



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2026 – 04:17 PM UTC

PDB ID : 2NUT / pdb_00002nut
Title : Crystal Structure of the human Sec23a/24a heterodimer, complexed with the SNARE protein Sec22b
Authors : Mancias, J.D.; Goldberg, J.
Deposited on : 2006-11-09
Resolution : 2.30 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

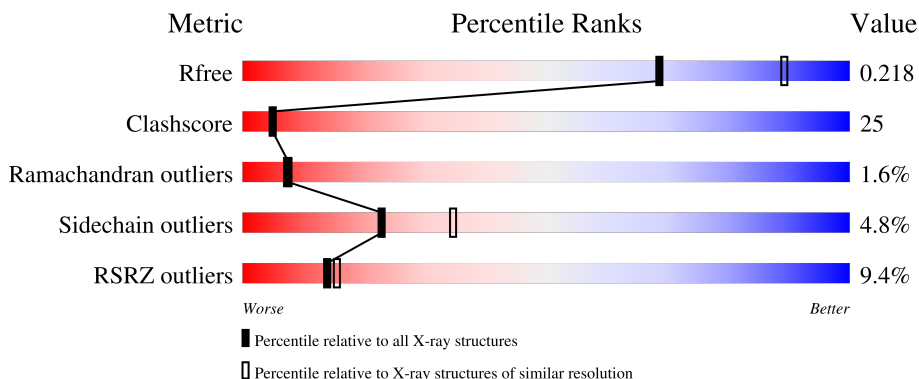
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	769	
2	B	753	
3	C	196	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12778 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			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	cloning artifact	UNP Q15436
A	-2	ALA	-	cloning artifact	UNP Q15436
A	-1	MET	-	cloning artifact	UNP Q15436
A	0	GLY	-	cloning artifact	UNP Q15436

- 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			

- 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
			1087	699	177	203	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	cloning artifact	UNP O75396

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

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

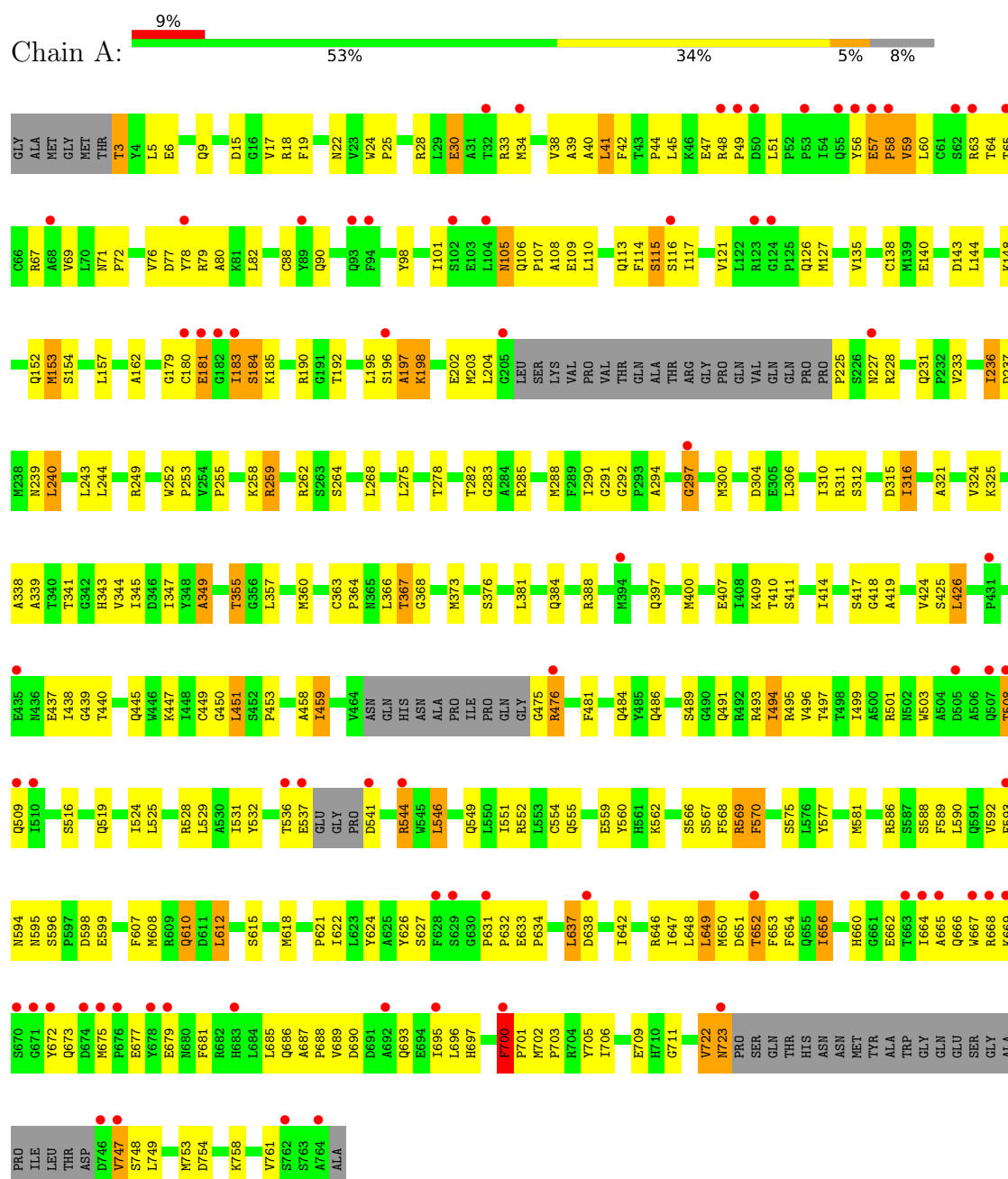
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	123	Total 123	O 123	0	0
5	B	167	Total 167	O 167	0	0
5	C	11	Total 11	O 11	0	0

3 Residue-property plots

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

• Molecule 1: Protein transport protein Sec23A



Chain B: 7% 63% 29% . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.28Å 97.58Å 129.80Å 90.00° 90.15° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 30.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	89.5 (30.00-2.30) 89.4 (30.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.268 0.221 , 0.218	Depositor DCC
R_{free} test set	4378 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12778	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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: 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	0.44	0/5758	0.99	26/7795 (0.3%)
2	B	0.47	1/5884 (0.0%)	0.95	25/7997 (0.3%)
3	C	0.40	0/1106	0.92	4/1489 (0.3%)
All	All	0.45	1/12748 (0.0%)	0.97	55/17281 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	789	MET	SD-CE	-5.24	1.66	1.79

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	N-CA-C	-12.86	91.24	110.28
1	A	652	THR	N-CA-C	-10.71	93.29	110.32
1	A	57	GLU	N-CA-C	-9.43	88.98	109.81
1	A	135	VAL	N-CA-C	9.22	121.01	108.11
2	B	954	ASP	N-CA-C	8.70	123.20	112.59
1	A	367	THR	N-CA-C	-8.58	97.82	110.52
1	A	198	LYS	N-CA-C	-8.34	101.23	111.40
1	A	700	PHE	CA-C-N	-8.15	110.53	119.98
1	A	700	PHE	C-N-CA	-8.15	110.53	119.98
1	A	592	VAL	N-CA-C	8.03	118.83	110.72
2	B	1019	GLN	CA-C-N	-7.78	110.11	119.84
2	B	1019	GLN	C-N-CA	-7.78	110.11	119.84
1	A	324	VAL	N-CA-C	7.40	117.92	110.23
3	C	3	LEU	N-CA-C	6.86	119.18	108.96
1	A	610	GLN	N-CA-C	6.69	119.36	110.53
1	A	228	ARG	N-CA-C	-6.63	105.00	113.23
1	A	325	LYS	N-CA-C	6.62	118.16	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	798	THR	N-CA-C	6.42	118.81	110.53
2	B	933	GLN	CA-C-N	6.39	126.15	119.76
2	B	933	GLN	C-N-CA	6.39	126.15	119.76
3	C	103	VAL	CB-CA-C	-6.33	107.68	113.70
2	B	631	GLY	N-CA-C	-6.32	103.33	112.17
2	B	569	ILE	N-CA-C	6.22	117.07	107.99
1	A	259	ARG	N-CA-C	-6.05	102.26	110.36
2	B	412	HIS	CA-C-N	5.96	125.83	119.28
2	B	412	HIS	C-N-CA	5.96	125.83	119.28
1	A	426	LEU	N-CA-C	-5.95	105.79	113.16
1	A	181	GLU	N-CA-C	5.93	123.44	110.80
1	A	575	SER	N-CA-C	5.91	118.51	111.71
1	A	679	GLU	N-CA-C	-5.88	105.95	113.01
1	A	237	ASP	N-CA-C	5.87	118.15	111.11
1	A	38	VAL	N-CA-C	-5.81	101.18	108.84
3	C	115	PHE	N-CA-C	-5.81	106.28	113.19
2	B	1065	PHE	N-CA-C	-5.72	105.12	111.36
1	A	656	ILE	N-CA-C	-5.66	99.60	107.80
1	A	259	ARG	CA-C-N	-5.64	114.44	120.03
1	A	259	ARG	C-N-CA	-5.64	114.44	120.03
2	B	413	PRO	N-CA-C	5.58	121.18	113.65
2	B	412	HIS	N-CA-C	-5.52	101.07	109.30
3	C	10	VAL	N-CA-C	5.50	115.70	110.42
2	B	840	VAL	N-CA-C	5.48	116.86	110.62
2	B	956	GLY	N-CA-C	5.37	120.84	112.31
2	B	1064	ASN	N-CA-C	-5.34	106.00	113.37
2	B	723	HIS	N-CA-C	5.32	117.99	111.82
2	B	584	LEU	N-CA-C	-5.29	105.64	112.68
1	A	41	LEU	N-CA-C	-5.28	99.18	108.20
2	B	943	HIS	CA-C-N	5.27	125.26	119.89
2	B	943	HIS	C-N-CA	5.27	125.26	119.89
2	B	348	LEU	N-CA-C	-5.24	105.34	112.26
2	B	1057	ASP	N-CA-C	-5.23	101.72	109.94
2	B	912	PHE	N-CA-C	5.14	120.40	113.72
2	B	511	ASP	N-CA-C	-5.07	101.70	109.76
1	A	411	SER	N-CA-C	-5.05	103.86	110.53
1	A	349	ALA	N-CA-C	5.05	116.86	108.02
2	B	1062	LYS	N-CA-C	-5.01	104.92	112.99

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	5574	291	0
2	B	5761	0	5812	269	0
3	C	1087	0	1091	77	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	123	0	0	33	0
5	B	167	0	0	30	0
5	C	11	0	0	0	0
All	All	12778	0	12477	625	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 25.

All (625) 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)
3:C:54:LEU:HD13	3:C:153:ILE:HD13	1.20	1.20
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.26	1.11
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.38	1.03
2:B:879:ARG:HH12	2:B:1092:ASN:HD22	1.04	0.98
2:B:874:SER:HB3	5:B:249:HOH:O	1.64	0.95
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.51	0.91
1:A:290:ILE:HB	5:A:910:HOH:O	1.69	0.91
2:B:382:ASN:ND2	2:B:384:GLU:H	1.70	0.90
2:B:879:ARG:NH1	2:B:1092:ASN:HD22	1.69	0.89
1:A:3:THR:HG22	1:A:6:GLU:H	1.37	0.88
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.37	0.88
2:B:872:ILE:HD13	2:B:1087:ILE:HG23	1.56	0.88
2:B:633:ARG:HB2	2:B:778:ASN:HD21	1.40	0.87
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.55	0.87
1:A:48:ARG:HB2	1:A:49:PRO:CD	2.04	0.86
2:B:573:ILE:HA	5:B:128:HOH:O	1.74	0.86
1:A:140:GLU:HA	1:A:249:ARG:HH21	1.39	0.86
1:A:297:GLY:H	1:A:300:MET:HE2	1.38	0.86
3:C:123:LYS:O	3:C:127:ILE:HD13	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLY:H	1:A:486:GLN:HE22	1.20	0.84
2:B:854:ARG:HH12	2:B:866:ALA:HB2	1.41	0.84
3:C:35:SER:O	3:C:39:GLN:HG2	1.77	0.83
2:B:358:ASN:HA	2:B:972:GLN:HE22	1.40	0.83
2:B:818:ILE:HD13	5:B:109:HOH:O	1.78	0.83
1:A:384:GLN:O	1:A:388:ARG:HG2	1.79	0.82
2:B:916:THR:HG22	2:B:917:ASN:H	1.45	0.81
2:B:567:MET:HG2	2:B:569:ILE:HD11	1.62	0.80
2:B:958:LEU:HA	2:B:964:THR:HA	1.62	0.80
2:B:666:MET:HE1	2:B:927:MET:HE1	1.61	0.80
1:A:493:ARG:C	1:A:494:ILE:HD12	2.06	0.80
2:B:1019:GLN:HB3	2:B:1020:PRO:CD	2.11	0.80
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.62	0.79
1:A:153:MET:HE2	1:A:154:SER:HA	1.63	0.79
2:B:916:THR:HB	5:B:281:HOH:O	1.84	0.78
1:A:440:THR:HB	5:A:892:HOH:O	1.83	0.78
2:B:1064:ASN:HA	5:B:274:HOH:O	1.83	0.77
2:B:351:VAL:HG23	5:B:240:HOH:O	1.83	0.77
2:B:960:ILE:HG21	2:B:963:ARG:HH12	1.47	0.77
2:B:382:ASN:HD22	2:B:384:GLU:H	1.31	0.77
1:A:121:VAL:HG12	5:A:900:HOH:O	1.85	0.77
2:B:433:SER:OG	2:B:457:ARG:HD3	1.85	0.76
2:B:872:ILE:HD11	2:B:1087:ILE:HA	1.66	0.76
2:B:609:THR:HG21	5:B:5:HOH:O	1.85	0.76
2:B:609:THR:HG22	2:B:611:GLU:H	1.49	0.76
1:A:357:LEU:HD12	1:A:373:MET:HE3	1.67	0.76
1:A:45:LEU:HA	1:A:495:ARG:NH1	2.01	0.76
1:A:459:ILE:HD13	1:A:481:PHE:HE2	1.50	0.76
1:A:310:ILE:HD12	1:A:310:ILE:H	1.50	0.76
2:B:916:THR:HG22	2:B:917:ASN:N	2.00	0.76
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.67	0.75
1:A:33:ARG:HB3	5:A:923:HOH:O	1.85	0.75
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.67	0.74
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.68	0.74
1:A:259:ARG:NH1	1:A:306:LEU:HD23	2.03	0.74
1:A:622:ILE:HD13	1:A:624:TYR:CE1	2.23	0.73
1:A:28:ARG:HH11	1:A:28:ARG:HB3	1.51	0.73
1:A:312:SER:O	1:A:316:ILE:HD13	1.89	0.73
2:B:1063:ALA:C	2:B:1065:PHE:H	1.96	0.72
1:A:297:GLY:H	1:A:300:MET:CE	2.01	0.72
3:C:113:ILE:O	3:C:116:ASP:HB2	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:GLN:HG3	1:A:618:MET:HE1	1.72	0.72
3:C:54:LEU:CD1	3:C:153:ILE:HD13	2.11	0.72
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.05	0.72
1:A:593:PHE:O	1:A:594:ASN:HB2	1.89	0.71
2:B:382:ASN:HD22	2:B:382:ASN:C	1.97	0.71
2:B:1059:SER:H	2:B:1060:PRO:HD3	1.55	0.71
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.05	0.71
1:A:311:ARG:HB2	1:A:316:ILE:HD11	1.71	0.71
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.72	0.71
2:B:359:MET:HE3	2:B:359:MET:H	1.55	0.71
1:A:673:GLN:HG2	1:A:685:LEU:HD12	1.73	0.71
1:A:449:CYS:HB2	5:A:831:HOH:O	1.91	0.71
2:B:760:HIS:CE1	2:B:788:GLN:HG2	2.26	0.71
3:C:113:ILE:HD13	3:C:113:ILE:H	1.56	0.71
1:A:115:SER:O	1:A:116:SER:HB3	1.89	0.70
1:A:283:GLY:N	1:A:486:GLN:HE22	1.88	0.70
1:A:44:PRO:O	1:A:495:ARG:NH1	2.23	0.70
1:A:652:THR:HG21	5:A:909:HOH:O	1.90	0.70
2:B:504:PRO:HG2	2:B:542:THR:HA	1.74	0.70
1:A:183:ILE:HD12	2:B:565:PRO:HG2	1.74	0.69
1:A:541:ASP:HB3	1:A:544:ARG:HD2	1.74	0.69
1:A:63:ARG:HD2	1:A:88:CYS:SG	2.33	0.69
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.22	0.69
2:B:412:HIS:HE1	2:B:781:PRO:O	1.76	0.68
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.74	0.68
1:A:484:GLN:HG2	1:A:494:ILE:HG13	1.74	0.68
2:B:915:GLY:HA3	2:B:1076:SER:HB2	1.76	0.68
1:A:76:VAL:HG12	1:A:77:ASP:H	1.58	0.68
1:A:419:ALA:HB3	5:A:892:HOH:O	1.94	0.68
1:A:622:ILE:HD13	1:A:624:TYR:HE1	1.57	0.68
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.23	0.67
2:B:602:LEU:HA	2:B:605:MET:HE3	1.75	0.67
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.76	0.67
2:B:1074:THR:HG23	2:B:1076:SER:H	1.59	0.67
2:B:654:GLU:OE2	2:B:919:ARG:HB3	1.95	0.67
2:B:496:TYR:HE1	5:B:109:HOH:O	1.76	0.66
2:B:879:ARG:NH1	2:B:1092:ASN:HB3	2.10	0.66
2:B:1021:MET:N	2:B:1055:ILE:HG12	2.09	0.66
1:A:686:GLN:HG2	1:A:690:ASP:OD1	1.96	0.66
1:A:722:VAL:O	1:A:723:ASN:HB2	1.96	0.66
2:B:671:ASP:OD2	2:B:675:LYS:HE3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:879:ARG:HH12	2:B:1092:ASN:ND2	1.88	0.66
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.78	0.66
2:B:641:LEU:HD21	2:B:649:LEU:HB2	1.78	0.65
1:A:283:GLY:H	1:A:486:GLN:NE2	1.94	0.65
1:A:297:GLY:N	1:A:300:MET:HE2	2.11	0.65
1:A:649:LEU:HD12	1:A:650:MET:N	2.11	0.65
1:A:60:LEU:HG	5:A:846:HOH:O	1.96	0.64
1:A:494:ILE:HD12	1:A:494:ILE:N	2.11	0.64
2:B:955:GLU:OE1	2:B:955:GLU:N	2.31	0.64
1:A:749:LEU:O	1:A:753:MET:HG2	1.97	0.64
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.80	0.64
2:B:634:MET:HE3	2:B:636:VAL:CG2	2.27	0.64
1:A:5:LEU:O	1:A:9:GLN:HG3	1.97	0.64
1:A:106:GLN:HB2	1:A:107:PRO:HD2	1.80	0.64
3:C:110:TYR:HB3	3:C:113:ILE:CG2	2.28	0.64
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.80	0.64
2:B:567:MET:HE2	2:B:569:ILE:HD11	1.80	0.64
2:B:779:VAL:HG21	2:B:807:LEU:HD21	1.79	0.64
1:A:121:VAL:HG23	1:A:494:ILE:HD13	1.79	0.64
2:B:525:VAL:HG22	2:B:735:LEU:HD11	1.80	0.64
2:B:1054:VAL:O	2:B:1056:ARG:N	2.30	0.64
1:A:126:GLN:HE22	1:A:491:GLN:HG2	1.62	0.63
2:B:915:GLY:HA3	2:B:1076:SER:CB	2.28	0.63
2:B:916:THR:CG2	2:B:917:ASN:H	2.10	0.63
2:B:1067:GLN:HG3	5:B:274:HOH:O	1.97	0.63
1:A:28:ARG:HB3	1:A:28:ARG:NH1	2.12	0.63
1:A:311:ARG:HB2	1:A:316:ILE:CD1	2.28	0.63
2:B:906:LEU:HD13	2:B:942:THR:HG21	1.80	0.63
2:B:634:MET:HE2	2:B:687:VAL:HG13	1.79	0.63
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.81	0.63
2:B:494:SER:HA	2:B:497:MET:HE3	1.79	0.63
1:A:345:ILE:HD13	1:A:367:THR:HG21	1.81	0.63
2:B:1048:PHE:HB2	5:B:154:HOH:O	1.99	0.63
1:A:116:SER:HA	1:A:496:VAL:O	1.99	0.62
2:B:641:LEU:HD23	2:B:642:PRO:HD2	1.81	0.62
1:A:76:VAL:HG12	1:A:77:ASP:N	2.13	0.62
3:C:110:TYR:O	3:C:113:ILE:HG23	1.98	0.62
3:C:127:ILE:N	3:C:127:ILE:HD12	2.14	0.62
1:A:153:MET:HE2	1:A:154:SER:CA	2.30	0.62
2:B:439:ASN:HB2	2:B:440:PRO:CD	2.29	0.62
1:A:624:TYR:CE2	1:A:634:PRO:HG3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:THR:HG22	5:A:810:HOH:O	1.99	0.62
2:B:382:ASN:HD22	2:B:383:PRO:N	1.98	0.62
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.29	0.62
2:B:634:MET:HE3	2:B:636:VAL:HG21	1.81	0.62
2:B:666:MET:HE1	2:B:927:MET:CE	2.30	0.62
1:A:58:PRO:O	1:A:59:VAL:HB	2.00	0.62
2:B:361:PRO:HG2	5:B:250:HOH:O	1.99	0.62
2:B:1020:PRO:HG3	2:B:1062:LYS:NZ	2.15	0.61
3:C:56:ALA:HB2	3:C:153:ILE:HG21	1.82	0.61
1:A:596:SER:OG	1:A:599:GLU:HG3	2.00	0.61
1:A:414:ILE:HD11	1:A:503:TRP:HH2	1.66	0.61
3:C:2:VAL:HG12	3:C:3:LEU:H	1.66	0.61
2:B:909:GLN:HG2	2:B:911:SER:H	1.65	0.61
1:A:63:ARG:HB2	1:A:90:GLN:HG2	1.83	0.61
1:A:696:LEU:CD1	1:A:703:PRO:HG2	2.29	0.61
1:A:475:GLY:O	1:A:476:ARG:HB2	2.00	0.61
2:B:1059:SER:H	2:B:1060:PRO:CD	2.14	0.61
1:A:381:LEU:HD12	1:A:702:MET:HE2	1.82	0.61
2:B:832:ASN:O	2:B:836:LEU:HG	2.00	0.61
2:B:633:ARG:HB2	2:B:778:ASN:ND2	2.14	0.60
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.81	0.60
1:A:259:ARG:NE	5:A:847:HOH:O	2.35	0.60
2:B:654:GLU:OE1	2:B:920:LEU:HB2	2.02	0.59
2:B:992:LEU:O	2:B:1052:LEU:HD12	2.02	0.59
1:A:414:ILE:HD11	1:A:503:TRP:CH2	2.37	0.59
2:B:991:VAL:HG22	5:B:149:HOH:O	2.02	0.59
1:A:536:THR:HB	5:A:919:HOH:O	2.03	0.59
1:A:80:ALA:O	1:A:82:LEU:HG	2.02	0.59
1:A:42:PHE:HB3	1:A:459:ILE:HD11	1.84	0.59
1:A:665:ALA:O	1:A:669:LYS:HG3	2.02	0.59
3:C:113:ILE:HD13	3:C:113:ILE:N	2.16	0.59
1:A:183:ILE:HG23	1:A:184:SER:N	2.17	0.58
1:A:116:SER:HA	1:A:497:THR:HA	1.84	0.58
2:B:987:ASP:HA	2:B:992:LEU:HD23	1.84	0.58
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.85	0.58
3:C:2:VAL:HG12	3:C:3:LEU:N	2.18	0.58
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.68	0.58
1:A:344:VAL:C	1:A:345:ILE:HD12	2.28	0.58
1:A:649:LEU:HD12	1:A:649:LEU:C	2.28	0.58
1:A:67:ARG:HG2	5:A:906:HOH:O	2.03	0.58
1:A:622:ILE:HD12	1:A:622:ILE:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:HIS:NE2	2:B:788:GLN:HG2	2.18	0.58
1:A:562:LYS:HB3	1:A:562:LYS:HZ2	1.69	0.58
1:A:622:ILE:HD12	1:A:622:ILE:C	2.29	0.58
2:B:605:MET:SD	5:B:220:HOH:O	2.57	0.58
1:A:368:GLY:N	5:A:831:HOH:O	2.26	0.58
2:B:909:GLN:HG2	2:B:910:LYS:N	2.19	0.58
3:C:148:ILE:N	3:C:148:ILE:HD12	2.19	0.57
1:A:227:ASN:HD21	1:A:278:THR:HB	1.68	0.57
2:B:347:GLY:HA3	5:B:130:HOH:O	2.03	0.57
2:B:1064:ASN:HA	5:B:78:HOH:O	2.04	0.57
1:A:524:ILE:HD12	1:A:615:SER:HB3	1.86	0.57
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.86	0.57
1:A:338:ALA:HB1	1:A:345:ILE:HD11	1.86	0.57
2:B:620:LEU:HD22	2:B:634:MET:HE1	1.86	0.57
2:B:960:ILE:HG21	2:B:963:ARG:NH1	2.18	0.57
3:C:1:MET:H2	3:C:76:GLU:H	1.51	0.57
1:A:711:GLY:HA2	5:A:889:HOH:O	2.04	0.57
1:A:297:GLY:CA	1:A:300:MET:HB2	2.34	0.57
1:A:338:ALA:CB	1:A:345:ILE:HD11	2.34	0.57
1:A:642:ILE:HD13	1:A:648:LEU:CD1	2.34	0.57
3:C:127:ILE:HG22	3:C:127:ILE:O	2.03	0.57
2:B:872:ILE:HD11	2:B:1087:ILE:HD13	1.87	0.57
3:C:127:ILE:N	3:C:127:ILE:CD1	2.66	0.57
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.39	0.56
2:B:958:LEU:HD23	2:B:958:LEU:O	2.06	0.56
1:A:528:ARG:HA	1:A:608:MET:HE1	1.86	0.56
2:B:446:ASP:HB2	2:B:449:ARG:HB2	1.86	0.56
2:B:696:TYR:CE1	2:B:920:LEU:HD23	2.41	0.56
1:A:311:ARG:CG	1:A:316:ILE:HD11	2.35	0.56
1:A:621:PRO:HD2	1:A:637:LEU:HD11	1.87	0.56
1:A:747:VAL:HG12	1:A:748:SER:N	2.21	0.56
2:B:602:LEU:N	2:B:605:MET:HE3	2.20	0.56
2:B:958:LEU:H	2:B:958:LEU:HD22	1.71	0.56
1:A:240:LEU:CD2	1:A:244:LEU:HG	2.36	0.56
1:A:647:ILE:HD12	1:A:660:HIS:ND1	2.20	0.56
2:B:1052:LEU:HG	2:B:1053:TYR:N	2.20	0.56
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.87	0.56
2:B:554:HIS:CD2	2:B:569:ILE:HD12	2.41	0.56
2:B:411:LEU:N	2:B:411:LEU:HD23	2.21	0.56
1:A:311:ARG:CB	1:A:316:ILE:HD11	2.36	0.55
2:B:750:ARG:HD2	5:B:44:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1059:SER:N	2:B:1060:PRO:CD	2.70	0.55
3:C:61:PHE:CZ	3:C:74:LEU:HD13	2.41	0.55
2:B:1019:GLN:CB	2:B:1020:PRO:CD	2.83	0.55
1:A:153:MET:HE3	1:A:157:LEU:CD1	2.36	0.55
1:A:15:ASP:OD1	1:A:116:SER:HB2	2.06	0.55
1:A:185:LYS:CB	2:B:567:MET:HB3	2.36	0.55
1:A:345:ILE:HD12	1:A:345:ILE:N	2.21	0.55
1:A:647:ILE:HD11	1:A:664:ILE:CG2	2.36	0.55
3:C:6:MET:O	3:C:7:ILE:HD13	2.07	0.55
2:B:854:ARG:NH1	2:B:866:ALA:HB2	2.19	0.54
2:B:1069:MET:HE2	2:B:1069:MET:HA	1.88	0.54
1:A:180:CYS:HB3	5:A:857:HOH:O	2.07	0.54
2:B:963:ARG:HB3	2:B:965:ILE:HD11	1.88	0.54
2:B:1054:VAL:C	2:B:1056:ARG:N	2.62	0.54
2:B:1051:ILE:N	2:B:1051:ILE:HD12	2.23	0.54
2:B:620:LEU:HD22	2:B:634:MET:CE	2.37	0.54
2:B:1022:THR:O	2:B:1023:ASP:HB2	2.08	0.54
1:A:24:TRP:HB3	1:A:25:PRO:HD2	1.90	0.54
1:A:626:TYR:CD2	1:A:632:PRO:HG3	2.43	0.54
2:B:601:THR:CG2	2:B:605:MET:HE2	2.38	0.54
1:A:162:ALA:O	1:A:233:VAL:HG23	2.08	0.53
1:A:364:PRO:O	1:A:367:THR:O	2.27	0.53
1:A:695:ILE:C	1:A:697:HIS:H	2.16	0.53
2:B:446:ASP:C	2:B:448:ARG:H	2.14	0.53
1:A:647:ILE:HD12	1:A:660:HIS:HA	1.91	0.53
3:C:30:LEU:O	3:C:34:GLN:HB2	2.08	0.53
1:A:121:VAL:CG2	1:A:494:ILE:HD13	2.39	0.53
1:A:438:ILE:HG21	1:A:529:LEU:HD21	1.90	0.53
1:A:673:GLN:HG2	1:A:685:LEU:CD1	2.37	0.53
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.89	0.53
2:B:1039:ILE:O	2:B:1043:ARG:HG2	2.07	0.53
1:A:519:GLN:HG2	5:A:812:HOH:O	2.07	0.53
1:A:642:ILE:HD13	1:A:648:LEU:HD11	1.89	0.53
2:B:351:VAL:HG13	2:B:356:GLU:HG3	1.90	0.53
3:C:33:TYR:CE2	3:C:59:MET:HG3	2.43	0.53
2:B:1087:ILE:O	2:B:1091:VAL:HG23	2.09	0.53
2:B:966:PRO:HG2	2:B:1038:PHE:HB2	1.90	0.53
3:C:50:THR:O	3:C:51:ARG:HG2	2.09	0.53
1:A:316:ILE:HD12	1:A:321:ALA:HB2	1.91	0.53
2:B:430:ARG:HD3	2:B:435:ARG:NH2	2.23	0.53
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.91	0.53
1:A:310:ILE:HD12	1:A:310:ILE:N	2.23	0.52
1:A:310:ILE:HG22	1:A:311:ARG:HD3	1.90	0.52
2:B:359:MET:H	2:B:359:MET:CE	2.21	0.52
2:B:445:LEU:C	2:B:447:GLN:H	2.15	0.52
2:B:879:ARG:NH1	5:B:232:HOH:O	2.41	0.52
3:C:101:LYS:HE3	3:C:101:LYS:HA	1.91	0.52
2:B:634:MET:HE2	2:B:687:VAL:CG1	2.39	0.52
1:A:687:ALA:N	1:A:688:PRO:HD2	2.24	0.52
2:B:958:LEU:HB3	2:B:964:THR:HG23	1.91	0.52
3:C:39:GLN:HE21	3:C:39:GLN:HA	1.74	0.52
3:C:61:PHE:CE2	3:C:74:LEU:HD13	2.45	0.52
2:B:872:ILE:CD1	2:B:1087:ILE:HA	2.38	0.52
1:A:76:VAL:C	5:A:882:HOH:O	2.53	0.52
1:A:373:MET:HE1	1:A:598:ASP:HB3	1.91	0.52
1:A:311:ARG:HG3	1:A:316:ILE:HD11	1.92	0.52
1:A:696:LEU:HD13	1:A:703:PRO:HG2	1.92	0.52
1:A:722:VAL:HG13	1:A:723:ASN:N	2.24	0.52
2:B:428:ILE:HD12	2:B:428:ILE:N	2.25	0.52
3:C:1:MET:N	3:C:76:GLU:HB2	2.24	0.52
1:A:297:GLY:N	1:A:300:MET:HB2	2.25	0.52
1:A:344:VAL:HG22	5:A:831:HOH:O	2.10	0.52
2:B:381:CYS:HB2	2:B:822:THR:O	2.09	0.52
2:B:641:LEU:HD23	2:B:642:PRO:CD	2.40	0.52
3:C:63:TYR:HB3	3:C:72:LEU:HD12	1.92	0.52
1:A:407:GLU:HG3	1:A:445:GLN:HG2	1.91	0.52
3:C:4:LEU:HD12	3:C:20:MET:HG2	1.91	0.51
1:A:316:ILE:CD1	1:A:316:ILE:N	2.73	0.51
2:B:602:LEU:CA	2:B:605:MET:HE3	2.40	0.51
3:C:114:GLU:C	3:C:116:ASP:H	2.16	0.51
1:A:349:ALA:CB	1:A:355:THR:HG21	2.41	0.51
2:B:412:HIS:HD2	5:B:10:HOH:O	1.93	0.51
2:B:936:VAL:O	2:B:940:LEU:HD23	2.11	0.51
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.91	0.51
1:A:262:ARG:NH1	5:A:860:HOH:O	2.41	0.51
2:B:964:THR:C	2:B:965:ILE:HD12	2.35	0.51
2:B:986:MET:HE1	2:B:1069:MET:HE3	1.93	0.51
1:A:25:PRO:HD3	1:A:34:MET:HE3	1.92	0.51
2:B:423:VAL:HG23	2:B:488:ILE:HD11	1.92	0.51
2:B:425:SER:HB3	2:B:427:THR:O	2.11	0.51
2:B:558:LEU:HD23	2:B:565:PRO:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:957:ALA:C	2:B:959:ASN:H	2.18	0.51
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.75	0.51
3:C:2:VAL:HG12	3:C:3:LEU:HD23	1.92	0.51
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.46	0.51
1:A:355:THR:HG22	1:A:357:LEU:HG	1.93	0.51
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.46	0.51
1:A:652:THR:HG22	1:A:654:PHE:H	1.76	0.51
2:B:437:TYR:HE1	5:B:109:HOH:O	1.93	0.51
2:B:993:MET:CE	2:B:1065:PHE:HA	2.41	0.51
3:C:148:ILE:HG22	3:C:149:MET:N	2.25	0.51
1:A:67:ARG:C	1:A:409:LYS:HZ3	2.19	0.50
3:C:54:LEU:HB3	3:C:153:ILE:HB	1.93	0.50
1:A:196:SER:O	1:A:197:ALA:HB2	2.12	0.50
1:A:410:THR:HB	1:A:414:ILE:HB	1.92	0.50
1:A:638:ASP:C	1:A:722:VAL:HG22	2.36	0.50
1:A:184:SER:HA	5:A:857:HOH:O	2.10	0.50
1:A:190:ARG:NH1	2:B:575:ASP:OD2	2.44	0.50
2:B:1019:GLN:CG	2:B:1020:PRO:HD3	2.41	0.50
1:A:140:GLU:CD	1:A:249:ARG:NH2	2.70	0.50
1:A:664:ILE:HD13	1:A:667:TRP:CE3	2.47	0.50
3:C:50:THR:C	3:C:51:ARG:HG2	2.36	0.50
1:A:114:PHE:HB3	1:A:117:ILE:HD12	1.93	0.50
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.94	0.50
1:A:528:ARG:HD2	5:A:876:HOH:O	2.12	0.50
1:A:673:GLN:HG3	1:A:681:PHE:CE2	2.47	0.50
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.94	0.50
1:A:180:CYS:SG	1:A:185:LYS:HE2	2.52	0.49
2:B:348:LEU:HG	2:B:348:LEU:O	2.11	0.49
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.41	0.49
1:A:183:ILE:O	2:B:565:PRO:O	2.30	0.49
1:A:290:ILE:CD1	1:A:360:MET:HE1	2.42	0.49
1:A:586:ARG:HB2	1:A:586:ARG:NH1	2.27	0.49
2:B:351:VAL:CG1	2:B:356:GLU:HG3	2.42	0.49
2:B:958:LEU:HD11	5:B:107:HOH:O	2.12	0.49
2:B:666:MET:HE3	2:B:856:MET:CE	2.42	0.49
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.76	0.49
2:B:1063:ALA:C	2:B:1065:PHE:N	2.63	0.49
1:A:183:ILE:HG23	1:A:184:SER:H	1.75	0.49
2:B:618:PRO:HB3	5:B:128:HOH:O	2.12	0.49
2:B:1055:ILE:CG2	2:B:1062:LYS:HD2	2.42	0.49
2:B:666:MET:CE	2:B:927:MET:HE1	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:730:LYS:NZ	5:B:257:HOH:O	2.44	0.49
1:A:19:PHE:CE1	1:A:499:ILE:HD12	2.47	0.48
1:A:259:ARG:CZ	5:A:847:HOH:O	2.61	0.48
2:B:439:ASN:HB2	2:B:440:PRO:HD2	1.94	0.48
2:B:1054:VAL:C	2:B:1056:ARG:H	2.20	0.48
3:C:6:MET:C	3:C:7:ILE:HD13	2.38	0.48
3:C:39:GLN:O	3:C:43:LYS:HG2	2.13	0.48
1:A:397:GLN:HE22	1:A:489:SER:CB	2.26	0.48
3:C:7:ILE:HD12	3:C:71:TYR:CD2	2.47	0.48
2:B:446:ASP:O	2:B:448:ARG:N	2.46	0.48
2:B:958:LEU:HD23	2:B:958:LEU:C	2.38	0.48
1:A:577:TYR:CZ	1:A:581:MET:HE3	2.47	0.48
1:A:668:ARG:HA	1:A:673:GLN:NE2	2.28	0.48
3:C:126:TYR:C	3:C:127:ILE:HD12	2.39	0.48
2:B:854:ARG:HH12	2:B:866:ALA:CB	2.19	0.48
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.93	0.48
1:A:495:ARG:NE	5:A:840:HOH:O	2.47	0.48
1:A:651:ASP:HA	1:A:656:ILE:HD13	1.95	0.48
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.49	0.48
3:C:33:TYR:HB3	3:C:74:LEU:HD22	1.96	0.48
1:A:153:MET:HE3	1:A:157:LEU:HD11	1.96	0.48
1:A:180:CYS:CB	5:A:857:HOH:O	2.61	0.48
3:C:63:TYR:CD1	3:C:63:TYR:C	2.91	0.48
1:A:115:SER:O	1:A:116:SER:CB	2.56	0.48
1:A:249:ARG:NH1	3:C:130:ARG:HB2	2.29	0.48
1:A:459:ILE:HD13	1:A:481:PHE:CE2	2.41	0.48
1:A:560:TYR:CD1	1:A:761:VAL:HG12	2.49	0.48
2:B:779:VAL:HA	5:B:52:HOH:O	2.14	0.48
3:C:55:GLU:O	3:C:152:ASN:ND2	2.46	0.48
2:B:956:GLY:HA2	2:B:967:GLN:HG2	1.96	0.47
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.78	0.47
1:A:259:ARG:HH11	1:A:306:LEU:HD23	1.76	0.47
1:A:531:ILE:HD13	1:A:590:LEU:CD2	2.44	0.47
2:B:483:VAL:O	2:B:483:VAL:HG12	2.13	0.47
2:B:958:LEU:HD22	2:B:958:LEU:N	2.29	0.47
1:A:148:LYS:O	1:A:152:GLN:HG3	2.14	0.47
2:B:677:ALA:HB2	2:B:705:ILE:HA	1.97	0.47
2:B:913:GLN:NE2	2:B:918:ALA:HB2	2.30	0.47
1:A:647:ILE:CD1	1:A:660:HIS:HA	2.45	0.47
2:B:734:GLU:HA	2:B:1048:PHE:HE2	1.79	0.47
1:A:42:PHE:CB	1:A:459:ILE:HD11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ASN:HB2	1:A:72:PRO:CD	2.44	0.47
2:B:359:MET:HE3	2:B:359:MET:N	2.26	0.47
2:B:446:ASP:C	2:B:448:ARG:N	2.73	0.47
2:B:602:LEU:HB2	2:B:603:PRO:HD3	1.96	0.47
2:B:872:ILE:HD12	2:B:1090:GLN:CB	2.33	0.47
1:A:417:SER:O	1:A:437:GLU:HA	2.15	0.47
1:A:622:ILE:HG13	1:A:651:ASP:HB3	1.97	0.47
2:B:382:ASN:HD22	2:B:384:GLU:N	2.06	0.47
2:B:1053:TYR:CD1	2:B:1055:ILE:HD12	2.50	0.47
2:B:936:VAL:HG13	2:B:937:TYR:N	2.29	0.47
2:B:965:ILE:HD12	2:B:965:ILE:N	2.30	0.47
3:C:64:ILE:C	3:C:64:ILE:HD12	2.40	0.47
1:A:56:TYR:CE1	1:A:98:TYR:OH	2.64	0.47
1:A:153:MET:HE2	1:A:154:SER:N	2.29	0.47
1:A:610:GLN:HG3	1:A:618:MET:CE	2.42	0.47
2:B:759:ILE:HD12	2:B:759:ILE:N	2.30	0.47
3:C:114:GLU:C	3:C:116:ASP:N	2.73	0.47
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.49	0.47
1:A:30:GLU:OE1	1:A:30:GLU:HA	2.15	0.46
1:A:559:GLU:O	1:A:568:PHE:HA	2.16	0.46
2:B:1047:PRO:HD2	5:B:154:HOH:O	2.14	0.46
1:A:290:ILE:HD13	1:A:360:MET:HE1	1.97	0.46
1:A:528:ARG:N	5:A:876:HOH:O	2.48	0.46
2:B:373:HIS:CD2	2:B:375:ASP:H	2.33	0.46
2:B:730:LYS:HD3	5:B:257:HOH:O	2.15	0.46
1:A:316:ILE:HD13	1:A:316:ILE:N	2.31	0.46
2:B:871:VAL:CG2	2:B:903:VAL:HG21	2.45	0.46
1:A:528:ARG:CD	5:A:876:HOH:O	2.63	0.46
1:A:549:GLN:HE22	1:A:552:ARG:HH11	1.63	0.46
2:B:439:ASN:ND2	2:B:822:THR:HG21	2.30	0.46
2:B:1062:LYS:C	2:B:1064:ASN:H	2.24	0.46
3:C:113:ILE:H	3:C:113:ILE:CD1	2.26	0.46
1:A:291:GLY:N	5:A:910:HOH:O	2.48	0.46
2:B:771:THR:O	2:B:771:THR:HG22	2.16	0.46
1:A:425:SER:HB2	1:A:440:THR:HG22	1.98	0.46
1:A:536:THR:HG22	1:A:536:THR:O	2.16	0.46
3:C:1:MET:HA	3:C:79:PHE:HB2	1.97	0.46
2:B:1005:LEU:HD13	2:B:1013:ASN:HA	1.96	0.46
2:B:1053:TYR:HB2	2:B:1055:ILE:HG13	1.96	0.46
1:A:259:ARG:HH11	1:A:259:ARG:HG2	1.81	0.46
1:A:476:ARG:HA	1:A:501:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HH12	3:C:130:ARG:HB2	1.81	0.46
1:A:190:ARG:NH1	2:B:575:ASP:CG	2.74	0.45
1:A:588:SER:OG	1:A:595:ASN:ND2	2.49	0.45
3:C:3:LEU:O	3:C:4:LEU:HB2	2.16	0.45
3:C:4:LEU:HD13	3:C:30:LEU:HD11	1.97	0.45
1:A:368:GLY:HA3	1:A:450:GLY:O	2.16	0.45
2:B:397:GLN:HE22	2:B:400:LEU:HD23	1.81	0.45
2:B:609:THR:HG22	2:B:610:LEU:N	2.30	0.45
2:B:890:LEU:HD23	2:B:1084:LEU:HD22	1.98	0.45
2:B:916:THR:CG2	2:B:917:ASN:N	2.67	0.45
2:B:956:GLY:HA3	2:B:965:ILE:O	2.16	0.45
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.81	0.45
1:A:153:MET:CE	1:A:157:LEU:HD12	2.46	0.45
1:A:754:ASP:O	1:A:758:LYS:HG3	2.16	0.45
2:B:959:ASN:O	2:B:961:SER:N	2.48	0.45
1:A:127:MET:HE1	1:A:225:PRO:HG3	1.97	0.45
2:B:1041:TRP:O	2:B:1045:GLN:HG2	2.17	0.45
2:B:666:MET:CE	2:B:855:SER:HB3	2.47	0.45
2:B:730:LYS:HE2	2:B:734:GLU:OE2	2.17	0.45
2:B:998:LYS:HB2	2:B:1058:GLU:OE1	2.16	0.45
2:B:1074:THR:CG2	2:B:1077:ALA:HB3	2.45	0.45
1:A:672:TYR:N	5:A:921:HOH:O	2.50	0.45
2:B:368:PRO:HD2	2:B:839:ASP:OD2	2.16	0.45
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.47	0.45
3:C:110:TYR:HB3	3:C:113:ILE:HG22	1.96	0.45
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.98	0.45
2:B:977:LYS:HE3	5:B:284:HOH:O	2.16	0.45
1:A:494:ILE:N	1:A:494:ILE:CD1	2.79	0.45
1:A:536:THR:O	1:A:537:GLU:C	2.60	0.45
1:A:607:PHE:HD2	1:A:608:MET:HE3	1.81	0.45
1:A:108:ALA:HB1	1:A:114:PHE:CD1	2.52	0.45
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.52	0.45
2:B:1060:PRO:O	2:B:1062:LYS:HG3	2.17	0.45
3:C:1:MET:H1	3:C:76:GLU:HB2	1.82	0.45
1:A:59:VAL:N	5:A:846:HOH:O	2.50	0.44
2:B:362:SER:O	2:B:970:ILE:HD13	2.16	0.44
2:B:382:ASN:ND2	2:B:382:ASN:C	2.69	0.44
2:B:642:PRO:HG2	2:B:702:LEU:HD21	1.98	0.44
2:B:1070:ILE:C	2:B:1070:ILE:HD12	2.42	0.44
1:A:631:PRO:O	1:A:633:GLU:HG3	2.16	0.44
2:B:423:VAL:CG2	2:B:488:ILE:HD11	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:970:ILE:HD12	2:B:970:ILE:N	2.32	0.44
3:C:51:ARG:HD3	3:C:64:ILE:HG22	1.99	0.44
2:B:1054:VAL:O	2:B:1055:ILE:C	2.61	0.44
1:A:47:GLU:HG3	1:A:453:PRO:HB3	1.99	0.44
1:A:204:LEU:HA	5:A:841:HOH:O	2.18	0.44
2:B:601:THR:C	2:B:605:MET:HE3	2.42	0.44
2:B:601:THR:HB	2:B:605:MET:HE2	1.99	0.44
2:B:661:ALA:HB3	2:B:861:SER:OG	2.18	0.44
1:A:19:PHE:HE1	1:A:499:ILE:HD12	1.82	0.44
1:A:28:ARG:HH11	1:A:28:ARG:CB	2.25	0.44
1:A:195:LEU:CD2	1:A:203:MET:HE1	2.41	0.44
1:A:560:TYR:CD2	1:A:560:TYR:N	2.85	0.44
2:B:601:THR:HB	2:B:605:MET:CE	2.47	0.44
3:C:4:LEU:CD1	3:C:20:MET:HG2	2.48	0.44
3:C:81:LYS:HE3	3:C:148:ILE:HG21	2.00	0.44
2:B:393:ILE:HA	2:B:394:PRO:HD3	1.91	0.44
1:A:700:PHE:O	1:A:701:PRO:C	2.53	0.43
2:B:367:PRO:HA	2:B:368:PRO:HD3	1.91	0.43
2:B:957:ALA:C	2:B:959:ASN:N	2.75	0.43
3:C:20:MET:C	3:C:21:GLN:HG3	2.44	0.43
1:A:101:ILE:O	1:A:101:ILE:HG13	2.19	0.43
1:A:705:TYR:O	1:A:706:ILE:HD13	2.16	0.43
1:A:198:LYS:O	1:A:202:GLU:HG3	2.17	0.43
2:B:358:ASN:HA	2:B:972:GLN:NE2	2.19	0.43
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.99	0.43
1:A:536:THR:CB	5:A:919:HOH:O	2.64	0.43
2:B:1051:ILE:HD12	2:B:1051:ILE:H	1.82	0.43
1:A:60:LEU:CD2	1:A:69:VAL:HG22	2.49	0.43
1:A:607:PHE:HD2	1:A:608:MET:CE	2.31	0.43
2:B:457:ARG:HG3	2:B:458:VAL:N	2.32	0.43
2:B:498:LEU:CD1	2:B:498:LEU:N	2.82	0.43
3:C:58:ALA:O	3:C:59:MET:HE2	2.19	0.43
1:A:567:SER:O	1:A:569:ARG:HG3	2.18	0.43
2:B:747:ALA:HB2	2:B:809:TYR:CB	2.48	0.43
1:A:113:GLN:H	1:A:113:GLN:HG3	1.53	0.43
2:B:567:MET:HG2	2:B:569:ILE:CD1	2.42	0.43
3:C:3:LEU:HD13	3:C:123:LYS:HD3	2.00	0.43
3:C:4:LEU:HD11	3:C:20:MET:SD	2.58	0.43
1:A:419:ALA:HA	1:A:458:ALA:O	2.19	0.43
3:C:53:THR:HG23	3:C:62:HIS:CE1	2.54	0.43
3:C:62:HIS:HB2	3:C:73:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:103:VAL:N	3:C:104:PRO:HD2	2.34	0.43
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.34	0.42
1:A:666:GLN:C	1:A:668:ARG:N	2.77	0.42
2:B:463:GLU:O	2:B:464:GLU:HG3	2.19	0.42
2:B:611:GLU:HG3	5:B:5:HOH:O	2.19	0.42
3:C:4:LEU:HD13	3:C:30:LEU:CD1	2.48	0.42
3:C:153:ILE:HD12	3:C:153:ILE:O	2.18	0.42
2:B:629:PRO:CG	3:C:23:ASP:HB2	2.29	0.42
1:A:3:THR:CG2	1:A:6:GLU:HG3	2.50	0.42
1:A:39:ALA:HB3	1:A:525:LEU:HD13	2.01	0.42
1:A:78:TYR:HD1	1:A:78:TYR:H	1.66	0.42
1:A:288:MET:HB3	1:A:347:ILE:HD13	2.00	0.42
1:A:316:ILE:HD12	1:A:321:ALA:CB	2.50	0.42
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.49	0.42
2:B:1057:ASP:C	2:B:1060:PRO:HD3	2.44	0.42
1:A:363:CYS:HB2	1:A:364:PRO:CD	2.49	0.42
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.84	0.42
1:A:622:ILE:HD11	1:A:651:ASP:HB3	2.02	0.42
2:B:480:ARG:HG3	2:B:481:PRO:HD2	2.02	0.42
2:B:601:THR:HG22	2:B:605:MET:HE2	1.99	0.42
1:A:107:PRO:HG2	1:A:110:LEU:HD12	2.01	0.42
2:B:567:MET:HE2	2:B:569:ILE:CD1	2.49	0.42
2:B:567:MET:CE	2:B:569:ILE:HD11	2.49	0.42
2:B:1055:ILE:HG22	2:B:1062:LYS:HD2	2.01	0.42
1:A:252:TRP:CE2	2:B:581:PRO:HD3	2.54	0.42
1:A:546:LEU:HD12	1:A:546:LEU:HA	1.90	0.42
1:A:577:TYR:CE2	1:A:581:MET:HE3	2.54	0.42
1:A:675:MET:HB3	1:A:677:GLU:OE2	2.20	0.42
2:B:522:LEU:HD22	2:B:526:CYS:SG	2.60	0.42
2:B:1055:ILE:HG13	2:B:1055:ILE:H	1.70	0.42
3:C:7:ILE:HD12	3:C:71:TYR:HA	2.00	0.42
1:A:183:ILE:O	1:A:184:SER:CB	2.68	0.42
1:A:341:THR:HG22	1:A:341:THR:O	2.19	0.42
1:A:76:VAL:CG1	1:A:77:ASP:N	2.82	0.42
1:A:418:GLY:HA3	1:A:438:ILE:O	2.20	0.42
3:C:54:LEU:HA	3:C:151:ALA:O	2.20	0.42
1:A:56:TYR:HE1	1:A:109:GLU:OE1	2.02	0.42
2:B:500:PRO:HG2	3:C:20:MET:HE3	2.02	0.42
2:B:674:LYS:O	2:B:678:LEU:HG	2.19	0.42
1:A:231:GLN:HB2	1:A:236:ILE:HG13	2.01	0.41
1:A:367:THR:HB	5:A:831:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ASN:HD21	2:B:453:ASN:ND2	2.17	0.41
2:B:447:GLN:O	2:B:447:GLN:HG2	2.20	0.41
2:B:564:GLN:HB2	2:B:565:PRO:HD2	2.02	0.41
3:C:4:LEU:HB3	3:C:74:LEU:HB3	2.01	0.41
3:C:39:GLN:HA	3:C:39:GLN:NE2	2.35	0.41
1:A:19:PHE:CE2	1:A:40:ALA:HB2	2.55	0.41
1:A:696:LEU:HD12	1:A:703:PRO:HG2	2.00	0.41
1:A:143:ASP:OD2	1:A:376:SER:OG	2.35	0.41
1:A:258:LYS:HA	1:A:304:ASP:O	2.20	0.41
1:A:339:ALA:HB1	1:A:424:VAL:HG21	2.02	0.41
1:A:700:PHE:O	1:A:702:MET:N	2.53	0.41
2:B:348:LEU:O	2:B:348:LEU:CG	2.68	0.41
2:B:654:GLU:HA	2:B:655:PRO:HD3	1.91	0.41
3:C:20:MET:SD	3:C:30:LEU:HD21	2.60	0.41
1:A:22:ASN:HB2	1:A:516:SER:HB2	2.02	0.41
1:A:689:VAL:O	1:A:693:GLN:HG2	2.20	0.41
1:A:722:VAL:O	1:A:723:ASN:CB	2.64	0.41
1:A:78:TYR:CD1	1:A:78:TYR:N	2.88	0.41
1:A:297:GLY:H	1:A:300:MET:HB2	1.85	0.41
1:A:312:SER:H	1:A:315:ASP:HB2	1.84	0.41
1:A:637:LEU:HD22	1:A:722:VAL:HA	2.02	0.41
2:B:358:ASN:CA	2:B:972:GLN:HE22	2.20	0.41
2:B:529:LEU:HD23	2:B:529:LEU:HA	1.88	0.41
2:B:628:SER:HB3	2:B:629:PRO:HD3	2.02	0.41
3:C:4:LEU:HD12	3:C:4:LEU:HA	1.70	0.41
3:C:82:LYS:H	3:C:82:LYS:HG2	1.68	0.41
1:A:140:GLU:OE2	1:A:249:ARG:NH2	2.54	0.41
1:A:310:ILE:H	1:A:310:ILE:CD1	2.26	0.41
1:A:339:ALA:O	1:A:447:LYS:HE3	2.21	0.41
1:A:700:PHE:CD1	1:A:700:PHE:C	2.96	0.41
2:B:515:ASN:O	2:B:519:THR:HG23	2.21	0.41
2:B:573:ILE:HG22	5:B:106:HOH:O	2.20	0.41
2:B:854:ARG:HH11	2:B:854:ARG:HG2	1.84	0.41
1:A:48:ARG:CZ	1:A:51:LEU:HD11	2.51	0.41
1:A:144:LEU:O	1:A:148:LYS:HG3	2.21	0.41
2:B:425:SER:C	2:B:427:THR:N	2.79	0.41
2:B:498:LEU:N	2:B:498:LEU:HD12	2.36	0.41
2:B:1053:TYR:HD1	2:B:1055:ILE:HB	1.85	0.41
3:C:40:LEU:HD23	3:C:72:LEU:HD13	2.03	0.41
1:A:3:THR:HG23	1:A:5:LEU:H	1.86	0.41
1:A:63:ARG:O	1:A:65:THR:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.92	0.41
1:A:531:ILE:HD13	1:A:590:LEU:HD21	2.03	0.41
1:A:662:GLU:O	1:A:665:ALA:HB3	2.21	0.41
2:B:407:LEU:HG	2:B:789:MET:HG3	2.03	0.41
2:B:592:LYS:O	2:B:596:GLN:HG3	2.21	0.41
3:C:62:HIS:O	3:C:73:VAL:HG12	2.21	0.41
1:A:63:ARG:HB2	1:A:90:GLN:CG	2.50	0.41
1:A:660:HIS:HB2	1:A:709:GLU:HB3	2.02	0.41
2:B:573:ILE:HD13	5:B:128:HOH:O	2.21	0.41
2:B:756:GLY:HA2	2:B:793:GLU:HB2	2.02	0.41
2:B:958:LEU:CA	2:B:964:THR:HA	2.42	0.41
3:C:54:LEU:HB2	3:C:61:PHE:HB2	2.03	0.41
1:A:747:VAL:HG12	1:A:748:SER:H	1.86	0.40
2:B:963:ARG:HB3	2:B:965:ILE:CD1	2.50	0.40
2:B:1021:MET:H	2:B:1055:ILE:CG1	2.20	0.40
3:C:128:ASP:OD1	3:C:130:ARG:HG2	2.21	0.40
1:A:283:GLY:CA	1:A:486:GLN:HE22	2.33	0.40
1:A:531:ILE:CD1	1:A:589:PHE:HB3	2.50	0.40
2:B:437:TYR:O	2:B:438:ILE:C	2.62	0.40
2:B:633:ARG:CB	2:B:778:ASN:HD21	2.19	0.40
2:B:641:LEU:HA	2:B:642:PRO:HD3	1.96	0.40
1:A:140:GLU:HB3	5:A:881:HOH:O	2.21	0.40
1:A:551:ILE:O	1:A:555:GLN:HG3	2.21	0.40
2:B:420:LEU:HA	2:B:421:PRO:HD3	1.96	0.40
1:A:586:ARG:CB	1:A:586:ARG:HH11	2.35	0.40
1:A:656:ILE:HD13	1:A:656:ILE:HA	1.92	0.40
2:B:719:TYR:CD2	2:B:719:TYR:C	3.00	0.40
2:B:747:ALA:HB2	2:B:809:TYR:HB3	2.03	0.40
1:A:183:ILE:CG2	1:A:184:SER:N	2.84	0.40
1:A:297:GLY:HA3	1:A:300:MET:HB2	2.02	0.40
2:B:732:GLN:NE2	5:B:126:HOH:O	2.55	0.40
2:B:1054:VAL:O	2:B:1054:VAL:HG12	2.21	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	698/769 (91%)	638 (91%)	46 (7%)	14 (2%)	6	5
2	B	721/753 (96%)	666 (92%)	46 (6%)	9 (1%)	10	12
3	C	129/196 (66%)	113 (88%)	14 (11%)	2 (2%)	7	7
All	All	1548/1718 (90%)	1417 (92%)	106 (7%)	25 (2%)	7	7

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	197	ALA
1	A	508	THR
1	A	509	GLN
2	B	1019	GLN
3	C	4	LEU
1	A	105	ASN
1	A	181	GLU
2	B	447	GLN
2	B	961	SER
2	B	1055	ILE
1	A	58	PRO
2	B	1059	SER
1	A	183	ILE
1	A	747	VAL
2	B	446	ASP
1	A	59	VAL
1	A	476	ARG
1	A	700	PHE
3	C	2	VAL
1	A	184	SER
2	B	960	ILE
2	B	965	ILE
1	A	297	GLY
2	B	1047	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	619/667 (93%)	589 (95%)	30 (5%)	23	35
2	B	660/684 (96%)	631 (96%)	29 (4%)	25	38
3	C	119/171 (70%)	111 (93%)	8 (7%)	15	21
All	All	1398/1522 (92%)	1331 (95%)	67 (5%)	23	35

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	17	VAL
1	A	30	GLU
1	A	41	LEU
1	A	57	GLU
1	A	105	ASN
1	A	153	MET
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	285	ARG
1	A	316	ILE
1	A	355	THR
1	A	400	MET
1	A	451	LEU
1	A	459	ILE
1	A	494	ILE
1	A	508	THR
1	A	544	ARG
1	A	546	LEU
1	A	566	SER
1	A	569	ARG
1	A	570	PHE
1	A	612	LEU

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Mol	Chain	Res	Type
1	A	637	LEU
1	A	649	LEU
1	A	722	VAL
1	A	723	ASN
2	B	359	MET
2	B	382	ASN
2	B	411	LEU
2	B	498	LEU
2	B	522	LEU
2	B	554	HIS
2	B	610	LEU
2	B	641	LEU
2	B	650	LYS
2	B	712	SER
2	B	713	VAL
2	B	773	LEU
2	B	787	VAL
2	B	789	MET
2	B	816	ARG
2	B	857	THR
2	B	906	LEU
2	B	920	LEU
2	B	935	LEU
2	B	955	GLU
2	B	958	LEU
2	B	964	THR
2	B	1001	THR
2	B	1002	GLN
2	B	1048	PHE
2	B	1052	LEU
2	B	1057	ASP
2	B	1075	GLU
2	B	1085	LEU
3	C	3	LEU
3	C	31	GLN
3	C	67	GLN
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS
3	C	127	ILE
3	C	153	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	113	GLN
1	A	126	GLN
1	A	174	GLN
1	A	227	ASN
1	A	248	GLN
1	A	296	GLN
1	A	314	HIS
1	A	320	ASN
1	A	330	HIS
1	A	397	GLN
1	A	436	ASN
1	A	486	GLN
1	A	509	GLN
1	A	549	GLN
1	A	579	GLN
1	A	583	HIS
1	A	595	ASN
1	A	614	GLN
1	A	620	GLN
1	A	666	GLN
1	A	673	GLN
1	A	710	HIS
1	A	714	GLN
1	A	723	ASN
2	B	355	GLN
2	B	358	ASN
2	B	373	HIS
2	B	382	ASN
2	B	412	HIS
2	B	439	ASN
2	B	515	ASN
2	B	559	GLN
2	B	566	GLN
2	B	589	ASN
2	B	604	GLN
2	B	621	GLN
2	B	683	GLN
2	B	732	GLN
2	B	760	HIS
2	B	778	ASN
2	B	788	GLN

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Mol	Chain	Res	Type
2	B	913	GLN
2	B	967	GLN
2	B	1090	GLN
2	B	1092	ASN
3	C	32	GLN
3	C	39	GLN
3	C	99	HIS
3	C	152	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	708/769 (92%)	0.53	73 (10%) 12 13	22, 44, 85, 115	0
2	B	729/753 (96%)	0.28	52 (7%) 22 24	20, 37, 80, 112	0
3	C	135/196 (68%)	1.14	22 (16%) 4 5	36, 66, 101, 122	0
All	All	1572/1718 (91%)	0.47	147 (9%) 14 15	20, 42, 86, 122	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	957	ALA	5.3
2	B	1055	ILE	5.2
1	A	49	PRO	5.2
2	B	446	ASP	5.1
3	C	2	VAL	4.8
1	A	56	TYR	4.6
2	B	1061	MET	4.6
1	A	180	CYS	4.3
2	B	1057	ASP	4.3
1	A	205	GLY	4.3
1	A	181	GLU	4.2
1	A	665	ALA	4.2
2	B	771	THR	4.2
2	B	427	THR	4.1
1	A	675	MET	4.0
1	A	672	TYR	3.9
2	B	959	ASN	3.9
1	A	182	GLY	3.7
1	A	678	TYR	3.7
1	A	670	SER	3.7
1	A	679	GLU	3.7
2	B	425	SER	3.7
1	A	695	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	958	LEU	3.6
2	B	1056	ARG	3.6
2	B	916	THR	3.6
1	A	94	PHE	3.5
1	A	667	TRP	3.4
2	B	915	GLY	3.4
2	B	881	SER	3.4
2	B	662	LYS	3.4
3	C	86	ALA	3.3
1	A	664	ILE	3.3
2	B	960	ILE	3.2
3	C	156	VAL	3.2
1	A	674	ASP	3.2
1	A	676	PRO	3.2
3	C	148	ILE	3.2
2	B	660	SER	3.2
1	A	510	ILE	3.2
2	B	426	SER	3.1
2	B	661	ALA	3.1
1	A	508	THR	3.1
2	B	464	GLU	3.0
1	A	764	ALA	3.0
2	B	462	PRO	3.0
2	B	609	THR	3.0
1	A	723	ASN	3.0
1	A	58	PRO	3.0
1	A	34	MET	2.9
1	A	57	GLU	2.9
2	B	954	ASP	2.9
1	A	631	PRO	2.9
3	C	127	ILE	2.9
2	B	1060	PRO	2.9
3	C	101	LYS	2.9
1	A	652	THR	2.9
2	B	1001	THR	2.9
2	B	1048	PHE	2.8
1	A	762	SER	2.8
1	A	507	GLN	2.8
1	A	104	LEU	2.8
2	B	1011	VAL	2.8
3	C	23	ASP	2.8
1	A	124	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	128	ASP	2.8
3	C	1	MET	2.8
1	A	671	GLY	2.7
1	A	541	ASP	2.7
2	B	424	THR	2.7
2	B	1058	GLU	2.7
3	C	30	LEU	2.7
1	A	692	ALA	2.7
2	B	882	VAL	2.7
1	A	628	PHE	2.7
1	A	50	ASP	2.7
1	A	65	THR	2.7
1	A	536	THR	2.6
2	B	956	GLY	2.6
1	A	53	PRO	2.6
2	B	445	LEU	2.6
1	A	663	THR	2.6
1	A	196	SER	2.6
1	A	509	GLN	2.5
2	B	976	GLU	2.5
1	A	63	ARG	2.5
1	A	544	ARG	2.5
3	C	149	MET	2.5
2	B	888	PRO	2.5
3	C	33	TYR	2.5
1	A	116	SER	2.5
1	A	435	GLU	2.4
2	B	798	THR	2.4
1	A	102	SER	2.4
2	B	348	LEU	2.4
1	A	505	ASP	2.4
3	C	80	PRO	2.4
3	C	81	LYS	2.4
1	A	683	HIS	2.4
1	A	476	ARG	2.4
2	B	347	GLY	2.4
1	A	700	PHE	2.4
1	A	747	VAL	2.4
2	B	569	ILE	2.4
2	B	955	GLU	2.4
3	C	76	GLU	2.4
2	B	770	SER	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	1063	ALA	2.3
3	C	77	ALA	2.3
3	C	151	ALA	2.3
1	A	593	PHE	2.3
2	B	461	VAL	2.3
2	B	1000	CYS	2.3
1	A	669	LYS	2.3
3	C	90	ASP	2.3
1	A	78	TYR	2.3
2	B	346	GLU	2.2
1	A	62	SER	2.2
2	B	1025	PRO	2.2
3	C	56	ALA	2.2
1	A	431	PRO	2.2
1	A	537	GLU	2.2
2	B	1019	GLN	2.2
1	A	89	TYR	2.2
1	A	394	MET	2.2
1	A	297	GLY	2.2
3	C	98	GLN	2.2
1	A	93	GLN	2.1
1	A	227	ASN	2.1
2	B	917	ASN	2.1
1	A	48	ARG	2.1
1	A	123	ARG	2.1
1	A	68	ALA	2.1
3	C	3	LEU	2.1
1	A	32	THR	2.1
1	A	629	SER	2.1
1	A	183	ILE	2.1
3	C	29	ASP	2.1
1	A	668	ARG	2.1
1	A	55	GLN	2.0
2	B	478	HIS	2.0
1	A	746	ASP	2.0
2	B	769	ARG	2.0
2	B	979	SER	2.0
2	B	1074	THR	2.0
2	B	604	GLN	2.0
1	A	638	ASP	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	ZN	A	800	1/1	0.99	0.06	54,54,54,54	0
4	ZN	B	1100	1/1	0.99	0.02	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.