



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:22 AM UTC

PDB ID : 1F3M / pdb_00001f3m
Title : CRYSTAL STRUCTURE OF HUMAN SERINE/THREONINE KINASE
PAK1
Authors : Lei, M.; Lu, W.; Meng, W.; Parrini, M.-C.; Eck, M.J.; Mayer, B.J.; Harrison,
S.C.
Deposited on : 2000-06-05
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

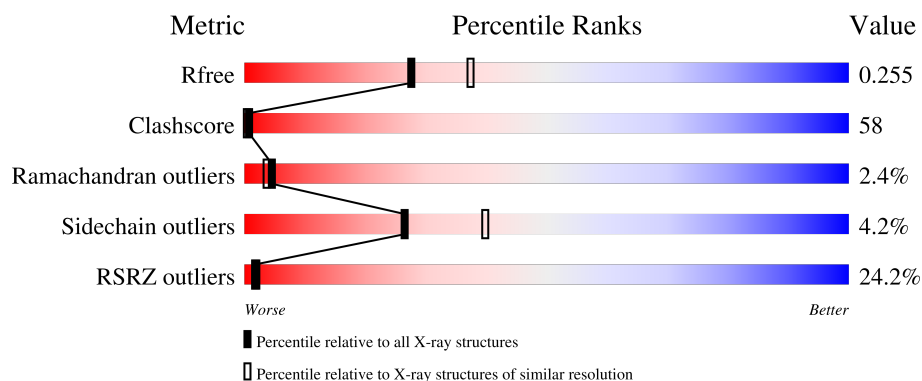
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	80	5% 44% 36% 8% 12%
1	B	80	24% 40% 36% 10% 12%
2	C	297	28% 44% 48% . .
2	D	297	23% 43% 45% 7% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	620	-	-	X	-
3	IOD	B	615	-	-	X	-
3	IOD	C	602	-	-	X	-
3	IOD	C	627	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6187 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 SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	70	Total	C	N	O	S	0	0	0
			563	355	93	113	2			
1	B	70	Total	C	N	O	S	0	0	0
			563	355	93	113	2			

- Molecule 2 is a protein called SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	287	Total	C	N	O	S	0	0	0
			2236	1420	373	427	16			
2	D	285	Total	C	N	O	S	0	0	0
			2215	1408	371	421	15			

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total	I	0	0
			6	6		
3	C	9	Total	I	0	0
			9	9		
3	B	6	Total	I	0	0
			6	6		
3	D	7	Total	I	0	0
			7	7		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	C	222	Total	O	0	0
			222	222		

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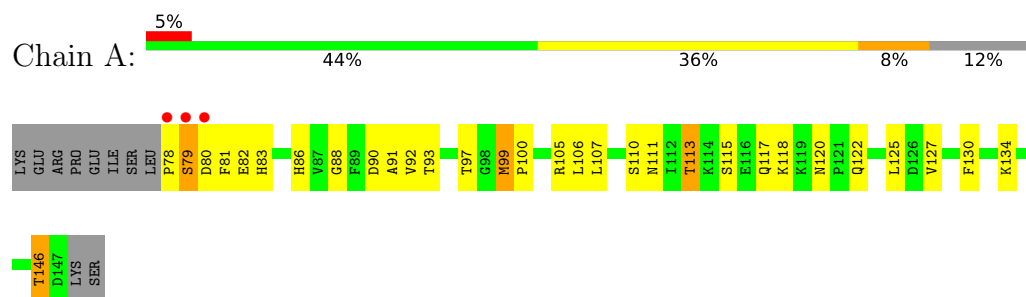
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	78	Total 78	O 78	0	0
4	D	188	Total 188	O 188	0	0

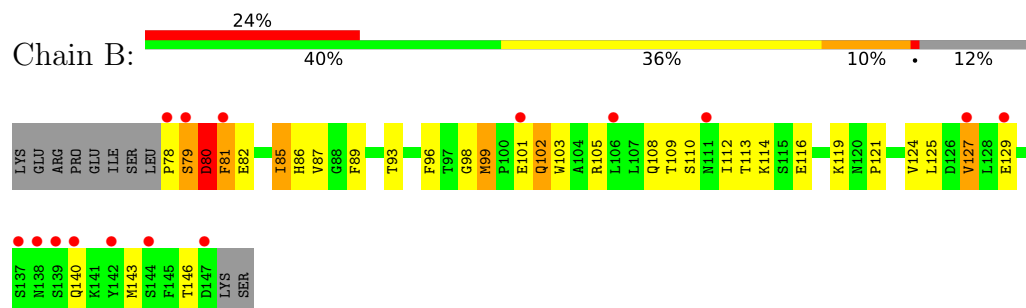
3 Residue-property plots

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.

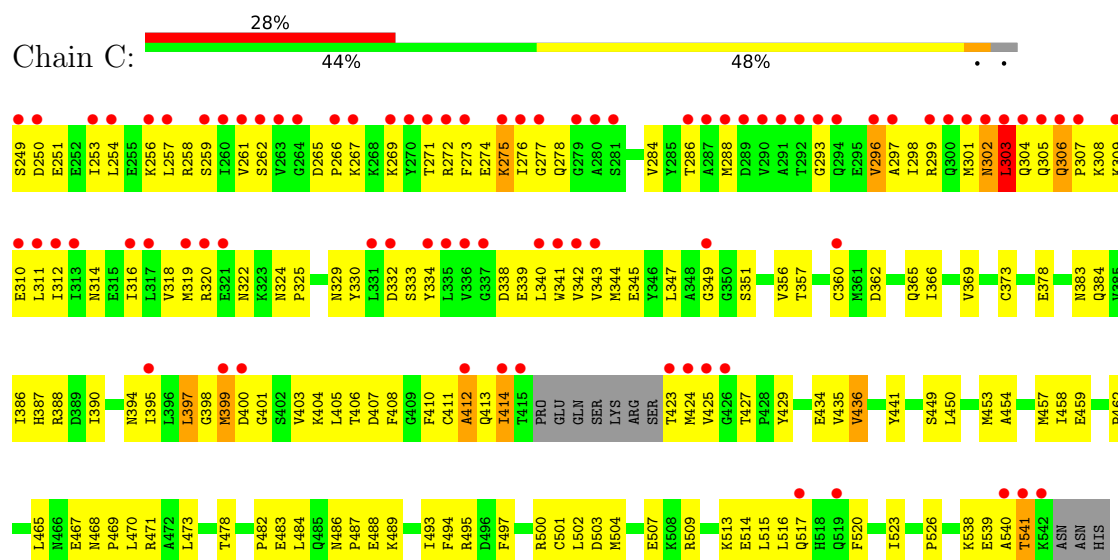
• Molecule 1: SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA



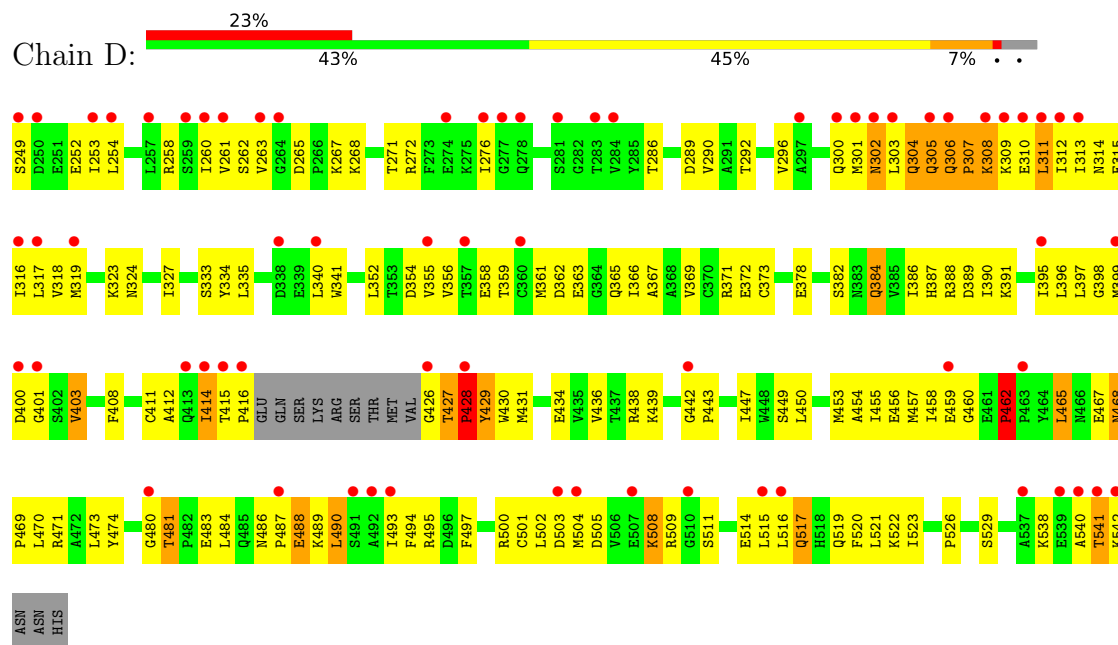
• Molecule 1: SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA



• Molecule 2: SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA



- Molecule 2: SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	94.58Å 94.58Å 147.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.08 – 2.30 34.08 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.6 (34.08-2.30) 98.1 (34.08-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.237 , 0.258 0.234 , 0.255	Depositor DCC
R_{free} test set	2857 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.037 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6187	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IOD

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	0.53	0/576	1.08	6/777 (0.8%)
1	B	0.48	0/576	1.03	4/777 (0.5%)
2	C	0.44	0/2272	0.98	9/3075 (0.3%)
2	D	0.41	0/2252	1.02	13/3049 (0.4%)
All	All	0.44	0/5676	1.01	32/7678 (0.4%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	N-CA-C	-8.33	102.67	112.92
2	C	540	ALA	N-CA-C	-8.11	103.88	113.21
2	C	401	GLY	N-CA-C	-7.86	104.70	114.92
1	B	133	SER	N-CA-C	-7.42	104.36	113.41
2	D	401	GLY	N-CA-C	-7.23	105.81	115.21
2	D	305	GLN	OE1-CD-NE2	-6.75	115.85	122.60
2	C	399	MET	N-CA-C	-6.67	104.87	112.87
2	D	508	LYS	N-CA-C	-6.28	105.62	113.28
2	D	311	LEU	N-CA-C	-6.22	103.81	112.45
2	D	399	MET	N-CA-C	-6.12	105.53	112.87
1	B	79	SER	N-CA-C	6.11	118.56	108.48
1	B	81	PHE	N-CA-C	6.05	119.03	109.96
1	A	120	ASN	CA-C-N	5.71	125.83	119.32
1	A	120	ASN	C-N-CA	5.71	125.83	119.32
2	D	306	GLN	CA-C-N	5.66	126.91	119.84
2	D	306	GLN	C-N-CA	5.66	126.91	119.84
1	A	140	GLN	OE1-CD-NE2	-5.65	116.95	122.60
2	D	296	VAL	N-CA-C	5.58	116.95	108.80
2	C	296	VAL	N-CA-C	5.51	116.63	108.65
1	A	78	PRO	CB-CA-C	5.45	120.46	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	VAL	N-CA-C	5.39	115.89	108.12
2	D	428	PRO	CA-N-CD	-5.37	104.48	112.00
2	C	403	VAL	N-CA-C	5.35	115.60	108.11
2	C	356	VAL	N-CA-C	5.26	115.47	110.42
1	B	80	ASP	N-CA-C	5.22	121.91	110.80
2	D	462	PRO	CB-CA-C	5.22	117.28	110.92
2	C	306	GLN	CA-C-N	5.21	126.35	119.84
2	C	306	GLN	C-N-CA	5.21	126.35	119.84
1	A	113	THR	N-CA-C	5.21	117.40	110.53
2	C	502	LEU	N-CA-C	5.18	118.42	112.57
2	D	442	GLY	CA-C-N	5.13	125.17	119.32
2	D	442	GLY	C-N-CA	5.13	125.17	119.32

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	563	0	537	45	0
1	B	563	0	537	83	0
2	C	2236	0	2261	284	0
2	D	2215	0	2234	244	0
3	A	6	0	0	4	0
3	B	6	0	0	5	0
3	C	9	0	0	8	0
3	D	7	0	0	2	0
4	A	94	0	0	42	0
4	B	78	0	0	47	0
4	C	222	0	0	184	0
4	D	188	0	0	133	0
All	All	6187	0	5569	648	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 58.

All (648) 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)
2:C:296:VAL:HG22	4:C:830:HOH:O	1.29	1.32
2:C:342:VAL:HA	4:C:831:HOH:O	1.29	1.27
2:D:514:GLU:HB3	4:D:812:HOH:O	1.31	1.26
1:A:115:SER:HB3	4:A:687:HOH:O	1.28	1.25
2:D:488:GLU:HG3	4:D:765:HOH:O	1.34	1.25
2:D:290:VAL:HB	4:D:797:HOH:O	1.31	1.25
2:C:275:LYS:HE2	4:C:845:HOH:O	1.33	1.24
3:B:617:IOD:I	4:B:660:HOH:O	2.21	1.23
2:D:319:MET:HB2	4:D:796:HOH:O	1.40	1.22
1:B:121:PRO:HA	4:B:701:HOH:O	1.36	1.21
2:C:301:MET:HE1	4:C:779:HOH:O	1.39	1.21
2:C:369:VAL:HB	4:C:750:HOH:O	1.39	1.21
2:C:388:ARG:HD3	4:C:762:HOH:O	1.34	1.21
1:B:79:SER:HA	4:B:695:HOH:O	1.42	1.17
2:C:395:ILE:CD1	2:C:453:MET:HE1	1.74	1.17
2:D:470:LEU:HB2	4:D:800:HOH:O	1.41	1.16
2:C:425:VAL:HG23	4:C:747:HOH:O	1.43	1.15
2:C:468:ASN:HB2	4:C:816:HOH:O	1.46	1.15
1:A:106:LEU:HD22	4:A:716:HOH:O	1.45	1.14
3:C:627:IOD:I	4:C:701:HOH:O	2.33	1.14
2:C:395:ILE:HD11	2:C:453:MET:HE1	1.19	1.13
2:D:382:SER:HB3	4:D:794:HOH:O	1.47	1.13
2:D:416:PRO:HB3	4:D:740:HOH:O	1.47	1.12
2:C:523:ILE:HG23	4:C:797:HOH:O	1.47	1.12
2:D:495:ARG:HG2	4:D:789:HOH:O	1.49	1.11
2:C:322:ASN:HB2	4:C:837:HOH:O	1.51	1.10
1:B:108:GLN:HG3	4:B:672:HOH:O	1.51	1.10
2:D:504:MET:HE1	4:D:714:HOH:O	1.48	1.10
2:C:500:ARG:HB3	4:C:819:HOH:O	1.52	1.10
1:B:79:SER:HB2	4:B:689:HOH:O	1.52	1.09
2:C:493:ILE:HB	4:C:784:HOH:O	1.52	1.09
1:B:80:ASP:HA	4:B:666:HOH:O	1.52	1.08
1:B:114:LYS:HD2	1:B:114:LYS:H	1.11	1.07
2:D:521:LEU:HD23	4:D:723:HOH:O	1.53	1.07
2:C:458:ILE:HG21	4:C:808:HOH:O	1.52	1.07
1:B:96:PHE:HZ	4:B:701:HOH:O	1.36	1.07
2:D:436:VAL:HB	4:D:778:HOH:O	1.52	1.07
2:D:361:MET:HE2	4:D:771:HOH:O	1.53	1.07
2:D:382:SER:HB2	4:D:806:HOH:O	1.52	1.06
2:D:263:VAL:HA	4:D:813:HOH:O	1.56	1.06
2:D:253:ILE:HG13	4:D:748:HOH:O	1.56	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:439:LYS:HE2	4:D:772:HOH:O	1.52	1.05
2:D:292:THR:HG23	4:D:757:HOH:O	1.57	1.04
1:A:90:ASP:HA	4:A:717:HOH:O	1.56	1.03
2:C:465:LEU:HD13	4:C:751:HOH:O	1.57	1.03
2:C:423:THR:HG22	4:C:771:HOH:O	1.56	1.03
2:C:486:ASN:HB3	4:C:749:HOH:O	1.56	1.03
1:A:118:LYS:HE2	4:A:696:HOH:O	1.59	1.01
2:C:347:LEU:HD13	4:C:829:HOH:O	1.59	1.01
2:C:395:ILE:HG12	4:C:753:HOH:O	1.61	0.99
2:C:465:LEU:HB3	4:C:765:HOH:O	1.61	0.98
2:C:503:ASP:HB2	4:C:710:HOH:O	1.63	0.98
2:C:397:LEU:HB2	4:C:804:HOH:O	1.64	0.98
2:D:497:PHE:HE1	4:D:784:HOH:O	1.46	0.98
2:C:388:ARG:HD2	4:C:661:HOH:O	1.63	0.97
2:C:395:ILE:CD1	2:C:453:MET:CE	2.41	0.97
2:D:372:GLU:HG3	4:D:785:HOH:O	1.64	0.97
2:C:538:LYS:HB3	4:C:824:HOH:O	1.63	0.96
1:B:105:ARG:HG2	4:B:668:HOH:O	1.63	0.95
2:C:468:ASN:OD1	3:C:602:IOD:I	2.54	0.95
2:C:269:LYS:HD3	4:C:844:HOH:O	1.64	0.95
2:C:347:LEU:HB2	4:C:829:HOH:O	1.67	0.94
2:C:484:LEU:HA	4:C:823:HOH:O	1.64	0.94
2:C:342:VAL:HB	4:C:752:HOH:O	1.68	0.94
2:C:302:ASN:HB2	2:C:305:GLN:HG3	1.50	0.94
2:D:310:GLU:HG2	2:D:313:ILE:HD12	1.46	0.93
2:D:493:ILE:HB	4:D:726:HOH:O	1.67	0.93
2:C:265:ASP:HB2	4:C:809:HOH:O	1.66	0.93
2:D:411:CYS:SG	4:D:783:HOH:O	2.25	0.93
2:D:486:ASN:HB2	2:D:489:LYS:HE2	1.49	0.92
2:D:361:MET:HB3	4:D:771:HOH:O	1.67	0.91
2:D:515:LEU:HB3	4:D:784:HOH:O	1.71	0.91
2:C:340:LEU:HD23	4:C:779:HOH:O	1.69	0.91
2:D:341:TRP:CG	4:D:799:HOH:O	2.22	0.91
4:B:665:HOH:O	2:D:438:ARG:HG3	1.70	0.91
2:D:252:GLU:HA	4:D:801:HOH:O	1.70	0.91
4:A:706:HOH:O	1:B:82:GLU:CG	2.20	0.90
4:A:711:HOH:O	1:B:78:PRO:HB3	1.70	0.90
2:C:424:MET:HE2	4:C:812:HOH:O	1.69	0.90
1:A:134:LYS:HE2	3:A:620:IOD:I	2.42	0.90
1:B:108:GLN:CB	4:B:702:HOH:O	2.20	0.90
4:A:718:HOH:O	1:B:81:PHE:CD2	2.25	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:640:HOH:O	3:C:616:IOD:I	2.60	0.89
2:C:515:LEU:HD22	4:C:770:HOH:O	1.72	0.89
1:A:99:MET:HE2	1:A:100:PRO:HD2	1.53	0.89
2:C:267:LYS:HA	4:C:786:HOH:O	1.71	0.89
2:C:538:LYS:HG3	4:C:793:HOH:O	1.73	0.89
2:C:334:TYR:CD2	4:C:760:HOH:O	2.24	0.88
2:D:447:ILE:HG12	4:D:701:HOH:O	1.74	0.88
2:C:347:LEU:HG	4:C:847:HOH:O	1.73	0.87
2:C:319:MET:SD	4:C:849:HOH:O	2.31	0.87
2:C:424:MET:HG2	4:C:771:HOH:O	1.74	0.86
2:C:330:TYR:CD1	4:C:833:HOH:O	2.29	0.85
1:B:108:GLN:HB3	4:B:702:HOH:O	1.75	0.85
1:B:114:LYS:H	1:B:114:LYS:CD	1.89	0.84
2:C:465:LEU:HB2	4:C:751:HOH:O	1.75	0.84
1:B:114:LYS:HG3	4:B:677:HOH:O	1.76	0.84
2:C:400:ASP:CB	4:C:777:HOH:O	2.24	0.84
2:C:397:LEU:C	4:C:847:HOH:O	2.21	0.84
2:C:497:PHE:HE2	4:C:839:HOH:O	1.60	0.84
1:B:136:THR:HG22	4:B:699:HOH:O	1.76	0.84
2:D:403:VAL:HG23	4:D:785:HOH:O	1.78	0.84
2:D:252:GLU:HG3	4:D:801:HOH:O	1.77	0.83
2:C:347:LEU:CD2	4:C:847:HOH:O	2.26	0.83
4:B:665:HOH:O	2:D:438:ARG:CG	2.25	0.83
4:A:706:HOH:O	1:B:82:GLU:HG3	1.79	0.83
2:C:250:ASP:CB	4:C:768:HOH:O	2.26	0.83
2:D:366:ILE:HG22	4:D:696:HOH:O	1.78	0.83
2:D:373:CYS:SG	2:D:395:ILE:HD13	2.19	0.82
2:C:312:ILE:HG21	4:C:779:HOH:O	1.79	0.82
2:C:395:ILE:HD11	2:C:453:MET:CE	2.04	0.82
4:A:691:HOH:O	2:C:308:LYS:HE2	1.78	0.82
2:D:415:THR:OG1	2:D:416:PRO:HD3	1.79	0.82
2:D:508:LYS:HB2	4:D:704:HOH:O	1.79	0.82
2:D:457:MET:SD	4:D:781:HOH:O	2.36	0.82
2:C:538:LYS:CE	4:C:748:HOH:O	2.27	0.82
2:C:507:GLU:CG	4:C:810:HOH:O	2.27	0.81
2:C:454:ALA:HB2	4:C:839:HOH:O	1.79	0.81
2:D:426:GLY:HA2	4:D:746:HOH:O	1.81	0.81
2:C:249:SER:HA	4:C:769:HOH:O	1.81	0.81
2:D:411:CYS:CB	4:D:783:HOH:O	2.27	0.80
1:A:118:LYS:HB3	4:A:696:HOH:O	1.82	0.80
2:C:450:LEU:HG	4:C:795:HOH:O	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:424:MET:HG3	4:C:812:HOH:O	1.80	0.80
4:A:711:HOH:O	1:B:78:PRO:CA	2.29	0.80
2:D:519:GLN:HB3	4:D:726:HOH:O	1.83	0.79
2:C:301:MET:CG	4:C:817:HOH:O	2.29	0.79
4:A:711:HOH:O	1:B:78:PRO:CB	2.29	0.79
2:D:436:VAL:CB	4:D:778:HOH:O	2.20	0.79
2:D:481:THR:HG23	4:D:685:HOH:O	1.81	0.79
2:D:308:LYS:HB3	4:D:736:HOH:O	1.83	0.79
2:C:399:MET:CE	4:C:813:HOH:O	2.30	0.79
2:C:408:PHE:CD2	4:C:814:HOH:O	2.35	0.78
2:C:271:THR:HG22	2:C:272:ARG:H	1.46	0.78
2:D:497:PHE:CE1	4:D:784:HOH:O	2.27	0.78
1:B:119:LYS:CG	3:B:615:IOD:I	3.02	0.78
1:B:119:LYS:HG3	3:B:615:IOD:I	2.53	0.78
2:C:400:ASP:HB3	4:C:777:HOH:O	1.82	0.78
2:D:300:GLN:HA	4:D:799:HOH:O	1.82	0.78
2:D:267:LYS:HE3	4:D:815:HOH:O	1.82	0.78
2:D:323:LYS:HB3	3:D:628:IOD:I	2.55	0.77
1:B:114:LYS:HD2	1:B:114:LYS:N	1.96	0.77
2:D:341:TRP:CD1	4:D:799:HOH:O	2.37	0.77
2:D:455:ILE:HD12	2:D:484:LEU:HD11	1.66	0.77
1:A:118:LYS:CB	4:A:696:HOH:O	2.32	0.77
2:C:269:LYS:HB3	4:C:844:HOH:O	1.84	0.77
2:D:493:ILE:CG2	4:D:726:HOH:O	2.32	0.77
2:D:523:ILE:CG2	4:D:791:HOH:O	2.32	0.77
2:C:538:LYS:HE2	4:C:748:HOH:O	1.84	0.77
2:D:481:THR:CG2	4:D:685:HOH:O	2.32	0.77
2:C:436:VAL:CG2	2:C:473:LEU:HD22	2.15	0.76
1:A:90:ASP:CA	4:A:717:HOH:O	2.22	0.76
2:D:403:VAL:CG2	4:D:785:HOH:O	2.33	0.76
2:C:395:ILE:CG1	4:C:753:HOH:O	2.22	0.76
2:D:253:ILE:CD1	4:D:748:HOH:O	2.34	0.76
2:D:300:GLN:HG2	4:D:799:HOH:O	1.86	0.76
4:A:711:HOH:O	1:B:78:PRO:HA	1.86	0.75
2:C:360:CYS:HB2	4:C:807:HOH:O	1.84	0.75
2:D:308:LYS:CB	4:D:736:HOH:O	2.33	0.75
2:D:366:ILE:HD12	2:D:457:MET:HB3	1.69	0.75
2:D:395:ILE:CD1	2:D:453:MET:HE1	2.17	0.75
2:C:538:LYS:CG	4:C:793:HOH:O	2.29	0.75
2:C:507:GLU:CD	4:C:810:HOH:O	2.30	0.75
2:D:542:LYS:CB	4:D:775:HOH:O	2.33	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:ASP:HB3	4:D:694:HOH:O	1.86	0.75
2:C:539:GLU:C	2:C:541:THR:H	1.93	0.74
2:C:484:LEU:HD23	4:C:842:HOH:O	1.88	0.74
2:D:523:ILE:HB	4:D:791:HOH:O	1.87	0.74
2:C:265:ASP:CB	4:C:809:HOH:O	2.29	0.74
2:D:517:GLN:HB2	4:D:728:HOH:O	1.86	0.74
2:D:490:LEU:HD12	4:D:789:HOH:O	1.86	0.74
2:C:414:ILE:CG2	4:C:826:HOH:O	2.36	0.73
2:D:362:ASP:O	2:D:366:ILE:HG12	1.88	0.73
1:A:139:SER:N	4:A:701:HOH:O	2.20	0.73
1:B:110:SER:OG	1:B:112:ILE:HG12	1.89	0.73
2:D:254:LEU:CD2	4:D:748:HOH:O	2.35	0.73
2:C:351:SER:N	4:C:825:HOH:O	2.20	0.73
2:C:407:ASP:N	4:C:814:HOH:O	2.22	0.73
2:C:435:VAL:HG13	4:C:799:HOH:O	1.89	0.73
2:C:494:PHE:CE2	4:C:808:HOH:O	2.39	0.73
2:C:465:LEU:CB	4:C:751:HOH:O	2.35	0.73
1:A:134:LYS:CE	3:A:620:IOD:I	3.06	0.73
2:C:487:PRO:HD2	2:C:488:GLU:OE2	1.89	0.73
2:D:541:THR:HA	4:D:759:HOH:O	1.88	0.73
2:C:330:TYR:HD1	4:C:833:HOH:O	1.65	0.72
2:D:361:MET:HE2	2:D:366:ILE:HD13	1.71	0.72
1:B:93:THR:CB	4:B:687:HOH:O	2.38	0.72
1:B:108:GLN:CG	4:B:702:HOH:O	2.36	0.72
2:C:450:LEU:CD2	4:C:795:HOH:O	2.38	0.72
1:B:85:ILE:HD13	1:B:86:HIS:N	2.05	0.72
2:D:416:PRO:CB	4:D:740:HOH:O	2.20	0.72
2:D:522:LYS:HE2	4:D:742:HOH:O	1.90	0.72
2:D:395:ILE:HD11	2:D:453:MET:HE1	1.72	0.72
2:D:484:LEU:HB2	2:D:487:PRO:HG3	1.72	0.72
2:C:538:LYS:HE2	4:C:824:HOH:O	1.88	0.72
2:D:493:ILE:CB	4:D:726:HOH:O	2.30	0.72
1:A:146:THR:HG23	2:C:386:ILE:HD11	1.71	0.71
2:C:507:GLU:HG2	4:C:810:HOH:O	1.89	0.71
2:D:490:LEU:HD21	4:D:780:HOH:O	1.89	0.71
1:B:78:PRO:CD	4:B:690:HOH:O	2.38	0.71
1:B:93:THR:HA	4:B:635:HOH:O	1.90	0.71
2:C:265:ASP:C	4:C:809:HOH:O	2.32	0.71
1:B:134:LYS:HG2	4:B:685:HOH:O	1.89	0.71
2:D:254:LEU:HD23	4:D:748:HOH:O	1.91	0.71
2:C:349:GLY:HA2	2:C:399:MET:SD	2.31	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:520:PHE:HA	4:C:784:HOH:O	1.89	0.71
3:D:603:IOD:I	4:D:631:HOH:O	2.77	0.71
2:D:523:ILE:HG22	4:D:791:HOH:O	1.89	0.71
1:B:108:GLN:HG2	4:B:702:HOH:O	1.91	0.71
2:C:467:GLU:OE2	2:C:471:ARG:HD3	1.90	0.70
2:C:303:LEU:HG	2:C:338:ASP:O	1.91	0.70
2:D:411:CYS:HB2	4:D:783:HOH:O	1.88	0.70
2:C:261:VAL:HG13	2:C:334:TYR:HA	1.73	0.70
2:D:276:ILE:HG13	2:D:286:THR:HG23	1.74	0.70
1:B:110:SER:HA	4:B:675:HOH:O	1.91	0.70
2:C:441:TYR:CE1	4:C:799:HOH:O	2.45	0.69
1:B:136:THR:CG2	4:B:699:HOH:O	2.36	0.69
2:D:468:ASN:ND2	2:D:471:ARG:H	1.90	0.69
2:C:299:ARG:HB3	4:C:752:HOH:O	1.92	0.69
2:C:465:LEU:CD1	4:C:751:HOH:O	2.27	0.69
2:C:278:GLN:HB2	4:C:845:HOH:O	1.92	0.69
2:C:319:MET:HA	4:C:837:HOH:O	1.93	0.69
2:D:276:ILE:CG1	2:D:286:THR:HG23	2.22	0.69
2:D:521:LEU:CD2	4:D:723:HOH:O	2.22	0.69
4:A:718:HOH:O	1:B:81:PHE:CG	2.43	0.69
2:D:365:GLN:HB2	4:D:771:HOH:O	1.92	0.68
2:C:504:MET:SD	4:C:778:HOH:O	2.51	0.68
1:A:86:HIS:HB3	1:B:79:SER:O	1.94	0.68
2:C:398:GLY:N	4:C:847:HOH:O	2.25	0.68
2:C:465:LEU:CG	4:C:751:HOH:O	2.40	0.68
2:D:267:LYS:CE	4:D:815:HOH:O	2.40	0.68
2:C:395:ILE:HD12	2:C:453:MET:SD	2.34	0.67
2:D:271:THR:HG22	2:D:272:ARG:H	1.58	0.67
2:D:517:GLN:NE2	4:D:728:HOH:O	2.24	0.67
1:B:93:THR:HG21	4:B:687:HOH:O	1.94	0.67
2:D:261:VAL:HG13	2:D:334:TYR:HA	1.75	0.67
2:C:500:ARG:NE	4:C:819:HOH:O	2.28	0.67
2:C:267:LYS:CA	4:C:786:HOH:O	2.35	0.67
2:D:366:ILE:HD13	4:D:771:HOH:O	1.95	0.67
2:D:457:MET:CE	4:D:781:HOH:O	2.43	0.66
4:A:691:HOH:O	2:C:308:LYS:CE	2.40	0.66
2:C:450:LEU:CG	4:C:795:HOH:O	2.39	0.66
1:A:97:THR:HB	1:B:78:PRO:HD3	1.77	0.66
2:D:382:SER:CA	4:D:794:HOH:O	2.42	0.66
2:D:486:ASN:CB	2:D:489:LYS:HE2	2.24	0.66
2:C:538:LYS:NZ	4:C:748:HOH:O	2.27	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:323:LYS:CE	4:D:786:HOH:O	2.42	0.66
2:D:517:GLN:CG	4:D:728:HOH:O	2.44	0.66
2:C:357:THR:HG22	4:C:725:HOH:O	1.96	0.66
2:C:497:PHE:CE1	4:C:770:HOH:O	2.49	0.66
2:C:538:LYS:CE	4:C:824:HOH:O	2.43	0.66
2:C:541:THR:HG21	4:C:754:HOH:O	1.95	0.66
2:D:382:SER:N	4:D:794:HOH:O	2.29	0.66
2:C:520:PHE:CA	4:C:784:HOH:O	2.41	0.65
2:C:484:LEU:CD2	4:C:842:HOH:O	2.44	0.65
2:C:395:ILE:HD12	2:C:453:MET:CE	2.25	0.65
2:D:427:THR:HG23	4:D:788:HOH:O	1.95	0.65
1:A:83:HIS:ND1	4:A:685:HOH:O	2.29	0.65
2:C:277:GLY:HA3	4:C:792:HOH:O	1.97	0.65
2:D:436:VAL:CG1	4:D:778:HOH:O	2.43	0.65
1:A:92:VAL:HG23	4:A:659:HOH:O	1.97	0.65
2:C:347:LEU:CD1	4:C:829:HOH:O	2.31	0.65
2:C:319:MET:CE	4:C:849:HOH:O	2.46	0.64
2:D:271:THR:OG1	2:D:290:VAL:HG22	1.97	0.64
2:C:344:MET:HE2	2:C:411:CYS:O	1.98	0.64
1:B:146:THR:HG22	2:D:386:ILE:HD11	1.79	0.64
2:C:526:PRO:HA	4:C:671:HOH:O	1.98	0.64
2:D:323:LYS:HE3	4:D:786:HOH:O	1.97	0.64
2:C:395:ILE:CD1	4:C:753:HOH:O	2.45	0.63
1:B:80:ASP:HB3	4:B:697:HOH:O	1.98	0.63
2:C:414:ILE:HG23	4:C:826:HOH:O	1.97	0.63
2:C:301:MET:HB3	4:C:817:HOH:O	1.99	0.62
2:D:352:LEU:O	2:D:356:VAL:HG23	2.00	0.62
2:C:465:LEU:HD22	4:C:751:HOH:O	1.97	0.62
2:C:406:THR:C	4:C:814:HOH:O	2.42	0.62
2:C:450:LEU:HD23	4:C:795:HOH:O	1.97	0.62
2:C:523:ILE:CG2	4:C:797:HOH:O	2.24	0.62
2:D:367:ALA:HA	4:D:723:HOH:O	2.00	0.62
2:C:253:ILE:HG13	2:C:254:LEU:HD12	1.82	0.62
2:D:515:LEU:HD22	4:D:784:HOH:O	1.99	0.62
2:C:340:LEU:CD2	4:C:779:HOH:O	2.38	0.62
2:D:263:VAL:HG12	4:D:813:HOH:O	1.98	0.62
2:C:347:LEU:CG	4:C:847:HOH:O	2.35	0.62
1:B:110:SER:HB2	2:D:468:ASN:ND2	2.14	0.62
2:D:436:VAL:HG13	2:D:473:LEU:HD22	1.80	0.62
4:A:691:HOH:O	2:C:308:LYS:CD	2.47	0.61
2:C:500:ARG:CZ	4:C:819:HOH:O	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLN:HB3	1:A:142:TYR:HE1	1.65	0.61
2:C:276:ILE:HB	2:C:284:VAL:HG23	1.82	0.61
1:B:109:THR:HG23	4:B:646:HOH:O	2.01	0.61
2:D:414:ILE:HG22	2:D:416:PRO:HD2	1.80	0.61
2:D:428:PRO:O	2:D:430:TRP:N	2.33	0.61
2:C:390:ILE:HB	2:C:449:SER:HB2	1.83	0.61
2:C:514:GLU:HG2	3:C:627:IOD:I	2.71	0.61
2:C:301:MET:HG2	4:C:817:HOH:O	1.95	0.61
2:C:399:MET:HE3	4:C:813:HOH:O	1.95	0.61
2:D:523:ILE:CB	4:D:791:HOH:O	2.43	0.61
2:C:378:GLU:OE2	2:C:513:LYS:HG3	2.01	0.61
2:D:391:LYS:HE2	4:D:694:HOH:O	2.00	0.61
2:C:468:ASN:ND2	4:C:816:HOH:O	2.26	0.60
2:D:300:GLN:CG	4:D:799:HOH:O	2.44	0.60
2:D:457:MET:HE1	4:D:781:HOH:O	2.01	0.60
3:B:624:IOD:I	4:B:631:HOH:O	2.86	0.60
1:A:113:THR:O	1:A:117:GLN:HG3	2.01	0.60
1:A:88:GLY:HA2	1:B:80:ASP:HB2	1.83	0.60
2:C:387:HIS:CD2	2:C:408:PHE:HB3	2.36	0.60
1:B:93:THR:HB	4:B:687:HOH:O	1.98	0.60
2:C:322:ASN:HA	4:C:785:HOH:O	2.00	0.60
1:B:110:SER:CA	4:B:675:HOH:O	2.47	0.60
1:B:89:PHE:HB3	4:B:643:HOH:O	2.01	0.59
4:A:706:HOH:O	1:B:82:GLU:CD	2.42	0.59
2:C:298:ILE:N	2:C:298:ILE:HD12	2.17	0.59
1:B:119:LYS:HG2	3:B:615:IOD:I	2.72	0.59
2:D:505:ASP:HB3	4:D:704:HOH:O	2.01	0.59
2:D:318:VAL:HG12	2:D:319:MET:HE2	1.85	0.59
2:D:517:GLN:CB	4:D:728:HOH:O	2.49	0.59
1:B:93:THR:CG2	4:B:687:HOH:O	2.50	0.59
1:B:110:SER:N	4:B:675:HOH:O	2.35	0.59
2:D:303:LEU:O	2:D:304:GLN:C	2.46	0.59
2:D:253:ILE:CG1	4:D:748:HOH:O	2.25	0.59
2:D:262:SER:CB	4:D:725:HOH:O	2.50	0.59
1:B:78:PRO:CG	4:B:690:HOH:O	2.51	0.59
4:B:651:HOH:O	2:D:468:ASN:HB3	2.03	0.59
2:D:467:GLU:OE2	2:D:471:ARG:HD3	2.02	0.59
2:C:256:LYS:HE3	2:C:310:GLU:OE1	2.03	0.58
2:C:267:LYS:CB	4:C:786:HOH:O	2.52	0.58
2:C:271:THR:HG22	2:C:272:ARG:N	2.16	0.58
2:D:263:VAL:CB	4:D:813:HOH:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:MET:HE3	1:A:99:MET:HA	1.84	0.58
2:C:399:MET:HE1	4:C:813:HOH:O	1.96	0.58
1:A:146:THR:CG2	2:C:386:ILE:HD11	2.33	0.58
2:D:289:ASP:CG	4:D:757:HOH:O	2.46	0.58
2:C:398:GLY:C	2:C:400:ASP:H	2.11	0.58
2:C:405:LEU:HD13	4:C:753:HOH:O	2.03	0.58
2:C:520:PHE:HB2	4:C:784:HOH:O	2.03	0.58
4:A:706:HOH:O	1:B:82:GLU:HB2	2.03	0.58
2:D:414:ILE:CG2	2:D:416:PRO:HD2	2.34	0.58
2:C:369:VAL:HG21	2:C:457:MET:SD	2.43	0.58
1:B:96:PHE:HD1	4:B:654:HOH:O	1.85	0.58
1:A:90:ASP:CB	4:A:717:HOH:O	2.47	0.58
2:C:541:THR:CG2	4:C:754:HOH:O	2.52	0.58
2:D:493:ILE:HG22	4:D:726:HOH:O	2.00	0.58
2:D:403:VAL:HG22	4:D:706:HOH:O	2.04	0.57
2:C:387:HIS:O	2:C:388:ARG:HB2	2.04	0.57
2:C:539:GLU:C	2:C:541:THR:N	2.62	0.57
2:C:333:SER:HA	4:C:831:HOH:O	2.05	0.57
2:C:262:SER:HB2	4:C:760:HOH:O	2.04	0.57
2:D:366:ILE:HA	4:D:781:HOH:O	2.04	0.57
1:A:105:ARG:HG2	4:A:669:HOH:O	2.03	0.57
4:A:718:HOH:O	1:B:81:PHE:CE2	2.51	0.57
1:B:78:PRO:HD2	4:B:690:HOH:O	2.03	0.57
2:D:366:ILE:HD12	2:D:457:MET:CB	2.34	0.57
2:D:398:GLY:C	2:D:400:ASP:N	2.62	0.56
1:A:138:ASN:C	4:A:701:HOH:O	2.48	0.56
2:C:493:ILE:CB	4:C:784:HOH:O	2.26	0.56
2:D:490:LEU:HD22	4:D:712:HOH:O	2.05	0.56
2:C:301:MET:CB	4:C:817:HOH:O	2.51	0.56
2:C:388:ARG:CD	4:C:661:HOH:O	2.36	0.56
2:C:397:LEU:CB	4:C:804:HOH:O	2.36	0.56
2:C:517:GLN:HG2	4:C:721:HOH:O	2.05	0.56
2:D:271:THR:HG22	2:D:272:ARG:N	2.19	0.56
2:D:428:PRO:HB3	2:D:431:MET:SD	2.45	0.56
1:B:108:GLN:HA	4:B:688:HOH:O	2.05	0.56
2:C:333:SER:HA	2:C:341:TRP:O	2.04	0.56
2:D:314:ASN:O	2:D:318:VAL:HG23	2.05	0.56
2:C:284:VAL:HG12	2:C:299:ARG:HA	1.87	0.56
2:D:520:PHE:HE2	4:D:696:HOH:O	1.89	0.56
2:C:322:ASN:CA	4:C:837:HOH:O	2.53	0.56
2:D:500:ARG:NH2	4:D:812:HOH:O	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:330:TYR:CE1	4:C:833:HOH:O	2.55	0.56
2:C:347:LEU:CB	4:C:829:HOH:O	2.41	0.56
2:C:515:LEU:CD2	4:C:770:HOH:O	2.43	0.56
2:D:249:SER:CB	4:D:798:HOH:O	2.54	0.56
2:C:398:GLY:C	2:C:400:ASP:N	2.61	0.55
2:D:366:ILE:CD1	2:D:457:MET:HB3	2.35	0.55
2:D:500:ARG:HD2	4:D:715:HOH:O	2.06	0.55
2:C:424:MET:CG	4:C:771:HOH:O	2.40	0.55
2:C:398:GLY:CA	4:C:847:HOH:O	2.53	0.55
1:A:107:LEU:HD22	4:A:668:HOH:O	2.06	0.55
2:C:489:LYS:HG3	4:C:749:HOH:O	2.06	0.55
2:D:361:MET:HA	2:D:365:GLN:NE2	2.21	0.55
2:D:453:MET:HG2	2:D:457:MET:HE2	1.89	0.55
2:C:308:LYS:HD3	2:C:311:LEU:CD1	2.37	0.55
2:C:411:CYS:O	2:C:412:ALA:HB2	2.06	0.55
2:C:482:PRO:HB2	4:C:742:HOH:O	2.07	0.55
2:C:319:MET:HG3	4:C:654:HOH:O	2.07	0.55
2:D:308:LYS:HB2	4:D:736:HOH:O	2.01	0.55
1:B:109:THR:C	4:B:675:HOH:O	2.50	0.55
2:D:303:LEU:O	2:D:305:GLN:N	2.39	0.54
2:D:398:GLY:C	2:D:400:ASP:H	2.15	0.54
2:C:303:LEU:HB2	2:C:339:GLU:HA	1.89	0.54
2:C:386:ILE:HG22	2:C:388:ARG:HG3	1.88	0.54
2:C:488:GLU:CD	2:C:488:GLU:H	2.13	0.54
2:C:471:ARG:HG3	2:C:471:ARG:HH11	1.71	0.54
2:D:387:HIS:CD2	2:D:408:PHE:HB3	2.43	0.54
2:C:454:ALA:CB	4:C:839:HOH:O	2.45	0.54
2:C:304:GLN:HA	2:C:309:LYS:NZ	2.23	0.54
2:C:459:GLU:CD	4:C:823:HOH:O	2.51	0.54
1:A:122:GLN:HB2	4:A:718:HOH:O	2.08	0.54
2:C:269:LYS:CD	4:C:844:HOH:O	2.38	0.54
2:D:459:GLU:OE2	2:D:484:LEU:HD12	2.08	0.54
1:A:110:SER:O	1:A:111:ASN:HB2	2.07	0.53
2:C:486:ASN:ND2	4:C:749:HOH:O	2.28	0.53
2:D:403:VAL:HB	4:D:785:HOH:O	2.08	0.53
2:D:427:THR:CG2	4:D:788:HOH:O	2.55	0.53
2:C:468:ASN:CG	3:C:602:IOD:I	3.20	0.53
2:D:319:MET:CB	4:D:796:HOH:O	2.21	0.53
2:C:253:ILE:HG13	2:C:254:LEU:CD1	2.39	0.53
2:C:343:VAL:HG22	4:C:715:HOH:O	2.09	0.53
1:B:85:ILE:HD12	1:B:98:GLY:HA3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:VAL:HG21	2:D:335:LEU:HG	1.89	0.53
2:D:395:ILE:HD12	2:D:453:MET:SD	2.48	0.53
1:A:140:GLN:HB3	1:A:142:TYR:CE1	2.42	0.53
1:B:124:VAL:HB	4:B:701:HOH:O	2.08	0.53
2:D:253:ILE:HG13	2:D:254:LEU:N	2.23	0.53
2:C:395:ILE:CD1	2:C:453:MET:SD	2.95	0.53
2:D:307:PRO:O	2:D:308:LYS:C	2.52	0.53
2:D:523:ILE:HG22	2:D:523:ILE:O	2.09	0.53
2:C:276:ILE:HD11	2:C:286:THR:OG1	2.08	0.53
1:A:79:SER:C	1:A:81:PHE:H	2.12	0.53
2:C:288:MET:CA	4:C:830:HOH:O	2.57	0.53
2:C:520:PHE:CB	4:C:784:HOH:O	2.57	0.53
1:B:99:MET:HE1	1:B:125:LEU:CD2	2.39	0.53
2:C:261:VAL:CG1	2:C:334:TYR:HA	2.40	0.52
2:C:308:LYS:HD3	2:C:311:LEU:HD12	1.91	0.52
2:D:262:SER:HB3	4:D:725:HOH:O	2.10	0.52
2:D:358:GLU:N	4:D:693:HOH:O	2.38	0.52
1:A:130:PHE:O	1:A:134:LYS:HG2	2.09	0.52
2:C:414:ILE:HG21	4:C:826:HOH:O	2.06	0.52
2:D:308:LYS:HG3	4:D:691:HOH:O	2.10	0.52
2:D:303:LEU:HG	2:D:304:GLN:H	1.73	0.52
2:C:278:GLN:HA	4:C:726:HOH:O	2.10	0.52
1:A:99:MET:HE1	1:A:125:LEU:CD2	2.39	0.52
1:A:107:LEU:HD21	1:A:117:GLN:OE1	2.10	0.52
2:C:398:GLY:HA2	4:C:847:HOH:O	2.07	0.52
2:C:470:LEU:HD12	3:C:602:IOD:I	2.79	0.52
2:C:395:ILE:HD11	4:C:753:HOH:O	2.05	0.51
2:C:424:MET:CG	4:C:812:HOH:O	2.50	0.51
1:B:116:GLU:HB3	2:D:474:TYR:CZ	2.46	0.51
2:D:397:LEU:HG	4:D:706:HOH:O	2.09	0.51
2:D:490:LEU:CD2	4:D:780:HOH:O	2.51	0.51
2:D:373:CYS:SG	2:D:395:ILE:CD1	2.96	0.51
2:C:301:MET:HB2	4:C:713:HOH:O	2.09	0.51
2:C:301:MET:SD	4:C:817:HOH:O	2.60	0.51
2:C:497:PHE:CD1	4:C:770:HOH:O	2.64	0.51
3:A:605:IOD:I	4:C:653:HOH:O	2.88	0.51
1:B:96:PHE:CZ	4:B:701:HOH:O	2.26	0.51
2:C:277:GLY:H	2:C:284:VAL:HG23	1.75	0.51
2:C:465:LEU:CD2	4:C:751:HOH:O	2.56	0.51
1:B:86:HIS:HD2	1:B:87:VAL:O	1.94	0.51
1:A:139:SER:C	4:A:701:HOH:O	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:288:MET:HA	4:C:830:HOH:O	2.11	0.51
2:C:288:MET:HE3	2:C:293:GLY:HA2	1.93	0.51
2:C:523:ILE:CG1	4:C:797:HOH:O	2.59	0.51
2:D:265:ASP:OD1	2:D:267:LYS:HB2	2.10	0.51
2:D:447:ILE:N	4:D:701:HOH:O	2.42	0.51
2:C:249:SER:C	2:C:251:GLU:H	2.19	0.50
2:C:366:ILE:O	2:C:369:VAL:HG22	2.11	0.50
2:C:410:PHE:O	2:C:413:GLN:HG3	2.10	0.50
1:B:116:GLU:HB3	2:D:474:TYR:OH	2.11	0.50
1:A:93:THR:HG23	4:A:660:HOH:O	2.11	0.50
2:C:494:PHE:HE2	4:C:808:HOH:O	1.87	0.50
2:D:403:VAL:CB	4:D:785:HOH:O	2.56	0.50
1:B:136:THR:HA	4:B:699:HOH:O	2.11	0.50
4:B:665:HOH:O	2:D:438:ARG:HG2	2.01	0.50
2:D:428:PRO:O	2:D:429:TYR:C	2.52	0.50
2:D:488:GLU:H	2:D:488:GLU:CD	2.20	0.50
2:C:257:LEU:O	2:C:261:VAL:HG23	2.11	0.50
2:C:296:VAL:HG23	2:C:298:ILE:HD11	1.94	0.50
2:D:261:VAL:CG1	2:D:334:TYR:HA	2.42	0.50
2:D:323:LYS:HE2	4:D:786:HOH:O	2.11	0.50
2:C:539:GLU:HA	2:C:539:GLU:OE1	2.11	0.50
2:D:455:ILE:O	2:D:458:ILE:HG22	2.12	0.49
2:D:503:ASP:O	2:D:509:ARG:HD3	2.12	0.49
2:D:390:ILE:HB	2:D:449:SER:CB	2.43	0.49
1:A:106:LEU:CD2	4:A:716:HOH:O	2.27	0.49
2:D:462:PRO:HB2	2:D:465:LEU:HD13	1.94	0.49
2:D:468:ASN:HD22	2:D:471:ARG:H	1.59	0.49
2:C:249:SER:CA	4:C:769:HOH:O	2.49	0.49
2:C:342:VAL:CB	4:C:752:HOH:O	2.42	0.49
2:C:424:MET:CE	4:C:812:HOH:O	2.45	0.49
1:A:92:VAL:N	4:A:659:HOH:O	2.40	0.49
1:B:143:MET:HG3	2:D:315:GLU:OE2	2.13	0.49
2:D:263:VAL:CA	4:D:813:HOH:O	2.29	0.49
2:D:352:LEU:HB2	2:D:397:LEU:HD11	1.93	0.49
1:A:122:GLN:CD	4:A:718:HOH:O	2.56	0.49
2:C:322:ASN:CB	4:C:837:HOH:O	2.29	0.49
2:D:366:ILE:CD1	4:D:771:HOH:O	2.59	0.49
2:C:314:ASN:O	2:C:318:VAL:HG23	2.13	0.49
2:D:359:THR:N	4:D:693:HOH:O	2.43	0.49
2:D:363:GLU:HG3	4:D:814:HOH:O	2.12	0.49
2:D:523:ILE:CG2	2:D:523:ILE:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:CYS:O	2:C:509:ARG:HD2	2.12	0.49
2:D:395:ILE:CD1	2:D:453:MET:CE	2.90	0.48
2:D:511:SER:OG	2:D:514:GLU:HG3	2.13	0.48
2:C:332:ASP:O	4:C:831:HOH:O	2.20	0.48
2:C:436:VAL:HG22	2:C:473:LEU:HD22	1.94	0.48
2:D:434:GLU:OE1	2:D:509:ARG:NH2	2.39	0.48
2:C:302:ASN:CB	2:C:305:GLN:HG3	2.35	0.48
2:C:504:MET:CE	4:C:705:HOH:O	2.61	0.48
2:C:297:ALA:C	2:C:298:ILE:HD12	2.38	0.48
2:D:258:ARG:HH11	2:D:258:ARG:HG2	1.77	0.48
2:D:501:CYS:O	2:D:509:ARG:HD2	2.13	0.48
2:D:319:MET:CG	4:D:796:HOH:O	2.55	0.48
2:D:355:VAL:C	4:D:693:HOH:O	2.55	0.48
2:D:494:PHE:O	2:D:497:PHE:HB3	2.13	0.48
2:C:298:ILE:HG13	4:C:715:HOH:O	2.12	0.48
2:C:332:ASP:H	2:C:343:VAL:HB	1.78	0.48
1:B:110:SER:HB2	2:D:468:ASN:HD21	1.76	0.48
2:D:254:LEU:HD21	4:D:680:HOH:O	2.12	0.48
2:D:412:ALA:N	4:D:734:HOH:O	2.21	0.48
2:D:490:LEU:N	2:D:490:LEU:HD23	2.29	0.48
1:A:118:LYS:HB2	4:A:696:HOH:O	2.07	0.48
2:D:387:HIS:O	2:D:388:ARG:HB2	2.14	0.48
2:D:361:MET:HA	2:D:365:GLN:HE22	1.79	0.47
4:A:691:HOH:O	2:C:308:LYS:HD2	2.11	0.47
2:D:253:ILE:HD11	4:D:680:HOH:O	2.13	0.47
2:D:305:GLN:O	2:D:305:GLN:HG3	2.15	0.47
2:D:371:ARG:NH1	2:D:372:GLU:OE2	2.42	0.47
2:D:390:ILE:HB	2:D:449:SER:HB2	1.95	0.47
1:A:146:THR:OG1	2:C:384:GLN:NE2	2.44	0.47
2:C:424:MET:C	4:C:747:HOH:O	2.57	0.47
2:D:378:GLU:CD	2:D:516:LEU:HD11	2.40	0.47
1:A:134:LYS:HE3	3:A:620:IOD:I	2.83	0.47
1:B:127:VAL:HG22	2:D:436:VAL:HG12	1.97	0.47
2:C:362:ASP:H	2:C:365:GLN:HE21	1.63	0.47
1:B:105:ARG:CG	4:B:668:HOH:O	2.39	0.47
2:D:312:ILE:O	2:D:316:ILE:HG12	2.15	0.46
4:A:706:HOH:O	1:B:82:GLU:CB	2.53	0.46
2:C:284:VAL:HA	2:C:298:ILE:O	2.16	0.46
1:A:82:GLU:OE2	4:A:690:HOH:O	2.20	0.46
2:D:301:MET:HE3	2:D:340:LEU:HD23	1.97	0.46
2:D:516:LEU:O	2:D:521:LEU:HD12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:322:ASN:ND2	2:C:383:ASN:HD21	2.14	0.46
2:D:382:SER:CB	4:D:806:HOH:O	2.30	0.46
2:D:468:ASN:OD1	2:D:469:PRO:HD2	2.16	0.46
2:C:342:VAL:HG13	4:C:831:HOH:O	2.16	0.46
2:C:483:GLU:C	4:C:742:HOH:O	2.59	0.46
2:C:523:ILE:HD12	2:C:523:ILE:C	2.40	0.46
2:D:311:LEU:HB2	4:D:691:HOH:O	2.15	0.46
2:C:462:PRO:HG2	4:C:751:HOH:O	2.16	0.46
1:B:129:GLU:HG2	4:D:655:HOH:O	2.16	0.46
2:C:373:CYS:SG	2:C:395:ILE:HD13	2.55	0.46
2:C:434:GLU:OE1	2:C:509:ARG:NH2	2.41	0.46
2:D:396:LEU:C	2:D:397:LEU:HD12	2.40	0.46
2:C:362:ASP:H	2:C:365:GLN:NE2	2.14	0.46
2:C:493:ILE:CG1	4:C:784:HOH:O	2.62	0.46
2:D:480:GLY:HA3	2:D:504:MET:HE2	1.98	0.46
1:B:114:LYS:CD	1:B:114:LYS:N	2.69	0.45
2:D:254:LEU:O	2:D:258:ARG:HG3	2.16	0.45
2:C:334:TYR:CG	4:C:760:HOH:O	2.59	0.45
1:B:114:LYS:HB3	4:B:663:HOH:O	2.15	0.45
2:D:481:THR:HG22	2:D:502:LEU:HB3	1.98	0.45
1:B:132:ASN:HB3	4:B:645:HOH:O	2.16	0.45
2:C:303:LEU:HD13	2:C:303:LEU:C	2.41	0.45
2:C:316:ILE:HG23	2:C:330:TYR:CE2	2.52	0.45
1:B:136:THR:CA	4:B:699:HOH:O	2.65	0.45
2:D:526:PRO:O	2:D:529:SER:HB3	2.16	0.45
2:C:273:PHE:O	2:C:274:GLU:HG3	2.17	0.45
1:B:105:ARG:CB	4:B:668:HOH:O	2.64	0.45
2:C:333:SER:O	4:C:760:HOH:O	2.21	0.45
2:C:436:VAL:HG21	2:C:473:LEU:HD22	1.96	0.45
2:C:471:ARG:HG3	2:C:471:ARG:NH1	2.31	0.45
2:C:320:ARG:HG3	2:C:320:ARG:HH11	1.82	0.45
2:C:266:PRO:N	4:C:809:HOH:O	2.46	0.44
1:B:146:THR:OG1	2:D:384:GLN:HG3	2.17	0.44
2:D:302:ASN:HD22	2:D:306:GLN:HE21	1.65	0.44
2:D:483:GLU:HB2	4:D:686:HOH:O	2.17	0.44
2:C:250:ASP:C	2:C:253:ILE:HG12	2.42	0.44
2:D:416:PRO:CA	4:D:740:HOH:O	2.61	0.44
2:C:320:ARG:HA	4:C:833:HOH:O	2.17	0.44
2:C:503:ASP:O	2:C:509:ARG:HD3	2.18	0.44
1:B:99:MET:HE2	1:B:103:TRP:HE3	1.82	0.44
2:D:395:ILE:CG2	2:D:403:VAL:HG13	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:249:SER:O	2:D:253:ILE:HG23	2.16	0.44
2:D:260:ILE:HD11	2:D:317:LEU:HD21	2.00	0.44
1:A:99:MET:HE1	1:A:125:LEU:HD22	1.98	0.44
2:D:309:LYS:O	2:D:313:ILE:HG13	2.18	0.44
2:C:394:ASN:O	2:C:406:THR:HG22	2.18	0.44
1:B:85:ILE:HD13	1:B:85:ILE:C	2.42	0.44
2:D:356:VAL:HG11	2:D:456:GLU:HG2	1.98	0.44
2:C:495:ARG:NH1	4:C:634:HOH:O	2.51	0.44
2:C:497:PHE:HE1	4:C:770:HOH:O	1.91	0.44
2:C:514:GLU:CG	3:C:627:IOD:I	3.36	0.44
1:B:113:THR:OG1	1:B:116:GLU:HG3	2.18	0.44
2:D:310:GLU:HA	2:D:313:ILE:HB	2.00	0.44
2:D:366:ILE:N	4:D:771:HOH:O	2.51	0.44
2:D:436:VAL:HG11	4:D:778:HOH:O	2.13	0.44
1:B:99:MET:HE1	1:B:125:LEU:HD21	2.00	0.43
2:D:265:ASP:HB3	2:D:268:LYS:HD2	2.00	0.43
2:D:354:ASP:HB2	4:D:750:HOH:O	2.18	0.43
1:A:90:ASP:CG	4:A:660:HOH:O	2.60	0.43
2:C:324:ASN:HA	2:C:325:PRO:HD3	1.87	0.43
2:C:390:ILE:HB	2:C:449:SER:CB	2.46	0.43
2:D:356:VAL:HG13	2:D:460:GLY:HA2	1.99	0.43
2:C:253:ILE:O	2:C:257:LEU:HG	2.18	0.43
2:C:267:LYS:HB3	4:C:786:HOH:O	2.17	0.43
2:D:450:LEU:HD12	2:D:453:MET:HE2	2.00	0.43
2:D:503:ASP:HB3	4:D:704:HOH:O	2.18	0.43
2:D:517:GLN:HG2	4:D:728:HOH:O	2.14	0.43
1:B:133:SER:C	1:B:135:LYS:H	2.26	0.43
2:D:306:GLN:HG3	2:D:307:PRO:HD2	2.01	0.43
2:D:327:ILE:O	2:D:327:ILE:HG13	2.17	0.43
2:C:253:ILE:HG13	2:C:254:LEU:N	2.33	0.43
2:C:468:ASN:ND2	3:C:602:IOD:I	3.22	0.43
2:C:478:THR:O	2:C:504:MET:HE1	2.18	0.43
2:C:500:ARG:NH2	4:C:803:HOH:O	2.28	0.43
2:D:365:GLN:CB	4:D:771:HOH:O	2.61	0.43
2:C:302:ASN:HB3	2:C:305:GLN:HE21	1.84	0.43
2:C:265:ASP:HA	2:C:266:PRO:HD3	1.91	0.43
2:D:302:ASN:HD22	2:D:306:GLN:NE2	2.17	0.43
2:C:397:LEU:CD2	4:C:804:HOH:O	2.66	0.42
2:C:504:MET:HE1	4:C:705:HOH:O	2.17	0.42
1:A:91:ALA:HB3	4:A:659:HOH:O	2.18	0.42
2:D:300:GLN:CA	4:D:799:HOH:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:254:LEU:HD23	2:C:258:ARG:NH2	2.34	0.42
2:C:329:ASN:HD22	2:C:345:GLU:CD	2.27	0.42
2:C:516:LEU:HD13	4:C:834:HOH:O	2.18	0.42
2:D:538:LYS:HE2	2:D:538:LYS:HB3	1.88	0.42
2:C:262:SER:N	4:C:760:HOH:O	2.53	0.42
2:C:404:LYS:CE	4:C:829:HOH:O	2.67	0.42
1:A:122:GLN:CB	4:A:718:HOH:O	2.66	0.42
2:C:316:ILE:O	2:C:320:ARG:HB3	2.19	0.42
2:C:538:LYS:HG2	4:C:793:HOH:O	2.05	0.42
2:D:324:ASN:HB3	2:D:327:ILE:HG12	2.02	0.42
2:C:469:PRO:O	2:C:473:LEU:HG	2.20	0.42
2:C:515:LEU:HB3	4:C:770:HOH:O	2.20	0.42
2:C:523:ILE:HG13	4:C:797:HOH:O	2.19	0.41
2:D:262:SER:HB2	4:D:725:HOH:O	2.19	0.41
2:D:292:THR:CG2	4:D:757:HOH:O	2.36	0.41
2:C:302:ASN:O	2:C:306:GLN:HB2	2.19	0.41
2:D:386:ILE:HD12	2:D:443:PRO:HA	2.02	0.41
1:B:101:GLU:HG3	1:B:102:GLN:N	2.35	0.41
2:D:306:GLN:HA	2:D:307:PRO:HD3	1.91	0.41
2:D:523:ILE:N	2:D:523:ILE:HD12	2.35	0.41
2:C:330:TYR:HB2	4:C:740:HOH:O	2.20	0.41
2:D:333:SER:HA	2:D:341:TRP:O	2.20	0.41
2:C:257:LEU:C	2:C:259:SER:H	2.29	0.41
2:C:342:VAL:CA	4:C:752:HOH:O	2.67	0.41
2:C:369:VAL:HG23	2:C:457:MET:HE1	2.03	0.41
1:B:80:ASP:CB	4:B:697:HOH:O	2.66	0.41
2:C:423:THR:C	2:C:425:VAL:H	2.27	0.40
2:D:397:LEU:HD12	2:D:397:LEU:N	2.37	0.40
2:D:454:ALA:HA	2:D:457:MET:HE3	2.02	0.40
2:D:356:VAL:CG1	2:D:460:GLY:HA2	2.51	0.40
2:D:382:SER:CB	4:D:794:HOH:O	2.21	0.40
2:C:500:ARG:HA	4:C:710:HOH:O	2.20	0.40
2:C:520:PHE:O	2:C:523:ILE:HG13	2.22	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	68/80 (85%)	66 (97%)	1 (2%)	1 (2%)	8	8
1	B	68/80 (85%)	60 (88%)	6 (9%)	2 (3%)	3	2
2	C	283/297 (95%)	261 (92%)	16 (6%)	6 (2%)	5	4
2	D	281/297 (95%)	254 (90%)	19 (7%)	8 (3%)	4	2
All	All	700/754 (93%)	641 (92%)	42 (6%)	17 (2%)	4	4

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	303	LEU
2	C	307	PRO
2	C	412	ALA
1	B	80	ASP
2	D	304	GLN
2	D	307	PRO
2	D	540	ALA
1	A	79	SER
2	C	414	ILE
2	C	541	THR
1	B	140	GLN
2	D	308	LYS
2	D	429	TYR
2	C	429	TYR
2	D	541	THR
2	D	414	ILE
2	D	428	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	64/74 (86%)	60 (94%)	4 (6%)	16	23
1	B	64/74 (86%)	59 (92%)	5 (8%)	11	16
2	C	245/258 (95%)	239 (98%)	6 (2%)	43	62
2	D	241/258 (93%)	230 (95%)	11 (5%)	24	36
All	All	614/664 (92%)	588 (96%)	26 (4%)	26	40

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	MET
1	A	127	VAL
1	A	138	ASN
1	A	146	THR
2	C	275	LYS
2	C	302	ASN
2	C	303	LEU
2	C	397	LEU
2	C	427	THR
2	C	436	VAL
1	B	85	ILE
1	B	99	MET
1	B	102	GLN
1	B	127	VAL
1	B	132	ASN
2	D	302	ASN
2	D	369	VAL
2	D	384	GLN
2	D	427	THR
2	D	462	PRO
2	D	465	LEU
2	D	468	ASN
2	D	481	THR
2	D	488	GLU
2	D	490	LEU
2	D	517	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	86	HIS
1	A	111	ASN
2	C	294	GLN
2	C	305	GLN
2	C	306	GLN
2	C	326	ASN
2	C	365	GLN
2	C	375	GLN
2	C	383	ASN
2	C	384	GLN
2	C	413	GLN
2	C	485	GLN
2	C	486	ASN
1	B	86	HIS
1	B	117	GLN
1	B	132	ASN
2	D	300	GLN
2	D	302	ASN
2	D	306	GLN
2	D	365	GLN
2	D	375	GLN
2	D	468	ASN
2	D	517	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 28 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	70/80 (87%)	0.71	4 (5%) 29 31	27, 40, 71, 81	0
1	B	70/80 (87%)	1.34	19 (27%) 1 1	31, 52, 93, 98	0
2	C	287/297 (96%)	1.25	82 (28%) 1 1	23, 45, 103, 113	0
2	D	285/297 (95%)	1.44	67 (23%) 2 2	35, 56, 89, 106	1 (0%)
All	All	712/754 (94%)	1.28	172 (24%) 2 2	23, 52, 96, 113	1 (0%)

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	319	MET	7.7
2	C	423	THR	6.2
1	A	78	PRO	5.9
2	C	277	GLY	5.6
2	D	250	ASP	5.4
2	C	254	LEU	5.1
2	C	276	ILE	5.1
2	C	414	ILE	5.0
2	C	303	LEU	4.8
1	A	79	SER	4.8
2	C	425	VAL	4.8
2	D	426	GLY	4.8
2	D	277	GLY	4.7
2	C	334	TYR	4.6
2	C	335	LEU	4.6
2	D	302	ASN	4.4
1	B	78	PRO	4.3
1	B	137	SER	4.3
2	D	306	GLN	4.2
2	C	541	THR	4.2
2	D	415	THR	4.2

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Mol	Chain	Res	Type	RSRZ
2	C	264	GLY	4.2
2	D	253	ILE	4.2
2	C	261	VAL	4.2
2	C	249	SER	4.0
2	C	302	ASN	4.0
2	D	395	ILE	4.0
2	C	424	MET	3.9
2	C	263	VAL	3.9
1	B	136	THR	3.9
2	C	306	GLN	3.8
1	B	139	SER	3.8
2	C	337	GLY	3.8
1	B	79	SER	3.7
2	C	271	THR	3.7
2	D	338	ASP	3.7
2	C	280	ALA	3.7
2	C	253	ILE	3.6
2	C	341	TRP	3.6
2	C	286	THR	3.6
2	D	492	ALA	3.6
2	D	493	ILE	3.6
2	D	516	LEU	3.5
2	C	313	ILE	3.4
2	C	399	MET	3.4
2	C	270	TYR	3.4
2	C	266	PRO	3.4
1	B	135	LYS	3.3
2	D	463	PRO	3.3
2	D	249	SER	3.3
2	D	276	ILE	3.3
2	C	426	GLY	3.2
1	A	80	ASP	3.2
2	D	303	LEU	3.2
2	D	414	ILE	3.2
2	D	283	THR	3.2
2	D	413	GLN	3.2
1	B	101	GLU	3.2
2	D	261	VAL	3.1
2	D	281	SER	3.1
2	C	250	ASP	3.1
2	D	305	GLN	3.1
2	C	273	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
2	C	332	ASP	3.0
2	C	257	LEU	3.0
2	C	340	LEU	3.0
2	C	342	VAL	2.9
2	D	263	VAL	2.9
2	D	542	LYS	2.9
2	C	316	ILE	2.9
1	A	142	TYR	2.9
2	C	262	SER	2.9
2	C	331	LEU	2.9
2	C	336	VAL	2.9
2	C	287	ALA	2.9
2	C	321	GLU	2.9
2	D	260	ILE	2.9
2	D	309	LYS	2.8
2	C	304	GLN	2.8
2	D	254	LEU	2.8
2	C	519	GLN	2.8
2	D	310	GLU	2.8
2	C	343	VAL	2.8
2	C	299	ARG	2.8
2	D	540	ALA	2.8
2	C	290	VAL	2.8
1	B	133	SER	2.8
2	C	259	SER	2.8
2	C	281	SER	2.8
2	C	412	ALA	2.8
2	D	316	ILE	2.7
2	D	360	CYS	2.7
2	C	256	LYS	2.7
2	C	291	ALA	2.7
2	C	312	ILE	2.7
2	C	317	LEU	2.7
2	C	540	ALA	2.7
2	D	313	ILE	2.7
2	D	507	GLU	2.7
2	C	269	LYS	2.7
1	B	140	GLN	2.6
2	D	297	ALA	2.6
2	C	289	ASP	2.6
2	D	400	ASP	2.5
2	D	264	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	296	VAL	2.5
2	D	308	LYS	2.5
2	C	542	LYS	2.5
2	D	257	LEU	2.5
2	C	288	MET	2.5
2	D	416	PRO	2.5
2	D	459	GLU	2.5
2	C	297	ALA	2.5
2	D	510	GLY	2.5
2	D	539	GLU	2.4
2	D	317	LEU	2.4
2	C	319	MET	2.4
1	B	147	ASP	2.4
2	D	480	GLY	2.4
2	D	301	MET	2.4
2	C	307	PRO	2.4
2	D	399	MET	2.4
2	D	541	THR	2.4
2	C	517	GLN	2.4
2	D	491	SER	2.3
2	C	310	GLU	2.3
2	C	415	THR	2.3
2	D	312	ILE	2.3
2	C	311	LEU	2.3
2	D	487	PRO	2.3
2	C	300	GLN	2.3
2	D	284	VAL	2.3
2	D	340	LEU	2.3
2	D	259	SER	2.3
2	C	400	ASP	2.2
2	C	293	GLY	2.2
2	C	320	ARG	2.2
2	C	292	THR	2.2
2	C	260	ILE	2.2
2	C	395	ILE	2.2
2	D	355	VAL	2.2
2	C	309	LYS	2.2
2	D	300	GLN	2.2
2	D	537	ALA	2.2
2	C	275	LYS	2.2
2	D	357	THR	2.2
1	B	106	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	129	GLU	2.1
2	C	279	GLY	2.1
2	D	442	GLY	2.1
2	D	504	MET	2.1
2	D	278	GLN	2.1
2	C	349	GLY	2.1
2	C	272	ARG	2.1
1	B	134	LYS	2.1
2	D	274	GLU	2.1
1	B	111	ASN	2.1
2	D	503	ASP	2.1
2	C	267	LYS	2.1
1	B	138	ASN	2.1
2	C	294	GLN	2.1
2	D	515	LEU	2.1
1	B	127	VAL	2.1
2	D	401	GLY	2.1
2	C	305	GLN	2.0
2	D	311	LEU	2.0
2	D	428	PRO	2.0
1	B	142	TYR	2.0
1	B	81	PHE	2.0
2	C	301	MET	2.0
1	B	144	SER	2.0
2	C	360	CYS	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IOD	B	606	1/1	0.87	0.20	61,61,61,61	1
3	IOD	D	625	1/1	0.88	0.16	58,58,58,58	1
3	IOD	C	618	1/1	0.89	0.19	68,68,68,68	1
3	IOD	D	628	1/1	0.89	0.15	58,58,58,58	1
3	IOD	A	620	1/1	0.94	0.13	64,64,64,64	1
3	IOD	D	621	1/1	0.94	0.15	64,64,64,64	1
3	IOD	D	622	1/1	0.94	0.16	64,64,64,64	1
3	IOD	C	613	1/1	0.94	0.17	42,42,42,42	1
3	IOD	A	605	1/1	0.94	0.17	56,56,56,56	1
3	IOD	D	604	1/1	0.95	0.09	49,49,49,49	1
3	IOD	A	626	1/1	0.95	0.15	50,50,50,50	1
3	IOD	A	614	1/1	0.95	0.08	47,47,47,47	1
3	IOD	B	615	1/1	0.95	0.07	49,49,49,49	1
3	IOD	B	624	1/1	0.95	0.10	58,58,58,58	1
3	IOD	C	616	1/1	0.96	0.11	51,51,51,51	1
3	IOD	C	627	1/1	0.96	0.14	58,58,58,58	1
3	IOD	B	617	1/1	0.96	0.08	51,51,51,51	1
3	IOD	C	623	1/1	0.97	0.10	55,55,55,55	1
3	IOD	A	607	1/1	0.98	0.04	44,44,44,44	1
3	IOD	D	603	1/1	0.98	0.13	60,60,60,60	1
3	IOD	C	611	1/1	0.98	0.07	39,39,39,39	1
3	IOD	D	619	1/1	0.98	0.12	58,58,58,58	1
3	IOD	A	601	1/1	0.99	0.03	40,40,40,40	0
3	IOD	B	612	1/1	0.99	0.08	41,41,41,41	1
3	IOD	C	609	1/1	0.99	0.08	46,46,46,46	1
3	IOD	C	610	1/1	0.99	0.05	40,40,40,40	1
3	IOD	B	608	1/1	1.00	0.05	43,43,43,43	1
3	IOD	C	602	1/1	1.00	0.03	34,34,34,34	1

6.5 Other polymers [i](#)

There are no such residues in this entry.