76
2:B:666:MET:HE1	2:B:927:MET:CE	2.15	0.76
2:B:620:LEU:HD22	2:B:634:MET:CE	2.16	0.75
2:B:437:TYR:CE2	4:D:29:GLU:OE2	2.39	0.75
2:B:382:ASN:HD22	2:B:383:PRO:N	1.84	0.75
1:A:51:LEU:HD13	1:A:117:ILE:HD12	1.69	0.75
2:B:879:ARG:C	2:B:881:SER:H	1.94	0.75
3:C:7:ILE:HD12	3:C:71:TYR:CD2	2.21	0.75
1:A:283:GLY:N	1:A:486:GLN:HE22	1.84	0.74
2:B:808:LEU:HD22	4:D:28:CYS:SG	2.27	0.74
2:B:592:LYS:O	2:B:596:GLN:HG3	1.87	0.74
1:A:622:ILE:HD13	1:A:624:TYR:CE1	2.22	0.74
2:B:808:LEU:CD2	4:D:28:CYS:SG	2.75	0.74
2:B:1019:GLN:O	2:B:1055:ILE:HG23	1.87	0.74
2:B:411:LEU:HD23	2:B:411:LEU:H	1.52	0.73
2:B:457:ARG:HG3	2:B:458:VAL:N	2.02	0.73
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.69	0.73
2:B:875:LEU:HD22	2:B:892:VAL:CG1	2.18	0.73
2:B:747:ALA:HB2	2:B:809:TYR:CB	2.18	0.73
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.69	0.73
1:A:592:VAL:HG23	1:A:593:PHE:N	2.03	0.73
2:B:435:ARG:HG3	4:D:30:GLU:O	1.88	0.73
1:A:171:ARG:HG2	1:A:172:MET:HE2	1.70	0.72
2:B:393:ILE:HD11	2:B:825:LEU:HD12	1.70	0.72
1:A:3:THR:HG22	1:A:5:LEU:H	1.54	0.72
2:B:437:TYR:CB	2:B:804:GLN:HE22	1.99	0.72
2:B:437:TYR:HE2	4:D:29:GLU:OE2	1.72	0.72
2:B:602:LEU:HA	2:B:605:MET:HE3	1.71	0.72
2:B:1051:ILE:N	2:B:1051:ILE:HD12	2.05	0.72
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.72	0.71
3:C:7:ILE:HD12	3:C:71:TYR:HD2	1.54	0.71
1:A:297:GLY:H	1:A:300:MET:HE2	1.54	0.71
2:B:389:THR:HB	2:B:843:ILE:HD13	1.73	0.71
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.26	0.71
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:LEU:HD23	3:C:74:LEU:HD22	1.73	0.71
1:A:25:PRO:HD3	1:A:34:MET:HE3	1.72	0.71
2:B:633:ARG:HB2	2:B:778:ASN:HD21	1.56	0.70
1:A:582:PHE:O	1:A:585:ARG:HG2	1.91	0.70
1:A:3:THR:HG22	1:A:5:LEU:N	2.06	0.70
2:B:748:VAL:HG22	2:B:808:LEU:HD23	1.73	0.70
2:B:747:ALA:HB2	2:B:809:TYR:HB2	1.74	0.70
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.20	0.70
1:A:147:LEU:O	1:A:151:MET:HG3	1.91	0.70
2:B:846:LEU:O	2:B:850:MET:HG3	1.92	0.70
2:B:423:VAL:HG23	2:B:488:ILE:HD11	1.74	0.70
2:B:955:GLU:OE1	2:B:955:GLU:N	2.24	0.70
1:A:528:ARG:HD2	1:A:608:MET:HE2	1.73	0.69
1:A:148:LYS:O	1:A:152:GLN:HG3	1.91	0.69
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.73	0.69
1:A:28:ARG:HB3	1:A:28:ARG:NH1	2.05	0.69
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.73	0.69
3:C:10:VAL:HG23	3:C:68:GLY:O	1.91	0.69
2:B:382:ASN:ND2	2:B:383:PRO:HD2	2.07	0.69
1:A:137:THR:OG1	1:A:169:PHE:O	2.10	0.69
2:B:508:PHE:CZ	2:B:529:LEU:HD21	2.27	0.69
3:C:127:ILE:HG22	3:C:127:ILE:O	1.92	0.69
2:B:750:ARG:HA	2:B:772:ASP:OD1	1.92	0.69
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.73	0.68
2:B:692:LEU:N	2:B:692:LEU:HD12	2.07	0.68
2:B:946:LEU:HG	2:B:971:LEU:HD12	1.75	0.68
2:B:502:GLN:HG2	2:B:746:GLU:CD	2.18	0.68
2:B:1079:SER:H	2:B:1082:GLU:HB2	1.59	0.68
1:A:593:PHE:O	1:A:594:ASN:HB2	1.93	0.68
3:C:50:THR:O	3:C:51:ARG:HG2	1.93	0.68
1:A:63:ARG:HD2	1:A:88:CYS:SG	2.34	0.68
1:A:148:LYS:HE3	1:A:244:LEU:O	1.94	0.68
2:B:548:THR:OG1	2:B:554:HIS:HB2	1.95	0.67
1:A:116:SER:HA	1:A:497:THR:HA	1.76	0.67
1:A:116:SER:HA	1:A:496:VAL:O	1.93	0.67
3:C:62:HIS:HB2	3:C:73:VAL:HG12	1.77	0.67
1:A:183:ILE:HD12	2:B:565:PRO:HG2	1.76	0.67
2:B:389:THR:HB	2:B:843:ILE:CD1	2.24	0.67
1:A:275:LEU:HA	1:A:278:THR:OG1	1.95	0.66
2:B:628:SER:HB3	2:B:629:PRO:HD3	1.76	0.66
2:B:430:ARG:NH2	2:B:435:ARG:HB3	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:814:GLY:HA3	3:C:113:ILE:HD13	1.77	0.66
1:A:76:VAL:HG12	1:A:77:ASP:H	1.60	0.66
1:A:312:SER:O	1:A:316:ILE:HD13	1.94	0.66
2:B:348:LEU:HG	2:B:348:LEU:O	1.95	0.66
2:B:854:ARG:HH12	2:B:866:ALA:HB2	1.61	0.66
2:B:666:MET:HE3	2:B:856:MET:CE	2.25	0.65
2:B:915:GLY:HA3	2:B:1076:SER:CB	2.26	0.65
1:A:51:LEU:HD13	1:A:117:ILE:CD1	2.27	0.65
2:B:1069:MET:HE2	2:B:1069:MET:HA	1.76	0.65
1:A:417:SER:CB	1:A:438:ILE:HD13	2.22	0.65
1:A:418:GLY:HA3	1:A:438:ILE:O	1.96	0.65
1:A:475:GLY:O	1:A:476:ARG:HB2	1.95	0.65
1:A:700:PHE:O	1:A:702:MET:N	2.29	0.65
1:A:106:GLN:HB2	1:A:107:PRO:HD2	1.79	0.65
1:A:58:PRO:O	1:A:59:VAL:HB	1.96	0.65
1:A:622:ILE:HD13	1:A:624:TYR:HE1	1.59	0.65
2:B:502:GLN:HG2	2:B:746:GLU:OE1	1.97	0.65
2:B:620:LEU:HD22	2:B:634:MET:HE3	1.77	0.65
1:A:673:GLN:H	1:A:673:GLN:NE2	1.95	0.65
2:B:772:ASP:OD1	2:B:772:ASP:O	2.14	0.65
2:B:916:THR:HG22	2:B:917:ASN:N	2.12	0.65
2:B:445:LEU:C	2:B:447:GLN:H	2.04	0.65
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.79	0.65
2:B:1043:ARG:HB3	2:B:1050:PRO:HD2	1.79	0.65
2:B:1054:VAL:O	2:B:1056:ALA:N	2.29	0.65
1:A:178:LEU:HD13	1:A:236:ILE:HG21	1.77	0.64
2:B:609:THR:HG22	2:B:611:GLU:H	1.60	0.64
2:B:1059:SER:H	2:B:1060:PRO:HD3	1.61	0.64
3:C:10:VAL:HG23	3:C:68:GLY:C	2.21	0.64
1:A:624:TYR:CE2	1:A:634:PRO:HG3	2.32	0.64
2:B:676:LEU:O	2:B:676:LEU:HD12	1.97	0.64
3:C:1:MET:H2	3:C:76:GLU:H	1.45	0.64
1:A:15:ASP:O	1:A:16:GLY:C	2.39	0.64
1:A:190:ARG:HH21	2:B:577:PHE:HB3	1.61	0.64
2:B:430:ARG:CZ	4:D:29:GLU:O	2.45	0.64
2:B:959:ASN:O	2:B:961:SER:N	2.31	0.64
2:B:1074:THR:HG22	2:B:1077:ALA:N	2.13	0.64
1:A:18:ARG:O	1:A:40:ALA:HA	1.97	0.64
1:A:571:SER:C	1:A:573:THR:H	2.06	0.64
2:B:879:ARG:NH1	2:B:1092:ASN:HD22	1.96	0.64
2:B:916:THR:HG22	2:B:917:ASN:H	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:TYR:CE2	3:C:59:MET:HG3	2.34	0.63
1:A:183:ILE:CG2	1:A:184:SER:H	2.10	0.63
2:B:620:LEU:HD22	2:B:634:MET:HE1	1.80	0.63
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.33	0.63
2:B:483:VAL:HG12	2:B:483:VAL:O	1.96	0.63
2:B:393:ILE:HD11	2:B:825:LEU:CD1	2.28	0.63
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.80	0.63
1:A:116:SER:HB2	1:A:497:THR:HG23	1.81	0.63
2:B:750:ARG:HD3	2:B:772:ASP:O	1.99	0.62
2:B:832:ASN:O	2:B:836:LEU:HG	1.99	0.62
1:A:115:SER:O	1:A:116:SER:HB3	1.99	0.62
3:C:115:PHE:O	3:C:119:ILE:HG13	2.00	0.62
1:A:461:PHE:CE2	1:A:479:ILE:HD13	2.34	0.62
1:A:266:VAL:HA	1:A:269:SER:OG	1.99	0.62
1:A:665:ALA:O	1:A:669:LYS:HG3	1.99	0.62
1:A:195:LEU:HD12	1:A:270:ILE:HD11	1.82	0.62
2:B:634:MET:HE2	2:B:687:VAL:HG22	1.82	0.62
1:A:494:ILE:N	1:A:494:ILE:HD12	2.15	0.62
2:B:760:HIS:HE1	2:B:788:GLN:HG2	1.64	0.62
2:B:989:GLY:HA2	2:B:1046:ARG:NH1	2.15	0.62
1:A:45:LEU:HA	1:A:495:ARG:NH1	2.15	0.61
1:A:571:SER:C	1:A:573:THR:N	2.53	0.61
1:A:541:ASP:HB3	1:A:544:ARG:HD2	1.81	0.61
1:A:548:ARG:O	1:A:551:ILE:HB	2.00	0.61
1:A:564:ASP:OD2	1:A:567:SER:HB3	2.00	0.61
1:A:297:GLY:CA	1:A:300:MET:HB2	2.30	0.61
1:A:370:TYR:HE1	1:A:389:VAL:HG13	1.65	0.61
1:A:407:GLU:HG3	1:A:445:GLN:CG	2.29	0.61
2:B:423:VAL:CG2	2:B:488:ILE:HD11	2.29	0.61
3:C:4:LEU:HD23	3:C:74:LEU:CD2	2.29	0.61
2:B:602:LEU:N	2:B:605:MET:HE3	2.14	0.61
2:B:909:GLN:HG2	2:B:910:LYS:N	2.16	0.61
1:A:88:CYS:SG	1:A:90:GLN:HB3	2.40	0.61
1:A:283:GLY:H	1:A:486:GLN:NE2	1.89	0.61
2:B:428:ILE:HD12	2:B:428:ILE:N	2.16	0.61
1:A:524:ILE:HD12	1:A:615:SER:HB3	1.80	0.61
1:A:63:ARG:O	1:A:65:THR:N	2.34	0.61
2:B:507:LEU:HD12	2:B:545:GLY:C	2.26	0.61
2:B:1054:VAL:C	2:B:1056:ALA:N	2.56	0.61
1:A:52:PRO:O	1:A:54:ILE:HD12	2.01	0.60
1:A:284:ALA:HB3	1:A:343:HIS:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:ARG:HB2	1:A:586:ARG:NH1	2.16	0.60
2:B:348:LEU:HD13	2:B:836:LEU:HD21	1.82	0.60
1:A:131:PHE:CE1	1:A:158:LEU:HD22	2.37	0.60
2:B:580:MET:HG2	2:B:582:GLU:O	2.01	0.60
2:B:430:ARG:HD2	2:B:437:TYR:CE1	2.36	0.60
2:B:1074:THR:HG23	2:B:1076:SER:N	2.13	0.60
3:C:3:LEU:CB	3:C:123:LYS:HZ3	2.11	0.60
3:C:44:LEU:HD13	3:C:65:ILE:HD11	1.83	0.60
2:B:498:LEU:N	2:B:498:LEU:HD12	2.15	0.60
2:B:559:GLN:HG2	2:B:583:ASN:OD1	2.02	0.60
2:B:770:SER:O	2:B:771:THR:C	2.43	0.60
2:B:1051:ILE:HG22	2:B:1052:LEU:N	2.15	0.60
2:B:634:MET:HE3	2:B:636:VAL:HG21	1.84	0.60
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.17	0.60
2:B:559:GLN:HG2	2:B:583:ASN:CG	2.26	0.60
1:A:190:ARG:NH2	2:B:577:PHE:HB3	2.17	0.59
2:B:457:ARG:HG3	2:B:458:VAL:H	1.67	0.59
1:A:108:ALA:HB1	1:A:114:PHE:CD1	2.38	0.59
3:C:30:LEU:O	3:C:34:GLN:HB2	2.02	0.59
3:C:79:PHE:CD1	3:C:80:PRO:HD2	2.37	0.59
1:A:164:VAL:O	1:A:230:LEU:HA	2.03	0.59
2:B:780:ASN:HD22	2:B:782:ASP:H	1.50	0.59
1:A:649:LEU:HD11	1:A:656:ILE:HG23	1.84	0.59
2:B:957:ALA:O	2:B:959:ASN:N	2.32	0.59
2:B:1051:ILE:HD12	2:B:1051:ILE:H	1.66	0.59
2:B:513:SER:O	2:B:517:VAL:HG23	2.02	0.59
2:B:554:HIS:N	2:B:554:HIS:CD2	2.70	0.59
2:B:854:ARG:NH1	2:B:866:ALA:HB2	2.16	0.59
2:B:964:THR:O	2:B:965:ILE:HB	2.03	0.59
2:B:642:PRO:CD	2:B:649:LEU:HD12	2.31	0.59
2:B:702:LEU:O	2:B:705:ILE:HG22	2.03	0.59
1:A:311:ARG:HG3	1:A:316:ILE:HD11	1.85	0.59
1:A:504:ALA:HB2	1:A:513:ILE:HD11	1.84	0.59
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.38	0.59
1:A:700:PHE:O	1:A:701:PRO:C	2.45	0.58
2:B:843:ILE:HG22	2:B:847:LEU:HD11	1.84	0.58
1:A:345:ILE:O	1:A:369:GLY:HA3	2.03	0.58
1:A:660:HIS:HB2	1:A:709:GLU:HB3	1.85	0.58
2:B:437:TYR:OH	2:B:818:ILE:HD13	2.02	0.58
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.67	0.58
2:B:352:ASN:O	2:B:356:GLU:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:615:ALA:O	2:B:618:PRO:HD2	2.03	0.58
2:B:641:LEU:HD11	2:B:651:PRO:HA	1.85	0.58
1:A:30:GLU:OE2	1:A:510:ILE:HD11	2.02	0.58
3:C:62:HIS:O	3:C:73:VAL:HG12	2.04	0.58
2:B:752:ARG:NH1	4:D:29:GLU:OE1	2.35	0.58
2:B:878:TYR:CD2	2:B:893:PRO:HD3	2.39	0.58
2:B:879:ARG:C	2:B:881:SER:N	2.58	0.58
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.69	0.58
1:A:76:VAL:HG12	1:A:77:ASP:N	2.18	0.58
1:A:331:PHE:O	1:A:334:LEU:HB2	2.04	0.58
1:A:297:GLY:N	1:A:300:MET:HB2	2.19	0.58
1:A:366:LEU:HD22	1:A:424:VAL:HG22	1.86	0.58
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.69	0.57
2:B:602:LEU:CA	2:B:605:MET:HE3	2.34	0.57
1:A:177:GLU:CD	1:A:185:LYS:HE2	2.29	0.57
2:B:768:VAL:HG22	2:B:774:LEU:CD2	2.33	0.57
1:A:495:ARG:HH11	1:A:495:ARG:HG2	1.69	0.57
2:B:444:PHE:CE1	2:B:450:TRP:HB3	2.39	0.57
1:A:28:ARG:HH11	1:A:28:ARG:CB	2.10	0.57
2:B:730:LYS:O	2:B:734:GLU:HG3	2.05	0.57
2:B:894:PHE:O	2:B:897:ARG:HG2	2.04	0.57
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.85	0.57
1:A:551:ILE:O	1:A:555:GLN:HG3	2.05	0.57
2:B:439:ASN:HB2	2:B:440:PRO:CD	2.34	0.57
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.85	0.57
1:A:673:GLN:H	1:A:673:GLN:CD	2.10	0.57
2:B:973:LEU:O	2:B:1071:GLU:HB2	2.04	0.57
2:B:409:LEU:C	2:B:410:LEU:HD12	2.29	0.57
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.86	0.57
2:B:1004:PHE:CE1	2:B:1008:VAL:HG11	2.40	0.57
3:C:64:ILE:HG23	3:C:88:LEU:CD1	2.35	0.57
1:A:408:ILE:HD13	1:A:459:ILE:HG21	1.87	0.57
2:B:411:LEU:N	2:B:411:LEU:CD2	2.59	0.57
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.86	0.57
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.86	0.56
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.87	0.56
2:B:401:ASN:O	2:B:404:LYS:N	2.35	0.56
2:B:752:ARG:HG3	2:B:752:ARG:HH11	1.70	0.56
1:A:98:TYR:O	1:A:101:ILE:HG12	2.04	0.56
1:A:154:SER:HB3	1:A:386:PHE:CE2	2.39	0.56
1:A:196:SER:OG	1:A:197:ALA:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:ASN:ND2	2:B:783:ALA:N	2.53	0.56
2:B:1019:GLN:HE21	2:B:1062:LYS:NZ	2.04	0.56
1:A:3:THR:HG22	1:A:6:GLU:H	1.70	0.56
1:A:286:ILE:HD12	1:A:286:ILE:N	2.19	0.56
2:B:929:GLN:O	2:B:933:GLN:HB2	2.04	0.56
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.86	0.56
2:B:580:MET:HG3	2:B:581:PRO:HD2	1.86	0.56
2:B:1057:ASP:C	2:B:1060:PRO:HD3	2.31	0.56
1:A:73:LEU:HD11	1:A:500:ALA:HB2	1.87	0.56
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.21	0.56
1:A:417:SER:HB3	1:A:438:ILE:CD1	2.28	0.56
2:B:439:ASN:HD21	2:B:453:ASN:HD21	1.54	0.56
2:B:440:PRO:HA	2:B:483:VAL:HG13	1.86	0.56
2:B:750:ARG:C	2:B:751:ILE:HD12	2.31	0.55
2:B:897:ARG:C	2:B:898:LEU:HD23	2.31	0.55
1:A:402:PHE:HA	1:A:449:CYS:O	2.06	0.55
1:A:406:LEU:O	1:A:445:GLN:HA	2.06	0.55
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.34	0.55
2:B:410:LEU:HD23	2:B:935:LEU:HG	1.88	0.55
2:B:843:ILE:O	2:B:847:LEU:HG	2.06	0.55
1:A:297:GLY:N	1:A:300:MET:HE2	2.21	0.55
1:A:389:VAL:HB	1:A:390:PHE:CE1	2.42	0.55
1:A:3:THR:HB	1:A:6:GLU:CG	2.36	0.55
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.89	0.55
1:A:443:THR:HG23	1:A:446:TRP:CE2	2.41	0.55
2:B:430:ARG:NH1	2:B:437:TYR:OH	2.40	0.55
2:B:890:LEU:HD23	2:B:1084:LEU:HD22	1.87	0.55
2:B:522:LEU:O	2:B:522:LEU:HD23	2.06	0.55
2:B:1054:VAL:C	2:B:1056:ALA:H	2.14	0.55
3:C:61:PHE:CZ	3:C:74:LEU:HD13	2.42	0.55
1:A:19:PHE:CD2	1:A:40:ALA:HB2	2.41	0.55
1:A:592:VAL:CG2	1:A:593:PHE:H	2.17	0.55
2:B:1041:TRP:O	2:B:1045:GLN:HG2	2.06	0.55
2:B:1049:PHE:C	2:B:1049:PHE:CD2	2.84	0.55
3:C:61:PHE:CE2	3:C:74:LEU:HD13	2.42	0.55
1:A:198:LYS:O	1:A:202:GLU:HG3	2.06	0.55
3:C:1:MET:N	3:C:76:GLU:HB2	2.21	0.55
1:A:130:ILE:HG21	1:A:275:LEU:HD21	1.89	0.54
1:A:240:LEU:O	1:A:244:LEU:HG	2.06	0.54
2:B:1011:VAL:HG12	2:B:1012:GLN:N	2.22	0.54
1:A:183:ILE:CG2	1:A:184:SER:N	2.67	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLN:HG2	1:A:494:ILE:HG13	1.88	0.54
2:B:411:LEU:HB2	2:B:413:PRO:HD3	1.89	0.54
2:B:634:MET:HE2	2:B:687:VAL:HG13	1.89	0.54
3:C:99:HIS:O	3:C:103:VAL:HG23	2.07	0.54
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.42	0.54
2:B:845:GLY:HA2	2:B:938:LEU:HD21	1.88	0.54
2:B:1039:ILE:HA	2:B:1042:LEU:HD12	1.88	0.54
3:C:110:TYR:O	3:C:113:ILE:HG23	2.08	0.54
1:A:606:HIS:CE1	1:A:701:PRO:HG2	2.42	0.54
1:A:408:ILE:CG2	1:A:416:ILE:HD11	2.38	0.54
2:B:639:THR:HG22	2:B:692:LEU:HB2	1.89	0.54
2:B:710:ALA:HA	2:B:765:ASN:O	2.08	0.54
2:B:1059:SER:N	2:B:1060:PRO:CD	2.71	0.54
1:A:76:VAL:HG11	1:A:78:TYR:CE1	2.43	0.54
2:B:382:ASN:HD22	2:B:382:ASN:C	2.13	0.54
2:B:958:LEU:HD23	2:B:958:LEU:O	2.08	0.54
2:B:840:VAL:HG13	2:B:841:GLN:N	2.22	0.54
1:A:180:CYS:O	1:A:181:GLU:HB2	2.08	0.54
2:B:1051:ILE:H	2:B:1051:ILE:CD1	2.21	0.54
2:B:491:MET:HE2	3:C:108:ARG:HD3	1.90	0.53
2:B:521:TYR:CG	2:B:522:LEU:N	2.75	0.53
3:C:35:SER:O	3:C:39:GLN:HG2	2.09	0.53
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.90	0.53
1:A:143:ASP:OD2	1:A:376:SER:HB2	2.08	0.53
1:A:411:SER:HB3	1:A:413:GLU:OE1	2.08	0.53
2:B:752:ARG:NH1	2:B:752:ARG:HG3	2.24	0.53
1:A:3:THR:HB	1:A:6:GLU:HG3	1.90	0.53
1:A:141:ASP:OD1	1:A:249:ARG:HD2	2.08	0.53
1:A:524:ILE:CD1	1:A:615:SER:HB3	2.37	0.53
2:B:348:LEU:CD1	2:B:836:LEU:HD21	2.38	0.53
2:B:957:ALA:C	2:B:959:ASN:H	2.17	0.53
2:B:1054:VAL:O	2:B:1054:VAL:HG12	2.08	0.53
1:A:25:PRO:HD3	1:A:34:MET:CE	2.38	0.53
1:A:543:LEU:HD22	1:A:585:ARG:HB2	1.91	0.53
2:B:439:ASN:O	2:B:442:VAL:HG22	2.09	0.53
2:B:634:MET:HE2	2:B:687:VAL:CG2	2.39	0.53
2:B:1051:ILE:N	2:B:1051:ILE:CD1	2.72	0.53
3:C:113:ILE:HG13	3:C:114:GLU:N	2.24	0.53
1:A:493:ARG:C	1:A:494:ILE:HD12	2.34	0.53
2:B:615:ALA:HB2	2:B:644:LEU:HB3	1.90	0.53
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ASP:HA	1:A:169:PHE:CE2	2.44	0.53
2:B:496:TYR:CD1	2:B:818:ILE:HD11	2.44	0.53
2:B:668:PRO:HA	2:B:701:SER:OG	2.07	0.53
2:B:948:ARG:HD2	2:B:984:PHE:CZ	2.44	0.53
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.90	0.53
1:A:456:THR:O	1:A:528:ARG:NH2	2.40	0.53
2:B:439:ASN:HB2	2:B:440:PRO:HD2	1.90	0.53
3:C:53:THR:HG23	3:C:62:HIS:CE1	2.44	0.53
1:A:404:GLY:HA2	1:A:484:GLN:O	2.09	0.52
1:A:452:SER:HB2	1:A:453:PRO:CD	2.39	0.52
1:A:624:TYR:O	1:A:648:LEU:HA	2.09	0.52
2:B:580:MET:HE3	2:B:583:ASN:HB2	1.91	0.52
1:A:535:GLU:HG3	1:A:604:ARG:HH11	1.74	0.52
2:B:878:TYR:CE2	2:B:893:PRO:HD3	2.45	0.52
3:C:64:ILE:HG23	3:C:88:LEU:HD12	1.90	0.52
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.92	0.52
2:B:666:MET:O	2:B:700:ALA:HB1	2.09	0.52
2:B:851:ALA:O	2:B:854:ARG:HB3	2.09	0.52
1:A:19:PHE:HA	1:A:39:ALA:O	2.09	0.52
1:A:657:LEU:C	1:A:658:ILE:HD12	2.35	0.52
2:B:1055:ILE:CG2	2:B:1062:LYS:HD2	2.38	0.52
3:C:54:LEU:HB3	3:C:153:ILE:HB	1.92	0.52
2:B:437:TYR:H	2:B:804:GLN:HE22	1.57	0.52
2:B:1059:SER:N	2:B:1060:PRO:HD3	2.24	0.52
2:B:1078:LEU:HB3	2:B:1082:GLU:HB3	1.92	0.52
1:A:579:GLN:O	1:A:582:PHE:HB3	2.10	0.52
1:A:612:LEU:O	1:A:613:THR:C	2.53	0.52
1:A:722:VAL:HG13	1:A:723:ASN:N	2.25	0.52
2:B:439:ASN:HD21	2:B:453:ASN:ND2	2.08	0.52
2:B:534:ASP:OD1	2:B:592:LYS:NZ	2.38	0.52
2:B:1049:PHE:C	2:B:1049:PHE:HD2	2.18	0.52
1:A:671:GLY:CA	1:A:673:GLN:HE22	2.23	0.52
2:B:550:ASP:O	2:B:614:SER:HA	2.10	0.52
1:A:411:SER:O	1:A:413:GLU:N	2.43	0.52
2:B:992:LEU:O	2:B:1052:LEU:HA	2.09	0.52
1:A:268:LEU:HD13	1:A:334:LEU:HD13	1.92	0.51
1:A:583:HIS:CD2	1:A:620:GLN:NE2	2.77	0.51
1:A:649:LEU:HD13	1:A:658:ILE:HD12	1.91	0.51
2:B:430:ARG:NH1	2:B:437:TYR:CZ	2.78	0.51
2:B:445:LEU:O	2:B:447:GLN:N	2.43	0.51
1:A:338:ALA:CB	1:A:345:ILE:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:699:LEU:HA	2:B:702:LEU:HB2	1.92	0.51
2:B:814:GLY:HA3	3:C:113:ILE:CD1	2.39	0.51
2:B:1029:THR:OG1	2:B:1032:SER:HB2	2.10	0.51
1:A:357:LEU:CD1	1:A:373:MET:HE3	2.35	0.51
1:A:382:PHE:O	1:A:383:LYS:C	2.54	0.51
1:A:722:VAL:HG22	1:A:723:ASN:N	2.10	0.51
2:B:375:ASP:HA	2:B:378:LYS:HG2	1.91	0.51
2:B:396:THR:HG22	2:B:794:SER:OG	2.10	0.51
2:B:605:MET:HB2	2:B:606:PHE:CE2	2.46	0.51
2:B:843:ILE:HG22	2:B:847:LEU:CD1	2.40	0.51
1:A:628:PHE:CE1	1:A:667:TRP:HZ3	2.29	0.51
3:C:2:VAL:HG12	3:C:3:LEU:HD23	1.93	0.51
1:A:3:THR:CG2	1:A:6:GLU:H	2.24	0.51
1:A:403:GLY:N	1:A:449:CYS:O	2.43	0.51
1:A:700:PHE:HB3	1:A:701:PRO:CD	2.39	0.51
2:B:415:LYS:HG2	2:B:416:ASP:N	2.26	0.51
2:B:751:ILE:H	2:B:772:ASP:CG	2.18	0.51
2:B:780:ASN:HD22	2:B:782:ASP:N	2.08	0.51
2:B:981:ASP:HA	2:B:999:ASN:O	2.11	0.51
1:A:118:GLU:CG	1:A:495:ARG:HD2	2.41	0.51
1:A:310:ILE:HD12	1:A:310:ILE:N	2.20	0.51
2:B:393:ILE:N	2:B:393:ILE:HD12	2.26	0.51
1:A:335:ALA:HB2	1:A:363:CYS:HA	1.92	0.51
2:B:385:LEU:CD2	2:B:415:LYS:HD3	2.41	0.51
2:B:810:THR:OG1	2:B:816:ARG:HD3	2.11	0.51
1:A:638:ASP:CA	1:A:722:VAL:HG22	2.41	0.50
1:A:711:GLY:O	1:A:712:GLY:C	2.54	0.50
2:B:511:ASP:HB2	2:B:549:PHE:CZ	2.46	0.50
2:B:989:GLY:HA2	2:B:1046:ARG:HH12	1.76	0.50
2:B:1020:PRO:HG3	2:B:1062:LYS:NZ	2.25	0.50
2:B:851:ALA:O	2:B:852:VAL:C	2.54	0.50
2:B:993:MET:CE	2:B:1065:PHE:HA	2.41	0.50
2:B:751:ILE:HD12	2:B:751:ILE:N	2.26	0.50
1:A:108:ALA:HB1	1:A:114:PHE:HD1	1.76	0.50
2:B:437:TYR:O	2:B:438:ILE:C	2.54	0.50
2:B:666:MET:CE	2:B:927:MET:HE1	2.28	0.50
2:B:808:LEU:CD1	4:D:28:CYS:SG	2.99	0.50
1:A:19:PHE:CE2	1:A:40:ALA:HB2	2.47	0.50
1:A:509:GLN:HB2	1:A:510:ILE:HD12	1.93	0.50
2:B:412:HIS:N	2:B:413:PRO:CD	2.75	0.50
2:B:493:PRO:HD2	2:B:496:TYR:CG	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.93	0.50
2:B:991:VAL:HG22	2:B:992:LEU:N	2.27	0.50
1:A:311:ARG:NH2	1:A:358:LEU:HB3	2.26	0.50
1:A:584:LEU:HB2	1:A:619:ILE:HD12	1.94	0.50
1:A:626:TYR:HD1	1:A:647:ILE:O	1.95	0.50
1:A:592:VAL:CG2	1:A:593:PHE:N	2.74	0.50
3:C:19:SER:C	3:C:20:MET:HG3	2.36	0.50
2:B:397:GLN:OE1	2:B:791:VAL:N	2.40	0.50
3:C:56:ALA:HB2	3:C:153:ILE:HG21	1.93	0.50
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.42	0.49
2:B:496:TYR:HD1	2:B:818:ILE:HD11	1.77	0.49
2:B:849:ASN:N	2:B:849:ASN:HD22	2.09	0.49
2:B:1053:TYR:HB2	2:B:1055:ILE:HG13	1.93	0.49
1:A:63:ARG:O	1:A:64:THR:C	2.55	0.49
2:B:438:ILE:O	2:B:438:ILE:HG23	2.12	0.49
3:C:65:ILE:O	3:C:66:GLU:HG2	2.12	0.49
1:A:596:SER:OG	1:A:599:GLU:HG3	2.12	0.49
1:A:349:ALA:CB	1:A:355:THR:HG21	2.43	0.49
1:A:262:ARG:CZ	1:A:292:GLY:HA3	2.43	0.49
1:A:656:ILE:HD12	1:A:696:LEU:HD13	1.94	0.49
2:B:449:ARG:CZ	2:B:460:ASP:OD1	2.59	0.49
2:B:864:ARG:O	2:B:867:LEU:HB2	2.12	0.49
2:B:437:TYR:N	2:B:804:GLN:HE22	2.09	0.49
1:A:297:GLY:HA2	1:A:298:PRO:C	2.37	0.49
1:A:652:THR:HG22	1:A:654:PHE:H	1.76	0.49
1:A:370:TYR:CE1	1:A:389:VAL:HG13	2.44	0.49
1:A:649:LEU:HD12	1:A:649:LEU:C	2.38	0.49
2:B:802:SER:HA	2:B:823:LEU:O	2.13	0.49
2:B:958:LEU:HB3	2:B:964:THR:CG2	2.38	0.49
1:A:577:TYR:HB3	1:A:578:PRO:HD3	1.94	0.49
2:B:498:LEU:N	2:B:498:LEU:CD1	2.75	0.49
2:B:666:MET:HE1	2:B:927:MET:SD	2.53	0.49
2:B:699:LEU:C	2:B:701:SER:N	2.67	0.49
2:B:1019:GLN:HE21	2:B:1062:LYS:HZ1	1.60	0.49
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.94	0.49
1:A:649:LEU:HA	1:A:657:LEU:O	2.13	0.49
2:B:634:MET:HE3	2:B:636:VAL:CG2	2.43	0.49
2:B:684:GLN:HG3	2:B:746:GLU:HB3	1.95	0.49
1:A:15:ASP:OD1	1:A:116:SER:HB2	2.13	0.48
1:A:88:CYS:SG	1:A:90:GLN:CB	3.01	0.48
1:A:622:ILE:HD12	1:A:622:ILE:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ILE:HD11	1:A:651:ASP:HB3	1.96	0.48
1:A:670:SER:HB3	1:A:672:TYR:HD1	1.77	0.48
3:C:60:THR:HG22	3:C:62:HIS:NE2	2.28	0.48
1:A:554:CYS:HA	1:A:570:PHE:HZ	1.76	0.48
2:B:348:LEU:O	2:B:348:LEU:CG	2.61	0.48
2:B:496:TYR:HB3	4:D:28:CYS:SG	2.54	0.48
3:C:50:THR:C	3:C:51:ARG:HG2	2.38	0.48
1:A:509:GLN:CB	1:A:510:ILE:HD12	2.43	0.48
1:A:596:SER:O	1:A:597:PRO:C	2.54	0.48
1:A:305:GLU:OE2	1:A:307:LYS:HE2	2.13	0.48
2:B:386:PHE:HE1	2:B:409:LEU:HD13	1.78	0.48
2:B:496:TYR:HD2	2:B:496:TYR:N	2.12	0.48
2:B:1079:SER:N	2:B:1082:GLU:HB2	2.28	0.48
1:A:136:ASP:O	1:A:139:MET:HE3	2.13	0.48
1:A:461:PHE:CZ	1:A:479:ILE:HD13	2.49	0.48
3:C:20:MET:SD	3:C:30:LEU:HD21	2.54	0.48
1:A:80:ALA:O	1:A:81:LYS:C	2.57	0.48
3:C:33:TYR:HB3	3:C:74:LEU:CD2	2.44	0.48
1:A:51:LEU:HD22	1:A:52:PRO:HD2	1.95	0.48
1:A:290:ILE:CD1	1:A:360:MET:HE1	2.43	0.48
1:A:622:ILE:C	1:A:622:ILE:CD1	2.77	0.48
2:B:780:ASN:ND2	2:B:782:ASP:H	2.10	0.48
2:B:1069:MET:HE2	2:B:1069:MET:CA	2.44	0.48
1:A:415:LYS:HB3	1:A:434:SER:HB2	1.94	0.48
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.95	0.48
2:B:496:TYR:N	2:B:496:TYR:CD2	2.81	0.48
1:A:153:MET:HE3	1:A:157:LEU:HD11	1.96	0.48
1:A:394:MET:HE3	1:A:394:MET:H	1.79	0.48
1:A:584:LEU:O	1:A:590:LEU:HD12	2.13	0.48
2:B:382:ASN:ND2	2:B:383:PRO:CD	2.64	0.48
2:B:499:ARG:O	2:B:500:PRO:C	2.56	0.48
2:B:634:MET:HE2	2:B:687:VAL:CG1	2.44	0.48
2:B:1057:ASP:O	2:B:1060:PRO:HD3	2.13	0.48
1:A:3:THR:HB	1:A:6:GLU:HB2	1.96	0.47
1:A:79:ARG:HG3	1:A:79:ARG:NH1	2.29	0.47
1:A:254:VAL:O	3:C:129:SER:OG	2.31	0.47
1:A:422:PRO:O	1:A:423:CYS:HB3	2.14	0.47
1:A:576:LEU:O	1:A:577:TYR:C	2.56	0.47
2:B:902:PHE:O	2:B:906:LEU:HB2	2.14	0.47
1:A:369:GLY:O	1:A:609:ARG:NH2	2.47	0.47
1:A:583:HIS:CD2	1:A:620:GLN:HE21	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:389:THR:CG2	2:B:843:ILE:HD13	2.44	0.47
2:B:389:THR:CB	2:B:843:ILE:HD13	2.42	0.47
2:B:437:TYR:CA	2:B:804:GLN:HE22	2.27	0.47
2:B:808:LEU:HD13	4:D:28:CYS:SG	2.55	0.47
1:A:648:LEU:HB2	1:A:659:TYR:HB3	1.96	0.47
1:A:678:TYR:C	1:A:680:ASN:H	2.23	0.47
2:B:808:LEU:HD21	4:D:28:CYS:SG	2.53	0.47
1:A:259:ARG:NH2	1:A:308:THR:O	2.47	0.47
2:B:382:ASN:ND2	2:B:384:GLU:H	2.12	0.47
2:B:776:LEU:O	2:B:777:PRO:C	2.57	0.47
2:B:1052:LEU:HG	2:B:1053:TYR:N	2.29	0.47
1:A:116:SER:CA	1:A:497:THR:HA	2.43	0.47
1:A:195:LEU:HD22	1:A:203:MET:CE	2.45	0.47
1:A:623:LEU:HD11	1:A:648:LEU:HB3	1.96	0.47
1:A:650:MET:HE1	1:A:718:LEU:HA	1.96	0.47
2:B:747:ALA:CB	2:B:809:TYR:HB3	2.44	0.47
2:B:941:THR:HG22	2:B:942:THR:N	2.29	0.47
3:C:20:MET:SD	3:C:30:LEU:HD11	2.54	0.47
2:B:729:GLN:O	2:B:730:LYS:C	2.56	0.47
2:B:946:LEU:HD11	2:B:984:PHE:HB3	1.97	0.47
3:C:80:PRO:HB2	3:C:83:LEU:HD12	1.96	0.47
1:A:448:ILE:O	1:A:449:CYS:C	2.57	0.47
1:A:560:TYR:CD2	1:A:560:TYR:N	2.83	0.47
2:B:385:LEU:HD21	2:B:415:LYS:HD3	1.96	0.47
2:B:934:PRO:O	2:B:935:LEU:C	2.58	0.47
2:B:994:LEU:HB3	2:B:1054:VAL:HG22	1.97	0.47
2:B:1074:THR:HG22	2:B:1077:ALA:H	1.78	0.47
3:C:73:VAL:HB	3:C:88:LEU:HD21	1.96	0.47
1:A:190:ARG:HH21	2:B:577:PHE:CB	2.27	0.47
1:A:268:LEU:HD13	1:A:334:LEU:CD1	2.44	0.47
2:B:357:ARG:NH2	2:B:1081:TYR:HB2	2.30	0.47
2:B:743:ILE:HD11	2:B:778:ASN:ND2	2.30	0.47
1:A:58:PRO:O	1:A:59:VAL:CB	2.61	0.47
1:A:130:ILE:HG21	1:A:275:LEU:CD2	2.44	0.47
1:A:671:GLY:H	1:A:673:GLN:HE22	1.61	0.47
2:B:1055:ILE:O	2:B:1057:ASP:N	2.46	0.47
1:A:282:THR:HG22	1:A:283:GLY:N	2.29	0.47
2:B:440:PRO:HA	2:B:483:VAL:CG1	2.45	0.47
2:B:493:PRO:HG2	2:B:496:TYR:CD2	2.49	0.47
2:B:752:ARG:NH2	4:D:29:GLU:OE1	2.45	0.47
2:B:780:ASN:ND2	2:B:782:ASP:HB2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:ARG:NE	1:A:359:GLU:OE2	2.39	0.46
1:A:371:MET:HB3	1:A:605:HIS:CD2	2.51	0.46
1:A:607:PHE:HD2	1:A:608:MET:HE3	1.80	0.46
2:B:405:LEU:HD23	2:B:405:LEU:HA	1.75	0.46
2:B:457:ARG:CG	2:B:458:VAL:N	2.76	0.46
2:B:557:GLY:O	2:B:558:LEU:HG	2.15	0.46
2:B:747:ALA:HB2	2:B:809:TYR:HB3	1.92	0.46
2:B:773:LEU:HA	2:B:773:LEU:HD12	1.44	0.46
1:A:44:PRO:O	1:A:45:LEU:HD23	2.16	0.46
1:A:342:GLY:HA2	1:A:449:CYS:SG	2.56	0.46
1:A:556:LYS:HB3	1:A:557:PHE:CE1	2.50	0.46
1:A:649:LEU:HD13	1:A:658:ILE:CD1	2.45	0.46
2:B:936:VAL:HG13	2:B:937:TYR:N	2.30	0.46
2:B:1074:THR:CG2	2:B:1077:ALA:N	2.78	0.46
1:A:657:LEU:HD23	1:A:658:ILE:N	2.30	0.46
1:A:700:PHE:CB	1:A:701:PRO:CD	2.94	0.46
1:A:101:ILE:HG21	1:A:107:PRO:HD3	1.98	0.46
1:A:248:GLN:O	1:A:249:ARG:C	2.58	0.46
1:A:397:GLN:HE22	1:A:489:SER:CB	2.28	0.46
2:B:622:ALA:O	2:B:623:ALA:C	2.57	0.46
3:C:65:ILE:C	3:C:66:GLU:HG2	2.40	0.46
1:A:289:PHE:CD1	1:A:289:PHE:N	2.83	0.46
1:A:420:ILE:HD13	1:A:439:GLY:HA3	1.98	0.46
1:A:536:THR:O	1:A:537:GLU:C	2.59	0.46
1:A:626:TYR:CD2	1:A:632:PRO:HG3	2.50	0.46
2:B:450:TRP:NE1	2:B:459:ASN:HB2	2.30	0.46
2:B:581:PRO:HG2	2:B:582:GLU:H	1.81	0.46
2:B:616:LEU:HD22	2:B:638:GLN:OE1	2.15	0.46
2:B:754:THR:HG21	2:B:801:VAL:HG12	1.97	0.46
2:B:879:ARG:O	2:B:881:SER:N	2.49	0.46
2:B:1005:LEU:HA	2:B:1009:LEU:HB2	1.97	0.46
1:A:57:GLU:O	1:A:57:GLU:HG2	2.14	0.46
1:A:561:HIS:O	1:A:562:LYS:C	2.55	0.46
2:B:960:ILE:HG21	2:B:963:ARG:HH12	1.81	0.46
1:A:297:GLY:H	1:A:300:MET:HB2	1.81	0.46
1:A:417:SER:O	1:A:437:GLU:HA	2.15	0.46
1:A:592:VAL:O	1:A:593:PHE:C	2.58	0.46
2:B:511:ASP:HA	2:B:549:PHE:CE2	2.51	0.46
2:B:533:LEU:HD12	2:B:533:LEU:HA	1.79	0.46
2:B:624:PHE:CE1	2:B:683:GLN:HG3	2.51	0.46
2:B:984:PHE:N	2:B:984:PHE:CD2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HA	1:A:495:ARG:HH12	1.81	0.46
1:A:250:ASP:OD2	1:A:251:PRO:HD2	2.16	0.46
2:B:521:TYR:CD1	2:B:522:LEU:N	2.84	0.46
2:B:864:ARG:HD2	2:B:914:THR:CG2	2.46	0.46
2:B:1019:GLN:CB	2:B:1020:PRO:CD	2.88	0.46
1:A:14:ARG:HG2	1:A:48:ARG:HH12	1.80	0.46
1:A:77:ASP:C	1:A:79:ARG:H	2.24	0.46
1:A:411:SER:C	1:A:413:GLU:H	2.24	0.46
1:A:586:ARG:HH11	1:A:586:ARG:CB	2.29	0.46
2:B:521:TYR:O	2:B:522:LEU:C	2.59	0.46
1:A:226:SER:CB	1:A:232:PRO:HD3	2.46	0.45
1:A:557:PHE:CD1	1:A:557:PHE:N	2.83	0.45
2:B:573:ILE:HG23	2:B:618:PRO:CG	2.45	0.45
2:B:766:PHE:CD1	2:B:766:PHE:C	2.94	0.45
2:B:807:LEU:O	2:B:818:ILE:HA	2.16	0.45
1:A:460:TYR:CE2	1:A:529:LEU:HD11	2.51	0.45
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.98	0.45
2:B:776:LEU:O	2:B:778:ASN:N	2.49	0.45
1:A:231:GLN:HB2	1:A:236:ILE:HG13	1.97	0.45
1:A:527:ALA:O	1:A:528:ARG:C	2.58	0.45
1:A:711:GLY:O	1:A:712:GLY:O	2.35	0.45
2:B:831:LEU:O	2:B:832:ASN:C	2.59	0.45
2:B:601:THR:CG2	2:B:605:MET:HE2	2.46	0.45
2:B:1033:ALA:O	2:B:1037:ALA:HB2	2.16	0.45
1:A:647:ILE:HD11	1:A:664:ILE:CG2	2.36	0.45
2:B:573:ILE:CG2	2:B:618:PRO:HG2	2.43	0.45
2:B:916:THR:CG2	2:B:917:ASN:H	2.27	0.45
2:B:1054:VAL:O	2:B:1055:ILE:C	2.60	0.45
1:A:258:LYS:HA	1:A:304:ASP:O	2.16	0.45
2:B:602:LEU:HB2	2:B:603:PRO:HD3	1.99	0.45
2:B:666:MET:HE3	2:B:856:MET:HE2	1.97	0.45
2:B:671:ASP:OD1	2:B:671:ASP:N	2.43	0.45
2:B:1064:ASN:O	2:B:1067:GLN:HB2	2.16	0.45
1:A:117:ILE:HD12	1:A:117:ILE:HA	1.80	0.45
2:B:391:THR:HG23	2:B:837:GLY:O	2.16	0.45
2:B:641:LEU:HD21	2:B:649:LEU:O	2.17	0.45
1:A:373:MET:HE1	1:A:598:ASP:HB3	1.98	0.45
2:B:358:ASN:HA	2:B:972:GLN:NE2	2.22	0.45
2:B:417:LEU:HD12	2:B:420:LEU:HD22	1.98	0.45
2:B:745:PHE:C	2:B:746:GLU:HG2	2.42	0.45
2:B:983:ALA:C	2:B:984:PHE:CD2	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:789:MET:HE1	2:B:803:PHE:CE1	2.52	0.45
2:B:958:LEU:HD23	2:B:958:LEU:C	2.42	0.45
3:C:19:SER:O	3:C:20:MET:HG3	2.17	0.45
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.52	0.45
1:A:577:TYR:CE2	1:A:581:MET:HE3	2.52	0.45
1:A:583:HIS:HA	1:A:586:ARG:HG2	1.99	0.45
1:A:671:GLY:N	1:A:673:GLN:HE22	2.15	0.45
2:B:620:LEU:HD21	2:B:636:VAL:HG21	1.99	0.45
3:C:63:TYR:CD1	3:C:63:TYR:C	2.95	0.45
3:C:103:VAL:N	3:C:104:PRO:HD2	2.31	0.45
1:A:117:ILE:N	1:A:496:VAL:O	2.48	0.44
1:A:177:GLU:HG3	1:A:228:ARG:HB3	1.98	0.44
1:A:268:LEU:O	1:A:272:VAL:HG23	2.17	0.44
1:A:297:GLY:HA3	1:A:300:MET:HB2	1.99	0.44
1:A:344:VAL:HG22	1:A:449:CYS:HB3	1.99	0.44
1:A:606:HIS:CE1	1:A:701:PRO:CG	3.00	0.44
2:B:528:SER:O	2:B:529:LEU:C	2.60	0.44
2:B:916:THR:CG2	2:B:917:ASN:N	2.79	0.44
1:A:652:THR:HG22	1:A:653:PHE:N	2.32	0.44
3:C:48:SER:HA	3:C:49:PRO:HD3	1.82	0.44
1:A:118:GLU:HG3	1:A:495:ARG:HD2	1.99	0.44
1:A:682:ARG:C	1:A:684:LEU:N	2.72	0.44
2:B:780:ASN:HD22	2:B:782:ASP:HB2	1.82	0.44
3:C:80:PRO:HG2	3:C:83:LEU:HD12	1.99	0.44
1:A:54:ILE:HG21	1:A:56:TYR:CD1	2.51	0.44
1:A:495:ARG:NH1	1:A:495:ARG:HG2	2.31	0.44
2:B:382:ASN:ND2	2:B:382:ASN:C	2.75	0.44
2:B:627:MET:O	2:B:628:SER:C	2.61	0.44
2:B:695:GLN:O	2:B:696:TYR:C	2.59	0.44
1:A:504:ALA:CB	1:A:513:ILE:HD11	2.48	0.44
2:B:730:LYS:HE2	2:B:734:GLU:OE2	2.18	0.44
2:B:780:ASN:HD21	2:B:783:ALA:N	2.15	0.44
2:B:972:GLN:HB3	2:B:1071:GLU:OE2	2.18	0.44
2:B:985:LEU:HD11	2:B:992:LEU:HB3	1.99	0.44
2:B:1051:ILE:CG2	2:B:1052:LEU:N	2.80	0.44
2:B:1055:ILE:O	2:B:1060:PRO:HG3	2.17	0.44
1:A:54:ILE:CG2	1:A:56:TYR:CG	3.01	0.44
1:A:147:LEU:HG	1:A:151:MET:HE2	2.00	0.44
1:A:411:SER:C	1:A:413:GLU:N	2.72	0.44
1:A:531:ILE:HD11	1:A:589:PHE:HB3	1.99	0.44
1:A:577:TYR:CZ	1:A:581:MET:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:558:LEU:HB2	2:B:586:VAL:HG11	1.99	0.44
2:B:1019:GLN:HG2	2:B:1062:LYS:HZ2	1.81	0.44
1:A:15:ASP:OD1	1:A:116:SER:CB	2.66	0.44
1:A:52:PRO:O	1:A:54:ILE:CD1	2.66	0.44
1:A:637:LEU:HD22	1:A:722:VAL:HA	1.98	0.44
2:B:389:THR:HB	2:B:843:ILE:HD11	2.00	0.44
2:B:539:ASN:OD1	2:B:541:ARG:HB2	2.18	0.44
2:B:699:LEU:C	2:B:701:SER:H	2.25	0.44
2:B:957:ALA:C	2:B:964:THR:O	2.60	0.44
1:A:687:ALA:N	1:A:688:PRO:HD2	2.33	0.44
2:B:375:ASP:C	2:B:378:LYS:HG2	2.43	0.44
2:B:830:THR:O	2:B:833:ASP:HB2	2.18	0.44
2:B:372:LEU:O	2:B:373:HIS:C	2.61	0.44
2:B:582:GLU:HG2	2:B:583:ASN:N	2.32	0.44
2:B:840:VAL:HG13	2:B:841:GLN:H	1.82	0.44
3:C:31:GLN:OE1	3:C:32:GLN:N	2.50	0.44
3:C:91:LEU:O	3:C:92:HIS:C	2.61	0.44
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.82	0.43
1:A:708:THR:OG1	1:A:709:GLU:N	2.51	0.43
1:A:24:TRP:CZ2	1:A:501:ARG:HG3	2.52	0.43
1:A:179:GLY:CA	1:A:239:ASN:HD22	2.28	0.43
2:B:620:LEU:CD2	2:B:634:MET:HE3	2.47	0.43
2:B:794:SER:HB3	2:B:796:THR:HG23	1.99	0.43
2:B:903:VAL:O	2:B:906:LEU:HB3	2.18	0.43
2:B:1021:MET:N	2:B:1055:ILE:HG12	2.26	0.43
2:B:1074:THR:HG22	2:B:1077:ALA:CB	2.47	0.43
1:A:358:LEU:HD22	1:A:597:PRO:HB3	2.00	0.43
1:A:534:ALA:C	1:A:536:THR:H	2.26	0.43
1:A:618:MET:HG2	1:A:653:PHE:HB3	2.00	0.43
2:B:749:MET:HG2	2:B:751:ILE:HD11	1.99	0.43
2:B:985:LEU:HG	2:B:986:MET:N	2.33	0.43
2:B:1092:ASN:O	2:B:1093:LYS:C	2.61	0.43
3:C:1:MET:H1	3:C:76:GLU:HB2	1.81	0.43
1:A:44:PRO:O	1:A:495:ARG:NH1	2.51	0.43
2:B:804:GLN:HG3	2:B:822:THR:OG1	2.19	0.43
1:A:236:ILE:O	1:A:236:ILE:CG2	2.65	0.43
1:A:628:PHE:HE1	1:A:667:TRP:HZ3	1.64	0.43
2:B:784:GLY:C	2:B:785:TYR:CD1	2.96	0.43
3:C:39:GLN:O	3:C:40:LEU:C	2.62	0.43
1:A:56:TYR:HE1	1:A:109:GLU:OE2	2.01	0.43
1:A:257:GLY:HA2	1:A:306:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:397:GLN:O	2:B:400:LEU:HB3	2.19	0.43
2:B:446:ASP:C	2:B:448:ARG:H	2.26	0.43
3:C:2:VAL:HG12	3:C:3:LEU:CD2	2.49	0.43
3:C:14:LEU:HD12	3:C:15:PRO:HD2	1.99	0.43
1:A:118:GLU:CD	1:A:495:ARG:HD2	2.44	0.43
2:B:825:LEU:HB3	2:B:826:PRO:HD2	2.01	0.43
2:B:879:ARG:HA	2:B:882:VAL:HG22	2.00	0.43
2:B:954:ASP:C	2:B:955:GLU:OE1	2.62	0.43
1:A:83:TRP:CH2	1:A:92:ASN:ND2	2.87	0.43
1:A:126:GLN:HE22	1:A:491:GLN:HG2	1.84	0.43
1:A:310:ILE:H	1:A:310:ILE:CD1	2.24	0.43
1:A:420:ILE:CD1	1:A:439:GLY:HA3	2.48	0.43
1:A:551:ILE:HD13	1:A:756:LEU:HD12	2.00	0.43
2:B:403:ALA:O	2:B:404:LYS:HB2	2.19	0.43
2:B:564:GLN:HB2	2:B:565:PRO:HD2	2.00	0.43
2:B:692:LEU:HB3	2:B:719:TYR:HB3	2.00	0.43
2:B:1032:SER:O	2:B:1035:ILE:HG22	2.18	0.43
2:B:1081:TYR:O	2:B:1085:LEU:HB2	2.19	0.43
1:A:551:ILE:HD13	1:A:756:LEU:CD1	2.49	0.43
2:B:497:MET:HE1	3:C:109:PRO:HB2	2.01	0.43
2:B:678:LEU:O	2:B:681:SER:HB3	2.19	0.43
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	2.00	0.43
1:A:88:CYS:O	1:A:89:TYR:HB2	2.19	0.43
1:A:657:LEU:C	1:A:657:LEU:HD23	2.43	0.43
2:B:375:ASP:O	2:B:378:LYS:HG2	2.18	0.43
2:B:897:ARG:HG3	2:B:898:LEU:HD23	2.00	0.43
1:A:171:ARG:HD3	1:A:252:TRP:CD2	2.53	0.42
2:B:360:LEU:HA	2:B:361:PRO:HD2	1.85	0.42
2:B:539:ASN:HB2	2:B:540:THR:H	1.70	0.42
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.49	0.42
2:B:1017:ILE:O	2:B:1018:PRO:C	2.61	0.42
1:A:324:VAL:O	1:A:325:LYS:C	2.61	0.42
2:B:634:MET:HG2	2:B:636:VAL:HG23	2.02	0.42
2:B:1055:ILE:HG21	2:B:1062:LYS:CD	2.49	0.42
1:A:311:ARG:HG2	1:A:311:ARG:HH11	1.85	0.42
1:A:574:PHE:O	1:A:575:SER:C	2.61	0.42
1:A:622:ILE:HD13	1:A:624:TYR:CD1	2.52	0.42
2:B:692:LEU:N	2:B:692:LEU:CD1	2.79	0.42
2:B:830:THR:O	2:B:831:LEU:C	2.61	0.42
3:C:7:ILE:O	3:C:16:LEU:HB2	2.20	0.42
1:A:131:PHE:HB3	1:A:287:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:HB3	1:A:386:PHE:HE2	1.82	0.42
1:A:236:ILE:HA	1:A:236:ILE:HD13	1.84	0.42
1:A:408:ILE:CD1	1:A:459:ILE:HG21	2.50	0.42
2:B:588:LEU:O	2:B:589:ASN:C	2.61	0.42
2:B:1011:VAL:CG1	2:B:1012:GLN:N	2.82	0.42
1:A:56:TYR:CD1	1:A:98:TYR:OH	2.70	0.42
1:A:612:LEU:O	1:A:615:SER:HB2	2.20	0.42
1:A:645:ASP:C	1:A:664:ILE:HD11	2.44	0.42
2:B:357:ARG:HH21	2:B:1081:TYR:HB2	1.84	0.42
2:B:397:GLN:O	2:B:400:LEU:N	2.53	0.42
2:B:957:ALA:C	2:B:959:ASN:N	2.74	0.42
2:B:1005:LEU:O	2:B:1010:GLY:N	2.53	0.42
1:A:81:LYS:C	1:A:94:PHE:HD1	2.27	0.42
1:A:359:GLU:N	1:A:359:GLU:OE1	2.50	0.42
1:A:623:LEU:HD11	1:A:648:LEU:HD13	2.01	0.42
1:A:638:ASP:O	1:A:639:SER:C	2.63	0.42
2:B:849:ASN:HD22	2:B:849:ASN:H	1.67	0.42
2:B:991:VAL:CG2	2:B:992:LEU:N	2.83	0.42
1:A:568:PHE:C	1:A:569:ARG:HG3	2.42	0.42
1:A:583:HIS:NE2	1:A:620:GLN:NE2	2.61	0.42
1:A:682:ARG:O	1:A:684:LEU:N	2.53	0.42
2:B:731:LEU:O	2:B:732:GLN:C	2.62	0.42
2:B:759:ILE:CG1	2:B:787:VAL:HG11	2.49	0.42
2:B:939:MET:O	2:B:940:LEU:C	2.62	0.42
2:B:958:LEU:CA	2:B:964:THR:HA	2.40	0.42
1:A:168:THR:HG21	1:A:247:LEU:HD11	2.00	0.42
1:A:185:LYS:HD2	2:B:569:ILE:HD11	2.01	0.42
1:A:622:ILE:CD1	1:A:651:ASP:HB3	2.49	0.42
2:B:393:ILE:HD12	2:B:393:ILE:H	1.83	0.42
2:B:505:VAL:HA	2:B:543:LYS:O	2.19	0.42
1:A:530:ALA:O	1:A:533:ARG:N	2.52	0.42
1:A:547:ASP:O	1:A:551:ILE:HG12	2.20	0.42
2:B:445:LEU:C	2:B:447:GLN:N	2.71	0.42
2:B:489:GLU:HG3	2:B:818:ILE:O	2.20	0.42
2:B:1060:PRO:O	2:B:1062:LYS:HG3	2.19	0.42
1:A:24:TRP:CH2	1:A:501:ARG:HB2	2.55	0.42
2:B:833:ASP:O	2:B:834:VAL:C	2.63	0.42
2:B:847:LEU:HA	2:B:850:MET:SD	2.60	0.42
2:B:871:VAL:HG11	2:B:1087:ILE:HD13	2.02	0.42
2:B:898:LEU:HD23	2:B:898:LEU:N	2.35	0.42
2:B:923:ARG:O	2:B:926:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:PHE:HE2	3:C:70:CYS:SG	2.43	0.42
1:A:546:LEU:HD12	1:A:546:LEU:HA	1.85	0.41
1:A:654:PHE:CD1	1:A:654:PHE:N	2.88	0.41
1:A:666:GLN:C	1:A:668:ARG:N	2.77	0.41
2:B:391:THR:O	2:B:826:PRO:HD2	2.20	0.41
2:B:641:LEU:CD1	2:B:651:PRO:HA	2.50	0.41
2:B:841:GLN:O	2:B:844:SER:HB2	2.19	0.41
2:B:911:SER:OG	2:B:926:ALA:HB1	2.20	0.41
2:B:964:THR:O	2:B:965:ILE:CB	2.67	0.41
1:A:67:ARG:C	1:A:409:LYS:HZ3	2.28	0.41
1:A:275:LEU:HA	1:A:278:THR:HG1	1.84	0.41
1:A:626:TYR:HB2	1:A:647:ILE:HB	2.02	0.41
1:A:638:ASP:HA	1:A:722:VAL:HG22	2.02	0.41
1:A:695:ILE:C	1:A:697:HIS:H	2.27	0.41
2:B:438:ILE:O	2:B:438:ILE:CG2	2.68	0.41
1:A:3:THR:HB	1:A:6:GLU:CB	2.51	0.41
1:A:5:LEU:O	1:A:9:GLN:HG3	2.20	0.41
2:B:381:CYS:SG	2:B:382:ASN:N	2.93	0.41
2:B:381:CYS:HB2	2:B:822:THR:O	2.20	0.41
1:A:393:ASP:O	1:A:395:HIS:N	2.53	0.41
2:B:1003:ASN:HD21	2:B:1031:GLU:HG2	1.85	0.41
1:A:183:ILE:O	1:A:184:SER:CB	2.68	0.41
1:A:249:ARG:O	1:A:250:ASP:C	2.62	0.41
2:B:932:ASN:O	2:B:932:ASN:CG	2.63	0.41
3:C:63:TYR:HB3	3:C:72:LEU:HD12	2.03	0.41
3:C:64:ILE:HG23	3:C:88:LEU:HD13	2.01	0.41
1:A:78:TYR:HD2	1:A:102:SER:C	2.29	0.41
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.84	0.41
1:A:723:ASN:HD22	1:A:723:ASN:HA	1.58	0.41
2:B:1030:PRO:O	2:B:1034:ARG:HG3	2.20	0.41
1:A:259:ARG:O	1:A:260:PRO:C	2.62	0.41
1:A:622:ILE:HG13	1:A:651:ASP:HB3	2.01	0.41
1:A:626:TYR:CE2	1:A:632:PRO:HG3	2.56	0.41
2:B:510:PHE:O	2:B:549:PHE:CD2	2.74	0.41
2:B:689:LEU:HD21	2:B:702:LEU:HB3	2.03	0.41
2:B:768:VAL:HG22	2:B:774:LEU:HD22	2.01	0.41
2:B:904:LEU:O	2:B:907:LEU:N	2.54	0.41
1:A:195:LEU:CD2	1:A:203:MET:HE1	2.51	0.41
1:A:265:GLY:HA3	1:A:298:PRO:O	2.20	0.41
1:A:452:SER:C	1:A:454:THR:H	2.29	0.41
2:B:500:PRO:HG2	3:C:20:MET:HE3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:780:ASN:HB2	2:B:781:PRO:HD2	2.03	0.41
4:D:30:GLU:O	4:D:31:GLU:C	2.64	0.41
1:A:129:LEU:HD11	1:A:488:SER:O	2.21	0.41
1:A:198:LYS:O	1:A:201:GLN:HB3	2.21	0.41
1:A:199:GLN:O	1:A:203:MET:HG3	2.21	0.41
1:A:312:SER:OG	1:A:315:ASP:OD2	2.34	0.41
1:A:407:GLU:HA	1:A:444:CYS:O	2.20	0.41
2:B:401:ASN:O	2:B:403:ALA:N	2.54	0.41
2:B:560:GLU:O	2:B:560:GLU:HG2	2.21	0.41
2:B:756:GLY:HA2	2:B:793:GLU:HB2	2.01	0.41
2:B:758:SER:O	2:B:789:MET:HA	2.21	0.41
2:B:762:PHE:CD2	2:B:774:LEU:HD21	2.55	0.41
2:B:879:ARG:NH1	2:B:1092:ASN:ND2	2.66	0.41
2:B:936:VAL:O	2:B:940:LEU:HD23	2.21	0.41
2:B:987:ASP:HA	2:B:992:LEU:HD23	2.02	0.41
2:B:1013:ASN:O	2:B:1014:TYR:C	2.63	0.41
2:B:1026:GLU:HG2	2:B:1036:ILE:HD13	2.03	0.41
2:B:1064:ASN:HB2	2:B:1067:GLN:NE2	2.36	0.41
3:C:152:ASN:O	3:C:153:ILE:C	2.64	0.41
4:D:31:GLU:O	4:D:31:GLU:HG3	2.21	0.41
1:A:48:ARG:CB	1:A:49:PRO:CD	2.90	0.41
1:A:115:SER:O	1:A:116:SER:CB	2.67	0.41
1:A:231:GLN:O	1:A:232:PRO:C	2.63	0.41
1:A:596:SER:O	1:A:599:GLU:N	2.54	0.41
2:B:617:GLY:O	2:B:618:PRO:C	2.64	0.41
2:B:703:GLY:O	2:B:704:CYS:C	2.64	0.41
2:B:906:LEU:HD12	2:B:906:LEU:HA	1.89	0.41
2:B:932:ASN:O	2:B:932:ASN:OD1	2.39	0.41
3:C:54:LEU:HB2	3:C:61:PHE:HB2	2.03	0.41
1:A:648:LEU:O	1:A:658:ILE:HA	2.21	0.40
2:B:350:VAL:HG12	2:B:351:VAL:N	2.35	0.40
2:B:577:PHE:CD1	2:B:577:PHE:C	2.99	0.40
2:B:909:GLN:OE1	2:B:911:SER:HB2	2.20	0.40
3:C:148:ILE:HG22	3:C:149:MET:N	2.35	0.40
1:A:63:ARG:O	1:A:63:ARG:HG2	2.21	0.40
1:A:107:PRO:HG2	1:A:110:LEU:HD12	2.04	0.40
1:A:153:MET:O	1:A:154:SER:C	2.64	0.40
1:A:161:THR:O	1:A:162:ALA:C	2.64	0.40
1:A:637:LEU:HD23	1:A:637:LEU:HA	1.94	0.40
1:A:682:ARG:O	1:A:683:HIS:C	2.64	0.40
2:B:389:THR:O	2:B:390:LEU:HD23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:579:PRO:HG2	2:B:584:LEU:HD11	2.03	0.40
1:A:678:TYR:C	1:A:680:ASN:N	2.77	0.40
2:B:401:ASN:O	2:B:402:LYS:C	2.63	0.40
2:B:404:LYS:HA	2:B:404:LYS:HD3	1.85	0.40
2:B:674:LYS:O	2:B:677:ALA:HB3	2.21	0.40
2:B:762:PHE:HB3	2:B:766:PHE:CZ	2.56	0.40
2:B:1039:ILE:HD13	2:B:1052:LEU:HD13	2.03	0.40
1:A:336:ASN:HD22	1:A:336:ASN:HA	1.67	0.40
1:A:361:LYS:HG3	1:A:362:CYS:N	2.36	0.40
1:A:542:VAL:O	1:A:543:LEU:C	2.64	0.40
2:B:641:LEU:HD23	2:B:642:PRO:HD2	2.04	0.40
2:B:807:LEU:HD12	2:B:807:LEU:HA	1.79	0.40
2:B:878:TYR:O	2:B:882:VAL:HG13	2.21	0.40
2:B:879:ARG:HH12	2:B:1092:ASN:ND2	2.20	0.40
1:A:332:GLU:HG3	1:A:362:CYS:SG	2.62	0.40
2:B:446:ASP:C	2:B:448:ARG:N	2.80	0.40
2:B:447:GLN:HG2	2:B:447:GLN:O	2.21	0.40
2:B:749:MET:HG2	2:B:751:ILE:CD1	2.52	0.40
2:B:986:MET:HE1	2:B:1069:MET:HE3	2.03	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	698/764 (91%)	583 (84%)	84 (12%)	31 (4%)	2	13
2	B	721/748 (96%)	608 (84%)	90 (12%)	23 (3%)	3	19
3	C	129/157 (82%)	106 (82%)	16 (12%)	7 (5%)	1	10
4	D	4/9 (44%)	3 (75%)	0	1 (25%)	0	0
All	All	1552/1678 (92%)	1300 (84%)	190 (12%)	62 (4%)	2	15

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	196	SER
1	A	324	VAL
1	A	509	GLN
1	A	700	PHE
1	A	722	VAL
2	B	446	ASP
2	B	456	TYR
2	B	769	ARG
2	B	771	THR
2	B	960	ILE
2	B	1019	GLN
3	C	4	LEU
1	A	16	GLY
1	A	50	ASP
1	A	197	ALA
1	A	249	ARG
1	A	394	MET
1	A	613	THR
1	A	712	GLY
2	B	447	GLN
2	B	797	ASP
2	B	1055	ILE
3	C	11	ALA
1	A	59	VAL
1	A	412	ARG
1	A	593	PHE
1	A	608	MET
2	B	894	PHE
2	B	935	LEU
2	B	1018	PRO
2	B	1056	ALA
3	C	2	VAL
3	C	117	THR
1	A	58	PRO
1	A	66	CYS
1	A	109	GLU
1	A	184	SER
1	A	697	HIS
2	B	539	ASN
2	B	696	TYR
2	B	880	SER

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Mol	Chain	Res	Type
2	B	958	LEU
3	C	80	PRO
3	C	92	HIS
4	D	31	GLU
1	A	78	TYR
1	A	562	LYS
1	A	566	SER
1	A	701	PRO
3	C	129	SER
1	A	476	ARG
1	A	510	ILE
1	A	592	VAL
2	B	628	SER
2	B	660	SER
2	B	777	PRO
2	B	965	ILE
2	B	1059	SER
1	A	747	VAL
2	B	725	PRO
1	A	170	GLY

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	619/666 (93%)	583 (94%)	36 (6%)	18	47
2	B	660/678 (97%)	621 (94%)	39 (6%)	18	46
3	C	119/138 (86%)	108 (91%)	11 (9%)	8	30
4	D	4/7 (57%)	3 (75%)	1 (25%)	0	3
All	All	1402/1489 (94%)	1315 (94%)	87 (6%)	16	45

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	SER

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Mol	Chain	Res	Type
1	A	28	ARG
1	A	30	GLU
1	A	105	ASN
1	A	135	VAL
1	A	137	THR
1	A	141	ASP
1	A	150	SER
1	A	153	MET
1	A	161	THR
1	A	164	VAL
1	A	180	CYS
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	261	LEU
1	A	268	LEU
1	A	286	ILE
1	A	302	VAL
1	A	328	THR
1	A	336	ASN
1	A	355	THR
1	A	414	ILE
1	A	451	LEU
1	A	457	LEU
1	A	495	ARG
1	A	510	ILE
1	A	544	ARG
1	A	569	ARG
1	A	570	PHE
1	A	612	LEU
1	A	673	GLN
1	A	685	LEU
1	A	723	ASN
1	A	754	ASP
2	B	359	MET
2	B	411	LEU
2	B	498	LEU
2	B	501	PRO
2	B	550	ASP
2	B	554	HIS
2	B	571	SER

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Mol	Chain	Res	Type
2	B	607	THR
2	B	610	LEU
2	B	635	SER
2	B	650	LYS
2	B	676	LEU
2	B	692	LEU
2	B	713	VAL
2	B	751	ILE
2	B	777	PRO
2	B	787	VAL
2	B	789	MET
2	B	816	ARG
2	B	826	PRO
2	B	829	SER
2	B	849	ASN
2	B	898	LEU
2	B	920	LEU
2	B	928	CYS
2	B	935	LEU
2	B	941	THR
2	B	955	GLU
2	B	958	LEU
2	B	990	SER
2	B	1000	CYS
2	B	1001	THR
2	B	1002	GLN
2	B	1048	PHE
2	B	1049	PHE
2	B	1051	ILE
2	B	1052	LEU
2	B	1057	ASP
2	B	1060	PRO
3	C	3	LEU
3	C	10	VAL
3	C	31	GLN
3	C	46	GLU
3	C	50	THR
3	C	64	ILE
3	C	67	GLN
3	C	90	ASP
3	C	101	LYS
3	C	121	LYS

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Mol	Chain	Res	Type
3	C	129	SER
4	D	28	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	105	ASN
1	A	106	GLN
1	A	113	GLN
1	A	126	GLN
1	A	201	GLN
1	A	239	ASN
1	A	248	GLN
1	A	320	ASN
1	A	336	ASN
1	A	378	ASN
1	A	384	GLN
1	A	397	GLN
1	A	436	ASN
1	A	486	GLN
1	A	509	GLN
1	A	579	GLN
1	A	595	ASN
1	A	606	HIS
1	A	620	GLN
1	A	655	GLN
1	A	666	GLN
1	A	673	GLN
1	A	714	GLN
1	A	723	ASN
1	A	755	HIS
2	B	355	GLN
2	B	358	ASN
2	B	382	ASN
2	B	439	ASN
2	B	559	GLN
2	B	564	GLN
2	B	566	GLN
2	B	587	ASN
2	B	589	ASN
2	B	656	ASN

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Mol	Chain	Res	Type
2	B	683	GLN
2	B	727	GLN
2	B	760	HIS
2	B	765	ASN
2	B	778	ASN
2	B	780	ASN
2	B	804	GLN
2	B	849	ASN
2	B	913	GLN
2	B	932	ASN
2	B	967	GLN
2	B	972	GLN
2	B	1002	GLN
2	B	1003	ASN
2	B	1019	GLN
2	B	1067	GLN
2	B	1092	ASN
3	C	32	GLN
3	C	36	GLN
3	C	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	708/764 (92%)	-0.44	0 100 100	6, 41, 90, 131	0
2	B	729/748 (97%)	-0.54	1 (0%) 92 90	2, 33, 81, 125	0
3	C	135/157 (85%)	-0.10	1 (0%) 84 70	14, 69, 106, 135	0
4	D	6/9 (66%)	1.47	1 (16%) 4 4	89, 99, 104, 107	0
All	All	1578/1678 (94%)	-0.45	3 (0%) 91 86	2, 39, 94, 135	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	27	ALA	2.8
2	B	772	ASP	2.3
3	C	127	ILE	2.1

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
5	ZN	A	765	1/1	0.99	0.03	34,34,34,34	0
5	ZN	B	1094	1/1	1.00	0.02	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.