



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2016 – 10:33 AM EDT

PDB ID : 5FRR
Title : Structure of the Pds5-Scc1 complex and implications for cohesin function
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Deposited on : 2015-12-22
Resolution : 5.80 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
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)	:	rb-20027939

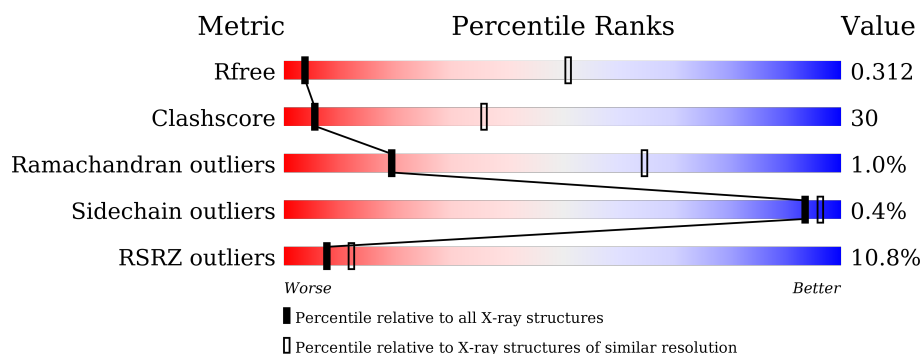
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.80 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	1013 (7.94-3.64)
Clashscore	102246	1043 (7.88-3.70)
Ramachandran outliers	100387	1018 (7.94-3.66)
Sidechain outliers	100360	1008 (7.94-3.64)
RSRZ outliers	91569	1012 (7.94-3.64)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	703	<div> <div>7%</div> <div>47%</div> <div>49%</div> <div>..</div> </div>
1	B	703	<div> <div>13%</div> <div>46%</div> <div>47%</div> <div>• 6%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10858 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 SISTER CHROMATID COHESION PROTEIN PDS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	677	Total	C	N	O	S	0	0	0
			5494	3526	914	1041	13			
1	B	660	Total	C	N	O	S	0	0	0
			5364	3455	889	1009	11			

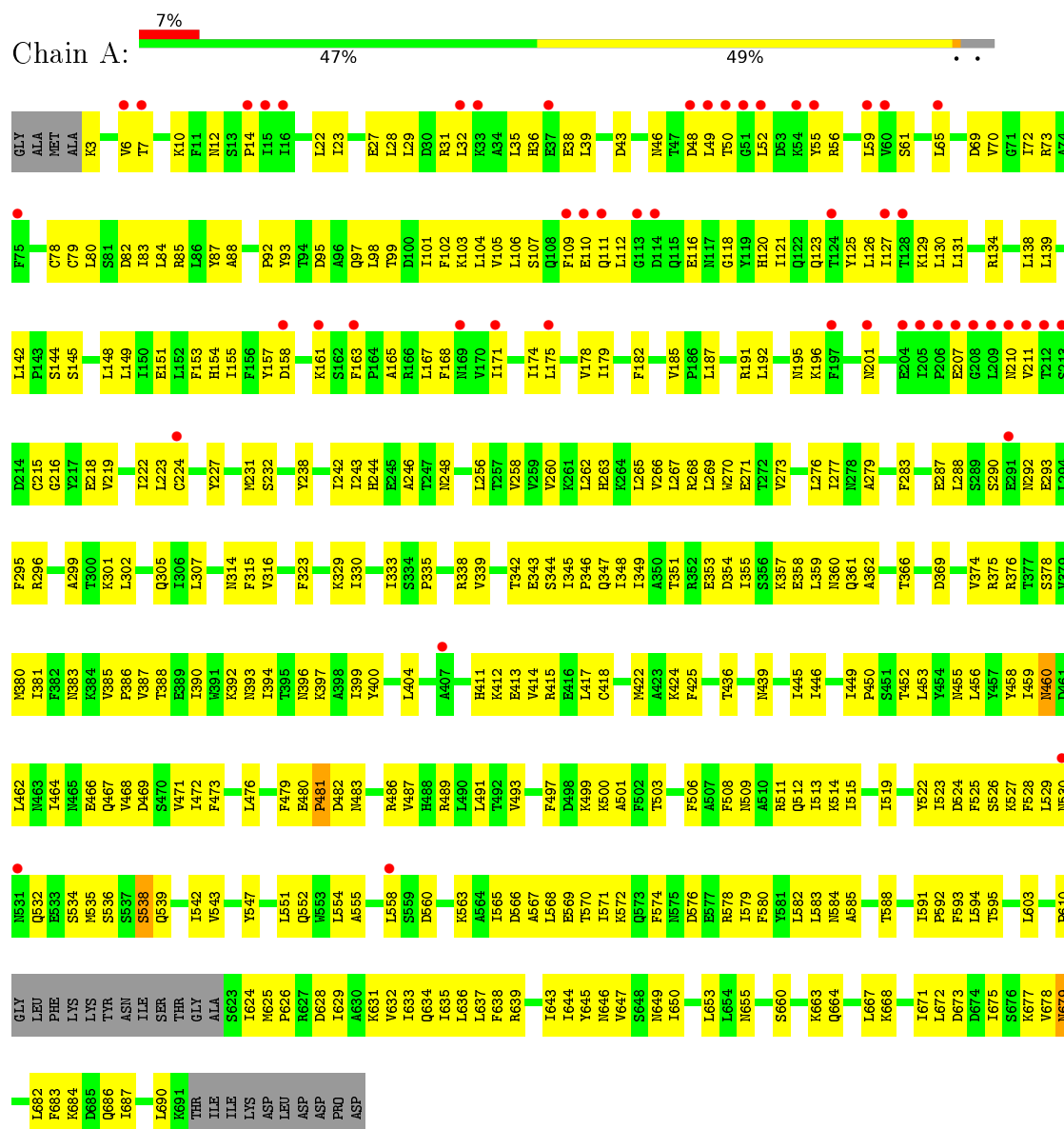
There are 4 discrepancies between the modelled and reference sequences:

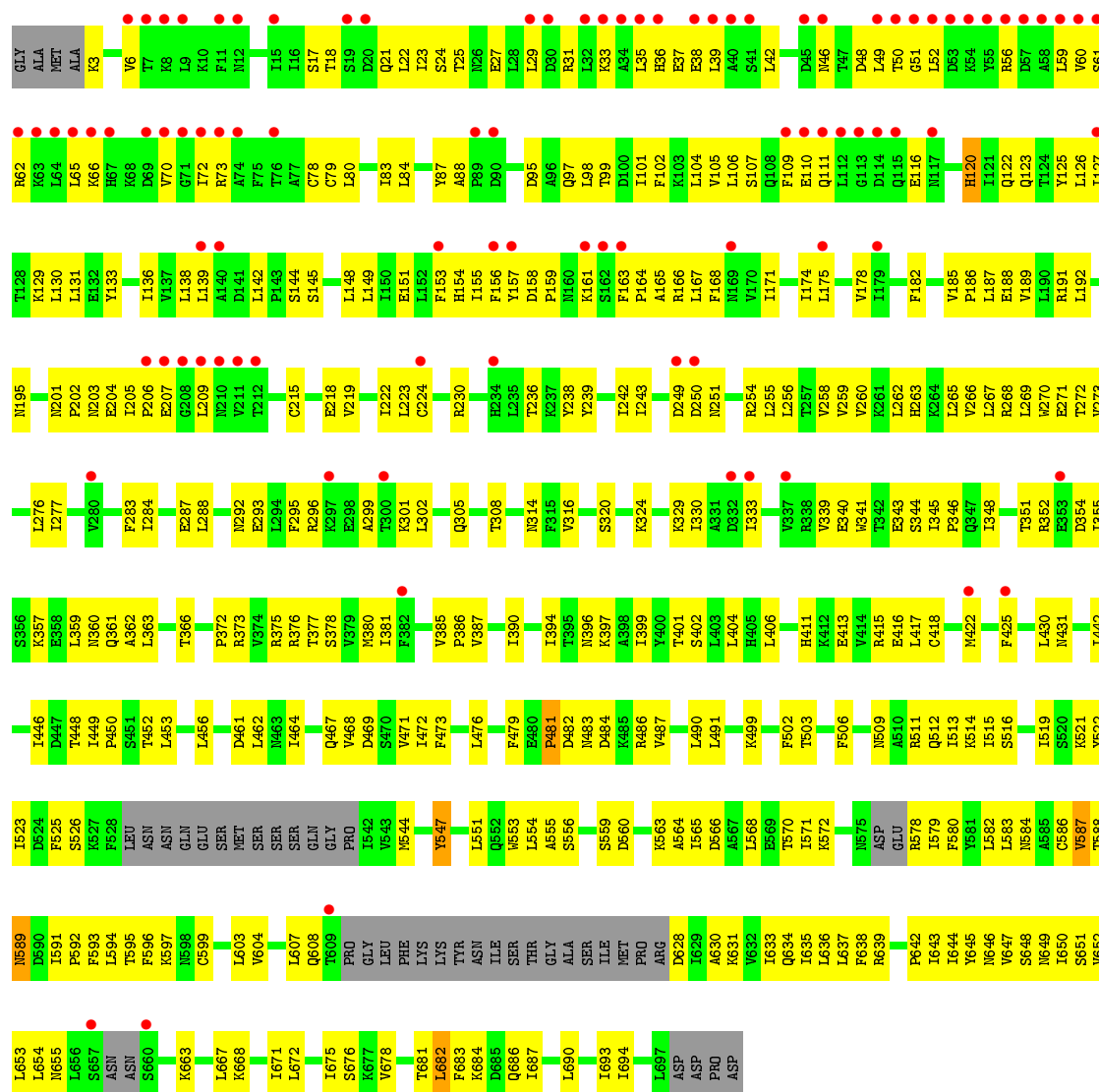
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q04264
A	0	ALA	-	EXPRESSION TAG	UNP Q04264
B	-1	GLY	-	EXPRESSION TAG	UNP Q04264
B	0	ALA	-	EXPRESSION TAG	UNP Q04264

3 Residue-property plots

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: SISTER CHROMATID COHESION PROTEIN PDS5





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	283.69 Å 283.69 Å 172.79 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 5.80 49.19 – 5.79	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-5.80) 99.6 (49.19-5.79)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 5.73 Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.311 0.251 , 0.312	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	383.9	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 402.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	10858	wwPDB-VP
Average B, all atoms (Å ²)	424.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.25	0/5600	0.42	0/7597
1	B	0.25	0/5464	0.41	0/7408
All	All	0.25	0/11064	0.41	0/15005

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5494	0	5551	334	0
1	B	5364	0	5435	324	1
All	All	10858	0	10986	647	1

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 30.

All (647) 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:B:333:ILE:HD12	1:B:333:ILE:H	1.29	0.97
1:A:98:LEU:HD23	1:A:142:LEU:HD21	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:ARG:HA	1:B:376:ARG:HH12	1.36	0.91
1:B:98:LEU:HD23	1:B:142:LEU:HD21	1.52	0.89
1:B:462:LEU:HD13	1:B:559:SER:HA	1.53	0.88
1:A:333:ILE:H	1:A:333:ILE:HD12	1.39	0.86
1:A:483:ASN:HA	1:A:486:ARG:NH1	1.94	0.82
1:B:523:ILE:HD13	1:B:580:PHE:HA	1.63	0.81
1:A:70:VAL:HG12	1:A:73:ARG:HH21	1.46	0.80
1:B:372:PRO:HA	1:B:375:ARG:HE	1.49	0.78
1:B:70:VAL:HG12	1:B:73:ARG:HH21	1.47	0.78
1:B:396:ASN:HB3	1:B:399:ILE:HG12	1.65	0.78
1:A:342:THR:HA	1:A:345:ILE:HD13	1.65	0.78
1:B:308:THR:HA	1:B:351:THR:HG21	1.66	0.78
1:B:105:VAL:HG23	1:B:126:LEU:HD21	1.64	0.77
1:A:682:LEU:H	1:A:682:LEU:HD23	1.50	0.77
1:A:293:GLU:HA	1:A:296:ARG:HE	1.51	0.76
1:A:610:PRO:HG3	1:A:626:PRO:HG2	1.66	0.76
1:A:105:VAL:HG23	1:A:126:LEU:HD21	1.66	0.75
1:B:351:THR:HG22	1:B:352:ARG:HG3	1.67	0.75
1:B:111:GLN:HB2	1:B:123:GLN:HE22	1.53	0.73
1:A:396:ASN:HB3	1:A:399:ILE:HG12	1.70	0.73
1:B:483:ASN:HA	1:B:486:ARG:NH1	2.03	0.73
1:B:242:ILE:HG21	1:B:262:LEU:HD21	1.70	0.73
1:A:480:GLU:HB2	1:A:481:PRO:HA	1.70	0.72
1:A:69:ASP:HB3	1:A:72:ILE:HD13	1.72	0.72
1:A:330:ILE:HG21	1:A:362:ALA:HB1	1.70	0.72
1:A:121:ILE:HD12	1:A:121:ILE:H	1.54	0.71
1:A:154:HIS:HD2	1:A:192:LEU:HD22	1.55	0.70
1:B:633:ILE:HD12	1:B:634:GLN:N	2.07	0.70
1:B:512:GLN:HA	1:B:639:ARG:O	1.92	0.70
1:A:56:ARG:HD2	1:A:92:PRO:HB2	1.74	0.69
1:B:373:ARG:HA	1:B:376:ARG:NH1	2.07	0.69
1:A:380:MET:HA	1:A:383:ASN:HD22	1.55	0.69
1:A:111:GLN:HB2	1:A:123:GLN:HE22	1.57	0.69
1:A:381:ILE:O	1:A:385:VAL:HG12	1.91	0.69
1:B:522:TYR:OH	1:B:572:LYS:HG3	1.93	0.69
1:B:263:HIS:HB3	1:B:302:LEU:HD13	1.74	0.69
1:A:196:LYS:HE3	1:A:216:GLY:HA3	1.74	0.68
1:A:473:PHE:HB3	1:A:479:PHE:HE1	1.57	0.68
1:B:381:ILE:O	1:B:385:VAL:HG12	1.94	0.67
1:A:263:HIS:HB3	1:A:302:LEU:HD13	1.77	0.67
1:B:339:VAL:HG13	1:B:377:THR:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:ILE:HD12	1:B:514:LYS:N	2.10	0.67
1:A:52:LEU:HD23	1:A:52:LEU:O	1.95	0.66
1:A:201:ASN:ND2	1:A:268:ARG:HE	1.93	0.66
1:B:272:THR:HG23	1:B:273:VAL:HG22	1.76	0.66
1:A:513:ILE:HD12	1:A:514:LYS:N	2.09	0.66
1:B:522:TYR:OH	1:B:571:ILE:HG13	1.95	0.66
1:A:411:HIS:HE1	1:A:413:GLU:HB3	1.61	0.65
1:B:164:PRO:HG2	1:B:167:LEU:HD13	1.78	0.65
1:A:349:ILE:HG23	1:A:393:ASN:ND2	2.12	0.65
1:B:99:THR:HG22	1:B:142:LEU:HD13	1.79	0.65
1:B:522:TYR:CE1	1:B:568:LEU:HB3	2.32	0.65
1:B:330:ILE:HG21	1:B:362:ALA:HB1	1.79	0.65
1:A:539:GLN:O	1:A:543:VAL:HG12	1.97	0.64
1:B:604:VAL:O	1:B:608:GLN:HG3	1.98	0.64
1:A:687:ILE:HD13	1:B:687:ILE:HG12	1.78	0.64
1:A:482:ASP:CG	1:A:483:ASN:H	2.00	0.64
1:B:415:ARG:NH1	1:B:464:ILE:HD11	2.13	0.64
1:A:360:ASN:HB3	1:A:396:ASN:HB2	1.79	0.63
1:A:683:PHE:HZ	1:B:690:LEU:HB3	1.61	0.63
1:B:102:PHE:HA	1:B:105:VAL:HG12	1.80	0.63
1:A:333:ILE:HD12	1:A:333:ILE:N	2.13	0.63
1:A:683:PHE:CZ	1:B:690:LEU:HD13	2.33	0.63
1:A:79:CYS:O	1:A:83:ILE:HG12	1.98	0.63
1:A:509:ASN:OD1	1:A:644:ILE:HD11	1.99	0.63
1:B:490:LEU:O	1:B:490:LEU:HD23	1.99	0.63
1:A:551:LEU:HD12	1:A:552:GLN:N	2.14	0.63
1:B:201:ASN:O	1:B:204:GLU:HG2	1.99	0.63
1:B:267:LEU:O	1:B:271:GLU:HG3	1.99	0.63
1:B:522:TYR:HH	1:B:572:LYS:HG3	1.64	0.63
1:A:102:PHE:O	1:A:106:LEU:HG	1.99	0.62
1:B:572:LYS:NZ	1:B:572:LYS:HB3	2.14	0.62
1:B:635:ILE:HD12	1:B:636:LEU:N	2.14	0.62
1:B:449:ILE:O	1:B:453:LEU:HD13	1.99	0.62
1:A:165:ALA:HA	1:A:168:PHE:CD1	2.35	0.62
1:A:151:GLU:O	1:A:155:ILE:HG13	2.00	0.62
1:A:256:LEU:O	1:A:260:VAL:HG23	2.00	0.62
1:B:394:ILE:HD12	1:B:394:ILE:O	2.00	0.62
1:A:568:LEU:HD12	1:A:569:GLU:N	2.14	0.61
1:B:650:ILE:HD12	1:B:651:SER:N	2.14	0.61
1:A:412:LYS:HB3	1:A:412:LYS:NZ	2.15	0.61
1:A:583:LEU:HD13	1:A:633:ILE:HD11	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:PHE:O	1:A:287:GLU:HG3	1.99	0.61
1:A:333:ILE:CD1	1:A:333:ILE:H	2.13	0.61
1:A:394:ILE:HD12	1:A:394:ILE:O	2.00	0.61
1:B:462:LEU:HB3	1:B:559:SER:CB	2.30	0.61
1:B:18:THR:HG23	1:B:21:GLN:H	1.65	0.61
1:B:547:TYR:OH	1:B:572:LYS:HE3	2.00	0.61
1:A:686:GLN:O	1:A:690:LEU:HG	2.01	0.61
1:A:3:LYS:HB3	1:A:50:THR:HG21	1.82	0.61
1:A:387:VAL:HA	1:A:390:ILE:HD12	1.82	0.60
1:A:524:ASP:HA	1:A:527:LYS:HE2	1.83	0.60
1:B:80:LEU:HD13	1:B:101:ILE:HG23	1.83	0.60
1:A:415:ARG:NH1	1:A:464:ILE:HD11	2.16	0.60
1:B:513:ILE:HG22	1:B:589:ASN:HD21	1.65	0.60
1:A:483:ASN:HA	1:A:486:ARG:HH12	1.66	0.60
1:B:462:LEU:HB3	1:B:559:SER:HB3	1.83	0.60
1:A:201:ASN:HD22	1:A:268:ARG:HE	1.49	0.60
1:B:655:ASN:OD1	1:B:668:LYS:HD2	2.01	0.60
1:A:290:SER:O	1:A:296:ARG:HD3	2.01	0.60
1:A:288:LEU:HB3	1:A:329:LYS:HE3	1.83	0.60
1:B:151:GLU:O	1:B:155:ILE:HG13	2.02	0.60
1:B:554:LEU:HD12	1:B:555:ALA:N	2.17	0.60
1:A:635:ILE:HA	1:A:638:PHE:HD2	1.66	0.59
1:A:584:ASN:O	1:A:588:THR:HG23	2.01	0.59
1:B:355:ILE:HD12	1:B:355:ILE:N	2.17	0.59
1:B:467:GLN:O	1:B:471:VAL:HG23	2.03	0.59
1:B:628:ASP:O	1:B:631:LYS:HG2	2.01	0.59
1:A:489:ARG:O	1:A:493:VAL:HG23	2.02	0.59
1:B:648:SER:O	1:B:652:VAL:HG23	2.03	0.59
1:A:49:LEU:HD23	1:A:49:LEU:O	2.02	0.59
1:B:156:PHE:HA	1:B:163:PHE:CE2	2.38	0.59
1:B:333:ILE:H	1:B:333:ILE:CD1	2.07	0.59
1:A:418:CYS:O	1:A:422:MET:HG2	2.02	0.59
1:A:635:ILE:HA	1:A:638:PHE:CD2	2.38	0.59
1:B:70:VAL:HG12	1:B:73:ARG:NH2	2.16	0.59
1:A:673:ASP:OD1	1:A:677:LYS:HE2	2.03	0.59
1:A:70:VAL:HG12	1:A:73:ARG:NH2	2.16	0.59
1:B:676:SER:HA	1:B:682:LEU:HD11	1.84	0.59
1:B:49:LEU:O	1:B:49:LEU:HD23	2.03	0.59
1:A:456:LEU:O	1:A:459:ILE:HG13	2.02	0.59
1:B:254:ARG:O	1:B:258:VAL:HG23	2.03	0.58
1:B:95:ASP:O	1:B:99:THR:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ILE:HG13	1:A:645:TYR:CD1	2.38	0.58
1:B:523:ILE:HD11	1:B:583:LEU:HD23	1.85	0.58
1:A:121:ILE:HD12	1:A:121:ILE:N	2.17	0.58
1:B:288:LEU:HB3	1:B:329:LYS:CE	2.33	0.58
1:B:314:ASN:OD1	1:B:316:VAL:HG22	2.03	0.58
1:A:110:GLU:HG3	1:A:161:LYS:NZ	2.18	0.58
1:B:288:LEU:HB3	1:B:329:LYS:HE3	1.84	0.58
1:B:139:LEU:HD23	1:B:139:LEU:O	2.04	0.58
1:B:22:LEU:O	1:B:22:LEU:HD12	2.04	0.58
1:B:333:ILE:HD12	1:B:333:ILE:N	2.11	0.58
1:B:646:ASN:OD1	1:B:647:VAL:HG13	2.03	0.58
1:A:355:ILE:HD12	1:A:355:ILE:N	2.19	0.57
1:B:116:GLU:HA	1:B:120:HIS:CE1	2.39	0.57
1:B:186:PRO:HG2	1:B:189:VAL:HG23	1.86	0.57
1:B:256:LEU:O	1:B:260:VAL:HG23	2.04	0.57
1:B:355:ILE:HG22	1:B:359:LEU:HG	1.84	0.57
1:B:554:LEU:HD11	1:B:568:LEU:HD11	1.86	0.57
1:A:139:LEU:HD23	1:A:139:LEU:O	2.04	0.57
1:B:110:GLU:HG3	1:B:161:LYS:HZ1	1.69	0.57
1:B:523:ILE:HG21	1:B:580:PHE:HB3	1.85	0.57
1:B:251:ASN:HB3	1:B:254:ARG:HB2	1.85	0.57
1:A:624:ILE:HG12	1:A:625:MET:N	2.19	0.57
1:A:571:ILE:HA	1:A:574:PHE:CD2	2.39	0.57
1:B:519:ILE:O	1:B:522:TYR:HB3	2.04	0.57
1:B:481:PRO:HG2	1:B:482:ASP:H	1.70	0.57
1:A:288:LEU:HB3	1:A:329:LYS:CE	2.35	0.57
1:A:187:LEU:HG	1:A:191:ARG:NH1	2.20	0.57
1:B:509:ASN:HD21	1:B:644:ILE:HD11	1.69	0.57
1:A:293:GLU:HA	1:A:296:ARG:NE	2.19	0.56
1:A:449:ILE:N	1:A:450:PRO:HD2	2.19	0.56
1:A:376:ARG:O	1:A:380:MET:HG2	2.03	0.56
1:B:449:ILE:HB	1:B:450:PRO:HD3	1.87	0.56
1:B:633:ILE:O	1:B:637:LEU:HG	2.04	0.56
1:A:110:GLU:HG3	1:A:161:LYS:HZ1	1.69	0.56
1:A:446:ILE:HD12	1:A:446:ILE:N	2.21	0.56
1:B:645:TYR:CE2	1:B:678:VAL:HG21	2.41	0.56
1:B:175:LEU:HD12	1:B:219:VAL:HG11	1.88	0.56
1:B:513:ILE:HG22	1:B:589:ASN:ND2	2.21	0.56
1:B:686:GLN:O	1:B:690:LEU:HG	2.04	0.56
1:A:397:LYS:NZ	1:A:445:ILE:HD11	2.21	0.56
1:B:78:CYS:SG	1:B:122:GLN:HB3	2.46	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:SER:HA	1:B:23:ILE:HD13	1.88	0.56
1:B:579:ILE:HG23	1:B:603:LEU:HD11	1.87	0.56
1:A:560:ASP:OD1	1:A:563:LYS:HB2	2.06	0.56
1:B:62:ARG:NH1	1:B:66:LYS:HD2	2.21	0.56
1:B:187:LEU:O	1:B:187:LEU:HD23	2.06	0.56
1:B:273:VAL:HB	1:B:276:LEU:HD13	1.86	0.56
1:A:453:LEU:HA	1:A:456:LEU:HD13	1.86	0.55
1:B:23:ILE:HD12	1:B:23:ILE:N	2.22	0.55
1:A:14:PRO:HG2	1:A:31:ARG:NH1	2.21	0.55
1:B:110:GLU:HG3	1:B:161:LYS:NZ	2.21	0.55
1:B:584:ASN:HA	1:B:587:VAL:HG12	1.88	0.55
1:A:22:LEU:C	1:A:23:ILE:HD12	2.27	0.55
1:A:633:ILE:O	1:A:637:LEU:HG	2.07	0.55
1:B:386:PRO:O	1:B:390:ILE:HG13	2.06	0.55
1:A:459:ILE:HD12	1:A:460:ASN:N	2.21	0.55
1:A:95:ASP:O	1:A:99:THR:HG23	2.07	0.55
1:B:131:LEU:HB2	1:B:174:ILE:HD11	1.89	0.55
1:B:283:PHE:O	1:B:287:GLU:HG3	2.07	0.55
1:A:565:ILE:HG13	1:A:566:ASP:OD1	2.06	0.55
1:B:592:PRO:O	1:B:595:THR:HG22	2.07	0.55
1:A:568:LEU:HA	1:A:571:ILE:HD12	1.88	0.55
1:A:664:GLN:HG2	1:A:668:LYS:HE3	1.88	0.55
1:B:219:VAL:O	1:B:223:LEU:HD13	2.07	0.55
1:B:663:LYS:O	1:B:667:LEU:HD13	2.07	0.55
1:B:188:GLU:O	1:B:192:LEU:HG	2.08	0.54
1:A:270:TRP:HE3	1:A:277:ILE:HG13	1.73	0.54
1:B:102:PHE:O	1:B:106:LEU:HG	2.08	0.54
1:B:288:LEU:HD12	1:B:299:ALA:HB1	1.89	0.54
1:B:654:LEU:C	1:B:655:ASN:HD22	2.11	0.54
1:A:335:PRO:HA	1:A:338:ARG:HD2	1.90	0.54
1:A:628:ASP:O	1:A:632:VAL:HG23	2.07	0.54
1:B:372:PRO:HB3	1:B:375:ARG:HH21	1.71	0.54
1:A:219:VAL:O	1:A:223:LEU:HD13	2.08	0.54
1:B:102:PHE:O	1:B:105:VAL:HG12	2.08	0.54
1:B:238:TYR:O	1:B:242:ILE:HG12	2.07	0.54
1:B:418:CYS:O	1:B:422:MET:HG2	2.08	0.54
1:B:453:LEU:HD22	1:B:476:LEU:HD21	1.90	0.54
1:B:560:ASP:OD1	1:B:563:LYS:HG3	2.07	0.54
1:A:690:LEU:HD13	1:B:683:PHE:CE2	2.43	0.54
1:B:376:ARG:O	1:B:380:MET:HG2	2.08	0.54
1:A:668:LYS:O	1:A:672:LEU:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:PHE:CZ	1:B:690:LEU:HB3	2.43	0.54
1:A:22:LEU:HD12	1:A:22:LEU:O	2.08	0.54
1:A:467:GLN:O	1:A:471:VAL:HG23	2.07	0.54
1:A:509:ASN:CG	1:A:644:ILE:HD11	2.29	0.53
1:B:165:ALA:HA	1:B:168:PHE:CD1	2.43	0.53
1:B:205:ILE:N	1:B:206:PRO:CD	2.71	0.53
1:B:316:VAL:HG11	1:B:355:ILE:HD11	1.90	0.53
1:A:157:TYR:HB2	1:A:192:LEU:HD21	1.89	0.53
1:A:585:ALA:O	1:A:591:ILE:HD13	2.07	0.53
1:B:396:ASN:HB3	1:B:399:ILE:CG1	2.37	0.53
1:B:411:HIS:HE1	1:B:413:GLU:HB3	1.72	0.53
1:A:23:ILE:N	1:A:23:ILE:HD12	2.23	0.53
1:A:84:LEU:O	1:A:88:ALA:HB2	2.08	0.53
1:A:635:ILE:HD12	1:A:636:LEU:N	2.24	0.53
1:B:156:PHE:HA	1:B:163:PHE:HE2	1.73	0.53
1:A:215:CYS:O	1:A:219:VAL:HG23	2.08	0.53
1:B:22:LEU:C	1:B:23:ILE:HD12	2.29	0.53
1:B:292:ASN:HB3	1:B:295:PHE:HD2	1.73	0.53
1:B:344:SER:O	1:B:348:ILE:HG13	2.09	0.53
1:B:516:SER:OG	1:B:587:VAL:HG22	2.09	0.53
1:A:154:HIS:O	1:A:158:ASP:HB2	2.09	0.53
1:A:646:ASN:OD1	1:A:647:VAL:HG13	2.09	0.53
1:B:479:PHE:HB3	1:B:597:LYS:HD3	1.90	0.53
1:A:571:ILE:HA	1:A:574:PHE:HD2	1.72	0.53
1:A:624:ILE:HG12	1:A:625:MET:H	1.73	0.53
1:B:205:ILE:O	1:B:207:GLU:HG2	2.09	0.53
1:A:380:MET:SD	1:A:417:LEU:HD21	2.49	0.52
1:A:411:HIS:CE1	1:A:413:GLU:HB3	2.43	0.52
1:A:673:ASP:O	1:A:677:LYS:HG3	2.09	0.52
1:B:566:ASP:O	1:B:570:THR:HG23	2.08	0.52
1:B:671:ILE:HG22	1:B:675:ILE:HD11	1.90	0.52
1:A:664:GLN:O	1:A:668:LYS:HG3	2.09	0.52
1:B:589:ASN:HA	1:B:642:PRO:HG3	1.91	0.52
1:B:84:LEU:O	1:B:88:ALA:HB2	2.10	0.52
1:A:339:VAL:O	1:A:343:GLU:HG3	2.09	0.52
1:A:449:ILE:O	1:A:453:LEU:HD13	2.09	0.52
1:A:551:LEU:HD22	1:A:568:LEU:HD11	1.91	0.52
1:B:254:ARG:HA	1:B:254:ARG:HE	1.74	0.52
1:B:643:ILE:HD12	1:B:643:ILE:N	2.25	0.52
1:A:644:ILE:HG13	1:A:645:TYR:HD1	1.75	0.52
1:A:72:ILE:N	1:A:72:ILE:HD12	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:LYS:HB3	1:B:525:PHE:CE2	2.44	0.52
1:B:380:MET:SD	1:B:417:LEU:HD21	2.50	0.52
1:B:3:LYS:HE3	1:B:50:THR:HG21	1.91	0.52
1:B:565:ILE:HG13	1:B:566:ASP:OD1	2.09	0.52
1:A:262:LEU:O	1:A:266:VAL:HG23	2.08	0.52
1:A:527:LYS:HA	1:A:530:ASN:OD1	2.10	0.52
1:A:121:ILE:CD1	1:A:121:ILE:H	2.20	0.52
1:A:238:TYR:O	1:A:242:ILE:HG12	2.10	0.52
1:A:396:ASN:HB3	1:A:399:ILE:CG1	2.40	0.52
1:A:99:THR:HG22	1:A:142:LEU:HD13	1.92	0.52
1:A:355:ILE:HG22	1:A:359:LEU:HG	1.92	0.51
1:A:27:GLU:O	1:A:31:ARG:HG3	2.10	0.51
1:A:523:ILE:HG23	1:A:580:PHE:HD2	1.75	0.51
1:B:649:ASN:O	1:B:653:LEU:HG	2.10	0.51
1:A:314:ASN:OD1	1:A:316:VAL:HG22	2.11	0.51
1:A:643:ILE:N	1:A:643:ILE:HD12	2.25	0.51
1:B:464:ILE:O	1:B:468:VAL:HG23	2.10	0.51
1:A:301:LYS:O	1:A:305:GLN:HG3	2.10	0.51
1:A:459:ILE:HD12	1:A:459:ILE:C	2.31	0.51
1:A:506:PHE:HA	1:A:509:ASN:HD22	1.74	0.51
1:B:215:CYS:O	1:B:219:VAL:HG23	2.11	0.51
1:B:607:LEU:HD23	1:B:633:ILE:HG12	1.92	0.51
1:B:693:ILE:HD12	1:B:694:ILE:N	2.26	0.51
1:A:87:TYR:HB3	1:A:92:PRO:HD3	1.92	0.51
1:A:265:LEU:O	1:A:269:LEU:HG	2.11	0.51
1:A:634:GLN:HG2	1:A:638:PHE:CE2	2.46	0.51
1:B:136:ILE:HG12	1:B:174:ILE:HG23	1.90	0.51
1:A:528:PHE:CE2	1:A:543:VAL:HG11	2.45	0.51
1:B:270:TRP:HE3	1:B:277:ILE:HG13	1.74	0.51
1:B:526:SER:CB	1:B:572:LYS:HE2	2.40	0.51
1:A:105:VAL:HG22	1:A:109:PHE:CE2	2.46	0.51
1:A:388:THR:O	1:A:392:LYS:HG2	2.10	0.51
1:A:576:ASP:OD2	1:A:578:ARG:HB3	2.10	0.51
1:B:415:ARG:HH11	1:B:464:ILE:HD11	1.74	0.51
1:A:663:LYS:O	1:A:667:LEU:HD13	2.11	0.51
1:B:360:ASN:HB3	1:B:396:ASN:HB2	1.92	0.51
1:B:397:LYS:HE3	1:B:401:THR:HG21	1.93	0.51
1:A:357:LYS:HB3	1:A:358:GLU:OE1	2.11	0.51
1:A:116:GLU:HG2	1:A:118:GLY:H	1.75	0.50
1:A:529:LEU:N	1:A:529:LEU:HD12	2.26	0.50
1:A:59:LEU:O	1:A:80:LEU:HD21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:PHE:HA	1:A:593:PHE:HZ	1.75	0.50
1:A:523:ILE:HG23	1:A:580:PHE:CD2	2.46	0.50
1:A:56:ARG:HD3	1:A:87:TYR:CE2	2.45	0.50
1:B:97:GLN:O	1:B:101:ILE:HG13	2.11	0.50
1:A:273:VAL:HB	1:A:276:LEU:HD13	1.94	0.50
1:A:566:ASP:O	1:A:570:THR:HG23	2.12	0.50
1:A:650:ILE:HG21	1:B:650:ILE:HD13	1.93	0.50
1:B:339:VAL:O	1:B:343:GLU:HG3	2.11	0.50
1:B:430:LEU:HD12	1:B:431:ASN:OD1	2.11	0.50
1:B:578:ARG:NE	1:B:582:LEU:HD11	2.27	0.50
1:B:584:ASN:O	1:B:587:VAL:HG12	2.11	0.50
1:A:592:PRO:HB2	1:A:595:THR:HG22	1.93	0.50
1:A:366:THR:HG22	1:A:378:SER:OG	2.11	0.50
1:A:487:VAL:O	1:A:491:LEU:HG	2.12	0.50
1:A:211:VAL:O	1:A:211:VAL:HG22	2.12	0.50
1:B:51:GLY:C	1:B:52:LEU:HD12	2.32	0.50
1:A:387:VAL:HG23	1:A:425:PHE:CE1	2.47	0.50
1:A:72:ILE:HD12	1:A:72:ILE:H	1.77	0.50
1:A:635:ILE:HD12	1:A:635:ILE:C	2.32	0.50
1:B:209:LEU:N	1:B:209:LEU:HD12	2.26	0.50
1:B:262:LEU:O	1:B:266:VAL:HG23	2.12	0.50
1:A:468:VAL:O	1:A:472:ILE:HG13	2.12	0.50
1:B:105:VAL:HG22	1:B:109:PHE:CE2	2.47	0.50
1:B:167:LEU:O	1:B:171:ILE:HG13	2.12	0.50
1:B:354:ASP:HB3	1:B:355:ILE:HD12	1.94	0.50
1:B:690:LEU:O	1:B:694:ILE:HG13	2.12	0.50
1:A:134:ARG:HH11	1:A:134:ARG:HG2	1.76	0.49
1:A:390:ILE:O	1:A:394:ILE:HG13	2.11	0.49
1:A:526:SER:C	1:A:528:PHE:H	2.14	0.49
1:B:6:VAL:CG1	1:B:46:ASN:HD21	2.24	0.49
1:B:572:LYS:HB3	1:B:572:LYS:HZ3	1.77	0.49
1:A:102:PHE:HA	1:A:105:VAL:HG12	1.93	0.49
1:B:482:ASP:O	1:B:486:ARG:HG3	2.12	0.49
1:B:265:LEU:O	1:B:269:LEU:HG	2.11	0.49
1:A:683:PHE:HZ	1:B:690:LEU:HD13	1.78	0.49
1:A:508:PHE:HE1	1:A:639:ARG:HG2	1.77	0.49
1:B:154:HIS:O	1:B:158:ASP:HB2	2.11	0.49
1:B:366:THR:HG22	1:B:378:SER:OG	2.13	0.49
1:A:628:ASP:HA	1:A:631:LYS:HG2	1.94	0.49
1:A:102:PHE:HZ	1:A:138:LEU:HB2	1.77	0.49
1:A:97:GLN:O	1:A:101:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:SER:HB3	1:B:182:PHE:HZ	1.76	0.49
1:B:579:ILE:HG23	1:B:603:LEU:CD1	2.43	0.49
1:A:515:ILE:HD12	1:A:639:ARG:O	2.13	0.49
1:B:301:LYS:HD3	1:B:340:GLU:OE2	2.12	0.49
1:A:276:LEU:N	1:A:276:LEU:HD12	2.27	0.49
1:A:52:LEU:HD22	1:A:87:TYR:HE1	1.78	0.49
1:A:678:VAL:O	1:A:679:ASN:CB	2.61	0.49
1:A:687:ILE:HA	1:A:690:LEU:HD12	1.95	0.49
1:B:276:LEU:N	1:B:276:LEU:HD12	2.28	0.49
1:B:25:THR:O	1:B:29:LEU:HG	2.13	0.49
1:B:387:VAL:HG23	1:B:425:PHE:CE1	2.48	0.49
1:B:515:ILE:HG22	1:B:519:ILE:HD13	1.93	0.49
1:A:292:ASN:HB3	1:A:295:PHE:HD2	1.77	0.48
1:A:534:SER:OG	1:A:538:SER:HB3	2.13	0.48
1:B:461:ASP:HB3	1:B:464:ILE:HB	1.95	0.48
1:B:588:THR:O	1:B:588:THR:HG22	2.13	0.48
1:B:218:GLU:O	1:B:222:ILE:HG13	2.13	0.48
1:B:442:ILE:HG22	1:B:446:ILE:HD13	1.94	0.48
1:B:523:ILE:CD1	1:B:583:LEU:HD23	2.43	0.48
1:A:515:ILE:HG22	1:A:519:ILE:HD13	1.94	0.48
1:A:6:VAL:HG13	1:A:7:THR:HG23	1.94	0.48
1:B:452:THR:O	1:B:456:LEU:HG	2.14	0.48
1:B:582:LEU:HD23	1:B:599:CYS:O	2.13	0.48
1:A:266:VAL:HG13	1:A:277:ILE:HD12	1.96	0.48
1:B:144:SER:O	1:B:148:LEU:HD13	2.13	0.48
1:B:165:ALA:HA	1:B:168:PHE:CE1	2.48	0.48
1:A:357:LYS:HG2	1:A:361:GLN:HE21	1.77	0.48
1:A:473:PHE:CE2	1:A:638:PHE:HB3	2.49	0.48
1:B:166:ARG:HG3	1:B:167:LEU:CD1	2.43	0.48
1:B:56:ARG:HD3	1:B:87:TYR:CE2	2.48	0.48
1:A:354:ASP:HB3	1:A:355:ILE:HD12	1.96	0.48
1:A:511:ARG:O	1:A:515:ILE:HG13	2.14	0.48
1:A:102:PHE:CZ	1:A:138:LEU:HB2	2.48	0.48
1:A:131:LEU:HB2	1:A:174:ILE:HD11	1.95	0.48
1:A:523:ILE:CD1	1:A:584:ASN:HB2	2.44	0.48
1:B:515:ILE:O	1:B:519:ILE:HD13	2.13	0.48
1:B:468:VAL:O	1:B:472:ILE:HG13	2.13	0.48
1:B:513:ILE:HD12	1:B:513:ILE:C	2.34	0.48
1:B:681:THR:HA	1:B:684:LYS:HE3	1.96	0.48
1:A:104:LEU:HD23	1:A:104:LEU:C	2.34	0.48
1:A:104:LEU:O	1:A:104:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:THR:HA	1:A:455:ASN:HD22	1.79	0.48
1:A:109:PHE:HE1	1:A:127:ILE:HB	1.79	0.48
1:A:464:ILE:O	1:A:468:VAL:HG23	2.14	0.48
1:B:411:HIS:CE1	1:B:413:GLU:HB3	2.49	0.48
1:B:676:SER:CB	1:B:682:LEU:HD11	2.44	0.48
1:A:107:SER:O	1:A:111:GLN:HG3	2.14	0.47
1:B:153:PHE:CE1	1:B:175:LEU:HB3	2.49	0.47
1:B:293:GLU:HA	1:B:296:ARG:HD2	1.95	0.47
1:B:650:ILE:C	1:B:650:ILE:HD12	2.33	0.47
1:A:551:LEU:HB2	1:A:568:LEU:HD21	1.96	0.47
1:B:635:ILE:HD12	1:B:635:ILE:C	2.34	0.47
1:A:569:GLU:O	1:A:572:LYS:HB3	2.14	0.47
1:B:487:VAL:O	1:B:491:LEU:HG	2.15	0.47
1:B:509:ASN:ND2	1:B:644:ILE:HD11	2.28	0.47
1:A:436:THR:HG23	1:A:439:ASN:HD21	1.80	0.47
1:B:448:THR:O	1:B:452:THR:HG23	2.14	0.47
1:B:564:ALA:O	1:B:568:LEU:HG	2.15	0.47
1:B:402:SER:O	1:B:406:LEU:HG	2.15	0.47
1:B:582:LEU:H	1:B:582:LEU:HD12	1.79	0.47
1:A:565:ILE:O	1:A:569:GLU:HB2	2.15	0.47
1:B:149:LEU:HD22	1:B:182:PHE:CE2	2.50	0.47
1:B:131:LEU:HB2	1:B:174:ILE:CD1	2.45	0.47
1:B:314:ASN:HD21	1:B:352:ARG:HH22	1.63	0.47
1:A:682:LEU:H	1:A:682:LEU:CD2	2.25	0.47
1:B:201:ASN:ND2	1:B:268:ARG:HE	2.13	0.47
1:B:60:VAL:HA	1:B:65:LEU:HD11	1.96	0.47
1:A:567:ALA:O	1:A:571:ILE:HG13	2.15	0.47
1:B:404:LEU:N	1:B:404:LEU:HD12	2.29	0.47
1:B:48:ASP:C	1:B:50:THR:H	2.18	0.47
1:A:218:GLU:O	1:A:222:ILE:HG13	2.15	0.47
1:A:36:HIS:CE1	1:A:78:CYS:HB3	2.50	0.47
1:A:569:GLU:OE2	1:A:572:LYS:HD3	2.15	0.47
1:B:607:LEU:CD2	1:B:633:ILE:HG12	2.45	0.47
1:A:157:TYR:HB3	1:A:192:LEU:HD11	1.98	0.47
1:A:232:SER:OG	1:A:279:ALA:HB2	2.15	0.47
1:A:513:ILE:C	1:A:513:ILE:HD12	2.35	0.47
1:A:690:LEU:HD13	1:B:683:PHE:CD2	2.50	0.47
1:B:647:VAL:O	1:B:650:ILE:HG13	2.15	0.47
1:B:36:HIS:CE1	1:B:78:CYS:HB3	2.50	0.47
1:A:369:ASP:HB3	1:A:374:VAL:HG21	1.96	0.46
1:A:80:LEU:HD13	1:A:101:ILE:HG23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:LEU:O	1:B:130:LEU:HG	2.15	0.46
1:B:416:GLU:HB3	1:B:467:GLN:HE22	1.80	0.46
1:B:594:LEU:HD13	1:B:594:LEU:C	2.35	0.46
1:A:112:LEU:HD21	1:A:167:LEU:HD13	1.97	0.46
1:A:386:PRO:O	1:A:390:ILE:HG13	2.14	0.46
1:A:592:PRO:O	1:A:595:THR:HG22	2.15	0.46
1:B:107:SER:O	1:B:111:GLN:HG3	2.14	0.46
1:B:59:LEU:O	1:B:80:LEU:HD21	2.15	0.46
1:B:630:ALA:O	1:B:634:GLN:HG3	2.15	0.46
1:A:462:LEU:HD13	1:A:558:LEU:O	2.15	0.46
1:B:109:PHE:HE1	1:B:127:ILE:HB	1.80	0.46
1:B:174:ILE:O	1:B:178:VAL:HG23	2.15	0.46
1:A:167:LEU:O	1:A:171:ILE:HG13	2.15	0.46
1:A:246:ALA:CB	1:A:258:VAL:HG21	2.46	0.46
1:A:243:ILE:HD11	1:A:262:LEU:HD12	1.97	0.46
1:A:539:GLN:C	1:A:543:VAL:HG12	2.36	0.46
1:A:678:VAL:HG23	1:A:679:ASN:N	2.30	0.46
1:B:104:LEU:C	1:B:104:LEU:HD23	2.36	0.46
1:B:582:LEU:N	1:B:582:LEU:HD12	2.30	0.46
1:A:10:LYS:HB2	1:A:38:GLU:OE2	2.15	0.46
1:A:153:PHE:HB3	1:A:192:LEU:HD23	1.95	0.46
1:A:267:LEU:O	1:A:271:GLU:HG3	2.16	0.46
1:B:102:PHE:HZ	1:B:138:LEU:HB2	1.80	0.46
1:B:357:LYS:O	1:B:361:GLN:HG3	2.15	0.46
1:B:345:ILE:HD13	1:B:363:LEU:HD21	1.97	0.46
1:A:404:LEU:N	1:A:404:LEU:HD12	2.30	0.46
1:B:476:LEU:HD12	1:B:476:LEU:N	2.29	0.46
1:B:526:SER:OG	1:B:572:LYS:HG2	2.15	0.46
1:B:687:ILE:HA	1:B:690:LEU:HD12	1.97	0.46
1:A:131:LEU:HB2	1:A:174:ILE:CD1	2.45	0.46
1:A:207:GLU:HG2	1:A:210:ASN:OD1	2.16	0.46
1:A:523:ILE:HD12	1:A:584:ASN:HB2	1.97	0.46
1:B:693:ILE:HD12	1:B:693:ILE:C	2.36	0.46
1:A:453:LEU:HD22	1:A:476:LEU:HD21	1.98	0.46
1:A:512:GLN:HA	1:A:639:ARG:O	2.16	0.46
1:B:166:ARG:NH1	1:B:167:LEU:HD11	2.31	0.46
1:A:288:LEU:HD12	1:A:299:ALA:HB1	1.97	0.45
1:A:532:GLN:HE22	1:A:535:MET:HB2	1.81	0.45
1:B:24:SER:HB3	1:B:27:GLU:HG3	1.98	0.45
1:A:125:TYR:CZ	1:A:129:LYS:HG3	2.51	0.45
1:A:168:PHE:CE2	1:A:215:CYS:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ASN:O	1:B:296:ARG:HG3	2.17	0.45
1:B:49:LEU:CA	1:B:52:LEU:HD13	2.46	0.45
1:A:390:ILE:HG22	1:A:394:ILE:HD11	1.97	0.45
1:A:476:LEU:N	1:A:476:LEU:HD12	2.31	0.45
1:A:542:ILE:HG13	1:A:543:VAL:N	2.31	0.45
1:A:83:ILE:HG21	1:A:93:TYR:OH	2.16	0.45
1:B:263:HIS:CG	1:B:302:LEU:HD22	2.51	0.45
1:A:145:SER:HB3	1:A:182:PHE:HZ	1.81	0.45
1:A:116:GLU:HA	1:A:120:HIS:NE2	2.32	0.45
1:A:629:ILE:O	1:A:633:ILE:HG22	2.16	0.45
1:A:165:ALA:HA	1:A:168:PHE:CE1	2.52	0.45
1:B:256:LEU:O	1:B:259:VAL:HG12	2.16	0.45
1:B:284:ILE:O	1:B:288:LEU:HD13	2.15	0.45
1:B:268:ARG:O	1:B:272:THR:HG22	2.16	0.45
1:B:586:CYS:HG	1:B:599:CYS:HG	1.63	0.45
1:B:635:ILE:HA	1:B:638:PHE:HD2	1.82	0.45
1:B:79:CYS:O	1:B:83:ILE:HD13	2.17	0.45
1:A:400:TYR:HB3	1:A:445:ILE:HG21	1.98	0.45
1:B:129:LYS:HD2	1:B:133:TYR:CE2	2.52	0.45
1:B:301:LYS:O	1:B:305:GLN:HG3	2.17	0.45
1:B:238:TYR:CE1	1:B:242:ILE:HD11	2.52	0.45
1:A:347:GLN:O	1:A:351:THR:HG23	2.17	0.44
1:A:411:HIS:CE1	1:A:414:VAL:HG23	2.52	0.44
1:A:519:ILE:O	1:A:522:TYR:HB3	2.17	0.44
1:A:558:LEU:HD13	1:A:632:VAL:HG13	2.00	0.44
1:A:149:LEU:HD22	1:A:182:PHE:CE2	2.52	0.44
1:A:191:ARG:HB3	1:A:195:ASN:HD21	1.82	0.44
1:A:594:LEU:HD13	1:A:594:LEU:C	2.37	0.44
1:B:243:ILE:HG23	1:B:255:LEU:HD11	1.99	0.44
1:B:61:SER:O	1:B:65:LEU:HD13	2.18	0.44
1:A:153:PHE:CE1	1:A:175:LEU:HB3	2.52	0.44
1:A:174:ILE:O	1:A:178:VAL:HG23	2.16	0.44
1:A:519:ILE:N	1:A:519:ILE:HD12	2.33	0.44
1:A:28:LEU:O	1:A:32:LEU:HG	2.18	0.44
1:A:345:ILE:HD12	1:A:345:ILE:N	2.32	0.44
1:B:345:ILE:HB	1:B:346:PRO:HD3	2.00	0.44
1:B:676:SER:CA	1:B:682:LEU:HD11	2.48	0.44
1:A:436:THR:OG1	1:A:439:ASN:ND2	2.51	0.44
1:A:52:LEU:HD22	1:A:87:TYR:CE1	2.52	0.44
1:B:387:VAL:HA	1:B:390:ILE:HD12	2.00	0.44
1:A:29:LEU:HD23	1:A:29:LEU:C	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ASP:HB2	1:A:46:ASN:OD1	2.18	0.44
1:B:482:ASP:OD1	1:B:484:ASP:HB2	2.17	0.44
1:B:589:ASN:N	1:B:591:ILE:HD11	2.32	0.44
1:B:646:ASN:OD1	1:B:647:VAL:N	2.50	0.44
1:B:29:LEU:HD23	1:B:72:ILE:HD13	1.98	0.44
1:A:273:VAL:O	1:A:273:VAL:HG23	2.17	0.44
1:A:358:GLU:OE1	1:A:358:GLU:N	2.48	0.44
1:A:374:VAL:HG23	1:A:375:ARG:N	2.32	0.44
1:B:239:TYR:CE1	1:B:243:ILE:HD11	2.53	0.44
1:B:645:TYR:CD2	1:B:678:VAL:HG21	2.52	0.44
1:A:35:LEU:O	1:A:39:LEU:HG	2.18	0.44
1:A:646:ASN:OD1	1:A:647:VAL:N	2.51	0.44
1:B:551:LEU:C	1:B:551:LEU:HD23	2.37	0.44
1:A:683:PHE:CZ	1:B:690:LEU:HD22	2.52	0.44
1:A:506:PHE:HA	1:A:509:ASN:ND2	2.33	0.44
1:A:528:PHE:HB3	1:A:529:LEU:HD12	2.00	0.44
1:A:554:LEU:C	1:A:554:LEU:HD12	2.39	0.44
1:B:644:ILE:HG13	1:B:645:TYR:CD1	2.53	0.44
1:A:529:LEU:HD11	1:A:572:LYS:HE3	1.98	0.43
1:B:514:LYS:HE2	1:B:553:TRP:CZ2	2.53	0.43
1:A:139:LEU:C	1:A:139:LEU:HD23	2.38	0.43
1:B:201:ASN:OD1	1:B:203:ASN:ND2	2.51	0.43
1:B:446:ILE:HD12	1:B:446:ILE:N	2.33	0.43
1:A:227:TYR:O	1:A:231:MET:HG2	2.18	0.43
1:A:224:CYS:O	1:A:276:LEU:HD11	2.17	0.43
1:A:48:ASP:O	1:A:49:LEU:HB3	2.18	0.43
1:A:567:ALA:CB	1:A:629:ILE:HG12	2.48	0.43
1:B:544:MET:O	1:B:544:MET:HE3	2.19	0.43
1:B:522:TYR:CZ	1:B:568:LEU:HD22	2.53	0.43
1:B:672:LEU:N	1:B:672:LEU:HD12	2.33	0.43
1:A:582:LEU:N	1:A:582:LEU:HD12	2.34	0.43
1:B:35:LEU:O	1:B:39:LEU:HG	2.18	0.43
1:B:589:ASN:C	1:B:591:ILE:HD12	2.37	0.43
1:A:126:LEU:O	1:A:130:LEU:HG	2.18	0.43
1:B:341:TRP:CZ3	1:B:345:ILE:HD11	2.53	0.43
1:B:582:LEU:CD1	1:B:582:LEU:H	2.32	0.43
1:A:355:ILE:CG2	1:A:359:LEU:HG	2.49	0.43
1:A:72:ILE:H	1:A:72:ILE:CD1	2.31	0.43
1:B:104:LEU:O	1:B:104:LEU:HD23	2.17	0.43
1:B:499:LYS:O	1:B:503:THR:HG23	2.17	0.43
1:B:591:ILE:HD12	1:B:591:ILE:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:CD2	1:A:192:LEU:HG	2.54	0.43
1:B:33:LYS:O	1:B:37:GLU:HG3	2.19	0.43
1:B:442:ILE:O	1:B:446:ILE:HD13	2.19	0.43
1:B:593:PHE:O	1:B:596:PHE:HB3	2.19	0.43
1:A:99:THR:O	1:A:103:LYS:HB2	2.18	0.43
1:A:116:GLU:HA	1:A:120:HIS:CD2	2.54	0.43
1:A:263:HIS:CG	1:A:302:LEU:HD22	2.54	0.43
1:A:482:ASP:CG	1:A:483:ASN:N	2.70	0.43
1:A:567:ALA:HB1	1:A:629:ILE:HG23	2.00	0.43
1:A:82:ASP:O	1:A:85:ARG:HB3	2.18	0.43
1:B:249:ASP:C	1:B:251:ASN:H	2.22	0.43
1:B:355:ILE:CG2	1:B:359:LEU:HG	2.47	0.43
1:B:139:LEU:C	1:B:139:LEU:HD23	2.38	0.42
1:B:273:VAL:HG23	1:B:273:VAL:O	2.18	0.42
1:B:686:GLN:N	1:B:686:GLN:OE1	2.47	0.42
1:B:80:LEU:O	1:B:84:LEU:HG	2.19	0.42
1:A:179:ILE:HG13	1:A:185:VAL:HG21	2.01	0.42
1:A:667:LEU:O	1:A:671:ILE:HG13	2.19	0.42
1:B:320:SER:O	1:B:324:LYS:HG3	2.19	0.42
1:A:508:PHE:O	1:A:512:GLN:HG3	2.20	0.42
1:A:48:ASP:C	1:A:50:THR:H	2.22	0.42
1:A:522:TYR:OH	1:A:568:LEU:HB2	2.18	0.42
1:A:671:ILE:HG22	1:A:675:ILE:HD11	2.02	0.42
1:B:292:ASN:HB3	1:B:295:PHE:CD2	2.51	0.42
1:A:383:ASN:OD1	1:A:424:LYS:HE2	2.19	0.42
1:A:480:GLU:HB2	1:A:481:PRO:CA	2.46	0.42
1:B:52:LEU:HD12	1:B:52:LEU:N	2.34	0.42
1:B:249:ASP:O	1:B:250:ASP:HB3	2.20	0.42
1:B:554:LEU:C	1:B:554:LEU:HD12	2.39	0.42
1:A:650:ILE:HD13	1:B:650:ILE:HB	2.01	0.42
1:A:307:LEU:HD21	1:A:315:PHE:HD2	1.84	0.42
1:A:539:GLN:HB3	1:A:542:ILE:HG13	2.01	0.42
1:B:652:VAL:HG12	1:B:672:LEU:HD11	2.02	0.42
1:A:497:PHE:CD2	1:A:501:ALA:HB1	2.55	0.42
1:A:525:PHE:O	1:A:528:PHE:HB2	2.19	0.42
1:B:481:PRO:HG2	1:B:482:ASP:N	2.33	0.42
1:B:49:LEU:C	1:B:49:LEU:HD23	2.40	0.42
1:A:112:LEU:HD21	1:A:167:LEU:CD1	2.49	0.42
1:A:292:ASN:HB3	1:A:295:PHE:CD2	2.54	0.42
1:A:462:LEU:O	1:A:466:GLU:HG3	2.19	0.42
1:A:499:LYS:O	1:A:503:THR:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:VAL:O	1:A:679:ASN:HB2	2.19	0.42
1:B:376:ARG:HB3	1:B:376:ARG:NH1	2.35	0.42
1:A:345:ILE:HB	1:A:346:PRO:HD3	2.02	0.42
1:A:568:LEU:C	1:A:568:LEU:HD12	2.40	0.42
1:A:671:ILE:O	1:A:675:ILE:HG13	2.20	0.42
1:A:678:VAL:O	1:A:679:ASN:ND2	2.52	0.42
1:B:154:HIS:CD2	1:B:192:LEU:HD11	2.54	0.42
1:B:511:ARG:HG2	1:B:515:ILE:HG13	2.00	0.42
1:B:509:ASN:O	1:B:512:GLN:HB3	2.19	0.42
1:A:191:ARG:HB3	1:A:195:ASN:ND2	2.34	0.42
1:A:376:ARG:HG2	1:A:376:ARG:HH11	1.85	0.41
1:A:671:ILE:HG22	1:A:675:ILE:CD1	2.49	0.41
1:B:224:CYS:O	1:B:276:LEU:HD11	2.20	0.41
1:B:48:ASP:O	1:B:49:LEU:HB3	2.20	0.41
1:B:125:TYR:CZ	1:B:129:LYS:HG3	2.55	0.41
1:B:164:PRO:CG	1:B:167:LEU:HD13	2.46	0.41
1:B:191:ARG:HB2	1:B:195:ASN:ND2	2.35	0.41
1:B:230:ARG:HH11	1:B:230:ARG:HG3	1.85	0.41
1:B:49:LEU:HA	1:B:52:LEU:HD13	2.01	0.41
1:A:3:LYS:HB3	1:A:50:THR:CG2	2.48	0.41
1:A:411:HIS:ND1	1:A:414:VAL:HG23	2.36	0.41
1:A:529:LEU:CD1	1:A:572:LYS:HE3	2.50	0.41
1:A:591:ILE:H	1:A:646:ASN:HD21	1.67	0.41
1:B:185:VAL:HG13	1:B:186:PRO:HD2	2.01	0.41
1:B:270:TRP:HB2	1:B:277:ILE:HG13	2.01	0.41
1:B:236:THR:HG23	1:B:283:PHE:CE2	2.56	0.41
1:B:523:ILE:HD13	1:B:580:PHE:CA	2.43	0.41
1:A:394:ILE:HD12	1:A:394:ILE:C	2.41	0.41
1:A:458:TYR:CE2	1:A:500:LYS:HB3	2.55	0.41
1:A:649:ASN:O	1:A:653:LEU:HB2	2.19	0.41
1:B:145:SER:HB3	1:B:182:PHE:CZ	2.54	0.41
1:B:157:TYR:O	1:B:159:PRO:HD3	2.21	0.41
1:B:523:ILE:CD1	1:B:580:PHE:HA	2.40	0.41
1:A:154:HIS:CD2	1:A:192:LEU:HD22	2.44	0.41
1:A:92:PRO:HG2	1:A:93:TYR:H	1.86	0.41
1:B:588:THR:O	1:B:589:ASN:HB2	2.20	0.41
1:B:65:LEU:O	1:B:73:ARG:HG2	2.21	0.41
1:B:390:ILE:CG2	1:B:394:ILE:HD11	2.51	0.41
1:A:144:SER:O	1:A:148:LEU:HG	2.21	0.41
1:A:161:LYS:HB3	1:A:163:PHE:CE1	2.56	0.41
1:A:335:PRO:HA	1:A:338:ARG:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:522:TYR:OH	1:B:568:LEU:O	2.37	0.41
1:A:353:GLU:O	1:A:353:GLU:HG2	2.19	0.41
1:A:49:LEU:C	1:A:49:LEU:HD23	2.41	0.41
1:A:579:ILE:HG23	1:A:603:LEU:HD11	2.01	0.41
1:A:686:GLN:CD	1:A:686:GLN:H	2.24	0.41
1:B:671:ILE:O	1:B:675:ILE:HG13	2.21	0.41
1:A:46:ASN:O	1:A:46:ASN:OD1	2.39	0.41
1:A:61:SER:O	1:A:65:LEU:HD13	2.21	0.41
1:B:348:ILE:O	1:B:351:THR:HB	2.21	0.41
1:B:38:GLU:O	1:B:42:LEU:HG	2.21	0.41
1:A:316:VAL:HG12	1:A:323:PHE:CD1	2.55	0.40
1:A:554:LEU:HD12	1:A:555:ALA:N	2.36	0.40
1:B:166:ARG:C	1:B:167:LEU:HD12	2.42	0.40
1:B:27:GLU:O	1:B:31:ARG:HG3	2.20	0.40
1:B:502:PHE:HB3	1:B:506:PHE:CE2	2.56	0.40
1:A:347:GLN:H	1:A:347:GLN:CD	2.24	0.40
1:A:12:ASN:HA	1:A:55:TYR:OH	2.21	0.40
1:B:416:GLU:CB	1:B:467:GLN:HE22	2.34	0.40
1:A:647:VAL:HG12	1:B:654:LEU:HD13	2.04	0.40
1:A:145:SER:HB3	1:A:182:PHE:CZ	2.56	0.40
1:A:244:HIS:CE1	1:A:248:ASN:ND2	2.90	0.40
1:A:344:SER:O	1:A:348:ILE:HG13	2.21	0.40
1:A:412:LYS:HZ2	1:A:412:LYS:HB3	1.86	0.40
1:B:272:THR:HG23	1:B:273:VAL:N	2.36	0.40
1:B:551:LEU:O	1:B:551:LEU:HD23	2.21	0.40
1:A:385:VAL:HG23	1:A:386:PRO:HD2	2.04	0.40
1:A:385:VAL:CG2	1:A:386:PRO:HD2	2.51	0.40
1:B:584:ASN:HA	1:B:587:VAL:CG1	2.50	0.40
1:B:473:PHE:CE2	1:B:638:PHE:HB3	2.56	0.40
1:A:560:ASP:CG	1:A:563:LYS:HB2	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:SER:CB	1:B:556:SER:CB[7_555]	2.12	0.08

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	673/703 (96%)	601 (89%)	64 (10%)	8 (1%)	16	61
1	B	650/703 (92%)	582 (90%)	63 (10%)	5 (1%)	24	69
All	All	1323/1406 (94%)	1183 (89%)	127 (10%)	13 (1%)	19	65

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	536	SER
1	A	538	SER
1	A	679	ASN
1	B	682	LEU
1	A	655	ASN
1	A	460	ASN
1	A	660	SER
1	A	684	LYS
1	B	481	PRO
1	B	589	ASN
1	B	587	VAL
1	B	202	PRO
1	A	481	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	629/650 (97%)	627 (100%)	2 (0%)	94	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	611/650 (94%)	608 (100%)	3 (0%)	92	96
All	All	1240/1300 (95%)	1235 (100%)	5 (0%)	93	96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	469	ASP
1	A	547	TYR
1	B	120	HIS
1	B	469	ASP
1	B	547	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	123	GLN
1	A	154	HIS
1	A	195	ASN
1	A	201	ASN
1	A	244	HIS
1	A	248	ASN
1	A	252	ASN
1	A	347	GLN
1	A	361	GLN
1	A	393	ASN
1	A	428	ASN
1	A	439	ASN
1	A	455	ASN
1	A	509	ASN
1	A	549	GLN
1	A	575	ASN
1	A	598	ASN
1	A	655	ASN
1	B	36	HIS
1	B	117	ASN
1	B	123	GLN
1	B	154	HIS
1	B	195	ASN
1	B	244	HIS
1	B	460	ASN

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Mol	Chain	Res	Type
1	B	467	GLN
1	B	509	ASN
1	B	589	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	677/703 (96%)	0.54	51 (7%) 17 20	217, 391, 564, 683	0
1	B	660/703 (93%)	0.81	94 (14%) 4 9	260, 428, 646, 847	0
All	All	1337/1406 (95%)	0.67	145 (10%) 8 12	217, 407, 606, 847	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	SER	9.3
1	B	208	GLY	8.3
1	B	65	LEU	8.2
1	B	114	ASP	7.6
1	B	209	LEU	7.5
1	A	15	ILE	7.3
1	B	113	GLY	7.3
1	A	213	SER	7.0
1	A	171	ILE	6.8
1	B	210	ASN	6.5
1	B	207	GLU	6.4
1	B	73	ARG	6.2
1	B	20	ASP	6.1
1	B	60	VAL	6.0
1	B	63	LYS	5.6
1	A	16	ILE	5.4
1	B	59	LEU	5.4
1	B	64	LEU	5.2
1	A	51	GLY	5.2
1	B	6	VAL	5.1
1	A	206	PRO	4.8
1	B	657	SER	4.7
1	B	19	SER	4.7
1	B	179	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	52	LEU	4.6
1	B	9	LEU	4.6
1	B	67	HIS	4.6
1	B	111	GLN	4.6
1	B	117	ASN	4.6
1	B	7	THR	4.5
1	B	115	GLN	4.5
1	B	70	VAL	4.4
1	B	11	PHE	4.4
1	A	211	VAL	4.4
1	B	69	ASP	4.3
1	A	52	LEU	4.3
1	B	66	LYS	4.3
1	B	112	LEU	4.2
1	B	35	LEU	4.1
1	B	175	LEU	4.1
1	B	12	ASN	4.1
1	B	153	PHE	4.1
1	A	55	TYR	4.1
1	A	212	THR	4.0
1	B	62	ARG	4.0
1	B	38	GLU	4.0
1	B	58	ALA	3.9
1	B	76	THR	3.8
1	A	33	LYS	3.8
1	B	56	ARG	3.7
1	A	163	PHE	3.7
1	B	55	TYR	3.6
1	B	337	VAL	3.5
1	A	124	THR	3.5
1	A	291	GLU	3.4
1	B	8	LYS	3.4
1	A	531	ASN	3.3
1	B	53	ASP	3.3
1	A	65	LEU	3.3
1	A	54	LYS	3.2
1	B	74	ALA	3.2
1	B	162	SER	3.2
1	B	51	GLY	3.2
1	B	140	ALA	3.1
1	A	127	ILE	3.1
1	A	14	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	49	LEU	3.1
1	B	39	LEU	3.1
1	A	111	GLN	3.0
1	B	157	TYR	3.0
1	B	163	PHE	3.0
1	B	212	THR	2.9
1	A	48	ASP	2.9
1	B	34	ALA	2.9
1	B	211	VAL	2.9
1	B	41	SER	2.9
1	A	109	PHE	2.9
1	A	530	ASN	2.9
1	B	72	ILE	2.8
1	B	422	MET	2.8
1	B	40	ALA	2.8
1	B	332	ASP	2.8
1	B	54	LYS	2.8
1	B	224	CYS	2.8
1	A	6	VAL	2.8
1	A	60	VAL	2.7
1	B	71	GLY	2.7
1	B	280	VAL	2.7
1	B	249	ASP	2.7
1	A	208	GLY	2.7
1	A	37	GLU	2.7
1	B	382	PHE	2.6
1	A	32	LEU	2.6
1	A	201	ASN	2.6
1	B	15	ILE	2.6
1	A	210	ASN	2.6
1	B	109	PHE	2.6
1	A	49	LEU	2.6
1	B	250	ASP	2.6
1	B	57	ASP	2.6
1	A	110	GLU	2.6
1	A	204	GLU	2.5
1	B	30	ASP	2.5
1	B	33	LYS	2.5
1	B	297	LYS	2.5
1	B	206	PRO	2.5
1	A	114	ASP	2.5
1	A	407	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	333	ILE	2.4
1	B	660	SER	2.4
1	A	207	GLU	2.4
1	B	90	ASP	2.4
1	B	169	ASN	2.4
1	A	169	ASN	2.3
1	B	156	PHE	2.3
1	B	425	PHE	2.3
1	A	209	LEU	2.3
1	A	205	ILE	2.3
1	B	353	GLU	2.3
1	A	197	PHE	2.3
1	B	609	THR	2.3
1	B	46	ASN	2.3
1	B	161	LYS	2.2
1	A	128	THR	2.2
1	B	50	THR	2.2
1	B	234	HIS	2.2
1	A	7	THR	2.2
1	B	29	LEU	2.2
1	A	224	CYS	2.2
1	B	110	GLU	2.2
1	A	175	LEU	2.2
1	B	139	LEU	2.1
1	A	75	PHE	2.1
1	A	161	LYS	2.1
1	B	300	THR	2.1
1	A	50	THR	2.1
1	B	127	ILE	2.1
1	B	45	ASP	2.1
1	A	113	GLY	2.1
1	A	158	ASP	2.0
1	A	59	LEU	2.0
1	B	36	HIS	2.0
1	B	89	PRO	2.0
1	B	32	LEU	2.0
1	A	558	LEU	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 [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.