



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:29 PM UTC

PDB ID : 5KYY / pdb_00005kyy
Title : Crystal structure of Sec23 and TANGO1 peptide4 complex
Authors : Ma, W.; Goldberg, J.
Deposited on : 2016-07-22
Resolution : 3.40 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

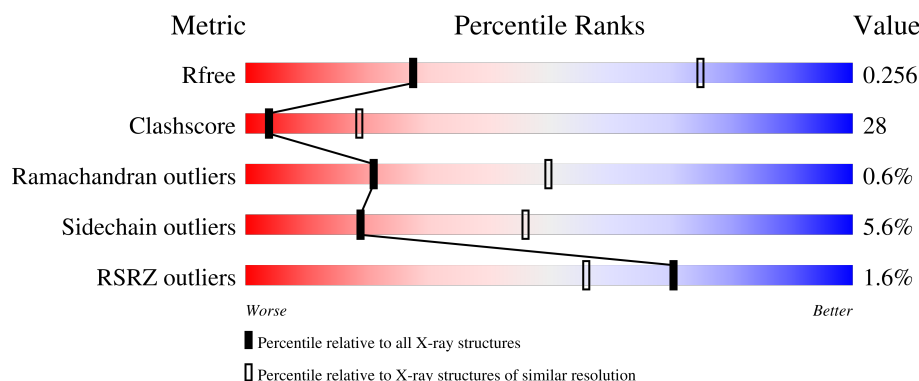
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	801	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11682 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
			5676	3619	975	1042	40			

- Molecule 2 is a protein called Protein transport protein Sec24D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	767	Total	C	N	O	S	0	0	0
			6004	3822	1014	1114	54			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP O94855
B	2	MET	-	expression tag	UNP O94855
B	3	GLY	-	expression tag	UNP O94855

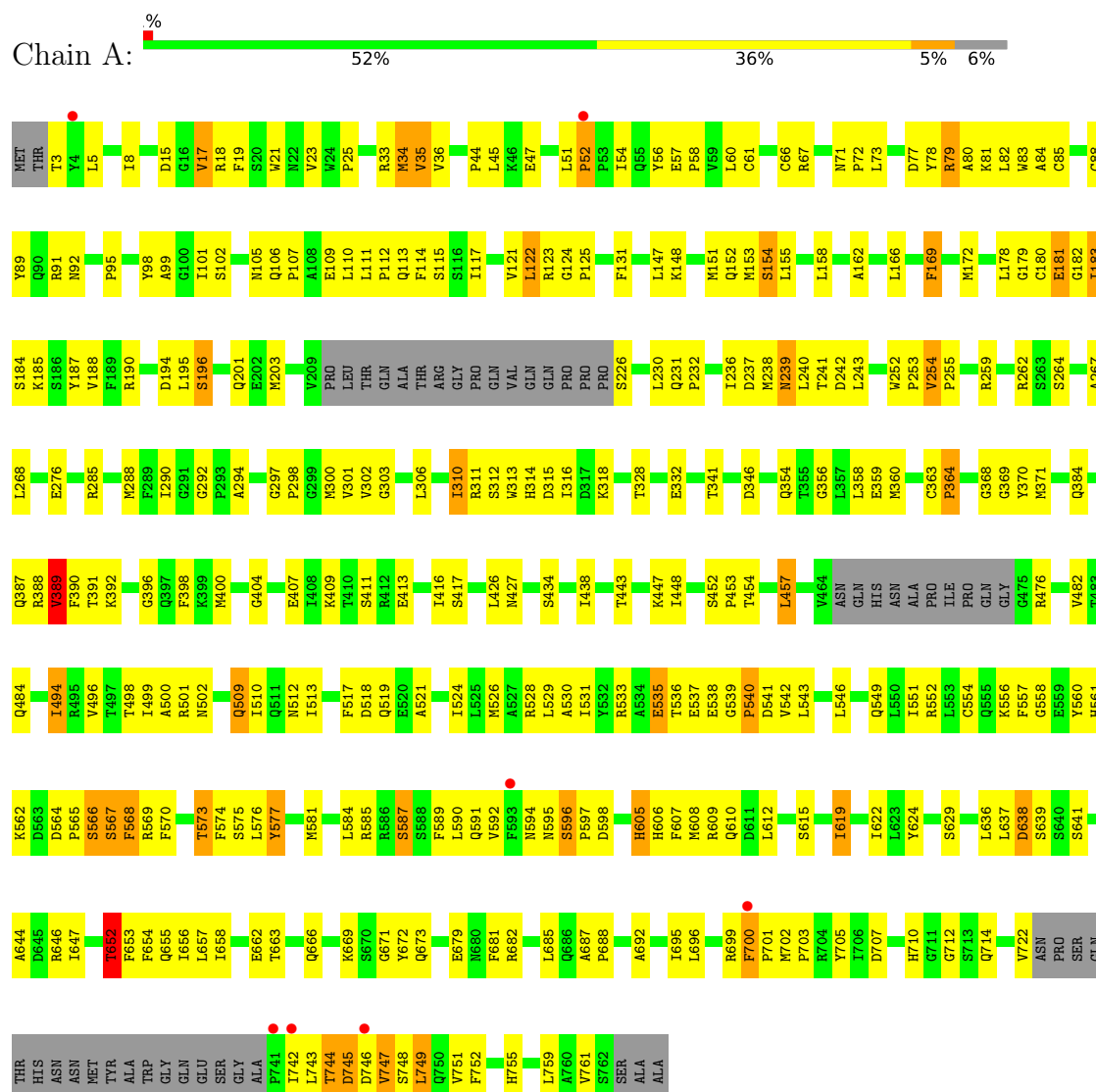
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

3 Residue-property plots

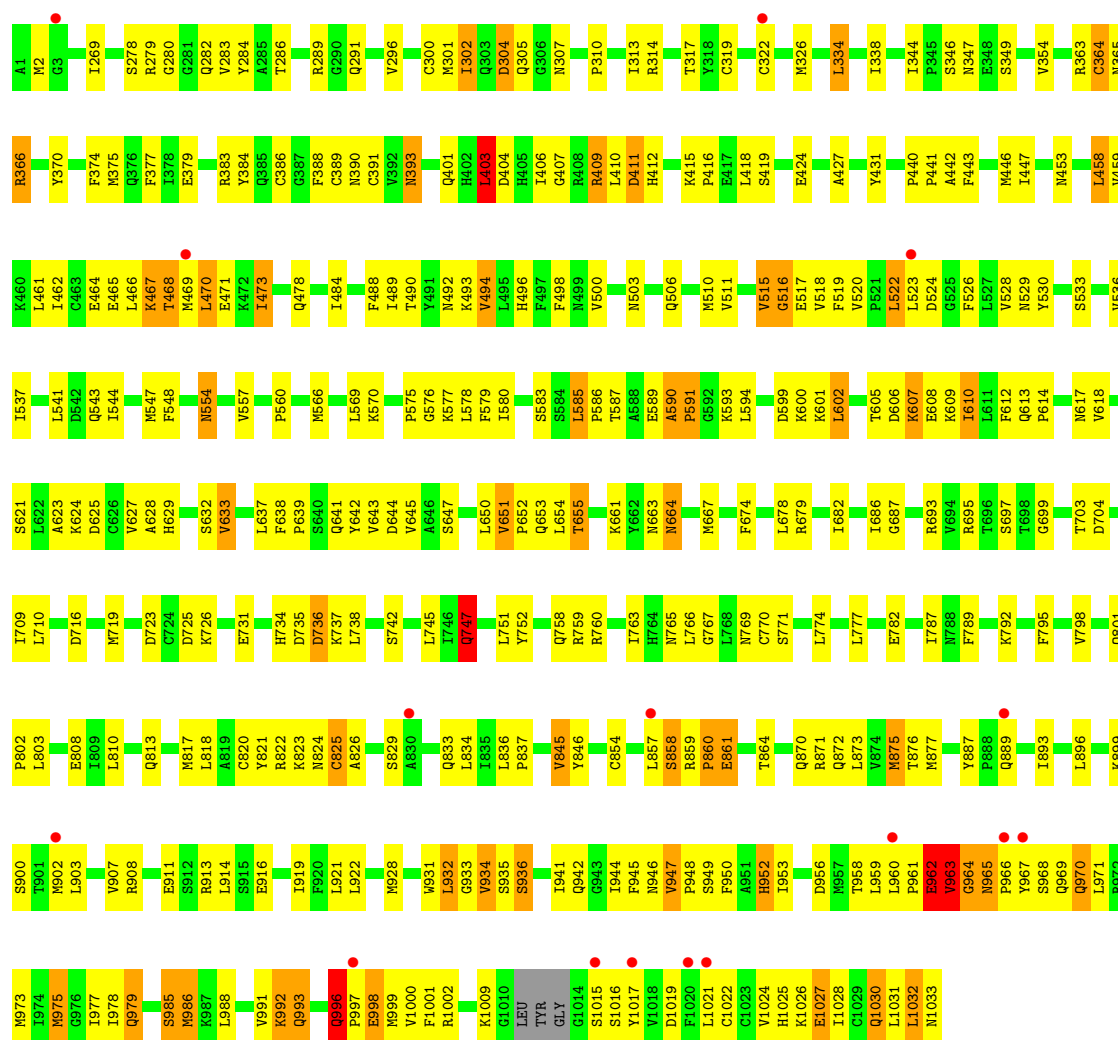
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Protein transport protein Sec23A



• Molecule 2: Protein transport protein Sec24D





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.39Å 139.06Å 149.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 3.40 48.01 – 3.40	Depositor EDS
% Data completeness (in resolution range)	83.9 (48.01-3.40) 81.4 (48.01-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.177 , 0.253 0.200 , 0.256	Depositor DCC
R_{free} test set	1985 reflections (6.70%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11682	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	0.82	0/5809	1.11	37/7868 (0.5%)
2	B	0.93	3/6132 (0.0%)	1.18	57/8309 (0.7%)
All	All	0.88	3/11941 (0.0%)	1.15	94/16177 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	409	ARG	CA-C	-9.70	1.43	1.53
2	B	515	VAL	CA-CB	-5.41	1.48	1.54
2	B	873	LEU	CA-C	-5.06	1.46	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	993	GLN	N-CA-C	10.92	123.19	111.28
2	B	467	LYS	N-CA-C	-8.85	100.50	111.11
2	B	861	GLU	N-CA-C	8.69	123.47	112.86
1	A	652	THR	N-CA-C	-8.03	99.18	110.50
2	B	1030	GLN	N-CA-C	-7.77	102.81	111.28
2	B	734	HIS	N-CA-C	7.62	120.94	108.52
1	A	577	TYR	CA-C-N	-7.33	112.24	119.64
1	A	577	TYR	C-N-CA	-7.33	112.24	119.64
1	A	566	SER	N-CA-C	-7.19	103.61	112.38
2	B	962	GLU	N-CA-C	7.16	119.08	111.28
2	B	936	SER	CA-C-N	7.12	127.72	120.38
2	B	936	SER	C-N-CA	7.12	127.72	120.38
1	A	154	SER	N-CA-C	-6.95	103.72	111.71
2	B	964	GLY	N-CA-C	-6.93	102.89	112.18
2	B	736	ASP	CB-CA-C	-6.84	108.69	116.63
2	B	985	SER	N-CA-C	-6.83	101.07	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	978	ILE	N-CA-C	6.80	117.59	110.72
1	A	509	GLN	N-CA-C	6.76	120.21	112.57
1	A	196	SER	N-CA-C	-6.75	99.68	110.14
2	B	975	MET	N-CA-C	-6.73	103.95	111.28
2	B	607	LYS	N-CA-C	-6.73	103.52	113.61
2	B	503	ASN	N-CA-C	6.71	121.08	113.02
2	B	591	PRO	N-CA-C	-6.59	100.85	111.14
2	B	516	GLY	N-CA-C	-6.58	106.10	113.79
2	B	963	VAL	N-CA-C	6.57	119.79	108.95
2	B	991	VAL	N-CA-C	6.53	117.43	107.77
2	B	887	TYR	CA-C-N	6.51	126.53	119.89
2	B	887	TYR	C-N-CA	6.51	126.53	119.89
1	A	183	ILE	N-CA-C	-6.49	98.84	108.45
2	B	858	SER	N-CA-C	6.44	120.13	110.14
1	A	79	ARG	N-CA-C	-6.31	101.61	110.50
2	B	1032	LEU	N-CA-C	6.30	119.46	109.50
1	A	169	PHE	N-CA-C	6.30	118.35	108.96
2	B	403	LEU	N-CA-C	-6.24	102.25	110.43
2	B	986	MET	N-CA-C	6.23	119.40	109.24
1	A	8	ILE	N-CA-C	6.21	116.88	110.36
1	A	364	PRO	N-CA-C	-6.12	105.20	113.40
2	B	494	VAL	N-CA-C	-6.07	99.74	108.42
2	B	522	LEU	N-CA-C	6.06	117.45	108.60
2	B	952	HIS	N-CA-C	6.03	117.86	111.28
1	A	254	VAL	CA-C-N	6.00	127.34	119.84
1	A	254	VAL	C-N-CA	6.00	127.34	119.84
2	B	366	ARG	N-CA-C	5.98	120.66	112.04
1	A	231	GLN	CA-C-N	5.95	125.97	119.90
1	A	231	GLN	C-N-CA	5.95	125.97	119.90
1	A	411	SER	N-CA-C	-5.95	102.64	110.43
1	A	654	PHE	N-CA-C	5.93	117.82	111.36
1	A	701	PRO	N-CA-C	-5.86	100.40	112.47
1	A	124	GLY	CA-C-N	-5.85	113.75	119.90
1	A	124	GLY	C-N-CA	-5.85	113.75	119.90
2	B	440	PRO	O-C-N	5.83	123.89	121.15
2	B	470	LEU	N-CA-C	-5.80	104.95	111.28
1	A	389	VAL	CB-CA-C	-5.71	101.93	111.29
2	B	511	VAL	N-CA-C	5.70	116.41	108.89
2	B	992	LYS	N-CA-C	-5.65	101.28	110.20
1	A	745	ASP	N-CA-C	-5.60	102.98	110.55
2	B	801	GLN	CA-C-N	5.58	125.34	119.76
2	B	801	GLN	C-N-CA	5.58	125.34	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	SER	N-CA-C	5.57	117.71	110.53
2	B	364	CYS	N-CA-C	-5.51	102.13	110.28
1	A	700	PHE	CA-C-N	-5.50	112.97	119.84
1	A	700	PHE	C-N-CA	-5.50	112.97	119.84
2	B	747	GLN	N-CA-C	-5.48	99.36	108.34
2	B	473	ILE	CA-C-N	-5.45	114.97	120.31
2	B	473	ILE	C-N-CA	-5.45	114.97	120.31
1	A	687	ALA	CA-C-N	-5.43	113.06	119.84
1	A	687	ALA	C-N-CA	-5.43	113.06	119.84
2	B	877	MET	N-CA-C	5.40	117.26	110.24
1	A	181	GLU	N-CA-C	5.37	118.86	110.32
2	B	515	VAL	N-CA-C	-5.34	102.69	109.80
2	B	651	VAL	CA-C-N	-5.34	113.12	119.05
2	B	651	VAL	C-N-CA	-5.34	113.12	119.05
2	B	349	SER	N-CA-C	5.33	117.34	109.50
2	B	590	ALA	N-CA-C	-5.32	103.33	108.07
2	B	860	PRO	N-CA-C	-5.32	102.59	111.26
1	A	184	SER	CA-C-N	-5.29	114.50	122.81
1	A	184	SER	C-N-CA	-5.29	114.50	122.81
2	B	934	VAL	N-CA-C	-5.28	105.24	110.62
2	B	623	ALA	N-CA-C	-5.27	105.53	111.28
2	B	736	ASP	N-CA-C	5.26	116.97	108.08
1	A	568	PHE	N-CA-C	5.25	117.84	110.23
2	B	585	LEU	CA-C-N	5.25	126.40	119.84
2	B	585	LEU	C-N-CA	5.25	126.40	119.84
1	A	457	LEU	N-CA-C	5.24	118.35	109.76
2	B	970	GLN	N-CA-C	-5.16	105.65	111.28
1	A	34	MET	CB-CA-C	5.12	120.14	109.95
1	A	35	VAL	CA-C-N	-5.11	118.91	122.59
1	A	35	VAL	C-N-CA	-5.11	118.91	122.59
2	B	996	GLN	N-CA-C	-5.11	98.53	109.81
2	B	344	ILE	CA-C-N	5.10	125.04	119.78
2	B	344	ILE	C-N-CA	5.10	125.04	119.78
1	A	535	GLU	N-CA-C	-5.08	107.73	114.04
2	B	956	ASP	N-CA-C	5.05	116.79	111.28
2	B	302	ILE	N-CA-C	5.02	115.14	108.11

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	5676	0	5627	317	0
2	B	6004	0	5968	356	0
3	A	1	0	0	2	0
3	B	1	0	0	0	0
All	All	11682	0	11595	663	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 (663) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:CD1	1:A:360:MET:HE1	1.94	0.97
2:B:469:MET:HE3	2:B:679:ARG:HA	1.45	0.96
1:A:51:LEU:HD21	1:A:117:ILE:HA	1.43	0.96
2:B:967:TYR:O	2:B:969:GLN:N	1.99	0.96
1:A:652:THR:HG23	1:A:655:GLN:H	1.29	0.94
2:B:366:ARG:NH2	2:B:391:CYS:HB2	1.83	0.93
2:B:931:TRP:CZ2	2:B:993:GLN:HG3	2.04	0.93
1:A:673:GLN:N	1:A:673:GLN:OE1	2.01	0.92
1:A:311:ARG:HG3	1:A:311:ARG:HH21	1.33	0.92
2:B:896:LEU:HD21	2:B:970:GLN:CG	2.00	0.92
1:A:290:ILE:HD13	1:A:360:MET:HE1	1.52	0.91
2:B:601:LYS:C	2:B:605:THR:HG21	1.96	0.90
2:B:996:GLN:HB3	2:B:997:PRO:HD2	1.52	0.90
1:A:564:ASP:HB3	1:A:567:SER:HB3	1.54	0.90
2:B:492:ASN:OD1	2:B:492:ASN:O	1.90	0.88
2:B:703:THR:O	2:B:704:ASP:OD1	1.91	0.88
1:A:66:CYS:HG	3:A:801:ZN:ZN	0.84	0.88
2:B:822:ARG:O	2:B:826:ALA:HB3	1.74	0.87
2:B:861:GLU:O	2:B:861:GLU:HG3	1.73	0.86
2:B:586:PRO:HG2	2:B:594:LEU:HD12	1.57	0.86
2:B:492:ASN:O	2:B:493:LYS:HB3	1.75	0.86
2:B:406:ILE:HG22	2:B:406:ILE:O	1.74	0.85
2:B:633:VAL:H	2:B:655:THR:HG21	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:934:VAL:N	2:B:993:GLN:OE1	2.10	0.85
2:B:617:ASN:O	2:B:617:ASN:ND2	2.09	0.85
1:A:35:VAL:HG21	1:A:552:ARG:HB3	1.58	0.84
1:A:564:ASP:O	1:A:567:SER:CB	2.25	0.84
2:B:932:LEU:O	2:B:993:GLN:HB2	1.77	0.84
2:B:1024:VAL:HG12	2:B:1028:ILE:HD11	1.58	0.83
2:B:375:MET:HE1	2:B:386:CYS:SG	2.18	0.83
1:A:749:LEU:HD12	1:A:749:LEU:O	1.77	0.83
2:B:500:VAL:HG11	2:B:537:ILE:HG12	1.62	0.82
1:A:35:VAL:HG13	1:A:549:GLN:NE2	1.94	0.81
1:A:673:GLN:O	1:A:682:ARG:CG	2.29	0.81
2:B:493:LYS:O	2:B:493:LYS:HG3	1.79	0.81
2:B:896:LEU:HD21	2:B:970:GLN:HG3	1.61	0.81
1:A:564:ASP:O	1:A:567:SER:HB3	1.81	0.81
2:B:998:GLU:O	2:B:1002:ARG:HG3	1.81	0.81
1:A:51:LEU:HD12	1:A:52:PRO:CD	2.11	0.81
2:B:384:TYR:CE1	2:B:393:ASN:HB2	2.15	0.81
1:A:179:GLY:CA	1:A:236:ILE:HD11	2.11	0.81
1:A:673:GLN:O	1:A:682:ARG:HG2	1.80	0.81
1:A:564:ASP:O	1:A:567:SER:N	2.13	0.80
2:B:747:GLN:NE2	2:B:765:ASN:OD1	2.14	0.80
1:A:238:MET:HE2	1:A:238:MET:HA	1.63	0.80
2:B:590:ALA:HB1	2:B:591:PRO:CD	2.12	0.80
2:B:493:LYS:O	2:B:493:LYS:CG	2.30	0.80
1:A:238:MET:HE2	1:A:238:MET:CA	2.12	0.80
2:B:944:ILE:HG22	2:B:945:PHE:CD1	2.17	0.79
2:B:490:THR:HG23	2:B:498:PHE:HE2	1.45	0.79
2:B:899:LYS:O	2:B:900:SER:OG	2.01	0.79
2:B:412:HIS:O	2:B:419:SER:HB3	1.83	0.78
2:B:470:LEU:HD12	2:B:530:TYR:CE1	2.19	0.78
2:B:590:ALA:HB1	2:B:591:PRO:HD2	1.66	0.78
1:A:551:ILE:HD11	1:A:743:LEU:HD13	1.66	0.78
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.65	0.78
2:B:469:MET:HE1	2:B:678:LEU:C	2.09	0.78
2:B:792:LYS:HE2	2:B:875:MET:O	1.84	0.77
2:B:466:LEU:O	2:B:467:LYS:C	2.24	0.77
2:B:795:PHE:O	2:B:871:ARG:NH1	2.17	0.77
2:B:1024:VAL:O	2:B:1028:ILE:HG13	1.86	0.76
1:A:179:GLY:HA2	1:A:236:ILE:HD11	1.66	0.76
2:B:522:LEU:HD12	2:B:522:LEU:C	2.11	0.76
1:A:311:ARG:HE	1:A:359:GLU:CD	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:469:MET:HE2	2:B:682:ILE:HD12	1.67	0.75
2:B:896:LEU:HD21	2:B:970:GLN:HG2	1.68	0.75
2:B:591:PRO:CD	2:B:591:PRO:O	2.30	0.75
2:B:934:VAL:HG13	2:B:993:GLN:OE1	1.86	0.75
2:B:468:THR:HG22	2:B:469:MET:N	2.02	0.75
1:A:744:THR:HG23	1:A:745:ASP:O	1.87	0.74
1:A:636:LEU:HG	1:A:638:ASP:HB2	1.68	0.74
1:A:745:ASP:O	1:A:747:VAL:HG22	1.86	0.74
1:A:564:ASP:CB	1:A:567:SER:HB3	2.18	0.74
1:A:179:GLY:O	1:A:181:GLU:HG3	1.86	0.74
2:B:469:MET:CE	2:B:679:ARG:HA	2.17	0.74
2:B:1024:VAL:HG12	2:B:1028:ILE:CD1	2.17	0.74
1:A:388:ARG:O	1:A:390:PHE:N	2.22	0.73
1:A:528:ARG:HA	1:A:608:MET:HE1	1.69	0.73
1:A:15:ASP:OD1	1:A:115:SER:OG	2.06	0.73
1:A:657:LEU:C	1:A:657:LEU:HD23	2.14	0.73
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.70	0.73
1:A:499:ILE:O	1:A:499:ILE:HD12	1.89	0.73
1:A:188:VAL:HG21	2:B:510:MET:HE2	1.71	0.72
1:A:681:PHE:CE2	1:A:685:LEU:HD11	2.23	0.72
2:B:366:ARG:NH2	2:B:391:CYS:CB	2.52	0.72
2:B:979:GLN:NE2	2:B:985:SER:HA	2.04	0.72
1:A:71:ASN:HB3	1:A:498:THR:HG21	1.70	0.72
2:B:489:ILE:HD11	2:B:526:PHE:HZ	1.53	0.72
2:B:528:VAL:HG11	2:B:533:SER:OG	1.89	0.72
1:A:312:SER:HG	1:A:315:ASP:CG	1.97	0.72
1:A:60:LEU:HB3	1:A:67:ARG:NH1	2.04	0.71
1:A:673:GLN:HB3	1:A:685:LEU:HD12	1.72	0.71
1:A:107:PRO:HD2	1:A:110:LEU:HD12	1.72	0.71
2:B:792:LYS:CE	2:B:875:MET:O	2.38	0.71
1:A:183:ILE:HD12	2:B:547:MET:HE1	1.72	0.71
2:B:587:THR:O	2:B:593:LYS:HE3	1.89	0.71
1:A:51:LEU:CD1	1:A:114:PHE:CE1	2.74	0.71
1:A:237:ASP:O	1:A:241:THR:HG22	1.90	0.71
2:B:470:LEU:CD1	2:B:530:TYR:CE1	2.73	0.71
1:A:54:ILE:HG21	1:A:56:TYR:CE2	2.25	0.71
2:B:639:PRO:HB3	2:B:643:VAL:HG21	1.72	0.71
2:B:921:LEU:HD11	2:B:975:MET:HG2	1.73	0.70
1:A:51:LEU:CD2	1:A:117:ILE:HA	2.19	0.70
2:B:379:GLU:OE1	2:B:383:ARG:HD2	1.91	0.70
1:A:51:LEU:HD12	1:A:52:PRO:HD2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:859:ARG:O	2:B:860:PRO:C	2.30	0.70
2:B:326:MET:HE3	2:B:774:LEU:HD23	1.73	0.70
2:B:758:GLN:OE1	2:B:760:ARG:NH2	2.23	0.70
2:B:591:PRO:HD2	2:B:591:PRO:O	1.91	0.69
1:A:499:ILE:HD12	1:A:499:ILE:C	2.18	0.69
1:A:123:ARG:HG3	1:A:125:PRO:HD2	1.73	0.69
2:B:469:MET:HE3	2:B:679:ARG:CA	2.22	0.68
2:B:586:PRO:CG	2:B:594:LEU:HD12	2.23	0.68
1:A:509:GLN:HB3	1:A:512:ASN:HB2	1.74	0.68
1:A:743:LEU:CD1	1:A:759:LEU:HD12	2.23	0.68
2:B:518:VAL:HG12	2:B:519:PHE:N	2.08	0.68
2:B:607:LYS:HE2	2:B:610:ILE:HD12	1.75	0.68
1:A:302:VAL:HG22	1:A:303:GLY:N	2.07	0.68
1:A:652:THR:HG23	1:A:655:GLN:N	2.08	0.68
2:B:403:LEU:HB3	2:B:407:GLY:HA2	1.75	0.68
2:B:602:LEU:N	2:B:605:THR:HG21	2.09	0.68
1:A:311:ARG:HG3	1:A:311:ARG:NH2	2.09	0.68
1:A:35:VAL:HG13	1:A:549:GLN:HE21	1.59	0.68
1:A:61:CYS:SG	1:A:85:CYS:HB2	2.34	0.67
1:A:185:LYS:NZ	1:A:187:TYR:OH	2.26	0.67
2:B:942:GLN:O	2:B:946:ASN:HA	1.94	0.67
2:B:992:LYS:CB	2:B:996:GLN:HG3	2.25	0.67
2:B:522:LEU:HD12	2:B:523:LEU:N	2.10	0.67
1:A:392:LYS:HD3	1:A:396:GLY:C	2.19	0.67
2:B:366:ARG:CZ	2:B:391:CYS:HB2	2.24	0.67
2:B:464:GLU:OE2	2:B:467:LYS:NZ	2.26	0.67
2:B:697:SER:HB3	2:B:745:LEU:HB2	1.76	0.67
1:A:743:LEU:O	1:A:755:HIS:ND1	2.27	0.67
1:A:743:LEU:O	1:A:755:HIS:CE1	2.48	0.66
2:B:946:ASN:CG	2:B:946:ASN:O	2.37	0.66
2:B:792:LYS:NZ	2:B:875:MET:O	2.28	0.66
1:A:370:TYR:HE2	1:A:389:VAL:HG13	1.60	0.66
2:B:958:THR:HG21	2:B:988:LEU:O	1.96	0.66
2:B:289:ARG:HH12	2:B:742:SER:C	2.04	0.65
1:A:749:LEU:HD12	1:A:749:LEU:C	2.18	0.65
1:A:482:VAL:HG13	1:A:496:VAL:HG22	1.77	0.65
2:B:406:ILE:O	2:B:406:ILE:CG2	2.43	0.65
2:B:1027:GLU:HA	2:B:1030:GLN:HB2	1.79	0.65
2:B:641:GLN:O	2:B:643:VAL:HG23	1.97	0.65
2:B:928:MET:HE3	2:B:986:MET:HE3	1.78	0.65
2:B:377:PHE:CE2	2:B:409:ARG:HD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:GLN:H	1:A:673:GLN:CD	2.03	0.65
2:B:304:ASP:O	2:B:305:GLN:HB2	1.96	0.65
2:B:469:MET:HE1	2:B:678:LEU:HG	1.79	0.64
2:B:820:CYS:HA	2:B:823:LYS:HE2	1.79	0.64
2:B:946:ASN:O	2:B:946:ASN:ND2	2.30	0.64
2:B:661:LYS:NZ	2:B:663:ASN:HD21	1.95	0.64
1:A:54:ILE:CG2	1:A:56:TYR:CE2	2.80	0.64
1:A:748:SER:OG	1:A:751:VAL:HG23	1.98	0.64
2:B:736:ASP:OD1	2:B:737:LYS:N	2.30	0.64
1:A:71:ASN:CB	1:A:498:THR:HG21	2.26	0.64
1:A:285:ARG:NH2	1:A:346:ASP:OD2	2.31	0.64
1:A:312:SER:OG	1:A:315:ASP:OD2	2.15	0.64
1:A:147:LEU:HG	1:A:151:MET:HE2	1.78	0.63
2:B:590:ALA:CB	2:B:591:PRO:HD2	2.28	0.63
1:A:102:SER:HB3	1:A:105:ASN:H	1.64	0.63
1:A:746:ASP:O	1:A:747:VAL:HG13	1.98	0.63
1:A:54:ILE:HG22	1:A:56:TYR:CD2	2.34	0.63
2:B:322:CYS:SG	2:B:771:SER:N	2.72	0.63
1:A:311:ARG:NH2	1:A:597:PRO:HB2	2.13	0.63
1:A:536:THR:HG22	1:A:537:GLU:H	1.61	0.63
2:B:533:SER:O	2:B:537:ILE:HG13	1.97	0.63
1:A:356:GLY:O	1:A:360:MET:HG3	1.98	0.63
1:A:565:PRO:HD3	1:A:761:VAL:HG21	1.81	0.62
2:B:314:ARG:NH1	2:B:782:GLU:OE2	2.33	0.62
2:B:386:CYS:SG	2:B:388:PHE:HD1	2.22	0.62
2:B:1000:VAL:HG13	2:B:1001:PHE:N	2.14	0.62
2:B:1032:LEU:HG	2:B:1033:ASN:N	2.15	0.62
1:A:311:ARG:NH1	1:A:598:ASP:OD1	2.27	0.61
2:B:699:GLY:HA3	2:B:738:LEU:HD23	1.82	0.61
2:B:590:ALA:CB	2:B:591:PRO:CD	2.74	0.61
2:B:992:LYS:HB2	2:B:996:GLN:HG3	1.82	0.61
1:A:696:LEU:HD23	1:A:703:PRO:HG2	1.83	0.60
1:A:388:ARG:NH1	1:A:699:ARG:O	2.34	0.60
2:B:523:LEU:C	2:B:523:LEU:HD23	2.26	0.60
2:B:599:ASP:HB3	2:B:601:LYS:HG3	1.83	0.60
1:A:312:SER:OG	1:A:315:ASP:CG	2.43	0.60
2:B:963:VAL:HG12	2:B:964:GLY:H	1.67	0.60
1:A:392:LYS:HD3	1:A:396:GLY:O	2.01	0.60
2:B:861:GLU:O	2:B:861:GLU:CG	2.42	0.60
1:A:66:CYS:SG	3:A:801:ZN:ZN	1.85	0.60
2:B:770:CYS:SG	2:B:771:SER:N	2.73	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:709:ILE:HG22	2:B:719:MET:HG2	1.84	0.60
1:A:671:GLY:C	1:A:673:GLN:OE1	2.45	0.60
1:A:389:VAL:HG12	1:A:389:VAL:O	2.01	0.59
2:B:523:LEU:O	2:B:524:ASP:HB2	2.02	0.59
2:B:518:VAL:CG1	2:B:519:PHE:N	2.65	0.59
2:B:307:ASN:HB3	2:B:766:LEU:HD12	1.83	0.59
2:B:289:ARG:NH1	2:B:742:SER:C	2.60	0.59
2:B:464:GLU:CD	2:B:467:LYS:HZ1	2.10	0.59
2:B:633:VAL:H	2:B:655:THR:CG2	2.14	0.59
2:B:2:MET:HG2	2:B:1017:TYR:OH	2.02	0.59
1:A:183:ILE:CD1	2:B:547:MET:CE	2.81	0.58
1:A:543:LEU:HD21	1:A:585:ARG:HB2	1.85	0.58
2:B:317:THR:HG22	2:B:319:CYS:H	1.67	0.58
2:B:493:LYS:HA	2:B:557:VAL:HG22	1.85	0.58
2:B:947:VAL:HG12	2:B:948:PRO:HD2	1.84	0.58
2:B:489:ILE:HD11	2:B:526:PHE:CZ	2.36	0.58
2:B:601:LYS:CA	2:B:605:THR:HG21	2.33	0.58
2:B:633:VAL:HG12	2:B:655:THR:HG21	1.86	0.58
1:A:652:THR:CG2	1:A:655:GLN:O	2.51	0.58
2:B:301:MET:HG3	2:B:347:ASN:HD21	1.68	0.58
2:B:591:PRO:O	2:B:591:PRO:CG	2.51	0.58
2:B:944:ILE:CG2	2:B:945:PHE:CE1	2.87	0.58
1:A:36:VAL:HG22	1:A:526:MET:HE2	1.85	0.58
1:A:681:PHE:O	1:A:685:LEU:HG	2.04	0.58
2:B:470:LEU:O	2:B:473:ILE:HG13	2.03	0.58
1:A:564:ASP:HB3	1:A:567:SER:CB	2.32	0.57
2:B:492:ASN:O	2:B:493:LYS:CB	2.49	0.57
2:B:464:GLU:CD	2:B:467:LYS:NZ	2.62	0.57
2:B:992:LYS:HB3	2:B:996:GLN:HG3	1.87	0.57
2:B:996:GLN:HB3	2:B:997:PRO:CD	2.28	0.57
2:B:289:ARG:CZ	2:B:742:SER:O	2.52	0.57
2:B:664:ASN:N	2:B:664:ASN:HD22	2.03	0.57
1:A:35:VAL:HG21	1:A:552:ARG:CB	2.34	0.57
2:B:289:ARG:NH1	2:B:742:SER:O	2.38	0.57
2:B:442:ALA:HA	2:B:484:ILE:HG23	1.86	0.57
2:B:643:VAL:HG12	2:B:643:VAL:O	2.02	0.57
1:A:673:GLN:HB3	1:A:685:LEU:CD1	2.34	0.57
2:B:446:MET:HE3	2:B:580:ILE:HG12	1.86	0.57
2:B:609:LYS:O	2:B:613:GLN:HG3	2.04	0.57
1:A:102:SER:HB3	1:A:105:ASN:CB	2.35	0.56
2:B:363:ARG:NE	2:B:370:TYR:CE1	2.72	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:TYR:OH	1:A:106:GLN:OE1	2.21	0.56
1:A:84:ALA:HB2	1:A:91:ARG:HD3	1.88	0.56
1:A:148:LYS:O	1:A:152:GLN:HG3	2.05	0.56
1:A:236:ILE:O	1:A:236:ILE:HG22	2.04	0.56
1:A:311:ARG:NH1	1:A:358:LEU:HB3	2.19	0.56
2:B:431:TYR:HB3	2:B:751:LEU:HD11	1.87	0.56
2:B:948:PRO:HG2	2:B:952:HIS:CD2	2.40	0.56
1:A:77:ASP:CG	1:A:79:ARG:O	2.49	0.56
1:A:102:SER:CB	1:A:105:ASN:H	2.18	0.56
1:A:155:LEU:HD21	1:A:240:LEU:HD23	1.88	0.56
1:A:290:ILE:HD11	1:A:360:MET:HE1	1.84	0.56
1:A:179:GLY:HA2	1:A:236:ILE:CD1	2.34	0.56
2:B:902:MET:O	2:B:903:LEU:HG	2.05	0.56
2:B:470:LEU:HD12	2:B:530:TYR:HE1	1.70	0.56
1:A:568:PHE:CD1	1:A:569:ARG:N	2.75	0.55
1:A:179:GLY:HA3	1:A:236:ILE:HD11	1.88	0.55
1:A:311:ARG:HH21	1:A:311:ARG:CG	2.12	0.55
2:B:377:PHE:HB3	2:B:403:LEU:HD21	1.88	0.55
2:B:465:GLU:O	2:B:468:THR:HB	2.06	0.55
1:A:310:ILE:HG22	1:A:311:ARG:H	1.69	0.55
1:A:363:CYS:HB2	1:A:364:PRO:CD	2.37	0.55
1:A:755:HIS:O	1:A:759:LEU:HG	2.07	0.55
1:A:81:LYS:HZ1	1:A:99:ALA:HB1	1.72	0.55
2:B:999:MET:SD	2:B:1002:ARG:CZ	2.95	0.55
1:A:652:THR:HG21	1:A:655:GLN:HB3	1.89	0.55
2:B:322:CYS:SG	2:B:771:SER:C	2.90	0.55
2:B:822:ARG:O	2:B:826:ALA:CB	2.52	0.55
1:A:369:GLY:O	1:A:609:ARG:NH2	2.39	0.54
1:A:607:PHE:HD2	1:A:608:MET:HE2	1.71	0.54
1:A:413:GLU:OE1	1:A:413:GLU:N	2.29	0.54
2:B:928:MET:HE3	2:B:986:MET:CE	2.37	0.54
1:A:313:TRP:CD1	1:A:592:VAL:O	2.60	0.54
1:A:85:CYS:O	1:A:89:TYR:HA	2.08	0.54
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.43	0.54
1:A:121:VAL:CG2	1:A:494:ILE:HG13	2.37	0.54
1:A:121:VAL:HG12	1:A:122:LEU:N	2.23	0.54
1:A:652:THR:HG22	1:A:655:GLN:O	2.08	0.54
1:A:153:MET:HG3	1:A:154:SER:N	2.22	0.54
1:A:183:ILE:HD12	2:B:547:MET:CE	2.38	0.54
1:A:183:ILE:CD1	2:B:547:MET:HE1	2.37	0.54
1:A:519:GLN:OE1	1:A:576:LEU:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LYS:HG2	1:A:557:PHE:CE2	2.43	0.54
2:B:941:ILE:HG23	2:B:953:ILE:HD11	1.90	0.54
1:A:311:ARG:NH2	1:A:354:GLN:OE1	2.39	0.54
1:A:404:GLY:HA2	1:A:484:GLN:O	2.08	0.54
1:A:107:PRO:CD	1:A:110:LEU:HD12	2.37	0.54
2:B:686:ILE:HG22	2:B:687:GLY:N	2.23	0.54
2:B:871:ARG:O	2:B:875:MET:CE	2.56	0.54
2:B:996:GLN:CB	2:B:997:PRO:HD2	2.30	0.54
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.88	0.54
1:A:606:HIS:O	1:A:610:GLN:HG2	2.08	0.54
1:A:700:PHE:C	1:A:700:PHE:CD1	2.85	0.54
2:B:644:ASP:OD1	2:B:647:SER:HB2	2.07	0.54
2:B:686:ILE:CG2	2:B:687:GLY:N	2.71	0.54
1:A:524:ILE:HG13	1:A:612:LEU:HD12	1.88	0.53
1:A:238:MET:HA	1:A:238:MET:CE	2.29	0.53
2:B:415:LYS:HB2	2:B:418:LEU:HD12	1.90	0.53
1:A:388:ARG:C	1:A:390:PHE:N	2.64	0.53
2:B:633:VAL:CG1	2:B:655:THR:HG21	2.39	0.53
2:B:307:ASN:OD1	2:B:767:GLY:N	2.35	0.53
2:B:469:MET:HE1	2:B:678:LEU:O	2.06	0.53
1:A:363:CYS:HB2	1:A:364:PRO:HD3	1.89	0.53
1:A:388:ARG:NH2	1:A:702:MET:HG3	2.24	0.53
2:B:963:VAL:HG12	2:B:964:GLY:N	2.24	0.53
1:A:311:ARG:NH1	1:A:356:GLY:HA2	2.23	0.53
1:A:388:ARG:C	1:A:390:PHE:H	2.17	0.53
1:A:573:THR:HG22	1:A:574:PHE:CD1	2.43	0.53
2:B:384:TYR:CZ	2:B:393:ASN:HB2	2.44	0.53
2:B:653:GLN:HB2	2:B:872:GLN:NE2	2.23	0.53
2:B:470:LEU:HD13	2:B:530:TYR:CD1	2.44	0.53
2:B:693:ARG:NH1	2:B:695:ARG:NE	2.56	0.53
1:A:388:ARG:O	1:A:391:THR:N	2.38	0.53
1:A:313:TRP:O	1:A:316:ILE:HG22	2.08	0.53
2:B:377:PHE:CD2	2:B:409:ARG:HD2	2.44	0.53
2:B:401:GLN:HB2	2:B:409:ARG:NH2	2.23	0.53
2:B:652:PRO:HA	2:B:655:THR:HG22	1.91	0.53
2:B:944:ILE:HG21	2:B:945:PHE:CE1	2.44	0.52
1:A:183:ILE:HD13	2:B:547:MET:SD	2.49	0.52
1:A:452:SER:C	1:A:454:THR:H	2.16	0.52
1:A:524:ILE:HG13	1:A:612:LEU:CD1	2.40	0.52
1:A:612:LEU:HA	1:A:615:SER:OG	2.09	0.52
1:A:652:THR:CG2	1:A:655:GLN:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:HB3	1:A:105:ASN:N	2.25	0.52
1:A:653:PHE:HA	1:A:699:ARG:NH1	2.24	0.52
2:B:899:LYS:O	2:B:900:SER:CB	2.57	0.52
1:A:33:ARG:O	1:A:556:LYS:HD3	2.09	0.52
2:B:500:VAL:CG1	2:B:537:ILE:HG12	2.38	0.52
2:B:605:THR:O	2:B:606:ASP:HB3	2.10	0.52
2:B:962:GLU:HB3	2:B:963:VAL:CG2	2.40	0.52
2:B:322:CYS:SG	2:B:771:SER:O	2.67	0.52
1:A:60:LEU:HB3	1:A:67:ARG:HH11	1.73	0.52
1:A:239:ASN:N	1:A:239:ASN:HD22	2.06	0.52
2:B:301:MET:HG3	2:B:347:ASN:ND2	2.24	0.52
2:B:492:ASN:O	2:B:492:ASN:CG	2.51	0.52
1:A:543:LEU:CD2	1:A:585:ARG:HB2	2.41	0.51
1:A:169:PHE:CD1	1:A:169:PHE:C	2.88	0.51
1:A:311:ARG:NH2	1:A:311:ARG:CG	2.73	0.51
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.91	0.51
1:A:384:GLN:O	1:A:388:ARG:HG2	2.09	0.51
1:A:656:ILE:HD11	1:A:695:ILE:HG21	1.90	0.51
2:B:699:GLY:O	2:B:735:ASP:O	2.28	0.51
1:A:476:ARG:HG2	1:A:502:ASN:OD1	2.10	0.51
2:B:944:ILE:CG2	2:B:945:PHE:CD1	2.92	0.51
1:A:166:LEU:HD23	1:A:243:LEU:CD2	2.40	0.51
1:A:564:ASP:O	1:A:567:SER:CA	2.59	0.51
1:A:591:GLN:HA	1:A:591:GLN:NE2	2.25	0.51
2:B:443:PHE:CG	2:B:579:PHE:HE2	2.28	0.51
2:B:834:LEU:HD11	2:B:1025:HIS:HB2	1.93	0.51
2:B:942:GLN:CG	2:B:948:PRO:HA	2.40	0.51
1:A:533:ARG:HD3	1:A:538:GLU:OE2	2.11	0.51
2:B:979:GLN:HE22	2:B:985:SER:HA	1.74	0.51
2:B:627:VAL:HG21	2:B:710:LEU:HD23	1.93	0.51
1:A:743:LEU:HD12	1:A:759:LEU:HD12	1.93	0.51
2:B:962:GLU:HB3	2:B:963:VAL:HG22	1.93	0.51
1:A:297:GLY:CA	1:A:300:MET:HB2	2.40	0.51
2:B:959:LEU:O	2:B:960:LEU:C	2.54	0.51
1:A:179:GLY:CA	1:A:236:ILE:CD1	2.87	0.51
2:B:453:ASN:ND2	2:B:583:SER:HB3	2.25	0.51
2:B:492:ASN:OD1	2:B:492:ASN:C	2.53	0.51
2:B:704:ASP:HB2	2:B:731:GLU:HB3	1.93	0.51
1:A:238:MET:CA	1:A:238:MET:CE	2.85	0.51
2:B:523:LEU:HD23	2:B:524:ASP:N	2.26	0.51
2:B:590:ALA:HB1	2:B:591:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:CD1	1:A:114:PHE:HE1	2.25	0.50
2:B:283:VAL:HG22	2:B:301:MET:HE2	1.93	0.50
2:B:607:LYS:HG2	2:B:610:ILE:HG13	1.93	0.50
1:A:290:ILE:CD1	1:A:360:MET:CE	2.80	0.50
1:A:612:LEU:C	1:A:615:SER:HG	2.18	0.50
1:A:51:LEU:HD12	1:A:52:PRO:HD3	1.92	0.50
1:A:313:TRP:HA	1:A:316:ILE:HG22	1.92	0.50
1:A:584:LEU:O	1:A:587:SER:OG	2.29	0.50
2:B:818:LEU:HD22	2:B:836:LEU:HD22	1.92	0.50
2:B:302:ILE:HD13	2:B:310:PRO:HD2	1.94	0.50
2:B:470:LEU:HD13	2:B:530:TYR:CE1	2.45	0.50
2:B:944:ILE:HG22	2:B:945:PHE:CE1	2.44	0.50
1:A:35:VAL:CG2	1:A:552:ARG:HB3	2.37	0.50
2:B:366:ARG:HH21	2:B:391:CYS:CB	2.21	0.50
2:B:949:SER:N	2:B:952:HIS:HD2	2.07	0.50
2:B:602:LEU:HA	2:B:608:GLU:HB2	1.94	0.50
2:B:947:VAL:HG11	2:B:952:HIS:HB3	1.93	0.50
1:A:18:ARG:HH21	1:A:518:ASP:CG	2.20	0.49
1:A:302:VAL:CG2	1:A:303:GLY:N	2.74	0.49
2:B:638:PHE:HZ	2:B:674:PHE:CE1	2.29	0.49
1:A:190:ARG:NH1	2:B:517:GLU:HG2	2.27	0.49
1:A:311:ARG:HH11	1:A:356:GLY:HA2	1.76	0.49
2:B:973:MET:O	2:B:977:ILE:N	2.46	0.49
1:A:18:ARG:NH2	1:A:518:ASP:OD1	2.42	0.49
1:A:51:LEU:HD13	1:A:114:PHE:CE1	2.47	0.49
2:B:554:ASN:N	2:B:554:ASN:ND2	2.60	0.49
1:A:77:ASP:OD1	1:A:79:ARG:O	2.29	0.49
1:A:426:LEU:HD21	1:A:447:LYS:HB2	1.93	0.49
2:B:363:ARG:CZ	2:B:370:TYR:CE1	2.83	0.49
2:B:365:ASN:N	2:B:393:ASN:OD1	2.44	0.49
2:B:942:GLN:HE21	2:B:948:PRO:HA	1.77	0.49
2:B:958:THR:O	2:B:958:THR:HG22	2.11	0.49
2:B:889:GLN:O	2:B:922:LEU:HA	2.12	0.49
1:A:239:ASN:N	1:A:239:ASN:ND2	2.60	0.49
1:A:448:ILE:HD11	1:A:457:LEU:HD11	1.94	0.49
2:B:726:LYS:CD	2:B:876:THR:HG21	2.43	0.49
2:B:945:PHE:O	2:B:946:ASN:HB3	2.11	0.49
2:B:971:LEU:CD2	2:B:975:MET:HE2	2.43	0.49
1:A:51:LEU:HD12	1:A:114:PHE:CE1	2.48	0.49
1:A:78:TYR:HD1	1:A:101:ILE:HG12	1.77	0.49
1:A:389:VAL:O	1:A:389:VAL:CG1	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:488:PHE:C	2:B:489:ILE:HG13	2.38	0.49
2:B:621:SER:O	2:B:624:LYS:HB2	2.12	0.49
2:B:928:MET:O	2:B:988:LEU:HD12	2.13	0.49
2:B:614:PRO:HA	2:B:647:SER:OG	2.13	0.48
1:A:577:TYR:CZ	1:A:581:MET:HE3	2.47	0.48
2:B:971:LEU:HD21	2:B:975:MET:HE2	1.94	0.48
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.95	0.48
2:B:528:VAL:HG12	2:B:529:ASN:N	2.27	0.48
1:A:123:ARG:HG3	1:A:125:PRO:CD	2.40	0.48
1:A:388:ARG:HH22	1:A:702:MET:HG3	1.78	0.48
2:B:389:CYS:O	2:B:390:ASN:HB2	2.13	0.48
2:B:523:LEU:CD2	2:B:524:ASP:CG	2.86	0.48
1:A:573:THR:HG22	1:A:574:PHE:CE1	2.49	0.48
2:B:289:ARG:HD2	2:B:769:ASN:OD1	2.13	0.48
1:A:540:PRO:C	1:A:542:VAL:H	2.21	0.48
1:A:564:ASP:N	1:A:565:PRO:CD	2.76	0.48
1:A:692:ALA:O	1:A:696:LEU:HG	2.13	0.48
2:B:523:LEU:HD23	2:B:524:ASP:CG	2.38	0.48
2:B:600:LYS:O	2:B:600:LYS:HG3	2.14	0.48
1:A:500:ALA:O	1:A:501:ARG:NH1	2.44	0.48
1:A:589:PHE:C	1:A:590:LEU:HD23	2.39	0.48
2:B:612:PHE:CD1	2:B:871:ARG:HD3	2.49	0.48
1:A:131:PHE:CD2	1:A:158:LEU:HD22	2.48	0.48
2:B:654:LEU:HD13	2:B:710:LEU:HD13	1.95	0.48
2:B:820:CYS:O	2:B:824:ASN:HB2	2.14	0.48
2:B:965:ASN:N	2:B:966:PRO:CD	2.77	0.48
2:B:1009:LYS:HG2	2:B:1016:SER:HB3	1.96	0.48
1:A:564:ASP:CG	1:A:567:SER:HB3	2.38	0.48
1:A:77:ASP:O	1:A:79:ARG:O	2.32	0.48
1:A:107:PRO:CG	1:A:110:LEU:HD12	2.44	0.47
1:A:183:ILE:HD13	2:B:547:MET:CE	2.44	0.47
1:A:262:ARG:CZ	1:A:292:GLY:HA3	2.44	0.47
2:B:427:ALA:HB3	2:B:759:ARG:HB3	1.96	0.47
2:B:469:MET:O	2:B:470:LEU:C	2.56	0.47
2:B:523:LEU:HD23	2:B:524:ASP:OD1	2.14	0.47
1:A:66:CYS:SG	1:A:88:CYS:SG	3.11	0.47
1:A:102:SER:HB3	1:A:105:ASN:CA	2.44	0.47
1:A:589:PHE:O	1:A:590:LEU:HD23	2.15	0.47
2:B:289:ARG:NH2	2:B:742:SER:O	2.47	0.47
2:B:537:ILE:HG22	2:B:541:LEU:HD12	1.96	0.47
2:B:949:SER:H	2:B:952:HIS:HD2	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:967:TYR:O	2:B:970:GLN:N	2.44	0.47
1:A:154:SER:O	1:A:158:LEU:HG	2.14	0.47
1:A:556:LYS:HG2	1:A:557:PHE:CZ	2.50	0.47
2:B:966:PRO:HG2	2:B:967:TYR:H	1.80	0.47
2:B:999:MET:SD	2:B:1002:ARG:NH1	2.88	0.47
2:B:1025:HIS:HA	2:B:1028:ILE:HD12	1.96	0.47
1:A:102:SER:HB3	1:A:105:ASN:HB2	1.96	0.47
1:A:751:VAL:O	1:A:752:PHE:C	2.57	0.47
2:B:470:LEU:O	2:B:471:GLU:C	2.55	0.47
2:B:522:LEU:HD11	2:B:526:PHE:HB2	1.97	0.47
2:B:642:TYR:OH	2:B:644:ASP:OD2	2.31	0.47
2:B:967:TYR:C	2:B:969:GLN:N	2.72	0.47
2:B:462:ILE:O	2:B:466:LEU:HB2	2.15	0.47
2:B:606:ASP:HA	2:B:802:PRO:HG3	1.97	0.47
2:B:461:LEU:HD22	2:B:667:MET:HE1	1.96	0.47
1:A:560:TYR:CD1	1:A:560:TYR:N	2.82	0.46
2:B:280:GLY:O	2:B:282:GLN:HG3	2.15	0.46
2:B:822:ARG:HD2	2:B:822:ARG:HA	1.73	0.46
1:A:44:PRO:O	1:A:45:LEU:HD23	2.15	0.46
1:A:195:LEU:CD2	1:A:203:MET:HE1	2.45	0.46
2:B:907:VAL:HG12	2:B:908:ARG:N	2.31	0.46
2:B:949:SER:O	2:B:950:PHE:C	2.57	0.46
1:A:363:CYS:CB	1:A:364:PRO:CD	2.93	0.46
1:A:591:GLN:HA	1:A:591:GLN:HE21	1.80	0.46
2:B:374:PHE:CD2	2:B:745:LEU:HD22	2.50	0.46
2:B:478:GLN:HE22	2:B:758:GLN:HE22	1.63	0.46
2:B:965:ASN:H	2:B:966:PRO:CD	2.29	0.46
1:A:113:GLN:H	1:A:113:GLN:HG2	1.52	0.46
1:A:166:LEU:HD23	1:A:243:LEU:HD21	1.97	0.46
1:A:276:GLU:HG3	1:A:341:THR:HG21	1.97	0.46
1:A:644:ALA:O	1:A:663:THR:HB	2.15	0.46
2:B:614:PRO:HG3	2:B:650:LEU:HD22	1.98	0.46
2:B:723:ASP:OD1	2:B:725:ASP:HB2	2.16	0.46
1:A:238:MET:O	1:A:242:ASP:OD2	2.34	0.46
1:A:612:LEU:O	1:A:615:SER:OG	2.28	0.46
1:A:622:ILE:HG21	1:A:624:TYR:CZ	2.51	0.46
2:B:617:ASN:HD22	2:B:617:ASN:C	2.15	0.46
2:B:625:ASP:O	2:B:628:ALA:HB3	2.16	0.46
2:B:637:LEU:HG	2:B:639:PRO:HD3	1.97	0.46
2:B:726:LYS:HD3	2:B:876:THR:HG21	1.96	0.46
1:A:81:LYS:HE2	1:A:99:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:SER:O	1:A:454:THR:N	2.49	0.46
1:A:705:TYR:HE1	1:A:707:ASP:HB2	1.81	0.46
2:B:354:VAL:HG22	2:B:416:PRO:HG2	1.98	0.46
2:B:916:GLU:O	2:B:935:SER:HB2	2.16	0.46
1:A:554:CYS:O	1:A:558:GLY:N	2.48	0.46
1:A:568:PHE:CD1	1:A:568:PHE:C	2.93	0.46
1:A:155:LEU:HD12	1:A:158:LEU:HD12	1.98	0.46
1:A:712:GLY:C	1:A:714:GLN:N	2.70	0.46
2:B:284:TYR:CZ	2:B:291:GLN:OE1	2.69	0.46
2:B:310:PRO:HA	2:B:313:ILE:O	2.16	0.46
2:B:606:ASP:OD1	2:B:802:PRO:HG3	2.16	0.46
1:A:499:ILE:C	1:A:499:ILE:CD1	2.85	0.45
1:A:712:GLY:C	1:A:714:GLN:H	2.23	0.45
2:B:286:THR:O	2:B:286:THR:OG1	2.33	0.45
2:B:854:CYS:SG	2:B:870:GLN:OE1	2.74	0.45
1:A:72:PRO:HD3	1:A:109:GLU:O	2.16	0.45
1:A:178:LEU:C	1:A:180:CYS:H	2.23	0.45
2:B:965:ASN:N	2:B:966:PRO:HD2	2.32	0.45
1:A:21:TRP:CZ3	1:A:517:PHE:HB2	2.51	0.45
1:A:388:ARG:O	1:A:389:VAL:C	2.56	0.45
1:A:653:PHE:O	1:A:699:ARG:NH1	2.45	0.45
1:A:657:LEU:HD23	1:A:658:ILE:N	2.31	0.45
1:A:662:GLU:HB2	1:A:710:HIS:ND1	2.32	0.45
2:B:518:VAL:HG21	2:B:560:PRO:HB3	1.98	0.45
1:A:79:ARG:O	1:A:80:ALA:HB3	2.16	0.45
1:A:162:ALA:O	1:A:232:PRO:HA	2.17	0.45
1:A:302:VAL:HG22	1:A:303:GLY:H	1.79	0.45
2:B:523:LEU:C	2:B:523:LEU:CD2	2.89	0.45
1:A:121:VAL:HG23	1:A:494:ILE:HG13	1.99	0.45
1:A:392:LYS:HD3	1:A:396:GLY:CA	2.47	0.45
1:A:452:SER:C	1:A:454:THR:N	2.75	0.45
1:A:745:ASP:O	1:A:746:ASP:C	2.58	0.45
2:B:458:LEU:O	2:B:462:ILE:HG13	2.17	0.45
2:B:893:ILE:HB	2:B:919:ILE:HG22	1.99	0.45
2:B:996:GLN:CB	2:B:997:PRO:CD	2.94	0.45
1:A:33:ARG:HA	1:A:33:ARG:HD3	1.73	0.45
1:A:652:THR:HG23	1:A:655:GLN:O	2.15	0.45
2:B:388:PHE:CD1	2:B:388:PHE:N	2.84	0.45
2:B:1022:CYS:O	2:B:1026:LYS:HG3	2.17	0.45
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.52	0.45
1:A:153:MET:HE1	1:A:387:GLN:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.88	0.45
1:A:605:HIS:CD2	1:A:605:HIS:C	2.94	0.45
2:B:364:CYS:SG	2:B:386:CYS:HB2	2.56	0.45
2:B:453:ASN:HD21	2:B:583:SER:HB3	1.82	0.45
2:B:601:LYS:HA	2:B:605:THR:HG21	1.98	0.45
2:B:664:ASN:N	2:B:664:ASN:ND2	2.65	0.45
2:B:726:LYS:HD2	2:B:876:THR:CG2	2.47	0.45
1:A:169:PHE:HE2	1:A:288:MET:HE2	1.82	0.44
1:A:568:PHE:HD1	1:A:569:ARG:N	2.14	0.44
2:B:284:TYR:CE1	2:B:291:GLN:CD	2.95	0.44
2:B:284:TYR:CE1	2:B:291:GLN:OE1	2.70	0.44
2:B:947:VAL:CG1	2:B:948:PRO:HD2	2.45	0.44
1:A:77:ASP:OD1	1:A:77:ASP:C	2.59	0.44
2:B:528:VAL:CG1	2:B:533:SER:OG	2.62	0.44
1:A:35:VAL:CG1	1:A:549:GLN:HE21	2.29	0.44
1:A:254:VAL:HA	1:A:255:PRO:HD2	1.66	0.44
1:A:565:PRO:C	1:A:567:SER:N	2.69	0.44
1:A:584:LEU:HD13	1:A:619:ILE:HD11	2.00	0.44
2:B:424:GLU:OE2	2:B:752:TYR:OH	2.29	0.44
2:B:282:GLN:O	2:B:300:CYS:HB2	2.18	0.44
2:B:602:LEU:N	2:B:605:THR:CG2	2.79	0.44
2:B:829:SER:HB2	2:B:833:GLN:OE1	2.17	0.44
2:B:1032:LEU:O	2:B:1033:ASN:HB2	2.17	0.44
1:A:700:PHE:CD1	1:A:700:PHE:O	2.70	0.44
1:A:371:MET:HE3	1:A:605:HIS:ND1	2.33	0.44
1:A:565:PRO:O	1:A:566:SER:C	2.58	0.44
2:B:813:GLN:O	2:B:817:MET:HG3	2.17	0.44
1:A:530:ALA:HB2	1:A:546:LEU:HD13	1.99	0.44
2:B:403:LEU:HD13	2:B:407:GLY:HA2	2.00	0.44
2:B:453:ASN:O	2:B:459:VAL:HG23	2.18	0.44
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.78	0.43
2:B:589:GLU:HG2	2:B:593:LYS:NZ	2.32	0.43
2:B:1000:VAL:CG1	2:B:1001:PHE:N	2.79	0.43
1:A:47:GLU:HG2	1:A:453:PRO:HB3	2.00	0.43
1:A:311:ARG:NE	1:A:359:GLU:OE2	2.49	0.43
1:A:60:LEU:CB	1:A:67:ARG:NH1	2.77	0.43
2:B:446:MET:HE2	2:B:578:LEU:HB3	2.00	0.43
2:B:520:VAL:HG12	2:B:522:LEU:H	1.83	0.43
2:B:466:LEU:C	2:B:468:THR:N	2.69	0.43
2:B:570:LYS:HE2	2:B:629:HIS:NE2	2.33	0.43
2:B:1024:VAL:CG1	2:B:1028:ILE:HD11	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:SER:H	1:A:315:ASP:HB2	1.82	0.43
1:A:314:HIS:HB3	1:A:318:LYS:NZ	2.33	0.43
1:A:518:ASP:HB3	1:A:521:ALA:HB3	1.99	0.43
1:A:561:HIS:O	1:A:562:LYS:C	2.59	0.43
2:B:404:ASP:OD1	2:B:404:ASP:C	2.61	0.43
1:A:102:SER:CB	1:A:105:ASN:HB2	2.48	0.43
1:A:413:GLU:H	1:A:413:GLU:CD	2.23	0.43
2:B:902:MET:O	2:B:903:LEU:CG	2.66	0.43
2:B:453:ASN:CG	2:B:583:SER:HB3	2.44	0.43
2:B:543:GLN:HB3	2:B:547:MET:CE	2.49	0.43
1:A:370:TYR:CE2	1:A:389:VAL:HG13	2.46	0.43
2:B:469:MET:SD	2:B:678:LEU:HG	2.59	0.43
2:B:933:GLY:O	2:B:936:SER:OG	2.30	0.43
1:A:297:GLY:HA3	1:A:300:MET:HB2	2.01	0.42
1:A:647:ILE:HG21	1:A:688:PRO:HG3	2.00	0.42
2:B:731:GLU:HB2	2:B:789:PHE:HE1	1.83	0.42
1:A:51:LEU:CD1	1:A:52:PRO:HD2	2.46	0.42
1:A:169:PHE:CE2	1:A:288:MET:HE2	2.54	0.42
1:A:3:THR:HG22	1:A:5:LEU:H	1.84	0.42
1:A:172:MET:HE3	1:A:172:MET:HB2	1.68	0.42
1:A:240:LEU:O	1:A:243:LEU:HB3	2.19	0.42
1:A:252:TRP:CD1	1:A:252:TRP:H	2.38	0.42
2:B:441:PRO:HA	2:B:575:PRO:O	2.18	0.42
2:B:469:MET:CE	2:B:678:LEU:HG	2.45	0.42
1:A:111:LEU:HA	1:A:112:PRO:HD3	1.92	0.42
1:A:672:TYR:N	1:A:673:GLN:OE1	2.53	0.42
2:B:496:HIS:CE1	2:B:548:PHE:CE2	3.08	0.42
2:B:911:GLU:HA	2:B:914:LEU:HD12	2.00	0.42
1:A:169:PHE:CD2	1:A:267:ALA:CB	3.03	0.42
1:A:194:ASP:OD1	1:A:195:LEU:N	2.53	0.42
1:A:416:ILE:O	1:A:434:SER:HB3	2.20	0.42
2:B:375:MET:SD	2:B:386:CYS:HA	2.59	0.42
2:B:1015:SER:HB2	2:B:1019:ASP:HB3	2.01	0.42
1:A:637:LEU:O	1:A:722:VAL:HG13	2.19	0.42
2:B:821:TYR:CD1	2:B:837:PRO:HD3	2.54	0.42
1:A:363:CYS:CB	1:A:364:PRO:HD3	2.49	0.42
2:B:410:LEU:O	2:B:411:ASP:CB	2.68	0.42
2:B:515:VAL:HG12	2:B:516:GLY:N	2.35	0.42
1:A:23:VAL:HG12	1:A:513:ILE:HG12	2.01	0.42
1:A:60:LEU:HD23	1:A:67:ARG:HG3	2.00	0.42
2:B:723:ASP:OD2	2:B:726:LYS:HE2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:845:VAL:HG13	2:B:1017:TYR:CD1	2.55	0.42
2:B:907:VAL:HG11	2:B:913:ARG:HB3	2.01	0.42
1:A:25:PRO:HG3	1:A:34:MET:SD	2.60	0.42
1:A:539:GLY:C	1:A:541:ASP:H	2.27	0.42
1:A:509:GLN:O	1:A:510:ILE:C	2.63	0.41
1:A:531:ILE:HB	1:A:608:MET:HE1	2.02	0.41
2:B:374:PHE:CE2	2:B:745:LEU:HD22	2.56	0.41
2:B:585:LEU:HA	2:B:586:PRO:HD2	1.80	0.41
2:B:600:LYS:HD2	2:B:602:LEU:HD23	2.02	0.41
2:B:810:LEU:HD23	2:B:810:LEU:HA	1.86	0.41
2:B:960:LEU:HA	2:B:961:PRO:HD3	1.62	0.41
2:B:547:MET:HB2	2:B:547:MET:HE3	1.75	0.41
2:B:661:LYS:HZ1	2:B:663:ASN:HD21	1.68	0.41
2:B:569:LEU:HD22	2:B:576:GLY:HA3	2.01	0.41
2:B:798:VAL:HG13	2:B:803:LEU:HD21	2.03	0.41
2:B:942:GLN:HG2	2:B:948:PRO:HA	2.01	0.41
2:B:960:LEU:HD12	2:B:960:LEU:H	1.85	0.41
1:A:666:GLN:HA	1:A:669:LYS:HB2	2.02	0.41
2:B:693:ARG:HD2	2:B:716:ASP:OD1	2.19	0.41
2:B:726:LYS:HA	2:B:876:THR:HG22	2.03	0.41
2:B:824:ASN:C	2:B:825:CYS:SG	3.01	0.41
2:B:947:VAL:CG1	2:B:952:HIS:CB	2.98	0.41
2:B:966:PRO:HG2	2:B:967:TYR:N	2.35	0.41
1:A:73:LEU:HD11	1:A:500:ALA:HB2	2.00	0.41
1:A:392:LYS:HD3	1:A:396:GLY:HA2	2.02	0.41
1:A:656:ILE:HD13	1:A:656:ILE:HA	1.94	0.41
1:A:673:GLN:CB	1:A:685:LEU:HD12	2.46	0.41
1:A:679:GLU:OE1	1:A:682:ARG:NH1	2.53	0.41
2:B:605:THR:O	2:B:606:ASP:CB	2.68	0.41
1:A:398:PHE:C	1:A:400:MET:H	2.29	0.41
2:B:947:VAL:HG11	2:B:952:HIS:CB	2.50	0.41
1:A:438:ILE:HG21	1:A:529:LEU:HD21	2.02	0.41
2:B:412:HIS:CD2	2:B:412:HIS:C	2.97	0.41
2:B:585:LEU:HD21	2:B:594:LEU:HB2	2.03	0.41
2:B:607:LYS:HE2	2:B:610:ILE:CD1	2.48	0.41
1:A:298:PRO:C	1:A:300:MET:H	2.28	0.41
2:B:469:MET:CE	2:B:679:ARG:CA	2.91	0.41
1:A:17:VAL:HG13	1:A:19:PHE:CD1	2.56	0.41
1:A:182:GLY:O	2:B:506:GLN:CD	2.63	0.41
1:A:658:ILE:HD12	1:A:705:TYR:OH	2.20	0.41
2:B:279:ARG:O	2:B:280:GLY:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:375:MET:CE	2:B:386:CYS:SG	3.02	0.41
2:B:441:PRO:HG2	2:B:484:ILE:HG12	2.02	0.41
1:A:368:GLY:C	1:A:609:ARG:HH21	2.28	0.41
2:B:787:ILE:HG13	2:B:846:TYR:HB3	2.03	0.41
1:A:123:ARG:CG	1:A:125:PRO:HD2	2.45	0.40
1:A:155:LEU:CD2	1:A:240:LEU:HD23	2.50	0.40
1:A:259:ARG:HG3	1:A:306:LEU:HD23	2.02	0.40
2:B:269:ILE:CD1	2:B:907:VAL:C	2.94	0.40
2:B:443:PHE:HB3	2:B:579:PHE:CE2	2.56	0.40
2:B:577:LYS:HA	2:B:632:SER:O	2.21	0.40
2:B:693:ARG:HH12	2:B:695:ARG:NE	2.19	0.40
2:B:942:GLN:O	2:B:946:ASN:CA	2.67	0.40
1:A:427:ASN:HA	1:A:443:THR:HB	2.03	0.40
2:B:645:VAL:O	2:B:645:VAL:HG12	2.20	0.40
1:A:576:LEU:HD23	1:A:576:LEU:HA	1.81	0.40
2:B:334:LEU:H	2:B:334:LEU:HD22	1.86	0.40
2:B:543:GLN:HB3	2:B:547:MET:HE3	2.03	0.40
2:B:651:VAL:O	2:B:655:THR:HB	2.21	0.40
2:B:787:ILE:HD13	2:B:787:ILE:HA	1.80	0.40
2:B:845:VAL:HG22	2:B:1017:TYR:CE1	2.55	0.40
1:A:407:GLU:OE2	1:A:409:LYS:HE3	2.21	0.40
1:A:594:ASN:O	1:A:595:ASN:ND2	2.50	0.40
1:A:596:SER:O	1:A:597:PRO:C	2.64	0.40
2:B:934:VAL:HG13	2:B:993:GLN:CD	2.47	0.40
1:A:190:ARG:NH1	2:B:517:GLU:O	2.54	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	708/765 (92%)	666 (94%)	39 (6%)	3 (0%)	30 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	763/770 (99%)	718 (94%)	39 (5%)	6 (1%)	16	44
All	All	1471/1535 (96%)	1384 (94%)	78 (5%)	9 (1%)	21	50

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	304	ASP
2	B	411	ASP
2	B	968	SER
2	B	998	GLU
1	A	389	VAL
1	A	52	PRO
2	B	965	ASN
2	B	996	GLN
1	A	540	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	624/666 (94%)	591 (95%)	33 (5%)	20	47
2	B	672/682 (98%)	633 (94%)	39 (6%)	18	45
All	All	1296/1348 (96%)	1224 (94%)	72 (6%)	19	46

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	82	LEU
1	A	122	LEU
1	A	196	SER
1	A	201	GLN
1	A	226	SER
1	A	230	LEU

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Mol	Chain	Res	Type
1	A	239	ASN
1	A	268	LEU
1	A	301	VAL
1	A	310	ILE
1	A	328	THR
1	A	332	GLU
1	A	417	SER
1	A	494	ILE
1	A	535	GLU
1	A	567	SER
1	A	570	PHE
1	A	573	THR
1	A	575	SER
1	A	596	SER
1	A	605	HIS
1	A	619	ILE
1	A	629	SER
1	A	638	ASP
1	A	639	SER
1	A	641	SER
1	A	646	ARG
1	A	652	THR
1	A	742	ILE
1	A	744	THR
1	A	747	VAL
1	A	749	LEU
2	B	278	SER
2	B	296	VAL
2	B	334	LEU
2	B	338	ILE
2	B	346	SER
2	B	393	ASN
2	B	403	LEU
2	B	447	ILE
2	B	458	LEU
2	B	468	THR
2	B	494	VAL
2	B	536	VAL
2	B	544	ILE
2	B	554	ASN
2	B	566	MET
2	B	602	LEU

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Mol	Chain	Res	Type
2	B	610	ILE
2	B	618	VAL
2	B	633	VAL
2	B	655	THR
2	B	664	ASN
2	B	747	GLN
2	B	763	ILE
2	B	777	LEU
2	B	808	GLU
2	B	825	CYS
2	B	845	VAL
2	B	857	LEU
2	B	858	SER
2	B	864	THR
2	B	875	MET
2	B	932	LEU
2	B	947	VAL
2	B	962	GLU
2	B	963	VAL
2	B	979	GLN
2	B	1021	LEU
2	B	1027	GLU
2	B	1031	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	227	ASN
1	A	330	HIS
1	A	397	GLN
1	A	436	ASN
1	A	509	GLN
1	A	512	ASN
1	A	591	GLN
1	A	595	ASN
1	A	655	GLN
1	A	693	GLN
1	A	697	HIS
2	B	305	GLN
2	B	385	GLN
2	B	405	HIS

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Mol	Chain	Res	Type
2	B	478	GLN
2	B	496	HIS
2	B	554	ASN
2	B	617	ASN
2	B	663	ASN
2	B	664	ASN
2	B	666	GLN
2	B	668	HIS
2	B	672	GLN
2	B	800	HIS
2	B	816	HIS
2	B	824	ASN
2	B	946	ASN
2	B	952	HIS
2	B	969	GLN
2	B	979	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [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	716/765 (93%)	-0.24	7 (0%) 79 66	26, 71, 129, 225	0
2	B	767/770 (99%)	-0.20	16 (2%) 63 48	31, 74, 160, 275	0
All	All	1483/1535 (96%)	-0.22	23 (1%) 70 56	26, 72, 149, 275	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	742	ILE	5.1
1	A	741	PRO	4.0
2	B	1015	SER	3.2
2	B	857	LEU	3.0
2	B	523	LEU	2.8
1	A	700	PHE	2.7
2	B	830	ALA	2.6
1	A	746	ASP	2.6
2	B	997	PRO	2.6
2	B	469	MET	2.5
2	B	902	MET	2.5
2	B	3	GLY	2.5
1	A	4	TYR	2.4
1	A	593	PHE	2.4
2	B	960	LEU	2.4
1	A	52	PRO	2.3
2	B	967	TYR	2.2
2	B	966	PRO	2.2
2	B	322	CYS	2.1
2	B	1020	PHE	2.1
2	B	1021	LEU	2.1
2	B	1017	TYR	2.0
2	B	889	GLN	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
3	ZN	B	1101	1/1	0.89	0.10	81,81,81,81	0
3	ZN	A	801	1/1	0.96	0.10	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.