



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 03:54 PM EDT

PDB ID : 3EG9 / pdb_00003eg9
Title : Crystal structure of the mammalian COPII-coat protein Sec23/24 bound to the transport signal sequence of membrin
Authors : Goldberg, J.; Mancias, J.D.
Deposited on : 2008-09-10
Resolution : 3.00 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

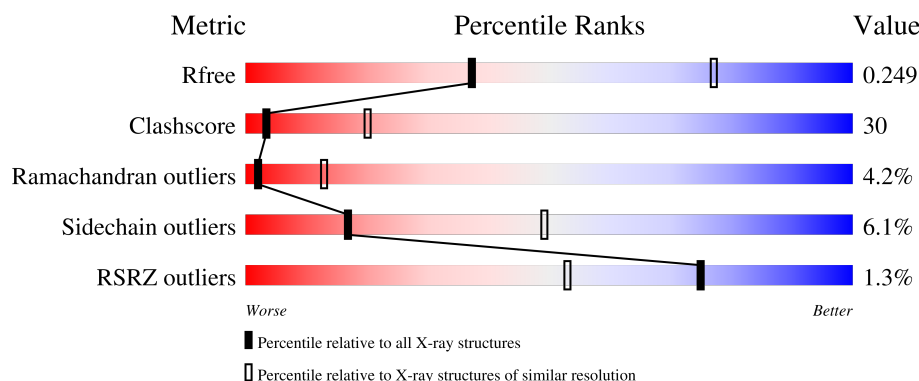
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	14% 49% 39% 5% • 5%
2	B	770	48% 42% 8% •
3	C	7	29% 57% 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11956 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	726	Total	C	N	O	S	0	0	0
			5764	3672	992	1060	40			

- Molecule 2 is a protein called SEC24 related gene family, member D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	767	Total	C	N	O	S	0	0	0
			6038	3841	1024	1119	54			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP Q8IYI7
B	2	MET	-	expression tag	UNP Q8IYI7
B	3	GLY	-	expression tag	UNP Q8IYI7

- Molecule 3 is a protein called peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	6	Total	C	N	O	S	0	0	0
			45	28	6	10	1			

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

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

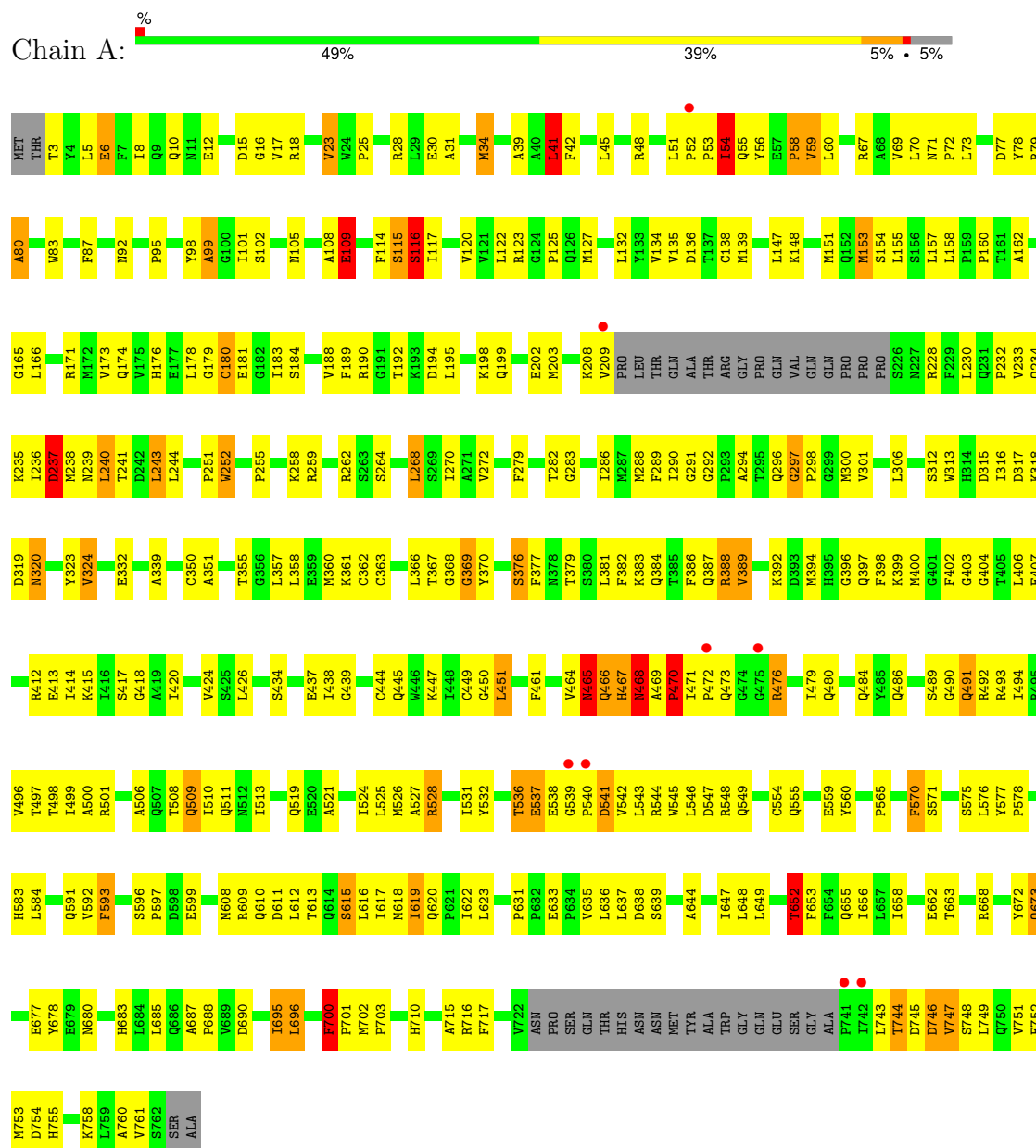
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total 51	O 51	0	0
5	B	55	Total 55	O 55	0	0
5	C	1	Total 1	O 1	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



• Molecule 2: SEC24 related gene family, member D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.13Å 140.75Å 152.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 95.8 (50.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.254 0.199 , 0.249	Depositor DCC
R_{free} test set	2241 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.636	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11956	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	0.45	0/5901	1.03	35/7995 (0.4%)
2	B	0.46	0/6166	1.02	38/8351 (0.5%)
3	C	0.54	0/45	0.74	0/61
All	All	0.46	0/12112	1.02	73/16407 (0.4%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	N-CA-C	-13.11	90.32	109.59
2	B	858	SER	N-CA-C	11.13	123.41	108.38
1	A	652	THR	N-CA-C	-10.52	95.84	110.35
2	B	543	GLN	N-CA-C	8.79	120.63	111.14
1	A	367	THR	N-CA-C	-8.52	96.78	110.32
1	A	228	ARG	N-CA-C	-8.23	103.24	113.28
1	A	55	GLN	N-CA-C	8.22	123.44	107.98
1	A	700	PHE	CA-C-N	-8.09	109.73	119.84
1	A	700	PHE	C-N-CA	-8.09	109.73	119.84
2	B	877	MET	N-CA-C	7.65	120.75	110.35
1	A	369	GLY	N-CA-C	7.46	122.24	112.25
1	A	541	ASP	N-CA-C	-7.27	104.41	113.20
2	B	339	LYS	CA-C-N	7.15	128.77	119.84
2	B	339	LYS	C-N-CA	7.15	128.77	119.84
1	A	135	VAL	N-CA-C	7.09	118.50	108.36
1	A	465	ASN	N-CA-C	-6.82	96.27	110.80
1	A	58	PRO	N-CA-C	6.80	122.83	113.65
2	B	730	VAL	N-CA-C	6.78	117.63	107.80
1	A	23	VAL	N-CA-C	-6.74	99.03	108.27
1	A	472	PRO	N-CA-C	-6.69	104.88	114.18
2	B	447	ILE	N-CA-C	6.64	117.69	107.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	454	ILE	N-CA-C	-6.36	104.84	111.58
2	B	864	THR	N-CA-C	-6.28	104.44	111.28
1	A	468	ASN	N-CA-C	6.28	124.17	110.80
2	B	996	GLN	CA-C-N	-6.26	113.23	119.56
2	B	996	GLN	C-N-CA	-6.26	113.23	119.56
2	B	859	ARG	N-CA-C	6.26	123.64	109.81
2	B	473	ILE	CA-C-N	6.12	126.14	119.90
2	B	473	ILE	C-N-CA	6.12	126.14	119.90
2	B	667	MET	N-CA-C	6.11	118.45	111.11
1	A	34	MET	N-CA-C	-6.09	104.48	113.61
1	A	592	VAL	N-CA-C	6.07	116.85	110.72
2	B	584	SER	N-CA-C	6.03	118.12	109.14
1	A	176	HIS	N-CA-C	6.00	118.96	109.96
2	B	338	ILE	N-CA-C	5.89	116.35	107.75
2	B	878	GLY	N-CA-C	-5.89	103.28	112.58
2	B	326	MET	N-CA-C	-5.84	104.60	110.97
2	B	948	PRO	N-CA-C	5.82	121.20	113.57
2	B	523	LEU	N-CA-C	-5.75	98.54	110.80
2	B	505	ALA	N-CA-C	-5.65	105.88	112.89
2	B	896	LEU	N-CA-C	5.62	118.47	110.10
2	B	618	VAL	N-CA-C	5.61	116.39	110.72
1	A	490	GLY	N-CA-C	-5.61	108.02	114.69
1	A	41	LEU	N-CA-C	-5.60	100.06	108.96
2	B	2	MET	N-CA-C	5.55	119.14	110.32
1	A	252	TRP	CA-C-N	5.52	125.46	119.78
1	A	252	TRP	C-N-CA	5.52	125.46	119.78
2	B	986	MET	N-CA-C	5.51	117.84	110.35
1	A	6	GLU	N-CA-C	-5.44	105.43	111.36
2	B	562	ILE	N-CA-C	-5.42	105.09	110.62
2	B	522	LEU	N-CA-C	5.38	116.97	108.96
1	A	444	CYS	N-CA-C	-5.37	105.36	112.94
1	A	42	PHE	N-CA-C	5.37	117.16	108.41
2	B	491	TYR	N-CA-C	5.35	116.28	108.14
1	A	363	CYS	CA-C-N	-5.35	114.16	119.56
1	A	363	CYS	C-N-CA	-5.35	114.16	119.56
1	A	593	PHE	N-CA-C	5.33	122.16	110.80
2	B	469	MET	N-CA-C	5.32	118.00	111.82
1	A	399	LYS	N-CA-C	-5.29	105.52	112.72
1	A	571	SER	N-CA-C	-5.29	103.50	110.43
2	B	949	SER	N-CA-C	5.29	117.02	109.14
2	B	409	ARG	N-CA-C	5.27	122.02	110.80
1	A	171	ARG	N-CA-C	-5.25	105.73	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	525	GLY	N-CA-C	-5.25	107.29	114.64
2	B	982	ARG	CA-C-N	5.24	124.42	118.97
2	B	982	ARG	C-N-CA	5.24	124.42	118.97
2	B	635	LEU	N-CA-C	5.23	117.05	108.52
1	A	715	ALA	N-CA-C	-5.23	105.70	111.71
2	B	685	LYS	N-CA-C	-5.20	101.95	109.59
2	B	1005	LEU	N-CA-C	-5.16	102.71	110.70
1	A	318	LYS	N-CA-C	-5.09	107.10	113.15
1	A	388	ARG	N-CA-C	-5.03	106.41	112.54
1	A	286	ILE	N-CA-C	-5.00	100.05	107.51

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	5764	0	5715	297	0
2	B	6038	0	6038	420	0
3	C	45	0	44	11	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	51	0	0	7	0
5	B	55	0	0	7	0
5	C	1	0	0	1	0
All	All	11956	0	11797	712	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 30.

All (712) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:MET:HE2	3:C:118:ILE:HD11	1.36	1.06
2:B:317:THR:HG22	2:B:319:CYS:H	1.23	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:SER:HB2	2:B:908:ARG:HE	1.22	1.01
1:A:147:LEU:HG	1:A:151:MET:HE2	1.43	0.99
2:B:639:PRO:HB3	2:B:643:VAL:HG21	1.42	0.97
2:B:469:MET:HE1	2:B:678:LEU:HG	1.48	0.96
1:A:54:ILE:HG13	1:A:54:ILE:O	1.65	0.95
2:B:996:GLN:HB3	2:B:997:PRO:HD2	1.47	0.94
1:A:51:LEU:HD12	1:A:52:PRO:HD2	1.51	0.93
2:B:633:VAL:H	2:B:655:THR:HG21	1.35	0.91
2:B:713:ASN:HD21	2:B:716:ASP:H	1.12	0.90
1:A:123:ARG:HG3	1:A:125:PRO:HD2	1.53	0.90
1:A:528:ARG:HA	1:A:608:MET:HE1	1.51	0.89
2:B:446:MET:HE3	2:B:561:VAL:HG12	1.53	0.89
2:B:453:ASN:ND2	2:B:583:SER:HB3	1.89	0.88
2:B:453:ASN:HD21	2:B:583:SER:HB3	1.36	0.88
1:A:381:LEU:HA	1:A:702:MET:HE2	1.57	0.87
2:B:901:THR:HG22	2:B:902:MET:H	1.36	0.87
2:B:743:GLY:HA2	2:B:770:CYS:HB2	1.57	0.87
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.56	0.86
2:B:802:PRO:HB2	2:B:805:VAL:HG23	1.55	0.85
1:A:3:THR:HB	1:A:6:GLU:HG3	1.58	0.85
1:A:283:GLY:H	1:A:486:GLN:HE22	1.20	0.85
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.59	0.85
1:A:381:LEU:HA	1:A:702:MET:CE	2.06	0.84
2:B:963:VAL:HG12	2:B:964:GLY:H	1.43	0.84
2:B:454:ILE:HD13	2:B:459:VAL:HG21	1.60	0.83
2:B:469:MET:HE3	2:B:679:ARG:HA	1.59	0.82
2:B:283:VAL:HG22	2:B:301:MET:HE2	1.61	0.82
2:B:469:MET:HE2	2:B:682:ILE:HD12	1.62	0.82
1:A:596:SER:OG	1:A:599:GLU:HG3	1.79	0.82
2:B:462:ILE:O	2:B:466:LEU:HB2	1.81	0.81
2:B:595:LYS:H	2:B:615:GLN:HE22	1.28	0.81
1:A:236:ILE:HG22	1:A:240:LEU:HB2	1.62	0.81
1:A:747:VAL:HG12	1:A:748:SER:H	1.43	0.81
1:A:153:MET:HE2	1:A:154:SER:HA	1.61	0.80
2:B:500:VAL:HG11	2:B:537:ILE:HG12	1.62	0.80
2:B:1030:GLN:C	2:B:1032:LEU:H	1.87	0.79
2:B:404:ASP:OD2	2:B:410:LEU:HB2	1.83	0.79
2:B:1000:VAL:HA	2:B:1003:GLN:HE21	1.45	0.79
2:B:2:MET:CE	2:B:836:LEU:HD12	2.13	0.78
1:A:115:SER:O	1:A:116:SER:HB2	1.83	0.78
2:B:355:ASN:ND2	2:B:357:GLY:H	1.80	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:ASN:ND2	2:B:716:ASP:H	1.81	0.78
2:B:996:GLN:HB3	2:B:997:PRO:CD	2.13	0.77
2:B:267:SER:HB2	2:B:908:ARG:NE	1.99	0.77
2:B:523:LEU:O	2:B:524:ASP:HB2	1.84	0.77
1:A:30:GLU:CD	1:A:506:ALA:HB3	2.10	0.76
2:B:633:VAL:H	2:B:655:THR:CG2	1.99	0.75
1:A:312:SER:O	1:A:316:ILE:HG22	1.87	0.75
1:A:656:ILE:HD11	1:A:695:ILE:HD13	1.68	0.75
2:B:2:MET:HG2	2:B:1017:TYR:OH	1.86	0.75
1:A:745:ASP:CG	1:A:746:ASP:H	1.96	0.74
2:B:269:ILE:HD11	2:B:907:VAL:C	2.12	0.74
1:A:511:GLN:CD	1:A:511:GLN:H	1.94	0.74
2:B:345:PRO:HB2	2:B:348:GLU:HG3	1.68	0.73
2:B:637:LEU:HG	2:B:639:PRO:HD3	1.69	0.73
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.70	0.73
2:B:356:HIS:HD2	2:B:362:VAL:H	1.36	0.73
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.03	0.72
1:A:238:MET:O	1:A:241:THR:HG22	1.90	0.72
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.72	0.72
2:B:600:LYS:O	2:B:600:LYS:HG3	1.90	0.71
2:B:852:LYS:HE3	2:B:1015:SER:O	1.90	0.71
1:A:407:GLU:HG3	1:A:445:GLN:HG3	1.70	0.71
2:B:600:LYS:HA	2:B:859:ARG:NH1	2.05	0.71
2:B:469:MET:HE1	2:B:678:LEU:CG	2.20	0.71
2:B:933:GLY:O	2:B:936:SER:HB2	1.89	0.71
2:B:795:PHE:HB3	2:B:875:MET:HE1	1.73	0.71
2:B:600:LYS:HD2	2:B:602:LEU:HD21	1.72	0.71
2:B:312:PHE:CZ	2:B:344:ILE:HD11	2.25	0.71
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.72	0.71
1:A:195:LEU:CD2	1:A:203:MET:HE1	2.21	0.70
2:B:378:ILE:HG12	2:B:383:ARG:O	1.91	0.70
2:B:901:THR:HB	2:B:973:MET:HE1	1.73	0.70
1:A:583:HIS:HD2	1:A:620:GLN:HE21	1.40	0.70
2:B:943:GLY:O	2:B:968:SER:HB2	1.91	0.70
2:B:686:ILE:HG22	2:B:723:ASP:HB3	1.73	0.70
1:A:283:GLY:N	1:A:486:GLN:HE22	1.89	0.70
1:A:190:ARG:HH12	2:B:519:PHE:HB3	1.57	0.70
2:B:2:MET:HE1	2:B:836:LEU:HD12	1.73	0.69
2:B:599:ASP:HB3	2:B:601:LYS:HG3	1.72	0.69
1:A:565:PRO:HG3	1:A:758:LYS:HA	1.75	0.69
2:B:605:THR:C	2:B:607:LYS:H	1.97	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:C	1:A:470:PRO:HD3	2.18	0.69
2:B:837:PRO:HG2	2:B:840:MET:HG3	1.74	0.69
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.29	0.68
1:A:3:THR:HG22	1:A:5:LEU:H	1.58	0.68
1:A:181:GLU:HG2	1:A:239:ASN:HD21	1.58	0.68
1:A:418:GLY:HA3	1:A:438:ILE:O	1.92	0.68
2:B:456:ASN:OD1	2:B:458:LEU:HB2	1.94	0.68
2:B:719:MET:SD	2:B:722:ILE:HD12	2.34	0.68
1:A:577:TYR:HB3	1:A:578:PRO:HD3	1.75	0.68
2:B:605:THR:HG22	2:B:607:LYS:HB3	1.75	0.67
2:B:269:ILE:HD11	2:B:908:ARG:N	2.10	0.67
2:B:616:THR:HB	2:B:618:VAL:HG22	1.77	0.67
1:A:179:GLY:O	1:A:181:GLU:HG3	1.95	0.67
1:A:466:GLN:O	1:A:468:ASN:N	2.27	0.67
2:B:500:VAL:HG11	2:B:537:ILE:CG1	2.25	0.67
2:B:842:VAL:HG12	2:B:842:VAL:O	1.95	0.67
2:B:963:VAL:O	2:B:964:GLY:O	2.13	0.67
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.77	0.67
2:B:601:LYS:HB3	2:B:605:THR:HG21	1.77	0.67
2:B:614:PRO:HG3	2:B:650:LEU:HD22	1.77	0.67
1:A:583:HIS:CD2	1:A:620:GLN:HG3	2.30	0.66
1:A:583:HIS:CD2	1:A:620:GLN:HE21	2.13	0.66
2:B:267:SER:CB	2:B:908:ARG:HE	2.05	0.66
2:B:501:LYS:CD	2:B:503:ASN:HD21	2.09	0.66
2:B:941:ILE:HG23	2:B:953:ILE:HD11	1.76	0.66
1:A:743:LEU:O	1:A:744:THR:HB	1.95	0.66
2:B:713:ASN:C	2:B:713:ASN:HD22	2.03	0.66
1:A:153:MET:HE2	1:A:154:SER:CA	2.25	0.66
1:A:153:MET:HE3	1:A:157:LEU:CD1	2.26	0.66
2:B:963:VAL:HG12	2:B:964:GLY:N	2.09	0.66
2:B:845:VAL:HG22	2:B:1017:TYR:CZ	2.31	0.66
1:A:673:GLN:HG2	1:A:685:LEU:HD12	1.77	0.65
2:B:2:MET:SD	2:B:3:GLY:N	2.69	0.65
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.78	0.65
1:A:30:GLU:OE1	1:A:506:ALA:HB3	1.96	0.65
1:A:369:GLY:O	1:A:609:ARG:NH2	2.29	0.65
2:B:775:ALA:O	2:B:779:LYS:HG3	1.96	0.65
2:B:835:ILE:HD13	3:C:117:THR:HG23	1.77	0.65
2:B:860:PRO:O	2:B:861:GLU:HB2	1.95	0.65
2:B:971:LEU:HD12	2:B:974:ILE:HD11	1.79	0.65
1:A:652:THR:HG23	1:A:655:GLN:H	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:MET:CE	2:B:678:LEU:HG	2.25	0.65
2:B:355:ASN:C	2:B:355:ASN:HD22	2.04	0.65
2:B:446:MET:CE	2:B:561:VAL:HG12	2.27	0.65
2:B:992:LYS:HD2	2:B:996:GLN:NE2	2.11	0.65
1:A:700:PHE:O	1:A:702:MET:N	2.30	0.64
2:B:802:PRO:HD2	2:B:805:VAL:HG21	1.78	0.64
1:A:190:ARG:NH1	2:B:519:PHE:HB3	2.13	0.64
2:B:334:LEU:H	2:B:334:LEU:HD22	1.62	0.64
2:B:974:ILE:HA	2:B:977:ILE:HG22	1.78	0.64
2:B:469:MET:HE3	2:B:679:ARG:CA	2.27	0.64
2:B:901:THR:HG22	2:B:902:MET:N	2.09	0.64
1:A:297:GLY:H	1:A:300:MET:HE3	1.63	0.64
2:B:901:THR:HG22	2:B:903:LEU:H	1.62	0.64
1:A:656:ILE:HG13	1:A:695:ILE:HG21	1.79	0.63
2:B:945:PHE:HE2	2:B:990:ILE:HD13	1.63	0.63
3:C:116:THR:N	5:C:4:HOH:O	2.31	0.63
1:A:492:ARG:HD3	5:A:811:HOH:O	1.98	0.63
1:A:297:GLY:CA	1:A:300:MET:HB2	2.29	0.63
2:B:633:VAL:HG13	2:B:655:THR:HG21	1.80	0.63
2:B:893:ILE:O	2:B:896:LEU:HB2	1.97	0.63
1:A:127:MET:HE2	1:A:127:MET:HA	1.80	0.63
2:B:602:LEU:N	2:B:605:THR:OG1	2.32	0.63
2:B:543:GLN:HB3	2:B:547:MET:HE3	1.80	0.62
2:B:602:LEU:HA	2:B:608:GLU:HB2	1.80	0.62
1:A:700:PHE:O	1:A:701:PRO:C	2.40	0.62
2:B:321:PRO:HG2	2:B:734:HIS:HE1	1.63	0.62
1:A:190:ARG:HB3	1:A:192:THR:HG22	1.80	0.62
2:B:601:LYS:O	2:B:608:GLU:HA	2.00	0.62
2:B:633:VAL:CG1	2:B:655:THR:HG21	2.29	0.62
2:B:602:LEU:N	2:B:602:LEU:HD23	2.13	0.62
1:A:199:GLN:HB3	1:A:203:MET:HE2	1.81	0.62
2:B:902:MET:O	2:B:902:MET:HG2	1.99	0.62
1:A:290:ILE:HD13	1:A:360:MET:HE1	1.82	0.61
2:B:374:PHE:CE2	2:B:765:ASN:HB3	2.35	0.61
2:B:641:GLN:HG2	2:B:642:TYR:N	2.16	0.61
1:A:746:ASP:HB3	5:A:840:HOH:O	1.99	0.61
2:B:453:ASN:O	2:B:459:VAL:HG23	2.01	0.61
1:A:25:PRO:CG	1:A:31:ALA:HB2	2.30	0.60
1:A:609:ARG:HG3	1:A:609:ARG:HH11	1.66	0.60
2:B:922:LEU:C	2:B:922:LEU:HD23	2.26	0.60
1:A:297:GLY:N	1:A:300:MET:HB2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:MET:HE3	2:B:836:LEU:HD12	1.82	0.60
1:A:116:SER:N	5:A:805:HOH:O	2.34	0.60
1:A:153:MET:HE3	1:A:157:LEU:HD11	1.83	0.60
1:A:160:PRO:HB3	1:A:234:GLN:HB3	1.83	0.60
2:B:492:ASN:O	2:B:493:LYS:HG2	2.01	0.60
2:B:602:LEU:HD11	2:B:859:ARG:HB2	1.84	0.60
1:A:638:ASP:OD1	1:A:639:SER:N	2.35	0.60
2:B:814:THR:HA	2:B:817:MET:HE3	1.82	0.60
1:A:155:LEU:HD12	1:A:158:LEU:HD12	1.83	0.60
2:B:600:LYS:HD2	2:B:602:LEU:CD2	2.31	0.60
1:A:123:ARG:HG2	5:A:811:HOH:O	2.01	0.60
1:A:412:ARG:HG3	1:A:413:GLU:OE2	2.02	0.60
2:B:835:ILE:O	2:B:836:LEU:HD23	2.01	0.60
1:A:116:SER:HA	1:A:496:VAL:O	2.02	0.59
2:B:403:LEU:HB3	2:B:407:GLY:HA2	1.84	0.59
2:B:470:LEU:HD12	2:B:473:ILE:HD11	1.84	0.59
1:A:559:GLU:O	1:A:560:TYR:HB3	2.02	0.59
2:B:690:ALA:HB2	2:B:752:TYR:HB3	1.83	0.59
2:B:992:LYS:HD2	2:B:996:GLN:HE21	1.67	0.59
2:B:997:PRO:O	2:B:999:MET:N	2.35	0.59
1:A:283:GLY:H	1:A:486:GLN:NE2	1.97	0.59
1:A:745:ASP:O	1:A:747:VAL:HG23	2.02	0.59
2:B:1030:GLN:C	2:B:1032:LEU:N	2.58	0.59
2:B:693:ARG:HG3	2:B:693:ARG:HH11	1.68	0.59
1:A:291:GLY:O	1:A:351:ALA:HB2	2.03	0.59
1:A:617:ILE:HG12	1:A:622:ILE:HD11	1.84	0.59
1:A:72:PRO:HD3	1:A:109:GLU:O	2.02	0.59
2:B:901:THR:HB	2:B:970:GLN:HE21	1.68	0.59
2:B:434:LYS:O	2:B:436:LYS:HG3	2.03	0.58
2:B:453:ASN:CG	2:B:583:SER:HB3	2.28	0.58
1:A:54:ILE:HD12	1:A:56:TYR:CZ	2.38	0.58
1:A:58:PRO:O	1:A:59:VAL:HB	2.02	0.58
1:A:148:LYS:HA	1:A:151:MET:HE3	1.84	0.58
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.84	0.58
1:A:536:THR:HG22	1:A:537:GLU:N	2.17	0.58
1:A:745:ASP:CG	1:A:746:ASP:N	2.61	0.58
2:B:406:ILE:HG22	2:B:406:ILE:O	2.03	0.58
1:A:312:SER:H	1:A:315:ASP:HB2	1.69	0.58
2:B:964:GLY:HA3	2:B:968:SER:HB3	1.86	0.58
1:A:53:PRO:O	1:A:54:ILE:C	2.47	0.58
2:B:356:HIS:CD2	2:B:361:PRO:HA	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:LYS:HD3	2:B:503:ASN:HD21	1.68	0.58
2:B:641:GLN:HG2	2:B:642:TYR:H	1.69	0.58
2:B:955:THR:C	2:B:957:MET:H	2.12	0.58
2:B:974:ILE:HA	2:B:977:ILE:CG2	2.33	0.58
1:A:183:ILE:HD11	2:B:509:MET:HB2	1.86	0.58
2:B:854:CYS:O	2:B:867:ARG:HD2	2.04	0.58
2:B:898:VAL:O	2:B:899:LYS:C	2.46	0.58
1:A:560:TYR:CD1	1:A:761:VAL:HG12	2.39	0.58
2:B:713:ASN:ND2	2:B:715:THR:H	2.02	0.58
2:B:492:ASN:O	2:B:492:ASN:OD1	2.22	0.58
2:B:898:VAL:HG22	2:B:967:TYR:CE2	2.39	0.58
1:A:134:VAL:HG11	1:A:288:MET:HE3	1.85	0.57
1:A:297:GLY:H	1:A:300:MET:HB2	1.68	0.57
2:B:494:VAL:HG22	2:B:513:THR:HA	1.86	0.57
2:B:845:VAL:HG22	2:B:1017:TYR:CE1	2.38	0.57
2:B:962:GLU:HG2	2:B:963:VAL:N	2.18	0.57
2:B:975:MET:HE1	2:B:988:LEU:HD22	1.86	0.57
1:A:696:LEU:HD12	1:A:703:PRO:HG2	1.87	0.57
2:B:371:MET:HB3	2:B:425:TYR:OH	2.04	0.57
2:B:835:ILE:CD1	3:C:117:THR:HG23	2.34	0.57
2:B:1027:GLU:O	2:B:1031:LEU:HG	2.05	0.57
1:A:539:GLY:O	1:A:542:VAL:HG23	2.04	0.57
2:B:665:PHE:HE2	2:B:667:MET:HE2	1.70	0.57
2:B:345:PRO:HD2	2:B:348:GLU:OE1	2.05	0.57
1:A:612:LEU:C	1:A:612:LEU:HD23	2.30	0.57
2:B:641:GLN:O	2:B:643:VAL:HG23	2.04	0.57
1:A:744:THR:HG21	1:A:752:PHE:HD1	1.70	0.57
2:B:854:CYS:HB3	2:B:862:ILE:HD13	1.87	0.57
1:A:162:ALA:O	1:A:233:VAL:HG23	2.05	0.56
1:A:466:GLN:OE1	1:A:466:GLN:HA	2.04	0.56
2:B:410:LEU:O	2:B:410:LEU:HG	2.05	0.56
2:B:493:LYS:HA	2:B:557:VAL:HG13	1.87	0.56
2:B:993:GLN:HG2	2:B:994:ARG:N	2.20	0.56
1:A:536:THR:C	1:A:538:GLU:H	2.14	0.56
2:B:356:HIS:HE1	2:B:417:GLU:OE2	1.88	0.56
2:B:605:THR:C	2:B:607:LYS:N	2.63	0.56
2:B:333:PRO:HD3	2:B:813:GLN:NE2	2.21	0.56
2:B:934:VAL:HG23	2:B:935:SER:N	2.19	0.56
2:B:965:ASN:HB3	2:B:966:PRO:HD3	1.86	0.56
2:B:775:ALA:HB1	2:B:779:LYS:HE3	1.87	0.56
1:A:545:TRP:O	1:A:549:GLN:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:616:THR:HG22	2:B:617:ASN:N	2.21	0.56
2:B:639:PRO:CB	2:B:643:VAL:HG21	2.28	0.56
1:A:77:ASP:OD2	1:A:80:ALA:HB3	2.06	0.55
1:A:506:ALA:O	1:A:510:ILE:HG13	2.06	0.55
2:B:766:LEU:CD2	2:B:768:LEU:HD21	2.36	0.55
2:B:948:PRO:HG2	2:B:952:HIS:ND1	2.21	0.55
2:B:838:ASP:HA	2:B:841:LYS:HG3	1.87	0.55
2:B:605:THR:HG22	2:B:607:LYS:CB	2.36	0.55
2:B:652:PRO:HA	2:B:655:THR:HG22	1.88	0.55
2:B:928:MET:O	2:B:988:LEU:HD12	2.06	0.55
1:A:8:ILE:HG21	1:A:18:ARG:NH2	2.21	0.55
2:B:948:PRO:HG2	2:B:952:HIS:CE1	2.42	0.55
2:B:963:VAL:CG1	2:B:964:GLY:H	2.15	0.55
2:B:852:LYS:HE2	2:B:1008:ASP:O	2.06	0.55
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.72	0.55
1:A:404:GLY:HA2	1:A:484:GLN:O	2.07	0.55
1:A:30:GLU:HB3	5:A:835:HOH:O	2.06	0.55
1:A:510:ILE:HB	1:A:511:GLN:NE2	2.22	0.55
1:A:673:GLN:HG2	1:A:685:LEU:CD1	2.36	0.55
2:B:616:THR:HG21	5:B:1107:HOH:O	2.06	0.55
2:B:854:CYS:CB	2:B:862:ILE:HD13	2.36	0.55
1:A:115:SER:O	1:A:116:SER:CB	2.52	0.55
1:A:290:ILE:CD1	1:A:360:MET:HE1	2.37	0.54
2:B:269:ILE:CD1	2:B:908:ARG:N	2.70	0.54
2:B:458:LEU:HD21	2:B:638:PHE:CD2	2.43	0.54
2:B:992:LYS:HB2	2:B:996:GLN:HE21	1.72	0.54
2:B:859:ARG:HB3	2:B:860:PRO:HD3	1.90	0.54
2:B:340:PRO:HB2	2:B:341:PHE:HD1	1.72	0.54
2:B:616:THR:HG22	2:B:617:ASN:H	1.73	0.54
2:B:971:LEU:O	2:B:974:ILE:HG12	2.07	0.54
1:A:350:CYS:HB2	1:A:377:PHE:CE1	2.42	0.54
2:B:833:GLN:CD	3:C:117:THR:HG21	2.33	0.54
1:A:491:GLN:HG2	1:A:493:ARG:HE	1.73	0.54
1:A:536:THR:O	1:A:538:GLU:N	2.41	0.54
2:B:606:ASP:HA	2:B:802:PRO:HG3	1.90	0.54
2:B:526:PHE:O	2:B:527:LEU:HB2	2.09	0.54
2:B:685:LYS:HG3	5:B:1116:HOH:O	2.07	0.53
2:B:355:ASN:HD22	2:B:356:HIS:N	2.06	0.53
2:B:974:ILE:O	2:B:978:ILE:HG13	2.07	0.53
2:B:529:ASN:HD21	2:B:531:GLN:HG2	1.73	0.53
2:B:901:THR:CG2	2:B:902:MET:H	2.14	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:312:PHE:HZ	2:B:344:ILE:HD11	1.71	0.53
2:B:465:GLU:HG2	2:B:675:LEU:HD22	1.90	0.53
2:B:334:LEU:HD22	2:B:334:LEU:N	2.24	0.53
2:B:958:THR:HG21	2:B:988:LEU:O	2.09	0.53
2:B:962:GLU:HG2	2:B:963:VAL:H	1.74	0.53
2:B:1000:VAL:HA	2:B:1003:GLN:NE2	2.21	0.53
2:B:267:SER:CB	2:B:908:ARG:HH21	2.22	0.53
1:A:386:PHE:O	1:A:389:VAL:HB	2.09	0.53
1:A:524:ILE:HD13	1:A:619:ILE:HD12	1.90	0.53
2:B:623:ALA:O	2:B:627:VAL:HG23	2.09	0.53
1:A:297:GLY:HA2	1:A:298:PRO:C	2.34	0.52
2:B:317:THR:HG22	2:B:319:CYS:N	2.08	0.52
2:B:955:THR:O	2:B:957:MET:N	2.42	0.52
2:B:992:LYS:HB2	2:B:996:GLN:HG3	1.91	0.52
1:A:696:LEU:CD1	1:A:703:PRO:HG2	2.38	0.52
2:B:917:GLU:HA	2:B:935:SER:O	2.08	0.52
1:A:28:ARG:HB3	1:A:466:GLN:OE1	2.09	0.52
1:A:297:GLY:HA3	1:A:300:MET:HB2	1.92	0.52
2:B:340:PRO:HB2	2:B:341:PHE:CD1	2.44	0.52
1:A:745:ASP:O	1:A:747:VAL:N	2.43	0.52
2:B:996:GLN:CB	2:B:997:PRO:HD2	2.31	0.52
1:A:236:ILE:CG2	1:A:240:LEU:HB2	2.38	0.52
1:A:313:TRP:CE2	1:A:597:PRO:HA	2.44	0.52
1:A:239:ASN:HB3	5:A:822:HOH:O	2.08	0.52
1:A:536:THR:HG22	1:A:537:GLU:H	1.75	0.52
1:A:236:ILE:O	1:A:237:ASP:C	2.53	0.52
1:A:521:ALA:HA	1:A:612:LEU:HD12	1.92	0.52
2:B:703:THR:HG21	2:B:733:LYS:HB2	1.92	0.52
2:B:743:GLY:HA2	2:B:770:CYS:CB	2.37	0.52
1:A:183:ILE:CD1	2:B:509:MET:HE3	2.40	0.52
1:A:415:LYS:HB3	1:A:434:SER:HB2	1.91	0.52
1:A:461:PHE:CE2	1:A:479:ILE:HD13	2.43	0.52
2:B:332:ILE:HD11	2:B:778:TYR:CE1	2.45	0.52
2:B:643:VAL:HG12	2:B:643:VAL:O	2.09	0.52
2:B:279:ARG:NH2	2:B:293:PRO:C	2.68	0.52
1:A:60:LEU:HB2	1:A:67:ARG:NH1	2.25	0.52
2:B:339:LYS:HD3	2:B:724:CYS:O	2.10	0.52
2:B:608:GLU:OE1	2:B:803:LEU:HG	2.10	0.52
1:A:509:GLN:O	1:A:510:ILE:C	2.54	0.51
2:B:529:ASN:ND2	2:B:531:GLN:H	2.08	0.51
1:A:53:PRO:O	1:A:54:ILE:O	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:LEU:HA	1:A:702:MET:HE1	1.92	0.51
2:B:2:MET:HB2	3:C:118:ILE:HD11	1.91	0.51
2:B:693:ARG:HG3	2:B:693:ARG:NH1	2.26	0.51
1:A:524:ILE:HD12	1:A:615:SER:HB3	1.92	0.51
2:B:600:LYS:O	2:B:600:LYS:CG	2.58	0.51
2:B:633:VAL:HG11	2:B:651:VAL:HG12	1.92	0.51
1:A:15:ASP:HB3	1:A:497:THR:HG21	1.93	0.51
1:A:51:LEU:HD21	1:A:117:ILE:HA	1.92	0.51
1:A:297:GLY:H	1:A:300:MET:CE	2.22	0.51
2:B:289:ARG:HD2	2:B:769:ASN:OD1	2.10	0.51
2:B:355:ASN:ND2	2:B:355:ASN:C	2.67	0.51
2:B:430:ASP:OD2	2:B:430:ASP:N	2.44	0.51
2:B:458:LEU:HD21	2:B:638:PHE:CG	2.45	0.51
2:B:570:LYS:HE2	2:B:629:HIS:CE1	2.45	0.51
2:B:633:VAL:N	2:B:655:THR:HG21	2.16	0.51
2:B:692:MET:HE1	2:B:728:VAL:HG11	1.93	0.51
1:A:183:ILE:HD12	2:B:547:MET:CE	2.40	0.51
2:B:1009:LYS:HE2	2:B:1019:ASP:OD2	2.10	0.51
1:A:25:PRO:HG2	1:A:31:ALA:HB2	1.93	0.51
1:A:368:GLY:HA3	1:A:450:GLY:O	2.11	0.51
2:B:713:ASN:HD21	2:B:716:ASP:N	1.94	0.51
1:A:755:HIS:CD2	1:A:758:LYS:HE2	2.45	0.51
2:B:492:ASN:C	2:B:494:VAL:H	2.19	0.51
2:B:605:THR:CG2	2:B:607:LYS:HB3	2.41	0.51
2:B:651:VAL:O	2:B:655:THR:HB	2.10	0.51
2:B:751:LEU:HD13	2:B:761:LEU:HD21	1.93	0.51
2:B:807:ARG:HG2	2:B:807:ARG:HH11	1.76	0.51
2:B:1015:SER:HB2	2:B:1019:ASP:HB2	1.92	0.51
2:B:339:LYS:HD2	2:B:342:ALA:HB2	1.93	0.51
1:A:524:ILE:CD1	1:A:615:SER:HB3	2.41	0.50
1:A:541:ASP:O	1:A:544:ARG:HB3	2.12	0.50
2:B:992:LYS:CB	2:B:996:GLN:HE21	2.23	0.50
1:A:370:TYR:HA	5:A:824:HOH:O	2.10	0.50
2:B:289:ARG:C	2:B:291:GLN:H	2.19	0.50
2:B:456:ASN:HB3	5:B:1135:HOH:O	2.10	0.50
2:B:919:ILE:HG12	2:B:932:LEU:HD23	1.93	0.50
2:B:370:TYR:HB3	2:B:425:TYR:HE1	1.76	0.50
2:B:523:LEU:HA	5:B:1109:HOH:O	2.10	0.50
2:B:766:LEU:HD21	2:B:768:LEU:HD21	1.93	0.50
1:A:71:ASN:OD1	1:A:73:LEU:HB2	2.11	0.50
1:A:662:GLU:HG3	1:A:710:HIS:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:304:ASP:O	2:B:305:GLN:CB	2.58	0.50
2:B:934:VAL:C	2:B:936:SER:H	2.19	0.50
2:B:992:LYS:CD	2:B:996:GLN:HE21	2.23	0.50
1:A:656:ILE:CD1	1:A:695:ILE:HG21	2.42	0.50
2:B:665:PHE:CE1	2:B:670:ASP:HB2	2.46	0.50
2:B:739:SER:C	2:B:741:ASP:H	2.19	0.50
1:A:190:ARG:C	1:A:192:THR:H	2.20	0.50
1:A:384:GLN:O	1:A:388:ARG:HG3	2.12	0.50
2:B:286:THR:OG1	2:B:304:ASP:O	2.25	0.50
2:B:356:HIS:CD2	2:B:362:VAL:H	2.24	0.50
1:A:747:VAL:HG11	1:A:751:VAL:HG11	1.93	0.50
2:B:338:ILE:O	2:B:340:PRO:HD3	2.12	0.50
2:B:363:ARG:NH2	2:B:368:LYS:HB3	2.27	0.50
2:B:529:ASN:HD22	2:B:530:TYR:N	2.10	0.50
2:B:795:PHE:CB	2:B:875:MET:HE1	2.40	0.50
2:B:934:VAL:HG23	2:B:935:SER:H	1.77	0.50
2:B:409:ARG:C	2:B:411:ASP:H	2.20	0.49
2:B:942:GLN:HG2	2:B:948:PRO:HA	1.94	0.49
1:A:178:LEU:C	1:A:180:CYS:H	2.20	0.49
2:B:570:LYS:HE2	2:B:629:HIS:NE2	2.27	0.49
1:A:120:VAL:HG11	1:A:491:GLN:OE1	2.12	0.49
1:A:134:VAL:HG11	1:A:288:MET:CE	2.42	0.49
1:A:339:ALA:HB1	1:A:424:VAL:HG21	1.95	0.49
2:B:526:PHE:O	2:B:527:LEU:CB	2.61	0.49
2:B:949:SER:O	2:B:952:HIS:HB2	2.13	0.49
1:A:656:ILE:CD1	1:A:695:ILE:HD13	2.40	0.49
2:B:661:LYS:NZ	2:B:661:LYS:HB3	2.26	0.49
1:A:3:THR:HG22	1:A:5:LEU:N	2.27	0.49
2:B:543:GLN:HB3	2:B:547:MET:CE	2.42	0.49
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.94	0.49
1:A:476:ARG:HB3	1:A:501:ARG:O	2.13	0.49
2:B:500:VAL:HG12	2:B:500:VAL:O	2.11	0.49
3:C:118:ILE:HG22	3:C:120:MET:CE	2.43	0.49
1:A:511:GLN:H	1:A:511:GLN:NE2	2.11	0.49
2:B:627:VAL:HG21	2:B:710:LEU:CD2	2.43	0.49
2:B:455:LYS:C	2:B:457:GLY:H	2.20	0.49
2:B:276:ARG:HA	2:B:298:THR:HG23	1.95	0.48
1:A:471:ILE:CG2	1:A:473:GLN:HB3	2.43	0.48
1:A:317:ASP:C	1:A:319:ASP:H	2.22	0.48
2:B:403:LEU:HA	2:B:409:ARG:HA	1.95	0.48
2:B:454:ILE:CD1	2:B:459:VAL:HG21	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PRO:HB2	1:A:235:LYS:HB3	1.95	0.48
2:B:751:LEU:HA	2:B:761:LEU:HD23	1.95	0.48
2:B:842:VAL:O	2:B:842:VAL:CG1	2.61	0.48
1:A:656:ILE:HG13	1:A:695:ILE:CG2	2.42	0.48
1:A:680:ASN:O	1:A:683:HIS:HB2	2.13	0.48
2:B:571:ALA:C	2:B:573:ASP:H	2.20	0.48
1:A:417:SER:HB3	1:A:438:ILE:HG13	1.96	0.48
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.95	0.48
2:B:296:VAL:HG12	2:B:314:ARG:NE	2.29	0.48
2:B:585:LEU:HD11	2:B:595:LYS:O	2.13	0.48
2:B:899:LYS:O	2:B:900:SER:HB3	2.13	0.48
2:B:941:ILE:HD13	2:B:950:PHE:HA	1.96	0.48
1:A:198:LYS:HE2	1:A:202:GLU:OE2	2.14	0.48
2:B:383:ARG:HD3	2:B:394:ASP:OD1	2.14	0.48
2:B:499:ASN:HB2	2:B:522:LEU:HD11	1.96	0.48
2:B:751:LEU:HD13	2:B:761:LEU:CD2	2.44	0.48
1:A:41:LEU:HD13	1:A:525:LEU:CD2	2.44	0.48
1:A:511:GLN:CD	1:A:511:GLN:N	2.67	0.48
2:B:560:PRO:O	2:B:563:GLN:HB3	2.14	0.48
2:B:955:THR:C	2:B:957:MET:N	2.72	0.48
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.95	0.47
1:A:25:PRO:HG3	1:A:31:ALA:HB2	1.96	0.47
1:A:290:ILE:HD12	1:A:355:THR:HB	1.95	0.47
1:A:749:LEU:O	1:A:753:MET:HG2	2.14	0.47
1:A:297:GLY:N	1:A:300:MET:HE3	2.29	0.47
1:A:208:LYS:O	1:A:209:VAL:HB	2.14	0.47
1:A:357:LEU:O	1:A:361:LYS:N	2.45	0.47
2:B:603:VAL:O	2:B:604:ASN:CG	2.58	0.47
2:B:651:VAL:N	2:B:652:PRO:HD2	2.29	0.47
2:B:996:GLN:CB	2:B:997:PRO:CD	2.90	0.47
1:A:59:VAL:C	1:A:60:LEU:HD23	2.40	0.47
2:B:288:THR:HG22	2:B:289:ARG:N	2.29	0.47
2:B:686:ILE:HD13	5:B:1113:HOH:O	2.14	0.47
2:B:834:LEU:HD21	2:B:836:LEU:HD21	1.96	0.47
1:A:547:ASP:HB3	1:A:743:LEU:HB2	1.97	0.47
2:B:355:ASN:HD22	2:B:357:GLY:H	1.61	0.47
2:B:873:LEU:HD22	2:B:984:TYR:CZ	2.50	0.47
2:B:813:GLN:O	2:B:817:MET:HG3	2.14	0.47
1:A:508:THR:C	1:A:509:GLN:HG2	2.39	0.47
1:A:716:ARG:NE	1:A:717:PHE:CE1	2.83	0.47
2:B:375:MET:HE1	2:B:386:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:ARG:HH21	1:A:549:GLN:NE2	2.12	0.47
1:A:716:ARG:CZ	1:A:717:PHE:HE1	2.28	0.47
2:B:901:THR:CB	2:B:970:GLN:HE21	2.27	0.47
1:A:41:LEU:HD23	1:A:612:LEU:HB2	1.96	0.46
2:B:409:ARG:C	2:B:411:ASP:N	2.73	0.46
2:B:516:GLY:HA2	2:B:591:PRO:CD	2.45	0.46
2:B:661:LYS:HB3	2:B:661:LYS:HZ2	1.79	0.46
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.50	0.46
2:B:2:MET:HB2	3:C:118:ILE:CD1	2.45	0.46
2:B:970:GLN:NE2	2:B:973:MET:SD	2.88	0.46
1:A:98:TYR:O	1:A:99:ALA:C	2.58	0.46
1:A:527:ALA:O	1:A:531:ILE:HG13	2.15	0.46
1:A:548:ARG:HH21	1:A:549:GLN:HE22	1.63	0.46
2:B:494:VAL:CG2	2:B:513:THR:HG22	2.46	0.46
1:A:73:LEU:HD11	1:A:500:ALA:HB2	1.98	0.46
2:B:411:ASP:O	2:B:412:HIS:C	2.58	0.46
2:B:319:CYS:HA	2:B:769:ASN:O	2.15	0.46
2:B:559:ALA:N	2:B:560:PRO:CD	2.78	0.46
2:B:739:SER:C	2:B:741:ASP:N	2.71	0.46
2:B:1015:SER:HB2	2:B:1019:ASP:CB	2.45	0.46
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.31	0.46
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.51	0.46
1:A:656:ILE:CG1	1:A:695:ILE:HG21	2.43	0.46
2:B:475:LYS:HB3	2:B:482:SER:HB2	1.97	0.46
2:B:585:LEU:CD2	2:B:594:LEU:HB2	2.46	0.46
2:B:303:GLN:O	2:B:304:ASP:O	2.34	0.45
2:B:415:LYS:HB2	2:B:418:LEU:HD12	1.98	0.45
2:B:515:VAL:CG1	2:B:590:ALA:HB1	2.46	0.45
2:B:639:PRO:HB3	2:B:643:VAL:CG2	2.30	0.45
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.97	0.45
1:A:279:PHE:O	1:A:282:THR:HG22	2.16	0.45
1:A:397:GLN:NE2	1:A:489:SER:HB3	2.31	0.45
2:B:528:VAL:HG11	2:B:533:SER:OG	2.15	0.45
2:B:2:MET:CE	3:C:118:ILE:HD11	2.27	0.45
2:B:901:THR:CB	2:B:973:MET:HE1	2.44	0.45
2:B:962:GLU:CG	2:B:963:VAL:H	2.26	0.45
1:A:18:ARG:HH11	1:A:612:LEU:HD22	1.76	0.45
1:A:45:LEU:CD1	1:A:451:LEU:HD13	2.46	0.45
1:A:153:MET:HE2	1:A:154:SER:N	2.31	0.45
1:A:402:PHE:CD1	1:A:402:PHE:N	2.85	0.45
1:A:609:ARG:HH11	1:A:609:ARG:CG	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:919:ILE:HG23	2:B:932:LEU:HD23	1.97	0.45
2:B:446:MET:HE3	2:B:561:VAL:CG1	2.37	0.45
2:B:726:LYS:HD3	2:B:876:THR:HG23	1.98	0.45
2:B:1009:LYS:CG	2:B:1016:SER:HB3	2.47	0.45
2:B:1009:LYS:HG2	2:B:1016:SER:HB3	1.97	0.45
1:A:467:HIS:O	1:A:470:PRO:HD3	2.17	0.45
1:A:672:TYR:HD2	1:A:678:TYR:CE2	2.34	0.45
2:B:267:SER:HA	2:B:908:ARG:HH21	1.82	0.45
2:B:726:LYS:HD3	2:B:876:THR:CG2	2.47	0.45
2:B:979:GLN:NE2	2:B:985:SER:HA	2.31	0.45
1:A:174:GLN:HG2	1:A:188:VAL:HG22	1.99	0.45
1:A:323:TYR:O	1:A:324:VAL:C	2.59	0.45
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.52	0.45
2:B:279:ARG:CZ	2:B:294:PRO:HG3	2.47	0.45
2:B:395:VAL:O	2:B:396:PRO:C	2.60	0.45
2:B:529:ASN:HD22	2:B:529:ASN:C	2.24	0.45
2:B:633:VAL:CG1	2:B:651:VAL:HG12	2.46	0.45
2:B:655:THR:O	2:B:720:ALA:HB3	2.17	0.45
1:A:78:TYR:CD2	1:A:101:ILE:HG12	2.52	0.45
1:A:136:ASP:O	1:A:139:MET:HE3	2.16	0.45
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.82	0.45
1:A:644:ALA:O	1:A:663:THR:HB	2.17	0.45
2:B:499:ASN:HA	2:B:525:GLY:O	2.16	0.45
2:B:958:THR:HG21	2:B:989:THR:HA	1.99	0.45
2:B:958:THR:HG23	2:B:990:ILE:HG13	1.98	0.45
1:A:12:GLU:CD	1:A:18:ARG:HD2	2.42	0.44
1:A:190:ARG:CB	1:A:192:THR:HG22	2.46	0.44
2:B:267:SER:HB2	2:B:908:ARG:HH21	1.81	0.44
2:B:312:PHE:CE1	2:B:344:ILE:HD11	2.51	0.44
2:B:665:PHE:CD1	2:B:670:ASP:HB2	2.53	0.44
2:B:974:ILE:HG13	2:B:975:MET:N	2.31	0.44
1:A:153:MET:SD	1:A:387:GLN:HB3	2.57	0.44
2:B:585:LEU:HD21	2:B:594:LEU:CB	2.46	0.44
2:B:618:VAL:HG23	2:B:619:TYR:N	2.32	0.44
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.45	0.44
2:B:747:GLN:HG3	2:B:765:ASN:OD1	2.17	0.44
1:A:268:LEU:HB2	1:A:288:MET:HE1	1.99	0.44
1:A:296:GLN:HA	1:A:300:MET:HE2	1.99	0.44
1:A:636:LEU:C	1:A:638:ASP:H	2.25	0.44
2:B:992:LYS:CB	2:B:996:GLN:HG3	2.47	0.44
1:A:618:MET:CE	1:A:653:PHE:CD2	3.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:OE1	1:A:18:ARG:HD2	2.17	0.44
2:B:644:ASP:OD2	2:B:647:SER:HB2	2.16	0.44
1:A:183:ILE:HD12	2:B:547:MET:SD	2.57	0.44
2:B:329:GLN:O	2:B:816:HIS:HE1	2.00	0.44
2:B:642:TYR:CZ	2:B:644:ASP:HB2	2.52	0.44
1:A:132:LEU:HD12	1:A:165:GLY:O	2.18	0.44
1:A:259:ARG:HG3	1:A:306:LEU:HD23	1.99	0.44
2:B:289:ARG:O	2:B:291:GLN:N	2.48	0.44
2:B:339:LYS:HD2	2:B:342:ALA:CB	2.48	0.44
2:B:612:PHE:O	2:B:646:ALA:HB1	2.18	0.44
2:B:690:ALA:HB2	2:B:752:TYR:CB	2.48	0.44
1:A:648:LEU:O	1:A:658:ILE:HA	2.18	0.44
1:A:668:ARG:HA	1:A:673:GLN:NE2	2.33	0.44
2:B:641:GLN:O	2:B:642:TYR:C	2.60	0.44
2:B:653:GLN:HE21	2:B:708:GLY:HA2	1.82	0.44
2:B:955:THR:HG23	2:B:990:ILE:O	2.18	0.44
2:B:692:MET:HE1	2:B:728:VAL:CB	2.48	0.43
1:A:23:VAL:HG12	1:A:513:ILE:HG12	2.00	0.43
2:B:706:PHE:CE2	2:B:793:SER:HA	2.52	0.43
1:A:743:LEU:O	1:A:755:HIS:ND1	2.52	0.43
2:B:1030:GLN:O	2:B:1032:LEU:N	2.47	0.43
1:A:392:LYS:HD3	1:A:396:GLY:HA2	2.00	0.43
1:A:519:GLN:OE1	1:A:576:LEU:HB2	2.16	0.43
1:A:543:LEU:HD11	1:A:591:GLN:HE22	1.84	0.43
2:B:317:THR:HG21	2:B:319:CYS:O	2.18	0.43
2:B:627:VAL:HG21	2:B:710:LEU:HD23	1.99	0.43
2:B:800:HIS:C	2:B:801:GLN:HG3	2.43	0.43
2:B:859:ARG:O	2:B:861:GLU:N	2.51	0.43
2:B:979:GLN:HE22	2:B:986:MET:H	1.67	0.43
2:B:1025:HIS:O	2:B:1028:ILE:HG22	2.19	0.43
1:A:6:GLU:O	1:A:10:GLN:HG3	2.18	0.43
1:A:79:ARG:O	1:A:80:ALA:HB2	2.18	0.43
2:B:704:ASP:HB3	2:B:731:GLU:HB3	1.99	0.43
2:B:988:LEU:HD12	2:B:989:THR:H	1.83	0.43
1:A:208:LYS:O	1:A:209:VAL:CB	2.66	0.43
1:A:499:ILE:C	1:A:499:ILE:HD12	2.43	0.43
1:A:747:VAL:HG12	1:A:748:SER:N	2.21	0.43
2:B:492:ASN:C	2:B:494:VAL:N	2.76	0.43
2:B:833:GLN:HB3	3:C:117:THR:CG2	2.49	0.43
2:B:958:THR:HG21	2:B:988:LEU:C	2.43	0.43
1:A:15:ASP:O	1:A:16:GLY:C	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ASN:C	1:A:470:PRO:CD	2.90	0.43
1:A:611:ASP:OD2	1:A:611:ASP:C	2.62	0.43
2:B:283:VAL:CG2	2:B:301:MET:HE2	2.40	0.43
1:A:48:ARG:HG3	1:A:48:ARG:HH11	1.84	0.43
1:A:179:GLY:O	1:A:181:GLU:N	2.51	0.43
1:A:376:SER:O	1:A:379:THR:HG23	2.18	0.43
1:A:464:VAL:O	1:A:465:ASN:HB2	2.18	0.43
2:B:902:MET:O	2:B:903:LEU:HB3	2.19	0.43
1:A:195:LEU:HD13	1:A:203:MET:HE1	2.01	0.43
1:A:403:GLY:HA2	1:A:449:CYS:HA	2.01	0.43
1:A:165:GLY:HA3	1:A:230:LEU:HD23	2.01	0.43
1:A:198:LYS:O	1:A:199:GLN:C	2.62	0.43
1:A:320:ASN:HD22	1:A:320:ASN:HA	1.63	0.43
1:A:382:PHE:O	1:A:383:LYS:C	2.62	0.43
1:A:547:ASP:OD2	1:A:743:LEU:HB3	2.18	0.43
1:A:631:PRO:O	1:A:633:GLU:HG3	2.19	0.43
1:A:633:GLU:O	1:A:635:VAL:HG13	2.19	0.43
1:A:754:ASP:O	1:A:755:HIS:C	2.62	0.43
2:B:854:CYS:O	2:B:867:ARG:CD	2.66	0.43
1:A:173:VAL:HG11	1:A:270:ILE:HD12	2.01	0.42
1:A:577:TYR:N	1:A:578:PRO:CD	2.82	0.42
1:A:678:TYR:CD1	1:A:678:TYR:N	2.87	0.42
2:B:364:CYS:O	2:B:368:LYS:HA	2.18	0.42
2:B:978:ILE:HG22	2:B:986:MET:HE1	2.01	0.42
2:B:269:ILE:CD1	2:B:907:VAL:C	2.87	0.42
2:B:272:ILE:HG23	2:B:297:THR:HB	2.00	0.42
2:B:494:VAL:HG21	2:B:513:THR:HG22	2.01	0.42
2:B:936:SER:HB3	2:B:941:ILE:HD11	2.00	0.42
1:A:536:THR:C	1:A:538:GLU:N	2.75	0.42
1:A:672:TYR:HD1	1:A:672:TYR:H	1.67	0.42
2:B:267:SER:CA	2:B:908:ARG:HH21	2.32	0.42
2:B:384:TYR:O	2:B:384:TYR:CD1	2.73	0.42
2:B:562:ILE:HB	2:B:622:LEU:HD21	2.01	0.42
2:B:676:ASN:O	2:B:680:ASN:HB2	2.20	0.42
2:B:766:LEU:HD23	2:B:768:LEU:HD21	2.01	0.42
1:A:255:PRO:HG2	1:A:258:LYS:CG	2.48	0.42
1:A:612:LEU:C	1:A:612:LEU:CD2	2.92	0.42
1:A:79:ARG:HG3	1:A:79:ARG:NH1	2.33	0.42
2:B:326:MET:O	2:B:327:ALA:C	2.62	0.42
2:B:529:ASN:ND2	2:B:529:ASN:C	2.77	0.42
1:A:58:PRO:O	1:A:59:VAL:CB	2.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ARG:CG	1:A:609:ARG:NH1	2.82	0.42
2:B:854:CYS:HB2	2:B:862:ILE:HG21	2.00	0.42
1:A:406:LEU:O	1:A:445:GLN:HA	2.20	0.42
2:B:271:VAL:HG21	2:B:842:VAL:HG23	2.00	0.42
2:B:354:VAL:CG2	2:B:416:PRO:HG2	2.49	0.42
2:B:415:LYS:HE2	5:B:1155:HOH:O	2.19	0.42
2:B:475:LYS:HD2	2:B:475:LYS:O	2.20	0.42
1:A:339:ALA:O	1:A:447:LYS:CE	2.68	0.42
2:B:709:ILE:HG22	2:B:719:MET:HG2	2.02	0.42
2:B:739:SER:OG	2:B:742:SER:HB2	2.20	0.42
2:B:439:ASN:HB3	2:B:440:PRO:HD2	2.01	0.42
2:B:486:VAL:O	2:B:527:LEU:HA	2.19	0.42
2:B:523:LEU:HD23	5:B:1109:HOH:O	2.19	0.42
2:B:945:PHE:CD1	2:B:945:PHE:N	2.88	0.42
1:A:420:ILE:HD13	1:A:532:TYR:HB2	2.02	0.42
1:A:536:THR:CG2	1:A:537:GLU:N	2.83	0.42
1:A:744:THR:HG21	1:A:752:PHE:CD1	2.54	0.42
2:B:316:THR:HA	2:B:785:ALA:HB3	2.01	0.42
2:B:723:ASP:OD1	2:B:726:LYS:HG2	2.20	0.42
2:B:992:LYS:O	2:B:996:GLN:HB2	2.19	0.42
2:B:1029:CYS:O	2:B:1032:LEU:HA	2.20	0.42
1:A:366:LEU:HA	1:A:366:LEU:HD23	1.77	0.41
1:A:687:ALA:HB3	1:A:688:PRO:CD	2.49	0.41
2:B:838:ASP:OD1	2:B:841:LYS:HE3	2.20	0.41
1:A:87:PHE:CZ	1:A:480:GLN:HB2	2.55	0.41
2:B:454:ILE:HD13	2:B:459:VAL:CG2	2.42	0.41
2:B:700:PHE:CZ	2:B:744:ALA:HB1	2.54	0.41
2:B:709:ILE:HD12	2:B:717:VAL:HG13	2.02	0.41
2:B:1025:HIS:ND1	3:C:120:MET:HG3	2.35	0.41
2:B:560:PRO:HA	2:B:563:GLN:HB3	2.02	0.41
2:B:665:PHE:HE2	2:B:667:MET:CE	2.33	0.41
2:B:692:MET:HE1	2:B:728:VAL:CG1	2.50	0.41
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.34	0.41
2:B:617:ASN:OD1	2:B:617:ASN:O	2.38	0.41
2:B:713:ASN:HD22	2:B:715:THR:H	1.66	0.41
2:B:964:GLY:HA3	2:B:968:SER:CB	2.50	0.41
2:B:993:GLN:O	2:B:994:ARG:C	2.62	0.41
1:A:78:TYR:CD2	1:A:102:SER:HA	2.56	0.41
1:A:251:PRO:O	1:A:252:TRP:C	2.63	0.41
1:A:542:VAL:O	1:A:543:LEU:C	2.63	0.41
2:B:624:LYS:HE2	2:B:624:LYS:HB3	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:696:THR:HB	2:B:700:PHE:CZ	2.55	0.41
1:A:69:VAL:O	1:A:70:LEU:C	2.64	0.41
1:A:108:ALA:HB1	1:A:114:PHE:CD1	2.55	0.41
1:A:183:ILE:HD12	2:B:547:MET:HE1	2.02	0.41
1:A:414:ILE:HG22	1:A:415:LYS:N	2.35	0.41
1:A:426:LEU:HD21	1:A:447:LYS:HB2	2.03	0.41
1:A:526:MET:HG3	1:A:577:TYR:OH	2.20	0.41
1:A:547:ASP:CG	1:A:743:LEU:HB3	2.45	0.41
2:B:377:PHE:CD2	2:B:409:ARG:HD2	2.55	0.41
2:B:441:PRO:HA	2:B:575:PRO:O	2.21	0.41
2:B:932:LEU:HD11	2:B:945:PHE:CZ	2.55	0.41
1:A:394:MET:SD	1:A:394:MET:N	2.84	0.41
1:A:297:GLY:HA2	1:A:298:PRO:O	2.21	0.41
2:B:486:VAL:HG12	2:B:487:GLY:N	2.36	0.41
2:B:820:CYS:HA	2:B:823:LYS:HE2	2.03	0.41
1:A:289:PHE:CD1	1:A:289:PHE:N	2.89	0.41
1:A:381:LEU:HD12	1:A:702:MET:HE2	2.02	0.41
2:B:356:HIS:CD2	2:B:362:VAL:HG23	2.56	0.41
2:B:407:GLY:C	2:B:409:ARG:H	2.28	0.41
2:B:441:PRO:HB3	2:B:575:PRO:HG2	2.02	0.41
2:B:458:LEU:HD12	2:B:461:LEU:HD23	2.03	0.41
2:B:536:VAL:O	2:B:539:ASN:HB3	2.21	0.41
2:B:643:VAL:CG1	2:B:648:LEU:HD12	2.50	0.41
2:B:707:GLY:O	2:B:709:ILE:HG12	2.21	0.41
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.56	0.40
1:A:154:SER:O	1:A:158:LEU:HG	2.21	0.40
1:A:612:LEU:HD23	1:A:613:THR:N	2.36	0.40
1:A:616:LEU:HD23	1:A:616:LEU:HA	1.83	0.40
1:A:623:LEU:HG	1:A:648:LEU:HD22	2.04	0.40
2:B:464:GLU:HA	2:B:467:LYS:HE3	2.03	0.40
2:B:857:LEU:HD12	2:B:857:LEU:HA	1.68	0.40
1:A:155:LEU:CD2	1:A:240:LEU:HD13	2.50	0.40
1:A:555:GLN:HG2	1:A:760:ALA:O	2.21	0.40
2:B:332:ILE:HD12	2:B:777:LEU:HD13	2.02	0.40
2:B:933:GLY:HA2	2:B:993:GLN:HB2	2.04	0.40
2:B:937:PRO:HG2	2:B:940:LEU:HD12	2.02	0.40
1:A:189:PHE:CD1	1:A:189:PHE:N	2.88	0.40
1:A:268:LEU:HD22	1:A:272:VAL:HG23	2.03	0.40
1:A:283:GLY:CA	1:A:486:GLN:HE22	2.33	0.40
1:A:376:SER:OG	1:A:379:THR:HG23	2.22	0.40
1:A:537:GLU:H	1:A:537:GLU:HG3	1.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:PRO:O	2:B:272:ILE:HG13	2.22	0.40
2:B:401:GLN:HG3	2:B:411:ASP:OD2	2.21	0.40
2:B:469:MET:C	2:B:471:GLU:N	2.79	0.40
2:B:602:LEU:HD21	2:B:859:ARG:HD3	2.02	0.40
2:B:692:MET:HE1	2:B:728:VAL:HB	2.02	0.40
2:B:967:TYR:O	2:B:968:SER:C	2.64	0.40
1:A:54:ILE:HD12	1:A:56:TYR:CE2	2.56	0.40
1:A:398:PHE:C	1:A:400:MET:H	2.29	0.40
2:B:289:ARG:HD3	2:B:768:LEU:O	2.20	0.40
2:B:649:GLY:HA2	2:B:652:PRO:CG	2.52	0.40
2:B:738:LEU:HB2	2:B:770:CYS:SG	2.61	0.40
1:A:546:LEU:HD21	1:A:584:LEU:CD2	2.52	0.40
2:B:854:CYS:HB3	2:B:862:ILE:CD1	2.49	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	720/764 (94%)	618 (86%)	76 (11%)	26 (4%)	2	16
2	B	763/770 (99%)	651 (85%)	76 (10%)	36 (5%)	2	11
3	C	4/7 (57%)	4 (100%)	0	0	100	100
All	All	1487/1541 (96%)	1273 (86%)	152 (10%)	62 (4%)	2	13

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ILE
1	A	80	ALA
1	A	237	ASP
1	A	465	ASN

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Mol	Chain	Res	Type
1	A	466	GLN
1	A	467	HIS
1	A	468	ASN
1	A	593	PHE
2	B	289	ARG
2	B	304	ASP
2	B	412	HIS
2	B	492	ASN
2	B	503	ASN
2	B	527	LEU
2	B	603	VAL
2	B	604	ASN
2	B	899	LYS
2	B	900	SER
2	B	902	MET
2	B	964	GLY
2	B	993	GLN
2	B	996	GLN
2	B	998	GLU
2	B	1032	LEU
1	A	180	CYS
1	A	297	GLY
1	A	324	VAL
1	A	537	GLU
1	A	575	SER
1	A	610	GLN
1	A	746	ASP
2	B	597	ARG
2	B	862	ILE
2	B	956	ASP
2	B	995	GLU
1	A	99	ALA
1	A	536	THR
1	A	700	PHE
1	A	744	THR
2	B	397	PRO
2	B	413	TYR
2	B	429	LEU
2	B	860	PRO
1	A	59	VAL
1	A	184	SER
2	B	398	PHE

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Mol	Chain	Res	Type
2	B	423	TYR
2	B	861	GLU
2	B	903	LEU
2	B	961	PRO
2	B	963	VAL
2	B	980	GLN
1	A	116	SER
2	B	859	ARG
2	B	966	PRO
1	A	109	GLU
1	A	469	ALA
1	A	470	PRO
2	B	524	ASP
1	A	540	PRO
2	B	290	GLY
2	B	1006	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	635/666 (95%)	595 (94%)	40 (6%)	16	48
2	B	680/682 (100%)	639 (94%)	41 (6%)	17	50
3	C	6/7 (86%)	6 (100%)	0	100	100
All	All	1321/1355 (98%)	1240 (94%)	81 (6%)	17	49

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	34	MET
1	A	41	LEU
1	A	54	ILE
1	A	105	ASN
1	A	109	GLU

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Mol	Chain	Res	Type
1	A	116	SER
1	A	122	LEU
1	A	153	MET
1	A	194	ASP
1	A	237	ASP
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	301	VAL
1	A	320	ASN
1	A	332	GLU
1	A	362	CYS
1	A	376	SER
1	A	389	VAL
1	A	437	GLU
1	A	451	LEU
1	A	470	PRO
1	A	476	ARG
1	A	491	GLN
1	A	498	THR
1	A	509	GLN
1	A	528	ARG
1	A	570	PHE
1	A	615	SER
1	A	619	ILE
1	A	637	LEU
1	A	649	LEU
1	A	652	THR
1	A	673	GLN
1	A	677	GLU
1	A	690	ASP
1	A	695	ILE
1	A	696	LEU
1	A	747	VAL
2	B	267	SER
2	B	313	ILE
2	B	334	LEU
2	B	376	GLN
2	B	383	ARG
2	B	391	CYS
2	B	401	GLN
2	B	409	ARG

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Mol	Chain	Res	Type
2	B	411	ASP
2	B	470	LEU
2	B	494	VAL
2	B	495	LEU
2	B	518	VAL
2	B	523	LEU
2	B	528	VAL
2	B	553	GLU
2	B	566	MET
2	B	585	LEU
2	B	599	ASP
2	B	620	ASP
2	B	633	VAL
2	B	647	SER
2	B	653	GLN
2	B	655	THR
2	B	661	LYS
2	B	691	ILE
2	B	693	ARG
2	B	713	ASN
2	B	777	LEU
2	B	799	LEU
2	B	807	ARG
2	B	834	LEU
2	B	845	VAL
2	B	876	THR
2	B	896	LEU
2	B	898	VAL
2	B	907	VAL
2	B	921	LEU
2	B	946	ASN
2	B	989	THR
2	B	1027	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	126	GLN
1	A	152	GLN
1	A	174	GLN
1	A	239	ASN

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Mol	Chain	Res	Type
1	A	320	ASN
1	A	330	HIS
1	A	397	GLN
1	A	436	ASN
1	A	468	ASN
1	A	486	GLN
1	A	509	GLN
1	A	511	GLN
1	A	549	GLN
1	A	579	GLN
1	A	583	HIS
1	A	591	GLN
1	A	595	ASN
1	A	620	GLN
1	A	655	GLN
1	A	673	GLN
1	A	697	HIS
1	A	710	HIS
2	B	347	ASN
2	B	355	ASN
2	B	356	HIS
2	B	385	GLN
2	B	402	HIS
2	B	492	ASN
2	B	503	ASN
2	B	508	GLN
2	B	529	ASN
2	B	615	GLN
2	B	653	GLN
2	B	663	ASN
2	B	668	HIS
2	B	672	GLN
2	B	712	ASN
2	B	713	ASN
2	B	773	GLN
2	B	813	GLN
2	B	816	HIS
2	B	942	GLN
2	B	946	ASN
2	B	952	HIS
2	B	954	ASN
2	B	970	GLN

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Mol	Chain	Res	Type
2	B	979	GLN
2	B	996	GLN
2	B	1003	GLN
2	B	1033	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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	726/764 (95%)	-0.36	8 (1%) 78 57	21, 48, 92, 144	0
2	B	767/770 (99%)	-0.31	11 (1%) 73 51	22, 50, 102, 128	0
3	C	6/7 (85%)	0.85	1 (16%) 4 3	59, 77, 90, 108	0
All	All	1499/1541 (97%)	-0.33	20 (1%) 75 53	21, 49, 98, 144	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	PRO	4.6
2	B	2	MET	4.0
1	A	741	PRO	4.0
1	A	742	ILE	3.7
2	B	3	GLY	3.5
2	B	960	LEU	3.4
1	A	209	VAL	3.1
1	A	472	PRO	3.0
2	B	1	ALA	2.9
2	B	997	PRO	2.9
2	B	1033	ASN	2.7
2	B	955	THR	2.5
1	A	52	PRO	2.5
1	A	539	GLY	2.4
1	A	475	GLY	2.3
3	C	121	ASP	2.3
2	B	901	THR	2.1
2	B	959	LEU	2.1
2	B	860	PRO	2.0
2	B	961	PRO	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	1.00	0.03	45,45,45,45	0
4	ZN	B	1100	1/1	1.00	0.04	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.