



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:02 AM UTC

PDB ID : 3EFO / pdb_00003efo
Title : Crystal Structure of the mammalian COPII-coat protein Sec23/24 bound to the transport signal sequence of syntaxin 5
Authors : Goldberg, J.; Mancias, J.D.
Deposited on : 2008-09-09
Resolution : 2.70 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

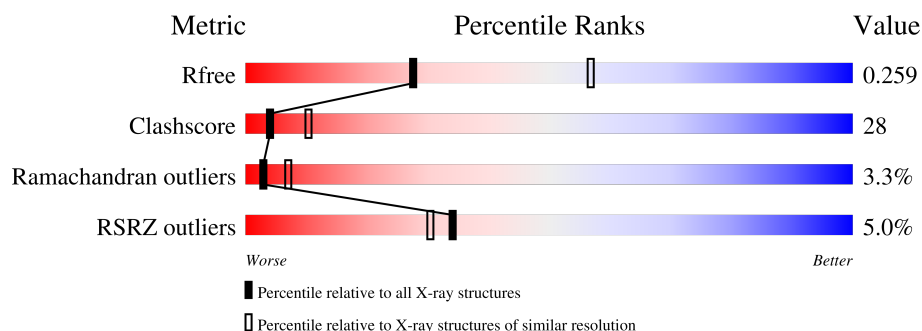
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	765	
2	B	770	
3	C	7	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11927 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	716	Total	C	N	O	S	0	0	0
			5684	3623	975	1046	40			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	GLY	LYS	conflict	UNP Q15436

- 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	7	Total	C	N	O	S	0	0	0
			53	32	7	12	2			

- 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		

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

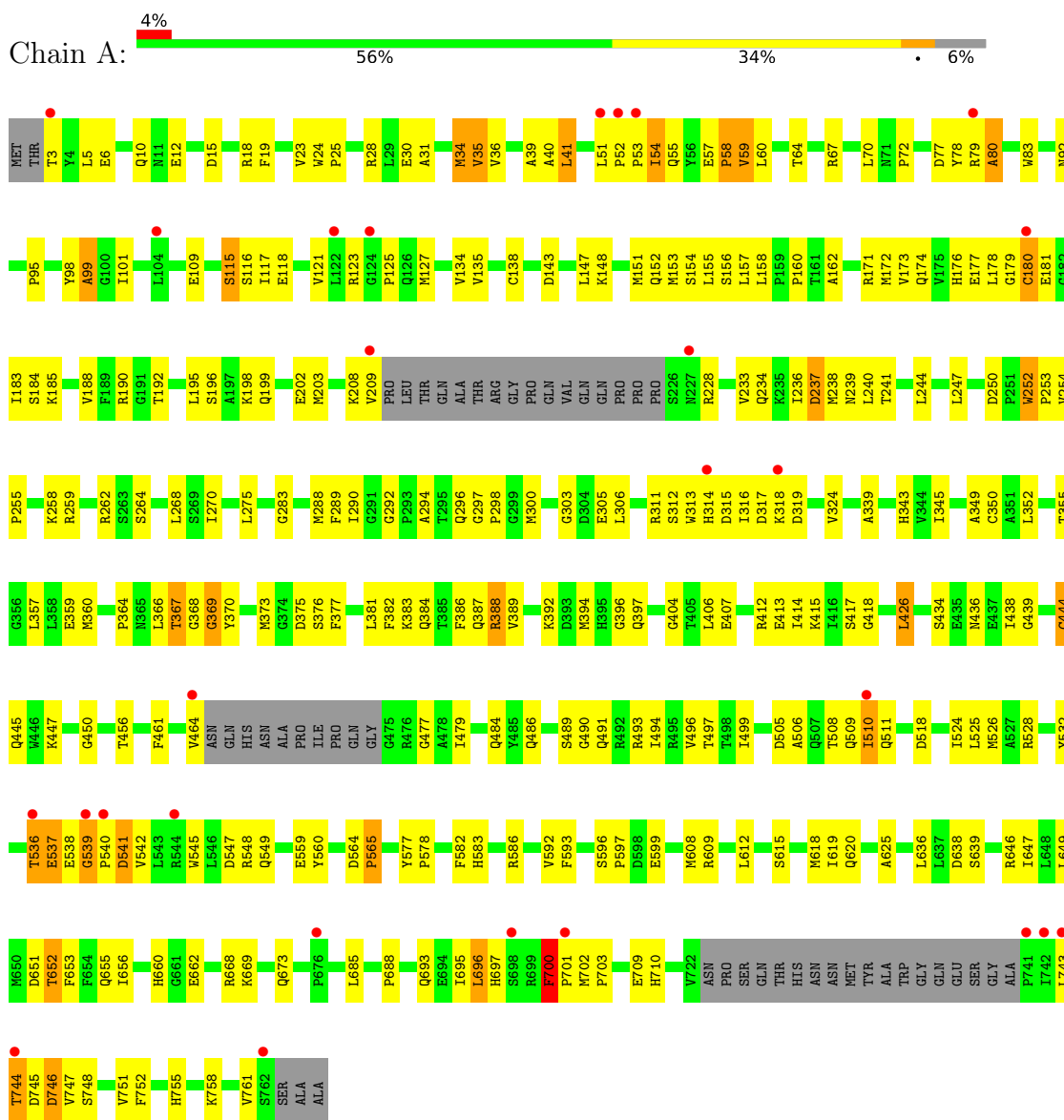
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total 79	O 79	0	0
5	B	71	Total 71	O 71	0	0

3 Residue-property plots

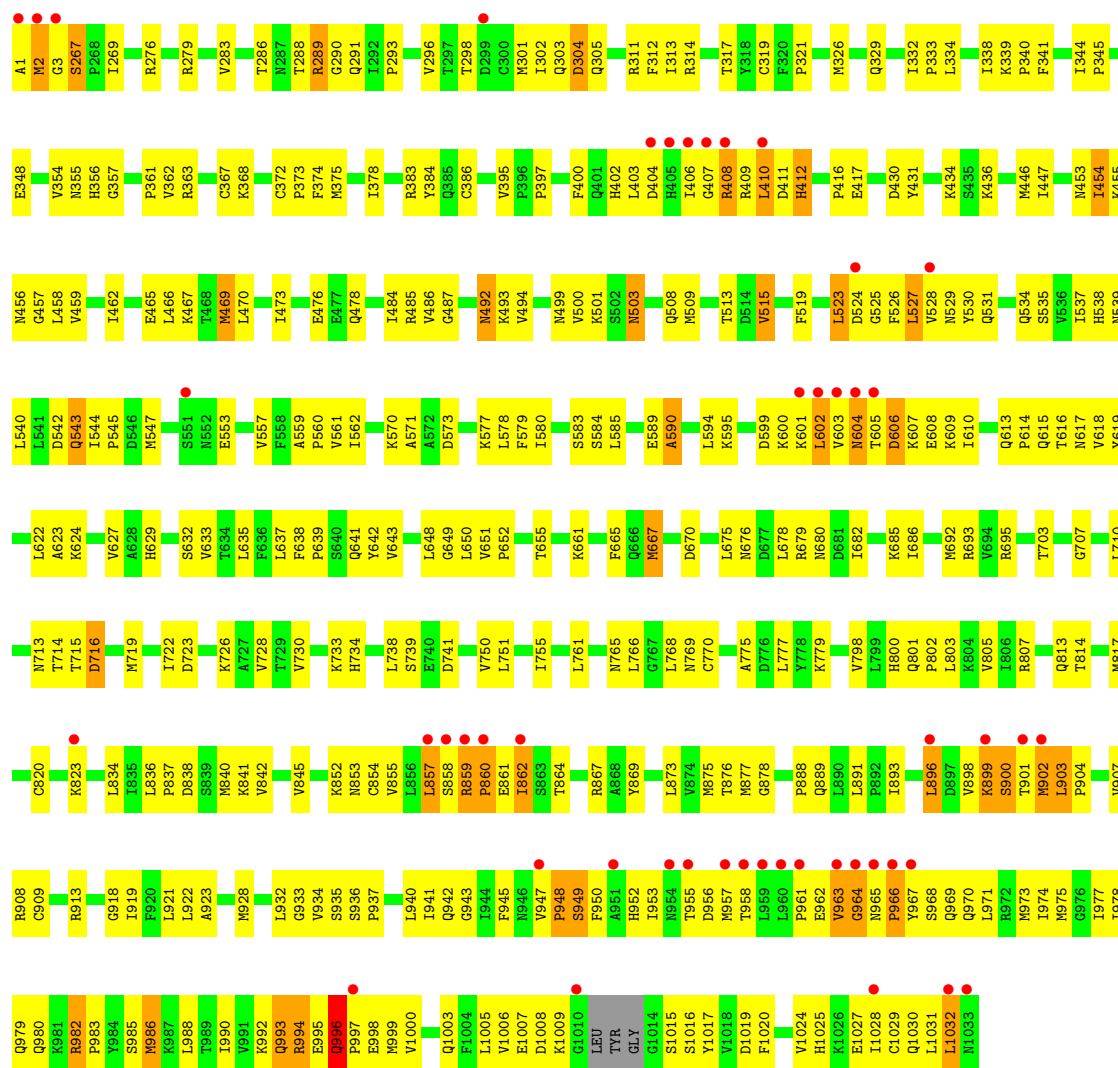
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 3: Peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.06Å 140.83Å 152.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 94.9 (50.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.13 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.261 0.210 , 0.259	Depositor DCC
R_{free} test set	3050 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	51.1	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.8	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	0.94	EDS
Total number of atoms	11927	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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	0/5817	1.01	28/7878 (0.4%)
2	B	0.44	0/6166	1.02	41/8351 (0.5%)
3	C	0.42	0/52	0.76	0/67
All	All	0.44	0/12035	1.01	69/16296 (0.4%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	N-CA-C	-13.22	90.40	110.10
1	A	652	THR	N-CA-C	-11.94	93.27	110.59
2	B	858	SER	N-CA-C	10.35	122.36	108.38
1	A	34	MET	N-CA-C	-10.29	99.61	112.88
2	B	877	MET	N-CA-C	9.47	122.56	110.24
1	A	367	THR	N-CA-C	-9.25	95.28	110.17
1	A	55	GLN	N-CA-C	9.23	123.47	109.62
1	A	58	PRO	N-CA-C	7.76	123.57	113.86
1	A	135	VAL	N-CA-C	7.60	118.81	108.17
2	B	543	GLN	N-CA-C	7.57	119.31	111.14
1	A	700	PHE	CA-C-N	-7.44	110.54	119.84
1	A	700	PHE	C-N-CA	-7.44	110.54	119.84
2	B	339	LYS	CA-C-N	7.31	127.95	119.47
2	B	339	LYS	C-N-CA	7.31	127.95	119.47
2	B	604	ASN	N-CA-C	-7.27	101.28	112.99
2	B	857	LEU	N-CA-C	7.14	114.64	108.78
2	B	523	LEU	N-CA-C	-6.51	96.93	110.80
1	A	228	ARG	N-CA-C	-6.45	104.89	112.89
2	B	1005	LEU	N-CA-C	-6.40	102.58	110.65
2	B	602	LEU	N-CA-C	6.32	124.27	110.80
1	A	41	LEU	N-CA-C	-6.27	98.99	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	447	ILE	N-CA-C	6.23	116.89	108.17
1	A	23	VAL	N-CA-C	-6.20	99.12	108.17
1	A	252	TRP	CA-C-N	6.17	126.13	119.78
1	A	252	TRP	C-N-CA	6.17	126.13	119.78
2	B	515	VAL	N-CA-C	-6.15	100.07	109.78
2	B	431	TYR	N-CA-C	-6.11	105.86	113.38
1	A	369	GLY	N-CA-C	6.08	119.02	112.33
2	B	730	VAL	N-CA-C	6.06	116.58	107.80
1	A	250	ASP	CA-C-N	5.94	125.15	118.97
1	A	250	ASP	C-N-CA	5.94	125.15	118.97
2	B	338	ILE	N-CA-C	5.86	116.31	107.75
2	B	982	ARG	N-CA-C	5.82	117.33	109.24
2	B	667	MET	N-CA-C	5.82	118.09	111.11
2	B	996	GLN	CA-C-N	-5.81	113.69	119.56
2	B	996	GLN	C-N-CA	-5.81	113.69	119.56
2	B	584	SER	N-CA-C	5.81	117.42	109.18
1	A	444	CYS	N-CA-C	-5.76	104.82	112.94
2	B	859	ARG	N-CA-C	5.68	122.36	109.81
2	B	864	THR	N-CA-C	-5.66	105.11	111.28
2	B	313	ILE	N-CA-C	5.66	116.02	108.27
2	B	635	LEU	N-CA-C	5.63	117.70	108.52
2	B	2	MET	N-CA-C	5.63	119.27	110.32
2	B	949	SER	N-CA-C	5.63	117.96	109.41
2	B	469	MET	N-CA-C	5.58	118.29	111.82
2	B	606	ASP	N-CA-C	-5.58	105.24	113.72
1	A	426	LEU	N-CA-C	-5.57	106.15	113.17
2	B	986	MET	N-CA-C	5.53	117.87	110.35
2	B	454	ILE	N-CA-C	-5.50	105.75	111.58
1	A	541	ASP	N-CA-C	-5.41	106.65	113.20
2	B	948	PRO	N-CA-C	5.40	120.64	113.40
2	B	685	LYS	N-CA-C	-5.31	101.99	109.96
1	A	24	TRP	N-CA-C	5.23	117.53	110.31
1	A	490	GLY	N-CA-C	-5.23	108.47	114.69
1	A	539	GLY	CA-C-N	5.20	126.34	119.84
1	A	539	GLY	C-N-CA	5.20	126.34	119.84
2	B	716	ASP	N-CA-C	5.18	117.07	108.20
2	B	267	SER	N-CA-C	5.17	117.65	110.20
2	B	896	LEU	N-CA-C	5.16	117.71	110.23
2	B	918	GLY	N-CA-C	5.15	121.31	112.51
2	B	982	ARG	CA-C-N	5.14	124.58	119.24
2	B	982	ARG	C-N-CA	5.14	124.58	119.24
2	B	525	GLY	N-CA-C	-5.13	107.90	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	878	GLY	N-CA-C	-5.13	104.47	112.58
1	A	477	GLY	N-CA-C	-5.13	102.76	112.51
1	A	176	HIS	N-CA-C	5.07	117.82	109.76
1	A	388	ARG	N-CA-C	-5.07	106.36	112.54
1	A	64	THR	N-CA-C	5.01	117.13	111.11
2	B	1006	VAL	N-CA-C	5.00	119.75	109.34

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	5684	0	5636	264	0
2	B	6038	0	6038	394	0
3	C	53	0	50	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	79	0	0	10	0
5	B	71	0	0	7	0
All	All	11927	0	11724	653	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 28.

All (653) 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:190:ILE:HD11	1.31	1.09
1:A:747:VAL:HG12	1:A:748:SER:H	1.25	1.01
1:A:123:ARG:HG3	1:A:125:PRO:HD2	1.39	1.01
2:B:639:PRO:HB3	2:B:643:VAL:HG21	1.40	1.00
2:B:601:LYS:HB3	2:B:605:THR:HG21	1.44	0.99
2:B:996:GLN:HB3	2:B:997:PRO:HD2	1.45	0.98
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.41	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.47	0.94
2:B:963:VAL:HG12	2:B:964:GLY:H	1.34	0.93
2:B:600:LYS:HD2	2:B:602:LEU:HD21	1.50	0.92
2:B:713:ASN:HD21	2:B:716:ASP:H	1.07	0.91
2:B:469:MET:HE1	2:B:678:LEU:HG	1.53	0.91
1:A:381:LEU:HA	1:A:702:MET:HE2	1.52	0.90
1:A:283:GLY:H	1:A:486:GLN:HE22	1.20	0.90
2:B:713:ASN:HD22	2:B:715:THR:H	1.17	0.89
2:B:469:MET:HE3	2:B:679:ARG:HA	1.54	0.89
1:A:51:LEU:HD12	1:A:52:PRO:HD2	1.54	0.88
1:A:745:ASP:CG	1:A:746:ASP:H	1.82	0.87
1:A:147:LEU:HG	1:A:151:MET:HE2	1.55	0.86
2:B:901:THR:HG22	2:B:902:MET:H	1.38	0.86
2:B:713:ASN:ND2	2:B:715:THR:H	1.74	0.85
2:B:453:ASN:HD21	2:B:583:SER:HB3	1.40	0.85
2:B:2:MET:HE1	2:B:836:LEU:HD12	1.57	0.84
2:B:2:MET:CE	2:B:836:LEU:HD12	2.06	0.84
1:A:528:ARG:HA	1:A:608:MET:HE1	1.61	0.83
2:B:453:ASN:ND2	2:B:583:SER:HB3	1.93	0.82
1:A:297:GLY:H	1:A:300:MET:HE3	1.45	0.81
2:B:1030:GLN:C	2:B:1032:LEU:H	1.89	0.80
2:B:469:MET:HE2	2:B:682:ILE:HD12	1.65	0.79
2:B:713:ASN:ND2	2:B:716:ASP:H	1.79	0.79
1:A:18:ARG:NH1	1:A:612:LEU:HD22	1.98	0.79
2:B:974:ILE:HA	2:B:977:ILE:HG22	1.66	0.78
2:B:996:GLN:HB3	2:B:997:PRO:CD	2.13	0.78
1:A:609:ARG:HG3	1:A:609:ARG:HH11	1.48	0.78
2:B:543:GLN:HB3	2:B:547:MET:HE3	1.64	0.78
1:A:297:GLY:H	1:A:300:MET:HB2	1.49	0.78
2:B:409:ARG:O	2:B:409:ARG:HG3	1.82	0.77
1:A:3:THR:HB	1:A:6:GLU:HG3	1.66	0.76
1:A:312:SER:O	1:A:316:ILE:HG22	1.85	0.76
1:A:297:GLY:N	1:A:300:MET:HB2	2.01	0.76
2:B:557:VAL:HA	5:B:1079:HOH:O	1.84	0.76
2:B:614:PRO:HG3	2:B:650:LEU:HD22	1.67	0.76
1:A:656:ILE:HG13	1:A:695:ILE:HG21	1.68	0.75
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.67	0.75
1:A:239:ASN:HB3	5:A:845:HOH:O	1.86	0.75
2:B:500:VAL:HG11	2:B:537:ILE:HG12	1.68	0.75
1:A:375:ASP:HA	5:A:843:HOH:O	1.87	0.74
1:A:511:GLN:CD	1:A:511:GLN:H	1.92	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:283:VAL:HG22	2:B:301:MET:HE2	1.70	0.74
2:B:356:HIS:HD2	2:B:362:VAL:H	1.36	0.74
1:A:381:LEU:HA	1:A:702:MET:CE	2.18	0.74
1:A:3:THR:HG22	1:A:5:LEU:H	1.51	0.74
2:B:1000:VAL:HA	2:B:1003:GLN:HE21	1.51	0.73
1:A:198:LYS:HE2	1:A:202:GLU:OE2	1.88	0.73
2:B:933:GLY:O	2:B:936:SER:HB2	1.88	0.73
1:A:296:GLN:HA	1:A:300:MET:HE2	1.70	0.73
2:B:889:GLN:HG2	2:B:891:LEU:HD21	1.70	0.73
1:A:153:MET:HE2	1:A:154:SER:HA	1.69	0.73
1:A:181:GLU:HG2	1:A:239:ASN:HD21	1.53	0.73
2:B:345:PRO:HB2	2:B:348:GLU:HG3	1.71	0.73
2:B:462:ILE:O	2:B:466:LEU:HB2	1.89	0.72
2:B:633:VAL:H	2:B:655:THR:HG21	1.54	0.72
2:B:637:LEU:HG	2:B:639:PRO:HD3	1.70	0.72
2:B:652:PRO:HA	2:B:655:THR:HG22	1.68	0.72
2:B:465:GLU:HG2	2:B:675:LEU:HD22	1.71	0.72
2:B:267:SER:HB3	2:B:908:ARG:HH21	1.55	0.72
1:A:596:SER:OG	1:A:599:GLU:HG3	1.88	0.72
2:B:595:LYS:H	2:B:615:GLN:HE22	1.36	0.72
2:B:901:THR:HB	2:B:970:GLN:HE21	1.53	0.72
1:A:583:HIS:CD2	1:A:620:GLN:HE21	2.08	0.71
2:B:600:LYS:HD2	2:B:602:LEU:CD2	2.19	0.70
2:B:454:ILE:HD13	2:B:459:VAL:HG21	1.73	0.70
1:A:583:HIS:HD2	1:A:620:GLN:HE21	1.39	0.70
2:B:963:VAL:HG12	2:B:964:GLY:N	2.07	0.70
1:A:369:GLY:O	1:A:609:ARG:NH2	2.24	0.70
2:B:997:PRO:O	2:B:999:MET:N	2.25	0.70
2:B:500:VAL:HG11	2:B:537:ILE:CG1	2.22	0.70
2:B:713:ASN:HD21	2:B:716:ASP:N	1.85	0.70
1:A:745:ASP:CG	1:A:746:ASP:N	2.50	0.69
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.72	0.69
2:B:992:LYS:HD2	2:B:996:GLN:HE21	1.58	0.69
1:A:236:ILE:HG22	1:A:240:LEU:HB2	1.74	0.69
1:A:506:ALA:O	1:A:510:ILE:HG13	1.93	0.69
2:B:469:MET:HE1	2:B:678:LEU:CG	2.22	0.69
2:B:407:GLY:O	2:B:409:ARG:N	2.26	0.69
1:A:115:SER:O	1:A:116:SER:HB3	1.91	0.68
1:A:560:TYR:CD1	1:A:761:VAL:HG12	2.28	0.68
2:B:585:LEU:HD21	2:B:594:LEU:HB2	1.74	0.68
2:B:901:THR:HB	2:B:973:MET:HE1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:802:PRO:HB2	2:B:805:VAL:HG23	1.76	0.68
2:B:992:LYS:HD2	2:B:996:GLN:NE2	2.08	0.68
1:A:283:GLY:N	1:A:486:GLN:HE22	1.92	0.68
2:B:312:PHE:CZ	2:B:344:ILE:HD11	2.28	0.68
2:B:501:LYS:HD3	2:B:503:ASN:HD21	1.59	0.68
1:A:12:GLU:OE1	1:A:18:ARG:HD2	1.94	0.68
1:A:636:LEU:HG	1:A:638:ASP:HB2	1.76	0.68
1:A:652:THR:HG23	1:A:655:GLN:H	1.58	0.67
1:A:51:LEU:HD21	1:A:117:ILE:HA	1.74	0.67
1:A:656:ILE:HD11	1:A:695:ILE:HD13	1.74	0.67
1:A:116:SER:HA	1:A:496:VAL:O	1.93	0.67
2:B:602:LEU:HD11	2:B:859:ARG:HB2	1.75	0.67
1:A:404:GLY:HA2	1:A:484:GLN:O	1.94	0.67
2:B:446:MET:HE3	2:B:561:VAL:HG12	1.77	0.67
2:B:842:VAL:HG12	2:B:842:VAL:O	1.94	0.67
2:B:901:THR:HG22	2:B:902:MET:N	2.09	0.67
1:A:30:GLU:CD	1:A:506:ALA:HB3	2.20	0.67
2:B:978:ILE:HG22	2:B:986:MET:HE1	1.77	0.66
2:B:493:LYS:HA	2:B:557:VAL:HG13	1.77	0.66
2:B:470:LEU:HD12	2:B:473:ILE:HD11	1.75	0.66
2:B:993:GLN:HG2	2:B:994:ARG:N	2.09	0.66
2:B:633:VAL:HG13	2:B:655:THR:HG21	1.78	0.66
1:A:747:VAL:HG12	1:A:748:SER:N	2.05	0.66
1:A:652:THR:CG2	1:A:655:GLN:H	2.10	0.65
2:B:317:THR:HG22	2:B:319:CYS:H	1.61	0.65
1:A:700:PHE:O	1:A:702:MET:N	2.30	0.65
2:B:807:ARG:HG2	2:B:807:ARG:HH11	1.62	0.65
2:B:269:ILE:HD11	2:B:907:VAL:C	2.22	0.65
1:A:195:LEU:CD2	1:A:203:MET:HE1	2.27	0.64
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.13	0.64
1:A:413:GLU:O	1:A:464:VAL:HG12	1.97	0.64
1:A:652:THR:HG21	1:A:655:GLN:HG2	1.79	0.64
2:B:267:SER:HB2	2:B:908:ARG:HE	1.61	0.64
2:B:469:MET:HE3	2:B:679:ARG:CA	2.26	0.64
2:B:485:ARG:HG3	5:B:1088:HOH:O	1.97	0.64
2:B:943:GLY:O	2:B:968:SER:HB2	1.97	0.64
2:B:948:PRO:HG2	2:B:952:HIS:ND1	2.12	0.64
2:B:627:VAL:HG21	2:B:710:LEU:HD23	1.79	0.64
2:B:600:LYS:O	2:B:600:LYS:HG3	1.98	0.64
2:B:605:THR:HG22	2:B:607:LYS:HB3	1.79	0.63
2:B:543:GLN:HB3	2:B:547:MET:CE	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ILE:HD12	1:A:615:SER:HB3	1.80	0.63
1:A:30:GLU:OE1	1:A:506:ALA:HB3	1.98	0.63
2:B:719:MET:SD	2:B:722:ILE:HD12	2.38	0.63
2:B:919:ILE:HG23	2:B:932:LEU:HD23	1.81	0.63
2:B:958:THR:HG21	2:B:988:LEU:O	1.98	0.63
2:B:403:LEU:HA	2:B:409:ARG:HA	1.80	0.63
2:B:543:GLN:HG3	5:B:1102:HOH:O	1.97	0.63
2:B:600:LYS:HA	2:B:859:ARG:NH1	2.13	0.63
1:A:743:LEU:O	1:A:744:THR:HB	1.97	0.63
2:B:529:ASN:HD22	2:B:530:TYR:N	1.96	0.63
2:B:492:ASN:C	2:B:494:VAL:H	2.05	0.62
2:B:934:VAL:HG23	2:B:935:SER:N	2.14	0.62
2:B:616:THR:HG21	5:B:1047:HOH:O	1.99	0.62
1:A:297:GLY:N	1:A:300:MET:HE3	2.13	0.62
1:A:297:GLY:CA	1:A:300:MET:HB2	2.30	0.62
2:B:500:VAL:HG12	2:B:500:VAL:O	2.00	0.62
2:B:355:ASN:ND2	2:B:357:GLY:H	1.96	0.62
2:B:456:ASN:OD1	2:B:458:LEU:HB2	1.99	0.62
2:B:974:ILE:HA	2:B:977:ILE:CG2	2.29	0.62
2:B:355:ASN:HD22	2:B:356:HIS:N	1.98	0.62
2:B:602:LEU:HD23	2:B:602:LEU:N	2.15	0.62
2:B:942:GLN:HG2	2:B:948:PRO:HA	1.81	0.62
2:B:289:ARG:HD2	2:B:769:ASN:OD1	2.00	0.62
1:A:524:ILE:HD13	1:A:619:ILE:HD12	1.82	0.61
1:A:199:GLN:O	1:A:203:MET:HG3	2.00	0.61
2:B:529:ASN:HD22	2:B:529:ASN:C	2.06	0.61
1:A:565:PRO:HG3	1:A:758:LYS:HA	1.83	0.61
2:B:2:MET:CE	3:C:190:ILE:HD11	2.19	0.61
2:B:922:LEU:C	2:B:922:LEU:HD23	2.25	0.61
2:B:501:LYS:CD	2:B:503:ASN:HD21	2.13	0.61
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.81	0.61
1:A:583:HIS:CD2	1:A:620:GLN:HG3	2.35	0.61
2:B:378:ILE:HG12	2:B:383:ARG:O	2.01	0.61
2:B:639:PRO:CB	2:B:643:VAL:HG21	2.24	0.61
2:B:852:LYS:HE3	2:B:1015:SER:O	1.99	0.61
2:B:585:LEU:CD2	2:B:594:LEU:HB2	2.30	0.61
1:A:238:MET:O	1:A:241:THR:HG22	2.01	0.61
2:B:632:SER:HA	2:B:655:THR:OG1	2.00	0.61
1:A:134:VAL:HG11	1:A:288:MET:HE3	1.82	0.60
1:A:190:ARG:HH12	2:B:519:PHE:HB3	1.65	0.60
2:B:692:MET:HE1	2:B:728:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:GLU:O	1:A:560:TYR:HB3	1.99	0.60
2:B:963:VAL:O	2:B:964:GLY:O	2.19	0.60
2:B:616:THR:HG22	2:B:617:ASN:H	1.66	0.60
1:A:115:SER:O	1:A:116:SER:CB	2.50	0.60
1:A:700:PHE:O	1:A:701:PRO:C	2.43	0.60
2:B:979:GLN:HE22	2:B:986:MET:H	1.50	0.60
2:B:406:ILE:HG22	2:B:406:ILE:O	2.02	0.60
2:B:975:MET:HE1	2:B:988:LEU:HD22	1.84	0.60
2:B:802:PRO:HD2	2:B:805:VAL:HG21	1.85	0.59
1:A:673:GLN:HG2	1:A:685:LEU:HD12	1.84	0.59
2:B:751:LEU:HA	2:B:761:LEU:HD23	1.85	0.59
1:A:303:GLY:HA3	5:A:823:HOH:O	2.02	0.59
2:B:340:PRO:HB2	2:B:341:PHE:CD1	2.36	0.59
2:B:889:GLN:HG2	2:B:891:LEU:CD2	2.32	0.59
2:B:909:CYS:O	2:B:1007:GLU:HB2	2.02	0.59
1:A:155:LEU:HD12	1:A:158:LEU:HD12	1.83	0.59
2:B:2:MET:HE3	2:B:836:LEU:HD12	1.84	0.59
2:B:321:PRO:HG2	2:B:734:HIS:HE1	1.68	0.59
2:B:529:ASN:ND2	2:B:531:GLN:H	2.01	0.59
1:A:386:PHE:O	1:A:389:VAL:HB	2.02	0.59
2:B:941:ILE:HG23	2:B:953:ILE:HD11	1.84	0.58
1:A:352:LEU:HA	5:A:843:HOH:O	2.02	0.58
1:A:745:ASP:O	1:A:747:VAL:N	2.36	0.58
2:B:838:ASP:OD1	2:B:841:LYS:HE3	2.03	0.58
2:B:901:THR:CB	2:B:970:GLN:HE21	2.16	0.58
1:A:412:ARG:HG3	1:A:413:GLU:OE2	2.03	0.58
1:A:153:MET:HE3	1:A:157:LEU:CD1	2.34	0.58
1:A:305:GLU:HG3	5:A:823:HOH:O	2.03	0.58
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.68	0.58
2:B:526:PHE:O	2:B:527:LEU:HB2	2.04	0.58
1:A:153:MET:SD	1:A:387:GLN:HB3	2.44	0.58
2:B:948:PRO:HG2	2:B:952:HIS:CE1	2.38	0.58
1:A:148:LYS:HE3	1:A:244:LEU:O	2.03	0.58
1:A:364:PRO:O	1:A:367:THR:O	2.22	0.58
2:B:852:LYS:HE2	2:B:1008:ASP:O	2.04	0.58
1:A:15:ASP:OD1	1:A:116:SER:HB2	2.04	0.58
2:B:633:VAL:HG11	2:B:651:VAL:HG12	1.86	0.58
1:A:407:GLU:HG3	1:A:445:GLN:HG3	1.85	0.57
2:B:492:ASN:OD1	2:B:492:ASN:O	2.22	0.57
2:B:523:LEU:O	2:B:524:ASP:HB2	2.02	0.57
2:B:355:ASN:HD22	2:B:355:ASN:C	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:THR:HG22	1:A:537:GLU:N	2.20	0.57
2:B:409:ARG:HG3	2:B:411:ASP:HB2	1.85	0.57
2:B:616:THR:HG22	2:B:617:ASN:N	2.20	0.57
1:A:153:MET:HE2	1:A:154:SER:CA	2.34	0.57
2:B:296:VAL:HG12	2:B:314:ARG:NE	2.20	0.57
2:B:859:ARG:HB3	2:B:860:PRO:HD3	1.87	0.57
2:B:652:PRO:HA	2:B:655:THR:CG2	2.33	0.57
1:A:147:LEU:HD11	1:A:289:PHE:CD2	2.40	0.57
1:A:183:ILE:HD11	2:B:509:MET:HB2	1.86	0.56
1:A:652:THR:HG22	1:A:655:GLN:O	2.05	0.56
2:B:404:ASP:OD2	2:B:410:LEU:HB2	2.05	0.56
2:B:633:VAL:CG1	2:B:655:THR:HG21	2.35	0.56
2:B:898:VAL:HG22	2:B:967:TYR:CE2	2.40	0.56
2:B:962:GLU:HG2	2:B:963:VAL:N	2.19	0.56
2:B:469:MET:CE	2:B:678:LEU:HG	2.32	0.56
2:B:608:GLU:OE1	2:B:803:LEU:HG	2.05	0.56
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.85	0.56
2:B:286:THR:OG1	2:B:304:ASP:O	2.20	0.56
2:B:332:ILE:HD12	2:B:777:LEU:HD13	1.88	0.56
2:B:553:GLU:OE1	2:B:553:GLU:HA	2.05	0.56
2:B:962:GLU:HG2	2:B:963:VAL:H	1.70	0.56
1:A:536:THR:HG22	1:A:537:GLU:H	1.70	0.56
2:B:934:VAL:HG23	2:B:935:SER:H	1.70	0.56
2:B:945:PHE:HE2	2:B:990:ILE:HD13	1.70	0.56
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.88	0.56
2:B:605:THR:C	2:B:607:LYS:H	2.14	0.56
1:A:317:ASP:C	1:A:319:ASP:H	2.12	0.56
1:A:418:GLY:HA3	1:A:438:ILE:O	2.06	0.56
2:B:1015:SER:HB2	2:B:1019:ASP:CB	2.35	0.56
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.87	0.55
1:A:28:ARG:HH22	1:A:436:ASN:HD21	1.54	0.55
2:B:2:MET:HG2	2:B:1017:TYR:OH	2.06	0.55
2:B:601:LYS:CB	2:B:605:THR:HG21	2.28	0.55
2:B:775:ALA:O	2:B:779:LYS:HG3	2.07	0.55
2:B:902:MET:O	2:B:902:MET:HG2	2.05	0.55
2:B:562:ILE:HB	2:B:622:LEU:HD21	1.88	0.55
2:B:276:ARG:HA	2:B:298:THR:HG23	1.88	0.55
2:B:492:ASN:O	2:B:493:LYS:HG2	2.06	0.55
2:B:345:PRO:HD2	2:B:348:GLU:OE1	2.06	0.55
2:B:739:SER:C	2:B:741:ASP:H	2.14	0.55
1:A:190:ARG:NH1	2:B:519:PHE:HB3	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:ALA:O	1:A:447:LYS:HE3	2.06	0.55
2:B:845:VAL:HG22	2:B:1017:TYR:CE1	2.42	0.55
2:B:854:CYS:HB3	2:B:862:ILE:HD13	1.88	0.55
2:B:633:VAL:H	2:B:655:THR:CG2	2.17	0.55
1:A:171:ARG:HD2	5:A:826:HOH:O	2.06	0.55
2:B:585:LEU:HD21	2:B:594:LEU:CB	2.37	0.55
1:A:609:ARG:HG3	1:A:609:ARG:NH1	2.21	0.54
2:B:374:PHE:CE2	2:B:765:ASN:HB3	2.42	0.54
1:A:116:SER:HB2	1:A:497:THR:HG23	1.88	0.54
1:A:117:ILE:HG12	1:A:118:GLU:N	2.22	0.54
2:B:901:THR:CG2	2:B:902:MET:H	2.15	0.54
2:B:992:LYS:HB2	2:B:996:GLN:HG3	1.88	0.54
1:A:160:PRO:HB3	1:A:234:GLN:HB3	1.89	0.54
2:B:269:ILE:CD1	2:B:908:ARG:N	2.70	0.54
2:B:993:GLN:HG2	2:B:994:ARG:H	1.71	0.54
2:B:1025:HIS:ND1	3:C:192:MET:HG3	2.23	0.54
1:A:536:THR:C	1:A:538:GLU:H	2.16	0.54
2:B:486:VAL:HG12	2:B:487:GLY:N	2.21	0.54
2:B:992:LYS:CD	2:B:996:GLN:HE21	2.19	0.54
2:B:356:HIS:CD2	2:B:362:VAL:H	2.21	0.54
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.43	0.54
1:A:77:ASP:OD2	1:A:80:ALA:HB3	2.07	0.54
1:A:577:TYR:HB3	1:A:578:PRO:HD3	1.89	0.54
2:B:333:PRO:HD3	2:B:813:GLN:NE2	2.22	0.54
2:B:845:VAL:HG22	2:B:1017:TYR:CZ	2.43	0.54
2:B:854:CYS:HB2	2:B:862:ILE:HG21	1.89	0.54
2:B:964:GLY:HA3	2:B:968:SER:HB3	1.90	0.54
1:A:755:HIS:CD2	1:A:758:LYS:HE2	2.44	0.53
2:B:616:THR:HB	2:B:618:VAL:HG22	1.91	0.53
1:A:172:MET:HE2	1:A:252:TRP:HE1	1.74	0.53
2:B:898:VAL:O	2:B:899:LYS:C	2.51	0.53
1:A:3:THR:HG22	1:A:5:LEU:N	2.20	0.53
2:B:693:ARG:HG3	2:B:693:ARG:HH11	1.72	0.53
2:B:641:GLN:HG2	2:B:642:TYR:N	2.24	0.53
2:B:834:LEU:HD21	2:B:836:LEU:HD21	1.90	0.53
2:B:860:PRO:O	2:B:861:GLU:HB2	2.09	0.53
1:A:312:SER:H	1:A:315:ASP:HB2	1.73	0.53
2:B:267:SER:HB3	2:B:908:ARG:NH2	2.21	0.53
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.91	0.53
2:B:602:LEU:HA	2:B:608:GLU:HB2	1.90	0.53
2:B:852:LYS:O	2:B:857:LEU:HD22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:745:ASP:O	1:A:747:VAL:HG23	2.08	0.53
2:B:641:GLN:O	2:B:643:VAL:HG23	2.09	0.53
2:B:738:LEU:HB2	2:B:770:CYS:SG	2.49	0.53
1:A:297:GLY:HA3	1:A:300:MET:HB2	1.90	0.52
1:A:509:GLN:O	1:A:510:ILE:C	2.52	0.52
2:B:288:THR:HG22	2:B:289:ARG:N	2.24	0.52
2:B:820:CYS:HA	2:B:823:LYS:HE2	1.91	0.52
2:B:375:MET:HE1	2:B:386:CYS:SG	2.49	0.52
2:B:965:ASN:HB3	2:B:966:PRO:HD3	1.90	0.52
1:A:199:GLN:HB3	1:A:203:MET:HE2	1.90	0.52
2:B:529:ASN:C	2:B:529:ASN:ND2	2.66	0.52
2:B:996:GLN:CB	2:B:997:PRO:HD2	2.30	0.52
1:A:173:VAL:HG11	1:A:270:ILE:HD12	1.92	0.52
2:B:602:LEU:HD21	2:B:859:ARG:HD3	1.92	0.52
2:B:633:VAL:CG1	2:B:651:VAL:HG12	2.39	0.52
1:A:127:MET:HE2	1:A:127:MET:HA	1.91	0.52
1:A:668:ARG:HA	1:A:673:GLN:NE2	2.25	0.52
2:B:661:LYS:NZ	2:B:661:LYS:HB3	2.25	0.52
2:B:279:ARG:NH2	2:B:293:PRO:C	2.68	0.51
1:A:397:GLN:NE2	1:A:489:SER:HB3	2.26	0.51
1:A:178:LEU:C	1:A:180:CYS:H	2.19	0.51
2:B:898:VAL:HG22	2:B:967:TYR:HE2	1.75	0.51
2:B:526:PHE:O	2:B:527:LEU:CB	2.59	0.51
2:B:627:VAL:HG21	2:B:710:LEU:CD2	2.39	0.51
2:B:1015:SER:HB2	2:B:1019:ASP:HB2	1.93	0.51
1:A:297:GLY:H	1:A:300:MET:CE	2.18	0.51
1:A:414:ILE:HG22	1:A:415:LYS:N	2.25	0.51
2:B:409:ARG:O	2:B:411:ASP:N	2.44	0.51
2:B:941:ILE:HD13	2:B:950:PHE:HA	1.93	0.51
1:A:696:LEU:HD12	1:A:703:PRO:HG2	1.93	0.51
1:A:259:ARG:HG3	1:A:306:LEU:HD23	1.91	0.51
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.76	0.50
1:A:547:ASP:HB3	1:A:743:LEU:HB2	1.93	0.50
2:B:269:ILE:HD11	2:B:908:ARG:N	2.26	0.50
2:B:523:LEU:HD23	5:B:1081:HOH:O	2.09	0.50
2:B:838:ASP:HA	2:B:841:LYS:HG3	1.93	0.50
2:B:937:PRO:HG2	2:B:940:LEU:HD12	1.92	0.50
2:B:589:GLU:O	2:B:590:ALA:HB2	2.10	0.50
2:B:641:GLN:HG2	2:B:642:TYR:H	1.77	0.50
2:B:739:SER:C	2:B:741:ASP:N	2.69	0.50
1:A:662:GLU:HG3	1:A:710:HIS:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:CYS:HB2	2:B:373:PRO:CD	2.41	0.50
1:A:6:GLU:O	1:A:10:GLN:HG3	2.12	0.50
1:A:456:THR:O	1:A:528:ARG:NH2	2.43	0.50
1:A:656:ILE:HG13	1:A:695:ILE:CG2	2.41	0.50
2:B:411:ASP:O	2:B:412:HIS:C	2.54	0.50
1:A:528:ARG:HG3	1:A:608:MET:CE	2.41	0.50
2:B:267:SER:CB	2:B:908:ARG:HH21	2.23	0.50
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.26	0.50
2:B:317:THR:HG21	2:B:777:LEU:HD23	1.94	0.50
2:B:686:ILE:HG22	2:B:723:ASP:HB3	1.93	0.50
1:A:183:ILE:CD1	2:B:509:MET:HE3	2.42	0.49
1:A:183:ILE:HD12	2:B:547:MET:CE	2.41	0.49
1:A:208:LYS:O	1:A:209:VAL:HB	2.12	0.49
1:A:392:LYS:HD3	1:A:396:GLY:HA2	1.94	0.49
1:A:696:LEU:CD1	1:A:703:PRO:HG2	2.42	0.49
1:A:511:GLN:CD	1:A:511:GLN:N	2.67	0.49
2:B:410:LEU:O	2:B:410:LEU:HG	2.11	0.49
2:B:544:ILE:HB	2:B:545:PRO:HD3	1.94	0.49
2:B:1025:HIS:CG	3:C:192:MET:HG3	2.47	0.49
1:A:53:PRO:O	1:A:54:ILE:O	2.30	0.49
2:B:643:VAL:HG12	2:B:643:VAL:O	2.12	0.49
1:A:596:SER:HG	1:A:599:GLU:HG3	1.78	0.49
2:B:407:GLY:C	2:B:409:ARG:N	2.71	0.49
2:B:893:ILE:O	2:B:896:LEU:HB2	2.12	0.49
1:A:179:GLY:O	1:A:181:GLU:HG3	2.12	0.49
1:A:673:GLN:HG2	1:A:685:LEU:CD1	2.42	0.49
2:B:703:THR:HG21	2:B:733:LYS:HB2	1.95	0.49
2:B:775:ALA:HB1	2:B:779:LYS:HE3	1.95	0.49
1:A:148:LYS:HA	1:A:151:MET:HE3	1.94	0.49
2:B:492:ASN:C	2:B:494:VAL:N	2.70	0.49
2:B:618:VAL:HG23	2:B:619:TYR:N	2.27	0.49
2:B:813:GLN:O	2:B:817:MET:HG3	2.12	0.49
1:A:153:MET:HE3	1:A:157:LEU:HD11	1.95	0.49
1:A:195:LEU:HD22	1:A:203:MET:CE	2.41	0.49
2:B:304:ASP:O	2:B:305:GLN:CB	2.61	0.49
2:B:974:ILE:CA	2:B:977:ILE:HG22	2.41	0.49
1:A:162:ALA:O	1:A:233:VAL:HG23	2.13	0.49
1:A:406:LEU:O	1:A:445:GLN:HA	2.13	0.49
1:A:536:THR:O	1:A:538:GLU:N	2.45	0.49
1:A:747:VAL:CG1	1:A:748:SER:H	2.08	0.49
2:B:455:LYS:C	2:B:457:GLY:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ASP:HB3	1:A:497:THR:CG2	2.43	0.48
2:B:375:MET:SD	2:B:386:CYS:HA	2.52	0.48
1:A:511:GLN:H	1:A:511:GLN:NE2	2.11	0.48
2:B:534:GLN:HG2	2:B:538:HIS:CD2	2.48	0.48
1:A:649:LEU:C	1:A:649:LEU:HD13	2.38	0.48
2:B:1:ALA:N	3:C:190:ILE:HG23	2.29	0.48
2:B:992:LYS:CB	2:B:996:GLN:HG3	2.43	0.48
2:B:993:GLN:O	2:B:994:ARG:C	2.57	0.48
1:A:78:TYR:CD2	1:A:101:ILE:HG12	2.48	0.48
1:A:609:ARG:HH11	1:A:609:ARG:CG	2.20	0.48
1:A:744:THR:HG21	1:A:752:PHE:HD1	1.78	0.48
2:B:372:CYS:HA	2:B:417:GLU:O	2.13	0.48
2:B:942:GLN:CG	2:B:948:PRO:HA	2.43	0.48
2:B:979:GLN:HE22	2:B:986:MET:N	2.10	0.48
2:B:1030:GLN:C	2:B:1032:LEU:N	2.61	0.48
2:B:485:ARG:NH2	5:B:1083:HOH:O	2.41	0.48
2:B:800:HIS:C	2:B:801:GLN:HG3	2.38	0.48
2:B:955:THR:HG23	2:B:990:ILE:O	2.13	0.48
1:A:252:TRP:HB3	5:A:826:HOH:O	2.12	0.48
1:A:609:ARG:NH1	5:A:771:HOH:O	2.47	0.48
2:B:607:LYS:HG2	2:B:610:ILE:HD12	1.95	0.48
2:B:289:ARG:HD3	2:B:768:LEU:O	2.14	0.48
2:B:528:VAL:HG12	2:B:529:ASN:H	1.78	0.48
2:B:602:LEU:N	2:B:605:THR:OG1	2.46	0.48
2:B:854:CYS:CB	2:B:862:ILE:HD13	2.44	0.48
1:A:58:PRO:O	1:A:59:VAL:HB	2.13	0.48
1:A:236:ILE:O	1:A:237:ASP:C	2.57	0.48
2:B:334:LEU:N	2:B:334:LEU:HD22	2.29	0.48
2:B:814:THR:HA	2:B:817:MET:HE2	1.95	0.48
1:A:695:ILE:C	1:A:697:HIS:H	2.22	0.47
2:B:446:MET:HE2	2:B:578:LEU:HB3	1.95	0.47
2:B:693:ARG:HG3	2:B:693:ARG:NH1	2.27	0.47
2:B:289:ARG:O	2:B:291:GLN:N	2.45	0.47
2:B:766:LEU:HD21	2:B:768:LEU:HD21	1.96	0.47
1:A:314:HIS:HB3	1:A:318:LYS:HE3	1.96	0.47
1:A:34:MET:C	1:A:35:VAL:CG1	2.87	0.47
2:B:356:HIS:CD2	2:B:361:PRO:HA	2.49	0.47
1:A:357:LEU:HD11	1:A:373:MET:HG3	1.95	0.47
2:B:649:GLY:O	2:B:652:PRO:HG2	2.14	0.47
1:A:19:PHE:CD2	1:A:40:ALA:HB2	2.50	0.47
1:A:143:ASP:OD2	1:A:376:SER:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ASP:O	1:A:565:PRO:C	2.57	0.47
2:B:515:VAL:CG1	2:B:560:PRO:HG2	2.45	0.47
2:B:534:GLN:HG2	2:B:538:HIS:HD2	1.80	0.47
2:B:842:VAL:O	2:B:842:VAL:CG1	2.62	0.47
2:B:559:ALA:HB3	2:B:560:PRO:HD3	1.97	0.47
2:B:1025:HIS:O	2:B:1028:ILE:HG22	2.15	0.47
1:A:345:ILE:O	1:A:369:GLY:HA3	2.15	0.47
1:A:539:GLY:O	1:A:542:VAL:HG23	2.15	0.47
2:B:979:GLN:NE2	2:B:985:SER:HA	2.30	0.47
2:B:269:ILE:CD1	2:B:907:VAL:C	2.87	0.47
2:B:807:ARG:HG2	2:B:807:ARG:NH1	2.29	0.47
1:A:370:TYR:HA	5:A:813:HOH:O	2.15	0.46
1:A:545:TRP:O	1:A:549:GLN:HG2	2.15	0.46
2:B:529:ASN:HD21	2:B:531:GLN:HG2	1.80	0.46
1:A:313:TRP:CE2	1:A:597:PRO:HA	2.50	0.46
2:B:639:PRO:HB3	2:B:643:VAL:CG2	2.28	0.46
2:B:652:PRO:CA	2:B:655:THR:HG22	2.41	0.46
2:B:971:LEU:O	2:B:974:ILE:HG12	2.15	0.46
2:B:994:ARG:O	2:B:996:GLN:HG2	2.16	0.46
1:A:198:LYS:O	1:A:202:GLU:HG3	2.15	0.46
1:A:625:ALA:HB1	1:A:646:ARG:HG2	1.97	0.46
2:B:571:ALA:C	2:B:573:ASP:H	2.23	0.46
2:B:319:CYS:HA	2:B:769:ASN:O	2.15	0.46
1:A:190:ARG:HB3	1:A:192:THR:HG22	1.98	0.46
1:A:413:GLU:C	1:A:464:VAL:HG12	2.41	0.46
2:B:605:THR:C	2:B:607:LYS:N	2.72	0.46
2:B:996:GLN:CB	2:B:997:PRO:CD	2.90	0.46
2:B:312:PHE:CE1	2:B:344:ILE:HD11	2.50	0.46
2:B:321:PRO:HB3	2:B:326:MET:HE2	1.98	0.46
2:B:888:PRO:HB3	2:B:922:LEU:HD21	1.97	0.46
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.98	0.46
2:B:559:ALA:N	2:B:560:PRO:CD	2.79	0.46
2:B:901:THR:HG22	2:B:903:LEU:H	1.80	0.46
2:B:446:MET:CE	2:B:561:VAL:HG12	2.45	0.46
2:B:949:SER:O	2:B:952:HIS:HB2	2.16	0.46
2:B:395:VAL:HG11	2:B:400:PHE:HA	1.97	0.46
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.51	0.45
1:A:536:THR:C	1:A:538:GLU:N	2.73	0.45
2:B:486:VAL:O	2:B:527:LEU:HA	2.16	0.45
2:B:499:ASN:HB3	2:B:508:GLN:HB2	1.98	0.45
2:B:1020:PHE:O	2:B:1024:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.51	0.45
1:A:290:ILE:CD1	1:A:360:MET:HE1	2.45	0.45
1:A:350:CYS:HB2	1:A:377:PHE:CE1	2.51	0.45
2:B:402:HIS:O	2:B:409:ARG:HA	2.15	0.45
2:B:500:VAL:HG11	2:B:537:ILE:HG13	1.97	0.45
1:A:491:GLN:HG2	1:A:493:ARG:HE	1.80	0.45
2:B:857:LEU:HD12	2:B:857:LEU:HA	1.69	0.45
1:A:196:SER:OG	1:A:199:GLN:HG3	2.17	0.45
1:A:505:ASP:O	1:A:509:GLN:N	2.50	0.45
1:A:638:ASP:OD1	1:A:639:SER:N	2.50	0.45
2:B:2:MET:CG	2:B:3:GLY:N	2.79	0.45
2:B:303:GLN:O	2:B:304:ASP:O	2.34	0.45
1:A:153:MET:CE	1:A:157:LEU:HD12	2.46	0.45
1:A:244:LEU:O	1:A:247:LEU:HB2	2.17	0.45
1:A:509:GLN:O	1:A:511:GLN:N	2.50	0.45
2:B:665:PHE:HE2	2:B:667:MET:HE2	1.81	0.45
2:B:751:LEU:HD13	2:B:761:LEU:HD21	1.99	0.45
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.46	0.45
1:A:60:LEU:HB2	1:A:67:ARG:NH1	2.32	0.45
1:A:660:HIS:HB2	1:A:709:GLU:HB3	1.98	0.45
2:B:599:ASP:HB3	2:B:601:LYS:HG3	1.98	0.45
2:B:643:VAL:CG1	2:B:648:LEU:HD12	2.46	0.45
2:B:834:LEU:HB2	2:B:1025:HIS:CD2	2.51	0.45
1:A:174:GLN:HG2	1:A:188:VAL:HG22	1.99	0.45
1:A:357:LEU:CD1	1:A:373:MET:HG3	2.47	0.45
2:B:515:VAL:HG13	2:B:560:PRO:CG	2.46	0.45
2:B:333:PRO:HD3	2:B:813:GLN:HE21	1.81	0.45
2:B:692:MET:HB2	2:B:750:VAL:HG22	1.98	0.45
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.81	0.45
2:B:922:LEU:HD23	2:B:923:ALA:N	2.31	0.45
2:B:955:THR:C	2:B:957:MET:H	2.25	0.45
2:B:1015:SER:HB2	2:B:1019:ASP:HB3	1.99	0.45
1:A:98:TYR:O	1:A:99:ALA:C	2.61	0.44
2:B:624:LYS:HE2	2:B:624:LYS:HB3	1.81	0.44
2:B:934:VAL:C	2:B:936:SER:H	2.25	0.44
1:A:407:GLU:HA	1:A:444:CYS:O	2.17	0.44
1:A:609:ARG:NH1	1:A:609:ARG:CG	2.78	0.44
1:A:647:ILE:HD11	1:A:685:LEU:HD23	2.00	0.44
2:B:356:HIS:HE1	2:B:417:GLU:OE2	2.00	0.44
2:B:798:VAL:HG22	2:B:803:LEU:HD22	2.00	0.44
2:B:928:MET:O	2:B:988:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:485:ARG:HB3	2:B:528:VAL:O	2.18	0.44
1:A:34:MET:O	1:A:36:VAL:N	2.47	0.44
2:B:476:GLU:HB3	2:B:478:GLN:HG3	2.00	0.44
2:B:603:VAL:HG12	2:B:604:ASN:ND2	2.32	0.44
2:B:605:THR:HG22	2:B:607:LYS:CB	2.48	0.44
2:B:891:LEU:HD12	2:B:904:PRO:O	2.17	0.44
2:B:899:LYS:O	2:B:900:SER:HB3	2.18	0.44
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.53	0.44
1:A:147:LEU:HD13	1:A:377:PHE:CD2	2.52	0.44
1:A:394:MET:SD	1:A:394:MET:N	2.87	0.44
1:A:582:PHE:O	1:A:586:ARG:HG2	2.18	0.44
1:A:417:SER:HB3	1:A:438:ILE:HG13	2.00	0.43
2:B:458:LEU:HD21	2:B:638:PHE:CG	2.53	0.43
1:A:747:VAL:HG11	1:A:751:VAL:HG11	2.00	0.43
2:B:312:PHE:HZ	2:B:344:ILE:HD11	1.79	0.43
2:B:535:SER:O	2:B:539:ASN:HB2	2.19	0.43
2:B:692:MET:HE1	2:B:728:VAL:CG1	2.48	0.43
2:B:713:ASN:HD22	2:B:714:THR:N	2.16	0.43
2:B:970:GLN:NE2	2:B:973:MET:SD	2.91	0.43
1:A:373:MET:HE1	1:A:599:GLU:HG2	2.00	0.43
2:B:409:ARG:C	2:B:411:ASP:N	2.76	0.43
2:B:869:TYR:CE2	2:B:873:LEU:HD11	2.53	0.43
2:B:962:GLU:CG	2:B:963:VAL:H	2.28	0.43
1:A:461:PHE:CE2	1:A:479:ILE:HD13	2.54	0.43
2:B:407:GLY:C	2:B:409:ARG:H	2.26	0.43
2:B:570:LYS:HE2	2:B:629:HIS:CE1	2.53	0.43
2:B:945:PHE:CD1	2:B:945:PHE:N	2.87	0.43
1:A:203:MET:HA	2:B:513:THR:HG21	2.01	0.43
1:A:319:ASP:OD1	1:A:319:ASP:O	2.36	0.43
1:A:693:GLN:O	1:A:697:HIS:CD2	2.71	0.43
1:A:311:ARG:HD2	5:A:833:HOH:O	2.19	0.43
1:A:652:THR:HG21	1:A:655:GLN:CG	2.47	0.43
2:B:609:LYS:O	2:B:613:GLN:HG3	2.19	0.43
2:B:837:PRO:HG2	2:B:840:MET:HB2	2.00	0.43
2:B:876:THR:CG2	5:B:1085:HOH:O	2.67	0.43
1:A:415:LYS:HB3	1:A:434:SER:HB2	2.01	0.43
1:A:618:MET:CE	1:A:653:PHE:CD2	3.02	0.43
2:B:453:ASN:O	2:B:459:VAL:HG23	2.19	0.43
2:B:993:GLN:CG	2:B:994:ARG:N	2.73	0.43
2:B:485:ARG:HB3	2:B:528:VAL:C	2.44	0.43
2:B:695:ARG:HG3	2:B:695:ARG:HH11	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:967:TYR:C	2:B:969:GLN:N	2.76	0.43
1:A:647:ILE:HG21	1:A:688:PRO:HG3	2.01	0.43
2:B:515:VAL:HG12	2:B:590:ALA:HB1	2.01	0.43
2:B:901:THR:HB	2:B:970:GLN:NE2	2.28	0.43
1:A:297:GLY:CA	1:A:298:PRO:C	2.92	0.42
1:A:359:GLU:OE1	1:A:359:GLU:N	2.48	0.42
1:A:651:ASP:OD1	1:A:652:THR:O	2.36	0.42
2:B:354:VAL:CG2	2:B:416:PRO:HG2	2.49	0.42
2:B:467:LYS:NZ	2:B:542:ASP:OD1	2.45	0.42
2:B:955:THR:O	2:B:957:MET:N	2.52	0.42
1:A:28:ARG:HH22	1:A:436:ASN:ND2	2.17	0.42
1:A:505:ASP:H	1:A:509:GLN:HG3	1.84	0.42
2:B:540:LEU:O	2:B:544:ILE:HG13	2.19	0.42
2:B:713:ASN:HD22	2:B:715:THR:N	1.99	0.42
2:B:907:VAL:HG11	2:B:913:ARG:HB3	2.01	0.42
1:A:508:THR:C	1:A:509:GLN:HG2	2.43	0.42
1:A:748:SER:OG	1:A:751:VAL:HG23	2.19	0.42
1:A:177:GLU:CD	1:A:185:LYS:HE2	2.45	0.42
2:B:430:ASP:OD2	2:B:430:ASP:N	2.46	0.42
2:B:1000:VAL:HA	2:B:1003:GLN:NE2	2.27	0.42
1:A:70:LEU:HD13	1:A:83:TRP:CD2	2.55	0.42
2:B:289:ARG:C	2:B:291:GLN:H	2.25	0.42
2:B:326:MET:O	2:B:329:GLN:HB2	2.20	0.42
2:B:486:VAL:CG1	2:B:487:GLY:N	2.82	0.42
2:B:577:LYS:HA	2:B:632:SER:O	2.18	0.42
2:B:304:ASP:O	2:B:305:GLN:HB2	2.19	0.42
2:B:907:VAL:CG1	2:B:913:ARG:HB3	2.49	0.42
1:A:526:MET:HG3	1:A:577:TYR:OH	2.19	0.42
2:B:2:MET:HG3	2:B:3:GLY:N	2.32	0.42
2:B:356:HIS:CD2	2:B:362:VAL:HG23	2.55	0.42
2:B:934:VAL:CG2	2:B:935:SER:N	2.82	0.42
1:A:121:VAL:HG12	1:A:123:ARG:N	2.35	0.42
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.87	0.42
1:A:636:LEU:CG	1:A:638:ASP:HB2	2.48	0.42
1:A:669:LYS:HE3	1:A:709:GLU:OE2	2.20	0.42
1:A:743:LEU:O	1:A:755:HIS:ND1	2.52	0.42
2:B:2:MET:HE3	2:B:836:LEU:CD1	2.50	0.42
2:B:361:PRO:O	2:B:363:ARG:HG3	2.20	0.42
2:B:600:LYS:CA	2:B:859:ARG:NH1	2.80	0.42
2:B:891:LEU:N	2:B:891:LEU:HD22	2.35	0.42
2:B:992:LYS:O	2:B:996:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:O	1:A:209:VAL:CB	2.68	0.42
2:B:853:ASN:ND2	2:B:855:VAL:HB	2.34	0.42
1:A:290:ILE:HD13	1:A:360:MET:HE1	2.02	0.42
2:B:854:CYS:O	2:B:867:ARG:HD2	2.19	0.42
1:A:72:PRO:HD3	1:A:109:GLU:O	2.20	0.41
1:A:116:SER:CB	1:A:497:THR:HG23	2.50	0.41
1:A:528:ARG:HG3	1:A:608:MET:HE1	2.00	0.41
2:B:616:THR:CG2	2:B:618:VAL:HG13	2.50	0.41
2:B:695:ARG:HG3	2:B:695:ARG:NH1	2.35	0.41
1:A:172:MET:HE2	1:A:252:TRP:NE1	2.36	0.41
1:A:384:GLN:O	1:A:388:ARG:HG3	2.20	0.41
2:B:367:CYS:O	2:B:368:LYS:HB2	2.21	0.41
2:B:409:ARG:C	2:B:411:ASP:H	2.28	0.41
2:B:1027:GLU:O	2:B:1031:LEU:HG	2.21	0.41
2:B:1029:CYS:O	2:B:1032:LEU:HA	2.20	0.41
2:B:570:LYS:HE2	2:B:629:HIS:NE2	2.35	0.41
2:B:798:VAL:HG22	2:B:803:LEU:CD2	2.51	0.41
1:A:297:GLY:HA2	1:A:298:PRO:C	2.45	0.41
1:A:382:PHE:O	1:A:383:LYS:C	2.64	0.41
2:B:372:CYS:HB2	2:B:373:PRO:HD2	2.02	0.41
2:B:484:ILE:HD11	2:B:755:ILE:HB	2.02	0.41
2:B:861:GLU:O	2:B:862:ILE:O	2.39	0.41
2:B:1009:LYS:CG	2:B:1016:SER:HB3	2.51	0.41
1:A:236:ILE:CG2	1:A:240:LEU:HB2	2.47	0.41
2:B:974:ILE:HG13	2:B:975:MET:N	2.36	0.41
1:A:148:LYS:O	1:A:152:GLN:HG3	2.20	0.41
1:A:195:LEU:HD13	1:A:203:MET:HE1	2.02	0.41
1:A:510:ILE:HB	1:A:511:GLN:NE2	2.36	0.41
2:B:434:LYS:O	2:B:436:LYS:HG3	2.20	0.41
2:B:446:MET:HE3	2:B:580:ILE:HG12	2.01	0.41
2:B:501:LYS:NZ	2:B:524:ASP:HB3	2.35	0.41
2:B:933:GLY:HA2	2:B:993:GLN:HB2	2.03	0.41
1:A:259:ARG:HG3	1:A:306:LEU:CD2	2.51	0.41
1:A:368:GLY:HA3	1:A:450:GLY:O	2.20	0.41
1:A:414:ILE:CG2	1:A:415:LYS:N	2.84	0.41
2:B:302:ILE:HD12	2:B:311:ARG:NE	2.36	0.41
2:B:665:PHE:CE1	2:B:670:ASP:HB2	2.55	0.41
2:B:723:ASP:OD2	2:B:726:LYS:HE2	2.21	0.41
1:A:313:TRP:HA	1:A:316:ILE:CG2	2.51	0.41
2:B:515:VAL:HG13	2:B:560:PRO:HG2	2.02	0.41
1:A:15:ASP:HB3	1:A:497:THR:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:PRO:CG	1:A:31:ALA:HB2	2.51	0.40
1:A:313:TRP:NE1	1:A:592:VAL:HB	2.36	0.40
2:B:407:GLY:O	2:B:408:ARG:C	2.64	0.40
2:B:627:VAL:CG2	2:B:710:LEU:HD23	2.49	0.40
1:A:18:ARG:HH21	1:A:518:ASP:CG	2.29	0.40
1:A:254:VAL:HA	1:A:255:PRO:HD2	1.83	0.40
1:A:313:TRP:NE1	1:A:597:PRO:HA	2.37	0.40
1:A:695:ILE:HG22	1:A:696:LEU:HD13	2.03	0.40
2:B:641:GLN:O	2:B:642:TYR:C	2.64	0.40
2:B:676:ASN:O	2:B:680:ASN:HB2	2.21	0.40
2:B:921:LEU:HD12	2:B:974:ILE:CD1	2.51	0.40
1:A:77:ASP:OD2	1:A:80:ALA:CB	2.68	0.40
1:A:153:MET:O	1:A:156:SER:OG	2.37	0.40
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.80	0.40
1:A:499:ILE:C	1:A:499:ILE:HD12	2.46	0.40
1:A:539:GLY:C	1:A:541:ASP:H	2.29	0.40
2:B:455:LYS:C	2:B:457:GLY:N	2.79	0.40
2:B:523:LEU:HD23	2:B:523:LEU:HA	1.82	0.40
2:B:605:THR:O	2:B:606:ASP:CB	2.70	0.40
1:A:548:ARG:HH21	1:A:549:GLN:HE22	1.69	0.40
2:B:465:GLU:HG2	2:B:675:LEU:CD2	2.45	0.40
2:B:982:ARG:HA	2:B:983:PRO:HD2	1.83	0.40
2:B:992:LYS:HB2	2:B:996:GLN:HE21	1.85	0.40
3:C:190:ILE:HB	3:C:192:MET:HE3	2.02	0.40
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.95	0.40
1:A:747:VAL:HG11	1:A:751:VAL:CB	2.52	0.40
2:B:384:TYR:CD1	2:B:384:TYR:C	2.98	0.40
2:B:577:LYS:HE2	2:B:579:PHE:CZ	2.57	0.40
2:B:623:ALA:O	2:B:627:VAL:HG23	2.20	0.40
2:B:707:GLY:HA2	2:B:875:MET:O	2.21	0.40
2:B:945:PHE:C	2:B:947:VAL:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	708/765 (92%)	635 (90%)	54 (8%)	19 (3%)	4	10
2	B	763/770 (99%)	659 (86%)	75 (10%)	29 (4%)	2	5
3	C	5/7 (71%)	5 (100%)	0	0	100	100
All	All	1476/1542 (96%)	1299 (88%)	129 (9%)	48 (3%)	3	7

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	746	ASP
2	B	289	ARG
2	B	304	ASP
2	B	408	ARG
2	B	412	HIS
2	B	492	ASN
2	B	900	SER
2	B	964	GLY
2	B	993	GLN
2	B	996	GLN
2	B	998	GLU
2	B	1032	LEU
1	A	54	ILE
1	A	80	ALA
1	A	180	CYS
1	A	237	ASP
1	A	537	GLU
1	A	593	PHE
2	B	410	LEU
2	B	527	LEU
2	B	862	ILE
2	B	899	LYS
2	B	902	MET
2	B	956	ASP
2	B	995	GLU
1	A	184	SER
1	A	540	PRO
1	A	700	PHE
1	A	744	THR
2	B	503	ASN

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Mol	Chain	Res	Type
2	B	860	PRO
2	B	963	VAL
2	B	980	GLN
1	A	536	THR
1	A	696	LEU
2	B	903	LEU
2	B	966	PRO
1	A	59	VAL
1	A	99	ALA
2	B	397	PRO
2	B	994	ARG
1	A	324	VAL
1	A	510	ILE
2	B	290	GLY
2	B	590	ALA
2	B	961	PRO
1	A	565	PRO

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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

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	716/765 (93%)	0.04	27 (3%)	44 40	26, 53, 94, 131	0
2	B	767/770 (99%)	0.14	47 (6%)	27 24	26, 54, 109, 141	0
3	C	7/7 (100%)	0.39	1 (14%)	6 5	56, 60, 91, 119	0
All	All	1490/1542 (96%)	0.09	75 (5%)	34 30	26, 54, 102, 141	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	PRO	6.9
2	B	960	LEU	5.3
1	A	742	ILE	5.0
2	B	1033	ASN	4.9
2	B	860	PRO	4.7
1	A	209	VAL	4.7
2	B	966	PRO	4.1
1	A	52	PRO	4.1
2	B	997	PRO	4.1
1	A	53	PRO	4.0
2	B	955	THR	4.0
1	A	741	PRO	3.9
2	B	2	MET	3.8
1	A	539	GLY	3.8
1	A	51	LEU	3.6
2	B	1010	GLY	3.5
2	B	3	GLY	3.5
2	B	857	LEU	3.5
2	B	963	VAL	3.4
2	B	1	ALA	3.2
2	B	959	LEU	3.2
2	B	901	THR	3.0
2	B	967	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	961	PRO	2.9
2	B	964	GLY	2.8
2	B	951	ALA	2.8
2	B	1028	ILE	2.8
2	B	947	VAL	2.7
1	A	510	ILE	2.7
2	B	965	ASN	2.7
2	B	410	LEU	2.7
1	A	314	HIS	2.7
2	B	406	ILE	2.6
2	B	957	MET	2.6
2	B	601	LYS	2.6
1	A	464	VAL	2.6
2	B	862	ILE	2.6
1	A	122	LEU	2.6
2	B	896	LEU	2.6
2	B	1032	LEU	2.6
2	B	405	HIS	2.6
1	A	762	SER	2.5
2	B	299	ASP	2.5
2	B	603	VAL	2.5
1	A	743	LEU	2.4
2	B	602	LEU	2.4
2	B	859	ARG	2.3
1	A	536	THR	2.3
2	B	858	SER	2.3
2	B	823	LYS	2.3
2	B	899	LYS	2.3
2	B	404	ASP	2.3
1	A	79	ARG	2.3
2	B	524	ASP	2.3
1	A	318	LYS	2.2
2	B	902	MET	2.2
1	A	701	PRO	2.2
2	B	407	GLY	2.2
2	B	551	SER	2.2
1	A	544	ARG	2.2
1	A	3	THR	2.2
3	C	193	MET	2.2
1	A	744	THR	2.1
1	A	180	CYS	2.1
1	A	698	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	528	VAL	2.1
2	B	958	THR	2.1
1	A	676	PRO	2.1
1	A	104	LEU	2.1
2	B	605	THR	2.0
1	A	124	GLY	2.0
1	A	227	ASN	2.0
2	B	604	ASN	2.0
2	B	954	ASN	2.0
2	B	408	ARG	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	766	1/1	1.00	0.04	46,46,46,46	0
4	ZN	B	1034	1/1	1.00	0.02	57,57,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.