Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2021 – 08:56 AM EDT

PDB ID	:	1F9W
Title	:	CRYSTAL STRUCTURES OF MUTANTS REVEAL A SIGNALLING PATHWAY FOR ACTIVATION OF THE KINESIN MOTOR ATPASE
Authors	:	Yun, M.; Zhang, X.; Park, C.G.; Park, H.W.; Endow, S.A.
Deposited on	:	2000-07-11
Resolution	:	2.50 Å(reported)

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

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

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

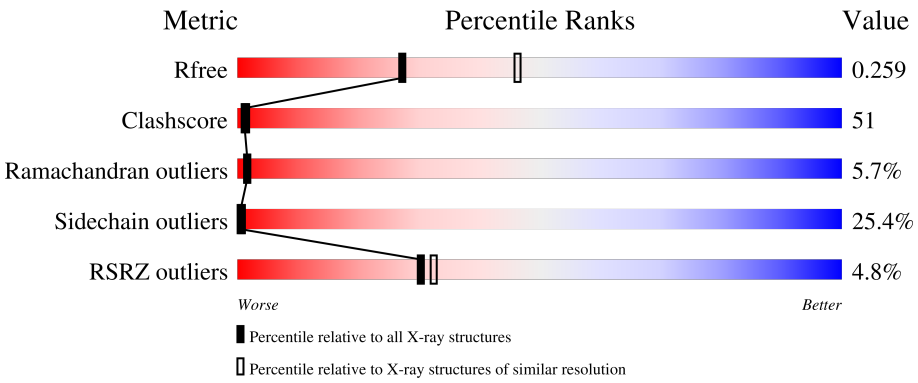
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	347	4% 23% 49% 14% • 14%
1	B	347	4% 22% 49% 15% • 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4935 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 KINESIN-LIKE PROTEIN KAR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	300	2372	1487	415	461	9	0	0	0
1	B	300	2372	1487	415	461	9	0	0	0

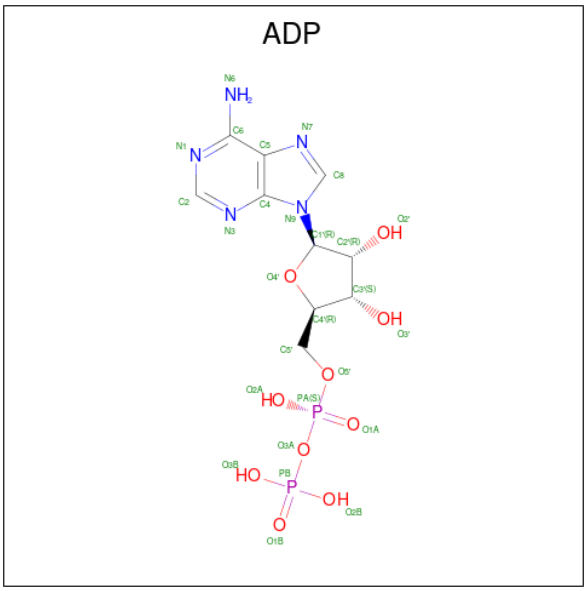
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	383	MET	LYS	engineered mutation	UNP P17119
A	631	ALA	GLU	engineered mutation	UNP P17119
B	383	MET	LYS	engineered mutation	UNP P17119
B	631	ALA	GLU	engineered mutation	UNP P17119

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

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

- 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.

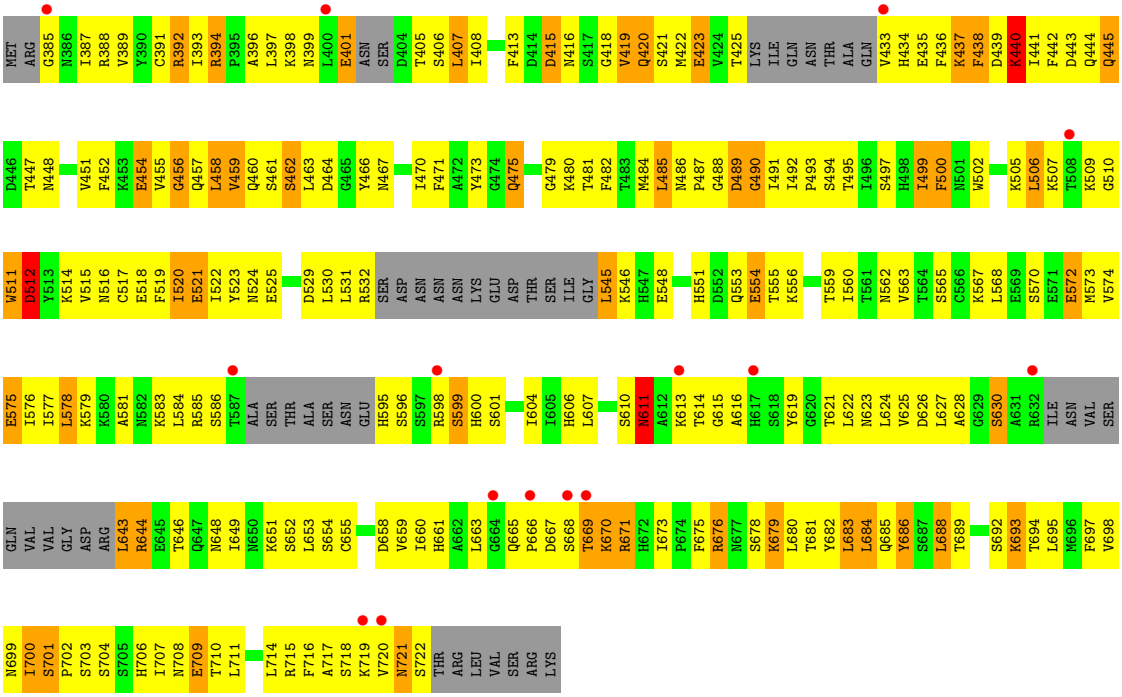
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	72	Total	O	0	0
			72	72		

3 Residue-property plots (i)

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

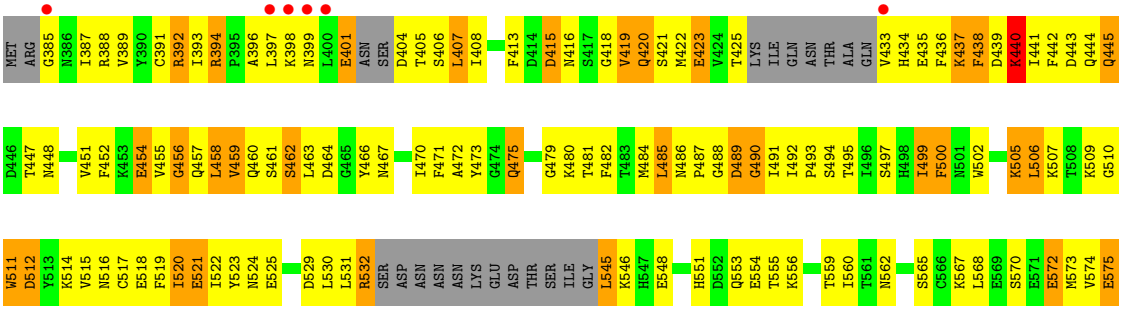
• Molecule 1: KINESIN-LIKE PROTEIN KAR3

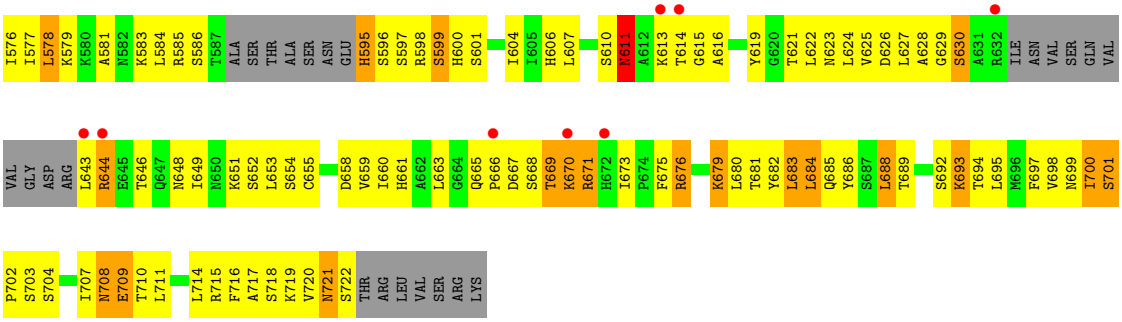
Chain A: 4% 23% 49% 14% • 14%



• Molecule 1: KINESIN-LIKE PROTEIN KAR3

Chain B: 4% 22% 49% 15% • 14%




I576 I577 L578 K579 K580 A581 N582 K583 L584 R585 S586 T587 ALA SER THR ALA SER ASN GLU H595 S596 S597 R598 S599 H600 S601
I604 I605 H606 L607
S610 N611 A612 K613 T614 G615 A616
Y619 G620 T621 L622 N623 L624 V625 D626 L627 A628 G629 S630 A631 R632 ILE ASN VAL SER GLN VAL
VAL GLY ASP ARG L643 R644 E645 T646 Q647 N648 I649 N650 K651 S652 L653 S654 C655
D658 V659 I660 H661 A662 L663 G664 Q665 P666 D667 S668 T669 K670 R671 H672 I673 P674 F675 R676
K679 L680 T681 Y682 L683 L684 Q685 Y686 S687 L688 T689
S692 K693 T694 L695 M696 F697 V698 N699 I700 S701
P702 S703 S704
I707 N708 E709 T710 L711
L714 R715 F716 A717 S718 K719 V720 N721 S722 THR ARG LEU VAL SER ARG LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	62.89Å 62.89Å 153.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.24 – 2.50	Depositor EDS
% Data completeness (in resolution range)	89.6 (20.00-2.50) 89.6 (19.24-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.80 (at 2.49Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.230 , 0.276 0.220 , 0.259	Depositor DCC
R_{free} test set	1802 reflections (9.78%)	wwPDB-VP
Wilson B-factor (Å^2)	39.3	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4935	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (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	0.48	0/2408	0.69	0/3245
1	B	0.48	0/2408	0.69	0/3245
All	All	0.48	0/4816	0.69	0/6490

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2372	0	2358	243	0
1	B	2372	0	2358	247	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	3	0
4	A	63	0	0	1	0
4	B	72	0	0	4	0
All	All	4935	0	4740	488	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 51.

All (488) 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:462:SER:HB2	1:B:607:LEU:HD12	1.31	1.10
1:A:668:SER:HA	1:A:671:ARG:HB3	1.32	1.08
1:B:394:ARG:HE	1:B:701:SER:HB2	1.15	1.07
1:A:462:SER:HB2	1:A:607:LEU:HD12	1.34	1.07
1:B:668:SER:HA	1:B:671:ARG:HB3	1.30	1.05
1:A:394:ARG:HE	1:A:701:SER:HB2	1.17	1.04
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.35	0.92
1:B:560:ILE:HD11	1:B:683:LEU:HD21	1.52	0.91
1:B:394:ARG:HG3	1:B:394:ARG:HH11	1.36	0.91
1:A:560:ILE:HD11	1:A:683:LEU:HD21	1.53	0.90
1:A:700:ILE:HG21	1:A:714:LEU:HD21	1.58	0.86
1:A:448:ASN:HD22	1:A:489:ASP:HB3	1.41	0.85
1:B:462:SER:HB2	1:B:607:LEU:CD1	2.05	0.85
1:B:698:VAL:HG21	1:B:717:ALA:HB2	1.59	0.85
1:A:462:SER:HB2	1:A:607:LEU:CD1	2.06	0.84
1:A:698:VAL:HG21	1:A:717:ALA:HB2	1.59	0.84
1:B:448:ASN:HD22	1:B:489:ASP:HB3	1.40	0.84
1:A:570:SER:OG	1:A:572:GLU:HG2	1.77	0.84
1:B:700:ILE:HG21	1:B:714:LEU:HD21	1.59	0.84
1:B:570:SER:OG	1:B:572:GLU:HG2	1.79	0.83
1:A:440:LYS:HD3	1:A:454:GLU:HG3	1.61	0.83
1:B:572:GLU:O	1:B:576:ILE:HD12	1.79	0.82
1:B:440:LYS:HD3	1:B:454:GLU:HG3	1.62	0.82
1:A:572:GLU:O	1:A:576:ILE:HD12	1.80	0.81
1:B:394:ARG:NE	1:B:701:SER:HB2	1.96	0.80
1:A:394:ARG:HE	1:A:701:SER:CB	1.94	0.80
1:B:521:GLU:HB3	1:B:530:LEU:HD11	1.64	0.79
1:B:521:GLU:OE1	1:B:599:SER:HB2	1.82	0.79
1:B:394:ARG:HE	1:B:701:SER:CB	1.92	0.79
1:B:419:VAL:HG23	1:B:420:GLN:N	1.98	0.79
1:B:458:LEU:HD23	1:B:459:VAL:N	1.98	0.79
1:A:524:ASN:HA	1:A:648:ASN:HD22	1.48	0.78
1:A:458:LEU:HD23	1:A:459:VAL:N	1.98	0.78
1:A:521:GLU:HB3	1:A:530:LEU:HD11	1.64	0.78
1:A:521:GLU:OE1	1:A:599:SER:HB2	1.84	0.78
1:B:394:ARG:HH11	1:B:394:ARG:CG	1.96	0.77
1:A:394:ARG:HH11	1:A:394:ARG:CG	1.96	0.77
1:B:425:THR:OG1	1:B:433:VAL:HG22	1.86	0.76
1:B:574:VAL:HG12	1:B:578:LEU:HD23	1.67	0.76
1:A:419:VAL:HG23	1:A:420:GLN:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:VAL:HG12	1:A:578:LEU:HD23	1.67	0.76
1:A:394:ARG:NE	1:A:701:SER:HB2	1.98	0.76
1:B:524:ASN:HA	1:B:648:ASN:HD22	1.49	0.75
1:A:459:VAL:HG12	1:A:622:LEU:CD2	2.18	0.74
1:A:425:THR:OG1	1:A:433:VAL:HG22	1.88	0.73
1:A:559:THR:HG22	1:A:560:ILE:H	1.53	0.73
1:A:669:THR:HG23	1:A:670:LYS:HG2	1.72	0.72
1:B:459:VAL:HG12	1:B:622:LEU:CD2	2.19	0.72
1:A:481:THR:HG21	1:A:585:ARG:O	1.90	0.72
1:B:669:THR:HG23	1:B:670:LYS:HG2	1.72	0.72
1:B:553:GLN:HA	1:B:686:TYR:OH	1.89	0.72
1:B:448:ASN:ND2	1:B:489:ASP:HB3	2.04	0.72
1:B:510:GLY:HA2	1:B:613:LYS:NZ	2.05	0.72
1:B:707:ILE:O	1:B:711:LEU:HG	1.89	0.72
1:A:448:ASN:ND2	1:A:489:ASP:HB3	2.04	0.71
1:A:553:GLN:HA	1:A:686:TYR:OH	1.88	0.71
1:A:510:GLY:HA2	1:A:613:LYS:NZ	2.06	0.71
1:A:715:ARG:O	1:A:719:LYS:HG2	1.91	0.70
1:B:481:THR:HG21	1:B:585:ARG:O	1.91	0.70
1:A:458:LEU:HD22	1:A:695:LEU:HD11	1.73	0.70
1:B:559:THR:HG22	1:B:560:ILE:H	1.55	0.70
1:A:524:ASN:HA	1:A:648:ASN:ND2	2.07	0.70
1:B:387:ILE:O	1:B:388:ARG:HD2	1.92	0.70
1:B:502:TRP:O	1:B:506:LEU:HD12	1.92	0.70
1:B:385:GLY:HA2	1:B:692:SER:O	1.91	0.69
1:A:707:ILE:O	1:A:711:LEU:HG	1.92	0.69
1:B:458:LEU:HD22	1:B:695:LEU:HD11	1.75	0.69
1:A:604:ILE:HG23	1:A:623:ASN:ND2	2.08	0.69
1:B:604:ILE:HG23	1:B:623:ASN:ND2	2.08	0.69
1:A:475:GLN:HB2	1:A:709:GLU:HG3	1.75	0.69
1:B:524:ASN:HA	1:B:648:ASN:ND2	2.07	0.69
1:A:442:PHE:CD2	1:A:451:VAL:HG22	2.29	0.68
1:A:502:TRP:O	1:A:506:LEU:HD12	1.93	0.68
1:A:387:ILE:O	1:A:388:ARG:HD2	1.93	0.68
1:B:413:PHE:HE1	1:B:415:ASP:HB3	1.59	0.68
1:B:475:GLN:HB2	1:B:709:GLU:HG3	1.76	0.68
1:B:510:GLY:HA2	1:B:613:LYS:HZ2	1.57	0.68
1:B:397:LEU:H	1:B:401:GLU:CG	2.07	0.68
1:A:385:GLY:HA2	1:A:692:SER:O	1.93	0.68
1:A:600:HIS:CD2	1:A:680:LEU:HD22	2.29	0.68
1:A:519:PHE:HB3	1:A:531:LEU:HG	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LEU:HD13	1:A:695:LEU:HD21	1.77	0.67
1:B:401:GLU:HA	1:B:703:SER:OG	1.95	0.67
1:A:401:GLU:HA	1:A:703:SER:OG	1.94	0.67
1:A:600:HIS:HD2	1:A:680:LEU:HD22	1.58	0.67
1:A:397:LEU:H	1:A:401:GLU:CG	2.07	0.67
1:B:715:ARG:O	1:B:719:LYS:HG2	1.95	0.67
1:A:413:PHE:HE1	1:A:415:ASP:HB3	1.59	0.66
1:B:442:PHE:CD2	1:B:451:VAL:HG22	2.31	0.66
1:B:600:HIS:CD2	1:B:680:LEU:HD22	2.30	0.66
1:B:600:HIS:HD2	1:B:680:LEU:HD22	1.60	0.66
1:A:423:GLU:HG2	4:A:1127:HOH:O	1.95	0.66
1:B:458:LEU:HD13	1:B:695:LEU:HD21	1.78	0.66
1:A:407:LEU:HD11	1:A:704:SER:HB3	1.78	0.65
1:A:515:VAL:HG12	1:A:568:LEU:HB2	1.79	0.65
1:B:519:PHE:HB3	1:B:531:LEU:HG	1.77	0.65
1:B:545:LEU:HD23	4:B:1161:HOH:O	1.96	0.65
1:A:495:THR:HG22	1:A:499:ILE:HD12	1.78	0.65
1:B:473:TYR:HB2	1:B:627:LEU:HD12	1.78	0.65
1:A:684:LEU:HB2	1:A:688:LEU:HD12	1.80	0.64
1:A:408:ILE:HD12	1:A:408:ILE:H	1.62	0.64
1:A:473:TYR:HB2	1:A:627:LEU:HD12	1.78	0.64
1:B:392:ARG:NH2	3:B:999:ADP:HN62	1.96	0.64
1:B:408:ILE:HD12	1:B:408:ILE:H	1.63	0.64
1:A:522:ILE:HB	1:A:600:HIS:HB2	1.80	0.63
1:A:574:VAL:CG1	1:A:578:LEU:HD23	2.27	0.63
1:A:518:GLU:HG3	1:A:565:SER:HA	1.81	0.63
1:B:407:LEU:HD11	1:B:704:SER:HB3	1.80	0.63
1:B:684:LEU:HB2	1:B:688:LEU:HD12	1.81	0.63
1:B:455:VAL:O	1:B:457:GLN:N	2.32	0.63
1:B:515:VAL:HG12	1:B:568:LEU:HB2	1.81	0.63
1:A:698:VAL:HG21	1:A:717:ALA:CB	2.29	0.62
1:B:495:THR:HG22	1:B:499:ILE:HD12	1.79	0.62
1:B:574:VAL:CG1	1:B:578:LEU:HD23	2.28	0.62
1:B:574:VAL:O	1:B:578:LEU:HB2	1.99	0.62
1:B:389:VAL:O	1:B:438:PHE:HB3	1.99	0.62
1:B:522:ILE:HB	1:B:600:HIS:HB2	1.81	0.62
1:B:518:GLU:HG3	1:B:565:SER:HA	1.81	0.62
1:A:392:ARG:NH2	3:A:998:ADP:HN62	1.96	0.62
1:A:574:VAL:O	1:A:578:LEU:HB2	1.99	0.62
1:B:461:SER:O	1:B:464:ASP:HB2	2.00	0.62
1:A:457:GLN:NE2	1:A:460:GLN:HE21	1.96	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:SER:O	1:A:464:ASP:HB2	1.99	0.62
1:A:715:ARG:HA	1:A:718:SER:HG	1.63	0.62
1:A:556:LYS:HG3	1:A:686:TYR:CE1	2.34	0.61
1:B:659:VAL:HG21	1:B:681:THR:HG21	1.82	0.61
1:A:458:LEU:HD23	1:A:459:VAL:HG22	1.81	0.61
1:A:458:LEU:HD12	1:A:693:LYS:HB3	1.83	0.61
1:B:676:ARG:HA	1:B:682:TYR:HB2	1.82	0.61
1:B:458:LEU:HD12	1:B:693:LYS:HB3	1.83	0.61
1:B:515:VAL:HG22	1:B:607:LEU:HD23	1.83	0.61
1:B:604:ILE:HG23	1:B:623:ASN:HD22	1.64	0.61
1:A:458:LEU:HD23	1:A:459:VAL:H	1.66	0.61
1:B:473:TYR:CE1	1:B:630:SER:HB2	2.36	0.61
1:B:698:VAL:HG21	1:B:717:ALA:CB	2.29	0.61
1:B:598:ARG:NH1	1:B:649:ILE:HD13	2.16	0.60
1:A:455:VAL:O	1:A:457:GLN:N	2.33	0.60
1:A:676:ARG:HA	1:A:682:TYR:HB2	1.83	0.60
1:B:490:GLY:O	1:B:493:PRO:HD2	2.02	0.60
1:A:667:ASP:CG	1:A:670:LYS:HG3	2.22	0.60
1:A:389:VAL:HG11	1:A:717:ALA:HB1	1.83	0.60
1:B:457:GLN:NE2	1:B:460:GLN:HE21	1.98	0.60
1:B:667:ASP:CG	1:B:670:LYS:HG3	2.22	0.60
1:A:473:TYR:CE1	1:A:630:SER:HB2	2.37	0.60
1:B:556:LYS:HG3	1:B:686:TYR:CE1	2.37	0.60
1:A:700:ILE:HD12	1:A:701:SER:O	2.02	0.60
1:B:545:LEU:HD22	1:B:546:LYS:H	1.66	0.60
1:A:471:PHE:O	1:A:697:PHE:HB2	2.01	0.59
1:A:545:LEU:HD22	1:A:546:LYS:H	1.66	0.59
1:B:458:LEU:HD23	1:B:459:VAL:HG22	1.84	0.59
1:A:694:THR:O	1:A:695:LEU:HD23	2.03	0.59
1:B:598:ARG:HD3	1:B:649:ILE:CD1	2.32	0.59
1:B:389:VAL:HG11	1:B:717:ALA:HB1	1.83	0.59
1:A:397:LEU:H	1:A:401:GLU:HG3	1.67	0.59
1:A:684:LEU:O	1:A:688:LEU:HD12	2.02	0.59
1:A:515:VAL:HG22	1:A:607:LEU:HD23	1.85	0.59
1:B:457:GLN:O	1:B:460:GLN:HG2	2.02	0.59
1:B:585:ARG:CZ	1:B:601:SER:HB3	2.33	0.59
1:A:457:GLN:O	1:A:460:GLN:HG2	2.02	0.59
1:A:604:ILE:HG23	1:A:623:ASN:HD22	1.66	0.59
1:A:585:ARG:CZ	1:A:601:SER:HB3	2.32	0.58
1:B:490:GLY:C	1:B:493:PRO:HD2	2.24	0.58
1:B:458:LEU:HD23	1:B:459:VAL:H	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:700:ILE:HG21	1:A:714:LEU:CD2	2.30	0.58
1:A:389:VAL:O	1:A:438:PHE:HB3	2.04	0.58
1:A:601:SER:OG	1:A:626:ASP:HB3	2.02	0.58
1:B:700:ILE:HG21	1:B:714:LEU:CD2	2.32	0.58
1:A:521:GLU:OE1	1:A:599:SER:CB	2.51	0.58
1:B:471:PHE:O	1:B:697:PHE:HB2	2.03	0.58
1:A:598:ARG:HD3	1:A:649:ILE:CD1	2.33	0.58
1:A:698:VAL:CG2	1:A:717:ALA:HB2	2.32	0.57
1:B:598:ARG:HD3	1:B:649:ILE:HD11	1.85	0.57
1:B:673:ILE:HB	1:B:675:PHE:CE2	2.39	0.57
1:A:490:GLY:C	1:A:493:PRO:HD2	2.25	0.57
1:A:545:LEU:HD21	1:B:572:GLU:HB2	1.87	0.57
1:B:521:GLU:OE1	1:B:599:SER:CB	2.50	0.57
1:A:485:LEU:O	1:A:486:ASN:C	2.43	0.57
1:A:598:ARG:NH1	1:A:649:ILE:HD13	2.20	0.57
1:B:684:LEU:O	1:B:688:LEU:HD12	2.04	0.57
1:B:694:THR:O	1:B:695:LEU:HD23	2.04	0.57
1:A:490:GLY:O	1:A:493:PRO:HD2	2.04	0.57
1:A:413:PHE:CE1	1:A:415:ASP:HB3	2.40	0.56
1:A:387:ILE:C	1:A:388:ARG:HD2	2.26	0.56
1:B:481:THR:CG2	1:B:585:ARG:HB2	2.35	0.56
1:B:668:SER:CA	1:B:671:ARG:HB3	2.21	0.56
1:B:397:LEU:H	1:B:401:GLU:HG3	1.68	0.56
1:B:700:ILE:HD12	1:B:701:SER:O	2.05	0.56
1:B:585:ARG:NH1	1:B:601:SER:HB3	2.21	0.56
1:B:719:LYS:HG3	1:B:720:VAL:N	2.21	0.56
1:A:585:ARG:NH1	1:A:601:SER:HB3	2.20	0.56
1:B:392:ARG:NH2	3:B:999:ADP:N6	2.54	0.56
1:B:601:SER:OG	1:B:626:ASP:HB3	2.04	0.56
1:A:523:TYR:HB2	1:A:599:SER:HB3	1.86	0.56
1:A:572:GLU:HB2	1:B:545:LEU:HD21	1.88	0.56
1:A:704:SER:HA	1:A:707:ILE:HG12	1.88	0.56
1:B:485:LEU:O	1:B:486:ASN:C	2.43	0.56
1:A:392:ARG:NH2	3:A:998:ADP:N6	2.54	0.55
1:A:407:LEU:HD12	1:A:407:LEU:H	1.72	0.55
1:A:659:VAL:HG21	1:A:681:THR:HG21	1.88	0.55
1:B:387:ILE:C	1:B:388:ARG:HD2	2.26	0.55
1:A:480:LYS:HA	1:A:699:ASN:ND2	2.22	0.55
1:B:407:LEU:HD12	1:B:407:LEU:H	1.71	0.55
1:A:719:LYS:HG3	1:A:720:VAL:N	2.22	0.55
1:A:599:SER:O	1:A:628:ALA:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ILE:HD12	1:B:393:ILE:H	1.72	0.55
1:B:704:SER:HA	1:B:707:ILE:HG12	1.88	0.55
1:A:511:TRP:HA	1:A:611:ASN:HB2	1.89	0.55
1:A:715:ARG:HA	1:A:718:SER:OG	2.06	0.55
1:B:391:CYS:HB3	1:B:441:ILE:HG23	1.86	0.55
1:B:480:LYS:HA	1:B:699:ASN:ND2	2.22	0.55
1:A:481:THR:CG2	1:A:585:ARG:HB2	2.37	0.54
1:B:437:LYS:O	1:B:437:LYS:HG3	2.07	0.54
1:B:523:TYR:HB2	1:B:599:SER:HB3	1.88	0.54
1:A:393:ILE:HD12	1:A:393:ILE:H	1.73	0.54
1:A:704:SER:HA	1:A:707:ILE:HD11	1.89	0.54
1:B:599:SER:O	1:B:628:ALA:HB2	2.08	0.54
1:B:698:VAL:CG2	1:B:717:ALA:HB2	2.33	0.54
1:A:704:SER:HA	1:A:707:ILE:CG1	2.38	0.54
1:B:667:ASP:OD2	1:B:670:LYS:HG3	2.08	0.54
1:A:598:ARG:HD3	1:A:649:ILE:HD11	1.88	0.54
1:B:679:LYS:O	1:B:683:LEU:HB2	2.08	0.54
1:B:394:ARG:HG3	1:B:394:ARG:NH1	2.13	0.54
1:A:673:ILE:HB	1:A:675:PHE:CE2	2.41	0.54
1:B:704:SER:HA	1:B:707:ILE:CG1	2.38	0.54
1:B:397:LEU:H	1:B:401:GLU:HG2	1.72	0.54
1:B:461:SER:O	1:B:464:ASP:N	2.40	0.54
1:A:397:LEU:H	1:A:401:GLU:HG2	1.73	0.53
1:A:667:ASP:OD2	1:A:670:LYS:HG3	2.09	0.53
1:B:715:ARG:HA	1:B:718:SER:OG	2.07	0.53
1:A:394:ARG:HH12	1:A:397:LEU:HD11	1.73	0.53
1:B:413:PHE:CE1	1:B:415:ASP:HB3	2.40	0.53
1:A:559:THR:HG22	1:A:560:ILE:N	2.23	0.53
1:A:679:LYS:O	1:A:683:LEU:HB2	2.08	0.53
1:A:648:ASN:O	1:A:651:LYS:HB3	2.09	0.53
1:B:572:GLU:O	1:B:576:ILE:CD1	2.56	0.53
1:A:510:GLY:HA2	1:A:613:LYS:HZ3	1.73	0.53
1:B:422:MET:HB3	1:B:441:ILE:CD1	2.39	0.53
1:A:401:GLU:HA	1:A:703:SER:CB	2.39	0.52
1:A:500:PHE:CE1	1:A:574:VAL:HG21	2.44	0.52
1:A:559:THR:O	1:A:560:ILE:HG13	2.10	0.52
1:B:521:GLU:HB3	1:B:530:LEU:CD1	2.38	0.52
1:B:606:HIS:ND1	1:B:619:TYR:OH	2.37	0.52
1:B:704:SER:HA	1:B:707:ILE:HD11	1.90	0.52
1:A:391:CYS:HB3	1:A:441:ILE:HG23	1.90	0.52
1:B:394:ARG:HH12	1:B:397:LEU:HD11	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLU:HB3	1:A:530:LEU:CD1	2.37	0.52
1:A:422:MET:HB3	1:A:441:ILE:CD1	2.39	0.52
1:B:443:ASP:HB3	1:B:445:GLN:NE2	2.25	0.52
1:A:518:GLU:OE1	1:A:606:HIS:NE2	2.38	0.52
1:A:684:LEU:C	1:A:688:LEU:HD12	2.30	0.52
1:B:500:PHE:CE1	1:B:574:VAL:HG21	2.43	0.52
1:A:437:LYS:HG3	1:A:437:LYS:O	2.10	0.52
1:A:492:ILE:HB	1:A:493:PRO:HD3	1.92	0.52
1:B:416:ASN:C	1:B:418:GLY:N	2.63	0.52
1:A:416:ASN:C	1:A:418:GLY:H	2.14	0.51
1:B:644:ARG:C	1:B:646:THR:N	2.64	0.51
1:B:511:TRP:HA	1:B:611:ASN:HB2	1.90	0.51
1:B:559:THR:HG22	1:B:560:ILE:N	2.24	0.51
1:B:559:THR:O	1:B:560:ILE:HG13	2.10	0.51
1:A:610:SER:OG	1:A:611:ASN:N	2.42	0.51
1:B:481:THR:HG21	1:B:585:ARG:HB2	1.92	0.51
1:A:443:ASP:HB3	1:A:445:GLN:NE2	2.26	0.51
1:A:458:LEU:CD1	1:A:693:LYS:HB3	2.41	0.51
1:B:663:LEU:HD21	1:B:689:THR:HG22	1.93	0.51
1:A:517:CYS:HA	1:A:604:ILE:O	2.11	0.51
1:A:644:ARG:C	1:A:646:THR:N	2.63	0.51
1:B:458:LEU:CD1	1:B:693:LYS:HB3	2.41	0.51
1:B:610:SER:OG	1:B:611:ASN:N	2.42	0.51
1:A:668:SER:CA	1:A:671:ARG:HB3	2.23	0.51
1:B:487:PRO:O	1:B:489:ASP:N	2.39	0.51
1:A:545:LEU:HD13	1:A:562:ASN:HB3	1.93	0.50
1:B:648:ASN:O	1:B:651:LYS:HB3	2.11	0.50
1:B:715:ARG:HA	1:B:718:SER:HG	1.76	0.50
1:A:457:GLN:HE21	1:A:460:GLN:HE21	1.57	0.50
1:B:684:LEU:C	1:B:688:LEU:HD12	2.31	0.50
1:A:495:THR:O	1:A:499:ILE:HB	2.11	0.50
1:B:416:ASN:C	1:B:418:GLY:H	2.14	0.50
1:B:545:LEU:HD13	1:B:562:ASN:HB3	1.93	0.50
1:A:704:SER:O	1:A:707:ILE:HG12	2.12	0.49
1:B:401:GLU:HA	1:B:703:SER:CB	2.41	0.49
1:A:573:MET:HE2	1:A:577:ILE:HG13	1.94	0.49
1:A:423:GLU:HA	1:A:434:HIS:O	2.12	0.49
1:B:467:ASN:HA	1:B:621:THR:O	2.12	0.49
1:B:520:ILE:HG22	1:B:529:ASP:HA	1.94	0.49
1:A:459:VAL:HG12	1:A:622:LEU:HD23	1.94	0.49
1:A:510:GLY:HA2	1:A:613:LYS:HZ2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:649:ILE:HG22	1:B:653:LEU:HD12	1.94	0.49
1:B:704:SER:O	1:B:707:ILE:HG12	2.13	0.49
1:B:423:GLU:HA	1:B:434:HIS:O	2.13	0.49
1:A:419:VAL:HG11	1:A:437:LYS:HE3	1.95	0.49
1:A:479:GLY:HA2	3:A:998:ADP:H8	1.78	0.49
1:A:416:ASN:C	1:A:418:GLY:N	2.63	0.49
1:A:663:LEU:HD21	1:A:689:THR:HG22	1.95	0.49
1:B:394:ARG:CD	1:B:701:SER:HA	2.42	0.49
1:A:438:PHE:CD2	1:A:438:PHE:N	2.80	0.49
1:B:517:CYS:HA	1:B:604:ILE:O	2.13	0.49
1:B:655:CYS:O	1:B:659:VAL:HG23	2.13	0.49
1:A:704:SER:HA	1:A:707:ILE:CD1	2.43	0.48
1:B:495:THR:O	1:B:499:ILE:HB	2.12	0.48
1:B:458:LEU:HD12	1:B:693:LYS:CG	2.44	0.48
1:A:649:ILE:HG22	1:A:653:LEU:HD12	1.96	0.48
1:B:505:LYS:HZ1	1:B:509:LYS:HD3	1.77	0.48
1:B:704:SER:HA	1:B:707:ILE:CD1	2.44	0.48
1:A:520:ILE:HG22	1:A:529:ASP:HA	1.94	0.48
1:B:419:VAL:HG11	1:B:437:LYS:HE3	1.94	0.48
1:B:439:ASP:O	1:B:440:LYS:CB	2.61	0.48
1:B:487:PRO:C	1:B:489:ASP:H	2.15	0.48
1:A:467:ASN:HA	1:A:621:THR:O	2.13	0.48
1:B:611:ASN:OD1	1:B:613:LYS:HB2	2.13	0.48
1:B:560:ILE:HD12	4:B:1210:HOH:O	2.12	0.48
1:B:492:ILE:HB	1:B:493:PRO:HD3	1.95	0.48
1:B:573:MET:HE2	1:B:577:ILE:HG13	1.94	0.48
1:A:458:LEU:HD12	1:A:693:LYS:CG	2.43	0.48
1:A:482:PHE:O	1:A:486:ASN:HB2	2.14	0.48
1:A:573:MET:CE	1:A:577:ILE:HG13	2.43	0.48
1:B:440:LYS:HG2	1:B:442:PHE:CE1	2.49	0.48
1:B:457:GLN:HE21	1:B:460:GLN:HE21	1.60	0.48
1:B:568:LEU:HD22	1:B:574:VAL:HG22	1.96	0.48
1:A:448:ASN:HB2	1:A:489:ASP:CG	2.33	0.47
1:B:448:ASN:HB2	1:B:489:ASP:CG	2.34	0.47
1:B:479:GLY:HA2	3:B:999:ADP:H8	1.79	0.47
1:B:492:ILE:HG12	1:B:624:LEU:CD1	2.44	0.47
1:B:644:ARG:HD3	1:B:644:ARG:HA	1.55	0.47
1:A:461:SER:O	1:A:464:ASP:N	2.44	0.47
1:A:481:THR:HG21	1:A:585:ARG:HB2	1.96	0.47
1:A:470:ILE:HG13	1:A:624:LEU:CD2	2.44	0.47
1:A:655:CYS:O	1:A:659:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:VAL:HG21	1:B:721:ASN:HB2	1.95	0.47
1:A:394:ARG:CD	1:A:701:SER:HA	2.43	0.47
1:A:439:ASP:O	1:A:440:LYS:CB	2.62	0.47
1:A:606:HIS:ND1	1:A:619:TYR:OH	2.40	0.47
1:A:644:ARG:HD3	1:A:644:ARG:HA	1.55	0.47
1:A:611:ASN:OD1	1:A:613:LYS:HB2	2.14	0.47
1:A:644:ARG:C	1:A:646:THR:H	2.16	0.47
1:B:598:ARG:HH11	1:B:649:ILE:CD1	2.28	0.47
1:A:568:LEU:HD22	1:A:574:VAL:HG22	1.96	0.47
1:A:572:GLU:H	1:A:572:GLU:CD	2.16	0.47
1:B:644:ARG:C	1:B:646:THR:H	2.17	0.47
1:A:394:ARG:HD3	1:A:702:PRO:HD3	1.97	0.47
1:B:518:GLU:OE1	1:B:606:HIS:NE2	2.39	0.47
1:A:421:SER:HA	1:A:436:PHE:O	2.15	0.46
1:B:421:SER:HA	1:B:436:PHE:O	2.14	0.46
1:B:545:LEU:CD2	1:B:546:LYS:H	2.28	0.46
1:B:599:SER:C	1:B:628:ALA:HB2	2.35	0.46
1:B:711:LEU:O	1:B:715:ARG:HB2	2.16	0.46
1:A:719:LYS:HG3	1:A:720:VAL:H	1.81	0.46
1:B:510:GLY:HA3	1:B:613:LYS:HD3	1.97	0.46
1:B:611:ASN:O	1:B:615:GLY:N	2.47	0.46
1:A:389:VAL:HG21	1:A:721:ASN:HB2	1.96	0.46
1:A:492:ILE:HG12	1:A:624:LEU:CD1	2.45	0.46
1:A:394:ARG:HG3	1:A:394:ARG:NH1	2.12	0.46
1:B:517:CYS:HB2	1:B:604:ILE:O	2.15	0.46
1:B:572:GLU:CD	1:B:572:GLU:H	2.18	0.46
1:A:611:ASN:O	1:A:615:GLY:N	2.49	0.46
1:A:684:LEU:HB2	1:A:688:LEU:CD1	2.45	0.46
1:B:500:PHE:HE1	1:B:574:VAL:HG21	1.81	0.46
1:A:572:GLU:O	1:A:576:ILE:CD1	2.57	0.46
1:B:394:ARG:HD3	1:B:702:PRO:HD3	1.97	0.46
1:B:455:VAL:O	1:B:456:GLY:C	2.54	0.46
1:A:455:VAL:O	1:A:456:GLY:C	2.54	0.46
1:A:555:THR:O	1:A:556:LYS:HB2	2.16	0.46
1:B:482:PHE:O	1:B:486:ASN:HB2	2.16	0.46
1:A:545:LEU:CD2	1:A:546:LYS:H	2.29	0.46
1:A:711:LEU:O	1:A:715:ARG:HB2	2.16	0.46
1:A:440:LYS:HG2	1:A:442:PHE:CE1	2.51	0.46
1:A:715:ARG:CA	1:A:718:SER:HG	2.28	0.46
1:B:438:PHE:CD2	1:B:438:PHE:N	2.81	0.46
1:B:472:ALA:O	1:B:480:LYS:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:PHE:CD1	1:A:494:SER:HB2	2.51	0.45
1:A:573:MET:HG3	1:A:577:ILE:HD12	1.97	0.45
1:A:422:MET:HB3	1:A:441:ILE:HD12	1.98	0.45
1:A:625:VAL:HG12	1:A:627:LEU:HD23	1.99	0.45
1:A:599:SER:C	1:A:628:ALA:HB2	2.36	0.45
1:B:401:GLU:N	1:B:401:GLU:OE2	2.49	0.45
1:B:445:GLN:H	1:B:445:GLN:HG3	1.42	0.45
1:B:452:PHE:CD1	1:B:494:SER:HB2	2.52	0.45
1:A:413:PHE:HE1	1:A:415:ASP:CB	2.29	0.45
1:A:487:PRO:C	1:A:489:ASP:H	2.18	0.45
1:A:401:GLU:N	1:A:401:GLU:OE2	2.50	0.45
1:A:654:SER:O	1:A:658:ASP:OD2	2.35	0.45
1:A:480:LYS:N	1:A:699:ASN:HD22	2.14	0.44
1:B:510:GLY:CA	1:B:613:LYS:HD3	2.46	0.44
1:B:719:LYS:HG3	1:B:720:VAL:H	1.81	0.44
1:A:510:GLY:HA3	1:A:613:LYS:HD3	2.00	0.44
1:A:598:ARG:HH11	1:A:649:ILE:CD1	2.31	0.44
1:B:459:VAL:HG12	1:B:622:LEU:HD23	1.95	0.44
1:B:573:MET:CE	1:B:577:ILE:HG13	2.47	0.44
1:A:510:GLY:CA	1:A:613:LYS:HD3	2.48	0.44
1:A:445:GLN:H	1:A:445:GLN:HG3	1.41	0.44
1:B:470:ILE:HG13	1:B:624:LEU:CD2	2.47	0.44
1:A:570:SER:HB2	1:A:572:GLU:OE2	2.18	0.44
1:A:394:ARG:CG	1:A:394:ARG:NH1	2.66	0.44
1:A:487:PRO:O	1:A:489:ASP:N	2.41	0.44
1:A:509:LYS:HB3	1:A:509:LYS:HE3	1.73	0.44
1:B:598:ARG:HH11	1:B:649:ILE:HD13	1.82	0.44
1:A:460:GLN:OE1	1:A:502:TRP:NE1	2.50	0.44
1:A:438:PHE:HE1	1:A:717:ALA:HB3	1.83	0.43
1:A:643:LEU:HB3	1:A:644:ARG:H	1.52	0.43
1:B:578:LEU:HD13	1:B:578:LEU:HA	1.79	0.43
1:B:684:LEU:HB2	1:B:688:LEU:CD1	2.46	0.43
1:A:716:PHE:CD1	1:A:717:ALA:N	2.87	0.43
1:B:458:LEU:HD12	1:B:693:LYS:CB	2.48	0.43
1:B:460:GLN:OE1	1:B:502:TRP:NE1	2.50	0.43
1:B:716:PHE:CD1	1:B:717:ALA:N	2.86	0.43
1:A:458:LEU:HD12	1:A:693:LYS:HG2	2.00	0.43
1:A:517:CYS:HB2	1:A:604:ILE:O	2.18	0.43
1:B:438:PHE:HE1	1:B:717:ALA:HB3	1.84	0.43
1:A:479:GLY:C	1:A:699:ASN:HD22	2.22	0.43
1:A:710:THR:HG22	1:A:714:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:VAL:HG12	1:B:438:PHE:HD1	1.83	0.43
1:B:479:GLY:C	1:B:699:ASN:HD22	2.22	0.43
1:B:611:ASN:O	1:B:611:ASN:CG	2.57	0.43
1:A:394:ARG:HE	1:A:701:SER:CA	2.31	0.43
1:A:570:SER:CB	1:A:572:GLU:HG2	2.47	0.43
1:B:570:SER:HB2	1:B:572:GLU:OE2	2.18	0.43
1:A:448:ASN:HD22	1:A:490:GLY:N	2.16	0.43
1:B:555:THR:O	1:B:556:LYS:HB2	2.19	0.43
1:B:621:THR:CG2	1:B:623:ASN:HD21	2.31	0.43
1:B:625:VAL:HG12	1:B:627:LEU:HD23	2.00	0.43
1:B:707:ILE:O	1:B:711:LEU:CG	2.63	0.43
1:B:480:LYS:N	1:B:699:ASN:HD22	2.16	0.43
1:B:573:MET:HG3	1:B:577:ILE:HD12	2.00	0.43
1:B:660:ILE:O	1:B:661:HIS:C	2.57	0.43
1:A:458:LEU:HD12	1:A:693:LYS:CB	2.47	0.43
1:A:393:ILE:HD13	1:A:443:ASP:HA	2.00	0.43
1:A:551:HIS:CE1	1:A:685:GLN:HG2	2.54	0.43
1:B:462:SER:HA	1:B:466:TYR:O	2.19	0.43
1:B:708:ASN:HD22	1:B:708:ASN:HA	1.58	0.42
1:B:393:ILE:HD13	1:B:443:ASP:HA	2.01	0.42
1:A:457:GLN:NE2	1:A:460:GLN:NE2	2.66	0.42
1:A:485:LEU:HD21	1:A:581:ALA:HB3	2.01	0.42
1:A:572:GLU:CD	1:A:572:GLU:N	2.72	0.42
1:A:470:ILE:HG13	1:A:624:LEU:HD22	2.02	0.42
1:A:500:PHE:HE1	1:A:574:VAL:HG21	1.82	0.42
1:A:554:GLU:HB2	1:A:555:THR:H	1.69	0.42
1:B:422:MET:HB3	1:B:441:ILE:HD12	2.02	0.42
1:B:509:LYS:HB3	1:B:509:LYS:HE3	1.72	0.42
1:A:660:ILE:O	1:A:661:HIS:C	2.58	0.42
1:B:710:THR:HG22	1:B:714:LEU:HD11	2.00	0.42
1:A:394:ARG:HD3	1:A:701:SER:HA	2.01	0.42
1:A:574:VAL:CG1	1:A:578:LEU:CD2	2.97	0.42
1:B:551:HIS:CE1	1:B:685:GLN:HG2	2.55	0.42
1:B:570:SER:CB	1:B:572:GLU:HG2	2.48	0.42
1:A:456:GLY:C	1:A:459:VAL:HG23	2.40	0.42
1:A:611:ASN:O	1:A:611:ASN:CG	2.57	0.42
1:A:671:ARG:HE	1:A:671:ARG:HB2	1.39	0.42
1:A:655:CYS:SG	1:A:678:SER:HB2	2.60	0.42
1:B:394:ARG:HE	1:B:701:SER:CA	2.31	0.42
1:B:654:SER:O	1:B:658:ASP:OD2	2.37	0.42
1:B:457:GLN:O	1:B:460:GLN:CG	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:LYS:O	1:B:437:LYS:CG	2.68	0.41
1:A:389:VAL:HG12	1:A:438:PHE:HD1	1.84	0.41
1:A:560:ILE:CG2	1:A:563:VAL:HG21	2.51	0.41
1:A:512:ASP:OD1	1:A:512:ASP:C	2.59	0.41
1:B:394:ARG:HD3	1:B:701:SER:HA	2.01	0.41
1:B:458:LEU:HD12	1:B:693:LYS:HG2	2.03	0.41
1:B:505:LYS:HD2	4:B:1133:HOH:O	2.20	0.41
1:B:595:HIS:C	1:B:597:SER:N	2.74	0.41
1:A:683:LEU:HD22	1:A:683:LEU:O	2.21	0.41
1:B:404:ASP:N	4:B:1138:HOH:O	2.53	0.41
1:B:448:ASN:HD22	1:B:490:GLY:N	2.18	0.41
1:B:532:ARG:O	1:B:532:ARG:HG3	2.19	0.41
1:A:575:GLU:O	1:A:579:LYS:HB2	2.20	0.41
1:A:462:SER:HA	1:A:466:TYR:O	2.20	0.41
1:B:407:LEU:HD13	1:B:707:ILE:HG13	2.02	0.41
1:B:667:ASP:OD1	1:B:670:LYS:HG3	2.21	0.41
1:B:456:GLY:C	1:B:459:VAL:HG23	2.40	0.41
1:B:581:ALA:HA	1:B:584:LEU:HD12	2.03	0.41
1:A:407:LEU:HD13	1:A:707:ILE:HG13	2.03	0.41
1:A:457:GLN:O	1:A:460:GLN:CG	2.68	0.41
1:A:610:SER:O	1:A:611:ASN:CB	2.68	0.41
1:B:572:GLU:CD	1:B:572:GLU:N	2.74	0.41
1:B:663:LEU:HD13	1:B:688:LEU:O	2.21	0.41
1:B:575:GLU:O	1:B:579:LYS:HB2	2.20	0.41
1:B:708:ASN:HA	1:B:711:LEU:HD12	2.03	0.40
1:B:574:VAL:CG1	1:B:578:LEU:CD2	2.97	0.40
1:A:425:THR:OG1	1:A:433:VAL:CG2	2.65	0.40
1:A:581:ALA:HA	1:A:584:LEU:HD12	2.02	0.40
1:A:614:THR:HG22	1:A:614:THR:O	2.22	0.40
1:B:439:ASP:O	1:B:440:LYS:HB2	2.22	0.40
1:B:614:THR:HG22	1:B:614:THR:O	2.21	0.40
1:B:455:VAL:C	1:B:457:GLN:N	2.74	0.40
1:B:470:ILE:HG13	1:B:624:LEU:HD22	2.04	0.40
1:A:475:GLN:HE22	1:A:706:HIS:HB3	1.87	0.40
1:A:598:ARG:HH11	1:A:649:ILE:HD13	1.85	0.40
1:B:663:LEU:HG	1:B:673:ILE:HD13	2.03	0.40
1:B:683:LEU:HD22	1:B:683:LEU:O	2.21	0.40
1:B:709:GLU:O	1:B:709:GLU:CD	2.60	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	288/347 (83%)	233 (81%)	39 (14%)	16 (6%)	2 1
1	B	288/347 (83%)	233 (81%)	38 (13%)	17 (6%)	1 1
All	All	576/694 (83%)	466 (81%)	77 (13%)	33 (6%)	1 1

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	THR
1	A	415	ASP
1	A	420	GLN
1	A	440	LYS
1	A	511	TRP
1	A	611	ASN
1	B	405	THR
1	B	415	ASP
1	B	420	GLN
1	B	440	LYS
1	B	511	TRP
1	B	611	ASN
1	A	396	ALA
1	A	419	VAL
1	A	438	PHE
1	A	456	GLY
1	A	490	GLY
1	A	512	ASP
1	A	525	GLU
1	A	666	PRO
1	B	396	ALA
1	B	419	VAL
1	B	438	PHE
1	B	456	GLY
1	B	490	GLY

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Mol	Chain	Res	Type
1	B	512	ASP
1	B	525	GLU
1	B	666	PRO
1	A	616	ALA
1	B	488	GLY
1	B	616	ALA
1	A	488	GLY
1	B	629	GLY

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	274/316 (87%)	204 (74%)	70 (26%)	0 1
1	B	274/316 (87%)	205 (75%)	69 (25%)	0 1
All	All	548/632 (87%)	409 (75%)	139 (25%)	0 1

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	ARG
1	A	394	ARG
1	A	398	LYS
1	A	399	ASN
1	A	401	GLU
1	A	406	SER
1	A	407	LEU
1	A	423	GLU
1	A	435	GLU
1	A	437	LYS
1	A	440	LYS
1	A	444	GLN
1	A	445	GLN
1	A	447	THR
1	A	454	GLU

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Mol	Chain	Res	Type
1	A	458	LEU
1	A	459	VAL
1	A	462	SER
1	A	463	LEU
1	A	475	GLN
1	A	484	MET
1	A	485	LEU
1	A	489	ASP
1	A	491	ILE
1	A	497	SER
1	A	499	ILE
1	A	500	PHE
1	A	505	LYS
1	A	506	LEU
1	A	507	LYS
1	A	512	ASP
1	A	514	LYS
1	A	516	ASN
1	A	520	ILE
1	A	521	GLU
1	A	532	ARG
1	A	545	LEU
1	A	548	GLU
1	A	554	GLU
1	A	567	LYS
1	A	572	GLU
1	A	575	GLU
1	A	578	LEU
1	A	583	LYS
1	A	586	SER
1	A	595	HIS
1	A	596	SER
1	A	599	SER
1	A	611	ASN
1	A	630	SER
1	A	643	LEU
1	A	644	ARG
1	A	652	SER
1	A	665	GLN
1	A	669	THR
1	A	670	LYS
1	A	671	ARG

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Mol	Chain	Res	Type
1	A	676	ARG
1	A	679	LYS
1	A	683	LEU
1	A	684	LEU
1	A	686	TYR
1	A	688	LEU
1	A	693	LYS
1	A	700	ILE
1	A	701	SER
1	A	708	ASN
1	A	709	GLU
1	A	721	ASN
1	A	722	SER
1	B	392	ARG
1	B	394	ARG
1	B	398	LYS
1	B	399	ASN
1	B	401	GLU
1	B	406	SER
1	B	407	LEU
1	B	423	GLU
1	B	435	GLU
1	B	437	LYS
1	B	440	LYS
1	B	444	GLN
1	B	445	GLN
1	B	447	THR
1	B	454	GLU
1	B	458	LEU
1	B	459	VAL
1	B	462	SER
1	B	463	LEU
1	B	475	GLN
1	B	484	MET
1	B	485	LEU
1	B	489	ASP
1	B	491	ILE
1	B	497	SER
1	B	499	ILE
1	B	500	PHE
1	B	505	LYS
1	B	506	LEU

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Mol	Chain	Res	Type
1	B	507	LYS
1	B	512	ASP
1	B	514	LYS
1	B	516	ASN
1	B	520	ILE
1	B	521	GLU
1	B	532	ARG
1	B	545	LEU
1	B	548	GLU
1	B	554	GLU
1	B	567	LYS
1	B	572	GLU
1	B	575	GLU
1	B	578	LEU
1	B	583	LYS
1	B	586	SER
1	B	595	HIS
1	B	596	SER
1	B	599	SER
1	B	611	ASN
1	B	630	SER
1	B	643	LEU
1	B	644	ARG
1	B	652	SER
1	B	665	GLN
1	B	669	THR
1	B	670	LYS
1	B	671	ARG
1	B	676	ARG
1	B	679	LYS
1	B	683	LEU
1	B	684	LEU
1	B	688	LEU
1	B	693	LYS
1	B	700	ILE
1	B	701	SER
1	B	708	ASN
1	B	709	GLU
1	B	721	ASN
1	B	722	SER

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

Mol	Chain	Res	Type
1	A	416	ASN
1	A	448	ASN
1	A	457	GLN
1	A	475	GLN
1	A	486	ASN
1	A	516	ASN
1	A	623	ASN
1	A	685	GLN
1	A	699	ASN
1	A	706	HIS
1	A	708	ASN
1	A	721	ASN
1	B	416	ASN
1	B	448	ASN
1	B	457	GLN
1	B	475	GLN
1	B	486	ASN
1	B	516	ASN
1	B	623	ASN
1	B	685	GLN
1	B	699	ASN
1	B	706	HIS
1	B	708	ASN
1	B	721	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are 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	B	999	2	24,29,29	1.21	3 (12%)	29,45,45	1.44	2 (6%)
3	ADP	A	998	2	24,29,29	1.16	3 (12%)	29,45,45	1.43	2 (6%)

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	B	999	2	-	5/12/32/32	0/3/3/3
3	ADP	A	998	2	-	5/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	ADP	O4'-C1'	2.92	1.45	1.41
3	A	998	ADP	O4'-C1'	2.75	1.44	1.41
3	B	999	ADP	C5-N7	-2.66	1.30	1.39
3	A	998	ADP	C5-N7	-2.44	1.30	1.39
3	A	998	ADP	C2-N3	2.16	1.35	1.32
3	B	999	ADP	PB-O2B	2.09	1.62	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	999	ADP	N3-C2-N1	-6.47	118.56	128.68
3	A	998	ADP	N3-C2-N1	-6.37	118.72	128.68
3	A	998	ADP	C4-C5-N7	-2.19	107.12	109.40
3	B	999	ADP	C4-C5-N7	-2.04	107.28	109.40

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	998	ADP	C5'-O5'-PA-O1A
3	A	998	ADP	C5'-O5'-PA-O2A
3	A	998	ADP	C5'-O5'-PA-O3A
3	B	999	ADP	C5'-O5'-PA-O1A
3	B	999	ADP	C5'-O5'-PA-O2A
3	B	999	ADP	C5'-O5'-PA-O3A
3	A	998	ADP	C3'-C4'-C5'-O5'
3	B	999	ADP	C3'-C4'-C5'-O5'
3	A	998	ADP	O4'-C4'-C5'-O5'
3	B	999	ADP	O4'-C4'-C5'-O5'

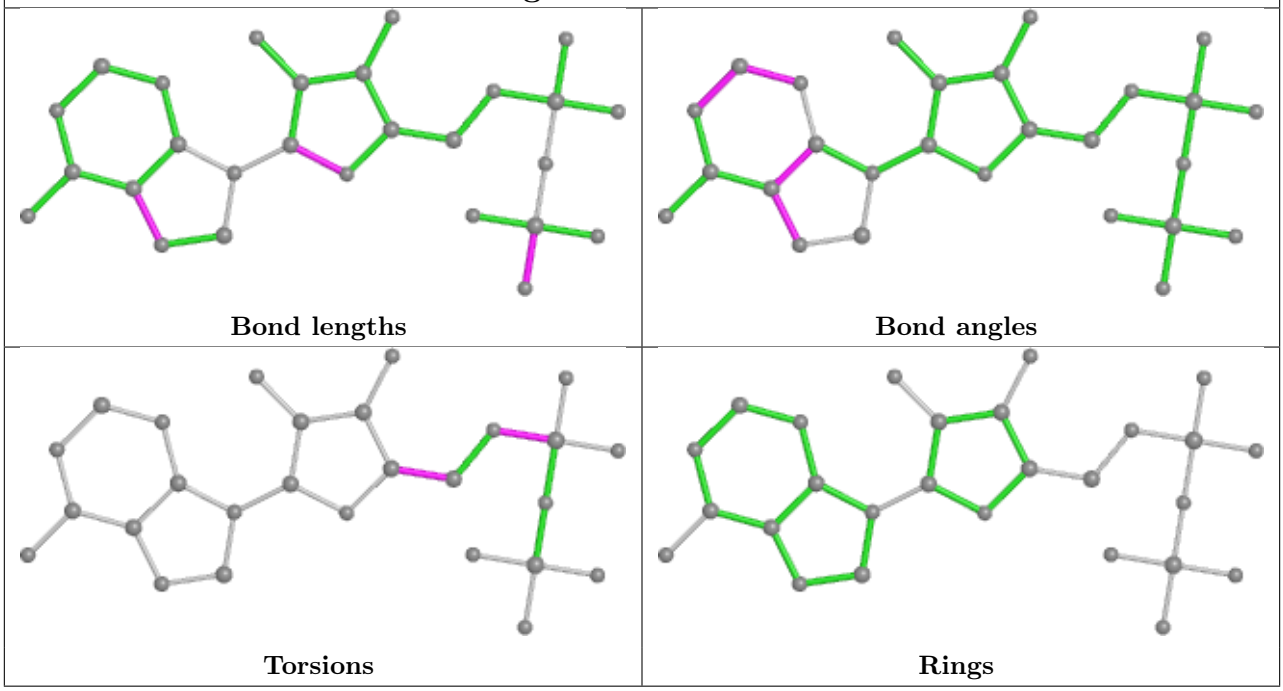
There are no ring outliers.

2 monomers are involved in 6 short contacts:

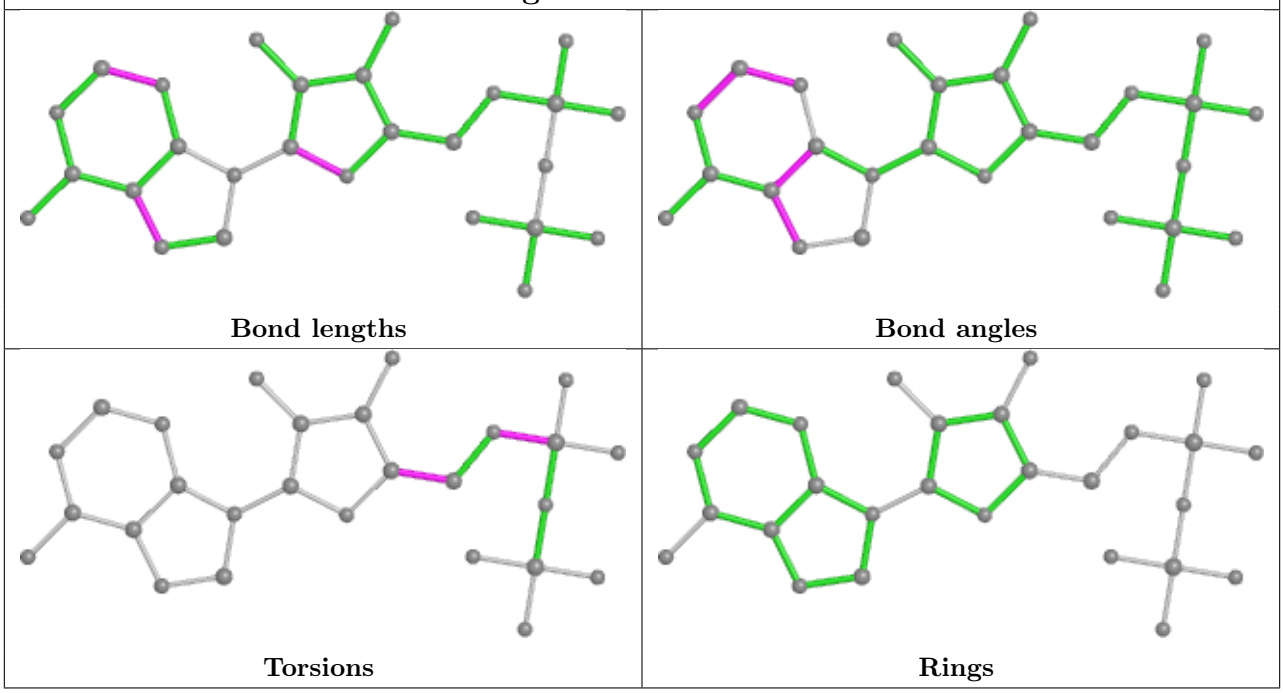
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	999	ADP	3	0
3	A	998	ADP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP B 999



Ligand ADP A 998



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(Å^2)	Q<0.9
1	A	300/347 (86%)	0.35	15 (5%)	28	30	16, 41, 75, 86	0
1	B	300/347 (86%)	0.31	14 (4%)	31	33	14, 41, 76, 84	0
All	All	600/694 (86%)	0.33	29 (4%)	30	32	14, 41, 76, 86	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	666	PRO	4.9
1	A	587	THR	4.5
1	B	632	ARG	4.4
1	A	385	GLY	4.2
1	A	666	PRO	4.2
1	B	643	LEU	4.1
1	A	664	GLY	4.0
1	A	632	ARG	3.9
1	A	400	LEU	3.7
1	A	669	THR	3.6
1	B	644	ARG	3.3
1	B	399	ASN	3.3
1	B	670	LYS	3.2
1	A	617	HIS	3.1
1	A	508	THR	3.0
1	B	433	VAL	2.9
1	A	668	SER	2.8
1	A	433	VAL	2.7
1	A	720	VAL	2.5
1	B	613	LYS	2.5
1	B	672	HIS	2.5
1	B	385	GLY	2.5
1	B	397	LEU	2.4
1	A	613	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	598	ARG	2.3
1	B	614	THR	2.2
1	B	400	LEU	2.2
1	A	719	LYS	2.1
1	B	398	LYS	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

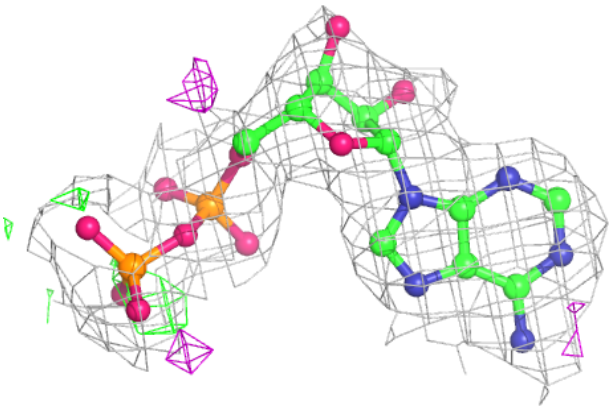
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

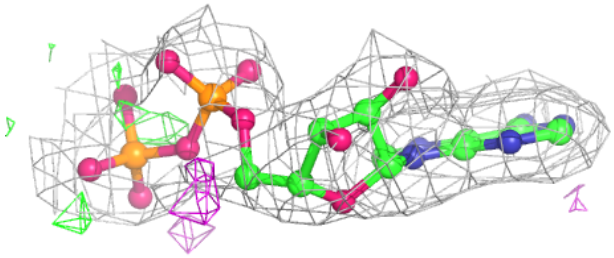
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	B	997	1/1	0.90	0.18	38,38,38,38	0
2	MG	A	996	1/1	0.92	0.20	36,36,36,36	0
3	ADP	A	998	27/27	0.94	0.17	27,42,53,57	0
3	ADP	B	999	27/27	0.95	0.15	28,40,55,58	0

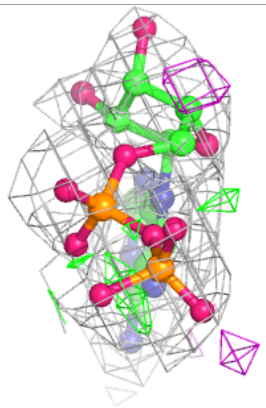
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 998:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

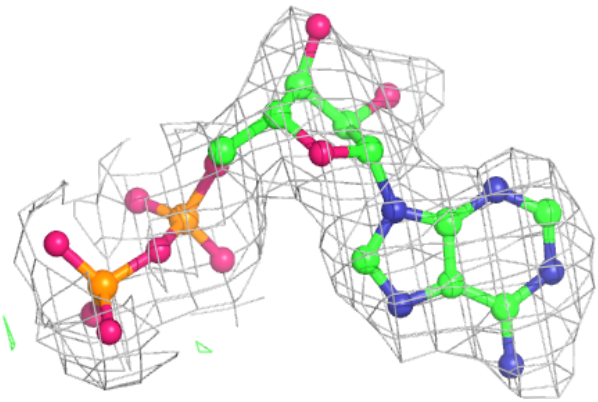


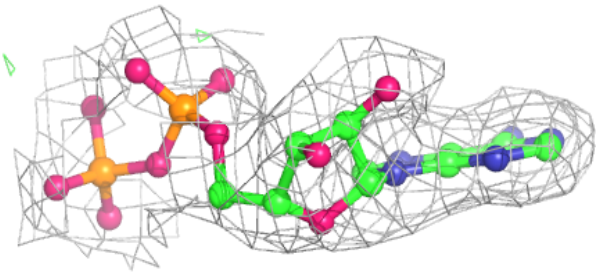


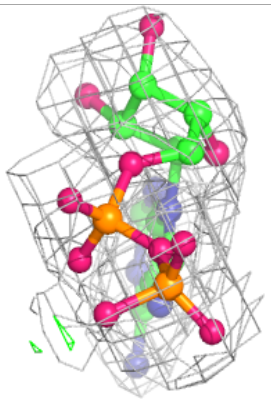


Electron density around ADP B 999:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.