WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:30 PM GMT

PDB ID	:	1TZD
Title	:	CRYSTAL STRUCTURE OF THE CATALYTIC CORE OF INOSITOL 1,4,5-TRISPHOSPHATE 3-KINASE
Authors	:	Miller, G.J.; Hurley, J.H.
Deposited on	:	2004-07-09
Resolution	:	2.20 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.273
Clashscore		84
Ramachandran outliers		4.9%
Sidechain outliers		6.8%
RSRZ outliers		16.6%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
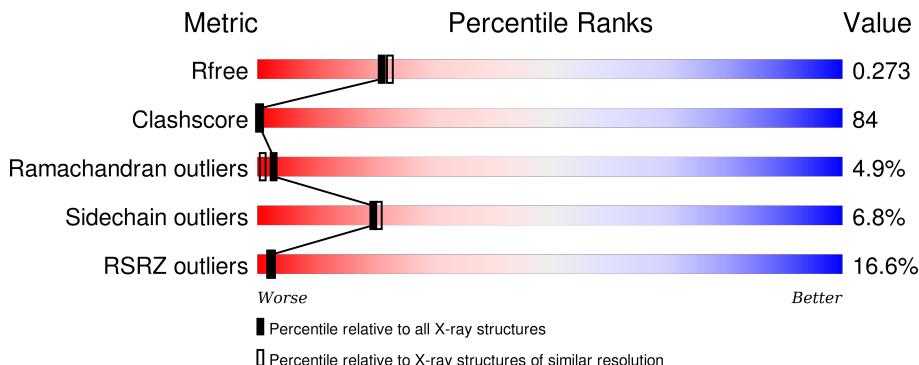
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	275	11% 28% 52% 7% • 12%
1	B	275	18% 31% 48% 7% • 12%
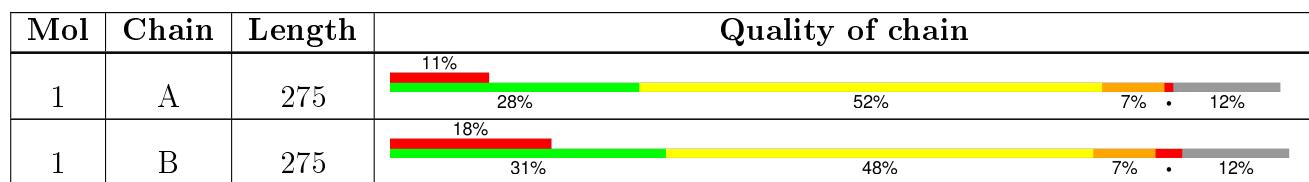
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4345 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 Inositol-trisphosphate 3-kinase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	243	Total	C	N	O	S	Se	7	0	0
			1961	1232	353	363	6	7			
1	B	242	Total	C	N	O	S	Se	0	0	0
			1952	1227	352	360	6	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	217	MSE	LEU	ENGINEERED	UNP P17105
A	423	ASN	ASP	ENGINEERED	UNP P17105
B	217	MSE	LEU	ENGINEERED	UNP P17105
B	423	ASN	ASP	ENGINEERED	UNP P17105

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
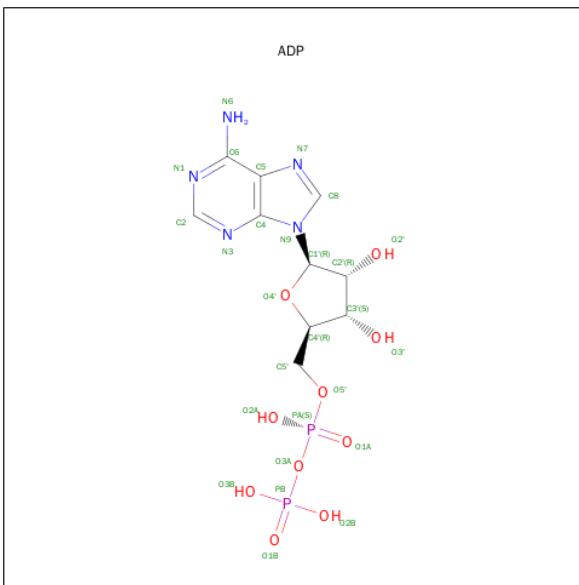
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

• Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total	O	0	0
			180	180		
4	B	197	Total	O	0	0
			197	197		

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: Inositol-trisphosphate 3-kinase A
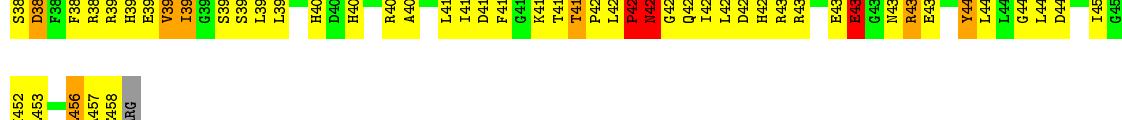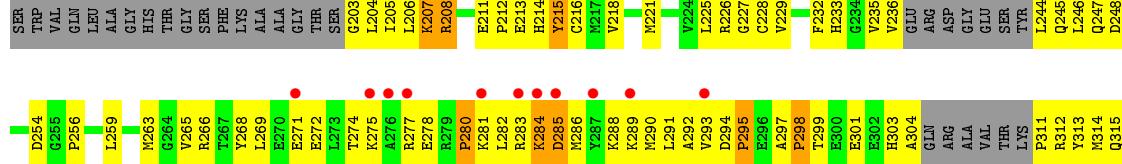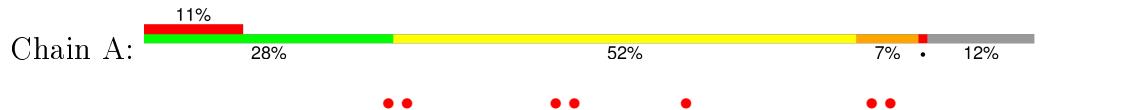
• Molecule 1: Inositol-trisphosphate 3-kinase A

L453 A454 N455 L456 A457 GLU ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	71.68Å 98.53Å 188.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.92 – 2.20 38.79 – 2.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.92-2.20) 94.8 (38.79-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.00 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.257 , 0.305 0.284 , 0.273	Depositor DCC
R_{free} test set	1641 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 54.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Outliers	0 of 32563 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4345	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, ADP

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	0.80	2/1991 (0.1%)	1.01	11/2666 (0.4%)
1	B	0.60	0/1982	1.17	16/2654 (0.6%)
All	All	0.71	2/3973 (0.1%)	1.09	27/5320 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	215	TYR	C-N	14.50	1.67	1.34
1	A	295	PRO	CA-C	5.57	1.64	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	PRO	CA-N-CD	-30.82	68.35	111.50
1	A	295	PRO	CA-N-CD	-8.32	99.86	111.50
1	B	279	ARG	CA-C-N	-8.11	94.39	117.10
1	B	279	ARG	C-N-CA	7.74	154.52	122.00
1	B	280	PRO	CA-CB-CG	-7.38	89.98	104.00
1	A	215	TYR	O-C-N	-7.25	111.10	122.70
1	A	208	ARG	N-CA-C	-7.06	91.94	111.00
1	A	208	ARG	N-CA-CB	7.00	123.19	110.60
1	B	279	ARG	O-C-N	6.89	134.19	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	284	LYS	N-CA-CB	6.63	122.54	110.60
1	B	386	ASP	CA-C-N	-6.53	102.84	117.20
1	A	284	LYS	C-N-CA	6.44	137.80	121.70
1	A	298	PRO	CA-N-CD	-6.42	102.51	111.50
1	B	282	LEU	C-N-CA	6.27	137.37	121.70
1	B	386	ASP	C-N-CA	6.21	137.23	121.70
1	A	280	PRO	CA-N-CD	-6.19	102.83	111.50
1	A	423	ASN	C-N-CA	-6.08	109.54	122.30
1	A	284	LYS	CA-C-N	-6.01	103.98	117.20
1	B	282	LEU	CA-C-N	-5.97	104.06	117.20
1	B	387	PHE	N-CA-CB	5.90	121.22	110.60
1	A	215	TYR	CA-C-N	5.64	129.60	117.20
1	B	326	LEU	N-CA-C	-5.58	95.92	111.00
1	B	387	PHE	N-CA-C	-5.56	95.98	111.00
1	B	321	SER	C-N-CA	-5.41	108.17	121.70
1	B	279	ARG	CA-C-O	5.39	131.42	120.10
1	B	244	LEU	CA-CB-CG	-5.15	103.44	115.30
1	B	321	SER	O-C-N	5.13	130.91	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	406	HIS	Mainchain

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	1961	0	1944	353	0
1	B	1952	0	1938	324	0
2	A	1	0	0	0	0
3	A	27	0	12	2	0
3	B	27	0	12	3	0
4	A	180	0	0	201	0
4	B	197	0	0	170	0
All	All	4345	0	3906	663	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 84.

All (663) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:VAL:O	1:B:244:LEU:N	1.68	1.26
1:A:215:TYR:HB2	4:A:557:HOH:O	1.36	1.25
1:B:208:ARG:HG3	4:B:601:HOH:O	1.37	1.21
1:A:336:ALA:HB1	1:B:292:ALA:HB1	1.22	1.21
1:B:361:MSE:HE1	1:B:371:TYR:CE1	1.77	1.20
1:A:419:THR:HB	4:A:497:HOH:O	1.42	1.19
1:B:292:ALA:HA	4:B:531:HOH:O	1.42	1.18
1:B:283:ARG:HG3	4:B:552:HOH:O	1.41	1.18
1:A:348:ARG:HD2	4:A:552:HOH:O	1.44	1.18
1:A:425:GLN:HB2	4:A:593:HOH:O	1.42	1.17
1:B:271:GLU:HB2	4:B:554:HOH:O	1.41	1.17
1:A:421:LEU:HD11	1:A:427:LEU:HG	1.26	1.16
1:A:328:PHE:HB2	4:A:577:HOH:O	1.43	1.16
1:B:394:ILE:HB	4:B:640:HOH:O	1.42	1.15
1:B:313:TYR:HA	4:B:602:HOH:O	1.45	1.13
1:A:297:ALA:HB2	4:A:518:HOH:O	1.48	1.13
1:B:288:LYS:HE2	4:B:636:HOH:O	1.47	1.13
1:A:263:MSE:SE	1:A:398:LEU:HD12	1.98	1.12
1:B:355:ARG:HA	4:B:533:HOH:O	1.48	1.11
1:B:211:GLU:HB3	4:B:631:HOH:O	1.50	1.10
1:A:355:ARG:HB3	4:A:628:HOH:O	1.50	1.10
1:A:394:ILE:HG22	1:A:417:LYS:HD3	1.32	1.10
1:A:277:ARG:HA	4:A:599:HOH:O	1.51	1.10
1:B:404:HIS:HB3	4:B:481:HOH:O	1.52	1.09
1:A:351:GLU:HG3	4:A:598:HOH:O	1.49	1.09
1:A:290:MSE:SE	1:A:312:ARG:NH1	2.36	1.09
1:B:236:VAL:HG12	1:B:236:VAL:O	1.53	1.08
1:A:389:ARG:HA	4:A:632:HOH:O	1.54	1.07
1:A:339:SER:HA	4:A:481:HOH:O	1.52	1.07
1:A:233:HIS:HD2	4:A:548:HOH:O	1.36	1.07
4:A:492:HOH:O	1:B:292:ALA:HB2	1.54	1.05
1:A:439:GLU:HG3	4:A:469:HOH:O	1.56	1.05
1:A:345:LYS:HE2	4:A:582:HOH:O	1.55	1.04
1:A:321:SER:HB2	4:A:488:HOH:O	1.55	1.04
1:B:389:ARG:HG2	4:B:646:HOH:O	1.57	1.04
1:B:425:GLN:HA	4:B:527:HOH:O	1.55	1.04
1:A:320:ILE:HA	1:A:348:ARG:HH21	1.20	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLY:HA2	4:A:466:HOH:O	1.58	1.03
1:A:266:ARG:HB2	4:A:505:HOH:O	1.55	1.03
1:A:361:MSE:HE1	1:A:368:LEU:HD13	1.38	1.03
1:B:270:GLU:HA	4:B:569:HOH:O	1.57	1.03
1:A:281:LYS:HB3	4:A:568:HOH:O	1.59	1.02
1:B:407:ARG:HA	4:B:628:HOH:O	1.57	1.02
1:A:297:ALA:HB1	4:A:531:HOH:O	1.58	1.01
1:A:412:LEU:HD21	4:A:603:HOH:O	1.58	1.01
1:B:346:THR:HB	4:B:589:HOH:O	1.59	1.01
1:B:421:LEU:HD11	1:B:427:LEU:HG	1.39	1.00
1:A:360:PHE:HB3	4:A:519:HOH:O	1.61	1.00
1:A:435:GLU:HA	4:A:498:HOH:O	1.58	1.00
1:A:317:ARG:HD2	4:A:488:HOH:O	1.62	0.99
1:A:396:SER:HA	1:A:414:ASP:HB2	1.41	0.99
1:A:389:ARG:HG3	4:A:604:HOH:O	1.63	0.99
1:A:367:VAL:HA	4:A:613:HOH:O	1.60	0.99
1:B:399:LEU:HG	4:B:647:HOH:O	1.59	0.99
1:A:421:LEU:HG	4:A:533:HOH:O	1.62	0.99
1:A:431:ARG:HD3	4:A:565:HOH:O	1.62	0.98
1:B:206:LEU:HD22	4:B:601:HOH:O	1.61	0.98
1:A:295:PRO:HA	4:A:545:HOH:O	1.61	0.98
1:B:250:LEU:HB3	4:B:491:HOH:O	1.61	0.98
1:A:336:ALA:CB	1:B:292:ALA:HB1	1.93	0.98
1:A:263:MSE:SE	4:A:577:HOH:O	2.32	0.98
1:A:414:ASP:HB3	4:A:513:HOH:O	1.63	0.97
1:B:321:SER:HB3	4:B:605:HOH:O	1.62	0.97
1:A:247:GLN:HA	4:A:584:HOH:O	1.65	0.96
1:B:290:MSE:HG2	4:B:614:HOH:O	1.66	0.96
1:B:383:GLU:HG2	4:B:622:HOH:O	1.66	0.96
1:A:204:LEU:HD23	4:A:584:HOH:O	1.66	0.95
1:B:270:GLU:HG2	4:B:569:HOH:O	1.66	0.95
1:A:425:GLN:HG3	4:A:532:HOH:O	1.65	0.94
1:B:282:LEU:HB3	4:B:590:HOH:O	1.66	0.94
1:B:315:GLN:HG3	4:B:542:HOH:O	1.66	0.94
1:A:443:LEU:HD13	4:A:506:HOH:O	1.64	0.94
1:A:204:LEU:HA	4:A:584:HOH:O	1.68	0.94
1:A:431:ARG:HB3	4:A:614:HOH:O	1.68	0.93
1:A:221:MSE:HE2	1:A:221:MSE:HA	1.49	0.93
1:B:361:MSE:HE1	1:B:371:TYR:HE1	1.23	0.93
1:B:312:ARG:HD2	4:B:550:HOH:O	1.69	0.93
1:B:333:ILE:HB	4:B:616:HOH:O	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:PRO:HD3	4:B:537:HOH:O	1.66	0.93
1:B:282:LEU:HD23	4:B:630:HOH:O	1.67	0.93
1:B:417:LYS:O	4:B:640:HOH:O	1.85	0.93
1:B:301:GLU:HB3	4:B:493:HOH:O	1.67	0.92
1:B:345:LYS:HG2	4:B:618:HOH:O	1.68	0.92
1:A:324:THR:HG22	4:A:622:HOH:O	1.69	0.91
1:B:361:MSE:HE1	1:B:371:TYR:CD1	2.03	0.91
1:A:394:ILE:CG2	1:A:417:LYS:HD3	2.00	0.90
1:A:438:ARG:HB3	1:A:438:ARG:HH21	1.35	0.90
1:A:345:LYS:HG2	4:A:634:HOH:O	1.70	0.90
1:B:219:ARG:HG3	4:B:603:HOH:O	1.70	0.90
1:B:269:LEU:HD11	1:B:417:LYS:HB2	1.52	0.89
1:A:313:TYR:HA	4:A:553:HOH:O	1.71	0.89
1:A:290:MSE:HE1	1:A:312:ARG:HD3	1.54	0.89
1:B:235:VAL:HA	4:B:517:HOH:O	1.72	0.89
1:B:286:MSE:HA	1:B:289:LYS:HD2	1.55	0.89
1:B:425:GLN:HG2	4:B:527:HOH:O	1.72	0.89
1:A:452:ILE:HG22	4:A:572:HOH:O	1.73	0.89
1:A:446:LEU:HD21	4:A:627:HOH:O	1.73	0.88
1:B:279:ARG:HB3	1:B:280:PRO:HD2	1.54	0.88
1:A:320:ILE:HA	1:A:348:ARG:NH2	1.88	0.88
1:A:214:HIS:HA	4:A:528:HOH:O	1.74	0.88
1:A:379:ARG:HB2	4:A:627:HOH:O	1.72	0.88
1:B:314:MSE:SE	4:B:540:HOH:O	2.42	0.88
1:A:290:MSE:SE	1:A:312:ARG:CZ	2.72	0.87
1:B:282:LEU:HD21	4:B:548:HOH:O	1.74	0.87
1:A:221:MSE:SE	4:A:556:HOH:O	2.41	0.87
1:B:358:GLU:HB3	4:B:533:HOH:O	1.74	0.87
1:A:293:VAL:HB	4:A:538:HOH:O	1.75	0.86
1:A:207:LYS:HD3	1:A:213:GLU:OE1	1.75	0.85
1:B:336:ALA:HB2	4:B:539:HOH:O	1.77	0.85
1:B:303:HIS:HB2	4:B:510:HOH:O	1.75	0.84
1:B:314:MSE:HA	4:B:540:HOH:O	1.77	0.84
1:A:286:MSE:O	1:A:289:LYS:HB2	1.78	0.84
1:A:367:VAL:HG22	4:A:613:HOH:O	1.76	0.84
1:A:336:ALA:HB1	1:B:292:ALA:CB	2.05	0.84
1:A:366:GLU:HG2	4:A:487:HOH:O	1.76	0.83
1:A:425:GLN:HG2	4:A:558:HOH:O	1.79	0.83
3:B:1:ADP:H5'2	4:B:634:HOH:O	1.79	0.83
1:B:383:GLU:HA	4:B:622:HOH:O	1.78	0.83
1:B:236:VAL:CG1	1:B:236:VAL:O	2.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:HG22	1:A:452:ILE:HG23	1.59	0.82
1:A:420:PRO:HB3	4:A:521:HOH:O	1.79	0.82
1:B:204:LEU:HB2	4:B:596:HOH:O	1.80	0.81
1:A:263:MSE:SE	1:A:398:LEU:CD1	2.79	0.81
1:B:426:ILE:HG12	4:B:646:HOH:O	1.81	0.81
1:A:317:ARG:HH11	1:A:317:ARG:HB2	1.46	0.81
1:B:211:GLU:HG2	4:B:623:HOH:O	1.81	0.80
1:A:394:ILE:O	1:A:417:LYS:HB2	1.80	0.80
1:B:325:THR:HG23	4:B:486:HOH:O	1.81	0.79
1:A:397:SER:HB2	4:A:626:HOH:O	1.80	0.79
1:B:215:TYR:HD1	4:B:568:HOH:O	1.66	0.79
1:A:283:ARG:HB2	4:A:562:HOH:O	1.82	0.79
1:A:304:ALA:HB3	4:A:561:HOH:O	1.83	0.78
1:B:443:LEU:HD13	4:B:546:HOH:O	1.83	0.78
1:B:215:TYR:CD1	4:B:568:HOH:O	2.35	0.78
1:A:393:VAL:HG22	1:A:418:THR:HG23	1.65	0.78
1:B:282:LEU:CB	4:B:590:HOH:O	2.27	0.78
1:B:288:LYS:HB2	4:B:591:HOH:O	1.82	0.78
1:B:276:ALA:CB	4:B:529:HOH:O	2.32	0.78
1:A:413:ILE:HD11	4:A:626:HOH:O	1.82	0.78
1:B:411:TRP:HD1	4:B:626:HOH:O	1.65	0.78
1:A:204:LEU:HD21	4:A:551:HOH:O	1.82	0.77
1:A:360:PHE:HD2	4:A:519:HOH:O	1.67	0.76
1:B:288:LYS:CB	4:B:591:HOH:O	2.33	0.76
1:B:390:ARG:HG2	4:B:489:HOH:O	1.84	0.76
1:A:215:TYR:CB	4:A:557:HOH:O	2.11	0.76
1:A:324:THR:CG2	4:A:622:HOH:O	2.32	0.76
1:B:275:LYS:HE3	4:B:523:HOH:O	1.85	0.76
1:B:207:LYS:O	1:B:244:LEU:HB3	1.85	0.76
1:B:346:THR:HG22	4:B:544:HOH:O	1.84	0.76
1:A:235:VAL:O	1:A:235:VAL:HG12	1.86	0.76
1:A:298:PRO:HD2	1:A:312:ARG:NH1	2.02	0.75
1:A:389:ARG:HG2	1:A:426:ILE:HG23	1.68	0.74
1:B:403:ASP:HB2	1:B:407:ARG:HB3	1.70	0.74
1:A:350:ARG:O	1:A:354:THR:HG23	1.87	0.74
1:A:361:MSE:HE1	1:A:368:LEU:CD1	2.17	0.74
1:A:370:ARG:HD2	4:A:487:HOH:O	1.87	0.74
1:B:405:CYS:SG	4:B:525:HOH:O	2.46	0.74
1:A:390:ARG:C	4:A:533:HOH:O	2.25	0.74
1:A:269:LEU:HB2	1:A:272:GLU:HG3	1.70	0.74
1:A:229:VAL:HB	4:A:583:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:N	4:B:561:HOH:O	2.21	0.73
1:A:228:CYS:HA	4:A:571:HOH:O	1.88	0.73
1:A:394:ILE:HG22	1:A:417:LYS:CD	2.16	0.73
1:A:203:GLY:HA3	4:A:639:HOH:O	1.88	0.73
1:B:326:LEU:HD21	1:B:350:ARG:NH1	2.03	0.73
1:A:421:LEU:HD13	4:A:558:HOH:O	1.87	0.73
1:B:403:ASP:OD2	1:B:405:CYS:HB2	1.89	0.73
1:A:361:MSE:SE	4:A:515:HOH:O	2.56	0.73
1:A:360:PHE:CD2	4:A:519:HOH:O	2.41	0.73
1:B:443:LEU:HD22	4:B:546:HOH:O	1.88	0.73
1:B:338:GLY:HA3	4:B:475:HOH:O	1.89	0.73
1:A:311:PRO:O	1:A:315:GLN:HG2	1.87	0.72
1:A:453:LEU:HG	4:A:572:HOH:O	1.88	0.72
1:B:390:ARG:CD	4:B:484:HOH:O	2.37	0.72
1:A:415:PHE:HA	4:A:563:HOH:O	1.90	0.72
1:A:254:ASP:O	1:A:256:PRO:HD3	1.90	0.72
1:B:287:TYR:CD1	4:B:645:HOH:O	2.43	0.72
1:B:421:LEU:CD1	1:B:427:LEU:HG	2.18	0.72
1:A:221:MSE:SE	1:A:232:PHE:H	2.23	0.72
1:B:255:GLY:HA3	4:B:481:HOH:O	1.89	0.71
1:A:334:LYS:HE3	4:A:594:HOH:O	1.89	0.71
1:B:361:MSE:CE	1:B:371:TYR:HE1	2.01	0.71
1:B:329:ARG:HG3	4:B:501:HOH:O	1.90	0.71
1:A:290:MSE:C	4:A:538:HOH:O	2.29	0.71
1:B:304:ALA:HB2	4:B:505:HOH:O	1.90	0.71
1:A:263:MSE:HE1	4:A:625:HOH:O	1.88	0.71
1:B:286:MSE:O	1:B:289:LYS:HB2	1.91	0.71
1:A:390:ARG:HD2	4:A:544:HOH:O	1.90	0.71
1:A:265:VAL:HG13	4:A:517:HOH:O	1.91	0.71
1:B:390:ARG:HD3	4:B:484:HOH:O	1.91	0.71
1:A:244:LEU:CD2	4:A:528:HOH:O	2.38	0.71
1:B:336:ALA:CB	4:B:539:HOH:O	2.35	0.70
1:A:244:LEU:HD22	4:A:528:HOH:O	1.91	0.70
1:A:211:GLU:HB2	4:A:592:HOH:O	1.89	0.70
1:B:413:ILE:HD12	1:B:414:ASP:H	1.56	0.70
1:B:279:ARG:CB	1:B:280:PRO:HD2	2.21	0.70
1:A:229:VAL:CG2	4:A:583:HOH:O	2.38	0.70
1:B:213:GLU:O	1:B:217:MSE:HG2	1.91	0.69
1:B:272:GLU:OE2	1:B:417:LYS:NZ	2.25	0.69
1:A:326:LEU:O	1:A:328:PHE:N	2.24	0.69
1:B:378:ILE:HG13	4:B:574:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:THR:HB	4:A:636:HOH:O	1.93	0.69
1:A:203:GLY:CA	4:A:639:HOH:O	2.38	0.69
1:A:423:ASN:HA	4:A:524:HOH:O	1.92	0.69
1:A:399:LEU:HB3	4:A:542:HOH:O	1.91	0.69
1:B:272:GLU:HG2	4:B:537:HOH:O	1.92	0.69
1:B:405:CYS:HA	4:B:525:HOH:O	1.93	0.69
1:B:326:LEU:HD11	4:B:520:HOH:O	1.92	0.69
1:B:206:LEU:HD23	1:B:207:LYS:N	2.07	0.69
1:A:263:MSE:CE	4:A:625:HOH:O	2.40	0.69
1:A:204:LEU:CD2	4:A:551:HOH:O	2.38	0.69
1:A:439:GLU:HG2	4:A:509:HOH:O	1.92	0.68
1:A:442:TYR:CZ	4:A:603:HOH:O	2.45	0.68
1:A:361:MSE:CG	4:A:515:HOH:O	2.40	0.68
1:B:275:LYS:CE	4:B:523:HOH:O	2.41	0.68
1:B:281:LYS:HD2	4:B:579:HOH:O	1.93	0.68
1:A:246:LEU:C	4:A:548:HOH:O	2.31	0.68
1:B:304:ALA:CB	4:B:505:HOH:O	2.41	0.68
1:A:430:ARG:NH2	4:A:506:HOH:O	2.26	0.68
1:A:228:CYS:CA	4:A:571:HOH:O	2.40	0.68
1:A:330:ILE:HD11	1:A:347:THR:HG21	1.75	0.68
1:B:215:TYR:CZ	4:B:603:HOH:O	2.47	0.68
1:B:422:PRO:HB3	4:B:624:HOH:O	1.93	0.67
1:B:208:ARG:H	1:B:208:ARG:HD2	1.59	0.67
1:B:346:THR:CG2	4:B:544:HOH:O	2.42	0.67
1:A:391:HIS:N	4:A:533:HOH:O	2.27	0.67
1:A:326:LEU:C	4:A:466:HOH:O	2.31	0.67
1:A:431:ARG:HG3	4:A:509:HOH:O	1.95	0.67
1:B:256:PRO:HB3	4:B:491:HOH:O	1.94	0.67
1:B:276:ALA:HB1	4:B:529:HOH:O	1.91	0.67
1:A:313:TYR:N	4:A:619:HOH:O	2.28	0.67
1:B:378:ILE:CG1	4:B:574:HOH:O	2.42	0.66
1:A:303:HIS:NE2	4:A:570:HOH:O	2.29	0.66
1:B:282:LEU:HA	4:B:630:HOH:O	1.94	0.66
1:A:216:CYS:SG	1:A:418:THR:CG2	2.84	0.66
1:B:370:ARG:NH1	4:B:628:HOH:O	2.25	0.66
1:A:227:GLY:C	4:A:571:HOH:O	2.34	0.66
1:A:321:SER:OG	1:A:329:ARG:HG3	1.95	0.66
1:A:438:ARG:CB	1:A:438:ARG:HH21	2.09	0.66
1:A:452:ILE:CG2	4:A:572:HOH:O	2.35	0.65
1:A:329:ARG:NH1	4:A:510:HOH:O	2.29	0.65
1:B:366:GLU:OE1	1:B:369:LYS:HE2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1:ADP:N7	4:B:508:HOH:O	2.29	0.65
1:B:369:LYS:HG3	1:B:370:ARG:N	2.10	0.65
1:A:290:MSE:HE2	4:A:553:HOH:O	1.97	0.65
1:B:229:VAL:N	4:B:626:HOH:O	2.29	0.65
1:B:422:PRO:HG2	4:B:570:HOH:O	1.97	0.65
1:A:263:MSE:HG3	1:A:398:LEU:HG	1.79	0.65
1:A:431:ARG:CD	4:A:565:HOH:O	2.32	0.65
1:B:374:ARG:CZ	4:B:574:HOH:O	2.45	0.64
1:B:269:LEU:HD11	1:B:417:LYS:CB	2.25	0.64
1:B:276:ALA:HB3	4:B:529:HOH:O	1.97	0.64
1:B:256:PRO:CB	4:B:491:HOH:O	2.46	0.64
1:A:283:ARG:HB3	1:A:285:ASP:OD1	1.96	0.64
1:A:379:ARG:HD2	4:A:470:HOH:O	1.98	0.64
1:B:413:ILE:CD1	4:B:526:HOH:O	2.45	0.64
1:A:268:TYR:CE2	4:A:615:HOH:O	2.50	0.64
1:B:375:LEU:HD13	1:B:449:LEU:HD22	1.81	0.64
1:A:221:MSE:HE2	1:A:221:MSE:CA	2.26	0.64
1:B:413:ILE:HD11	4:B:508:HOH:O	1.98	0.64
1:A:204:LEU:CG	4:A:551:HOH:O	2.46	0.63
1:A:342:THR:OG1	1:B:339:SER:CB	2.45	0.63
1:A:304:ALA:CB	4:A:561:HOH:O	2.44	0.63
1:A:314:MSE:O	1:A:318:GLU:HG3	1.98	0.63
1:A:226:ARG:HD2	4:A:473:HOH:O	1.96	0.63
1:B:284:LYS:HD2	1:B:287:TYR:HB2	1.80	0.63
1:B:321:SER:C	1:B:348:ARG:HB2	2.19	0.63
1:A:414:ASP:CB	4:A:513:HOH:O	2.33	0.63
1:A:389:ARG:HG2	1:A:426:ILE:CG2	2.28	0.63
1:A:425:GLN:CG	4:A:532:HOH:O	2.32	0.63
1:A:291:LEU:CD1	4:A:545:HOH:O	2.45	0.63
1:A:413:ILE:HG23	4:A:542:HOH:O	1.99	0.63
1:B:217:MSE:SE	4:B:495:HOH:O	2.67	0.62
1:B:284:LYS:HZ2	1:B:287:TYR:HB3	1.63	0.62
1:B:215:TYR:HB2	4:B:610:HOH:O	1.99	0.62
1:A:439:GLU:CG	4:A:509:HOH:O	2.47	0.62
1:B:287:TYR:CG	4:B:586:HOH:O	2.51	0.62
1:A:362:GLN:HG2	4:A:624:HOH:O	2.00	0.62
1:A:389:ARG:NH1	4:A:604:HOH:O	2.33	0.62
1:A:211:GLU:HB3	1:A:212:PRO:HD3	1.82	0.62
1:A:342:THR:OG1	1:B:339:SER:HB2	2.00	0.62
1:B:346:THR:HG22	1:B:346:THR:O	1.98	0.62
1:B:206:LEU:CD2	4:B:601:HOH:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:LEU:C	1:B:259:LEU:HD23	2.20	0.61
1:A:290:MSE:SE	1:A:312:ARG:HH12	2.32	0.61
1:B:229:VAL:C	4:B:626:HOH:O	2.38	0.61
1:A:338:GLY:C	4:B:618:HOH:O	2.37	0.61
1:A:311:PRO:N	4:A:619:HOH:O	2.33	0.61
1:A:204:LEU:HG	4:A:551:HOH:O	1.99	0.61
1:B:286:MSE:HA	1:B:289:LYS:CD	2.29	0.61
1:A:450:ILE:HD11	4:A:627:HOH:O	2.00	0.61
1:B:297:ALA:CB	4:B:627:HOH:O	2.48	0.60
1:B:361:MSE:HB2	4:B:597:HOH:O	2.01	0.60
1:B:285:ASP:O	1:B:289:LYS:HG3	2.00	0.60
1:A:413:ILE:CG2	4:A:542:HOH:O	2.48	0.60
1:A:413:ILE:CG1	4:A:626:HOH:O	2.50	0.60
1:A:345:LYS:CD	4:A:634:HOH:O	2.49	0.60
1:A:278:GLU:CG	4:A:559:HOH:O	2.49	0.60
1:B:230:PRO:HG3	1:B:249:LEU:HD11	1.84	0.60
1:A:225:LEU:HD21	1:A:382:LEU:HD23	1.83	0.60
1:B:312:ARG:CD	4:B:550:HOH:O	2.36	0.60
1:A:379:ARG:O	1:A:383:GLU:HG3	2.02	0.60
1:A:357:PHE:HA	4:A:519:HOH:O	2.01	0.60
1:A:311:PRO:C	4:A:619:HOH:O	2.41	0.59
3:A:1:ADP:H5'2	4:A:500:HOH:O	2.01	0.59
1:B:401:VAL:CG2	4:B:647:HOH:O	2.50	0.59
1:B:413:ILE:CD1	1:B:414:ASP:H	2.15	0.59
1:A:399:LEU:CB	4:A:542:HOH:O	2.48	0.59
1:B:303:HIS:N	4:B:510:HOH:O	2.35	0.59
1:B:265:VAL:HA	1:B:323:SER:O	2.02	0.59
1:A:446:LEU:CG	4:A:627:HOH:O	2.50	0.59
1:A:266:ARG:HD3	4:A:505:HOH:O	2.02	0.59
1:A:407:ARG:HD2	4:A:465:HOH:O	2.03	0.59
1:B:271:GLU:HG3	1:B:272:GLU:N	2.17	0.58
1:B:271:GLU:HG3	1:B:272:GLU:H	1.68	0.58
1:A:228:CYS:N	4:A:571:HOH:O	2.36	0.58
1:A:361:MSE:HG2	4:A:515:HOH:O	2.03	0.58
1:A:265:VAL:HG22	4:A:517:HOH:O	2.03	0.58
1:B:262:LYS:HE2	1:B:395:GLY:HA2	1.84	0.58
1:A:430:ARG:NE	4:A:506:HOH:O	2.37	0.57
1:B:297:ALA:HB1	4:B:627:HOH:O	2.04	0.57
1:A:389:ARG:NH2	4:A:620:HOH:O	2.38	0.57
1:A:446:LEU:CD2	4:A:627:HOH:O	2.41	0.57
1:A:374:ARG:NH1	4:A:571:HOH:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LYS:CE	4:A:594:HOH:O	2.50	0.57
1:B:284:LYS:HG3	1:B:288:LYS:HG3	1.85	0.57
1:B:361:MSE:O	1:B:362:GLN:HB2	2.04	0.57
1:A:452:ILE:CB	4:A:572:HOH:O	2.52	0.57
1:A:351:GLU:HG2	1:A:355:ARG:CZ	2.34	0.57
1:B:301:GLU:HG2	4:B:505:HOH:O	2.04	0.56
1:B:388:PHE:CE2	1:B:429:HIS:CD2	2.93	0.56
1:A:277:ARG:HH22	1:A:435:GLU:HG2	1.70	0.56
1:A:298:PRO:HD2	1:A:312:ARG:HH12	1.70	0.56
1:B:386:ASP:HA	1:B:389:ARG:HB3	1.87	0.56
1:B:415:PHE:HA	4:B:469:HOH:O	2.05	0.56
1:B:443:LEU:CD2	4:B:546:HOH:O	2.52	0.56
1:A:338:GLY:HA2	4:B:618:HOH:O	2.04	0.56
1:A:229:VAL:CB	4:A:583:HOH:O	2.49	0.56
1:A:424:GLY:N	4:A:524:HOH:O	2.39	0.56
1:B:322:SER:HB3	1:B:348:ARG:HA	1.88	0.56
1:A:317:ARG:NH1	1:A:317:ARG:HB2	2.19	0.56
1:B:390:ARG:HD2	4:B:484:HOH:O	2.01	0.55
1:B:293:VAL:O	1:B:294:ASP:HB2	2.05	0.55
1:B:224:VAL:CG2	1:B:385:SER:HA	2.36	0.55
1:B:286:MSE:HE2	1:B:313:TYR:CE2	2.42	0.55
1:A:278:GLU:HG3	4:A:559:HOH:O	2.05	0.55
1:B:329:ARG:NH2	4:B:605:HOH:O	2.29	0.55
1:A:295:PRO:CA	4:A:545:HOH:O	2.35	0.55
1:B:400:PHE:HZ	1:B:449:LEU:HD21	1.71	0.55
1:A:354:THR:CB	4:A:636:HOH:O	2.53	0.55
1:B:349:SER:HB3	1:B:352:GLN:HG3	1.87	0.55
1:A:328:PHE:CE2	4:A:496:HOH:O	2.60	0.55
1:A:415:PHE:CA	4:A:563:HOH:O	2.51	0.55
1:B:350:ARG:CA	4:B:520:HOH:O	2.55	0.55
1:B:372:LEU:HD21	1:B:453:LEU:HB2	1.88	0.55
1:B:443:LEU:CD1	4:B:546:HOH:O	2.47	0.54
1:B:275:LYS:HE2	1:B:279:ARG:HB2	1.88	0.54
1:B:311:PRO:CD	4:B:537:HOH:O	2.37	0.54
1:B:350:ARG:CB	4:B:520:HOH:O	2.53	0.54
1:A:349:SER:HB3	1:A:352:GLN:HE21	1.71	0.54
1:B:413:ILE:HD11	4:B:526:HOH:O	2.06	0.54
1:A:345:LYS:CG	4:A:634:HOH:O	2.39	0.54
1:A:342:THR:OG1	1:B:339:SER:HB3	2.07	0.54
1:B:284:LYS:HZ1	1:B:304:ALA:HB3	1.72	0.54
1:A:244:LEU:HD21	4:A:528:HOH:O	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HG22	1:A:303:HIS:NE2	2.23	0.54
1:B:272:GLU:CG	4:B:537:HOH:O	2.55	0.54
1:A:286:MSE:HA	1:A:289:LYS:CG	2.37	0.54
1:A:452:ILE:HB	4:A:572:HOH:O	2.07	0.54
1:A:271:GLU:HB3	4:A:611:HOH:O	2.07	0.54
1:A:288:LYS:HD3	1:B:254:ASP:O	2.07	0.54
1:A:235:VAL:O	1:A:235:VAL:CG1	2.56	0.53
1:A:221:MSE:CE	1:A:221:MSE:HA	2.29	0.53
1:B:276:ALA:HA	1:B:279:ARG:O	2.07	0.53
1:A:284:LYS:NZ	4:A:480:HOH:O	2.26	0.53
1:A:317:ARG:HH21	1:A:345:LYS:NZ	2.07	0.53
1:A:248:ASP:N	4:A:584:HOH:O	2.39	0.53
1:B:413:ILE:HG13	1:B:414:ASP:N	2.23	0.53
1:A:254:ASP:OD1	1:A:404:HIS:HE1	1.91	0.53
1:A:299:THR:HG22	1:A:303:HIS:CD2	2.43	0.53
1:B:284:LYS:NZ	1:B:304:ALA:HB3	2.24	0.53
1:A:434:GLU:N	1:A:437:ASN:HD22	2.06	0.53
1:A:338:GLY:CA	4:B:618:HOH:O	2.57	0.53
1:B:207:LYS:HE2	1:B:213:GLU:OE1	2.09	0.53
1:A:328:PHE:CE1	4:A:496:HOH:O	2.62	0.53
1:B:401:VAL:HG22	4:B:647:HOH:O	2.08	0.53
1:A:412:LEU:CD2	4:A:603:HOH:O	2.32	0.52
1:A:407:ARG:HG3	4:A:617:HOH:O	2.08	0.52
1:B:346:THR:CG2	4:B:589:HOH:O	2.55	0.52
1:B:413:ILE:HD12	4:B:526:HOH:O	2.06	0.52
1:A:430:ARG:NH1	1:A:447:ASP:OD2	2.42	0.52
1:A:207:LYS:HD3	1:A:213:GLU:CD	2.30	0.52
1:B:384:ILE:C	1:B:384:ILE:HD12	2.29	0.52
1:B:346:THR:HB	4:B:494:HOH:O	2.10	0.52
1:A:336:ALA:HB3	1:B:292:ALA:O	2.09	0.52
1:A:316:TRP:HB3	4:A:553:HOH:O	2.09	0.52
1:B:330:ILE:HD12	1:B:331:GLU:N	2.25	0.52
1:A:421:LEU:CD1	4:A:533:HOH:O	2.58	0.52
1:B:321:SER:O	1:B:348:ARG:HB2	2.09	0.52
1:A:216:CYS:SG	1:A:418:THR:HB	2.50	0.52
1:A:317:ARG:CD	4:A:488:HOH:O	2.37	0.52
1:B:375:LEU:CD1	1:B:449:LEU:HD22	2.40	0.52
1:A:446:LEU:HD11	4:A:627:HOH:O	2.10	0.52
1:A:299:THR:CG2	4:A:570:HOH:O	2.58	0.52
1:A:292:ALA:HB3	1:B:336:ALA:HB1	1.92	0.51
1:B:431:ARG:CG	1:B:439:GLU:HG3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:NH2	4:B:566:HOH:O	2.42	0.51
1:B:329:ARG:CG	4:B:501:HOH:O	2.51	0.51
1:B:205:ILE:HG22	1:B:206:LEU:N	2.26	0.51
1:A:431:ARG:HG3	1:A:439:GLU:HG2	1.92	0.51
1:A:266:ARG:CD	4:A:505:HOH:O	2.57	0.51
1:B:421:LEU:HA	1:B:438:ARG:HH21	1.75	0.51
1:A:430:ARG:CZ	4:A:506:HOH:O	2.56	0.51
1:A:216:CYS:SG	1:A:418:THR:HG21	2.51	0.51
1:B:413:ILE:CG1	1:B:414:ASP:N	2.73	0.51
1:A:285:ASP:O	1:A:289:LYS:HG3	2.10	0.51
1:B:288:LYS:C	4:B:591:HOH:O	2.48	0.51
1:B:389:ARG:HG2	1:B:426:ILE:HG12	1.93	0.51
1:A:397:SER:CB	4:A:626:HOH:O	2.50	0.51
1:B:326:LEU:HD21	1:B:350:ARG:HH12	1.75	0.51
1:B:255:GLY:CA	4:B:481:HOH:O	2.55	0.51
1:A:214:HIS:NE2	1:A:235:VAL:CG2	2.74	0.51
1:B:389:ARG:C	4:B:646:HOH:O	2.50	0.50
1:B:211:GLU:HG3	4:B:610:HOH:O	2.11	0.50
1:B:253:PHE:HA	1:B:403:ASP:OD1	2.10	0.50
1:A:339:SER:OG	1:B:342:THR:HB	2.10	0.50
1:A:413:ILE:CD1	4:A:626:HOH:O	2.47	0.50
1:B:287:TYR:CE1	4:B:645:HOH:O	2.64	0.50
1:B:326:LEU:CD2	1:B:350:ARG:NH1	2.73	0.50
1:B:284:LYS:N	4:B:630:HOH:O	2.45	0.50
1:B:421:LEU:HA	1:B:438:ARG:NH2	2.26	0.50
1:B:330:ILE:HD12	1:B:330:ILE:C	2.32	0.50
1:A:339:SER:CB	1:B:342:THR:HB	2.42	0.50
1:B:383:GLU:CG	4:B:622:HOH:O	2.38	0.50
1:B:235:VAL:CA	4:B:517:HOH:O	2.44	0.50
1:B:421:LEU:HD23	1:B:438:ARG:NH2	2.27	0.50
1:B:282:LEU:CD2	4:B:548:HOH:O	2.47	0.49
1:A:390:ARG:NH2	4:A:629:HOH:O	2.45	0.49
1:A:345:LYS:HE2	4:A:634:HOH:O	2.12	0.49
1:B:298:PRO:HD2	4:B:493:HOH:O	2.11	0.49
1:B:323:SER:HB2	4:B:605:HOH:O	2.13	0.49
1:A:288:LYS:CD	1:B:254:ASP:O	2.60	0.49
1:A:415:PHE:C	4:A:563:HOH:O	2.50	0.49
1:B:346:THR:CB	4:B:589:HOH:O	2.35	0.49
1:A:206:LEU:HA	1:A:244:LEU:O	2.12	0.49
1:B:317:ARG:HA	1:B:320:ILE:HD11	1.95	0.49
1:A:297:ALA:CB	4:A:531:HOH:O	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:ARG:CD	1:B:208:ARG:H	2.23	0.49
1:A:313:TYR:OH	1:A:317:ARG:NH2	2.45	0.49
1:A:362:GLN:NE2	4:A:585:HOH:O	2.45	0.49
1:B:401:VAL:HG23	4:B:647:HOH:O	2.12	0.49
1:B:279:ARG:HB3	1:B:280:PRO:CD	2.34	0.49
1:B:330:ILE:HD11	1:B:344:PHE:CD1	2.47	0.49
1:B:236:VAL:C	1:B:244:LEU:N	2.66	0.49
1:A:328:PHE:CD2	4:A:496:HOH:O	2.65	0.49
1:B:315:GLN:O	1:B:318:GLU:HB2	2.13	0.48
1:A:283:ARG:CB	4:A:562:HOH:O	2.53	0.48
1:B:411:TRP:CD1	4:B:626:HOH:O	2.50	0.48
1:B:351:GLU:HG3	4:B:507:HOH:O	2.12	0.48
1:B:254:ASP:HB3	1:B:404:HIS:CE1	2.48	0.48
1:B:318:GLU:HA	1:B:323:SER:HB2	1.95	0.48
1:B:403:ASP:HB3	1:B:406:HIS:H	1.78	0.48
1:A:338:GLY:O	1:B:343:ASP:HA	2.14	0.48
1:B:378:ILE:HG12	4:B:574:HOH:O	2.12	0.48
1:B:266:ARG:NH2	1:B:394:ILE:HD11	2.29	0.48
1:A:327:GLY:N	4:A:466:HOH:O	2.47	0.48
1:B:303:HIS:CA	4:B:510:HOH:O	2.61	0.48
1:A:413:ILE:HG12	4:A:626:HOH:O	2.12	0.48
1:A:393:VAL:HA	1:A:418:THR:HA	1.96	0.48
1:B:269:LEU:CD1	1:B:417:LYS:HD3	2.44	0.48
1:A:263:MSE:SE	4:A:625:HOH:O	2.80	0.48
1:B:252:GLY:O	1:B:407:ARG:CD	2.62	0.48
1:A:312:ARG:HA	1:A:315:GLN:OE1	2.14	0.48
1:B:275:LYS:NZ	1:B:279:ARG:HD2	2.28	0.48
1:B:330:ILE:HG23	4:B:488:HOH:O	2.13	0.48
1:B:235:VAL:HG23	1:B:236:VAL:N	2.28	0.47
1:B:290:MSE:CG	4:B:614:HOH:O	2.41	0.47
1:B:205:ILE:CG2	1:B:206:LEU:N	2.77	0.47
1:A:266:ARG:HG3	4:A:615:HOH:O	2.14	0.47
1:A:207:LYS:NZ	1:A:213:GLU:OE2	2.38	0.47
1:A:435:GLU:CA	4:A:498:HOH:O	2.34	0.47
1:A:281:LYS:CB	4:A:568:HOH:O	2.36	0.47
1:A:206:LEU:N	1:A:206:LEU:HD12	2.30	0.47
1:A:292:ALA:CB	1:B:336:ALA:HB1	2.44	0.47
1:A:328:PHE:CD1	4:A:496:HOH:O	2.67	0.47
1:A:266:ARG:NH2	1:A:394:ILE:CD1	2.78	0.47
1:A:286:MSE:HA	1:A:289:LYS:HG3	1.97	0.47
1:A:317:ARG:HH21	1:A:345:LYS:HZ1	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ILE:HG13	1:B:248:ASP:OD2	2.15	0.47
1:A:336:ALA:O	1:A:337:ASP:HB2	2.14	0.47
1:B:321:SER:OG	1:B:329:ARG:HG3	2.14	0.47
1:A:330:ILE:CD1	1:A:347:THR:HG21	2.42	0.47
1:B:283:ARG:HD3	1:B:283:ARG:HA	1.79	0.47
1:B:384:ILE:O	1:B:384:ILE:HD12	2.15	0.47
1:A:288:LYS:HB2	1:A:288:LYS:HE3	1.66	0.47
1:A:286:MSE:SE	1:A:313:TYR:CD2	3.18	0.47
1:A:254:ASP:OD1	1:A:404:HIS:CE1	2.68	0.47
1:B:214:HIS:HD2	4:B:637:HOH:O	1.98	0.47
1:A:266:ARG:NH2	1:A:394:ILE:HD13	2.29	0.46
1:B:383:GLU:HG3	4:B:546:HOH:O	2.14	0.46
1:A:407:ARG:CG	4:A:617:HOH:O	2.61	0.46
1:A:215:TYR:HA	4:A:557:HOH:O	2.14	0.46
1:B:389:ARG:HD3	1:B:426:ILE:HD13	1.96	0.46
1:B:256:PRO:CG	4:B:491:HOH:O	2.63	0.46
1:B:346:THR:O	1:B:346:THR:CG2	2.61	0.46
1:A:431:ARG:CB	4:A:614:HOH:O	2.41	0.46
1:A:291:LEU:HD12	4:A:545:HOH:O	2.10	0.46
1:B:250:LEU:HD22	4:B:491:HOH:O	2.15	0.46
1:A:221:MSE:HA	4:A:556:HOH:O	2.14	0.46
1:A:453:LEU:N	4:A:572:HOH:O	2.48	0.46
1:A:330:ILE:O	1:A:330:ILE:HG13	2.16	0.46
1:A:389:ARG:NE	1:A:426:ILE:HD13	2.31	0.46
1:A:312:ARG:HA	1:A:315:GLN:CG	2.45	0.46
1:B:286:MSE:HE2	1:B:313:TYR:HE2	1.80	0.46
1:A:298:PRO:HD2	1:A:312:ARG:CZ	2.45	0.46
1:B:400:PHE:CZ	1:B:449:LEU:HD21	2.49	0.46
1:A:313:TYR:OH	1:A:317:ARG:NH1	2.48	0.46
1:A:236:VAL:HB	1:A:245:GLN:NE2	2.31	0.46
1:B:400:PHE:C	4:B:647:HOH:O	2.55	0.46
1:A:325:THR:HG23	4:A:622:HOH:O	2.15	0.46
1:A:438:ARG:NH1	4:A:497:HOH:O	2.33	0.46
1:A:204:LEU:O	1:A:205:ILE:HD13	2.16	0.46
1:B:279:ARG:CB	1:B:280:PRO:CD	2.91	0.46
1:B:284:LYS:O	1:B:288:LYS:N	2.44	0.45
1:A:391:HIS:O	1:A:427:LEU:HD12	2.15	0.45
1:B:207:LYS:HE2	1:B:213:GLU:CD	2.36	0.45
1:B:290:MSE:HE2	4:B:602:HOH:O	2.16	0.45
1:A:393:VAL:H	1:A:418:THR:HA	1.82	0.45
1:A:456:LEU:C	1:A:458:GLU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:ASP:O	1:A:390:ARG:HG2	2.17	0.45
1:B:315:GLN:CG	4:B:542:HOH:O	2.41	0.45
1:B:404:HIS:C	1:B:404:HIS:CD2	2.90	0.45
1:A:221:MSE:CG	1:A:232:PHE:HB3	2.46	0.45
1:B:311:PRO:O	1:B:315:GLN:HG2	2.15	0.45
1:A:263:MSE:SE	1:A:398:LEU:CG	3.15	0.45
1:A:286:MSE:HA	1:A:289:LYS:CD	2.47	0.45
1:A:313:TYR:CZ	1:A:317:ARG:NH1	2.59	0.45
1:B:386:ASP:CG	1:B:389:ARG:HD2	2.37	0.45
1:B:350:ARG:N	4:B:520:HOH:O	2.50	0.45
1:B:426:ILE:CG2	1:B:427:LEU:N	2.79	0.45
1:B:335:LYS:O	1:B:337:ASP:N	2.49	0.45
1:B:207:LYS:HE2	1:B:213:GLU:OE2	2.16	0.45
1:B:392:GLU:OE1	1:B:438:ARG:HD2	2.16	0.45
1:A:299:THR:O	1:A:303:HIS:CD2	2.70	0.45
1:A:385:SER:O	1:A:389:ARG:HB2	2.16	0.45
1:A:408:ALA:HB2	4:A:613:HOH:O	2.15	0.45
1:A:329:ARG:HD2	1:A:331:GLU:OE2	2.16	0.45
1:A:335:LYS:HB2	1:A:338:GLY:H	1.82	0.45
1:A:442:TYR:C	1:A:442:TYR:CD2	2.90	0.45
1:A:367:VAL:CG2	4:A:613:HOH:O	2.48	0.45
1:A:393:VAL:N	1:A:418:THR:HA	2.32	0.44
1:B:221:MSE:O	1:B:226:ARG:HD3	2.18	0.44
1:B:217:MSE:CE	4:B:495:HOH:O	2.66	0.44
1:A:328:PHE:CG	4:A:496:HOH:O	2.70	0.44
1:A:439:GLU:HB2	4:A:509:HOH:O	2.16	0.44
1:B:390:ARG:CD	4:B:489:HOH:O	2.66	0.44
1:B:392:GLU:OE1	1:B:438:ARG:NH1	2.51	0.44
1:A:313:TYR:HB3	4:A:619:HOH:O	2.17	0.44
1:B:258:VAL:HG12	1:B:259:LEU:N	2.32	0.44
1:A:221:MSE:HG3	1:A:232:PHE:HB3	1.98	0.44
1:B:224:VAL:HG21	1:B:385:SER:HA	1.99	0.44
1:B:345:LYS:CG	4:B:618:HOH:O	2.45	0.44
1:B:431:ARG:HG3	1:B:439:GLU:HG3	1.99	0.44
1:A:228:CYS:SG	4:A:571:HOH:O	2.62	0.44
1:B:285:ASP:CG	1:B:286:MSE:H	2.21	0.44
1:B:318:GLU:HA	4:B:605:HOH:O	2.17	0.44
1:A:272:GLU:OE2	1:A:417:LYS:HE3	2.18	0.44
1:A:437:ASN:HB3	1:A:439:GLU:H	1.82	0.44
1:B:253:PHE:CD2	1:B:407:ARG:HD3	2.53	0.44
1:A:213:GLU:HA	1:A:216:CYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:PRO:HG3	4:B:595:HOH:O	2.17	0.43
1:A:389:ARG:CZ	4:A:604:HOH:O	2.64	0.43
1:B:405:CYS:O	1:B:406:HIS:CG	2.71	0.43
1:A:371:TYR:OH	1:A:402:HIS:HD2	2.01	0.43
1:B:206:LEU:C	1:B:206:LEU:HD23	2.38	0.43
1:B:284:LYS:C	4:B:586:HOH:O	2.56	0.43
1:B:293:VAL:HG12	1:B:293:VAL:O	2.19	0.43
1:A:434:GLU:H	1:A:437:ASN:HB2	1.83	0.43
1:B:390:ARG:N	4:B:646:HOH:O	2.51	0.43
1:A:372:LEU:HD21	1:A:453:LEU:HB2	2.01	0.43
1:A:349:SER:OG	1:A:352:GLN:HG3	2.19	0.43
1:B:232:PHE:CE2	1:B:234:GLY:O	2.71	0.43
1:B:203:GLY:HA3	1:B:251:ASP:OD2	2.19	0.43
1:A:297:ALA:CB	4:A:518:HOH:O	2.31	0.43
1:B:290:MSE:SE	1:B:297:ALA:HB2	2.69	0.43
1:A:428:ASP:CB	1:A:431:ARG:NH1	2.82	0.43
1:B:407:ARG:NH2	4:B:585:HOH:O	2.29	0.43
1:B:374:ARG:NH1	4:B:574:HOH:O	2.48	0.43
1:B:233:HIS:O	1:B:245:GLN:NE2	2.51	0.43
1:A:339:SER:CA	4:A:481:HOH:O	2.33	0.43
1:B:420:PRO:CA	4:B:561:HOH:O	2.67	0.43
1:B:275:LYS:HZ3	1:B:279:ARG:HD2	1.84	0.43
1:A:266:ARG:CB	4:A:505:HOH:O	2.33	0.43
1:A:259:LEU:C	1:A:259:LEU:HD23	2.39	0.43
1:A:392:GLU:HB2	1:A:438:ARG:HH22	1.84	0.42
1:B:229:VAL:CA	4:B:626:HOH:O	2.65	0.42
1:B:297:ALA:HA	1:B:298:PRO:HD3	1.88	0.42
1:B:315:GLN:NE2	4:B:542:HOH:O	2.50	0.42
1:A:263:MSE:HE3	1:A:263:MSE:HB3	1.90	0.42
1:A:274:THR:O	1:A:277:ARG:HB2	2.20	0.42
1:A:291:LEU:C	1:A:293:VAL:H	2.21	0.42
1:B:443:LEU:HD11	4:B:622:HOH:O	2.18	0.42
1:A:335:LYS:HD2	1:B:343:ASP:OD1	2.20	0.42
1:B:455:ASN:ND2	4:B:652:HOH:O	2.51	0.42
1:B:252:GLY:O	1:B:407:ARG:HD2	2.19	0.42
1:B:258:VAL:HG13	4:B:647:HOH:O	2.20	0.42
1:A:211:GLU:HA	1:A:211:GLU:OE1	2.19	0.42
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.78	0.42
1:A:322:SER:OG	1:A:329:ARG:HA	2.20	0.42
1:A:236:VAL:HG12	1:A:236:VAL:O	2.19	0.42
1:B:235:VAL:CG2	1:B:236:VAL:N	2.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:ARG:C	4:B:630:HOH:O	2.58	0.42
1:A:328:PHE:CB	4:A:625:HOH:O	2.68	0.42
1:B:286:MSE:HB3	1:B:313:TYR:CD2	2.54	0.42
1:A:437:ASN:C	1:A:439:GLU:N	2.73	0.42
1:A:429:HIS:N	1:A:439:GLU:OE2	2.42	0.42
1:B:296:GLU:HB2	4:B:614:HOH:O	2.18	0.42
1:A:388:PHE:CE2	1:A:429:HIS:CD2	3.08	0.42
1:B:361:MSE:O	1:B:362:GLN:CB	2.67	0.42
1:A:386:ASP:O	1:A:389:ARG:HB3	2.19	0.42
1:A:328:PHE:HB3	4:A:625:HOH:O	2.19	0.42
1:B:329:ARG:NE	4:B:605:HOH:O	2.43	0.41
1:A:339:SER:HB3	1:B:342:THR:HB	2.01	0.41
1:A:361:MSE:CE	1:A:368:LEU:HD13	2.27	0.41
1:B:399:LEU:CG	4:B:647:HOH:O	2.38	0.41
1:A:426:ILE:HG22	1:A:427:LEU:N	2.35	0.41
1:B:211:GLU:N	1:B:212:PRO:CD	2.84	0.41
1:A:266:ARG:HA	4:A:615:HOH:O	2.20	0.41
1:A:313:TYR:HD1	4:A:553:HOH:O	2.02	0.41
1:A:413:ILE:HG21	4:A:542:HOH:O	2.18	0.41
1:B:260:ASP:HB2	3:B:1:ADP:O3'	2.21	0.41
1:B:225:LEU:HD21	1:B:382:LEU:HD23	2.02	0.41
1:B:217:MSE:HE3	1:B:246:LEU:HD21	2.01	0.41
1:B:313:TYR:CZ	1:B:317:ARG:HD3	2.56	0.41
1:A:392:GLU:CG	1:A:438:ARG:HH22	2.33	0.41
1:A:437:ASN:C	1:A:439:GLU:H	2.22	0.41
1:A:434:GLU:H	1:A:437:ASN:HD22	1.68	0.41
1:A:266:ARG:NH1	1:A:439:GLU:O	2.47	0.41
1:B:284:LYS:NZ	1:B:287:TYR:HB3	2.34	0.41
1:A:423:ASN:CA	4:A:524:HOH:O	2.56	0.41
1:B:422:PRO:CB	4:B:624:HOH:O	2.63	0.41
1:B:285:ASP:CG	1:B:286:MSE:N	2.74	0.41
1:B:211:GLU:H	1:B:212:PRO:CD	2.33	0.41
1:A:414:ASP:CG	3:A:1:ADP:O2A	2.58	0.41
1:A:216:CYS:CB	1:A:415:PHE:HB3	2.51	0.41
1:B:413:ILE:CG1	1:B:414:ASP:H	2.33	0.41
1:A:275:LYS:HE3	4:A:611:HOH:O	2.20	0.41
1:A:426:ILE:CG2	1:A:427:LEU:N	2.83	0.41
1:B:404:HIS:CE1	1:B:405:CYS:HG	2.38	0.41
1:A:295:PRO:CB	4:A:545:HOH:O	2.67	0.41
1:A:233:HIS:O	1:A:245:GLN:HB3	2.20	0.41
1:B:328:PHE:CZ	1:B:353:VAL:HG11	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ARG:CD	1:A:331:GLU:OE2	2.69	0.40
1:B:350:ARG:HB2	4:B:520:HOH:O	2.19	0.40
1:A:422:PRO:HB2	4:A:593:HOH:O	2.21	0.40
1:B:421:LEU:HD11	1:B:427:LEU:CG	2.29	0.40
1:A:214:HIS:O	1:A:218:VAL:HG23	2.21	0.40
1:B:284:LYS:CD	1:B:287:TYR:HB2	2.49	0.40
1:A:247:GLN:N	4:A:548:HOH:O	2.54	0.40
1:A:371:TYR:O	1:A:375:LEU:HG	2.21	0.40
1:A:337:ASP:OD2	1:B:289:LYS:HG2	2.22	0.40
1:B:396:SER:HA	1:B:414:ASP:O	2.21	0.40
1:B:326:LEU:CD2	1:B:350:ARG:HH12	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	237/275 (86%)	198 (84%)	28 (12%)	11 (5%)	3	1
1	B	236/275 (86%)	193 (82%)	31 (13%)	12 (5%)	2	1
All	All	473/550 (86%)	391 (83%)	59 (12%)	23 (5%)	3	1

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	207	LYS
1	A	208	ARG
1	A	327	GLY
1	A	337	ASP
1	A	435	GLU
1	B	211	GLU
1	B	280	PRO

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Mol	Chain	Res	Type
1	B	283	ARG
1	B	294	ASP
1	B	406	HIS
1	B	423	ASN
1	A	282	LEU
1	A	285	ASP
1	A	393	VAL
1	B	336	ALA
1	B	435	GLU
1	A	457	ALA
1	B	362	GLN
1	A	422	PRO
1	A	423	ASN
1	B	276	ALA
1	B	235	VAL
1	B	422	PRO

5.3.2 Protein sidechains (i)

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	213/230 (93%)	199 (93%)	14 (7%)	21	22
1	B	212/230 (92%)	197 (93%)	15 (7%)	18	19
All	All	425/460 (92%)	396 (93%)	29 (7%)	20	21

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	280	PRO
1	A	294	ASP
1	A	301	GLU
1	A	317	ARG
1	A	326	LEU
1	A	349	SER
1	A	386	ASP

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Mol	Chain	Res	Type
1	A	394	ILE
1	A	419	THR
1	A	422	PRO
1	A	435	GLU
1	A	438	ARG
1	A	442	TYR
1	A	456	LEU
1	B	208	ARG
1	B	215	TYR
1	B	235	VAL
1	B	244	LEU
1	B	245	GLN
1	B	254	ASP
1	B	280	PRO
1	B	281	LYS
1	B	294	ASP
1	B	330	ILE
1	B	348	ARG
1	B	362	GLN
1	B	417	LYS
1	B	422	PRO
1	B	435	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	GLN
1	A	402	HIS
1	A	437	ASN
1	A	448	ASN
1	B	245	GLN
1	B	362	GLN
1	B	402	HIS
1	B	404	HIS

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	ADP	A	1	-	22,29,29	1.28	4 (18%)	27,45,45	1.33	2 (7%)
3	ADP	B	1	2	22,29,29	1.27	4 (18%)	27,45,45	1.32	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1	-	-	0/12/32/32	0/3/3/3
3	ADP	B	1	2	-	0/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	ADP	O4'-C1'	2.01	1.43	1.41
3	A	1	ADP	C2-N3	2.18	1.36	1.32
3	A	1	ADP	C2-N1	2.23	1.38	1.33
3	B	1	ADP	C2-N3	2.25	1.36	1.32
3	B	1	ADP	C2-N1	2.29	1.38	1.33
3	B	1	ADP	C4-N3	2.43	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	ADP	C4-N3	2.52	1.39	1.35
3	B	1	ADP	O4'-C1'	2.61	1.44	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	ADP	N3-C2-N1	-2.28	127.15	128.89
3	A	1	ADP	N3-C2-N1	-2.20	127.21	128.89
3	B	1	ADP	O2B-PB-O1B	2.20	117.67	110.58
3	B	1	ADP	C1'-N9-C4	4.36	133.52	126.94
3	A	1	ADP	C1'-N9-C4	4.69	134.02	126.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	ADP	2	0
3	B	1	ADP	3	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	236/275 (85%)	0.86	29 (12%)	5	5	22, 46, 79, 92	1 (0%)
1	B	235/275 (85%)	1.27	49 (20%)	1	1	20, 42, 90, 98	0
All	All	471/550 (85%)	1.06	78 (16%)	2	2	20, 43, 87, 98	1 (0%)

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	210	SER	9.8
1	A	284	LYS	9.0
1	B	303	HIS	9.0
1	B	282	LEU	8.8
1	B	293	VAL	8.6
1	B	281	LYS	8.2
1	B	277	ARG	8.1
1	B	287	TYR	6.9
1	B	299	THR	6.8
1	B	304	ALA	6.6
1	B	280	PRO	6.4
1	B	236	VAL	6.1
1	B	279	ARG	5.3
1	A	206	LEU	5.2
1	A	336	ALA	5.0
1	B	283	ARG	4.9
1	B	386	ASP	4.8
1	A	337	ASP	4.6
1	A	205	ILE	4.5
1	B	298	PRO	4.4
1	A	277	ARG	4.4
1	A	236	VAL	4.4
1	B	313	TYR	4.1
1	B	300	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	235	VAL	3.9
1	B	278	GLU	3.9
1	B	339	SER	3.8
1	A	287	TYR	3.8
1	B	457	ALA	3.6
1	B	288	LYS	3.6
1	B	209	SER	3.5
1	B	295	PRO	3.5
1	B	289	LYS	3.5
1	A	235	VAL	3.4
1	B	285	ASP	3.3
1	B	302	GLU	3.3
1	B	337	ASP	3.3
1	A	281	LYS	3.2
1	B	405	CYS	2.9
1	A	285	ASP	2.9
1	B	275	LYS	2.9
1	A	283	ARG	2.9
1	B	413	ILE	2.8
1	A	289	LYS	2.8
1	A	215	TYR	2.8
1	A	330	ILE	2.6
1	B	271	GLU	2.6
1	A	216	CYS	2.6
1	B	326	LEU	2.6
1	B	327	GLY	2.6
1	B	274	THR	2.6
1	B	292	ALA	2.5
1	B	252	GLY	2.5
1	A	271	GLU	2.5
1	B	205	ILE	2.5
1	B	291	LEU	2.5
1	B	276	ALA	2.4
1	A	412	LEU	2.4
1	A	334	LYS	2.3
1	B	284	LYS	2.3
1	B	294	ASP	2.3
1	A	423	ASN	2.3
1	A	275	LYS	2.3
1	A	418	THR	2.3
1	B	204	LEU	2.3
1	B	417	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	443	LEU	2.3
1	A	348	ARG	2.2
1	A	224	VAL	2.2
1	B	301	GLU	2.2
1	A	435	GLU	2.2
1	A	293	VAL	2.1
1	B	351	GLU	2.1
1	A	276	ALA	2.1
1	B	316	TRP	2.1
1	B	207	LYS	2.0
1	A	422	PRO	2.0
1	A	338	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
3	ADP	B	1	27/27	0.83	0.21	0.49	59,62,75,75	0
3	ADP	A	1	27/27	0.90	0.13	-0.88	50,54,58,60	0
2	MG	A	2	1/1	0.88	0.15	-	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.