Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 12:26 PM EDT

PDB ID	:	3EWE
Title	:	Crystal Structure of the Nup85/Seh1 Complex
Authors	:	Brohawn, S.G.; Leksa, N.C.; Rajashankar, K.R.; Schwartz, T.U.
Deposited on	:	2008-10-14
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

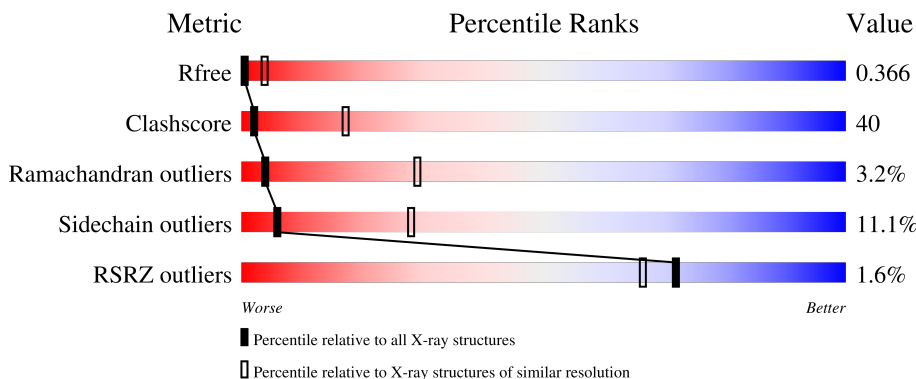|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	Percentile Ranks	Value
Rfree		0.366
Clashscore		40
Ramachandran outliers		3.2%
Sidechain outliers		11.1%
RSRZ outliers		1.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	349	% / 30% / 41% / • / 27%
1	C	349	3% / 31% / 39% / • / 27%
2	B	564	% / 31% / 34% / 5% / 30%
2	D	564	% / 35% / 30% / 6% / 30%

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 9689 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 Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1869	1198	304	358	9			
1	C	255	Total	C	N	O	S	0	0	0
			1872	1201	304	358	9			

- Molecule 2 is a protein called Nucleoporin NUP85.

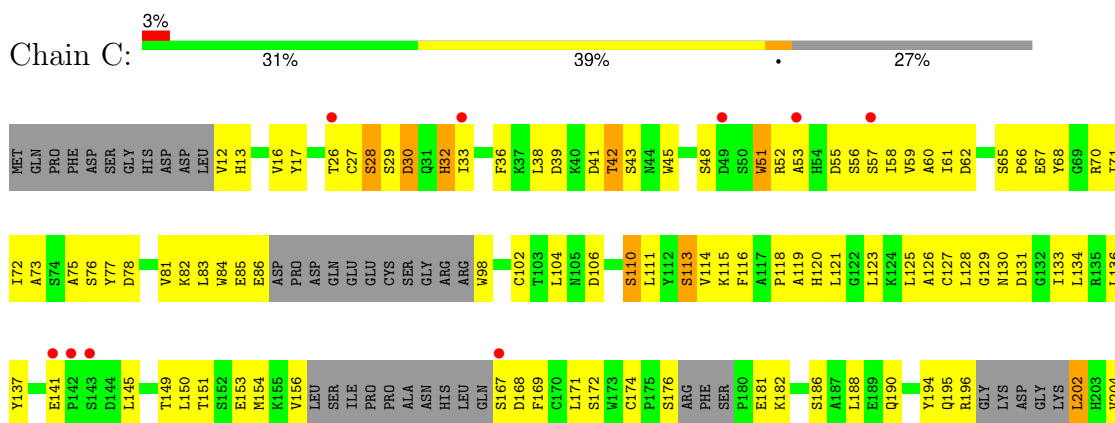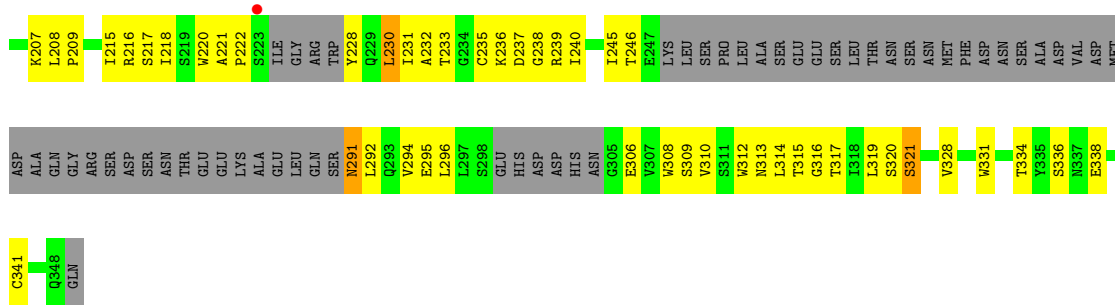| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	395	Total	C	N	O	S	0	0	0
			2974	1941	452	560	21			
2	D	395	Total	C	N	O	S	0	0	0
			2974	1941	452	560	21			

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
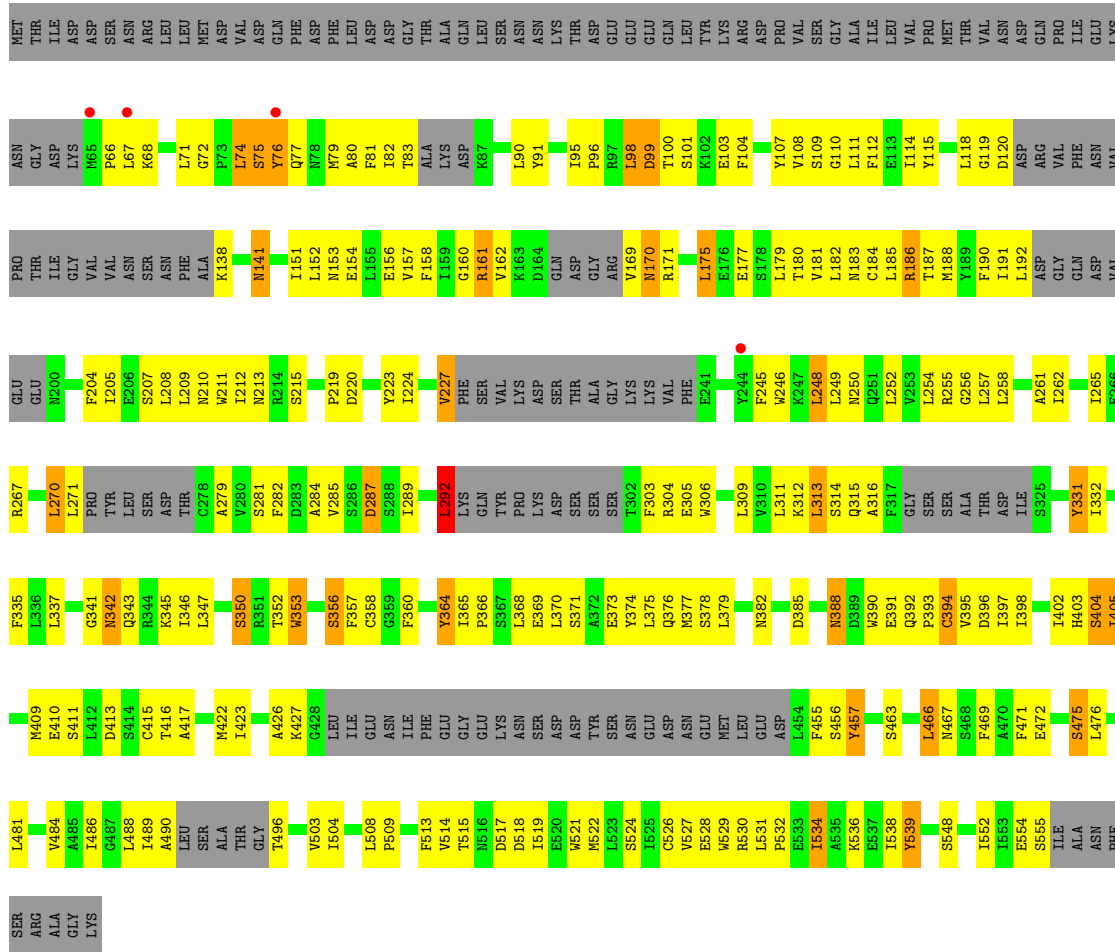
- Molecule 1: Nucleoporin SEH1
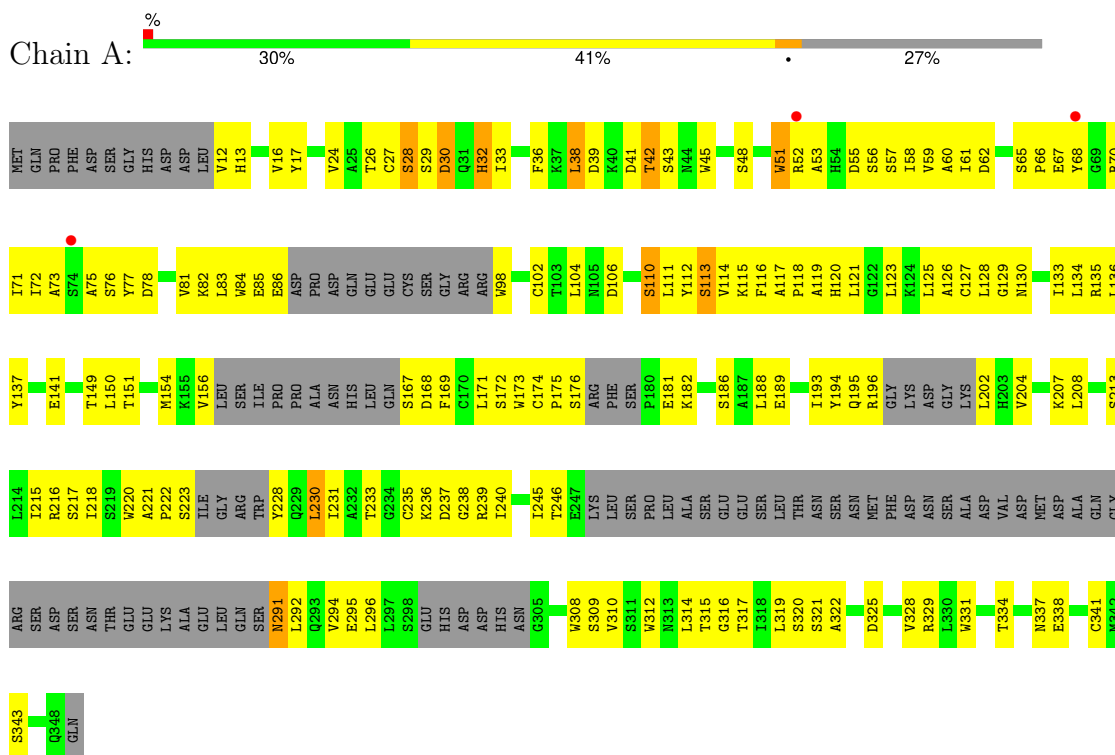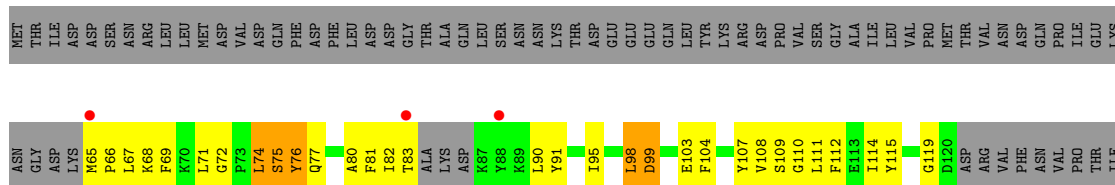

- Molecule 1: Nucleoporin SEH1

Molecule 2: Nucleoporin NUP85

Chain B:

Molecule 2: Nucleoporin NUP85

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	112.56Å 112.56Å 350.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 3.50 39.80 – 3.13	Depositor EDS
% Data completeness (in resolution range)	96.4 (29.75-3.50) 95.4 (39.80-3.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.17 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.326 , 0.369 0.315 , 0.366	Depositor DCC
R_{free} test set	1955 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	117.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 102.3	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9689	wwPDB-VP
Average B, all atoms (Å^2)	156.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.41	0/1909	0.60	0/2610
1	C	0.39	0/1912	0.59	0/2614
2	B	0.41	0/3033	0.59	2/4137 (0.0%)
2	D	0.42	0/3033	0.60	0/4137
All	All	0.41	0/9887	0.59	2/13498 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	313	LEU	CA-CB-CG	5.25	127.38	115.30
2	B	292	LEU	CA-CB-CG	5.11	127.06	115.30

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	1869	0	1709	171	0
1	C	1872	0	1718	169	0
2	B	2974	0	2765	228	0
2	D	2974	0	2765	210	0
All	All	9689	0	8957	750	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 40.

All (750) 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:239:ARG:HD3	1:A:296:LEU:HD11	1.17	1.15
1:C:239:ARG:HD3	1:C:296:LEU:HD11	1.25	1.09
2:B:279:ALA:HA	2:B:282:PHE:HD2	1.22	1.03
1:C:118:PRO:HB2	1:C:120:HIS:HD2	1.23	1.03
1:C:154:MET:CB	1:C:202:LEU:HD13	1.89	1.02
1:C:154:MET:HB2	1:C:202:LEU:CD1	1.89	1.02
1:A:118:PRO:HB2	1:A:120:HIS:HD2	1.23	1.01
2:D:262:ILE:HA	2:D:265:ILE:HD12	1.40	0.99
2:D:279:ALA:HA	2:D:282:PHE:HD2	1.29	0.98
1:C:154:MET:HB2	1:C:202:LEU:HD13	0.98	0.97
1:A:58:ILE:HD13	1:A:76:SER:HB2	1.45	0.97
2:D:413:ASP:OD2	2:D:416:THR:HG23	1.65	0.94
2:B:413:ASP:OD2	2:B:416:THR:HG23	1.69	0.93
1:C:60:ALA:HB3	1:C:75:ALA:HB3	1.52	0.92
2:D:360:PHE:HB3	2:D:374:TYR:CE1	2.04	0.92
2:B:74:LEU:HD23	2:B:475:SER:O	1.69	0.92
2:D:74:LEU:HG	2:D:75:SER:H	1.34	0.92
1:A:51:TRP:N	1:A:51:TRP:HE3	1.69	0.90
2:B:370:LEU:HB3	2:B:374:TYR:CE2	2.06	0.90
2:B:262:ILE:HA	2:B:265:ILE:HD12	1.52	0.90
2:B:74:LEU:HG	2:B:75:SER:H	1.35	0.90
2:D:360:PHE:HB3	2:D:374:TYR:CD1	2.08	0.88
1:A:60:ALA:HB3	1:A:75:ALA:HB3	1.56	0.88
2:B:370:LEU:CB	2:B:374:TYR:HE2	1.87	0.88
2:B:67:LEU:HA	2:B:82:ILE:HG13	1.55	0.87
1:C:58:ILE:HD13	1:C:76:SER:HB2	1.54	0.87
1:A:239:ARG:HD3	1:A:296:LEU:CD1	2.03	0.87
1:C:154:MET:HG3	1:C:202:LEU:HD22	1.55	0.87
1:A:81:VAL:HG23	1:A:111:LEU:HD12	1.55	0.86
2:D:258:LEU:HD13	2:D:289:ILE:HG23	1.56	0.86
2:D:74:LEU:HD11	2:D:98:LEU:HG	1.58	0.86
1:C:27:CYS:HB2	1:C:58:ILE:HB	1.56	0.86
1:A:118:PRO:HB2	1:A:120:HIS:CD2	2.11	0.85
2:B:74:LEU:HG	2:B:75:SER:N	1.92	0.84
1:C:51:TRP:HE3	1:C:51:TRP:N	1.75	0.84
1:C:169:PHE:HB2	1:C:186:SER:O	1.77	0.84
2:D:74:LEU:HG	2:D:75:SER:N	1.93	0.83
1:A:51:TRP:HE3	1:A:51:TRP:H	1.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:220:ASP:HA	2:D:223:TYR:HD2	1.44	0.82
2:B:74:LEU:HD11	2:B:98:LEU:HG	1.61	0.82
2:B:220:ASP:HA	2:B:223:TYR:HD2	1.44	0.82
1:A:169:PHE:HB2	1:A:186:SER:O	1.81	0.80
2:B:509:PRO:HD3	2:B:534:ILE:HD11	1.63	0.80
1:A:51:TRP:N	1:A:51:TRP:CE3	2.50	0.80
2:B:258:LEU:HD13	2:B:289:ILE:HG23	1.64	0.80
2:D:245:PHE:CE2	2:D:249:LEU:HD11	2.17	0.80
1:C:118:PRO:HB2	1:C:120:HIS:CD2	2.12	0.79
1:A:331:TRP:CZ3	1:A:341:CYS:HB2	2.18	0.79
1:C:239:ARG:HD3	1:C:296:LEU:CD1	2.09	0.79
2:B:107:TYR:OH	2:B:416:THR:HG22	1.83	0.78
2:D:292:LEU:C	2:D:292:LEU:HD23	2.03	0.78
1:C:331:TRP:CZ3	1:C:341:CYS:HB2	2.19	0.78
1:A:27:CYS:HB2	1:A:58:ILE:HB	1.64	0.77
1:C:32:HIS:C	1:C:33:ILE:HD13	2.05	0.77
1:C:60:ALA:HB1	1:C:114:VAL:HG12	1.67	0.77
2:D:220:ASP:HA	2:D:223:TYR:CD2	2.19	0.76
2:B:279:ALA:HA	2:B:282:PHE:CD2	2.14	0.76
1:C:51:TRP:HE3	1:C:51:TRP:H	1.32	0.76
1:C:291:ASN:O	1:C:292:LEU:HD23	1.85	0.75
2:B:98:LEU:HD22	2:B:99:ASP:N	2.00	0.75
2:D:67:LEU:HA	2:D:82:ILE:HG13	1.66	0.75
2:B:220:ASP:HA	2:B:223:TYR:CD2	2.21	0.74
1:C:51:TRP:N	1:C:51:TRP:CE3	2.56	0.74
2:B:360:PHE:HB3	2:B:374:TYR:CD1	2.22	0.74
1:C:81:VAL:HG23	1:C:111:LEU:HD12	1.68	0.74
2:B:368:LEU:HD23	2:B:368:LEU:H	1.51	0.74
2:B:360:PHE:HB3	2:B:374:TYR:CE1	2.22	0.74
1:A:291:ASN:O	1:A:292:LEU:HD23	1.87	0.73
1:A:315:THR:HB	2:B:471:PHE:HB3	1.70	0.73
1:A:56:SER:CB	1:A:77:TYR:HB2	2.19	0.73
2:D:279:ALA:HA	2:D:282:PHE:CD2	2.20	0.72
1:C:26:THR:HG21	2:D:90:LEU:HD11	1.71	0.72
2:D:250:ASN:HD21	2:D:335:PHE:HD1	1.37	0.72
2:B:422:MET:SD	2:B:466:LEU:HD11	2.29	0.72
2:B:370:LEU:HB2	2:B:374:TYR:HE2	1.54	0.72
2:B:385:ASP:HB2	2:B:391:GLU:OE1	1.88	0.71
1:A:33:ILE:HD11	1:A:58:ILE:HG13	1.71	0.71
2:B:370:LEU:CB	2:B:374:TYR:CE2	2.68	0.71
2:D:98:LEU:HD22	2:D:99:ASP:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:HG12	1:A:17:TYR:H	1.54	0.71
1:C:315:THR:HB	2:D:471:PHE:HB3	1.72	0.70
1:C:33:ILE:HD11	1:C:58:ILE:HG13	1.73	0.70
2:D:537:GLU:O	2:D:541:THR:HG23	1.92	0.70
1:A:27:CYS:SG	1:A:61:ILE:HD11	2.32	0.70
2:B:353:TRP:HE1	2:B:391:GLU:HG2	1.55	0.70
2:D:368:LEU:HD23	2:D:368:LEU:H	1.56	0.70
2:B:504:ILE:HG22	2:B:531:LEU:HD21	1.72	0.70
2:B:74:LEU:HD13	2:B:95:ILE:HD12	1.73	0.69
2:D:422:MET:SD	2:D:466:LEU:HD11	2.32	0.69
1:C:16:VAL:HG12	1:C:17:TYR:H	1.57	0.69
2:D:360:PHE:CB	2:D:374:TYR:CD1	2.76	0.69
1:A:45:TRP:CZ2	2:B:77:GLN:HG2	2.28	0.69
1:A:45:TRP:HZ2	2:B:77:GLN:HG2	1.57	0.69
2:B:245:PHE:CE2	2:B:249:LEU:HD11	2.28	0.69
2:D:285:VAL:HG23	2:D:313:LEU:HD21	1.74	0.69
2:D:541:THR:HA	2:D:544:ASN:HD22	1.58	0.68
1:A:32:HIS:C	1:A:33:ILE:HD13	2.14	0.68
2:D:74:LEU:CD1	2:D:98:LEU:HG	2.23	0.68
1:C:56:SER:CB	1:C:77:TYR:HB2	2.24	0.68
2:D:524:SER:O	2:D:527:VAL:HG12	1.93	0.68
2:B:185:LEU:HD23	2:B:190:PHE:CE1	2.29	0.68
2:B:248:LEU:HD12	2:B:248:LEU:O	1.94	0.68
1:C:150:LEU:H	1:C:150:LEU:HD23	1.57	0.67
1:A:26:THR:HG21	2:B:90:LEU:HD11	1.76	0.67
1:C:310:VAL:HA	1:C:320:SER:O	1.94	0.67
2:D:114:ILE:HD11	2:D:154:GLU:HG3	1.75	0.67
1:A:51:TRP:CZ2	1:A:98:TRP:HB2	2.30	0.67
2:B:67:LEU:HD22	2:B:82:ILE:HG12	1.76	0.67
2:B:246:TRP:CZ3	2:B:249:LEU:HD12	2.30	0.67
1:C:114:VAL:O	1:C:115:LYS:HG3	1.94	0.67
2:D:481:LEU:O	2:D:484:VAL:HB	1.94	0.67
2:D:370:LEU:CB	2:D:374:TYR:HE2	2.08	0.67
2:B:177:GLU:CG	2:B:390:TRP:HB3	2.25	0.67
1:A:167:SER:HA	1:A:188:LEU:HD21	1.76	0.66
2:B:67:LEU:O	2:B:68:LYS:HG2	1.95	0.66
2:B:515:THR:HG22	2:B:517:ASP:H	1.59	0.66
2:D:107:TYR:OH	2:D:416:THR:HG22	1.95	0.66
1:C:334:THR:HG23	1:C:338:GLU:O	1.95	0.66
2:D:67:LEU:HD22	2:D:82:ILE:HG12	1.76	0.66
2:B:81:PHE:C	2:B:82:ILE:HD12	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:LEU:CD2	2:B:190:PHE:HE1	2.08	0.66
2:D:74:LEU:HD23	2:D:475:SER:O	1.94	0.66
1:A:60:ALA:HB1	1:A:114:VAL:HG12	1.78	0.66
2:D:74:LEU:HD13	2:D:95:ILE:HD12	1.77	0.66
1:A:126:ALA:HB2	1:A:136:LEU:HD12	1.76	0.66
2:B:185:LEU:HD23	2:B:190:PHE:HE1	1.60	0.66
2:D:370:LEU:HB2	2:D:374:TYR:HE2	1.60	0.66
2:D:341:GLY:HA2	2:D:346:ILE:HD11	1.78	0.66
1:A:174:CYS:HB2	1:A:220:TRP:CE2	2.31	0.66
1:A:51:TRP:CD1	1:A:84:TRP:HZ3	2.13	0.65
1:A:83:LEU:HD12	1:A:102:CYS:HB2	1.77	0.65
1:C:195:GLN:HG2	1:C:196:ARG:H	1.61	0.65
1:C:167:SER:HA	1:C:188:LEU:HD21	1.76	0.65
2:D:385:ASP:HB2	2:D:391:GLU:OE1	1.96	0.65
2:D:246:TRP:CZ3	2:D:249:LEU:HD12	2.32	0.65
2:B:250:ASN:HD21	2:B:335:PHE:HD1	1.43	0.65
2:B:285:VAL:HG23	2:B:313:LEU:HD21	1.77	0.65
2:B:375:LEU:HD22	2:B:398:ILE:HB	1.79	0.65
1:C:45:TRP:HZ2	2:D:77:GLN:HG2	1.61	0.65
1:C:65:SER:CB	1:C:119:ALA:HB2	2.27	0.65
1:C:125:LEU:O	1:C:136:LEU:HD12	1.96	0.65
1:A:310:VAL:HA	1:A:320:SER:O	1.96	0.65
2:B:341:GLY:HA2	2:B:346:ILE:HD11	1.79	0.65
2:B:529:TRP:HB3	2:B:531:LEU:HD11	1.79	0.65
2:D:110:GLY:O	2:D:114:ILE:HG13	1.97	0.65
1:A:65:SER:CB	1:A:119:ALA:HB2	2.27	0.64
2:B:185:LEU:CD2	2:B:190:PHE:CE1	2.80	0.64
1:A:53:ALA:HB2	1:A:84:TRP:CH2	2.32	0.64
1:C:45:TRP:CZ2	2:D:77:GLN:HG2	2.33	0.64
1:C:208:LEU:HD23	1:C:292:LEU:HD13	1.80	0.64
2:B:114:ILE:HD11	2:B:154:GLU:HG3	1.79	0.64
2:B:526:CYS:SG	2:B:534:ILE:CG2	2.86	0.64
2:B:527:VAL:HG13	2:B:528:GLU:N	2.12	0.64
1:C:27:CYS:SG	1:C:61:ILE:HD11	2.38	0.64
2:B:279:ALA:CA	2:B:282:PHE:HD2	2.07	0.63
2:D:75:SER:O	2:D:76:TYR:HB3	1.97	0.63
2:B:74:LEU:CD1	2:B:98:LEU:HG	2.26	0.63
2:D:248:LEU:HD12	2:D:248:LEU:O	1.99	0.63
2:D:107:TYR:CZ	2:D:111:LEU:HD11	2.34	0.63
1:A:195:GLN:HG2	1:A:196:ARG:H	1.62	0.63
1:A:174:CYS:HB2	1:A:220:TRP:CD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LEU:HD13	2:B:95:ILE:CD1	2.28	0.62
1:C:51:TRP:CZ2	1:C:98:TRP:HB2	2.33	0.62
2:D:212:ILE:HD13	2:D:358:CYS:SG	2.39	0.62
1:A:245:ILE:HG12	1:A:292:LEU:CD2	2.30	0.62
2:D:375:LEU:HD22	2:D:398:ILE:HB	1.80	0.62
1:A:13:HIS:HB2	1:A:59:VAL:HA	1.81	0.62
1:C:86:GLU:HA	1:C:98:TRP:HA	1.82	0.62
1:C:110:SER:O	1:C:129:GLY:HA3	2.00	0.62
2:D:530:ARG:C	2:D:532:PRO:HD3	2.21	0.61
1:A:60:ALA:C	1:A:61:ILE:HG13	2.20	0.61
1:A:106:ASP:HB2	1:A:137:TYR:OH	1.99	0.61
1:C:312:TRP:CZ3	1:C:317:THR:HG22	2.35	0.61
2:D:393:PRO:HB3	2:D:405:ILE:HD12	1.81	0.61
1:C:245:ILE:HG12	1:C:292:LEU:CD2	2.30	0.61
1:A:334:THR:HG23	1:A:338:GLU:O	2.00	0.61
2:D:219:PRO:HB2	2:D:223:TYR:CZ	2.36	0.61
1:A:125:LEU:O	1:A:136:LEU:HD12	2.00	0.61
1:A:58:ILE:CD1	1:A:76:SER:HB2	2.27	0.61
2:B:75:SER:O	2:B:76:TYR:HB3	2.01	0.61
1:A:150:LEU:H	1:A:150:LEU:HD23	1.65	0.61
1:C:28:SER:HB2	1:C:30:ASP:OD1	2.01	0.61
2:D:360:PHE:CG	2:D:374:TYR:HD1	2.18	0.61
1:A:114:VAL:O	1:A:115:LYS:HG3	2.01	0.60
1:C:55:ASP:OD1	1:C:78:ASP:HB3	2.01	0.60
1:C:83:LEU:HD12	1:C:102:CYS:HB2	1.83	0.60
1:A:308:TRP:CE2	2:B:66:PRO:HB3	2.36	0.60
1:A:55:ASP:OD1	1:A:78:ASP:HB3	2.01	0.60
1:A:312:TRP:CZ3	1:A:317:THR:HG22	2.37	0.60
2:D:303:PHE:O	2:D:306:TRP:N	2.34	0.60
2:B:524:SER:O	2:B:527:VAL:HG12	2.02	0.60
2:B:82:ILE:CG2	2:B:83:THR:N	2.65	0.60
2:D:471:PHE:HE2	2:D:489:ILE:HD11	1.66	0.60
2:D:67:LEU:O	2:D:68:LYS:HG2	2.02	0.60
2:D:99:ASP:N	2:D:99:ASP:OD1	2.34	0.60
2:B:373:GLU:O	2:B:377:MET:HG3	2.02	0.59
1:A:221:ALA:HB2	1:A:230:LEU:HD12	1.84	0.59
2:B:115:TYR:CE2	2:B:488:LEU:HD23	2.37	0.59
1:C:126:ALA:HB2	1:C:136:LEU:HD12	1.83	0.59
2:D:185:LEU:O	2:D:185:LEU:HD23	2.02	0.59
1:A:110:SER:O	1:A:129:GLY:HA3	2.02	0.59
1:A:111:LEU:HD13	1:A:127:CYS:SG	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:107:TYR:CZ	2:B:111:LEU:HD11	2.38	0.59
2:B:187:THR:OG1	2:B:207:SER:HB3	2.03	0.59
2:B:394:CYS:HA	2:B:397:ILE:HD12	1.85	0.59
2:B:536:LYS:O	2:B:539:TYR:HB3	2.03	0.59
1:C:27:CYS:CB	1:C:58:ILE:HB	2.30	0.59
2:D:74:LEU:CG	2:D:75:SER:H	2.13	0.59
2:D:152:LEU:O	2:D:156:GLU:HG3	2.03	0.59
1:A:86:GLU:HA	1:A:98:TRP:HA	1.85	0.58
2:B:99:ASP:N	2:B:99:ASP:OD1	2.36	0.58
1:C:174:CYS:HB2	1:C:220:TRP:CE2	2.38	0.58
1:C:308:TRP:CE2	2:D:66:PRO:HB3	2.37	0.58
2:D:81:PHE:C	2:D:82:ILE:HD12	2.23	0.58
1:C:42:THR:O	1:C:43:SER:HB2	2.03	0.58
2:D:402:ILE:O	2:D:404:SER:N	2.37	0.58
2:B:393:PRO:HB3	2:B:405:ILE:HD12	1.84	0.58
1:C:27:CYS:CB	1:C:61:ILE:HD11	2.33	0.58
2:D:279:ALA:CA	2:D:282:PHE:HD2	2.12	0.58
2:B:303:PHE:O	2:B:306:TRP:N	2.36	0.58
2:B:530:ARG:C	2:B:532:PRO:HD3	2.24	0.58
2:D:250:ASN:ND2	2:D:335:PHE:HD1	2.02	0.58
2:B:177:GLU:HG2	2:B:390:TRP:HB3	1.85	0.58
2:D:392:GLN:HB3	2:D:393:PRO:HD3	1.85	0.58
1:A:295:GLU:N	1:A:295:GLU:OE1	2.37	0.58
2:D:360:PHE:CB	2:D:374:TYR:HD1	2.15	0.58
1:C:291:ASN:C	1:C:292:LEU:HD23	2.24	0.57
1:C:77:TYR:HA	1:C:110:SER:OG	2.03	0.57
2:B:250:ASN:ND2	2:B:335:PHE:HD1	2.03	0.57
2:D:115:TYR:CE2	2:D:488:LEU:HD23	2.38	0.57
2:B:82:ILE:CG2	2:B:83:THR:HG23	2.35	0.57
1:C:51:TRP:CD1	1:C:84:TRP:HZ3	2.22	0.57
2:B:98:LEU:HD22	2:B:99:ASP:H	1.69	0.57
1:C:27:CYS:HB3	1:C:61:ILE:HD11	1.85	0.57
1:C:316:GLY:O	1:C:317:THR:C	2.42	0.57
2:D:74:LEU:HD13	2:D:95:ILE:CD1	2.35	0.57
2:B:409:MET:HB3	2:B:417:ALA:HB2	1.86	0.57
1:C:295:GLU:N	1:C:295:GLU:OE1	2.38	0.57
1:A:208:LEU:HD23	1:A:292:LEU:HD13	1.86	0.57
2:B:385:ASP:HB2	2:B:388:ASN:HD21	1.70	0.57
1:A:60:ALA:O	1:A:61:ILE:HG13	2.05	0.56
1:C:13:HIS:HB2	1:C:59:VAL:HA	1.87	0.56
2:D:370:LEU:HB3	2:D:374:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:393:PRO:O	2:D:405:ILE:HD11	2.06	0.56
2:B:303:PHE:O	2:B:306:TRP:HB3	2.05	0.56
2:D:508:LEU:HD22	2:D:522:MET:HG3	1.87	0.56
2:D:541:THR:HA	2:D:544:ASN:ND2	2.18	0.56
1:A:27:CYS:CB	1:A:61:ILE:HD11	2.34	0.56
1:A:28:SER:HB2	1:A:30:ASP:OD1	2.06	0.56
1:C:77:TYR:HA	1:C:110:SER:CB	2.35	0.56
1:C:133:ILE:O	1:C:133:ILE:HG23	2.05	0.56
1:C:60:ALA:CB	1:C:114:VAL:HG12	2.36	0.56
1:C:65:SER:OG	1:C:119:ALA:HB2	2.05	0.56
1:C:120:HIS:NE2	1:C:121:LEU:HG	2.20	0.56
1:C:217:SER:HB3	1:C:310:VAL:HG12	1.86	0.56
1:C:104:LEU:HD13	1:C:137:TYR:CD2	2.40	0.56
2:D:245:PHE:CE2	2:D:249:LEU:CD1	2.88	0.56
2:B:171:ARG:O	2:B:175:LEU:HB2	2.06	0.56
1:A:320:SER:OG	2:B:71:LEU:HD11	2.06	0.56
1:C:174:CYS:HB2	1:C:220:TRP:CD2	2.40	0.56
2:D:82:ILE:CG2	2:D:83:THR:N	2.68	0.56
2:B:353:TRP:HE1	2:B:391:GLU:CG	2.19	0.56
1:C:194:TYR:CE1	1:C:204:VAL:HG22	2.40	0.56
2:D:82:ILE:CG2	2:D:83:THR:HG23	2.36	0.56
2:B:393:PRO:O	2:B:405:ILE:HD11	2.06	0.55
1:C:33:ILE:CD1	1:C:58:ILE:HG13	2.35	0.55
1:A:68:TYR:CE1	1:A:123:LEU:HG	2.41	0.55
1:A:240:ILE:O	1:A:296:LEU:HD12	2.06	0.55
2:B:152:LEU:O	2:B:156:GLU:HG3	2.05	0.55
2:D:530:ARG:O	2:D:532:PRO:HD3	2.06	0.55
1:A:42:THR:HG23	1:A:42:THR:O	2.07	0.55
2:B:392:GLN:HB3	2:B:393:PRO:HD3	1.87	0.55
2:D:75:SER:O	2:D:76:TYR:CB	2.54	0.55
2:D:292:LEU:C	2:D:292:LEU:CD2	2.74	0.55
1:A:51:TRP:NE1	1:A:84:TRP:CZ3	2.74	0.55
1:C:33:ILE:HD13	1:C:33:ILE:N	2.20	0.55
1:A:134:LEU:HB3	1:A:154:MET:O	2.06	0.55
1:C:53:ALA:HB2	1:C:84:TRP:CH2	2.41	0.55
1:C:85:GLU:HG2	1:C:86:GLU:H	1.71	0.55
1:A:217:SER:HB3	1:A:310:VAL:HG12	1.88	0.55
1:C:104:LEU:HD13	1:C:137:TYR:CG	2.42	0.55
2:D:394:CYS:O	2:D:398:ILE:HG13	2.07	0.55
1:A:39:ASP:C	1:A:41:ASP:H	2.09	0.55
2:B:463:SER:O	2:B:467:ASN:ND2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:508:LEU:HD22	2:B:522:MET:HG3	1.89	0.55
2:D:177:GLU:HG2	2:D:390:TRP:HB3	1.87	0.55
1:C:60:ALA:HB2	1:C:113:SER:HA	1.88	0.55
2:D:177:GLU:CG	2:D:390:TRP:HB3	2.37	0.55
2:B:410:GLU:HG3	2:B:411:SER:N	2.22	0.54
2:D:527:VAL:HG13	2:D:528:GLU:N	2.23	0.54
1:A:56:SER:O	1:A:57:SER:C	2.46	0.54
1:A:120:HIS:NE2	1:A:121:LEU:HG	2.22	0.54
2:D:303:PHE:O	2:D:306:TRP:HB3	2.07	0.54
2:D:529:TRP:HB3	2:D:531:LEU:HD11	1.89	0.54
1:A:33:ILE:CD1	1:A:58:ILE:HG13	2.37	0.54
1:A:60:ALA:HB2	1:A:113:SER:HA	1.88	0.54
2:B:81:PHE:O	2:B:82:ILE:HD12	2.08	0.54
2:B:160:GLY:O	2:B:162:VAL:N	2.41	0.54
2:B:188:MET:CE	2:B:398:ILE:HG23	2.38	0.54
1:C:60:ALA:C	1:C:61:ILE:HG13	2.28	0.54
2:D:356:SER:HB2	2:D:378:SER:OG	2.08	0.53
1:A:42:THR:O	1:A:43:SER:HB2	2.08	0.53
2:D:250:ASN:ND2	2:D:335:PHE:CD1	2.75	0.53
2:D:370:LEU:CB	2:D:374:TYR:CE2	2.90	0.53
1:C:68:TYR:CE1	1:C:123:LEU:HG	2.43	0.53
1:A:27:CYS:HB3	1:A:61:ILE:HD11	1.90	0.53
2:D:490:ALA:CB	2:D:529:TRP:HZ2	2.22	0.53
1:A:53:ALA:HB2	1:A:84:TRP:CZ2	2.44	0.53
2:D:246:TRP:CD1	2:D:331:TYR:CG	2.96	0.53
1:C:106:ASP:HB2	1:C:137:TYR:OH	2.08	0.53
2:B:346:ILE:O	2:B:350:SER:HB2	2.09	0.53
2:B:282:PHE:CE1	2:B:332:ILE:HD13	2.44	0.53
1:C:111:LEU:HD23	1:C:129:GLY:HA3	1.91	0.53
1:C:111:LEU:HD13	1:C:127:CYS:SG	2.48	0.53
2:D:179:LEU:O	2:D:183:ASN:N	2.41	0.53
1:A:65:SER:OG	1:A:119:ALA:HB2	2.09	0.52
1:C:85:GLU:C	1:C:98:TRP:HE3	2.12	0.52
2:D:342:ASN:O	2:D:345:LYS:N	2.36	0.52
2:B:212:ILE:HD13	2:B:358:CYS:SG	2.49	0.52
1:C:39:ASP:C	1:C:41:ASP:H	2.10	0.52
2:D:353:TRP:HE1	2:D:391:GLU:HG2	1.75	0.52
2:D:375:LEU:HD11	2:D:395:VAL:HG13	1.92	0.52
1:A:27:CYS:CB	1:A:58:ILE:HB	2.36	0.52
1:A:27:CYS:HA	1:A:33:ILE:HG23	1.91	0.52
1:A:316:GLY:O	1:A:317:THR:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ASP:HB2	2:B:104:PHE:CD1	2.44	0.52
2:B:224:ILE:HA	2:B:227:VAL:HG23	1.90	0.52
1:A:33:ILE:HD13	1:A:33:ILE:N	2.24	0.52
2:B:95:ILE:O	2:B:98:LEU:CB	2.57	0.52
2:D:187:THR:OG1	2:D:207:SER:HB3	2.10	0.52
2:D:68:LYS:HD2	2:D:81:PHE:CZ	2.44	0.52
2:B:481:LEU:O	2:B:484:VAL:HB	2.09	0.52
2:B:402:ILE:O	2:B:404:SER:N	2.43	0.52
2:D:185:LEU:CD2	2:D:190:PHE:CE1	2.93	0.52
2:D:248:LEU:HD12	2:D:248:LEU:C	2.31	0.52
1:A:186:SER:HB2	1:A:218:ILE:HG13	1.92	0.52
2:B:527:VAL:HG13	2:B:528:GLU:H	1.75	0.52
2:D:98:LEU:HD22	2:D:99:ASP:H	1.74	0.51
2:B:82:ILE:HG22	2:B:83:THR:HG23	1.92	0.51
2:B:158:PHE:CE1	2:B:175:LEU:HD21	2.45	0.51
2:B:281:SER:HB2	2:B:313:LEU:HD11	1.93	0.51
2:B:284:ALA:O	2:B:287:ASP:HB2	2.10	0.51
2:B:360:PHE:CB	2:B:374:TYR:CD1	2.93	0.51
2:D:188:MET:CE	2:D:398:ILE:HG23	2.40	0.51
1:A:51:TRP:NE1	1:A:84:TRP:HZ3	2.09	0.51
1:A:310:VAL:HG22	1:A:319:LEU:HD11	1.92	0.51
1:C:154:MET:CG	1:C:202:LEU:HD22	2.33	0.51
1:A:56:SER:HB3	1:A:77:TYR:HB2	1.89	0.51
1:A:228:TYR:HE1	2:B:457:TYR:HE2	1.58	0.51
1:C:174:CYS:HB3	1:C:182:LYS:O	2.09	0.51
2:B:292:LEU:C	2:B:292:LEU:HD12	2.30	0.51
1:C:67:GLU:O	1:C:67:GLU:HG2	2.11	0.51
1:A:126:ALA:HB2	1:A:136:LEU:CD1	2.40	0.51
1:A:194:TYR:CE1	1:A:204:VAL:HG22	2.45	0.51
2:B:422:MET:SD	2:B:466:LEU:HD21	2.50	0.51
2:B:548:SER:O	2:B:552:ILE:HG12	2.10	0.51
2:B:370:LEU:O	2:B:374:TYR:HD2	1.93	0.51
1:A:32:HIS:HB3	1:A:52:ARG:CA	2.40	0.51
2:B:250:ASN:ND2	2:B:335:PHE:CD1	2.79	0.51
1:C:42:THR:O	1:C:42:THR:HG23	2.11	0.51
1:C:168:ASP:H	1:C:188:LEU:HD11	1.75	0.51
2:D:157:VAL:O	2:D:161:ARG:HG2	2.11	0.51
1:C:70:ARG:O	1:C:98:TRP:HZ3	1.94	0.51
2:D:394:CYS:HA	2:D:397:ILE:HD12	1.93	0.51
2:B:75:SER:O	2:B:76:TYR:CB	2.59	0.50
1:C:56:SER:O	1:C:57:SER:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:GLU:C	1:C:98:TRP:CE3	2.84	0.50
2:D:306:TRP:O	2:D:310:VAL:HG23	2.11	0.50
1:A:32:HIS:HB3	1:A:52:ARG:HA	1.91	0.50
1:A:85:GLU:HG2	1:A:86:GLU:H	1.76	0.50
2:B:471:PHE:HE2	2:B:489:ILE:HD11	1.75	0.50
2:D:423:ILE:O	2:D:426:ALA:HB3	2.11	0.50
1:A:70:ARG:O	1:A:98:TRP:HZ3	1.95	0.50
2:B:394:CYS:O	2:B:398:ILE:HG13	2.11	0.50
1:C:134:LEU:HB3	1:C:154:MET:O	2.12	0.50
1:A:56:SER:HB2	1:A:77:TYR:H	1.76	0.50
2:D:270:LEU:N	2:D:270:LEU:HD23	2.27	0.50
2:D:463:SER:O	2:D:467:ASN:ND2	2.44	0.50
2:B:415:CYS:HA	2:B:469:PHE:CE1	2.46	0.50
2:D:185:LEU:CD2	2:D:190:PHE:HE1	2.24	0.50
2:D:393:PRO:O	2:D:397:ILE:HG13	2.11	0.50
1:C:104:LEU:HD21	1:C:149:THR:HG21	1.94	0.50
1:C:320:SER:OG	2:D:71:LEU:HD11	2.12	0.50
2:D:158:PHE:CE1	2:D:175:LEU:HD21	2.46	0.50
1:A:120:HIS:CD2	1:A:121:LEU:HG	2.46	0.50
2:B:74:LEU:CG	2:B:75:SER:H	2.14	0.50
2:B:179:LEU:O	2:B:183:ASN:N	2.43	0.50
1:C:83:LEU:C	1:C:84:TRP:CD1	2.85	0.50
1:A:53:ALA:CB	1:A:84:TRP:CZ2	2.94	0.49
2:B:246:TRP:HA	2:B:246:TRP:CE3	2.47	0.49
2:D:360:PHE:HB3	2:D:374:TYR:HE1	1.71	0.49
2:D:112:PHE:CD2	2:D:484:VAL:HG22	2.47	0.49
1:A:83:LEU:C	1:A:84:TRP:CD1	2.86	0.49
2:B:79:MET:HE2	2:B:90:LEU:HD22	1.93	0.49
2:D:356:SER:O	2:D:357:PHE:C	2.50	0.49
2:B:526:CYS:SG	2:B:534:ILE:HG21	2.52	0.49
1:C:51:TRP:NE1	1:C:84:TRP:CZ3	2.80	0.49
2:D:184:CYS:HB2	2:D:211:TRP:NE1	2.27	0.49
2:D:245:PHE:CZ	2:D:249:LEU:HD11	2.48	0.49
2:B:112:PHE:CD2	2:B:484:VAL:HG22	2.47	0.49
2:D:330:ASP:C	2:D:330:ASP:OD1	2.50	0.49
1:C:120:HIS:CD2	1:C:121:LEU:HG	2.48	0.49
2:D:80:ALA:HB3	2:D:91:TYR:HB2	1.94	0.49
2:D:82:ILE:HG22	2:D:83:THR:HG23	1.94	0.49
1:A:106:ASP:OD2	1:A:151:THR:HG21	2.12	0.49
2:B:74:LEU:HD13	2:B:95:ILE:CG1	2.42	0.49
2:B:368:LEU:H	2:B:368:LEU:CD2	2.22	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:394:CYS:SG	2:B:397:ILE:HD12	2.52	0.49
1:C:195:GLN:CG	1:C:196:ARG:H	2.25	0.49
1:A:12:VAL:N	1:A:29:SER:HG	2.11	0.49
1:A:77:TYR:HA	1:A:110:SER:CB	2.43	0.49
1:A:174:CYS:HB3	1:A:182:LYS:O	2.12	0.49
1:A:320:SER:OG	2:B:71:LEU:CD1	2.61	0.49
2:B:270:LEU:O	2:B:271:LEU:HD23	2.13	0.49
2:D:158:PHE:O	2:D:162:VAL:HG23	2.12	0.49
2:B:490:ALA:CB	2:B:529:TRP:HZ2	2.25	0.48
2:B:527:VAL:CG1	2:B:528:GLU:N	2.76	0.48
1:C:215:ILE:HG22	1:C:216:ARG:N	2.27	0.48
2:B:82:ILE:HG23	2:B:83:THR:N	2.28	0.48
2:B:305:GLU:O	2:B:309:LEU:HG	2.13	0.48
1:C:128:LEU:HG	1:C:171:LEU:HD23	1.95	0.48
2:D:346:ILE:HG22	2:D:346:ILE:O	2.13	0.48
1:A:85:GLU:C	1:A:98:TRP:HE3	2.17	0.48
1:A:291:ASN:C	1:A:292:LEU:HD23	2.34	0.48
2:D:181:VAL:O	2:D:184:CYS:HB3	2.13	0.48
2:B:529:TRP:CB	2:B:531:LEU:HD11	2.43	0.48
2:D:311:LEU:HA	2:D:314:SER:OG	2.13	0.48
2:D:410:GLU:HG3	2:D:411:SER:N	2.29	0.48
2:D:285:VAL:CG2	2:D:313:LEU:HD21	2.42	0.48
2:B:213:ASN:ND2	2:B:257:LEU:HD21	2.29	0.48
2:D:68:LYS:HD2	2:D:81:PHE:CE1	2.49	0.48
1:A:67:GLU:O	1:A:67:GLU:HG2	2.14	0.48
2:B:423:ILE:O	2:B:426:ALA:HB3	2.14	0.48
2:B:365:ILE:HA	2:B:366:PRO:HD3	1.75	0.48
1:C:208:LEU:HD23	1:C:292:LEU:CD1	2.43	0.48
2:D:153:ASN:O	2:D:157:VAL:HG23	2.14	0.48
2:B:246:TRP:CE3	2:B:249:LEU:HD12	2.49	0.47
2:B:248:LEU:HD12	2:B:248:LEU:C	2.33	0.47
1:A:104:LEU:HD13	1:A:137:TYR:CD2	2.48	0.47
1:C:154:MET:CB	1:C:202:LEU:CD1	2.68	0.47
2:D:152:LEU:CD1	2:D:186:ARG:HD3	2.45	0.47
2:D:246:TRP:HA	2:D:246:TRP:CE3	2.48	0.47
1:A:17:TYR:OH	2:B:79:MET:HG2	2.14	0.47
1:A:85:GLU:C	1:A:98:TRP:CE3	2.87	0.47
2:D:152:LEU:HD23	2:D:152:LEU:HA	1.67	0.47
2:B:281:SER:HB2	2:B:313:LEU:CD1	2.45	0.47
1:C:310:VAL:HG22	1:C:319:LEU:HD11	1.95	0.47
2:D:95:ILE:O	2:D:98:LEU:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:LEU:CD1	2:D:289:ILE:HG23	2.37	0.47
1:A:42:THR:O	1:A:42:THR:CG2	2.62	0.47
1:A:86:GLU:O	1:A:86:GLU:HG3	2.14	0.47
1:C:126:ALA:HB2	1:C:136:LEU:CD1	2.44	0.47
2:D:390:TRP:C	2:D:393:PRO:HD2	2.35	0.47
2:B:138:LYS:O	2:B:141:ASN:HB2	2.15	0.47
2:D:284:ALA:O	2:D:287:ASP:HB2	2.15	0.47
2:D:337:LEU:HD23	2:D:337:LEU:HA	1.55	0.47
2:D:345:LYS:C	2:D:347:LEU:H	2.18	0.47
2:D:541:THR:O	2:D:545:GLN:HG3	2.15	0.47
1:A:67:GLU:CD	1:A:68:TYR:CE1	2.88	0.47
1:A:171:LEU:HD12	1:A:171:LEU:O	2.14	0.47
1:C:56:SER:HB2	1:C:77:TYR:H	1.79	0.47
2:D:490:ALA:HB2	2:D:529:TRP:HZ2	1.78	0.47
2:D:508:LEU:N	2:D:509:PRO:HD2	2.30	0.47
1:A:27:CYS:CA	1:A:33:ILE:HG23	2.45	0.47
2:B:356:SER:O	2:B:357:PHE:C	2.53	0.47
2:D:373:GLU:O	2:D:377:MET:HG3	2.15	0.47
2:D:246:TRP:CD1	2:D:331:TYR:CD1	3.02	0.47
1:A:112:TYR:HE1	1:A:168:ASP:HA	1.80	0.46
2:B:170:ASN:HD22	2:B:170:ASN:HA	1.56	0.46
1:C:240:ILE:HG12	1:C:321:SER:HB2	1.97	0.46
2:B:292:LEU:C	2:B:292:LEU:CD1	2.84	0.46
2:D:364:TYR:CD2	2:D:365:ILE:HG12	2.49	0.46
2:B:152:LEU:HD21	2:B:182:LEU:HG	1.98	0.46
2:B:211:TRP:CE3	2:B:212:ILE:HG13	2.51	0.46
2:B:315:GLN:HE21	1:C:207:LYS:H	1.63	0.46
2:D:151:ILE:HD12	2:D:423:ILE:HD11	1.97	0.46
1:A:117:ALA:HB2	1:A:173:TRP:CZ2	2.51	0.46
2:B:531:LEU:N	2:B:531:LEU:HD12	2.31	0.46
1:C:32:HIS:HB3	1:C:52:ARG:HA	1.96	0.46
2:B:99:ASP:HB2	2:B:104:PHE:CE1	2.51	0.46
1:C:129:GLY:O	1:C:131:ASP:N	2.48	0.46
1:C:172:SER:HB3	1:C:218:ILE:HG22	1.98	0.46
2:D:81:PHE:O	2:D:82:ILE:HD12	2.16	0.46
2:B:152:LEU:HD23	2:B:152:LEU:HA	1.69	0.46
1:C:120:HIS:CE1	1:C:121:LEU:HD21	2.51	0.46
2:D:515:THR:HB	2:D:518:ASP:H	1.80	0.46
1:A:137:TYR:CD1	1:A:151:THR:HB	2.51	0.46
1:C:73:ALA:HB2	1:C:116:PHE:CZ	2.51	0.46
2:D:160:GLY:O	2:D:162:VAL:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:211:TRP:CE3	2:D:212:ILE:HG13	2.51	0.46
2:B:258:LEU:O	2:B:262:ILE:HG13	2.16	0.46
1:C:32:HIS:HB3	1:C:52:ARG:CA	2.45	0.46
1:C:125:LEU:HG	1:C:126:ALA:N	2.30	0.46
1:C:190:GLN:O	1:C:215:ILE:HD12	2.16	0.46
2:D:474:CYS:SG	2:D:507:LEU:HD13	2.56	0.46
1:A:128:LEU:HG	1:A:171:LEU:HD23	1.98	0.46
2:B:160:GLY:C	2:B:162:VAL:N	2.69	0.46
1:C:171:LEU:HD12	1:C:171:LEU:O	2.15	0.46
2:D:99:ASP:HB2	2:D:104:PHE:CD1	2.50	0.46
2:D:151:ILE:HD12	2:D:423:ILE:CD1	2.46	0.46
1:A:24:VAL:HG13	1:A:36:PHE:HB2	1.97	0.45
1:A:322:ALA:HB2	1:A:328:VAL:HG22	1.99	0.45
2:D:246:TRP:CE3	2:D:249:LEU:HD12	2.51	0.45
2:D:521:TRP:O	2:D:524:SER:HB3	2.16	0.45
1:A:104:LEU:HD13	1:A:137:TYR:CG	2.52	0.45
2:B:110:GLY:O	2:B:114:ILE:HG13	2.16	0.45
1:A:60:ALA:O	1:A:61:ILE:CG1	2.64	0.45
1:A:71:ILE:HA	1:A:84:TRP:O	2.16	0.45
1:A:215:ILE:HG22	1:A:216:ARG:N	2.31	0.45
2:B:95:ILE:O	2:B:98:LEU:HB2	2.16	0.45
1:C:120:HIS:CE1	1:C:121:LEU:CD2	2.99	0.45
1:C:186:SER:HB2	1:C:218:ILE:HG13	1.98	0.45
2:D:346:ILE:O	2:D:350:SER:HB2	2.16	0.45
2:D:353:TRP:HE1	2:D:391:GLU:CG	2.28	0.45
2:D:385:ASP:HB2	2:D:388:ASN:HD21	1.80	0.45
1:A:189:GLU:HA	1:A:213:SER:O	2.16	0.45
2:B:80:ALA:HB3	2:B:91:TYR:HB2	1.98	0.45
2:B:246:TRP:CD1	2:B:331:TYR:CG	3.04	0.45
1:C:62:ASP:HB3	1:C:116:PHE:CD2	2.51	0.45
1:C:72:ILE:N	1:C:72:ILE:HD12	2.32	0.45
2:D:422:MET:SD	2:D:466:LEU:HD21	2.56	0.45
1:A:60:ALA:CB	1:A:114:VAL:HG12	2.44	0.45
1:A:62:ASP:HB3	1:A:116:PHE:CD2	2.52	0.45
1:A:82:LYS:CB	1:A:84:TRP:HE1	2.30	0.45
2:B:521:TRP:O	2:B:524:SER:HB3	2.17	0.45
2:B:527:VAL:CG1	2:B:528:GLU:H	2.30	0.45
1:A:16:VAL:HG12	1:A:17:TYR:N	2.28	0.45
1:A:39:ASP:C	1:A:41:ASP:N	2.71	0.45
1:A:208:LEU:HD23	1:A:292:LEU:CD1	2.46	0.45
2:B:153:ASN:O	2:B:157:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:LEU:HG	2:B:212:ILE:CD1	2.46	0.45
1:C:328:VAL:HG11	2:D:69:PHE:CD1	2.52	0.45
2:D:360:PHE:CG	2:D:374:TYR:CD1	3.01	0.45
1:A:207:LYS:O	1:A:292:LEU:CD1	2.65	0.45
2:D:249:LEU:O	2:D:253:VAL:HG23	2.17	0.45
2:D:390:TRP:O	2:D:390:TRP:CE3	2.69	0.45
1:A:77:TYR:HA	1:A:110:SER:HB2	1.99	0.45
1:A:81:VAL:HG23	1:A:111:LEU:CD1	2.37	0.45
1:C:58:ILE:CD1	1:C:76:SER:HB2	2.36	0.45
1:C:67:GLU:CD	1:C:68:TYR:CE1	2.90	0.45
1:C:39:ASP:C	1:C:41:ASP:N	2.71	0.44
1:C:315:THR:C	1:C:317:THR:H	2.20	0.44
2:D:74:LEU:HD13	2:D:95:ILE:CG1	2.47	0.44
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.78	0.44
2:B:254:LEU:C	2:B:256:GLY:H	2.20	0.44
1:C:153:GLU:O	1:C:154:MET:HG2	2.18	0.44
2:D:65:MET:HA	2:D:66:PRO:HD3	1.77	0.44
2:D:171:ARG:O	2:D:175:LEU:HB2	2.17	0.44
2:D:219:PRO:HB2	2:D:223:TYR:CE2	2.53	0.44
2:B:151:ILE:HD12	2:B:423:ILE:HD11	1.98	0.44
1:A:218:ILE:HD13	1:A:233:THR:HG22	1.98	0.44
1:C:27:CYS:HA	1:C:33:ILE:HG23	2.00	0.44
2:B:311:LEU:O	2:B:312:LYS:C	2.55	0.44
2:B:530:ARG:O	2:B:532:PRO:HD3	2.16	0.44
1:C:42:THR:O	1:C:42:THR:CG2	2.66	0.44
2:D:365:ILE:HA	2:D:366:PRO:HD3	1.74	0.44
1:A:104:LEU:HD21	1:A:149:THR:HG21	2.00	0.44
2:B:282:PHE:CZ	2:B:332:ILE:HD13	2.52	0.44
2:D:82:ILE:HG23	2:D:83:THR:N	2.33	0.44
2:D:224:ILE:HA	2:D:227:VAL:HG23	1.98	0.44
2:D:315:GLN:O	2:D:316:ALA:C	2.55	0.44
2:D:529:TRP:O	2:D:531:LEU:HD12	2.17	0.44
1:A:168:ASP:H	1:A:188:LEU:HD11	1.83	0.44
1:C:235:CYS:HB3	1:C:237:ASP:OD1	2.18	0.44
2:D:95:ILE:O	2:D:98:LEU:HB3	2.18	0.44
2:D:152:LEU:HD12	2:D:186:ARG:HD3	1.99	0.44
1:C:51:TRP:NE1	1:C:84:TRP:HZ3	2.15	0.44
1:C:222:PRO:HG2	1:C:313:ASN:O	2.18	0.44
2:D:388:ASN:C	2:D:390:TRP:H	2.21	0.44
1:A:112:TYR:CE1	1:A:168:ASP:HA	2.53	0.43
1:A:309:SER:CB	2:B:68:LYS:HA	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:GLU:HG3	2:B:390:TRP:HB3	2.00	0.43
2:B:508:LEU:N	2:B:509:PRO:HD2	2.33	0.43
1:C:12:VAL:N	1:C:29:SER:HG	2.16	0.43
1:C:82:LYS:CB	1:C:84:TRP:HE1	2.31	0.43
1:C:309:SER:HB3	2:D:68:LYS:HA	2.00	0.43
2:D:158:PHE:O	2:D:158:PHE:CD2	2.71	0.43
2:D:334:ASP:O	2:D:337:LEU:N	2.51	0.43
2:B:315:GLN:O	2:B:316:ALA:C	2.55	0.43
2:B:364:TYR:CD2	2:B:365:ILE:HG12	2.52	0.43
2:B:515:THR:HB	2:B:518:ASP:H	1.83	0.43
1:C:77:TYR:N	1:C:77:TYR:CD2	2.86	0.43
1:A:133:ILE:HG23	1:A:133:ILE:O	2.18	0.43
1:A:309:SER:HB3	2:B:68:LYS:HA	2.01	0.43
1:C:128:LEU:HD23	1:C:128:LEU:HA	1.80	0.43
2:D:212:ILE:CD1	2:D:358:CYS:SG	3.06	0.43
2:D:249:LEU:HD23	2:D:249:LEU:HA	1.60	0.43
1:A:325:ASP:OD2	1:A:329:ARG:NH2	2.52	0.43
2:B:74:LEU:HD13	2:B:95:ILE:HG13	1.99	0.43
2:B:337:LEU:HA	2:B:337:LEU:HD23	1.80	0.43
1:C:118:PRO:HG2	1:C:174:CYS:O	2.19	0.43
2:B:423:ILE:H	2:B:423:ILE:HG13	1.57	0.43
1:C:53:ALA:CB	1:C:84:TRP:CZ2	3.02	0.43
1:A:228:TYR:CE1	2:B:457:TYR:HE2	2.35	0.43
1:A:236:LYS:C	1:A:238:GLY:H	2.22	0.43
2:B:337:LEU:HD22	2:B:342:ASN:ND2	2.34	0.43
2:D:368:LEU:H	2:D:368:LEU:CD2	2.28	0.43
1:A:126:ALA:HA	1:A:135:ARG:O	2.18	0.43
1:A:239:ARG:CD	1:A:296:LEU:HD11	2.13	0.43
1:C:86:GLU:O	1:C:86:GLU:HG3	2.18	0.43
1:C:145:LEU:HD12	1:C:145:LEU:HA	1.86	0.43
2:D:531:LEU:HD12	2:D:531:LEU:N	2.33	0.43
1:A:73:ALA:HB2	1:A:116:PHE:CZ	2.53	0.43
1:C:36:PHE:CD1	1:C:36:PHE:N	2.86	0.43
1:C:60:ALA:O	1:C:61:ILE:HG13	2.19	0.43
1:C:133:ILE:O	1:C:133:ILE:CG2	2.65	0.43
1:C:236:LYS:C	1:C:238:GLY:H	2.21	0.43
1:C:334:THR:C	1:C:336:SER:H	2.22	0.43
2:B:68:LYS:HD2	2:B:81:PHE:CZ	2.54	0.43
2:B:249:LEU:HD23	2:B:249:LEU:HA	1.59	0.43
1:C:77:TYR:HA	1:C:110:SER:HB2	1.99	0.43
1:C:221:ALA:HB2	1:C:230:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:SER:OG	2:D:71:LEU:CD1	2.67	0.43
2:D:213:ASN:ND2	2:D:257:LEU:HD21	2.34	0.43
1:A:310:VAL:CG2	1:A:319:LEU:HD11	2.49	0.43
2:B:74:LEU:CD2	2:B:475:SER:O	2.55	0.43
2:B:393:PRO:O	2:B:397:ILE:HG13	2.18	0.43
2:D:390:TRP:C	2:D:390:TRP:CD2	2.92	0.43
1:A:217:SER:OG	1:A:309:SER:HA	2.19	0.42
2:B:152:LEU:CD1	2:B:186:ARG:HD3	2.48	0.42
1:C:334:THR:C	1:C:336:SER:N	2.73	0.42
2:D:71:LEU:HB3	2:D:72:GLY:H	1.60	0.42
1:A:343:SER:OG	2:B:96:PRO:HG2	2.18	0.42
2:B:99:ASP:CB	2:B:104:PHE:CD1	3.03	0.42
2:B:508:LEU:HD23	2:B:508:LEU:HA	1.86	0.42
1:C:240:ILE:O	1:C:296:LEU:HD12	2.18	0.42
2:D:205:ILE:H	2:D:205:ILE:HG13	1.44	0.42
2:D:490:ALA:HB2	2:D:529:TRP:CZ2	2.53	0.42
1:A:195:GLN:O	1:A:202:LEU:N	2.53	0.42
1:A:216:ARG:NH1	1:A:308:TRP:CE2	2.87	0.42
2:B:191:ILE:O	2:B:192:LEU:HB2	2.19	0.42
2:B:261:ALA:O	2:B:265:ILE:HG13	2.20	0.42
2:B:271:LEU:HD23	2:B:271:LEU:HA	1.82	0.42
2:D:258:LEU:HD22	2:D:289:ILE:HG23	2.02	0.42
2:B:204:PHE:CD2	2:B:204:PHE:C	2.93	0.42
2:B:356:SER:HB2	2:B:378:SER:OG	2.19	0.42
2:B:471:PHE:N	2:B:471:PHE:CD2	2.87	0.42
1:C:53:ALA:HB2	1:C:84:TRP:CZ2	2.55	0.42
2:D:182:LEU:O	2:D:182:LEU:HD12	2.19	0.42
2:D:282:PHE:CE1	2:D:332:ILE:HD13	2.54	0.42
1:A:38:LEU:HD21	2:B:77:GLN:NE2	2.34	0.42
2:B:219:PRO:HB2	2:B:223:TYR:CZ	2.55	0.42
1:A:71:ILE:C	1:A:72:ILE:HD12	2.40	0.42
1:A:193:ILE:HD11	1:A:231:ILE:HD12	2.01	0.42
2:B:90:LEU:HD23	2:B:90:LEU:HA	1.85	0.42
2:B:118:LEU:O	2:B:120:ASP:N	2.53	0.42
2:B:151:ILE:HD12	2:B:423:ILE:CD1	2.50	0.42
1:C:56:SER:HB3	1:C:77:TYR:HB2	1.98	0.42
2:D:357:PHE:CE1	2:D:398:ILE:HG21	2.55	0.42
2:B:375:LEU:HD11	2:B:395:VAL:HG13	2.01	0.42
2:D:248:LEU:O	2:D:249:LEU:C	2.57	0.42
2:B:345:LYS:C	2:B:347:LEU:H	2.23	0.42
1:C:216:ARG:NH1	1:C:308:TRP:CE2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ILE:HG22	1:C:232:ALA:N	2.34	0.42
2:B:476:LEU:HD12	2:B:476:LEU:O	2.20	0.42
1:C:309:SER:CB	2:D:68:LYS:HA	2.50	0.42
1:A:27:CYS:HB2	1:A:33:ILE:HD12	2.01	0.42
1:A:27:CYS:SG	1:A:27:CYS:O	2.78	0.42
1:A:337:ASN:HD22	1:A:337:ASN:HA	1.66	0.42
2:B:180:THR:HG21	2:B:215:SER:HA	2.00	0.42
2:B:252:LEU:HD23	2:B:252:LEU:HA	1.86	0.42
1:C:56:SER:HB2	1:C:76:SER:OG	2.20	0.42
1:C:68:TYR:CZ	1:C:123:LEU:HG	2.55	0.42
2:B:71:LEU:HB3	2:B:72:GLY:H	1.64	0.41
2:B:152:LEU:HD12	2:B:186:ARG:HD3	2.01	0.41
2:B:554:GLU:O	2:B:555:SER:O	2.37	0.41
1:C:71:ILE:HA	1:C:84:TRP:O	2.20	0.41
1:C:208:LEU:HA	1:C:209:PRO:HD3	1.82	0.41
1:A:292:LEU:O	2:D:311:LEU:HD13	2.20	0.41
2:B:514:VAL:HG12	2:B:515:THR:N	2.35	0.41
1:C:65:SER:HA	1:C:66:PRO:HD3	1.89	0.41
1:A:66:PRO:C	1:A:68:TYR:H	2.23	0.41
2:B:99:ASP:O	2:B:101:SER:N	2.48	0.41
2:B:181:VAL:O	2:B:184:CYS:HB3	2.20	0.41
2:B:208:LEU:O	2:B:209:LEU:C	2.59	0.41
2:B:209:LEU:CD2	2:B:256:GLY:HA3	2.50	0.41
2:B:469:PHE:O	2:B:472:GLU:HB2	2.20	0.41
2:B:513:PHE:CD1	2:B:519:ILE:HD11	2.55	0.41
2:B:554:GLU:O	2:B:555:SER:C	2.58	0.41
1:C:106:ASP:OD2	1:C:151:THR:HG21	2.20	0.41
2:D:138:LYS:O	2:D:141:ASN:HB2	2.20	0.41
1:A:66:PRO:C	1:A:68:TYR:N	2.73	0.41
1:A:68:TYR:CZ	1:A:123:LEU:HG	2.55	0.41
1:C:77:TYR:N	1:C:77:TYR:HD2	2.18	0.41
2:D:375:LEU:HD12	2:D:379:LEU:CD2	2.51	0.41
2:D:536:LYS:O	2:D:540:THR:HG23	2.21	0.41
1:A:308:TRP:NE1	2:B:66:PRO:HB3	2.35	0.41
2:B:184:CYS:HB2	2:B:211:TRP:NE1	2.36	0.41
2:B:342:ASN:O	2:B:343:GLN:C	2.59	0.41
2:B:360:PHE:CB	2:B:374:TYR:HD1	2.33	0.41
1:C:228:TYR:HE1	2:D:457:TYR:HE2	1.67	0.41
2:D:201:ARG:O	2:D:205:ILE:HD11	2.21	0.41
1:A:16:VAL:O	1:A:24:VAL:HG23	2.20	0.41
2:B:179:LEU:O	2:B:183:ASN:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:LEU:HG	2:B:212:ILE:HD11	2.01	0.41
2:B:392:GLN:NE2	2:B:396:ASP:OD1	2.54	0.41
1:C:86:GLU:OE1	1:C:98:TRP:CD1	2.74	0.41
2:D:254:LEU:C	2:D:256:GLY:H	2.24	0.41
2:D:290:GLU:O	2:D:290:GLU:HG2	2.20	0.41
1:A:77:TYR:N	1:A:77:TYR:CD2	2.88	0.41
2:B:95:ILE:O	2:B:98:LEU:HB3	2.20	0.41
1:A:125:LEU:HG	1:A:126:ALA:N	2.35	0.41
1:A:172:SER:HB3	1:A:218:ILE:HG22	2.02	0.41
2:B:370:LEU:HB3	2:B:374:TYR:CD2	2.54	0.41
1:C:111:LEU:HA	1:C:129:GLY:HA3	2.02	0.41
2:D:252:LEU:HD23	2:D:252:LEU:HA	1.78	0.41
1:A:36:PHE:CD1	1:A:36:PHE:N	2.88	0.41
1:A:125:LEU:HG	1:A:126:ALA:H	1.85	0.41
1:A:315:THR:C	1:A:317:THR:H	2.20	0.41
2:B:68:LYS:HD2	2:B:81:PHE:CE1	2.55	0.41
2:B:303:PHE:O	2:B:306:TRP:CB	2.69	0.41
2:B:311:LEU:HD23	2:B:311:LEU:HA	1.85	0.41
2:B:471:PHE:N	2:B:471:PHE:HD2	2.19	0.41
2:B:534:ILE:O	2:B:538:ILE:HG12	2.20	0.41
1:C:71:ILE:C	1:C:72:ILE:HD12	2.42	0.41
1:C:125:LEU:HG	1:C:126:ALA:H	1.84	0.41
2:D:67:LEU:HD22	2:D:82:ILE:CG1	2.49	0.41
2:D:261:ALA:O	2:D:265:ILE:HG13	2.20	0.41
2:D:311:LEU:O	2:D:312:LYS:C	2.59	0.41
2:D:543:GLY:O	2:D:544:ASN:C	2.60	0.41
2:B:370:LEU:O	2:B:374:TYR:CD2	2.74	0.41
1:C:218:ILE:HD13	1:C:233:THR:HG22	2.02	0.41
2:D:75:SER:O	2:D:75:SER:OG	2.39	0.41
1:A:235:CYS:HB3	1:A:237:ASP:OD1	2.21	0.40
1:C:236:LYS:HA	1:C:306:GLU:HG3	2.03	0.40
2:D:311:LEU:HA	2:D:311:LEU:HD23	1.82	0.40
2:D:345:LYS:C	2:D:347:LEU:N	2.74	0.40
2:D:536:LYS:C	2:D:538:ILE:N	2.74	0.40
1:A:28:SER:HB2	1:A:30:ASP:CG	2.42	0.40
1:A:217:SER:O	1:A:233:THR:HA	2.21	0.40
2:B:303:PHE:CG	2:B:304:ARG:N	2.89	0.40
2:B:390:TRP:CD2	2:B:390:TRP:C	2.95	0.40
1:C:236:LYS:C	1:C:238:GLY:N	2.75	0.40
2:D:514:VAL:HG12	2:D:515:THR:N	2.36	0.40
2:D:522:MET:HE3	2:D:538:ILE:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LEU:HD12	1:C:171:LEU:C	2.42	0.40
2:D:537:GLU:O	2:D:537:GLU:HG2	2.22	0.40
1:A:195:GLN:CG	1:A:196:ARG:H	2.28	0.40
1:A:221:ALA:HA	1:A:222:PRO:HD3	1.86	0.40
2:B:67:LEU:HD23	2:B:67:LEU:N	2.36	0.40
2:B:160:GLY:O	2:B:161:ARG:C	2.60	0.40
2:B:360:PHE:CG	2:B:374:TYR:HD1	2.39	0.40
2:B:529:TRP:C	2:B:531:LEU:HD12	2.41	0.40
2:D:281:SER:HB2	2:D:313:LEU:CD1	2.52	0.40
2:D:281:SER:HB2	2:D:313:LEU:HD11	2.04	0.40
1:A:68:TYR:N	1:A:68:TYR:CD1	2.90	0.40
1:A:222:PRO:O	1:A:223:SER:C	2.59	0.40
2:B:270:LEU:N	2:B:270:LEU:HD23	2.36	0.40
1:C:172:SER:HB2	1:C:218:ILE:O	2.22	0.40
2:D:342:ASN:O	2:D:343:GLN:C	2.60	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	239/349 (68%)	201 (84%)	33 (14%)	5 (2%)	7	38
1	C	239/349 (68%)	204 (85%)	30 (13%)	5 (2%)	7	38
2	B	373/564 (66%)	293 (79%)	64 (17%)	16 (4%)	2	22
2	D	373/564 (66%)	298 (80%)	62 (17%)	13 (4%)	3	27
All	All	1224/1826 (67%)	996 (81%)	189 (15%)	39 (3%)	4	29

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
2	B	270	LEU
2	B	364	TYR
2	B	403	HIS
1	C	130	ASN
2	D	270	LEU
2	D	364	TYR
2	D	403	HIS
2	D	141	ASN
1	A	28	SER
2	B	76	TYR
2	B	100	THR
2	B	141	ASN
2	B	161	ARG
2	B	353	TRP
2	B	539	TYR
1	C	28	SER
1	C	181	GLU
2	D	74	LEU
2	D	76	TYR
2	D	119	GLY
2	D	161	ARG
1	A	110	SER
1	A	141	GLU
1	A	181	GLU
2	B	74	LEU
2	B	119	GLY
2	B	210	ASN
2	D	371	SER
2	D	389	ASP
2	B	108	VAL
2	B	331	TYR
1	C	110	SER
2	D	108	VAL
2	D	524	SER
2	B	255	ARG
2	B	267	ARG
1	C	141	GLU
2	D	402	ILE

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	188/305 (62%)	172 (92%)	16 (8%)	10	39
1	C	189/305 (62%)	173 (92%)	16 (8%)	10	39
2	B	304/504 (60%)	266 (88%)	38 (12%)	4	23
2	D	304/504 (60%)	265 (87%)	39 (13%)	4	22
All	All	985/1618 (61%)	876 (89%)	109 (11%)	6	28

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
1	A	32	HIS
1	A	38	LEU
1	A	42	THR
1	A	48	SER
1	A	51	TRP
1	A	113	SER
1	A	156	VAL
1	A	175	PRO
1	A	176	SER
1	A	230	LEU
1	A	246	THR
1	A	291	ASN
1	A	294	VAL
1	A	314	LEU
1	A	321	SER
2	B	75	SER
2	B	98	LEU
2	B	99	ASP
2	B	103	GLU
2	B	109	SER
2	B	169	VAL
2	B	170	ASN
2	B	175	LEU

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Mol	Chain	Res	Type
2	B	186	ARG
2	B	205	ILE
2	B	227	VAL
2	B	248	LEU
2	B	287	ASP
2	B	292	LEU
2	B	314	SER
2	B	342	ASN
2	B	350	SER
2	B	352	THR
2	B	356	SER
2	B	369	GLU
2	B	371	SER
2	B	376	GLN
2	B	379	LEU
2	B	382	ASN
2	B	388	ASN
2	B	394	CYS
2	B	404	SER
2	B	405	ILE
2	B	427	LYS
2	B	455	PHE
2	B	456	SER
2	B	457	TYR
2	B	466	LEU
2	B	475	SER
2	B	486	ILE
2	B	496	THR
2	B	503	VAL
2	B	534	ILE
1	C	30	ASP
1	C	32	HIS
1	C	38	LEU
1	C	42	THR
1	C	48	SER
1	C	51	TRP
1	C	113	SER
1	C	156	VAL
1	C	176	SER
1	C	202	LEU
1	C	230	LEU
1	C	246	THR

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Mol	Chain	Res	Type
1	C	291	ASN
1	C	294	VAL
1	C	314	LEU
1	C	321	SER
2	D	75	SER
2	D	98	LEU
2	D	99	ASP
2	D	103	GLU
2	D	109	SER
2	D	169	VAL
2	D	170	ASN
2	D	175	LEU
2	D	180	THR
2	D	186	ARG
2	D	227	VAL
2	D	248	LEU
2	D	287	ASP
2	D	292	LEU
2	D	314	SER
2	D	334	ASP
2	D	342	ASN
2	D	350	SER
2	D	352	THR
2	D	356	SER
2	D	369	GLU
2	D	371	SER
2	D	376	GLN
2	D	378	SER
2	D	379	LEU
2	D	382	ASN
2	D	383	VAL
2	D	388	ASN
2	D	394	CYS
2	D	404	SER
2	D	405	ILE
2	D	427	LYS
2	D	455	PHE
2	D	456	SER
2	D	457	TYR
2	D	466	LEU
2	D	475	SER
2	D	486	ILE

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Mol	Chain	Res	Type
2	D	496	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	HIS
1	A	337	ASN
2	B	78	ASN
2	B	145	ASN
2	B	170	ASN
2	B	250	ASN
2	B	315	GLN
2	B	376	GLN
2	B	382	ASN
2	B	388	ASN
1	C	120	HIS
1	C	337	ASN
2	D	78	ASN
2	D	145	ASN
2	D	170	ASN
2	D	250	ASN
2	D	376	GLN
2	D	382	ASN
2	D	388	ASN
2	D	403	HIS
2	D	544	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	255/349 (73%)	-0.17	3 (1%)	79	73	113, 154, 229, 288	0
1	C	255/349 (73%)	0.03	10 (3%)	39	35	124, 191, 259, 320	0
2	B	395/564 (70%)	-0.48	4 (1%)	82	77	106, 137, 205, 278	0
2	D	395/564 (70%)	-0.51	4 (1%)	82	77	97, 134, 201, 267	0
All	All	1300/1826 (71%)	-0.33	21 (1%)	72	66	97, 148, 235, 320	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	142	PRO	7.6
2	B	76	TYR	3.9
2	B	65	MET	3.4
1	C	141	GLU	3.3
1	C	49	ASP	3.2
1	C	143	SER	2.9
1	C	53	ALA	2.9
2	B	244	TYR	2.8
1	C	57	SER	2.4
2	D	88	TYR	2.4
1	A	52	ARG	2.3
2	D	65	MET	2.3
2	B	67	LEU	2.2
1	C	167	SER	2.2
1	A	74	SER	2.2
2	D	83	THR	2.2
1	C	223	SER	2.1
2	D	455	PHE	2.1
1	A	68	TYR	2.1
1	C	33	ILE	2.1
1	C	26	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.