



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2017 – 04:29 PM EST

PDB ID : 1F3M  
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,  
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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](mailto: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.

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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-20028442
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-20028442

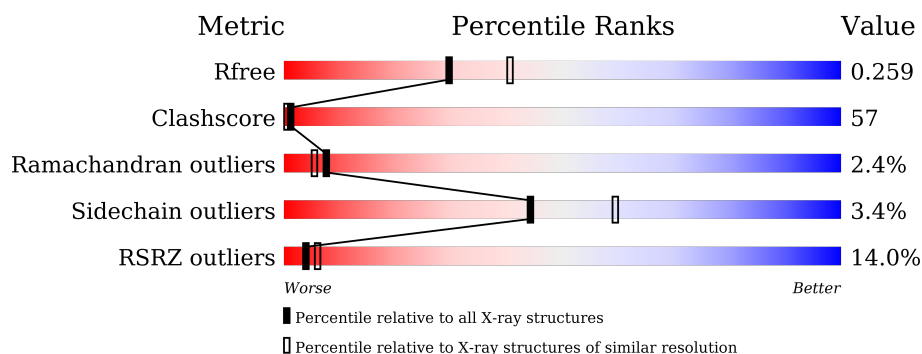
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	80	<div> <div>5%</div> <div> <div>49%</div> <div>34%</div> <div>5%</div> <div>13%</div> </div> </div>
1	B	80	<div> <div>14%</div> <div> <div>44%</div> <div>38%</div> <div>6%</div> <div>13%</div> </div> </div>
2	C	297	<div> <div>15%</div> <div> <div>48%</div> <div>46%</div> <div>• •</div> </div> </div>
2	D	297	<div> <div>13%</div> <div> <div>46%</div> <div>45%</div> <div>• •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	A	605	-	-	-	X
3	IOD	A	620	-	-	X	-
3	IOD	B	615	-	-	X	-
3	IOD	C	602	-	-	X	-
3	IOD	C	616	-	-	X	-
3	IOD	C	627	-	-	X	-
3	IOD	D	622	-	-	-	X
3	IOD	D	625	-	-	-	X
3	IOD	D	628	-	-	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 (three-letter code: IOD) (formula: I).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	78	Total	O	0	0
			78	78		

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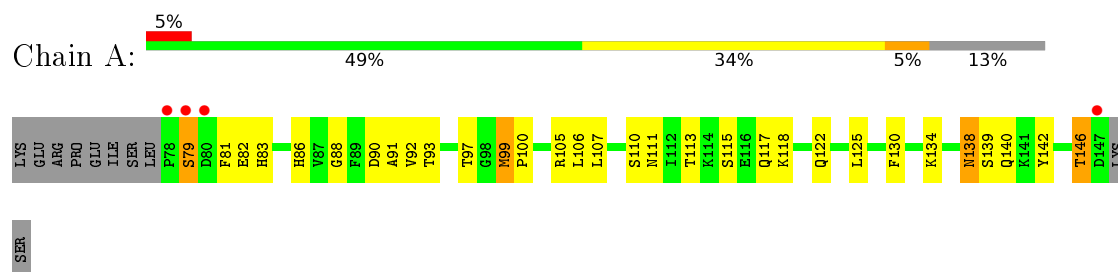
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	222	Total 222	O 222	0	0
4	D	188	Total 188	O 188	0	0

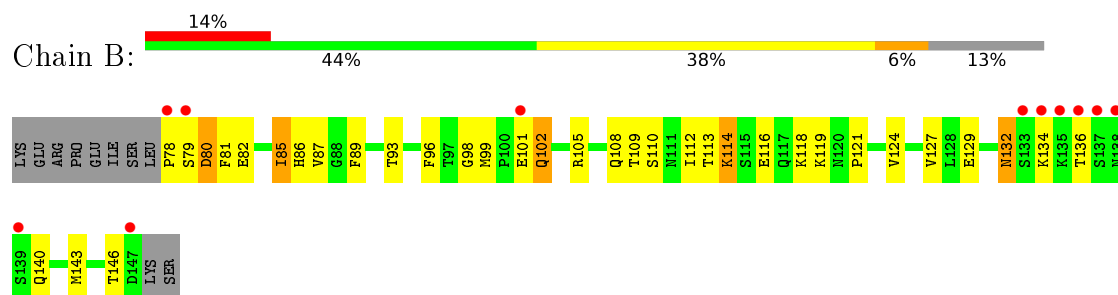
### 3 Residue-property plots

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.

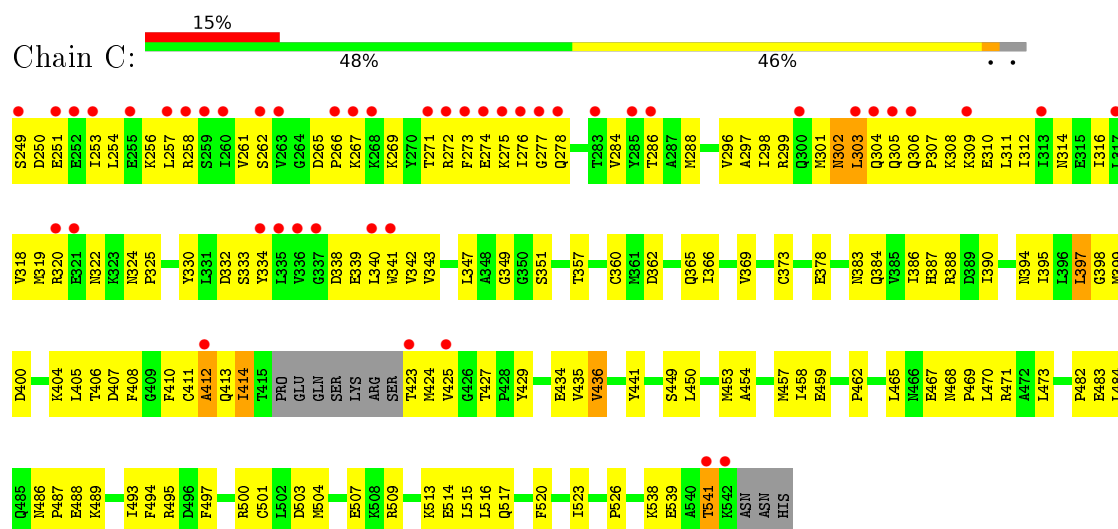
- Molecule 1: SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA



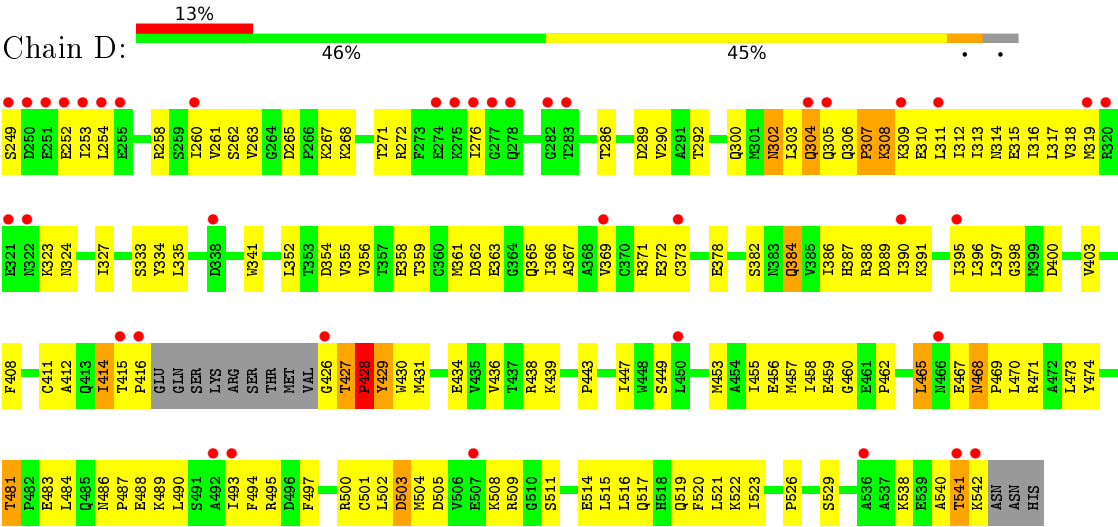
- Molecule 1: SERINE/THREONINE-PROTEIN KINASE PAK-ALPHA



- 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, $\alpha$ , $\beta$ , $\gamma$	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) 98.2 (34.08-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 2.29Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.237 , 0.258 0.237 , 0.259	Depositor DCC
$R_{free}$ test set	2857 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

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	0.44	0/576	0.67	0/777
1	B	0.40	0/576	0.65	0/777
2	C	0.35	0/2272	0.64	0/3075
2	D	0.33	0/2252	0.64	1/3049 (0.0%)
All	All	0.36	0/5676	0.64	1/7678 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	428	PRO	CA-N-CD	-5.02	104.48	111.50

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	563	0	537	44	0
1	B	563	0	537	78	0
2	C	2236	0	2261	278	0
2	D	2215	0	2234	239	0
3	A	6	0	0	4	0
3	B	6	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	9	0	0	9	0
3	D	7	0	0	3	0
4	A	94	0	0	41	0
4	B	78	0	0	47	0
4	C	222	0	0	184	0
4	D	188	0	0	135	0
All	All	6187	0	5569	633	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 57.

All (633) 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)
3:D:604:IOD:I	3:D:628:IOD:I	1.65	1.64
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: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: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: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
1:B:108:GLN:HG3	4:B:672:HOH:O	1.51	1.10
2:C:322:ASN:HB2	4:C:837:HOH:O	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:B:114:LYS:HD2	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:382:SER:HB2	4:D:806:HOH:O	1.52	1.06
2:C:301:MET:HE1	4:C:779:HOH:O	1.55	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
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
2:C:465:LEU:HD13	4:C:751:HOH:O	1.57	1.03
1:A:90:ASP:HA	4:A:717:HOH:O	1.56	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:395:ILE:HD11	2:C:453:MET:HE1	1.42	0.99
2:C:395:ILE:CD1	2:C:453:MET:CE	2.41	0.98
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: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:D:361:MET:HE2	4:D:771:HOH:O	1.65	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:C:399:MET:HE3	4:C:813:HOH:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:252:GLU:HA	4:D:801:HOH:O	1.70	0.91
4:B:665:HOH:O	2:D:438:ARG:HG3	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
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:D:504:MET:HE1	4:D:714:HOH:O	1.74	0.88
2:C:395:ILE:HD11	2:C:453:MET:CE	2.04	0.87
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
1:B:114:LYS:HG3	4:B:677:HOH:O	1.76	0.84
2:C:465:LEU:HB2	4:C:751:HOH:O	1.75	0.84
2:C:400:ASP:CB	4:C:777:HOH:O	2.24	0.84
1:B:136:THR:HG22	4:B:699:HOH:O	1.76	0.84
2:C:497:PHE:HE2	4:C:839:HOH:O	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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
2:C:397:LEU:C	4:C:847:HOH:O	2.21	0.78
1:B:119:LYS:HG3	3:B:615:IOD:I	2.53	0.78
1:B:119:LYS:CG	3:B:615:IOD:I	3.02	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:N	1:B:114:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:538:LYS:CG	4:C:793:HOH:O	2.29	0.75
2:D:542:LYS:CB	4:D:775:HOH:O	2.33	0.75
2:D:389:ASP:HB3	4:D:694:HOH:O	1.86	0.75
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
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
1:B:85:ILE:HD13	1:B:86:HIS:N	2.05	0.72
2:C:450:LEU:CD2	4:C:795:HOH:O	2.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:C:395:ILE:CD1	2:C:453:MET:HE3	2.19	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:C:507:GLU:CD	4:C:810:HOH:O	2.30	0.70
2:D:276:ILE:HG13	2:D:286:THR:HG23	1.74	0.70
2:D:504:MET:CE	4:D:714:HOH:O	2.34	0.70
2:C:539:GLU:C	2:C:541:THR:H	1.93	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:D:457:MET:HE3	4:D:781:HOH:O	1.92	0.69
2:C:319:MET:HA	4:C:837:HOH:O	1.93	0.69
2:C:278:GLN:HB2	4:C:845:HOH:O	1.92	0.69
2:C:399:MET:CE	4:C:813:HOH:O	2.30	0.69
2:C:395:ILE:CD1	2:C:453:MET:HE1	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:265:ASP:C	4:C:809:HOH:O	2.32	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:436:VAL:HG13	2:D:473:LEU:HD22	1.80	0.62
1:B:110:SER:HB2	2:D:468:ASN:ND2	2.14	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
1:A:140:GLN:HB3	1:A:142:TYR:HE1	1.65	0.61
1:B:109:THR:HG23	4:B:646:HOH:O	2.01	0.61
2:C:276:ILE:HB	2:C:284:VAL:HG23	1.82	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:504:MET:HE3	4:C:705:HOH:O	1.99	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: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
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
1:B:93:THR:HB	4:B:687:HOH:O	1.98	0.60
2:C:387:HIS:CD2	2:C:408:PHE:HB3	2.36	0.60
1:B:110:SER:CA	4:B:675:HOH:O	2.47	0.60
2:C:322:ASN:HA	4:C:785:HOH:O	2.00	0.60
1:B:89:PHE:HB3	4:B:643:HOH:O	2.01	0.59
1:B:119:LYS:HG2	3:B:615:IOD:I	2.72	0.59
2:C:298:ILE:N	2:C:298:ILE:HD12	2.17	0.59
2:D:505:ASP:HB3	4:D:704:HOH:O	2.01	0.59
2:D:517:GLN:CB	4:D:728:HOH:O	2.49	0.59
1:B:110:SER:N	4:B:675:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:THR:CG2	4:B:687:HOH:O	2.50	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
2:D:467:GLU:OE2	2:D:471:ARG:HD3	2.02	0.59
4:B:651:HOH:O	2:D:468:ASN:HB3	2.03	0.59
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:C:256:LYS:HE3	2:C:310:GLU:OE1	2.03	0.58
2:D:263:VAL:CB	4:D:813:HOH:O	2.51	0.58
1:A:99:MET:HE3	1:A:99:MET:HA	1.84	0.58
1:A:146:THR:CG2	2:C:386:ILE:HD11	2.33	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: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: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: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:428:PRO:HB3	2:D:431:MET:SD	2.45	0.56
2:C:388:ARG:CD	4:C:661:HOH:O	2.36	0.56
2:D:271:THR:HG22	2:D:272:ARG:N	2.19	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:C:406:THR:C	4:C:814:HOH:O	2.42	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
4:A:706:HOH:O	1:B:82:GLU:CD	2.42	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
2:D:289:ASP:CG	4:D:757:HOH:O	2.46	0.54
2:D:303:LEU:O	2:D:305:GLN:N	2.39	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:D:303:LEU:O	2:D:304:GLN:C	2.46	0.54
2:C:471:ARG:HH11	2:C:471:ARG:HG3	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:398:GLY:C	2:C:400:ASP:N	2.61	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:C:398:GLY:C	2:C:400:ASP:H	2.11	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:523:ILE:O	2:D:523:ILE:HG22	2.09	0.53
2:C:276:ILE:HD11	2:C:286:THR:OG1	2.08	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
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
2:D:398:GLY:C	2:D:400:ASP:N	2.62	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:107:LEU:HD21	1:A:117:GLN:OE1	2.10	0.52
1:A:99:MET:HE1	1:A:125:LEU:CD2	2.39	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
2:D:397:LEU:HG	4:D:706:HOH:O	2.09	0.51
1:B:116:GLU:HB3	2:D:474:TYR:CZ	2.46	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
1:B:86:HIS:HD2	1:B:87:VAL:O	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASN:C	4:A:701:HOH:O	2.48	0.51
2:C:288:MET:HA	4:C:830:HOH:O	2.11	0.51
2:C:488:GLU:H	2:C:488:GLU:CD	2.13	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: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: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
3:C:602:IOD:I	3:C:616:IOD:I	3.69	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
1:B:109:THR:C	4:B:675:HOH:O	2.50	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
2:C:459:GLU:CD	4:C:823:HOH:O	2.51	0.49
2:D:263:VAL:CA	4:D:813:HOH:O	2.29	0.49
1:B:143:MET:HG3	2:D:315:GLU:OE2	2.13	0.49
2:D:352:LEU:HB2	2:D:397:LEU:HD11	1.93	0.49
2:D:395:ILE:CD1	2:D:453:MET:CE	2.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:523:ILE:O	2:D:523:ILE:CG2	2.60	0.49
2:C:301:MET:CE	4:C:779:HOH:O	2.33	0.49
2:C:468:ASN:CG	3:C:602:IOD:I	3.20	0.49
2:C:501:CYS:O	2:C:509:ARG:HD2	2.12	0.49
2:D:361:MET:HE1	2:D:366:ILE:HD13	1.93	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:398:GLY:C	2:D:400:ASP:H	2.15	0.48
2:D:434:GLU:OE1	2:D:509:ARG:NH2	2.39	0.48
1:A:79:SER:C	1:A:81:PHE:H	2.12	0.48
2:C:302:ASN:CB	2:C:305:GLN:HG3	2.35	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:307:PRO:O	2:D:308:LYS:C	2.52	0.48
2:D:319:MET:CG	4:D:796: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
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
1:B:110:SER:HB2	2:D:468:ASN:HD21	1.76	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:HG3	2:D:305:GLN:O	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:139:SER:C	4:A:701:HOH:O	2.52	0.47
1:A:146:THR:OG1	2:C:384:GLN:NE2	2.44	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
1:B:105:ARG:CG	4:B:668:HOH:O	2.39	0.47
2:C:362:ASP:H	2:C:365:GLN:HE21	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:516:LEU:O	2:D:521:LEU:HD12	2.16	0.46
2:C:249:SER:C	2:C:251:GLU:H	2.19	0.46
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:D:311:LEU:HB2	4:D:691:HOH:O	2.15	0.46
1:B:129:GLU:HG2	4:D:655:HOH:O	2.16	0.46
2:C:462:PRO:HG2	4:C:751:HOH:O	2.16	0.46
2:D:361:MET:CE	4:D:771:HOH:O	2.39	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: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
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
1:B:114:LYS:HB3	4:B:663:HOH:O	2.15	0.45
2:C:334:TYR:CG	4:C:760:HOH:O	2.59	0.45
2:D:428:PRO:O	2:D:429:TYR:C	2.52	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: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
1:B:105:ARG:CB	4:B:668:HOH:O	2.64	0.45
2:C:273:PHE:O	2:C:274:GLU:HG3	2.17	0.45
2:C:333:SER:O	4:C:760:HOH:O	2.21	0.45
2:C:471:ARG:HG3	2:C:471:ARG:NH1	2.31	0.45
2:C:436:VAL:HG21	2:C:473:LEU:HD22	1.96	0.45
2:C:320:ARG:HG3	2:C:320:ARG:HH11	1.82	0.45
2:D:488:GLU:CD	2:D:488:GLU:H	2.20	0.45
1:B:146:THR:OG1	2:D:384:GLN:HG3	2.17	0.44
2:C:266:PRO:N	4:C:809:HOH:O	2.46	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: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
2:D:395:ILE:CG2	2:D:403:VAL:HG13	2.48	0.44
1:A:122:GLN:CD	4:A:718:HOH:O	2.56	0.44
2:D:249:SER:O	2:D:253:ILE:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:356:VAL:HG11	2:D:456:GLU:HG2	1.98	0.44
1:B:113:THR:OG1	1:B:116:GLU:HG3	2.18	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
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
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
2:C:297:ALA:C	2:C:298:ILE:HD12	2.38	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:355:VAL:C	4:D:693:HOH:O	2.55	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:C:504:MET:CE	4:C:705:HOH:O	2.61	0.43
2:C:539:GLU:C	2:C:541:THR:N	2.62	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
2:D:306:GLN:HG3	2:D:307:PRO:HD2	2.01	0.43
2:D:327:ILE:HG13	2:D:327:ILE:O	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: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:D:395:ILE:CD1	2:D:453:MET:HE3	2.49	0.43
2:C:424:MET:C	4:C:747:HOH:O	2.57	0.43
2:C:397:LEU:CD2	4:C:804:HOH:O	2.66	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
2:C:254:LEU:HD23	2:C:258:ARG:NH2	2.34	0.42
2:C:516:LEU:HD13	4:C:834:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:378:GLU:CD	2:D:516:LEU:HD11	2.40	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:HD12	2:D:523:ILE:N	2.35	0.41
2:C:523:ILE:HD12	2:C:523:ILE:C	2.40	0.41
2:C:330:TYR:HB2	4:C:740:HOH:O	2.20	0.41
2:C:395:ILE:HD12	2:C:453:MET:HE3	1.96	0.41
2:D:333:SER:HA	2:D:341:TRP:O	2.20	0.41
2:C:342:VAL:CA	4:C:752:HOH:O	2.67	0.41
1:B:80:ASP:CB	4:B:697:HOH:O	2.66	0.41
2:D:396:LEU:C	2:D:397:LEU:HD12	2.40	0.41
2:C:483:GLU:C	4:C:742:HOH:O	2.59	0.41
2:C:303:LEU:HD13	2:C:303:LEU:C	2.41	0.40
2:D:397:LEU:HD12	2:D:397:LEU:N	2.37	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%)	13	12
1	B	68/80 (85%)	60 (88%)	6 (9%)	2 (3%)	6	3
2	C	283/297 (95%)	261 (92%)	16 (6%)	6 (2%)	9	7
2	D	281/297 (95%)	254 (90%)	19 (7%)	8 (3%)	6	4
All	All	700/754 (93%)	641 (92%)	42 (6%)	17 (2%)	7	5

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%)	61 (95%)	3 (5%)	32	43
1	B	64/74 (86%)	58 (91%)	6 (9%)	11	12
2	C	245/258 (95%)	241 (98%)	4 (2%)	70	84
2	D	241/258 (93%)	233 (97%)	8 (3%)	45	61
All	All	614/664 (92%)	593 (97%)	21 (3%)	44	59

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	MET
1	A	138	ASN
1	A	146	THR
2	C	302	ASN
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	114	LYS
1	B	118	LYS
1	B	132	ASN
2	D	302	ASN
2	D	369	VAL
2	D	384	GLN
2	D	427	THR
2	D	465	LEU
2	D	468	ASN
2	D	481	THR
2	D	503	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	HIS
1	A	111	ASN
2	C	294	GLN
2	C	300	GLN
2	C	305	GLN
2	C	306	GLN

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Mol	Chain	Res	Type
2	C	365	GLN
2	C	383	ASN
2	C	384	GLN
2	C	413	GLN
2	C	485	GLN
1	B	86	HIS
1	B	132	ASN
2	D	294	GLN
2	D	300	GLN
2	D	302	ASN
2	D	306	GLN
2	D	365	GLN
2	D	468	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](#)

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	70/80 (87%)	0.37	4 (5%) 27 36	27, 40, 71, 81	0
1	B	70/80 (87%)	1.06	11 (15%) 3 4	31, 52, 93, 98	0
2	C	287/297 (96%)	1.00	46 (16%) 3 4	23, 45, 103, 113	0
2	D	285/297 (95%)	0.92	39 (13%) 4 6	36, 56, 89, 106	1 (0%)
All	All	712/754 (94%)	0.91	100 (14%) 4 6	23, 52, 96, 113	1 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	PRO	10.8
2	C	423	THR	7.2
1	B	136	THR	7.2
1	B	135	LYS	6.6
2	D	426	GLY	6.3
2	C	251	GLU	6.3
2	C	337	GLY	6.2
1	B	78	PRO	6.0
2	C	542	LYS	5.9
2	C	336	VAL	5.8
2	D	305	GLN	5.4
1	B	79	SER	5.4
2	C	305	GLN	5.3
2	D	253	ILE	5.3
2	C	334	TYR	5.1
2	C	262	SER	5.0
2	C	340	LEU	4.9
2	D	277	GLY	4.8
1	B	137	SER	4.8
2	D	542	LYS	4.7
2	C	276	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
2	C	541	THR	4.6
2	D	541	THR	4.6
2	C	277	GLY	4.5
2	D	249	SER	4.5
2	C	278	GLN	4.4
2	C	268	LYS	4.2
1	A	80	ASP	4.1
2	C	255	GLU	4.0
2	C	266	PRO	3.8
1	B	138	ASN	3.8
2	D	250	ASP	3.8
2	D	338	ASP	3.8
1	B	147	ASP	3.7
2	D	321	GLU	3.7
2	C	274	GLU	3.7
1	A	79	SER	3.7
2	D	251	GLU	3.6
1	B	134	LYS	3.6
2	C	304	GLN	3.6
1	A	147	ASP	3.5
2	C	263	VAL	3.5
2	D	369	VAL	3.5
2	C	320	ARG	3.4
2	D	276	ILE	3.2
2	D	254	LEU	3.2
2	C	425	VAL	3.2
2	D	466	ASN	3.2
2	D	322	ASN	3.2
2	C	309	LYS	3.1
2	D	274	GLU	3.1
2	D	275	LYS	3.1
2	C	283	THR	3.1
2	C	313	ILE	3.1
2	C	249	SER	3.0
2	D	260	ILE	3.0
2	D	252	GLU	3.0
2	C	267	LYS	3.0
2	D	390	ILE	2.9
2	C	271	THR	2.9
2	D	493	ILE	2.9
2	C	341	TRP	2.9
2	C	321	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	258	ARG	2.9
2	D	395	ILE	2.8
2	D	309	LYS	2.7
2	C	252	GLU	2.7
2	D	415	THR	2.7
2	D	278	GLN	2.6
2	D	319	MET	2.6
2	C	412	ALA	2.6
2	D	507	GLU	2.6
2	C	260	ILE	2.5
2	D	311	LEU	2.5
2	D	304	GLN	2.5
2	D	416	PRO	2.5
2	C	272	ARG	2.5
2	C	257	LEU	2.5
1	B	133	SER	2.4
2	D	283	THR	2.4
2	C	273	PHE	2.4
2	C	286	THR	2.4
2	D	492	ALA	2.4
2	C	253	ILE	2.3
2	C	285	TYR	2.3
2	C	303	LEU	2.3
2	D	450	LEU	2.3
2	D	373	CYS	2.3
2	C	259	SER	2.2
2	C	275	LYS	2.2
2	C	335	LEU	2.2
2	D	255	GLU	2.2
2	D	320	ARG	2.2
2	C	306	GLN	2.2
2	D	282	GLY	2.2
2	C	300	GLN	2.2
1	B	101	GLU	2.1
2	D	536	ALA	2.1
1	B	139	SER	2.1
2	C	317	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 ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	IOD	A	605	1/1	0.93	0.31	5.89	56,56,56,56	1
3	IOD	D	625	1/1	0.88	0.32	4.07	58,58,58,58	1
3	IOD	D	622	1/1	0.96	0.29	3.14	64,64,64,64	1
3	IOD	C	616	1/1	0.98	0.21	0.69	51,51,51,51	1
3	IOD	B	612	1/1	0.98	0.16	0.48	41,41,41,41	1
3	IOD	B	606	1/1	0.86	0.21	-0.45	61,61,61,61	1
3	IOD	C	602	1/1	1.00	0.14	-0.64	34,34,34,34	1
3	IOD	A	601	1/1	0.99	0.12	-1.21	40,40,40,40	0
3	IOD	C	623	1/1	0.98	0.13	-	55,55,55,55	1
3	IOD	B	615	1/1	0.97	0.17	-	49,49,49,49	1
3	IOD	C	611	1/1	0.98	0.14	-	39,39,39,39	1
3	IOD	B	624	1/1	0.88	0.16	-	58,58,58,58	1
3	IOD	D	603	1/1	0.97	0.18	-	60,60,60,60	1
3	IOD	C	613	1/1	0.96	0.25	-	42,42,42,42	1
3	IOD	C	610	1/1	0.98	0.17	-	40,40,40,40	1
3	IOD	A	614	1/1	0.96	0.17	-	47,47,47,47	1
3	IOD	A	607	1/1	0.99	0.13	-	44,44,44,44	1
3	IOD	B	608	1/1	0.99	0.15	-	43,43,43,43	1
3	IOD	D	621	1/1	0.94	0.13	-	64,64,64,64	1
3	IOD	D	619	1/1	0.94	0.18	-	58,58,58,58	1
3	IOD	A	626	1/1	0.88	0.24	-	50,50,50,50	1
3	IOD	D	604	1/1	0.96	0.18	-	49,49,49,49	1
3	IOD	B	617	1/1	0.97	0.22	-	51,51,51,51	1
3	IOD	C	627	1/1	0.92	0.25	-	58,58,58,58	1
3	IOD	C	609	1/1	0.99	0.15	-	46,46,46,46	1
3	IOD	C	618	1/1	0.91	0.16	-	68,68,68,68	1
3	IOD	A	620	1/1	0.94	0.22	-	64,64,64,64	1
3	IOD	D	628	1/1	0.98	0.13	-	58,58,58,58	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.