Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:41 AM GMT

PDB ID	:	2NUP
Title	:	Crystal Structure of the human Sec23a/24a heterodimer, complexed with the SNARE protein Sec22b
Authors	:	Mancias, J.D.; Goldberg, J.
Deposited on	:	2006-11-09
Resolution	:	2.80 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:

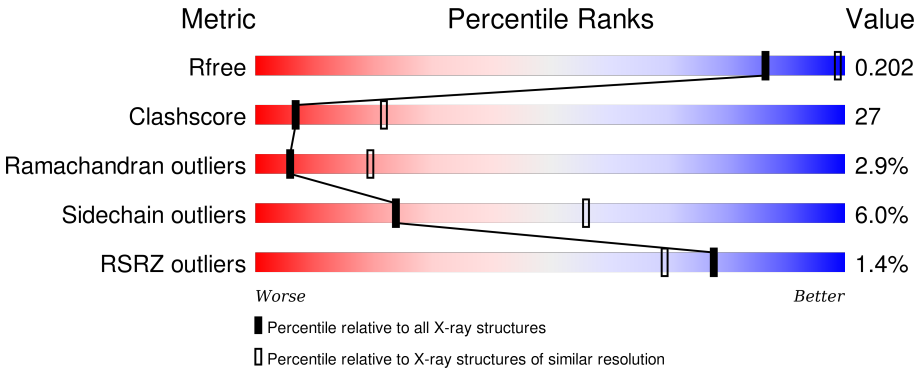
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	769	% 51% 35% 5% 9%
2	B	753	% 54% 37% 6% .
3	C	196	2% 36% 27% 7% 30%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12641 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	699	Total	C	N	O	S	0	0	0
			5536	3527	953	1017	39			

There are 4 discrepancies between the modelled and reference sequences:

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

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

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

- 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
			1103	708	182	205	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	SER	-	CLONING ARTIFACT	UNP O75396

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 5 is water.

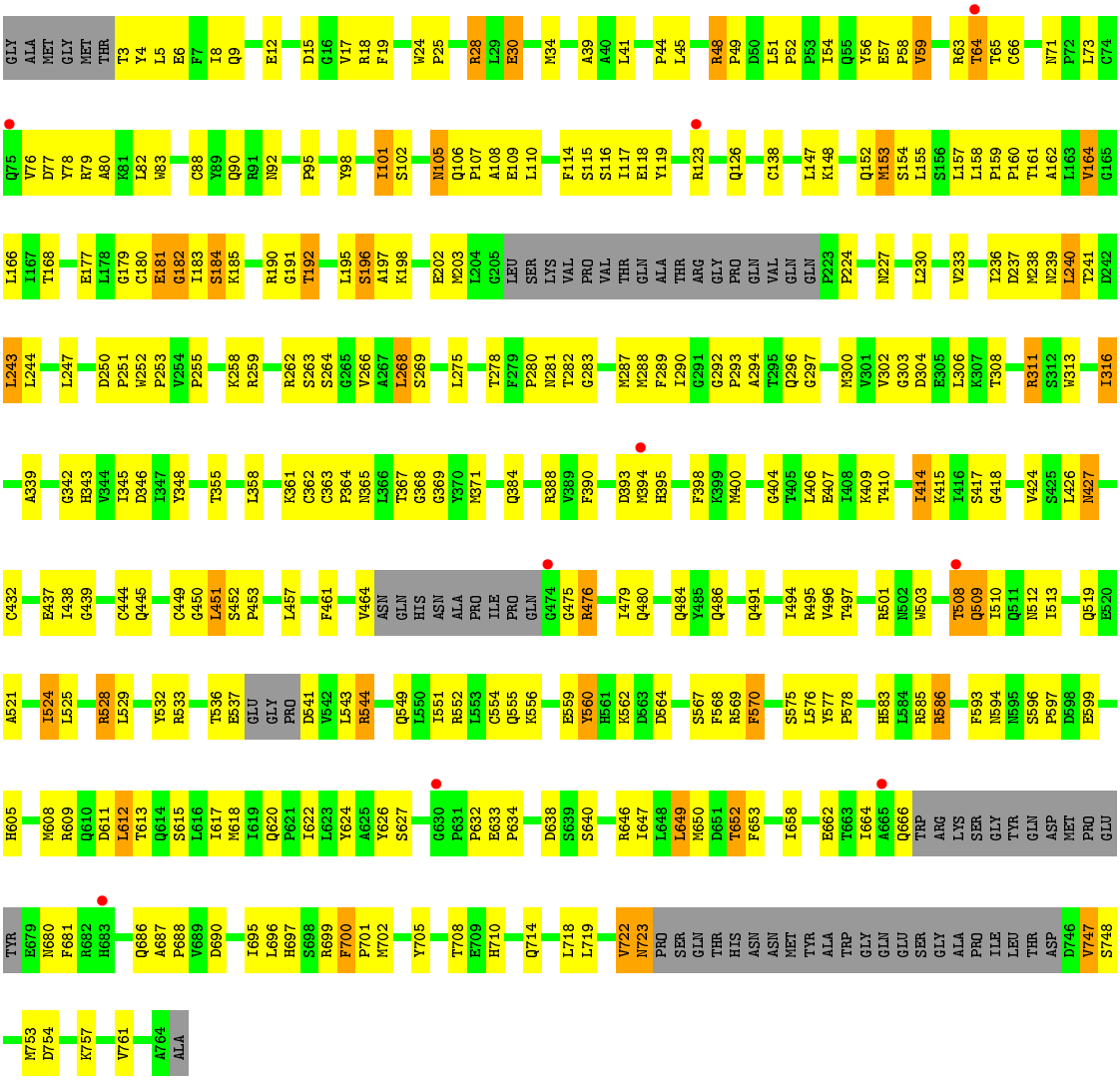
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	92	Total O 92 92	0	0
5	B	118	Total O 118 118	0	0
5	C	10	Total O 10 10	0	0

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.

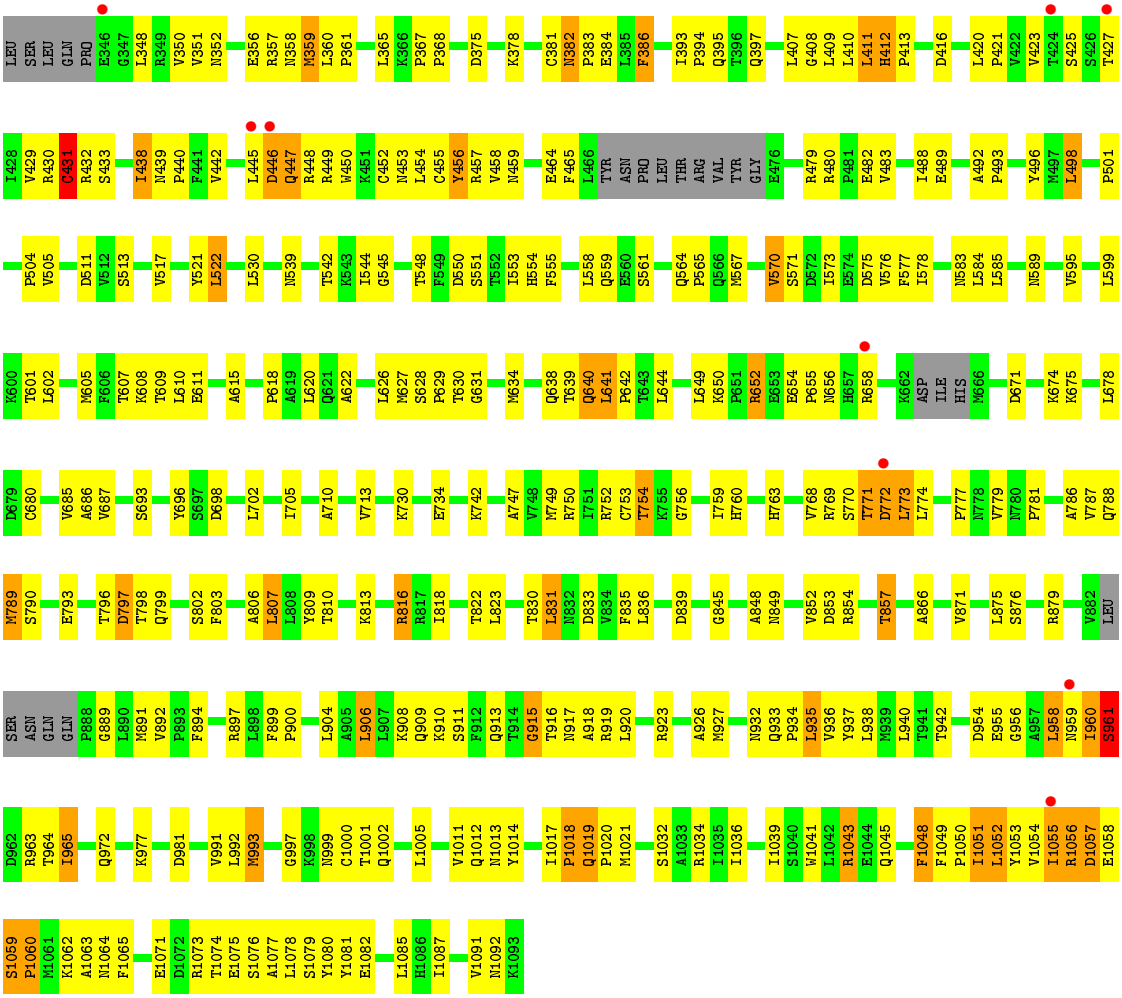
- Molecule 1: Protein transport protein Sec23A

Chain A:



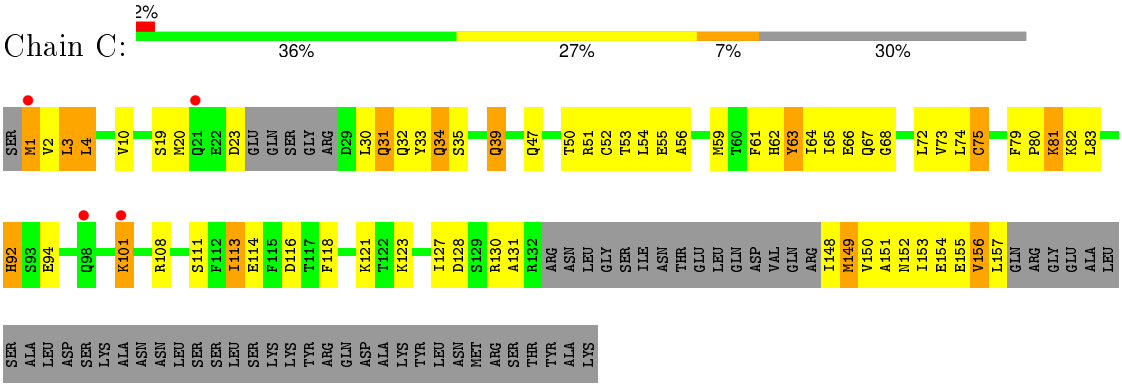
- Molecule 2: Protein transport protein Sec24A

Chain B:



• Molecule 3: Vesicle-trafficking protein SEC22b

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.20Å 97.40Å 129.62Å 90.00° 90.23° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 29.73 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.1 (20.00-2.80) 93.1 (29.73-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.202 , 0.275 0.205 , 0.202	Depositor DCC
R_{free} test set	2143 reflections (5.06%)	DCC
Wilson B-factor (Å^2)	38.7	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 59.5	EDS
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 44196 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12641	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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	0.39	0/5663	0.68	4/7667 (0.1%)
2	B	0.38	0/5904	0.65	0/8024
3	C	0.37	0/1122	0.62	0/1510
All	All	0.38	0/12689	0.66	4/17201 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	SER	N-CA-C	-8.06	89.24	111.00
1	A	652	THR	N-CA-C	-5.92	95.00	111.00
1	A	509	GLN	N-CA-C	5.06	124.67	111.00
1	A	182	GLY	N-CA-C	5.02	125.65	113.10

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	5536	0	5494	283	0
2	B	5780	0	5832	316	0
3	C	1103	0	1109	76	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	92	0	0	6	0
5	B	118	0	0	12	0
5	C	10	0	0	1	0
All	All	12641	0	12435	666	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 27.

All (666) 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:45:LEU:HA	1:A:495:ARG:HH12	1.07	1.09
3:C:2:VAL:HG12	3:C:3:LEU:H	1.19	1.08
1:A:48:ARG:HB2	1:A:49:PRO:CD	1.89	1.03
1:A:48:ARG:HB2	1:A:49:PRO:HD2	1.39	1.02
2:B:958:LEU:HB3	2:B:964:THR:HG23	1.39	1.02
1:A:15:ASP:OD1	1:A:116:SER:HB2	1.62	1.00
1:A:45:LEU:HA	1:A:495:ARG:NH1	1.76	1.00
1:A:3:THR:HG22	1:A:6:GLU:H	1.28	0.98
2:B:609:THR:HG22	2:B:611:GLU:H	1.30	0.96
2:B:879:ARG:NH1	2:B:1092:ASN:HD22	1.66	0.94
2:B:854:ARG:HH12	2:B:866:ALA:HB2	1.33	0.92
2:B:620:LEU:HD22	2:B:634:MET:HE3	1.46	0.92
1:A:432:CYS:HB2	1:A:444:CYS:SG	2.10	0.92
3:C:39:GLN:HE21	3:C:39:GLN:HA	1.32	0.91
1:A:290:ILE:HG21	1:A:355:THR:HG23	1.54	0.90
2:B:1019:GLN:HB3	2:B:1020:PRO:HD3	1.50	0.90
2:B:573:ILE:HG23	2:B:618:PRO:HG2	1.55	0.89
2:B:629:PRO:HG3	3:C:23:ASP:HB2	1.55	0.88
2:B:446:ASP:HB2	2:B:449:ARG:HB2	1.55	0.87
1:A:508:THR:HB	1:A:512:ASN:HD21	1.38	0.87
2:B:1021:MET:H	2:B:1055:ILE:HG12	1.40	0.87
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.56	0.86
1:A:722:VAL:HG22	1:A:723:ASN:H	1.41	0.85
3:C:2:VAL:HG12	3:C:3:LEU:N	1.92	0.84
2:B:759:ILE:HG23	2:B:787:VAL:HG13	1.58	0.84
3:C:2:VAL:CG1	3:C:3:LEU:H	1.91	0.83
2:B:992:LEU:O	2:B:1052:LEU:HD12	1.78	0.83
1:A:118:GLU:HB2	1:A:495:ARG:HD2	1.60	0.83
1:A:407:GLU:HG3	1:A:445:GLN:HG2	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:SER:HB3	1:A:646:ARG:HG3	1.62	0.82
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.61	0.82
2:B:760:HIS:NE2	2:B:788:GLN:HG2	1.94	0.81
2:B:1019:GLN:HB3	2:B:1020:PRO:CD	2.10	0.81
2:B:1073:ARG:HB3	2:B:1079:SER:HB3	1.62	0.80
1:A:238:MET:O	1:A:241:THR:HG22	1.81	0.80
2:B:955:GLU:N	2:B:955:GLU:OE1	2.15	0.80
2:B:879:ARG:HH12	2:B:1092:ASN:HD22	1.29	0.79
2:B:553:ILE:HB	2:B:570:VAL:HG13	1.65	0.79
2:B:382:ASN:ND2	2:B:384:GLU:H	1.81	0.78
3:C:113:ILE:O	3:C:116:ASP:HB2	1.83	0.78
1:A:583:HIS:CD2	1:A:620:GLN:HE21	2.01	0.78
2:B:423:VAL:HG23	2:B:488:ILE:HD11	1.65	0.77
2:B:1074:THR:HG23	2:B:1076:SER:H	1.47	0.77
1:A:181:GLU:O	1:A:183:ILE:N	2.16	0.77
2:B:576:VAL:HG11	2:B:622:ALA:HB2	1.66	0.77
1:A:313:TRP:O	1:A:316:ILE:HG22	1.84	0.77
2:B:854:ARG:NH1	2:B:866:ALA:HB2	1.99	0.76
1:A:296:GLN:HA	1:A:300:MET:HE2	1.66	0.76
3:C:56:ALA:HB2	3:C:153:ILE:HG21	1.69	0.75
1:A:297:GLY:H	1:A:300:MET:CE	1.99	0.75
1:A:63:ARG:HD2	1:A:88:CYS:SG	2.27	0.75
2:B:382:ASN:HD22	2:B:384:GLU:H	1.33	0.75
2:B:1074:THR:HG22	2:B:1077:ALA:HB3	1.68	0.74
2:B:760:HIS:CE1	2:B:788:GLN:HG2	2.23	0.74
2:B:916:THR:HG22	2:B:917:ASN:N	2.03	0.74
2:B:671:ASP:OD2	2:B:675:LYS:HE3	1.86	0.74
1:A:168:THR:HG21	1:A:247:LEU:HD21	1.70	0.73
2:B:1019:GLN:CB	2:B:1020:PRO:HD3	2.18	0.73
2:B:875:LEU:HD22	2:B:892:VAL:HG12	1.69	0.73
1:A:508:THR:HB	1:A:512:ASN:ND2	2.02	0.73
2:B:642:PRO:HD2	2:B:649:LEU:HD12	1.71	0.73
3:C:81:LYS:HD3	3:C:81:LYS:H	1.54	0.73
2:B:1057:ASP:H	2:B:1060:PRO:HG3	1.54	0.72
1:A:596:SER:OG	1:A:599:GLU:HG3	1.88	0.72
1:A:5:LEU:O	1:A:9:GLN:HG3	1.88	0.72
2:B:438:ILE:HD12	2:B:442:VAL:HG11	1.71	0.72
1:A:101:ILE:HD11	1:A:107:PRO:CD	2.20	0.71
1:A:183:ILE:HD12	2:B:565:PRO:HG2	1.72	0.71
2:B:492:ALA:HB3	2:B:816:ARG:HB3	1.73	0.70
1:A:543:LEU:HD22	1:A:585:ARG:HB2	1.71	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LYS:HD2	1:A:464:VAL:HG21	1.72	0.70
1:A:153:MET:HE1	1:A:154:SER:HA	1.74	0.70
2:B:993:MET:HE2	2:B:1065:PHE:HA	1.74	0.70
1:A:106:GLN:HB2	1:A:107:PRO:HD2	1.74	0.70
2:B:750:ARG:HD3	2:B:772:ASP:O	1.91	0.70
2:B:1059:SER:H	2:B:1060:PRO:HD3	1.57	0.69
1:A:290:ILE:HG21	1:A:355:THR:CG2	2.22	0.69
2:B:358:ASN:HA	2:B:972:GLN:HE22	1.56	0.69
2:B:879:ARG:HH12	2:B:1092:ASN:ND2	1.90	0.69
2:B:634:MET:HE2	2:B:687:VAL:HG13	1.74	0.69
1:A:559:GLU:O	1:A:568:PHE:HA	1.93	0.69
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.75	0.68
2:B:620:LEU:CD2	2:B:634:MET:HE3	2.23	0.68
1:A:287:MET:HA	1:A:346:ASP:HB2	1.74	0.68
1:A:101:ILE:HD11	1:A:107:PRO:HD3	1.75	0.68
1:A:58:PRO:O	1:A:59:VAL:HB	1.92	0.68
2:B:759:ILE:HG23	2:B:787:VAL:CG1	2.24	0.68
3:C:33:TYR:CZ	3:C:59:MET:HG3	2.29	0.68
3:C:20:MET:SD	3:C:30:LEU:HD11	2.34	0.68
1:A:368:GLY:HA3	1:A:450:GLY:O	1.94	0.68
2:B:425:SER:HB3	2:B:427:THR:O	1.94	0.68
3:C:113:ILE:HD13	3:C:113:ILE:H	1.60	0.67
2:B:1055:ILE:CG2	2:B:1062:LYS:HD2	2.24	0.67
2:B:830:THR:HG22	2:B:833:ASP:H	1.57	0.67
2:B:747:ALA:HB2	2:B:809:TYR:CB	2.25	0.67
2:B:909:GLN:HG2	2:B:911:SER:H	1.59	0.67
2:B:407:LEU:HG	2:B:789:MET:HG3	1.76	0.67
2:B:964:THR:O	2:B:965:ILE:HB	1.94	0.67
1:A:28:ARG:HB3	1:A:28:ARG:HH11	1.60	0.66
2:B:958:LEU:O	2:B:958:LEU:HD23	1.95	0.66
1:A:80:ALA:O	1:A:82:LEU:HG	1.96	0.66
2:B:411:LEU:HD23	2:B:411:LEU:N	2.11	0.66
1:A:297:GLY:H	1:A:300:MET:HE3	1.57	0.66
1:A:398:PHE:HB3	1:A:400:MET:HG2	1.77	0.66
2:B:496:TYR:HD1	2:B:818:ILE:HD11	1.61	0.66
1:A:195:LEU:HD22	1:A:203:MET:HE1	1.78	0.66
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.11	0.65
1:A:98:TYR:O	1:A:101:ILE:HB	1.96	0.65
1:A:624:TYR:CE2	1:A:634:PRO:HG3	2.32	0.64
2:B:1020:PRO:HG3	2:B:1062:LYS:NZ	2.13	0.64
2:B:954:ASP:C	2:B:956:GLY:H	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:770:SER:O	2:B:771:THR:C	2.36	0.64
2:B:496:TYR:CD1	2:B:818:ILE:HD11	2.33	0.64
2:B:652:ARG:HB2	2:B:696:TYR:CE2	2.32	0.64
2:B:879:ARG:NH1	2:B:1092:ASN:ND2	2.42	0.64
1:A:316:ILE:HD13	1:A:316:ILE:O	1.96	0.64
2:B:412:HIS:HE1	2:B:781:PRO:O	1.80	0.64
2:B:1063:ALA:C	2:B:1065:PHE:H	1.99	0.64
1:A:524:ILE:CG1	1:A:615:SER:HB3	2.28	0.64
3:C:33:TYR:CE2	3:C:59:MET:HG3	2.34	0.63
1:A:371:MET:HB3	1:A:605:HIS:CD2	2.33	0.63
1:A:4:TYR:O	1:A:8:ILE:HG13	1.99	0.63
2:B:620:LEU:HD22	2:B:634:MET:CE	2.24	0.63
2:B:382:ASN:HD22	2:B:382:ASN:C	2.03	0.63
1:A:198:LYS:O	1:A:202:GLU:HG3	1.99	0.63
1:A:116:SER:HA	1:A:496:VAL:O	1.98	0.62
1:A:224:PRO:HB2	5:A:869:HOH:O	1.99	0.62
1:A:3:THR:HG22	1:A:6:GLU:N	2.09	0.62
2:B:628:SER:HB3	2:B:629:PRO:HD3	1.82	0.62
2:B:1041:TRP:O	2:B:1045:GLN:HG2	1.98	0.62
1:A:148:LYS:O	1:A:152:GLN:HG3	1.99	0.62
2:B:348:LEU:O	2:B:348:LEU:HG	1.99	0.62
2:B:504:PRO:HG2	2:B:542:THR:HA	1.81	0.62
1:A:695:ILE:HD11	1:A:699:ARG:NH2	2.15	0.62
1:A:410:THR:HB	1:A:414:ILE:HB	1.81	0.61
2:B:423:VAL:CG2	2:B:488:ILE:HD11	2.30	0.61
1:A:404:GLY:HA2	1:A:484:GLN:O	2.01	0.61
3:C:128:ASP:OD1	3:C:130:ARG:HG2	2.01	0.61
1:A:179:GLY:HA2	1:A:239:ASN:HD22	1.64	0.61
2:B:454:LEU:HG	2:B:754:THR:H	1.65	0.61
3:C:35:SER:O	3:C:39:GLN:HG2	2.01	0.60
2:B:578:ILE:HD11	2:B:626:LEU:HA	1.82	0.60
1:A:583:HIS:HD2	1:A:620:GLN:HE21	1.45	0.60
1:A:259:ARG:NH2	1:A:308:THR:O	2.34	0.60
1:A:195:LEU:HD22	1:A:203:MET:CE	2.31	0.60
1:A:439:GLY:HA2	1:A:532:TYR:CZ	2.36	0.60
2:B:352:ASN:O	2:B:356:GLU:HG2	2.02	0.60
2:B:652:ARG:NH2	5:B:218:HOH:O	2.34	0.60
2:B:958:LEU:HA	2:B:964:THR:HA	1.83	0.60
2:B:438:ILE:O	2:B:438:ILE:HG23	2.00	0.60
1:A:649:LEU:C	1:A:649:LEU:HD12	2.21	0.60
1:A:593:PHE:O	1:A:594:ASN:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:959:ASN:O	2:B:961:SER:N	2.33	0.60
1:A:611:ASP:HB2	5:A:819:HOH:O	2.00	0.60
1:A:288:MET:HG2	1:A:290:ILE:CD1	2.32	0.60
1:A:227:ASN:HD21	1:A:278:THR:HB	1.67	0.60
1:A:452:SER:HB2	1:A:453:PRO:CD	2.32	0.59
1:A:268:LEU:HG	1:A:288:MET:SD	2.42	0.59
2:B:1054:VAL:O	2:B:1056:ARG:N	2.35	0.59
2:B:382:ASN:HD22	2:B:383:PRO:N	2.01	0.59
3:C:2:VAL:CG1	3:C:3:LEU:N	2.59	0.59
1:A:475:GLY:O	1:A:476:ARG:HB2	2.02	0.59
2:B:1011:VAL:HG12	2:B:1013:ASN:H	1.68	0.59
1:A:339:ALA:HB1	1:A:424:VAL:HG21	1.85	0.59
1:A:549:GLN:HE22	1:A:552:ARG:HH11	1.49	0.59
2:B:916:THR:CG2	2:B:917:ASN:N	2.65	0.59
2:B:936:VAL:O	2:B:940:LEU:HD23	2.02	0.59
1:A:407:GLU:HG3	1:A:445:GLN:CG	2.32	0.58
1:A:560:TYR:CD2	1:A:560:TYR:N	2.71	0.58
2:B:747:ALA:HB2	2:B:809:TYR:HB3	1.84	0.58
2:B:1021:MET:N	2:B:1055:ILE:HG12	2.14	0.58
1:A:475:GLY:HA2	1:A:503:TRP:HB2	1.84	0.58
2:B:558:LEU:CD2	2:B:565:PRO:HB3	2.33	0.58
2:B:1064:ASN:HA	5:B:89:HOH:O	2.01	0.58
2:B:916:THR:HG22	2:B:917:ASN:H	1.66	0.58
2:B:410:LEU:CD2	2:B:935:LEU:HG	2.33	0.58
1:A:293:PRO:HA	1:A:355:THR:O	2.04	0.58
1:A:18:ARG:NH1	1:A:612:LEU:HD22	2.18	0.58
3:C:127:ILE:O	3:C:127:ILE:HG22	2.04	0.58
1:A:185:LYS:HB3	2:B:567:MET:HB3	1.85	0.58
1:A:560:TYR:HD2	1:A:560:TYR:N	2.01	0.58
2:B:871:VAL:HG11	2:B:1087:ILE:HD13	1.84	0.58
1:A:240:LEU:HD22	1:A:244:LEU:HG	1.86	0.58
2:B:1051:ILE:H	2:B:1051:ILE:HD13	1.69	0.57
2:B:439:ASN:HB2	2:B:440:PRO:CD	2.34	0.57
2:B:1020:PRO:HA	2:B:1055:ILE:HG12	1.86	0.57
2:B:1055:ILE:HG21	2:B:1062:LYS:HD2	1.86	0.57
2:B:433:SER:OG	2:B:457:ARG:HD3	2.03	0.57
2:B:412:HIS:HD2	5:B:22:HOH:O	1.87	0.57
2:B:879:ARG:CZ	2:B:1092:ASN:HB3	2.35	0.57
2:B:702:LEU:O	2:B:705:ILE:HG22	2.04	0.57
2:B:899:PHE:HB3	2:B:900:PRO:HD3	1.86	0.57
2:B:576:VAL:HG12	2:B:577:PHE:N	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:HB	1:A:6:GLU:HG3	1.87	0.57
2:B:916:THR:CG2	2:B:917:ASN:H	2.17	0.57
1:A:45:LEU:CD1	1:A:451:LEU:HD13	2.36	0.56
2:B:641:LEU:HD23	2:B:642:PRO:HD2	1.86	0.56
3:C:39:GLN:CA	3:C:39:GLN:HE21	2.09	0.56
2:B:1019:GLN:CB	2:B:1020:PRO:CD	2.81	0.56
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.87	0.56
3:C:50:THR:O	3:C:51:ARG:HG2	2.06	0.56
1:A:48:ARG:HE	1:A:49:PRO:HD2	1.70	0.56
2:B:558:LEU:HD23	2:B:565:PRO:HB3	1.87	0.56
2:B:649:LEU:HD13	2:B:698:ASP:HB3	1.87	0.56
1:A:519:GLN:HG2	5:A:810:HOH:O	2.04	0.56
2:B:854:ARG:HH12	2:B:866:ALA:CB	2.14	0.56
1:A:54:ILE:HG23	1:A:56:TYR:CE2	2.41	0.56
2:B:772:ASP:O	2:B:773:LEU:HB2	2.06	0.56
2:B:375:ASP:O	2:B:378:LYS:HG2	2.06	0.56
1:A:45:LEU:CA	1:A:495:ARG:HH12	1.99	0.56
2:B:958:LEU:HB3	2:B:964:THR:CG2	2.27	0.56
3:C:30:LEU:O	3:C:34:GLN:HB2	2.06	0.56
2:B:410:LEU:HD22	2:B:935:LEU:HG	1.86	0.56
1:A:686:GLN:HG2	1:A:690:ASP:OD1	2.06	0.56
2:B:964:THR:O	2:B:965:ILE:CB	2.54	0.56
2:B:1055:ILE:HG22	2:B:1062:LYS:HD2	1.88	0.56
1:A:562:LYS:NZ	1:A:562:LYS:HB3	2.21	0.56
3:C:20:MET:SD	3:C:30:LEU:HD21	2.46	0.56
2:B:492:ALA:HB1	2:B:496:TYR:HB2	1.87	0.56
3:C:4:LEU:HD23	3:C:74:LEU:CB	2.36	0.56
1:A:76:VAL:HG21	1:A:110:LEU:HD13	1.88	0.56
1:A:108:ALA:HB1	1:A:114:PHE:CD1	2.40	0.56
1:A:44:PRO:O	1:A:495:ARG:NH1	2.39	0.55
1:A:495:ARG:HG2	1:A:495:ARG:HH11	1.71	0.55
2:B:429:VAL:HB	2:B:438:ILE:CG2	2.36	0.55
1:A:56:TYR:HD1	1:A:57:GLU:O	1.89	0.55
2:B:1039:ILE:O	2:B:1043:ARG:HG2	2.06	0.55
1:A:345:ILE:HG21	1:A:363:CYS:HB3	1.87	0.55
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.41	0.55
1:A:108:ALA:HB1	1:A:114:PHE:HD1	1.71	0.55
1:A:78:TYR:H	1:A:78:TYR:HD1	1.53	0.55
3:C:94:GLU:HG2	3:C:118:PHE:CD2	2.42	0.55
1:A:647:ILE:HG21	1:A:688:PRO:HG3	1.89	0.55
1:A:101:ILE:HD13	1:A:102:SER:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:686:ALA:HB2	2:B:777:PRO:HB2	1.88	0.55
1:A:155:LEU:HD22	1:A:240:LEU:HD13	1.88	0.54
2:B:1032:SER:O	2:B:1036:ILE:HG12	2.07	0.54
1:A:418:GLY:HA3	1:A:438:ILE:O	2.07	0.54
2:B:360:LEU:HB3	2:B:972:GLN:HG2	1.88	0.54
3:C:63:TYR:CD1	3:C:63:TYR:C	2.81	0.54
2:B:1074:THR:HG23	2:B:1076:SER:N	2.21	0.54
3:C:4:LEU:HB3	3:C:74:LEU:HB3	1.90	0.54
2:B:513:SER:O	2:B:517:VAL:HG23	2.08	0.54
3:C:56:ALA:HB2	3:C:153:ILE:CG2	2.36	0.54
1:A:528:ARG:HA	1:A:608:MET:HE1	1.90	0.54
2:B:915:GLY:HA3	2:B:1076:SER:OG	2.07	0.54
2:B:615:ALA:O	2:B:618:PRO:HD2	2.08	0.54
3:C:61:PHE:CZ	3:C:74:LEU:HD13	2.43	0.54
1:A:101:ILE:HD11	1:A:107:PRO:HD2	1.87	0.54
1:A:24:TRP:HB3	1:A:25:PRO:HD2	1.90	0.54
2:B:351:VAL:CG1	2:B:356:GLU:HG3	2.38	0.54
1:A:687:ALA:N	1:A:688:PRO:HD2	2.23	0.54
1:A:529:LEU:O	1:A:533:ARG:HG3	2.08	0.54
1:A:190:ARG:NH2	2:B:577:PHE:HB3	2.23	0.53
3:C:4:LEU:HD12	3:C:20:MET:HG2	1.90	0.53
2:B:348:LEU:CD1	2:B:836:LEU:HD21	2.39	0.53
2:B:446:ASP:O	2:B:448:ARG:N	2.42	0.53
2:B:1074:THR:HG22	2:B:1077:ALA:CB	2.35	0.53
2:B:936:VAL:HG13	2:B:937:TYR:N	2.23	0.53
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.38	0.53
1:A:76:VAL:HG12	1:A:77:ASP:N	2.23	0.53
2:B:480:ARG:HG3	2:B:480:ARG:HH11	1.73	0.53
2:B:932:ASN:ND2	5:B:2:HOH:O	2.40	0.53
2:B:779:VAL:HA	5:B:82:HOH:O	2.08	0.53
2:B:631:GLY:HA2	2:B:685:VAL:HG22	1.89	0.53
2:B:991:VAL:HG12	2:B:1051:ILE:HD11	1.91	0.53
2:B:997:GLY:O	2:B:1000:CYS:HB2	2.07	0.53
3:C:81:LYS:HD3	3:C:81:LYS:N	2.22	0.53
2:B:445:LEU:C	2:B:447:GLN:H	2.12	0.53
1:A:393:ASP:O	1:A:395:HIS:N	2.40	0.53
2:B:845:GLY:HA2	2:B:938:LEU:CD2	2.38	0.53
2:B:423:VAL:HG12	2:B:425:SER:H	1.73	0.53
3:C:62:HIS:O	3:C:73:VAL:HG12	2.08	0.53
2:B:734:GLU:HG2	2:B:1048:PHE:CE2	2.44	0.53
1:A:524:ILE:HG13	1:A:615:SER:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:VAL:HG13	5:B:111:HOH:O	2.08	0.53
1:A:346:ASP:HB3	1:A:348:TYR:CE1	2.44	0.53
1:A:41:LEU:HD21	1:A:524:ILE:HG21	1.90	0.53
1:A:393:ASP:C	1:A:395:HIS:H	2.12	0.53
2:B:430:ARG:O	2:B:431:CYS:C	2.47	0.53
1:A:461:PHE:CE2	1:A:479:ILE:HD13	2.44	0.53
2:B:654:GLU:OE2	2:B:919:ARG:HB3	2.09	0.53
1:A:166:LEU:HD23	1:A:243:LEU:HD13	1.91	0.53
1:A:3:THR:CG2	1:A:6:GLU:HG3	2.38	0.53
2:B:420:LEU:HD21	2:B:489:GLU:HB2	1.90	0.53
2:B:454:LEU:HD11	2:B:802:SER:HB2	1.90	0.53
2:B:429:VAL:HB	2:B:438:ILE:HG21	1.91	0.52
2:B:548:THR:OG1	2:B:554:HIS:HB2	2.09	0.52
2:B:696:TYR:CE1	2:B:920:LEU:HD23	2.44	0.52
1:A:179:GLY:CA	1:A:239:ASN:HD22	2.22	0.52
2:B:539:ASN:ND2	2:B:813:LYS:HA	2.24	0.52
1:A:283:GLY:H	1:A:486:GLN:NE2	2.07	0.52
1:A:58:PRO:HA	1:A:119:TYR:CE2	2.45	0.52
2:B:1020:PRO:HG3	2:B:1062:LYS:HZ1	1.73	0.52
3:C:81:LYS:CD	3:C:81:LYS:H	2.16	0.52
1:A:45:LEU:O	1:A:453:PRO:HA	2.09	0.52
2:B:1019:GLN:CG	2:B:1020:PRO:HD3	2.39	0.52
1:A:126:GLN:NE2	1:A:491:GLN:HG2	2.25	0.52
1:A:288:MET:HG2	1:A:290:ILE:HD11	1.90	0.52
1:A:476:ARG:HA	1:A:501:ARG:O	2.10	0.52
1:A:652:THR:O	1:A:653:PHE:C	2.47	0.52
2:B:395:GLN:NE2	2:B:796:THR:HA	2.24	0.52
1:A:3:THR:CG2	1:A:6:GLU:H	2.12	0.52
2:B:1060:PRO:O	2:B:1062:LYS:HG3	2.10	0.52
2:B:550:ASP:OD1	2:B:551:SER:N	2.42	0.52
2:B:641:LEU:HD21	2:B:649:LEU:HB2	1.92	0.52
2:B:465:PHE:CE1	2:B:480:ARG:HG2	2.44	0.52
3:C:31:GLN:CG	3:C:32:GLN:N	2.72	0.52
1:A:586:ARG:NH1	1:A:586:ARG:HB2	2.25	0.52
1:A:45:LEU:HD11	1:A:451:LEU:HD13	1.91	0.51
1:A:153:MET:HE3	1:A:157:LEU:HD11	1.91	0.51
1:A:262:ARG:HG2	1:A:264:SER:OG	2.10	0.51
1:A:250:ASP:OD2	1:A:251:PRO:HD2	2.10	0.51
3:C:4:LEU:HD23	3:C:74:LEU:HB2	1.92	0.51
2:B:916:THR:HG22	2:B:918:ALA:H	1.75	0.51
2:B:483:VAL:HG12	2:B:483:VAL:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:THR:HG21	5:B:24:HOH:O	2.10	0.51
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.75	0.51
3:C:55:GLU:HB2	3:C:152:ASN:HD22	1.75	0.51
1:A:289:PHE:C	1:A:290:ILE:HD12	2.31	0.51
2:B:1053:TYR:HB2	2:B:1055:ILE:HG13	1.93	0.51
2:B:960:ILE:HG21	2:B:963:ARG:HH12	1.76	0.51
1:A:426:LEU:O	1:A:427:ASN:C	2.49	0.51
2:B:573:ILE:HG22	5:B:136:HOH:O	2.11	0.51
3:C:61:PHE:HD2	3:C:72:LEU:HD11	1.74	0.51
1:A:76:VAL:HG12	1:A:77:ASP:H	1.76	0.51
3:C:148:ILE:HG22	3:C:149:MET:N	2.24	0.51
1:A:384:GLN:O	1:A:388:ARG:HG2	2.10	0.51
1:A:58:PRO:O	1:A:59:VAL:CB	2.57	0.51
2:B:447:GLN:HG2	2:B:447:GLN:O	2.11	0.51
2:B:981:ASP:OD1	2:B:999:ASN:ND2	2.43	0.51
2:B:753:CYS:HB3	2:B:803:PHE:HD1	1.76	0.50
1:A:126:GLN:HE22	1:A:491:GLN:HG2	1.76	0.50
2:B:831:LEU:HD22	2:B:835:PHE:CE1	2.46	0.50
2:B:634:MET:HE2	2:B:687:VAL:CG1	2.40	0.50
2:B:1074:THR:HG22	2:B:1077:ALA:N	2.27	0.50
3:C:62:HIS:HB2	3:C:73:VAL:CG1	2.40	0.50
1:A:183:ILE:CD1	2:B:565:PRO:HG2	2.41	0.50
2:B:381:CYS:HB2	2:B:822:THR:O	2.11	0.50
1:A:168:THR:HG21	1:A:247:LEU:CD2	2.40	0.50
2:B:638:GLN:HE21	2:B:640:GLN:H	1.60	0.50
2:B:360:LEU:HB3	2:B:972:GLN:CG	2.42	0.50
1:A:180:CYS:SG	1:A:185:LYS:HE2	2.52	0.50
2:B:348:LEU:HD13	2:B:836:LEU:HD21	1.93	0.50
2:B:409:LEU:C	2:B:410:LEU:HD12	2.32	0.50
2:B:763:HIS:HB2	2:B:786:ALA:HB3	1.93	0.50
2:B:1079:SER:OG	2:B:1082:GLU:HG3	2.11	0.50
3:C:153:ILE:HG23	3:C:154:GLU:N	2.27	0.50
2:B:498:LEU:HD12	2:B:498:LEU:N	2.26	0.50
3:C:108:ARG:HB2	3:C:111:SER:OG	2.12	0.50
1:A:406:LEU:O	1:A:445:GLN:HA	2.12	0.50
1:A:180:CYS:O	1:A:181:GLU:CG	2.60	0.50
1:A:618:MET:HG2	1:A:653:PHE:HB3	1.94	0.50
3:C:10:VAL:HG23	3:C:68:GLY:O	2.11	0.50
1:A:658:ILE:HD12	1:A:705:TYR:OH	2.11	0.50
3:C:39:GLN:NE2	3:C:39:GLN:HA	2.13	0.49
1:A:313:TRP:HE3	1:A:316:ILE:HG21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:THR:HG22	1:A:536:THR:O	2.12	0.49
2:B:1055:ILE:HG21	2:B:1062:LYS:CD	2.42	0.49
1:A:266:VAL:HA	1:A:269:SER:OG	2.12	0.49
1:A:162:ALA:O	1:A:233:VAL:HG23	2.11	0.49
3:C:79:PHE:CD1	3:C:80:PRO:HD2	2.47	0.49
2:B:1063:ALA:C	2:B:1065:PHE:N	2.66	0.49
2:B:578:ILE:CD1	2:B:626:LEU:HA	2.42	0.49
1:A:71:ASN:OD1	1:A:73:LEU:HB2	2.12	0.49
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.28	0.49
2:B:963:ARG:HH11	2:B:963:ARG:HB2	1.77	0.49
1:A:626:TYR:CD2	1:A:632:PRO:HG3	2.48	0.49
2:B:906:LEU:HD13	2:B:942:THR:HG21	1.94	0.49
1:A:583:HIS:HD2	1:A:620:GLN:NE2	2.09	0.49
1:A:575:SER:O	1:A:578:PRO:HD2	2.12	0.49
1:A:190:ARG:NH1	2:B:575:ASP:OD1	2.46	0.49
2:B:954:ASP:C	2:B:956:GLY:N	2.65	0.49
1:A:364:PRO:O	1:A:367:THR:O	2.31	0.49
1:A:3:THR:CG2	1:A:5:LEU:H	2.26	0.49
2:B:420:LEU:HD12	2:B:421:PRO:HD2	1.94	0.49
2:B:411:LEU:HB2	2:B:413:PRO:HD3	1.95	0.48
1:A:88:CYS:SG	1:A:90:GLN:HB3	2.53	0.48
2:B:439:ASN:O	2:B:442:VAL:HG13	2.13	0.48
1:A:583:HIS:CD2	1:A:620:GLN:HG3	2.49	0.48
2:B:753:CYS:HB2	2:B:803:PHE:CD1	2.48	0.48
1:A:369:GLY:O	1:A:609:ARG:NH2	2.46	0.48
1:A:259:ARG:NH1	1:A:306:LEU:HD23	2.27	0.48
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.94	0.48
1:A:510:ILE:HD13	1:A:556:LYS:HE2	1.94	0.48
2:B:802:SER:HA	2:B:823:LEU:O	2.13	0.48
1:A:719:LEU:O	1:A:722:VAL:HG12	2.13	0.48
2:B:1055:ILE:O	2:B:1057:ASP:N	2.47	0.48
2:B:352:ASN:HD21	2:B:889:GLY:HA3	1.79	0.48
2:B:498:LEU:N	2:B:498:LEU:CD1	2.77	0.48
2:B:641:LEU:CD2	2:B:649:LEU:HB2	2.43	0.48
2:B:773:LEU:HA	2:B:773:LEU:HD12	1.71	0.48
1:A:753:MET:O	1:A:757:LYS:HG3	2.14	0.48
1:A:695:ILE:C	1:A:697:HIS:H	2.16	0.48
1:A:495:ARG:HG2	1:A:495:ARG:NH1	2.29	0.48
1:A:297:GLY:CA	1:A:300:MET:HB2	2.43	0.48
2:B:913:GLN:NE2	2:B:916:THR:HG21	2.29	0.48
3:C:80:PRO:HB3	3:C:82:LYS:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ASP:OD2	1:A:567:SER:HB3	2.14	0.47
2:B:1059:SER:N	2:B:1060:PRO:HD3	2.26	0.47
2:B:958:LEU:H	2:B:958:LEU:HD22	1.79	0.47
2:B:1057:ASP:C	2:B:1060:PRO:HD3	2.35	0.47
2:B:358:ASN:CA	2:B:972:GLN:HE22	2.24	0.47
1:A:79:ARG:HH11	1:A:79:ARG:HG3	1.78	0.47
3:C:53:THR:O	3:C:150:VAL:HA	2.14	0.47
2:B:386:PHE:CE1	2:B:409:LEU:HD13	2.49	0.47
2:B:573:ILE:CG2	2:B:618:PRO:HG2	2.35	0.47
2:B:450:TRP:CE2	2:B:459:ASN:HB2	2.50	0.47
1:A:722:VAL:HG22	1:A:723:ASN:N	2.19	0.47
2:B:916:THR:HG22	2:B:918:ALA:N	2.30	0.47
1:A:78:TYR:N	1:A:78:TYR:CD1	2.82	0.47
2:B:710:ALA:HB3	2:B:777:PRO:HD2	1.97	0.47
2:B:559:GLN:HG2	2:B:583:ASN:ND2	2.29	0.47
2:B:756:GLY:HA2	2:B:793:GLU:HB2	1.97	0.47
1:A:524:ILE:HG12	1:A:615:SER:HB3	1.94	0.47
2:B:1011:VAL:HG12	2:B:1012:GLN:N	2.29	0.47
1:A:577:TYR:N	1:A:578:PRO:CD	2.78	0.47
1:A:51:LEU:HD22	1:A:52:PRO:HD2	1.96	0.47
2:B:879:ARG:NH1	2:B:1092:ASN:HB3	2.30	0.47
2:B:493:PRO:HD2	2:B:496:TYR:CG	2.50	0.47
1:A:282:THR:HG22	5:A:825:HOH:O	2.15	0.47
2:B:368:PRO:HD2	2:B:839:ASP:OD2	2.14	0.47
1:A:417:SER:O	1:A:437:GLU:HA	2.15	0.47
2:B:1055:ILE:HG21	2:B:1062:LYS:NZ	2.30	0.47
2:B:423:VAL:HG21	2:B:482:GLU:HG3	1.96	0.47
2:B:452:CYS:O	2:B:456:TYR:HA	2.15	0.47
2:B:674:LYS:O	2:B:678:LEU:HG	2.15	0.47
2:B:1059:SER:N	2:B:1060:PRO:CD	2.78	0.46
1:A:313:TRP:CE2	1:A:597:PRO:HA	2.49	0.46
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.50	0.46
2:B:807:LEU:O	2:B:818:ILE:HA	2.15	0.46
2:B:505:VAL:HG21	2:B:630:THR:OG1	2.15	0.46
1:A:664:ILE:O	1:A:664:ILE:HG22	2.15	0.46
2:B:854:ARG:HH11	2:B:854:ARG:HG2	1.79	0.46
1:A:185:LYS:CB	2:B:567:MET:HB3	2.45	0.46
2:B:1005:LEU:HD13	2:B:1013:ASN:HA	1.97	0.46
1:A:617:ILE:HG12	1:A:622:ILE:CD1	2.45	0.46
2:B:752:ARG:HA	5:B:184:HOH:O	2.15	0.46
1:A:39:ALA:CB	1:A:525:LEU:HD13	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:641:LEU:HD23	2:B:642:PRO:CD	2.46	0.46
1:A:536:THR:O	1:A:537:GLU:C	2.53	0.46
1:A:191:GLY:HA3	1:A:263:SER:CB	2.45	0.46
2:B:1059:SER:H	2:B:1060:PRO:CD	2.27	0.46
3:C:33:TYR:HB3	3:C:74:LEU:HD22	1.97	0.46
2:B:913:GLN:HE22	2:B:916:THR:HG21	1.79	0.46
2:B:909:GLN:HG2	2:B:910:LYS:N	2.31	0.46
1:A:19:PHE:HA	1:A:39:ALA:O	2.15	0.46
2:B:768:VAL:HG22	2:B:774:LEU:HD22	1.97	0.46
1:A:757:LYS:O	1:A:761:VAL:HG22	2.16	0.46
2:B:753:CYS:O	2:B:754:THR:O	2.33	0.46
2:B:991:VAL:HG12	2:B:1051:ILE:CD1	2.45	0.46
1:A:554:CYS:HA	1:A:570:PHE:CZ	2.51	0.46
2:B:576:VAL:CG1	2:B:577:PHE:N	2.78	0.46
2:B:439:ASN:HB2	2:B:440:PRO:HD2	1.97	0.46
1:A:609:ARG:HG3	5:A:805:HOH:O	2.16	0.46
2:B:1054:VAL:C	2:B:1056:ARG:N	2.65	0.46
2:B:656:ASN:OD1	2:B:658:ARG:HB3	2.15	0.46
3:C:3:LEU:HD22	3:C:127:ILE:HD13	1.98	0.46
1:A:649:LEU:HD12	1:A:650:MET:N	2.30	0.46
2:B:763:HIS:HB3	2:B:849:ASN:OD1	2.16	0.46
2:B:521:TYR:CG	2:B:522:LEU:N	2.84	0.46
2:B:555:PHE:HE2	2:B:570:VAL:HG11	1.81	0.46
1:A:559:GLU:O	1:A:560:TYR:HB3	2.16	0.46
1:A:101:ILE:HD13	1:A:102:SER:N	2.31	0.45
2:B:753:CYS:CB	2:B:803:PHE:HD1	2.29	0.45
2:B:457:ARG:HG3	2:B:458:VAL:N	2.31	0.45
3:C:94:GLU:HG2	3:C:118:PHE:CE2	2.51	0.45
1:A:15:ASP:OD1	1:A:497:THR:HG23	2.16	0.45
2:B:854:ARG:NH1	2:B:866:ALA:CB	2.76	0.45
1:A:183:ILE:O	2:B:565:PRO:O	2.34	0.45
2:B:734:GLU:HA	2:B:1048:PHE:HE2	1.81	0.45
2:B:631:GLY:HA2	2:B:685:VAL:CG2	2.46	0.45
3:C:19:SER:O	3:C:20:MET:HG3	2.16	0.45
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.52	0.45
1:A:302:VAL:HG22	1:A:303:GLY:H	1.81	0.45
2:B:923:ARG:O	2:B:927:MET:HG3	2.17	0.45
1:A:63:ARG:HH11	1:A:88:CYS:HB2	1.82	0.45
1:A:700:PHE:CB	1:A:701:PRO:HD3	2.46	0.45
2:B:642:PRO:HG2	2:B:702:LEU:HD21	1.99	0.45
1:A:560:TYR:HD1	1:A:761:VAL:HG12	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:LEU:C	1:A:649:LEU:CD1	2.85	0.45
2:B:779:VAL:O	2:B:779:VAL:HG13	2.15	0.45
2:B:749:MET:HA	2:B:806:ALA:O	2.16	0.45
2:B:1051:ILE:N	2:B:1051:ILE:HD13	2.32	0.45
1:A:457:LEU:HD22	1:A:457:LEU:N	2.32	0.45
1:A:183:ILE:HG23	1:A:184:SER:N	2.32	0.44
2:B:639:THR:O	2:B:693:SER:HA	2.17	0.44
3:C:92:HIS:CD2	3:C:92:HIS:C	2.91	0.44
1:A:180:CYS:O	1:A:181:GLU:HG2	2.18	0.44
1:A:250:ASP:OD2	1:A:252:TRP:HD1	1.99	0.44
1:A:302:VAL:HG22	1:A:303:GLY:N	2.32	0.44
2:B:397:GLN:OE1	2:B:790:SER:HB2	2.17	0.44
2:B:446:ASP:C	2:B:448:ARG:N	2.71	0.44
2:B:425:SER:C	2:B:427:THR:H	2.20	0.44
2:B:425:SER:C	2:B:427:THR:N	2.71	0.44
2:B:993:MET:CE	2:B:1065:PHE:HA	2.45	0.44
1:A:275:LEU:HA	1:A:278:THR:OG1	2.18	0.44
2:B:395:GLN:HE21	2:B:796:THR:HA	1.83	0.44
1:A:638:ASP:HB3	1:A:640:SER:OG	2.17	0.44
1:A:508:THR:O	1:A:512:ASN:ND2	2.51	0.44
2:B:1078:LEU:HB3	2:B:1082:GLU:HB2	1.99	0.44
3:C:61:PHE:CD1	3:C:153:ILE:HD12	2.52	0.44
1:A:747:VAL:HG12	1:A:748:SER:N	2.32	0.44
1:A:342:GLY:HA2	1:A:449:CYS:SG	2.57	0.44
3:C:3:LEU:HD13	3:C:123:LYS:HD3	2.00	0.44
2:B:449:ARG:HA	2:B:459:ASN:O	2.18	0.44
1:A:313:TRP:CZ2	1:A:597:PRO:HA	2.52	0.44
1:A:297:GLY:H	1:A:300:MET:HE2	1.81	0.44
2:B:913:GLN:NE2	2:B:918:ALA:HB2	2.32	0.44
2:B:1064:ASN:CA	5:B:89:HOH:O	2.63	0.44
2:B:972:GLN:HB3	2:B:1071:GLU:OE2	2.18	0.44
1:A:700:PHE:O	1:A:702:MET:N	2.51	0.44
1:A:153:MET:HE3	1:A:157:LEU:CD1	2.47	0.44
2:B:747:ALA:CB	2:B:809:TYR:HB3	2.45	0.44
2:B:753:CYS:CB	2:B:803:PHE:CD1	3.01	0.44
1:A:63:ARG:O	1:A:64:THR:C	2.56	0.44
1:A:196:SER:HA	5:A:842:HOH:O	2.17	0.44
2:B:420:LEU:HA	2:B:421:PRO:HD3	1.89	0.43
2:B:551:SER:HA	2:B:644:LEU:HD23	1.99	0.43
1:A:509:GLN:O	1:A:513:ILE:HG13	2.17	0.43
1:A:666:GLN:H	1:A:666:GLN:HG3	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:853:ASP:O	2:B:857:THR:HB	2.18	0.43
1:A:159:PRO:HD3	1:A:398:PHE:CE1	2.53	0.43
3:C:50:THR:C	3:C:51:ARG:HG2	2.38	0.43
2:B:561:SER:HB3	5:B:122:HOH:O	2.18	0.43
2:B:1057:ASP:O	2:B:1060:PRO:HD3	2.18	0.43
1:A:177:GLU:OE1	1:A:185:LYS:HE3	2.19	0.43
1:A:88:CYS:SG	1:A:90:GLN:CB	3.07	0.43
1:A:560:TYR:CD1	1:A:761:VAL:HA	2.54	0.43
2:B:412:HIS:CE1	2:B:781:PRO:O	2.67	0.43
2:B:350:VAL:HG12	2:B:351:VAL:N	2.33	0.43
2:B:680:CYS:HB3	2:B:685:VAL:O	2.19	0.43
3:C:52:CYS:SG	3:C:53:THR:N	2.91	0.43
2:B:894:PHE:O	2:B:897:ARG:HD3	2.17	0.43
2:B:544:ILE:HG13	2:B:545:GLY:N	2.33	0.43
1:A:311:ARG:NH2	1:A:358:LEU:HB3	2.33	0.43
2:B:958:LEU:HD23	2:B:958:LEU:C	2.39	0.43
1:A:88:CYS:C	1:A:90:GLN:H	2.22	0.43
2:B:652:ARG:HB2	2:B:696:TYR:CZ	2.52	0.43
2:B:351:VAL:O	2:B:891:MET:HA	2.18	0.43
1:A:114:PHE:HB3	1:A:117:ILE:HD12	2.00	0.43
1:A:662:GLU:HG3	1:A:710:HIS:HD2	1.83	0.43
1:A:362:CYS:HA	1:A:365:ASN:HB2	2.00	0.43
3:C:54:LEU:HA	3:C:151:ALA:O	2.18	0.43
2:B:393:ILE:HA	2:B:394:PRO:HD3	1.90	0.43
2:B:584:LEU:HA	2:B:584:LEU:HD23	1.79	0.43
2:B:848:ALA:O	2:B:852:VAL:HG23	2.19	0.43
1:A:650:MET:CE	1:A:718:LEU:HA	2.48	0.43
1:A:17:VAL:O	1:A:18:ARG:HG3	2.19	0.43
3:C:65:ILE:C	3:C:66:GLU:HG2	2.39	0.43
2:B:1014:TYR:HH	2:B:1058:GLU:H	1.65	0.43
2:B:609:THR:HG22	2:B:610:LEU:N	2.33	0.43
2:B:564:GLN:HB2	2:B:565:PRO:HD2	2.00	0.43
3:C:19:SER:C	3:C:20:MET:HG3	2.39	0.43
1:A:126:GLN:H	1:A:126:GLN:HG3	1.54	0.43
3:C:10:VAL:HG23	3:C:68:GLY:C	2.39	0.43
2:B:602:LEU:HA	2:B:605:MET:CE	2.47	0.43
1:A:12:GLU:OE1	1:A:18:ARG:HD2	2.19	0.43
1:A:25:PRO:HD3	1:A:34:MET:CE	2.49	0.43
2:B:479:ARG:HA	2:B:479:ARG:HD2	1.68	0.43
1:A:297:GLY:HA3	1:A:300:MET:HB2	2.01	0.42
1:A:159:PRO:HA	1:A:160:PRO:HD3	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:PRO:HB3	2:B:810:THR:HG23	2.01	0.42
1:A:255:PRO:HG2	1:A:258:LYS:CG	2.39	0.42
3:C:4:LEU:HD23	3:C:74:LEU:HB3	2.01	0.42
2:B:871:VAL:CG1	2:B:1087:ILE:HD13	2.47	0.42
3:C:63:TYR:HD1	3:C:64:ILE:N	2.17	0.42
2:B:445:LEU:O	2:B:447:GLN:N	2.51	0.42
3:C:80:PRO:HB2	3:C:83:LEU:HG	2.01	0.42
2:B:357:ARG:HA	2:B:359:MET:HE2	2.00	0.42
3:C:30:LEU:HG	3:C:34:GLN:HE21	1.83	0.42
3:C:61:PHE:CE1	3:C:74:LEU:HD13	2.54	0.42
3:C:1:MET:HA	3:C:79:PHE:CD1	2.54	0.42
1:A:3:THR:HG22	1:A:5:LEU:N	2.35	0.42
3:C:20:MET:CG	3:C:30:LEU:HD11	2.49	0.42
3:C:74:LEU:O	3:C:75:CYS:HB3	2.20	0.42
1:A:227:ASN:HD22	1:A:230:LEU:HD12	1.85	0.42
1:A:541:ASP:HB3	1:A:544:ARG:HD2	2.01	0.42
2:B:876:SER:HA	2:B:1091:VAL:HG13	2.00	0.42
2:B:977:LYS:HE3	5:B:114:HOH:O	2.19	0.42
2:B:440:PRO:HA	2:B:483:VAL:HG13	2.02	0.42
1:A:264:SER:HB2	1:A:294:ALA:HB2	2.02	0.42
1:A:612:LEU:O	1:A:613:THR:C	2.55	0.42
1:A:409:LYS:HB2	1:A:480:GLN:HB3	2.01	0.42
1:A:30:GLU:OE1	1:A:30:GLU:HA	2.19	0.42
3:C:128:ASP:OD1	3:C:130:ARG:CG	2.66	0.42
1:A:521:ALA:HA	1:A:612:LEU:HD12	2.01	0.42
2:B:601:THR:C	2:B:605:MET:HE3	2.40	0.42
1:A:63:ARG:O	1:A:65:THR:N	2.53	0.42
1:A:157:LEU:HD12	1:A:390:PHE:HB2	2.02	0.42
1:A:361:LYS:O	1:A:364:PRO:HD2	2.19	0.42
3:C:148:ILE:CG2	3:C:149:MET:N	2.83	0.42
3:C:101:LYS:HA	3:C:101:LYS:HE3	2.01	0.42
1:A:238:MET:C	1:A:241:THR:HG22	2.40	0.42
1:A:191:GLY:HA3	1:A:263:SER:HB3	2.01	0.42
2:B:1049:PHE:CD2	2:B:1049:PHE:C	2.92	0.42
3:C:3:LEU:CD2	3:C:127:ILE:HD13	2.50	0.42
1:A:147:LEU:HD11	1:A:289:PHE:CD2	2.54	0.42
3:C:72:LEU:HD12	3:C:73:VAL:H	1.84	0.42
2:B:654:GLU:HA	2:B:655:PRO:HD3	1.89	0.42
1:A:17:VAL:HG22	1:A:18:ARG:N	2.34	0.42
1:A:519:GLN:NE2	1:A:576:LEU:HB2	2.35	0.42
1:A:363:CYS:HB2	1:A:364:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:GLN:HG2	3:C:32:GLN:N	2.32	0.42
2:B:360:LEU:CB	2:B:972:GLN:HG2	2.50	0.41
2:B:453:ASN:C	2:B:454:LEU:HD12	2.39	0.41
1:A:164:VAL:O	1:A:230:LEU:HA	2.20	0.41
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.91	0.41
1:A:452:SER:CB	1:A:453:PRO:CD	2.99	0.41
1:A:3:THR:HB	1:A:6:GLU:CG	2.49	0.41
2:B:412:HIS:N	2:B:413:PRO:CD	2.82	0.41
1:A:258:LYS:HA	1:A:304:ASP:O	2.20	0.41
3:C:39:GLN:CB	3:C:157:LEU:HD22	2.50	0.41
2:B:530:LEU:HD21	2:B:599:LEU:HB2	2.02	0.41
1:A:203:MET:HB3	2:B:571:SER:OG	2.21	0.41
1:A:280:PRO:O	1:A:281:ASN:HB2	2.20	0.41
2:B:904:LEU:CD2	2:B:1080:TYR:HA	2.50	0.41
2:B:361:PRO:HG3	2:B:365:LEU:CD2	2.51	0.41
2:B:627:MET:O	2:B:628:SER:C	2.59	0.41
2:B:1078:LEU:HA	2:B:1082:GLU:OE1	2.21	0.41
2:B:558:LEU:HD13	2:B:595:VAL:HG12	2.02	0.41
2:B:408:GLY:HA2	2:B:789:MET:HG2	2.03	0.41
1:A:633:GLU:HA	1:A:634:PRO:HD3	1.84	0.41
2:B:655:PRO:HD3	2:B:920:LEU:HD13	2.02	0.41
3:C:130:ARG:HG3	3:C:130:ARG:O	2.21	0.41
1:A:12:GLU:CD	1:A:18:ARG:HD2	2.40	0.41
1:A:158:LEU:HA	1:A:159:PRO:HD3	1.89	0.41
1:A:680:ASN:CG	1:A:681:PHE:H	2.24	0.41
1:A:290:ILE:HD12	1:A:290:ILE:N	2.36	0.41
1:A:259:ARG:HB2	1:A:304:ASP:HA	2.03	0.41
2:B:911:SER:OG	2:B:926:ALA:HB1	2.21	0.41
1:A:686:GLN:HG2	1:A:686:GLN:O	2.21	0.41
3:C:80:PRO:HB3	3:C:82:LYS:CE	2.51	0.41
2:B:357:ARG:NH2	2:B:1081:TYR:HB2	2.36	0.41
2:B:904:LEU:HD11	2:B:908:LYS:HE3	2.02	0.41
2:B:933:GLN:HA	2:B:934:PRO:HD3	1.82	0.41
1:A:551:ILE:O	1:A:555:GLN:HG3	2.21	0.41
1:A:708:THR:HB	1:A:714:GLN:HB2	2.03	0.41
2:B:416:ASP:OD1	2:B:742:LYS:NZ	2.54	0.41
2:B:411:LEU:CD2	2:B:411:LEU:N	2.81	0.40
2:B:420:LEU:HD12	2:B:421:PRO:CD	2.51	0.40
2:B:367:PRO:HA	2:B:368:PRO:HD3	1.93	0.40
3:C:155:GLU:HG2	3:C:156:VAL:N	2.35	0.40
2:B:1043:ARG:HB3	2:B:1050:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:831:LEU:HD22	2:B:835:PHE:HE1	1.84	0.40
1:A:680:ASN:CG	1:A:681:PHE:N	2.74	0.40
2:B:585:LEU:HD23	2:B:585:LEU:HA	1.89	0.40
2:B:1017:ILE:HA	2:B:1018:PRO:HD2	1.80	0.40
1:A:3:THR:HG23	1:A:5:LEU:H	1.86	0.40
2:B:1019:GLN:O	2:B:1055:ILE:HG23	2.21	0.40
2:B:348:LEU:CG	2:B:348:LEU:O	2.64	0.40
1:A:722:VAL:HG13	1:A:723:ASN:N	2.37	0.40
1:A:297:GLY:N	1:A:300:MET:CE	2.78	0.40
1:A:398:PHE:HB3	1:A:400:MET:CG	2.49	0.40
1:A:687:ALA:N	1:A:688:PRO:CD	2.84	0.40
1:A:586:ARG:HH11	1:A:586:ARG:CB	2.33	0.40
2:B:963:ARG:HB2	2:B:963:ARG:NH1	2.37	0.40
3:C:114:GLU:HG3	5:C:201:HOH:O	2.21	0.40
1:A:3:THR:CB	1:A:6:GLU:HG3	2.49	0.40
1:A:237:ASP:O	1:A:241:THR:HB	2.22	0.40
1:A:190:ARG:C	1:A:192:THR:H	2.24	0.40
1:A:700:PHE:O	1:A:701:PRO:C	2.57	0.40
1:A:57:GLU:CG	1:A:58:PRO:HD2	2.51	0.40
2:B:432:ARG:HD2	2:B:457:ARG:NH2	2.36	0.40
2:B:730:LYS:HE2	2:B:734:GLU:OE2	2.21	0.40
3:C:155:GLU:O	3:C:156:VAL:C	2.59	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	687/769 (89%)	607 (88%)	61 (9%)	19 (3%)	6 21
2	B	723/753 (96%)	638 (88%)	64 (9%)	21 (3%)	6 19
3	C	131/196 (67%)	107 (82%)	19 (14%)	5 (4%)	4 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1541/1718 (90%)	1352 (88%)	144 (9%)	45 (3%)	6 19

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	64	THR
1	A	105	ASN
1	A	182	GLY
1	A	197	ALA
1	A	394	MET
2	B	447	GLN
2	B	754	THR
2	B	769	ARG
2	B	773	LEU
2	B	961	SER
2	B	1019	GLN
3	C	4	LEU
3	C	131	ALA
1	A	59	VAL
1	A	66	CYS
1	A	196	SER
1	A	747	VAL
2	B	446	ASP
2	B	456	TYR
2	B	960	ILE
2	B	1055	ILE
2	B	1056	ARG
1	A	123	ARG
1	A	181	GLU
1	A	427	ASN
1	A	696	LEU
2	B	772	ASP
2	B	797	ASP
2	B	1059	SER
3	C	92	HIS
1	A	109	GLU
1	A	184	SER
1	A	476	ARG
1	A	700	PHE
2	B	431	CYS
2	B	464	GLU

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Mol	Chain	Res	Type
2	B	771	THR
2	B	965	ILE
2	B	1018	PRO
3	C	75	CYS
1	A	722	VAL
2	B	438	ILE
2	B	915	GLY
3	C	156	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	610/667 (92%)	582 (95%)	28 (5%)	33 67
2	B	662/684 (97%)	620 (94%)	42 (6%)	22 53
3	C	120/171 (70%)	107 (89%)	13 (11%)	8 23
All	All	1392/1522 (92%)	1309 (94%)	83 (6%)	24 56

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	30	GLU
1	A	101	ILE
1	A	105	ASN
1	A	153	MET
1	A	161	THR
1	A	164	VAL
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	316	ILE

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Mol	Chain	Res	Type
1	A	414	ILE
1	A	451	LEU
1	A	508	THR
1	A	524	ILE
1	A	528	ARG
1	A	544	ARG
1	A	560	TYR
1	A	569	ARG
1	A	570	PHE
1	A	586	ARG
1	A	612	LEU
1	A	649	LEU
1	A	723	ASN
1	A	754	ASP
2	B	359	MET
2	B	382	ASN
2	B	386	PHE
2	B	411	LEU
2	B	412	HIS
2	B	431	CYS
2	B	455	CYS
2	B	498	LEU
2	B	511	ASP
2	B	522	LEU
2	B	570	VAL
2	B	589	ASN
2	B	607	THR
2	B	608	LYS
2	B	640	GLN
2	B	641	LEU
2	B	650	LYS
2	B	652	ARG
2	B	789	MET
2	B	797	ASP
2	B	798	THR
2	B	799	GLN
2	B	807	LEU
2	B	816	ARG
2	B	831	LEU
2	B	857	THR
2	B	906	LEU
2	B	935	LEU

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Mol	Chain	Res	Type
2	B	958	LEU
2	B	961	SER
2	B	993	MET
2	B	1001	THR
2	B	1002	GLN
2	B	1034	ARG
2	B	1043	ARG
2	B	1048	PHE
2	B	1051	ILE
2	B	1052	LEU
2	B	1057	ASP
2	B	1060	PRO
2	B	1075	GLU
2	B	1085	LEU
3	C	1	MET
3	C	3	LEU
3	C	31	GLN
3	C	34	GLN
3	C	39	GLN
3	C	47	GLN
3	C	63	TYR
3	C	67	GLN
3	C	81	LYS
3	C	101	LYS
3	C	113	ILE
3	C	121	LYS
3	C	149	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	106	GLN
1	A	227	ASN
1	A	239	ASN
1	A	256	GLN
1	A	296	GLN
1	A	320	ASN
1	A	397	GLN
1	A	436	ASN
1	A	486	GLN
1	A	502	ASN

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Mol	Chain	Res	Type
1	A	512	ASN
1	A	519	GLN
1	A	549	GLN
1	A	579	GLN
1	A	583	HIS
1	A	591	GLN
1	A	595	ASN
1	A	606	HIS
1	A	710	HIS
1	A	723	ASN
2	B	355	GLN
2	B	382	ASN
2	B	412	HIS
2	B	439	ASN
2	B	502	GLN
2	B	514	HIS
2	B	589	ASN
2	B	640	GLN
2	B	683	GLN
2	B	721	HIS
2	B	778	ASN
2	B	841	GLN
2	B	913	GLN
2	B	932	ASN
2	B	1003	ASN
2	B	1088	GLN
2	B	1092	ASN
3	C	39	GLN
3	C	152	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	699/769 (90%)	-0.37	9 (1%)	79	71	10, 35, 75, 103	0
2	B	731/753 (97%)	-0.48	9 (1%)	81	73	8, 29, 74, 98	0
3	C	137/196 (69%)	0.05	4 (2%)	55	43	24, 63, 91, 111	0
All	All	1567/1718 (91%)	-0.38	22 (1%)	78	69	8, 33, 79, 111	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	346	GLU	3.5
2	B	1055	ILE	3.2
1	A	394	MET	3.2
1	A	123	ARG	3.1
2	B	772	ASP	2.9
3	C	1	MET	2.8
2	B	445	LEU	2.5
1	A	508	THR	2.5
2	B	424	THR	2.4
3	C	21	GLN	2.3
2	B	658	ARG	2.3
2	B	427	THR	2.3
2	B	959	ASN	2.3
3	C	101	LYS	2.3
1	A	630	GLY	2.3
1	A	683	HIS	2.2
1	A	75	GLN	2.2
2	B	446	ASP	2.1
1	A	665	ALA	2.1
1	A	474	GLY	2.1
1	A	64	THR	2.1
3	C	98	GLN	2.1

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
4	ZN	A	800	1/1	0.99	0.07	-1.73	47,47,47,47	0
4	ZN	B	1100	1/1	0.99	0.06	-1.90	34,34,34,34	0

6.5 Other polymers (i)

There are no such residues in this entry.