Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:23 AM GMT

PDB ID	:	3EGD
Title	:	Crystal structure of the mammalian COPII-coat protein Sec23a/24a complexed with the SNARE protein Sec22 and bound to the transport signal sequence of vesicular stomatitis virus glycoprotein
Authors	:	Goldberg, J.; Mancias, J.D.
Deposited on	:	2008-09-10
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

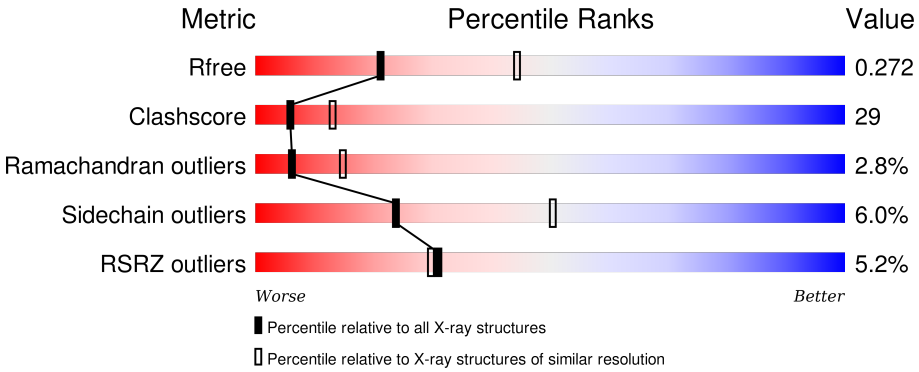
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	764	5% 47% 40% 5% 7%
2	B	748	3% 57% 35% 5% •
3	C	157	13% 44% 38% 6% 13%
4	D	10	30% 40% 30% 30%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12754 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	711	Total	C	N	O	S	0	0	0
			5645	3597	971	1037	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	731	Total	C	N	O	S	0	0	0
			5780	3690	983	1073	34			

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	137	Total	C	N	O	S	0	0	0
			1104	708	182	206	8			

- Molecule 4 is a protein called 10 residue peptide from VSV glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	7	Total	C	N	O	S	0	0	0
			60	34	11	14	1			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

- Molecule 6 is water.

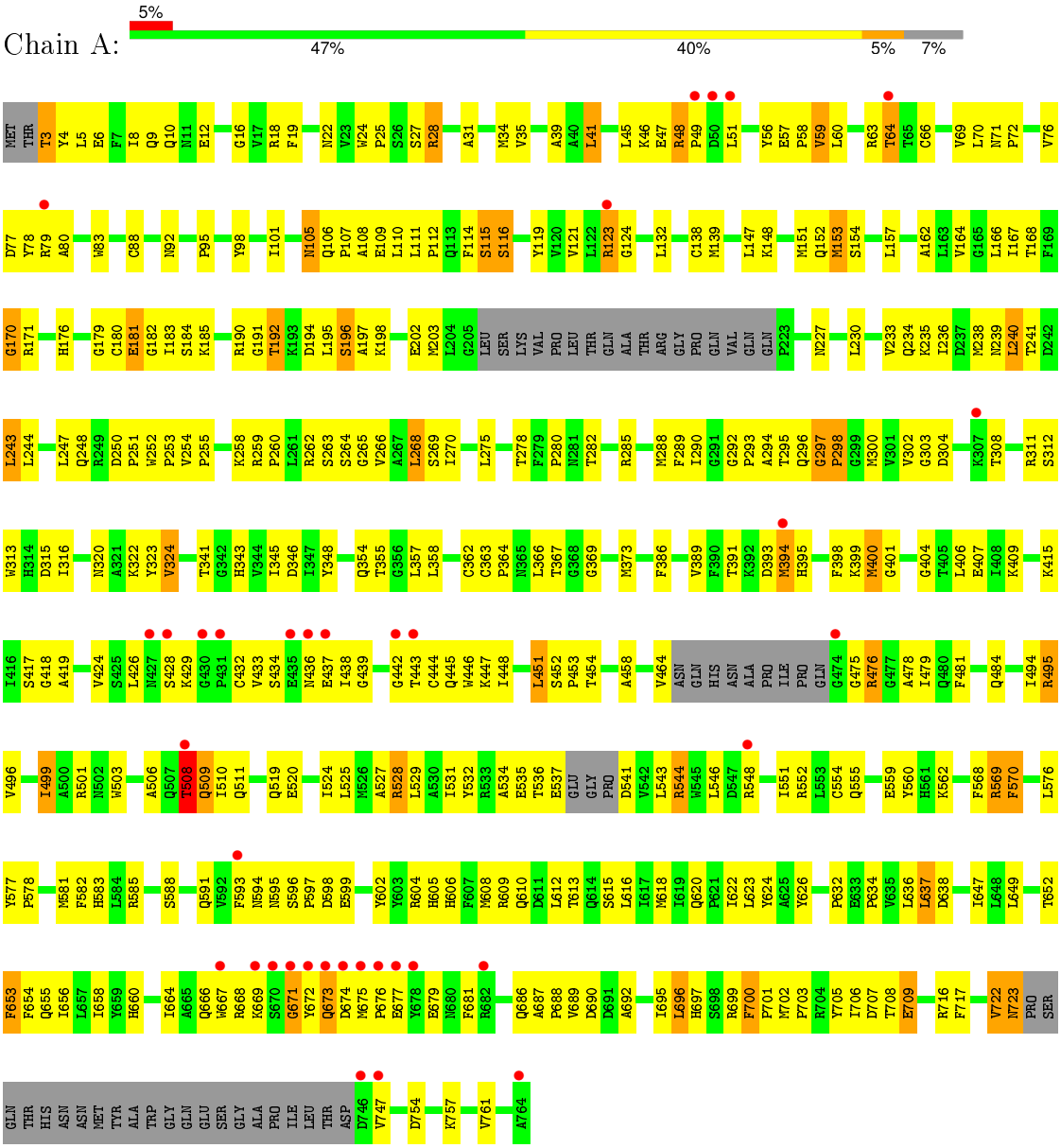
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	74	Total O 74 74	0	0
6	B	84	Total O 84 84	0	0
6	C	5	Total O 5 5	0	0

3 Residue-property plots (i)

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

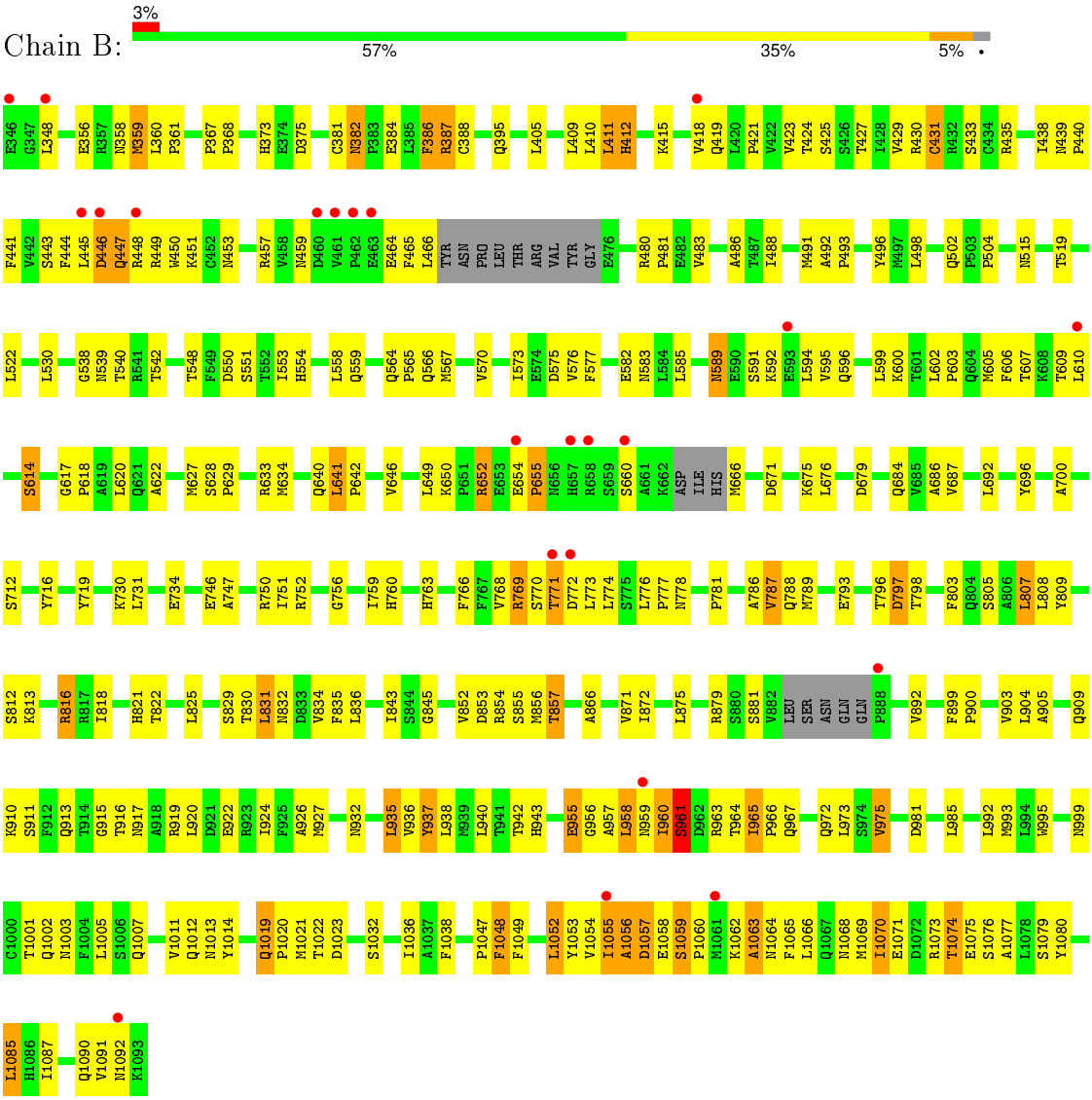
- Molecule 1: Protein transport protein Sec23A

Chain A:



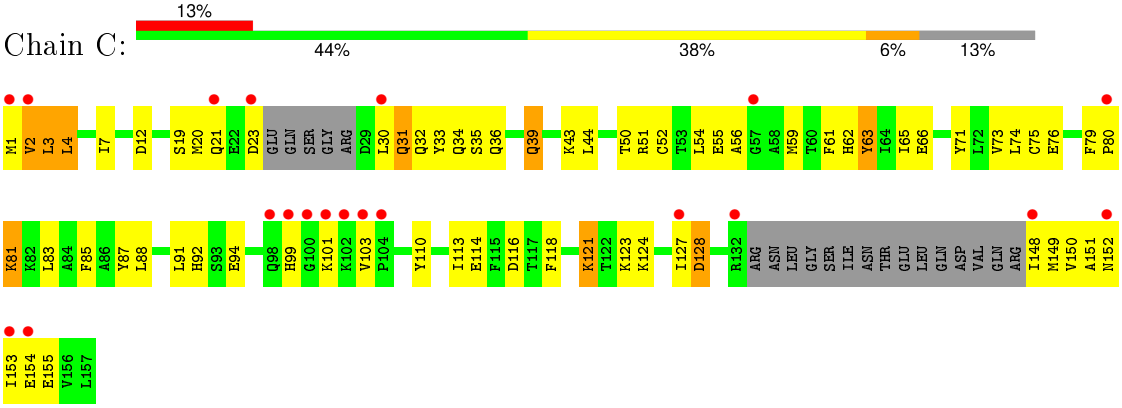
- Molecule 2: Protein transport protein Sec24A

Chain B:



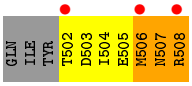
• Molecule 3: Vesicle-trafficking protein SEC22b

Chain C:



• Molecule 4: 10 residue peptide from VSV glycoprotein

Chain D:


GLN
ILE
TYR
T502
D503
I504
E505
M506
N507
R508

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.75Å 97.63Å 129.12Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 29.60 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.70) 91.7 (29.60-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.274 0.205 , 0.272	Depositor DCC
R_{free} test set	2291 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.6	EDS
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 48031 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12754	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.38	0/5778	0.65	2/7824 (0.0%)
2	B	0.38	0/5904	0.65	0/8024
3	C	0.34	0/1123	0.57	0/1510
4	D	0.72	0/59	1.18	0/76
All	All	0.38	0/12864	0.65	2/17434 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	SER	N-CA-C	-7.96	89.51	111.00
1	A	170	GLY	N-CA-C	-5.23	100.03	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	937	TYR	Sidechain

5.2 Too-close contacts (i)

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	5645	0	5591	334	0
2	B	5780	0	5835	318	0
3	C	1104	0	1109	77	0
4	D	60	0	55	16	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	74	0	0	24	0
6	B	84	0	0	29	0
6	C	5	0	0	0	0
All	All	12754	0	12590	721	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 29.

All (721) 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:48:ARG:HB2	1:A:49:PRO:HD2	1.17	1.15
2:B:435:ARG:HH21	4:D:507:ASN:HB3	1.07	1.14
1:A:417:SER:HB3	1:A:438:ILE:HD13	1.31	1.08
1:A:647:ILE:HD11	1:A:664:ILE:HG21	1.31	1.07
1:A:48:ARG:HB2	1:A:49:PRO:CD	1.84	1.05
1:A:479:ILE:HB	1:A:499:ILE:HD11	1.41	1.03
1:A:366:LEU:HD22	1:A:424:VAL:HG22	1.41	1.02
1:A:3:THR:HG22	1:A:6:GLU:H	1.25	1.01
1:A:723:ASN:HA	6:A:811:HOH:O	1.62	0.99
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.44	0.96
1:A:722:VAL:HG22	1:A:723:ASN:H	1.29	0.96
2:B:909:GLN:HG2	2:B:911:SER:H	1.29	0.95
1:A:28:ARG:HB3	1:A:28:ARG:HH11	1.31	0.95
1:A:45:LEU:HA	1:A:495:ARG:NH1	1.81	0.95
2:B:879:ARG:NH1	2:B:1092:ASN:HD22	1.64	0.95
1:A:596:SER:OG	1:A:599:GLU:HG3	1.68	0.93
3:C:39:GLN:HE21	3:C:39:GLN:HA	1.33	0.92
2:B:358:ASN:HA	2:B:972:GLN:HE22	1.32	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.51	0.91
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.34	0.91
2:B:1048:PHE:HB2	6:B:128:HOH:O	1.71	0.90
2:B:443:SER:HB2	2:B:451:LYS:HB3	1.52	0.90
2:B:797:ASP:HB2	6:B:113:HOH:O	1.73	0.87
1:A:313:TRP:O	1:A:316:ILE:HG22	1.75	0.86
2:B:1074:THR:HG23	2:B:1076:SER:H	1.39	0.86
1:A:132:LEU:HD11	1:A:167:ILE:HD13	1.57	0.86
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.41	0.86
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.58	0.85
2:B:435:ARG:NH2	4:D:507:ASN:HB3	1.91	0.85
1:A:34:MET:HA	6:A:782:HOH:O	1.77	0.84
2:B:382:ASN:HD22	2:B:384:GLU:H	1.24	0.84
1:A:238:MET:O	1:A:241:THR:HG22	1.75	0.84
2:B:1048:PHE:HB3	6:B:3:HOH:O	1.77	0.84
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.60	0.84
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.60	0.83
3:C:148:ILE:HG22	3:C:149:MET:H	1.42	0.83
2:B:760:HIS:NE2	2:B:788:GLN:HG2	1.93	0.83
2:B:769:ARG:HB2	2:B:773:LEU:HB3	1.61	0.83
2:B:955:GLU:N	2:B:955:GLU:OE1	2.13	0.82
2:B:965:ILE:HA	6:B:40:HOH:O	1.78	0.82
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.62	0.82
2:B:1019:GLN:HB3	2:B:1020:PRO:CD	2.09	0.81
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.59	0.81
1:A:510:ILE:HD12	1:A:510:ILE:H	1.43	0.81
1:A:49:PRO:HA	6:A:805:HOH:O	1.79	0.81
1:A:297:GLY:H	1:A:300:MET:HB2	1.47	0.79
1:A:652:THR:O	1:A:654:PHE:N	2.15	0.79
2:B:1056:ALA:HB2	6:B:143:HOH:O	1.83	0.79
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.65	0.79
4:D:506:MET:HG2	4:D:508:ARG:OXT	1.82	0.78
2:B:642:PRO:HD2	2:B:649:LEU:HD12	1.66	0.78
2:B:879:ARG:NH1	2:B:1092:ASN:ND2	2.31	0.77
2:B:356:GLU:HB2	6:B:123:HOH:O	1.84	0.77
2:B:916:THR:HG22	2:B:917:ASN:N	2.00	0.77
2:B:361:PRO:HG2	6:B:149:HOH:O	1.84	0.76
2:B:1054:VAL:O	2:B:1056:ALA:N	2.18	0.76
1:A:671:GLY:C	1:A:673:GLN:H	1.89	0.75
2:B:958:LEU:HA	2:B:964:THR:HA	1.66	0.75
2:B:423:VAL:HG12	2:B:425:SER:H	1.52	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1064:ASN:HA	6:B:82:HOH:O	1.85	0.74
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.18	0.74
2:B:1074:THR:CG2	2:B:1076:SER:H	2.01	0.74
2:B:872:ILE:HD12	2:B:1090:GLN:HB2	1.67	0.74
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.69	0.74
2:B:879:ARG:HH12	2:B:1092:ASN:ND2	1.86	0.74
1:A:45:LEU:HA	1:A:495:ARG:HH12	1.52	0.74
2:B:772:ASP:HB3	6:B:23:HOH:O	1.86	0.74
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.70	0.74
2:B:504:PRO:HG2	2:B:542:THR:HA	1.69	0.74
2:B:395:GLN:HE21	2:B:796:THR:HA	1.50	0.73
1:A:180:CYS:O	1:A:181:GLU:HG3	1.88	0.73
2:B:854:ARG:NH1	2:B:866:ALA:HB2	2.04	0.73
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.69	0.73
1:A:652:THR:O	1:A:655:GLN:N	2.22	0.73
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.29	0.73
1:A:583:HIS:CD2	1:A:620:GLN:HE21	2.07	0.72
1:A:354:GLN:HE22	1:A:597:PRO:HD2	1.54	0.72
2:B:854:ARG:HH12	2:B:866:ALA:HB2	1.53	0.72
4:D:507:ASN:O	4:D:508:ARG:HB2	1.88	0.72
1:A:647:ILE:HD12	1:A:660:HIS:ND1	2.04	0.72
1:A:8:ILE:CD1	1:A:22:ASN:HD21	2.01	0.72
2:B:966:PRO:HD2	6:B:40:HOH:O	1.90	0.72
3:C:81:LYS:HD3	3:C:81:LYS:H	1.54	0.72
1:A:475:GLY:HA2	1:A:503:TRP:HB2	1.71	0.72
3:C:110:TYR:HB3	3:C:113:ILE:HG23	1.70	0.72
2:B:756:GLY:HA2	2:B:793:GLU:HB2	1.71	0.71
2:B:419:GLN:HG2	6:B:147:HOH:O	1.90	0.71
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.71	0.71
1:A:499:ILE:H	1:A:499:ILE:HD13	1.54	0.71
1:A:527:ALA:O	1:A:531:ILE:HD13	1.90	0.70
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.73	0.70
2:B:1019:GLN:HG2	2:B:1062:LYS:HZ2	1.55	0.70
1:A:610:GLN:HG3	1:A:618:MET:HE1	1.72	0.70
1:A:198:LYS:O	1:A:202:GLU:HG3	1.92	0.70
1:A:181:GLU:O	1:A:183:ILE:N	2.25	0.70
1:A:183:ILE:HD12	2:B:605:MET:SD	2.32	0.70
2:B:602:LEU:HD23	2:B:605:MET:HE1	1.72	0.70
1:A:290:ILE:HG21	1:A:355:THR:HG23	1.74	0.69
1:A:297:GLY:N	1:A:300:MET:HB2	2.08	0.69
2:B:872:ILE:CD1	2:B:1087:ILE:HD13	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:ILE:O	3:C:116:ASP:HB2	1.92	0.69
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.23	0.69
1:A:647:ILE:HD11	1:A:664:ILE:CG2	2.16	0.68
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.73	0.68
3:C:39:GLN:NE2	3:C:39:GLN:HA	2.07	0.68
1:A:348:TYR:HD1	6:A:795:HOH:O	1.75	0.68
1:A:357:LEU:HD12	1:A:373:MET:HE3	1.75	0.68
2:B:1074:THR:HG22	2:B:1077:ALA:N	2.09	0.68
1:A:652:THR:HB	1:A:655:GLN:HG2	1.74	0.68
2:B:750:ARG:NH2	4:D:503:ASP:OD2	2.25	0.68
2:B:348:LEU:HD13	2:B:836:LEU:HD21	1.76	0.68
1:A:121:VAL:HG12	6:A:775:HOH:O	1.93	0.67
2:B:633:ARG:HB2	2:B:778:ASN:HD21	1.59	0.67
3:C:113:ILE:HD12	3:C:114:GLU:HG3	1.76	0.67
1:A:116:SER:HA	1:A:496:VAL:O	1.94	0.67
1:A:297:GLY:HA3	1:A:300:MET:HB2	1.77	0.67
3:C:1:MET:H2	3:C:76:GLU:H	1.43	0.67
3:C:3:LEU:HD13	3:C:123:LYS:HZ2	1.58	0.67
1:A:108:ALA:HB1	1:A:114:PHE:CD1	2.30	0.66
1:A:407:GLU:HG3	1:A:445:GLN:HG2	1.76	0.66
1:A:58:PRO:HA	1:A:119:TYR:CE2	2.30	0.66
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.77	0.66
1:A:610:GLN:CG	1:A:618:MET:HE1	2.26	0.66
1:A:58:PRO:O	1:A:59:VAL:HB	1.95	0.66
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.76	0.66
2:B:395:GLN:NE2	2:B:796:THR:HA	2.11	0.66
1:A:297:GLY:CA	1:A:300:MET:HB2	2.27	0.65
3:C:148:ILE:HG22	3:C:149:MET:N	2.11	0.65
2:B:602:LEU:HD23	2:B:605:MET:CE	2.27	0.65
2:B:808:LEU:HD23	4:D:504:ILE:HG23	1.78	0.65
1:A:108:ALA:HB1	1:A:114:PHE:HD1	1.61	0.65
1:A:162:ALA:O	1:A:233:VAL:HG23	1.97	0.65
2:B:559:GLN:HG2	2:B:583:ASN:ND2	2.12	0.65
2:B:382:ASN:ND2	2:B:384:GLU:H	1.92	0.64
2:B:1064:ASN:HA	6:B:106:HOH:O	1.97	0.64
2:B:964:THR:O	2:B:965:ILE:HB	1.97	0.64
1:A:190:ARG:HH21	2:B:577:PHE:HB3	1.63	0.64
1:A:197:ALA:N	6:A:770:HOH:O	2.31	0.64
2:B:466:LEU:HD23	6:B:27:HOH:O	1.97	0.64
2:B:429:VAL:HB	2:B:438:ILE:HG21	1.78	0.64
3:C:62:HIS:O	3:C:73:VAL:HG12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.13	0.64
1:A:48:ARG:CZ	1:A:51:LEU:HD11	2.28	0.64
1:A:660:HIS:CD2	1:A:668:ARG:HH21	2.16	0.64
1:A:190:ARG:NH2	2:B:577:PHE:HB3	2.13	0.64
1:A:519:GLN:HG2	6:A:784:HOH:O	1.98	0.64
2:B:423:VAL:CG1	2:B:425:SER:HB2	2.29	0.63
1:A:417:SER:CB	1:A:438:ILE:HD13	2.21	0.63
1:A:479:ILE:HB	1:A:499:ILE:CD1	2.21	0.63
3:C:99:HIS:O	3:C:103:VAL:HG23	1.98	0.63
1:A:316:ILE:HD13	1:A:324:VAL:HG21	1.79	0.63
3:C:21:GLN:HE21	3:C:123:LYS:NZ	1.97	0.63
3:C:55:GLU:HB2	3:C:152:ASN:HD22	1.62	0.63
1:A:528:ARG:HA	1:A:608:MET:HE1	1.81	0.63
2:B:418:VAL:HB	6:B:147:HOH:O	1.99	0.63
2:B:958:LEU:HD23	2:B:958:LEU:C	2.19	0.63
2:B:348:LEU:CD1	2:B:836:LEU:HD21	2.29	0.63
2:B:916:THR:HG22	2:B:917:ASN:H	1.62	0.63
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.80	0.63
2:B:412:HIS:HD2	6:B:5:HOH:O	1.81	0.63
1:A:115:SER:O	1:A:116:SER:HB2	1.99	0.62
2:B:440:PRO:HA	2:B:483:VAL:HG13	1.81	0.62
2:B:916:THR:CG2	2:B:917:ASN:N	2.62	0.62
3:C:2:VAL:HG12	3:C:3:LEU:H	1.64	0.62
2:B:1021:MET:N	2:B:1055:ILE:HG12	2.09	0.62
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.81	0.62
1:A:148:LYS:HE3	1:A:244:LEU:O	1.99	0.62
1:A:692:ALA:O	1:A:696:LEU:HB2	1.99	0.62
2:B:913:GLN:NE2	2:B:916:THR:HG21	2.14	0.62
3:C:52:CYS:HB3	3:C:63:TYR:CE2	2.35	0.62
1:A:297:GLY:H	1:A:300:MET:CB	2.12	0.62
2:B:450:TRP:CE2	2:B:459:ASN:HB2	2.35	0.62
1:A:722:VAL:HG22	1:A:723:ASN:N	2.09	0.61
3:C:113:ILE:HD12	3:C:114:GLU:N	2.15	0.61
1:A:266:VAL:O	1:A:270:ILE:HD13	2.00	0.61
2:B:992:LEU:HB2	2:B:1052:LEU:HD12	1.83	0.61
2:B:750:ARG:HA	2:B:772:ASP:OD1	2.01	0.61
2:B:493:PRO:HG2	2:B:496:TYR:CD2	2.35	0.61
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.31	0.61
2:B:916:THR:CG2	2:B:917:ASN:H	2.12	0.61
1:A:357:LEU:HD12	1:A:373:MET:CE	2.29	0.61
1:A:656:ILE:HD12	1:A:696:LEU:HD13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:HD2	1:A:88:CYS:SG	2.40	0.61
2:B:446:ASP:HB2	2:B:449:ARG:HB2	1.82	0.60
2:B:831:LEU:HD22	2:B:835:PHE:CE1	2.36	0.60
1:A:196:SER:C	6:A:770:HOH:O	2.40	0.60
1:A:313:TRP:HE3	1:A:316:ILE:HG21	1.66	0.60
2:B:573:ILE:CG2	2:B:618:PRO:HG2	2.31	0.60
2:B:958:LEU:HB3	2:B:964:THR:HG23	1.82	0.60
1:A:268:LEU:HG	1:A:288:MET:SD	2.42	0.60
2:B:853:ASP:O	2:B:857:THR:HB	2.01	0.60
1:A:3:THR:HG22	1:A:6:GLU:N	2.08	0.60
1:A:536:THR:O	1:A:536:THR:HG22	2.01	0.60
2:B:620:LEU:HD22	2:B:634:MET:CE	2.31	0.60
1:A:653:PHE:HA	1:A:699:ARG:NH1	2.16	0.60
2:B:498:LEU:HD12	2:B:498:LEU:H	1.65	0.60
2:B:956:GLY:HA2	2:B:967:GLN:HG2	1.82	0.60
1:A:437:GLU:C	1:A:438:ILE:HD12	2.21	0.60
1:A:652:THR:O	1:A:653:PHE:C	2.39	0.60
2:B:573:ILE:HG23	2:B:618:PRO:CG	2.31	0.60
2:B:614:SER:HB2	2:B:640:GLN:HE21	1.67	0.60
2:B:430:ARG:HB2	2:B:435:ARG:NH1	2.17	0.60
1:A:8:ILE:HD11	1:A:22:ASN:ND2	2.16	0.60
2:B:596:GLN:O	2:B:600:LYS:HG3	2.02	0.60
2:B:913:GLN:HE22	2:B:916:THR:HG21	1.67	0.59
2:B:1057:ASP:C	2:B:1060:PRO:HD3	2.21	0.59
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.67	0.59
1:A:8:ILE:HD11	1:A:22:ASN:HD21	1.66	0.59
1:A:24:TRP:HB3	1:A:25:PRO:HD2	1.85	0.59
3:C:110:TYR:HB3	3:C:113:ILE:CG2	2.33	0.59
3:C:94:GLU:HG2	3:C:118:PHE:CD2	2.37	0.59
1:A:60:LEU:CD2	1:A:69:VAL:HG22	2.33	0.59
1:A:322:LYS:HE3	1:A:323:TYR:CZ	2.38	0.59
1:A:475:GLY:O	1:A:476:ARG:HB2	2.03	0.59
2:B:429:VAL:HB	2:B:438:ILE:CG2	2.32	0.59
1:A:262:ARG:CZ	1:A:292:GLY:HA3	2.33	0.59
2:B:1003:ASN:O	2:B:1007:GLN:HB2	2.03	0.58
2:B:972:GLN:HB3	2:B:1071:GLU:OE2	2.03	0.58
2:B:498:LEU:HD12	2:B:498:LEU:N	2.18	0.58
2:B:558:LEU:CD2	2:B:565:PRO:HB3	2.33	0.58
2:B:412:HIS:HE1	2:B:781:PRO:O	1.86	0.58
1:A:48:ARG:HE	1:A:49:PRO:HD2	1.68	0.58
2:B:1019:GLN:HG2	2:B:1062:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:LEU:HD22	2:B:634:MET:HE1	1.86	0.58
1:A:582:PHE:O	1:A:585:ARG:HG2	2.03	0.58
1:A:510:ILE:HD12	1:A:510:ILE:N	2.17	0.58
1:A:255:PRO:O	1:A:258:LYS:HB2	2.03	0.58
2:B:975:VAL:HG23	2:B:1069:MET:HG3	1.85	0.58
2:B:1060:PRO:O	2:B:1062:LYS:HG3	2.04	0.57
2:B:1052:LEU:HG	2:B:1053:TYR:N	2.20	0.57
1:A:593:PHE:O	1:A:594:ASN:HB2	2.04	0.57
1:A:524:ILE:HD12	1:A:615:SER:HB3	1.87	0.57
1:A:366:LEU:HD22	1:A:424:VAL:CG2	2.27	0.57
2:B:760:HIS:CE1	2:B:788:GLN:HG2	2.38	0.57
1:A:506:ALA:HA	1:A:509:GLN:HG3	1.87	0.57
1:A:56:TYR:HD1	1:A:57:GLU:O	1.88	0.57
1:A:166:LEU:CD2	1:A:243:LEU:HD13	2.35	0.57
2:B:628:SER:HB3	2:B:629:PRO:HD3	1.86	0.57
2:B:423:VAL:HG23	2:B:488:ILE:HD11	1.85	0.57
1:A:132:LEU:HD11	1:A:167:ILE:CD1	2.31	0.57
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.20	0.57
3:C:21:GLN:HE21	3:C:123:LYS:HZ2	1.52	0.56
4:D:502:THR:O	4:D:502:THR:HG22	2.05	0.56
1:A:5:LEU:O	1:A:9:GLN:HG3	2.05	0.56
1:A:723:ASN:ND2	6:A:804:HOH:O	2.33	0.56
1:A:705:TYR:C	1:A:706:ILE:HD12	2.25	0.56
3:C:56:ALA:HB2	3:C:153:ILE:HG21	1.86	0.56
1:A:190:ARG:NH1	2:B:575:ASP:OD2	2.39	0.56
3:C:35:SER:O	3:C:39:GLN:HG2	2.05	0.56
1:A:610:GLN:HG3	1:A:618:MET:CE	2.35	0.56
2:B:450:TRP:NE1	2:B:459:ASN:HB2	2.20	0.56
1:A:543:LEU:HD22	1:A:585:ARG:HB2	1.87	0.56
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.41	0.56
2:B:985:LEU:C	2:B:985:LEU:HD23	2.26	0.56
1:A:653:PHE:N	6:A:767:HOH:O	2.39	0.56
2:B:830:THR:O	2:B:834:VAL:HG23	2.05	0.56
2:B:684:GLN:HG3	2:B:746:GLU:HB3	1.87	0.56
1:A:153:MET:HE1	1:A:154:SER:HA	1.88	0.56
1:A:3:THR:CG2	1:A:6:GLU:HG3	2.36	0.55
2:B:439:ASN:HD21	2:B:453:ASN:ND2	2.04	0.55
2:B:435:ARG:HG3	4:D:508:ARG:OXT	2.06	0.55
2:B:750:ARG:HG3	2:B:751:ILE:N	2.21	0.55
1:A:479:ILE:O	1:A:499:ILE:HD13	2.06	0.55
1:A:671:GLY:C	1:A:673:GLN:N	2.57	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:TYR:O	1:A:101:ILE:HB	2.06	0.55
2:B:1063:ALA:C	2:B:1065:PHE:H	2.09	0.55
2:B:411:LEU:N	2:B:411:LEU:HD23	2.22	0.55
1:A:45:LEU:CD1	1:A:451:LEU:HD13	2.36	0.55
1:A:348:TYR:CD1	6:A:795:HOH:O	2.53	0.55
2:B:750:ARG:HH22	4:D:503:ASP:CG	2.10	0.55
1:A:107:PRO:HG2	1:A:110:LEU:HD12	1.88	0.55
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.42	0.55
2:B:920:LEU:HD23	6:B:99:HOH:O	2.06	0.55
2:B:1059:SER:H	2:B:1060:PRO:HD3	1.70	0.55
2:B:576:VAL:HG11	2:B:622:ALA:CB	2.36	0.55
1:A:369:GLY:O	1:A:609:ARG:NH2	2.39	0.55
1:A:302:VAL:HG22	1:A:303:GLY:H	1.72	0.55
1:A:535:GLU:HG3	1:A:604:ARG:HH11	1.71	0.55
2:B:558:LEU:HD23	2:B:565:PRO:HB3	1.88	0.55
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.42	0.55
3:C:33:TYR:CE2	3:C:59:MET:HG3	2.42	0.55
1:A:541:ASP:HB3	1:A:544:ARG:HD2	1.88	0.55
1:A:417:SER:HB3	1:A:438:ILE:CD1	2.22	0.54
1:A:559:GLU:O	1:A:568:PHE:HA	2.07	0.54
3:C:59:MET:HB3	3:C:74:LEU:HD11	1.89	0.54
2:B:1038:PHE:HA	6:B:40:HOH:O	2.07	0.54
2:B:553:ILE:HD12	2:B:553:ILE:N	2.22	0.54
1:A:185:LYS:CB	2:B:567:MET:HB3	2.36	0.54
2:B:602:LEU:HA	2:B:605:MET:HE3	1.90	0.54
3:C:113:ILE:CD1	3:C:114:GLU:HG3	2.38	0.54
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.38	0.54
1:A:265:GLY:HA3	1:A:298:PRO:O	2.08	0.54
1:A:433:VAL:HG13	1:A:442:GLY:HA2	1.88	0.54
2:B:1059:SER:N	2:B:1060:PRO:CD	2.71	0.54
2:B:582:GLU:N	6:B:22:HOH:O	2.41	0.54
1:A:708:THR:OG1	1:A:709:GLU:N	2.41	0.54
1:A:407:GLU:HG3	1:A:445:GLN:CG	2.38	0.54
1:A:524:ILE:CD1	1:A:615:SER:HB3	2.38	0.53
1:A:76:VAL:HG21	1:A:110:LEU:HD13	1.91	0.53
3:C:30:LEU:O	3:C:34:GLN:HB2	2.07	0.53
2:B:550:ASP:OD2	2:B:554:HIS:HE1	1.92	0.53
1:A:8:ILE:CD1	1:A:22:ASN:ND2	2.70	0.53
1:A:70:LEU:HD11	1:A:110:LEU:HD21	1.91	0.53
1:A:56:TYR:CE1	1:A:98:TYR:OH	2.59	0.53
1:A:658:ILE:HD13	1:A:705:TYR:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:LEU:HA	3:C:151:ALA:O	2.07	0.53
2:B:551:SER:O	2:B:573:ILE:HD11	2.09	0.53
1:A:114:PHE:HA	6:A:787:HOH:O	2.09	0.53
1:A:35:VAL:N	6:A:820:HOH:O	2.42	0.53
3:C:55:GLU:HB2	3:C:152:ASN:ND2	2.23	0.53
1:A:722:VAL:O	1:A:723:ASN:HB2	2.08	0.53
1:A:316:ILE:CD1	1:A:324:VAL:HG21	2.38	0.53
3:C:81:LYS:N	3:C:81:LYS:HD3	2.23	0.53
2:B:830:THR:HG22	2:B:832:ASN:N	2.24	0.53
1:A:28:ARG:CB	1:A:28:ARG:HH11	2.13	0.52
2:B:872:ILE:HD11	2:B:1087:ILE:HD13	1.90	0.52
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.75	0.52
2:B:358:ASN:CA	2:B:972:GLN:HE22	2.15	0.52
2:B:770:SER:O	2:B:771:THR:O	2.27	0.52
1:A:438:ILE:HD12	1:A:438:ILE:N	2.24	0.52
2:B:576:VAL:HG12	2:B:577:PHE:N	2.23	0.52
4:D:504:ILE:HG23	4:D:505:GLU:N	2.25	0.52
1:A:686:GLN:HG2	1:A:690:ASP:OD1	2.10	0.52
1:A:184:SER:HA	6:A:800:HOH:O	2.08	0.52
3:C:123:LYS:HG2	3:C:127:ILE:HD12	1.91	0.52
1:A:254:VAL:HG21	1:A:260:PRO:HG3	1.90	0.52
2:B:609:THR:HG21	6:B:43:HOH:O	2.10	0.52
1:A:250:ASP:OD2	1:A:251:PRO:HD2	2.09	0.52
2:B:359:MET:HG3	6:B:123:HOH:O	2.10	0.52
2:B:879:ARG:C	2:B:881:SER:H	2.13	0.52
3:C:1:MET:N	3:C:76:GLU:HB2	2.24	0.52
3:C:21:GLN:NE2	3:C:123:LYS:HZ2	2.08	0.52
2:B:1005:LEU:HD13	2:B:1013:ASN:HA	1.92	0.52
2:B:957:ALA:C	2:B:959:ASN:H	2.13	0.52
1:A:520:GLU:HB3	1:A:616:LEU:HD11	1.91	0.52
2:B:770:SER:O	2:B:771:THR:C	2.48	0.52
3:C:79:PHE:CD1	3:C:80:PRO:HD2	2.45	0.52
1:A:519:GLN:NE2	1:A:576:LEU:HD12	2.25	0.51
3:C:118:PHE:HA	3:C:121:LYS:HG2	1.92	0.51
2:B:387:ARG:HG3	2:B:388:CYS:N	2.24	0.51
2:B:642:PRO:CD	2:B:649:LEU:HD12	2.39	0.51
1:A:63:ARG:HH11	1:A:88:CYS:HB2	1.75	0.51
1:A:658:ILE:HD12	1:A:658:ILE:N	2.25	0.51
1:A:543:LEU:HD11	1:A:591:GLN:HE22	1.76	0.51
2:B:655:PRO:HD3	2:B:920:LEU:HD13	1.92	0.51
1:A:364:PRO:O	1:A:367:THR:O	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:439:ASN:HB2	2:B:440:PRO:CD	2.40	0.51
1:A:259:ARG:NH2	1:A:308:THR:O	2.43	0.51
3:C:2:VAL:HG12	3:C:3:LEU:N	2.25	0.51
2:B:1066:LEU:C	2:B:1068:ASN:H	2.14	0.51
2:B:1032:SER:O	2:B:1036:ILE:HG12	2.11	0.51
1:A:313:TRP:CE3	1:A:316:ILE:HG21	2.44	0.51
2:B:964:THR:O	2:B:965:ILE:CB	2.57	0.51
1:A:183:ILE:CD1	2:B:567:MET:HB2	2.40	0.51
1:A:176:HIS:ND1	1:A:243:LEU:HD11	2.26	0.51
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.41	0.51
1:A:106:GLN:HB2	1:A:107:PRO:HD2	1.93	0.51
1:A:124:GLY:HA3	6:A:785:HOH:O	2.09	0.51
1:A:12:GLU:HG2	1:A:46:LYS:NZ	2.26	0.51
1:A:669:LYS:C	1:A:671:GLY:H	2.14	0.51
1:A:476:ARG:HA	1:A:501:ARG:O	2.11	0.51
1:A:696:LEU:HD13	1:A:703:PRO:HG2	1.93	0.51
2:B:750:ARG:HD3	2:B:772:ASP:O	2.11	0.51
1:A:695:ILE:O	1:A:697:HIS:N	2.37	0.51
2:B:700:ALA:HA	2:B:924:ILE:HG21	1.92	0.51
2:B:425:SER:C	2:B:427:THR:H	2.14	0.50
1:A:660:HIS:CD2	1:A:668:ARG:NH2	2.80	0.50
1:A:415:LYS:HB3	1:A:434:SER:HB2	1.94	0.50
1:A:438:ILE:HG21	1:A:529:LEU:HD21	1.93	0.50
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.93	0.50
1:A:652:THR:HG23	6:A:824:HOH:O	2.11	0.50
1:A:406:LEU:O	1:A:445:GLN:HA	2.12	0.50
2:B:439:ASN:HD21	2:B:453:ASN:HD21	1.60	0.50
2:B:440:PRO:HA	2:B:483:VAL:CG1	2.41	0.50
1:A:559:GLU:HB2	1:A:569:ARG:HD2	1.92	0.50
1:A:6:GLU:O	1:A:10:GLN:HG3	2.12	0.50
1:A:56:TYR:OH	1:A:109:GLU:OE2	2.29	0.50
3:C:33:TYR:CZ	3:C:59:MET:HG3	2.46	0.50
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.93	0.50
2:B:803:PHE:HE2	2:B:825:LEU:HD12	1.77	0.50
2:B:1021:MET:H	2:B:1055:ILE:CG1	2.17	0.50
1:A:58:PRO:O	1:A:59:VAL:CB	2.60	0.50
1:A:692:ALA:O	1:A:696:LEU:CB	2.58	0.50
2:B:671:ASP:OD2	2:B:675:LYS:HE3	2.11	0.50
2:B:548:THR:OG1	2:B:554:HIS:HB2	2.10	0.50
2:B:582:GLU:HG3	3:C:124:LYS:NZ	2.26	0.50
1:A:695:ILE:C	1:A:697:HIS:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:TRP:NE1	1:A:92:ASN:HB2	2.26	0.50
1:A:393:ASP:O	1:A:395:HIS:N	2.44	0.50
2:B:684:GLN:HA	2:B:684:GLN:OE1	2.12	0.49
1:A:687:ALA:N	1:A:688:PRO:HD2	2.27	0.49
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.93	0.49
1:A:227:ASN:HD21	1:A:278:THR:HB	1.76	0.49
2:B:1053:TYR:CD1	2:B:1055:ILE:HD12	2.47	0.49
1:A:166:LEU:C	1:A:167:ILE:HD12	2.33	0.49
1:A:290:ILE:HG21	1:A:355:THR:CG2	2.42	0.49
2:B:956:GLY:HA2	2:B:967:GLN:CG	2.42	0.49
2:B:415:LYS:NZ	6:B:156:HOH:O	2.45	0.49
2:B:830:THR:HG22	2:B:832:ASN:H	1.77	0.49
2:B:480:ARG:HG3	2:B:481:PRO:HD2	1.94	0.49
2:B:943:HIS:CD2	2:B:973:LEU:HD12	2.48	0.49
2:B:910:LYS:HD3	2:B:922:GLU:OE2	2.11	0.49
3:C:44:LEU:HD13	3:C:65:ILE:HD11	1.94	0.49
2:B:441:PHE:O	2:B:453:ASN:HB3	2.13	0.49
2:B:493:PRO:HG2	2:B:496:TYR:CE2	2.48	0.49
1:A:700:PHE:O	1:A:702:MET:N	2.45	0.49
3:C:31:GLN:HG2	3:C:32:GLN:N	2.28	0.49
2:B:750:ARG:O	2:B:805:SER:HA	2.12	0.49
1:A:638:ASP:C	1:A:722:VAL:CG2	2.81	0.49
1:A:183:ILE:HD12	2:B:605:MET:CE	2.43	0.49
2:B:360:LEU:CD2	2:B:972:GLN:HG2	2.42	0.48
2:B:911:SER:OG	2:B:926:ALA:HB1	2.12	0.48
1:A:183:ILE:O	2:B:565:PRO:O	2.32	0.48
2:B:1022:THR:O	2:B:1023:ASP:HB2	2.13	0.48
1:A:391:THR:HG22	1:A:399:LYS:HE3	1.95	0.48
3:C:81:LYS:O	3:C:85:PHE:HD1	1.96	0.48
2:B:446:ASP:O	2:B:448:ARG:N	2.46	0.48
1:A:153:MET:HE3	1:A:157:LEU:CD1	2.44	0.48
1:A:393:ASP:C	1:A:395:HIS:H	2.17	0.48
1:A:191:GLY:HA3	1:A:263:SER:CB	2.44	0.48
2:B:936:VAL:HG13	2:B:937:TYR:N	2.29	0.48
1:A:255:PRO:HG2	1:A:258:LYS:CG	2.39	0.48
2:B:423:VAL:CG2	2:B:488:ILE:HD11	2.43	0.48
1:A:312:SER:H	1:A:315:ASP:HB2	1.78	0.48
1:A:45:LEU:O	1:A:453:PRO:HA	2.13	0.48
1:A:194:ASP:OD1	1:A:195:LEU:N	2.46	0.48
3:C:7:ILE:N	3:C:7:ILE:HD12	2.28	0.48
2:B:1053:TYR:HD1	2:B:1055:ILE:HB	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:478:ALA:O	1:A:479:ILE:HD13	2.14	0.48
1:A:443:THR:HG23	1:A:446:TRP:CE2	2.49	0.48
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.96	0.48
1:A:296:GLN:O	1:A:297:GLY:O	2.31	0.48
2:B:958:LEU:H	2:B:958:LEU:HD22	1.78	0.48
1:A:297:GLY:N	1:A:300:MET:HE2	2.29	0.48
1:A:606:HIS:O	1:A:610:GLN:HG2	2.13	0.48
3:C:19:SER:O	3:C:20:MET:HG3	2.13	0.48
2:B:550:ASP:OD2	2:B:554:HIS:CE1	2.67	0.47
2:B:446:ASP:C	2:B:448:ARG:N	2.66	0.47
3:C:31:GLN:CG	3:C:32:GLN:N	2.77	0.47
2:B:591:SER:HB3	2:B:594:LEU:HD12	1.96	0.47
2:B:666:MET:HB3	2:B:856:MET:CE	2.44	0.47
2:B:751:ILE:O	2:B:772:ASP:OD2	2.31	0.47
1:A:295:THR:C	1:A:300:MET:HG3	2.34	0.47
1:A:183:ILE:HD11	2:B:567:MET:HB2	1.95	0.47
2:B:716:TYR:CZ	2:B:731:LEU:HD13	2.49	0.47
2:B:960:ILE:HG22	6:B:122:HOH:O	2.14	0.47
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.50	0.47
2:B:498:LEU:H	2:B:498:LEU:CD1	2.27	0.47
2:B:1066:LEU:C	2:B:1068:ASN:N	2.66	0.47
1:A:180:CYS:O	1:A:181:GLU:CG	2.62	0.47
1:A:541:ASP:CB	1:A:544:ARG:HD2	2.43	0.47
1:A:541:ASP:HB3	1:A:544:ARG:HB2	1.97	0.47
2:B:405:LEU:HD22	2:B:843:ILE:HD13	1.96	0.47
2:B:992:LEU:CB	2:B:1052:LEU:HD12	2.45	0.47
2:B:734:GLU:HA	2:B:1048:PHE:HE2	1.79	0.47
2:B:492:ALA:HB1	2:B:496:TYR:HB2	1.95	0.47
3:C:149:MET:HG2	3:C:150:VAL:N	2.30	0.47
1:A:696:LEU:CD1	1:A:703:PRO:HG2	2.44	0.47
1:A:27:SER:CB	1:A:509:GLN:HE22	2.27	0.47
2:B:904:LEU:CD2	2:B:1080:TYR:HA	2.44	0.47
1:A:551:ILE:O	1:A:555:GLN:HG3	2.14	0.47
1:A:609:ARG:HG3	6:A:823:HOH:O	2.15	0.47
2:B:1014:TYR:OH	2:B:1058:GLU:N	2.46	0.47
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.49	0.47
1:A:316:ILE:HD11	1:A:324:VAL:HG11	1.97	0.47
1:A:652:THR:C	6:A:767:HOH:O	2.53	0.47
2:B:438:ILE:O	2:B:438:ILE:HG23	2.13	0.47
2:B:1049:PHE:N	6:B:46:HOH:O	2.47	0.47
2:B:441:PHE:HB2	2:B:453:ASN:ND2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:GLN:HE21	2:B:746:GLU:HG2	1.80	0.46
2:B:465:PHE:CE1	2:B:480:ARG:HG2	2.50	0.46
1:A:667:TRP:HB3	1:A:681:PHE:CZ	2.50	0.46
2:B:845:GLY:HA2	2:B:938:LEU:HD21	1.96	0.46
1:A:373:MET:CE	1:A:598:ASP:HB3	2.45	0.46
1:A:302:VAL:HG22	1:A:303:GLY:N	2.29	0.46
3:C:33:TYR:HB3	3:C:74:LEU:HD22	1.97	0.46
3:C:80:PRO:HB2	3:C:83:LEU:HD12	1.96	0.46
2:B:515:ASN:O	2:B:519:THR:HG23	2.16	0.46
3:C:20:MET:HG2	3:C:30:LEU:HD11	1.98	0.46
2:B:936:VAL:HG22	2:B:940:LEU:HD23	1.96	0.46
1:A:71:ASN:HB2	1:A:72:PRO:CD	2.45	0.46
2:B:1019:GLN:CB	2:B:1020:PRO:CD	2.82	0.46
1:A:76:VAL:HG12	1:A:77:ASP:N	2.30	0.46
1:A:418:GLY:HA3	1:A:438:ILE:O	2.16	0.46
1:A:700:PHE:O	1:A:701:PRO:C	2.51	0.46
1:A:153:MET:CE	1:A:154:SER:HA	2.46	0.46
2:B:692:LEU:HD23	2:B:719:TYR:CD1	2.50	0.46
1:A:3:THR:HG23	1:A:5:LEU:H	1.81	0.46
3:C:36:GLN:O	3:C:39:GLN:HB2	2.15	0.46
1:A:248:GLN:HE22	2:B:559:GLN:HE22	1.64	0.46
1:A:168:THR:HG21	1:A:247:LEU:HD21	1.97	0.46
2:B:773:LEU:HA	2:B:773:LEU:HD12	1.70	0.46
2:B:1054:VAL:C	2:B:1056:ALA:N	2.69	0.46
1:A:716:ARG:HG3	1:A:717:PHE:N	2.31	0.46
2:B:1038:PHE:CA	6:B:40:HOH:O	2.63	0.46
1:A:666:GLN:O	1:A:669:LYS:N	2.48	0.46
2:B:410:LEU:HD12	2:B:410:LEU:N	2.31	0.46
1:A:248:GLN:NE2	2:B:559:GLN:HE22	2.14	0.46
2:B:614:SER:HB2	2:B:640:GLN:NE2	2.28	0.46
2:B:592:LYS:O	2:B:596:GLN:HG3	2.16	0.46
1:A:417:SER:O	1:A:437:GLU:HA	2.16	0.46
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.98	0.46
1:A:672:TYR:HA	1:A:675:MET:HG3	1.97	0.46
3:C:63:TYR:C	3:C:63:TYR:CD1	2.89	0.45
1:A:404:GLY:O	1:A:448:ILE:N	2.48	0.45
1:A:168:THR:HG21	1:A:247:LEU:CD2	2.46	0.45
2:B:747:ALA:HB2	2:B:809:TYR:CB	2.46	0.45
1:A:401:GLY:HA3	1:A:451:LEU:CD1	2.46	0.45
2:B:913:GLN:NE2	2:B:916:THR:CG2	2.80	0.45
2:B:504:PRO:HG2	2:B:542:THR:CA	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:92:HIS:CD2	3:C:92:HIS:C	2.90	0.45
1:A:297:GLY:H	1:A:300:MET:CG	2.30	0.45
2:B:913:GLN:NE2	2:B:916:THR:CB	2.80	0.45
2:B:871:VAL:HG12	2:B:1087:ILE:HD12	1.99	0.45
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.43	0.45
3:C:81:LYS:CD	3:C:81:LYS:H	2.18	0.45
2:B:993:MET:CE	2:B:1065:PHE:HA	2.46	0.45
1:A:76:VAL:HG21	1:A:110:LEU:CD1	2.47	0.45
1:A:508:THR:HG22	1:A:511:GLN:NE2	2.31	0.45
1:A:3:THR:CG2	1:A:6:GLU:H	2.11	0.45
2:B:1053:TYR:CD1	2:B:1055:ILE:HB	2.51	0.45
2:B:831:LEU:HD22	2:B:835:PHE:HE1	1.78	0.45
2:B:433:SER:OG	2:B:457:ARG:HD3	2.16	0.45
1:A:192:THR:O	1:A:192:THR:HG23	2.16	0.45
1:A:48:ARG:NH1	1:A:51:LEU:HD11	2.31	0.45
1:A:447:LYS:C	1:A:448:ILE:HD12	2.37	0.45
1:A:419:ALA:HA	1:A:458:ALA:O	2.17	0.45
2:B:852:VAL:O	2:B:855:SER:HB2	2.17	0.45
3:C:148:ILE:CG2	3:C:149:MET:H	2.23	0.45
2:B:583:ASN:N	6:B:22:HOH:O	2.28	0.45
3:C:12:ASP:OD2	3:C:12:ASP:N	2.47	0.45
2:B:1062:LYS:C	2:B:1064:ASN:H	2.20	0.45
2:B:879:ARG:NH1	2:B:1092:ASN:HB3	2.32	0.45
2:B:576:VAL:CG1	2:B:577:PHE:N	2.80	0.45
2:B:752:ARG:NH2	4:D:505:GLU:OE1	2.50	0.45
2:B:446:ASP:C	2:B:448:ARG:H	2.21	0.45
1:A:626:TYR:CD2	1:A:632:PRO:HG3	2.52	0.45
1:A:548:ARG:O	1:A:552:ARG:HG3	2.16	0.45
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.99	0.44
2:B:1059:SER:H	2:B:1060:PRO:CD	2.30	0.44
2:B:395:GLN:OE1	2:B:829:SER:HB3	2.17	0.44
2:B:959:ASN:O	2:B:961:SER:N	2.50	0.44
2:B:666:MET:HE3	2:B:927:MET:SD	2.57	0.44
2:B:768:VAL:HG22	2:B:774:LEU:HD22	1.99	0.44
2:B:431:CYS:O	2:B:435:ARG:HA	2.17	0.44
2:B:550:ASP:OD1	2:B:551:SER:N	2.51	0.44
1:A:296:GLN:HG2	1:A:296:GLN:O	2.18	0.44
1:A:4:TYR:O	1:A:8:ILE:HG12	2.16	0.44
1:A:476:ARG:H	1:A:503:TRP:H	1.65	0.44
2:B:956:GLY:CA	2:B:967:GLN:HG2	2.46	0.44
1:A:577:TYR:HB3	1:A:578:PRO:HD3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:ASN:C	6:A:808:HOH:O	2.55	0.44
2:B:530:LEU:HD23	2:B:599:LEU:HD12	1.98	0.44
1:A:266:VAL:HA	1:A:269:SER:OG	2.16	0.44
1:A:107:PRO:HG2	1:A:110:LEU:CD1	2.48	0.44
1:A:183:ILE:HG23	1:A:184:SER:N	2.32	0.44
3:C:3:LEU:N	3:C:3:LEU:HD23	2.32	0.44
1:A:452:SER:C	1:A:454:THR:H	2.20	0.44
2:B:445:LEU:C	2:B:447:GLN:H	2.20	0.44
2:B:564:GLN:HB2	2:B:565:PRO:HD2	2.00	0.44
1:A:293:PRO:HA	1:A:355:THR:O	2.18	0.44
2:B:620:LEU:HD22	2:B:634:MET:HE3	1.99	0.44
1:A:535:GLU:HG3	1:A:604:ARG:NH1	2.33	0.44
2:B:807:LEU:O	2:B:818:ILE:HA	2.17	0.44
1:A:147:LEU:O	1:A:151:MET:HG3	2.17	0.44
1:A:668:ARG:NH2	1:A:707:ASP:OD1	2.41	0.44
1:A:41:LEU:HD23	1:A:612:LEU:HB2	1.98	0.44
1:A:153:MET:HE3	1:A:157:LEU:HD11	2.00	0.44
2:B:905:ALA:HB1	2:B:942:THR:HG22	2.00	0.44
2:B:538:GLY:HA2	2:B:812:SER:O	2.17	0.44
2:B:367:PRO:HA	2:B:368:PRO:HD3	1.90	0.44
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.99	0.44
1:A:358:LEU:O	1:A:358:LEU:HD12	2.17	0.44
1:A:656:ILE:HD11	1:A:695:ILE:HG23	1.99	0.44
2:B:449:ARG:HA	2:B:459:ASN:O	2.18	0.44
1:A:56:TYR:C	1:A:56:TYR:CD1	2.91	0.44
2:B:995:TRP:CZ2	2:B:1058:GLU:OE1	2.71	0.44
1:A:345:ILE:HG21	1:A:363:CYS:HB3	2.00	0.44
1:A:562:LYS:HB3	1:A:562:LYS:HZ2	1.83	0.44
2:B:634:MET:HE2	2:B:687:VAL:CG2	2.47	0.44
1:A:77:ASP:OD2	1:A:80:ALA:HB3	2.18	0.44
1:A:757:LYS:O	1:A:761:VAL:HG22	2.18	0.44
1:A:675:MET:C	1:A:677:GLU:N	2.70	0.43
2:B:1070:ILE:HD12	2:B:1070:ILE:C	2.37	0.43
2:B:576:VAL:CG1	2:B:622:ALA:HB2	2.44	0.43
1:A:559:GLU:O	1:A:560:TYR:HB3	2.17	0.43
2:B:666:MET:HB3	2:B:856:MET:HE1	1.99	0.43
2:B:617:GLY:HA3	2:B:646:VAL:O	2.18	0.43
3:C:74:LEU:HG	3:C:75:CYS:N	2.33	0.43
2:B:1019:GLN:CG	2:B:1020:PRO:HD3	2.48	0.43
2:B:716:TYR:CE2	2:B:731:LEU:HD13	2.53	0.43
3:C:114:GLU:C	3:C:116:ASP:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:PHE:CZ	3:C:74:LEU:HD13	2.53	0.43
1:A:686:GLN:HG3	1:A:689:VAL:HB	2.00	0.43
1:A:354:GLN:N	6:A:818:HOH:O	2.48	0.43
1:A:12:GLU:CD	1:A:18:ARG:HD2	2.39	0.43
1:A:123:ARG:N	6:A:775:HOH:O	2.50	0.43
3:C:62:HIS:O	3:C:88:LEU:HD11	2.19	0.43
1:A:63:ARG:O	1:A:64:THR:C	2.56	0.43
2:B:540:THR:HG22	2:B:589:ASN:OD1	2.18	0.43
2:B:1085:LEU:HD12	2:B:1085:LEU:HA	1.89	0.43
2:B:766:PHE:CD1	2:B:766:PHE:C	2.92	0.43
4:D:507:ASN:HA	4:D:507:ASN:HD22	1.66	0.43
2:B:915:GLY:HA3	2:B:1076:SER:OG	2.18	0.43
2:B:421:PRO:O	2:B:488:ILE:HG13	2.19	0.43
3:C:153:ILE:HG23	3:C:154:GLU:N	2.33	0.43
1:A:259:ARG:HB2	1:A:304:ASP:HA	2.01	0.43
1:A:448:ILE:HD12	1:A:448:ILE:N	2.34	0.43
2:B:766:PHE:HB3	2:B:776:LEU:CD2	2.49	0.43
2:B:373:HIS:CD2	2:B:375:ASP:H	2.37	0.43
2:B:424:THR:HG22	2:B:491:MET:HG3	1.99	0.43
2:B:435:ARG:HD2	2:B:435:ARG:HA	1.80	0.43
2:B:1062:LYS:O	2:B:1064:ASN:N	2.46	0.43
2:B:1074:THR:HG23	2:B:1075:GLU:N	2.34	0.43
2:B:686:ALA:HB2	2:B:777:PRO:HB2	2.01	0.43
1:A:534:ALA:C	1:A:536:THR:H	2.21	0.43
2:B:692:LEU:HD12	2:B:692:LEU:N	2.33	0.43
1:A:234:GLN:HG3	1:A:235:LYS:HG3	2.00	0.43
2:B:386:PHE:CE1	2:B:409:LEU:HD13	2.54	0.43
2:B:606:PHE:HB3	2:B:609:THR:OG1	2.19	0.43
2:B:981:ASP:OD1	2:B:999:ASN:ND2	2.49	0.42
2:B:958:LEU:O	2:B:958:LEU:HD23	2.18	0.42
1:A:386:PHE:O	1:A:389:VAL:HB	2.18	0.42
2:B:654:GLU:OE2	2:B:919:ARG:HB3	2.19	0.42
1:A:3:THR:CG2	1:A:5:LEU:H	2.32	0.42
2:B:1055:ILE:HG21	2:B:1062:LYS:HD3	2.01	0.42
3:C:4:LEU:HD23	3:C:74:LEU:CD2	2.49	0.42
3:C:71:TYR:CE2	3:C:92:HIS:HA	2.54	0.42
2:B:381:CYS:HB2	2:B:822:THR:O	2.19	0.42
2:B:730:LYS:HD3	6:B:142:HOH:O	2.19	0.42
2:B:750:ARG:NH1	4:D:503:ASP:OD2	2.53	0.42
1:A:664:ILE:O	1:A:664:ILE:HG22	2.19	0.42
3:C:148:ILE:CG2	3:C:149:MET:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:56:ALA:HB2	3:C:153:ILE:CG2	2.48	0.42
1:A:289:PHE:CD1	1:A:289:PHE:N	2.87	0.42
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.82	0.42
4:D:505:GLU:CD	4:D:505:GLU:O	2.58	0.42
1:A:588:SER:OG	1:A:595:ASN:ND2	2.52	0.42
2:B:872:ILE:HD12	2:B:1090:GLN:CB	2.41	0.42
3:C:127:ILE:HG22	3:C:127:ILE:O	2.20	0.42
2:B:759:ILE:HD12	2:B:759:ILE:N	2.35	0.42
1:A:531:ILE:N	1:A:531:ILE:HD12	2.35	0.42
2:B:348:LEU:O	2:B:348:LEU:HG	2.20	0.42
1:A:554:CYS:HA	1:A:570:PHE:HZ	1.81	0.42
1:A:138:CYS:SG	1:A:170:GLY:HA2	2.59	0.42
1:A:66:CYS:O	1:A:409:LYS:NZ	2.48	0.42
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.55	0.42
2:B:1055:ILE:O	2:B:1060:PRO:HG3	2.19	0.42
1:A:48:ARG:NH2	1:A:51:LEU:HD21	2.35	0.42
2:B:1019:GLN:HE21	2:B:1062:LYS:NZ	2.17	0.42
1:A:47:GLU:HG3	1:A:453:PRO:HB3	2.01	0.42
2:B:1087:ILE:O	2:B:1091:VAL:HG23	2.19	0.42
3:C:4:LEU:HD23	3:C:74:LEU:HD22	2.02	0.42
1:A:282:THR:HG22	6:A:769:HOH:O	2.19	0.42
1:A:602:TYR:O	1:A:605:HIS:HB3	2.20	0.42
1:A:12:GLU:O	1:A:16:GLY:HA2	2.19	0.41
1:A:63:ARG:NH1	1:A:88:CYS:HB2	2.34	0.41
1:A:285:ARG:NE	1:A:346:ASP:OD2	2.52	0.41
2:B:539:ASN:ND2	2:B:813:LYS:HA	2.35	0.41
2:B:871:VAL:CG2	2:B:903:VAL:HG21	2.50	0.41
1:A:253:PRO:HB3	3:C:128:ASP:HB2	2.02	0.41
2:B:483:VAL:HG12	2:B:483:VAL:O	2.20	0.41
2:B:1011:VAL:HG12	2:B:1012:GLN:N	2.35	0.41
1:A:398:PHE:HB3	1:A:400:MET:CG	2.50	0.41
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.85	0.41
2:B:585:LEU:HD23	2:B:585:LEU:HA	1.95	0.41
4:D:503:ASP:OD1	4:D:506:MET:HB2	2.20	0.41
1:A:637:LEU:HD22	1:A:722:VAL:HA	2.03	0.41
3:C:39:GLN:O	3:C:43:LYS:HG2	2.20	0.41
2:B:956:GLY:CA	6:B:102:HOH:O	2.69	0.41
3:C:54:LEU:HD13	3:C:153:ILE:HG13	2.02	0.41
1:A:191:GLY:HA3	1:A:263:SER:OG	2.20	0.41
1:A:546:LEU:HA	1:A:546:LEU:HD12	1.92	0.41
2:B:872:ILE:HD13	2:B:1087:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:O	1:A:152:GLN:HG3	2.20	0.41
1:A:164:VAL:O	1:A:230:LEU:HA	2.21	0.41
1:A:25:PRO:HD3	1:A:34:MET:HE1	2.03	0.41
1:A:31:ALA:O	1:A:34:MET:HB2	2.20	0.41
2:B:686:ALA:CB	2:B:778:ASN:HB2	2.51	0.41
2:B:808:LEU:HD23	4:D:504:ILE:CG2	2.47	0.41
3:C:50:THR:C	3:C:51:ARG:HG2	2.41	0.41
3:C:127:ILE:O	3:C:128:ASP:HB2	2.20	0.41
1:A:171:ARG:HB3	1:A:252:TRP:CD1	2.56	0.41
2:B:1055:ILE:O	2:B:1057:ASP:N	2.53	0.41
1:A:519:GLN:HE22	1:A:576:LEU:HD12	1.85	0.41
1:A:622:ILE:HG22	1:A:623:LEU:N	2.36	0.41
1:A:280:PRO:HA	1:A:341:THR:CG2	2.51	0.41
1:A:19:PHE:HA	1:A:39:ALA:O	2.21	0.41
1:A:180:CYS:C	1:A:181:GLU:CG	2.89	0.41
2:B:992:LEU:O	2:B:1052:LEU:HA	2.20	0.40
2:B:1064:ASN:CA	6:B:82:HOH:O	2.58	0.40
2:B:1047:PRO:HD2	6:B:128:HOH:O	2.22	0.40
2:B:618:PRO:HD3	2:B:646:VAL:O	2.20	0.40
1:A:56:TYR:O	1:A:56:TYR:CD1	2.74	0.40
1:A:428:SER:O	1:A:429:LYS:HD3	2.20	0.40
1:A:510:ILE:H	1:A:510:ILE:CD1	2.19	0.40
2:B:627:MET:O	2:B:628:SER:C	2.59	0.40
2:B:602:LEU:HB2	2:B:603:PRO:HD3	2.01	0.40
1:A:288:MET:C	6:A:795:HOH:O	2.60	0.40
2:B:444:PHE:CE1	2:B:450:TRP:HB3	2.56	0.40
2:B:957:ALA:C	2:B:959:ASN:N	2.74	0.40
1:A:624:TYR:CE2	1:A:634:PRO:HG3	2.56	0.40
1:A:674:ASP:O	1:A:676:PRO:HD3	2.21	0.40
1:A:111:LEU:HA	1:A:112:PRO:HD3	1.92	0.40
1:A:139:MET:HB2	6:A:796:HOH:O	2.21	0.40
2:B:964:THR:HG22	2:B:965:ILE:N	2.36	0.40
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.36	0.40
3:C:3:LEU:CD1	3:C:123:LYS:HZ2	2.32	0.40
1:A:536:THR:O	1:A:537:GLU:C	2.59	0.40
1:A:524:ILE:HA	1:A:524:ILE:HD13	1.88	0.40
1:A:675:MET:C	1:A:677:GLU:H	2.24	0.40
1:A:481:PHE:HE1	1:A:499:ILE:HD12	1.86	0.40
2:B:1020:PRO:HG3	2:B:1062:LYS:NZ	2.36	0.40
3:C:114:GLU:C	3:C:116:ASP:H	2.20	0.40
3:C:21:GLN:NE2	3:C:123:LYS:NZ	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:LEU:HD22	1:A:244:LEU:HG	2.03	0.40
2:B:620:LEU:HB3	2:B:676:LEU:HD21	2.03	0.40
3:C:87:TYR:CZ	3:C:91:LEU:HD11	2.56	0.40
2:B:486:ALA:O	2:B:821:HIS:HA	2.21	0.40
1:A:78:TYR:N	1:A:78:TYR:CD1	2.89	0.40
3:C:66:GLU:HA	3:C:66:GLU:OE1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	701/764 (92%)	620 (88%)	58 (8%)	23 (3%)	5 11
2	B	723/748 (97%)	648 (90%)	59 (8%)	16 (2%)	8 22
3	C	131/157 (83%)	106 (81%)	21 (16%)	4 (3%)	5 12
4	D	5/10 (50%)	2 (40%)	3 (60%)	0	100 100
All	All	1560/1679 (93%)	1376 (88%)	141 (9%)	43 (3%)	6 15

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	A	181	GLU
1	A	182	GLY
1	A	196	SER
1	A	653	PHE
2	B	771	THR
2	B	1019	GLN
2	B	1055	ILE
3	C	4	LEU

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Mol	Chain	Res	Type
1	A	48	ARG
1	A	59	VAL
1	A	297	GLY
1	A	394	MET
1	A	508	THR
1	A	671	GLY
1	A	696	LEU
2	B	447	GLN
2	B	769	ARG
2	B	960	ILE
2	B	961	SER
3	C	128	ASP
1	A	105	ASN
1	A	123	ARG
1	A	509	GLN
1	A	673	GLN
2	B	1063	ALA
1	A	324	VAL
1	A	722	VAL
2	B	660	SER
2	B	1056	ALA
1	A	476	ARG
1	A	700	PHE
2	B	446	ASP
2	B	464	GLU
2	B	1059	SER
3	C	155	GLU
1	A	116	SER
2	B	655	PRO
2	B	1070	ILE
3	C	2	VAL
1	A	747	VAL
2	B	965	ILE
1	A	298	PRO

5.3.2 Protein sidechains (i)

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	621/666 (93%)	588 (95%)	33 (5%)	28 57
2	B	662/678 (98%)	620 (94%)	42 (6%)	22 48
3	C	120/138 (87%)	113 (94%)	7 (6%)	25 52
4	D	7/10 (70%)	4 (57%)	3 (43%)	0 0
All	All	1410/1492 (94%)	1325 (94%)	85 (6%)	24 50

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	28	ARG
1	A	41	LEU
1	A	105	ASN
1	A	153	MET
1	A	192	THR
1	A	236	ILE
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	311	ARG
1	A	320	ASN
1	A	362	CYS
1	A	394	MET
1	A	400	MET
1	A	436	ASN
1	A	451	LEU
1	A	495	ARG
1	A	499	ILE
1	A	508	THR
1	A	528	ARG
1	A	544	ARG
1	A	569	ARG
1	A	570	PHE
1	A	581	MET
1	A	613	THR
1	A	636	LEU
1	A	637	LEU
1	A	649	LEU
1	A	679	GLU
1	A	709	GLU
1	A	723	ASN
1	A	754	ASP

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Mol	Chain	Res	Type
2	B	359	MET
2	B	382	ASN
2	B	386	PHE
2	B	387	ARG
2	B	411	LEU
2	B	412	HIS
2	B	431	CYS
2	B	522	LEU
2	B	566	GLN
2	B	570	VAL
2	B	589	ASN
2	B	595	VAL
2	B	607	THR
2	B	610	LEU
2	B	614	SER
2	B	641	LEU
2	B	650	LYS
2	B	652	ARG
2	B	679	ASP
2	B	712	SER
2	B	787	VAL
2	B	789	MET
2	B	797	ASP
2	B	798	THR
2	B	807	LEU
2	B	816	ARG
2	B	831	LEU
2	B	857	THR
2	B	932	ASN
2	B	935	LEU
2	B	955	GLU
2	B	958	LEU
2	B	961	SER
2	B	963	ARG
2	B	975	VAL
2	B	1001	THR
2	B	1002	GLN
2	B	1048	PHE
2	B	1052	LEU
2	B	1057	ASP
2	B	1074	THR
2	B	1085	LEU

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Mol	Chain	Res	Type
3	C	3	LEU
3	C	31	GLN
3	C	39	GLN
3	C	63	TYR
3	C	81	LYS
3	C	101	LYS
3	C	121	LYS
4	D	506	MET
4	D	507	ASN
4	D	508	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	22	ASN
1	A	105	ASN
1	A	227	ASN
1	A	239	ASN
1	A	248	GLN
1	A	320	ASN
1	A	397	GLN
1	A	436	ASN
1	A	486	GLN
1	A	509	GLN
1	A	511	GLN
1	A	512	ASN
1	A	579	GLN
1	A	583	HIS
1	A	595	ASN
1	A	620	GLN
1	A	723	ASN
2	B	355	GLN
2	B	373	HIS
2	B	382	ASN
2	B	395	GLN
2	B	412	HIS
2	B	439	ASN
2	B	502	GLN
2	B	566	GLN
2	B	583	ASN
2	B	640	GLN

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Mol	Chain	Res	Type
2	B	732	GLN
2	B	765	ASN
2	B	778	ASN
2	B	788	GLN
2	B	913	GLN
2	B	932	ASN
2	B	1003	ASN
2	B	1019	GLN
2	B	1092	ASN
3	C	21	GLN
3	C	34	GLN
3	C	39	GLN
3	C	92	HIS
3	C	152	ASN
4	D	507	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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, 95^{th} 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	711/764 (93%)	0.01	36 (5%) 32 30	12, 36, 80, 119	0
2	B	731/748 (97%)	-0.16	23 (3%) 52 52	11, 30, 73, 102	0
3	C	137/157 (87%)	0.72	20 (14%) 3 2	27, 61, 92, 104	0
4	D	7/10 (70%)	2.10	3 (42%) 0 0	74, 87, 96, 103	0
All	All	1586/1679 (94%)	-0.00	82 (5%) 31 30	11, 35, 83, 119	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	1	MET	7.1
4	D	502	THR	6.2
1	A	672	TYR	5.5
2	B	1055	ILE	5.3
1	A	675	MET	4.7
4	D	508	ARG	4.5
3	C	132	ARG	4.5
1	A	676	PRO	4.4
1	A	678	TYR	4.4
3	C	57	GLY	4.3
2	B	346	GLU	4.3
2	B	772	ASP	4.2
3	C	98	GLN	4.0
1	A	674	ASP	4.0
3	C	23	ASP	3.9
1	A	670	SER	3.6
2	B	348	LEU	3.6
3	C	102	LYS	3.5
1	A	437	GLU	3.4
2	B	446	ASP	3.4
1	A	394	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	764	ALA	3.2
2	B	460	ASP	3.2
1	A	123	ARG	3.2
3	C	103	VAL	3.2
1	A	442	GLY	3.1
1	A	436	ASN	3.1
1	A	307	LYS	3.0
1	A	430	GLY	3.0
1	A	682	ARG	3.0
3	C	2	VAL	3.0
1	A	669	LYS	3.0
3	C	148	ILE	3.0
1	A	746	ASP	2.9
1	A	79	ARG	2.9
1	A	428	SER	2.9
1	A	474	GLY	2.9
1	A	427	ASN	2.9
1	A	677	GLU	2.8
1	A	431	PRO	2.8
1	A	64	THR	2.8
1	A	435	GLU	2.7
1	A	50	ASP	2.7
1	A	51	LEU	2.7
2	B	610	LEU	2.7
4	D	506	MET	2.7
1	A	671	GLY	2.7
2	B	448	ARG	2.7
1	A	747	VAL	2.7
1	A	548	ARG	2.6
2	B	657	HIS	2.6
2	B	888	PRO	2.6
2	B	418	VAL	2.6
2	B	959	ASN	2.5
3	C	127	ILE	2.4
3	C	101	LYS	2.4
1	A	49	PRO	2.4
3	C	100	GLY	2.4
2	B	1061	MET	2.4
2	B	654	GLU	2.4
3	C	153	ILE	2.3
2	B	463	GLU	2.3
3	C	154	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	667	TRP	2.3
1	A	593	PHE	2.2
2	B	658	ARG	2.2
1	A	673	GLN	2.2
2	B	593	GLU	2.2
2	B	445	LEU	2.2
2	B	1092	ASN	2.2
2	B	461	VAL	2.2
2	B	660	SER	2.2
3	C	99	HIS	2.1
1	A	443	THR	2.1
3	C	80	PRO	2.1
2	B	771	THR	2.1
2	B	462	PRO	2.1
3	C	30	LEU	2.1
3	C	152	ASN	2.1
1	A	508	THR	2.0
3	C	21	GLN	2.0
3	C	104	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	ZN	A	765	1/1	0.98	0.07	-1.49	49,49,49,49	0
5	ZN	B	1094	1/1	0.99	0.06	-2.14	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.