



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 03:06 am GMT

PDB ID : 3L1C  
Title : Kinesin-14 Protein Ncd, T436S Mutant  
Authors : Kull, F.J.  
Deposited on : 2009-12-11  
Resolution : 2.75 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

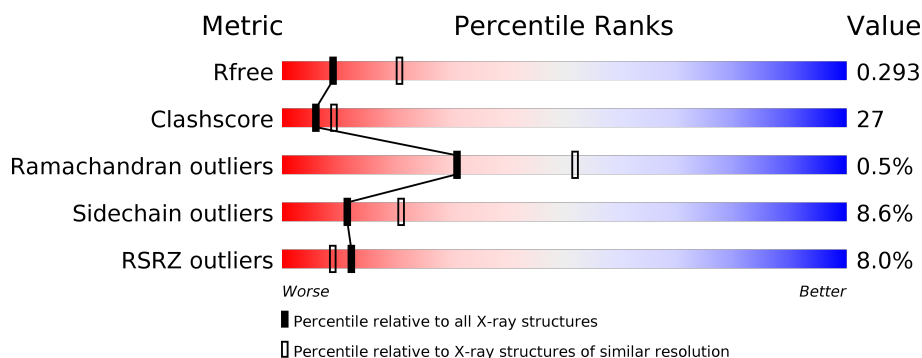
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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))
$R_{free}$	111664	4013 (2.80-2.72)
Clashscore	122126	1029 (2.78-2.74)
Ramachandran outliers	120053	1013 (2.78-2.74)
Sidechain outliers	120020	1013 (2.78-2.74)
RSRZ outliers	108989	3920 (2.80-2.72)

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

Mol	Chain	Length	Quality of chain
1	A	383	<div> <div>3%</div> <div> <div></div> <div>53%</div> <div>34%</div> <div>6%</div> <div>7%</div> </div> </div>
1	B	383	<div> <div>11%</div> <div> <div></div> <div>39%</div> <div>42%</div> <div>• •</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5768 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-14 Ncd.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	0	0	0
			2833	1767	495	551	20			
1	B	331	Total	C	N	O	S	0	0	0
			2636	1648	461	507	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	MET	-	EXPRESSION TAG	UNP P20480
A	436	SER	THR	ENGINEERED MUTATION	UNP P20480

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

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

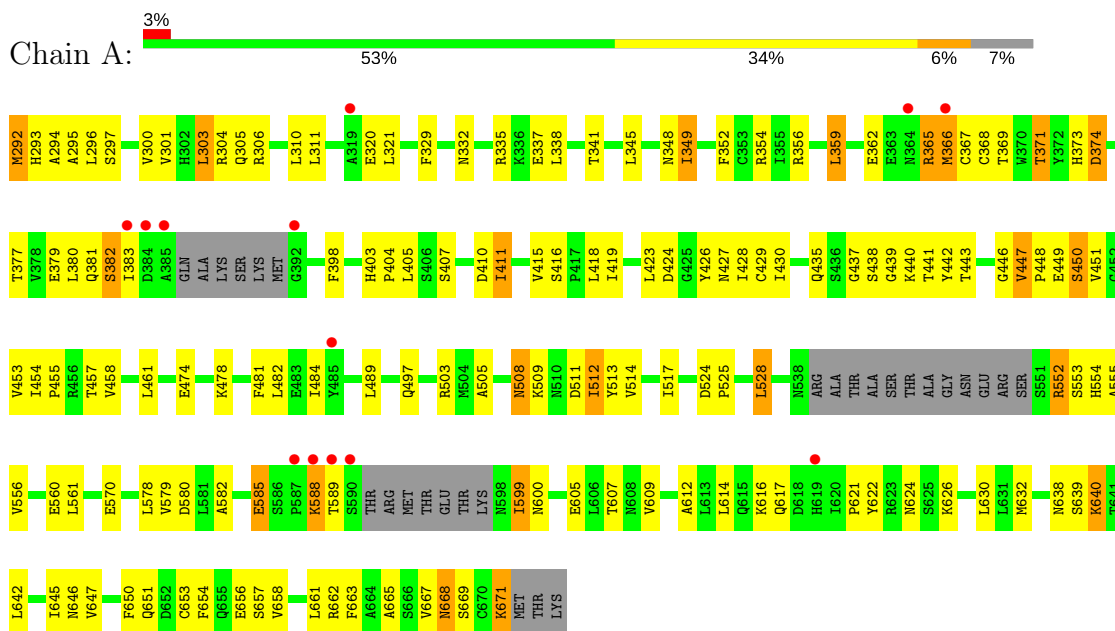
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total	O	0	0
			134	134		
4	B	109	Total	O	0	0
			109	109		

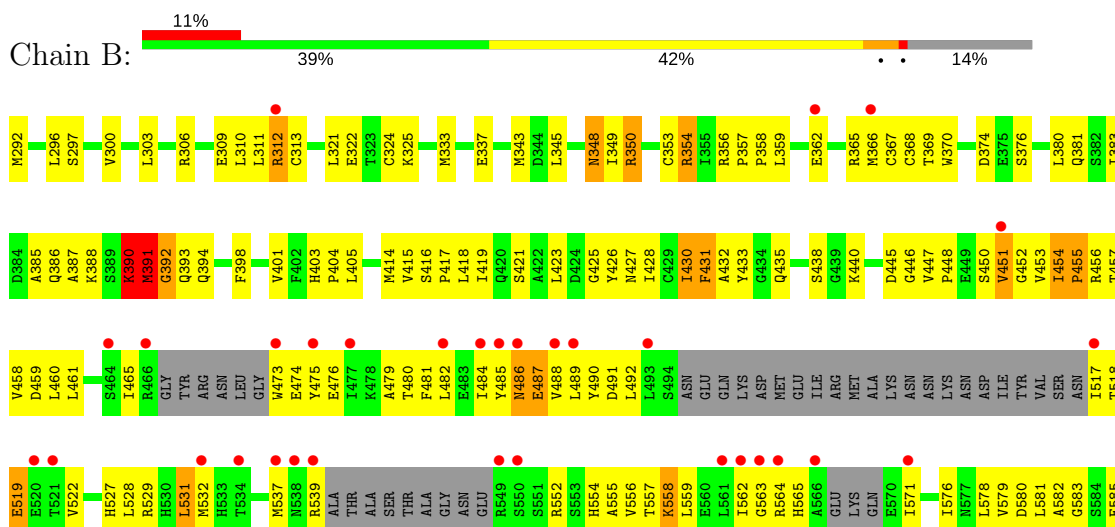
### 3 Residue-property plots

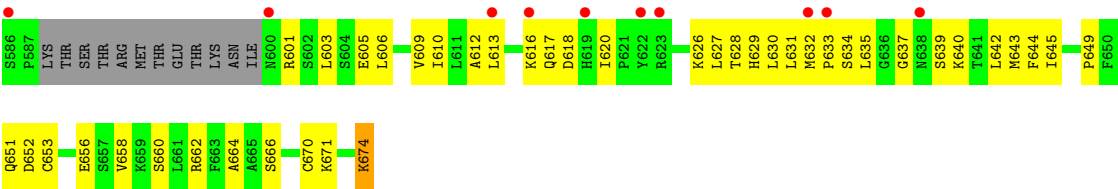
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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-14 Ncd



#### • Molecule 1: Kinesin-14 Ncd





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	162.01 Å   66.42 Å   93.57 Å 90.00°   98.20°   90.00°	Depositor
Resolution (Å)	19.34 – 2.75 19.34 – 2.75	Depositor EDS
% Data completeness (in resolution range)	86.2 (19.34-2.75) 86.4 (19.34-2.75)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.94 (at 2.75 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.238   ,   0.292 0.238   ,   0.293	Depositor DCC
$R_{free}$ test set	1535 reflections (6.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 60.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.54	5/2879 (0.2%)	0.74	4/3884 (0.1%)
1	B	0.61	7/2678 (0.3%)	0.72	8/3609 (0.2%)
All	All	0.57	12/5557 (0.2%)	0.73	12/7493 (0.2%)

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	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	455	PRO	C-N	-11.97	1.06	1.34
1	A	367	CYS	C-O	-10.60	1.03	1.23
1	B	391	MET	CA-C	-9.13	1.29	1.52
1	B	390	LYS	C-O	-7.80	1.08	1.23
1	A	367	CYS	CB-SG	-7.59	1.69	1.82
1	B	454	ILE	C-N	-7.21	1.20	1.34
1	A	292	MET	C-N	-6.48	1.19	1.34
1	B	390	LYS	CG-CD	-6.42	1.30	1.52
1	B	390	LYS	CB-CG	-6.17	1.35	1.52
1	A	367	CYS	C-N	-5.78	1.20	1.34
1	B	391	MET	C-O	-5.53	1.12	1.23
1	A	367	CYS	CA-C	-5.30	1.39	1.52

All (12) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	366	MET	N-CA-CB	-16.71	80.52	110.60
1	A	365	ARG	N-CA-C	-12.67	76.78	111.00
1	B	486	ASN	N-CA-C	-11.45	80.08	111.00
1	B	487	GLU	N-CA-CB	-10.06	92.49	110.60
1	B	391	MET	CB-CG-SD	-8.40	87.18	112.40
1	A	367	CYS	N-CA-CB	8.15	125.28	110.60
1	B	392	GLY	C-N-CA	6.82	138.74	121.70
1	B	618	ASP	CB-CA-C	-6.68	97.03	110.40
1	B	391	MET	CB-CA-C	-6.09	98.23	110.40
1	A	639	SER	CB-CA-C	-5.94	98.82	110.10
1	B	618	ASP	N-CA-C	5.72	126.44	111.00
1	B	348	ASN	CB-CA-C	-5.58	99.25	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	390	LYS	Peptide
1	B	391	MET	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2833	0	2790	146	1
1	B	2636	0	2607	152	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	5	0
3	B	27	0	12	1	0
4	A	134	0	0	5	0
4	B	109	0	0	6	1
All	All	5768	0	5421	291	2

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 27.

All (291) 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:A:362:GLU:HG2	1:A:365:ARG:HB2	1.26	1.11
1:A:362:GLU:CG	1:A:365:ARG:HB2	1.82	1.08
1:A:366:MET:HG2	1:A:651:GLN:HB3	1.34	1.03
1:B:454:ILE:HB	1:B:455:PRO:HD3	1.41	1.02
1:A:447:VAL:HG22	1:A:448:PRO:HD2	1.42	0.99
1:B:579:VAL:HG21	1:B:631:LEU:HD21	1.52	0.91
1:B:455:PRO:HG3	1:B:532:MET:CE	2.03	0.88
1:A:359:LEU:H	1:A:359:LEU:HD13	1.39	0.88
1:B:440:LYS:NZ	3:B:999:ADP:O1B	2.06	0.88
1:B:455:PRO:HG3	1:B:532:MET:HE1	1.57	0.86
1:A:654:PHE:O	1:A:658:VAL:HG23	1.75	0.86
1:A:304:ARG:NH1	1:B:303:LEU:HD11	1.90	0.86
1:A:366:MET:CG	1:A:651:GLN:HB3	2.07	0.83
1:A:356:ARG:HH12	1:A:359:LEU:HD12	1.43	0.83
1:B:376:SER:HB2	1:B:398:PHE:O	1.79	0.82
1:A:354:ARG:HH12	3:A:998:ADP:HN61	1.28	0.81
1:A:454:ILE:HB	1:A:455:PRO:HD3	1.62	0.81
1:A:554:HIS:HD2	1:A:582:ALA:H	1.27	0.81
1:B:386:GLN:O	1:B:390:LYS:HD2	1.85	0.76
1:B:446:GLY:HA3	1:B:451:VAL:O	1.87	0.74
1:B:454:ILE:HG23	1:B:578:LEU:HD13	1.70	0.73
1:B:485:TYR:C	1:B:486:ASN:O	2.11	0.73
1:B:366:MET:SD	1:B:383:ILE:HG13	2.28	0.72
1:A:304:ARG:HH11	1:B:303:LEU:HD11	1.53	0.72
1:A:447:VAL:HG13	1:A:449:GLU:H	1.53	0.72
1:B:387:ALA:O	1:B:390:LYS:O	2.07	0.72
1:B:454:ILE:CB	1:B:455:PRO:HD3	2.11	0.72
1:A:310:LEU:HD23	1:B:310:LEU:HB3	1.72	0.71
1:A:418:LEU:HB3	1:A:428:ILE:HG12	1.73	0.71
1:A:292:MET:N	4:A:679:HOH:O	2.23	0.70
1:B:454:ILE:O	1:B:457:THR:HB	1.91	0.70
1:B:555:ALA:HB3	1:B:580:ASP:HB3	1.74	0.70
1:B:391:MET:HG2	1:B:391:MET:O	1.91	0.70
1:A:484:ILE:HG12	1:A:489:LEU:HD23	1.75	0.69
1:A:354:ARG:HE	1:A:411:ILE:HG12	1.56	0.69
1:A:354:ARG:HH12	3:A:998:ADP:N6	1.90	0.69
1:A:362:GLU:HG3	1:A:365:ARG:HB2	1.72	0.69
1:A:301:VAL:O	1:A:305:GLN:HG3	1.93	0.68
1:B:613:LEU:HD11	1:B:635:LEU:HD12	1.76	0.68
1:A:435:GLN:HE22	1:A:653:CYS:HB3	1.57	0.68
1:A:622:TYR:CG	1:A:632:MET:HG3	2.27	0.68
1:B:367:CYS:O	1:B:383:ILE:HD11	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:MET:HG2	1:A:651:GLN:CB	2.18	0.67
1:A:403:HIS:HD2	1:A:405:LEU:HB2	1.59	0.66
1:A:366:MET:CG	1:A:651:GLN:CB	2.73	0.66
1:B:383:ILE:HG12	1:B:651:GLN:OE1	1.96	0.66
1:A:443:THR:O	1:A:453:VAL:HG23	1.96	0.66
1:B:610:ILE:HA	1:B:613:LEU:HD12	1.78	0.65
1:B:455:PRO:HG3	1:B:532:MET:HE3	1.77	0.65
1:A:585:GLU:HA	1:A:656:GLU:CD	2.18	0.64
1:A:614:LEU:HD11	1:A:667:VAL:HG13	1.79	0.64
1:A:369:THR:HB	1:A:381:GLN:HB2	1.80	0.64
1:A:663:PHE:O	1:A:667:VAL:HG23	1.98	0.63
1:B:357:PRO:HB3	1:B:404:PRO:HB2	1.80	0.63
1:A:403:HIS:CD2	1:A:405:LEU:HB2	2.34	0.63
1:B:558:LYS:HE2	1:B:630:LEU:HD11	1.81	0.63
1:A:303:LEU:HD23	1:B:303:LEU:HB2	1.80	0.62
1:A:461:LEU:HD21	1:A:561:LEU:HD21	1.81	0.61
1:B:419:ILE:HG23	1:B:576:ILE:HD13	1.82	0.61
1:B:645:ILE:HG13	1:B:664:ALA:HB1	1.82	0.61
1:B:674:LYS:HA	1:B:674:LYS:HE3	1.83	0.61
1:B:343:MET:SD	1:B:350:ARG:HG2	2.40	0.61
1:B:393:GLN:HE21	1:B:393:GLN:HA	1.66	0.61
1:B:385:ALA:HA	1:B:388:LYS:HD3	1.82	0.61
1:B:557:THR:HB	1:B:578:LEU:HB2	1.82	0.61
1:A:371:THR:HG23	1:A:379:GLU:HB3	1.83	0.60
1:A:442:TYR:O	1:A:446:GLY:HA2	2.00	0.60
1:A:366:MET:O	1:A:650:PHE:HD1	1.85	0.60
1:A:554:HIS:CD2	1:A:582:ALA:H	2.14	0.60
1:B:416:SER:HB3	1:B:417:PRO:HD3	1.83	0.59
1:B:423:LEU:HD11	1:B:461:LEU:HD12	1.84	0.59
1:B:465:ILE:HG23	1:B:475:TYR:HD2	1.68	0.59
1:B:563:GLY:O	1:B:571:ILE:HA	2.01	0.59
1:A:329:PHE:CZ	1:A:570:GLU:HG3	2.38	0.59
1:A:348:ASN:HB2	4:A:41:HOH:O	2.03	0.59
1:B:419:ILE:HD13	1:B:457:THR:HG23	1.84	0.59
1:A:671:LYS:H	1:A:671:LYS:HD2	1.67	0.59
1:A:555:ALA:HB3	1:A:580:ASP:HB3	1.85	0.58
1:B:643:MET:SD	1:B:645:ILE:HD11	2.43	0.58
1:B:292:MET:HE2	1:B:296:LEU:HG	1.84	0.58
1:B:306:ARG:HA	1:B:309:GLU:HG2	1.84	0.58
1:A:359:LEU:N	1:A:359:LEU:HD13	2.16	0.58
1:B:476:GLU:HB3	1:B:562:ILE:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:TRP:CG	1:B:565:HIS:HB2	2.39	0.58
1:B:306:ARG:O	1:B:310:LEU:HB2	2.04	0.57
1:A:403:HIS:HB2	1:A:404:PRO:CD	2.35	0.57
1:B:632:MET:N	1:B:633:PRO:HD2	2.19	0.57
1:B:312:ARG:HH21	1:B:313:CYS:HB2	1.70	0.57
1:B:430:ILE:HA	1:B:642:LEU:O	2.04	0.57
1:A:599:ILE:HD13	1:A:599:ILE:H	1.69	0.56
1:B:605:GLU:O	1:B:609:VAL:HG23	2.05	0.56
1:A:428:ILE:HD12	1:A:428:ILE:N	2.20	0.56
1:B:585:GLU:HA	1:B:656:GLU:OE2	2.06	0.56
1:A:352:PHE:HE2	1:A:642:LEU:HD22	1.71	0.55
1:A:304:ARG:HG3	1:A:304:ARG:HH11	1.71	0.55
1:B:418:LEU:O	1:B:428:ILE:HG12	2.06	0.55
1:A:524:ASP:HB2	1:A:525:PRO:HD2	1.87	0.55
1:B:473:TRP:HE1	1:B:563:GLY:C	2.10	0.55
1:A:505:ALA:CB	1:A:511:ASP:HB2	2.37	0.55
1:A:292:MET:CG	1:A:295:ALA:H	2.20	0.55
1:B:435:GLN:NE2	1:B:656:GLU:HG2	2.21	0.55
1:A:441:THR:HB	3:A:998:ADP:O2A	2.08	0.54
1:B:447:VAL:HG23	1:B:450:SER:H	1.72	0.54
1:B:482:LEU:HD12	1:B:489:LEU:HD22	1.90	0.54
1:B:579:VAL:CG2	1:B:631:LEU:HD21	2.32	0.54
1:A:292:MET:HG3	1:A:295:ALA:H	1.72	0.54
1:A:668:ASN:HD22	1:A:669:SER:N	2.06	0.54
1:B:451:VAL:HB	1:B:456:ARG:CZ	2.37	0.54
1:A:419:ILE:HD11	1:A:457:THR:HG23	1.90	0.54
1:B:393:GLN:NE2	1:B:393:GLN:HA	2.22	0.54
1:A:478:LYS:HB2	1:A:560:GLU:HB3	1.90	0.53
1:A:447:VAL:CG2	1:A:448:PRO:HD2	2.30	0.53
1:A:553:SER:O	1:A:582:ALA:HB2	2.08	0.53
1:B:415:VAL:HG13	1:B:642:LEU:HD23	1.91	0.53
1:B:354:ARG:HG3	1:B:354:ARG:HH11	1.74	0.53
1:A:605:GLU:O	1:A:609:VAL:HG23	2.09	0.53
1:A:451:VAL:HB	1:A:455:PRO:HB2	1.90	0.53
1:B:480:THR:HB	1:B:558:LYS:HB2	1.90	0.53
1:A:292:MET:HE3	1:A:294:ALA:H	1.74	0.53
1:A:356:ARG:NE	1:A:437:GLY:O	2.42	0.53
1:B:431:PHE:HB3	1:B:579:VAL:HB	1.92	0.52
1:A:552:ARG:O	1:A:599:ILE:HG21	2.09	0.52
1:B:492:LEU:HB3	1:B:518:THR:O	2.09	0.52
1:A:458:VAL:HG13	1:A:528:LEU:HD13	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:ILE:HG23	1:A:513:TYR:N	2.24	0.52
1:B:403:HIS:CD2	1:B:405:LEU:H	2.28	0.52
1:A:296:LEU:O	1:A:300:VAL:HG23	2.09	0.52
1:B:356:ARG:HG2	1:B:438:SER:O	2.09	0.52
1:B:564:ARG:HE	1:B:571:ILE:HD13	1.73	0.52
1:A:439:GLY:HA2	3:A:998:ADP:O1A	2.09	0.52
1:A:458:VAL:CG1	1:A:528:LEU:HD13	2.40	0.52
1:B:374:ASP:HB2	4:B:680:HOH:O	2.09	0.52
1:A:474:GLU:HA	1:A:474:GLU:OE2	2.10	0.52
1:B:403:HIS:HD2	1:B:405:LEU:HB2	1.75	0.52
1:B:645:ILE:HG13	1:B:664:ALA:CB	2.39	0.51
1:A:665:ALA:O	1:A:669:SER:HB3	2.09	0.51
1:A:293:HIS:O	1:A:297:SER:HB2	2.11	0.51
1:B:391:MET:CG	1:B:392:GLY:N	2.65	0.51
1:A:671:LYS:N	1:A:671:LYS:HD2	2.25	0.51
1:B:428:ILE:N	1:B:428:ILE:HD12	2.26	0.51
1:A:382:SER:HA	1:A:651:GLN:OE1	2.10	0.51
1:A:356:ARG:NH1	1:A:359:LEU:HD12	2.20	0.51
1:A:435:GLN:NE2	1:A:653:CYS:HB3	2.26	0.51
1:A:622:TYR:CD1	1:A:632:MET:HG3	2.47	0.50
1:A:552:ARG:HD3	1:A:552:ARG:N	2.26	0.50
1:A:599:ILE:N	1:A:599:ILE:HD13	2.27	0.50
1:B:479:ALA:HA	1:B:559:LEU:HD23	1.93	0.50
1:A:349:ILE:O	1:A:349:ILE:HG23	2.11	0.50
1:B:306:ARG:HG2	4:B:692:HOH:O	2.12	0.50
1:B:383:ILE:N	1:B:651:GLN:OE1	2.42	0.50
1:A:366:MET:SD	1:A:383:ILE:HD12	2.52	0.50
1:B:484:ILE:HG12	1:B:489:LEU:HD23	1.93	0.50
1:B:554:HIS:CD2	1:B:627:LEU:HD22	2.46	0.50
1:B:556:VAL:HG11	1:B:630:LEU:CD2	2.42	0.49
1:B:632:MET:C	1:B:634:SER:H	2.16	0.49
1:A:647:VAL:HG21	1:A:661:LEU:HD21	1.95	0.49
1:B:353:CYS:HB3	1:B:401:VAL:HG22	1.93	0.49
1:A:332:ASN:OD1	1:A:335:ARG:NH1	2.46	0.49
1:B:658:VAL:O	1:B:662:ARG:HB2	2.11	0.49
1:A:621:PRO:HB2	1:A:624:ASN:CG	2.33	0.49
1:A:426:TYR:CE1	1:A:638:ASN:HB3	2.47	0.49
1:B:475:TYR:HA	1:B:562:ILE:O	2.12	0.49
1:B:653:CYS:HA	4:B:28:HOH:O	2.12	0.48
1:B:348:ASN:HA	1:B:670:CYS:O	2.12	0.48
1:B:451:VAL:HB	1:B:456:ARG:NE	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:LEU:N	1:B:482:LEU:HD23	2.28	0.48
1:B:612:ALA:HB3	1:B:620:ILE:HG23	1.95	0.48
1:B:354:ARG:HG3	1:B:354:ARG:NH1	2.28	0.48
1:B:556:VAL:HG11	1:B:630:LEU:HD21	1.96	0.48
1:B:556:VAL:HG12	1:B:557:THR:N	2.28	0.48
1:A:359:LEU:HD23	1:A:362:GLU:HB3	1.95	0.48
1:A:482:LEU:HD21	1:A:630:LEU:HD21	1.95	0.48
1:B:585:GLU:HA	1:B:656:GLU:CD	2.34	0.48
1:A:348:ASN:O	1:A:640:LYS:HA	2.13	0.48
1:B:473:TRP:HE1	1:B:564:ARG:N	2.10	0.48
1:A:514:VAL:HG12	1:A:517:ILE:HB	1.96	0.47
1:B:365:ARG:HH21	1:B:652:ASP:CG	2.18	0.47
1:A:337:GLU:HG2	4:A:722:HOH:O	2.13	0.47
1:B:487:GLU:OE2	1:B:626:LYS:HB2	2.14	0.47
1:A:447:VAL:HG13	1:A:449:GLU:N	2.27	0.47
1:B:296:LEU:O	1:B:300:VAL:HG23	2.15	0.47
1:B:612:ALA:CB	1:B:620:ILE:HG23	2.45	0.47
1:B:432:ALA:O	1:B:440:LYS:HD2	2.15	0.46
1:A:329:PHE:HZ	1:A:570:GLU:HG3	1.79	0.46
1:B:643:MET:HG2	1:B:644:PHE:N	2.30	0.46
1:A:306:ARG:O	1:A:310:LEU:HB2	2.15	0.46
1:A:481:PHE:N	1:A:481:PHE:CD1	2.82	0.46
1:A:553:SER:C	1:A:582:ALA:HB2	2.36	0.46
1:B:421:SER:O	1:B:426:TYR:HB2	2.15	0.46
1:B:481:PHE:HE2	1:B:532:MET:HG3	1.80	0.46
1:A:426:TYR:HE1	1:A:638:ASN:HB3	1.80	0.46
1:B:403:HIS:HD2	1:B:405:LEU:H	1.63	0.46
1:A:508:ASN:HD22	1:A:509:LYS:N	2.14	0.46
1:B:430:ILE:HG23	1:B:578:LEU:HD23	1.98	0.46
1:A:374:ASP:OD1	1:A:377:THR:N	2.46	0.46
1:B:431:PHE:HA	1:B:579:VAL:O	2.16	0.46
1:B:482:LEU:HD11	1:B:630:LEU:HD22	1.97	0.46
1:A:356:ARG:HH12	1:A:359:LEU:CD1	2.23	0.46
1:A:419:ILE:CG1	1:A:457:THR:HG23	2.46	0.46
1:B:423:LEU:C	1:B:425:GLY:H	2.19	0.45
1:B:380:LEU:HD23	1:B:380:LEU:H	1.80	0.45
1:A:668:ASN:N	1:A:668:ASN:HD22	2.13	0.45
1:B:393:GLN:NE2	4:B:43:HOH:O	2.49	0.45
1:B:492:LEU:HD23	1:B:519:GLU:HA	1.99	0.45
1:B:527:HIS:O	1:B:531:LEU:HB2	2.15	0.45
1:B:473:TRP:HE1	1:B:563:GLY:CA	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ILE:HG23	1:B:578:LEU:CD1	2.43	0.45
1:A:335:ARG:NH2	1:A:424:ASP:OD2	2.49	0.45
1:A:503:ARG:HH11	1:A:503:ARG:HG2	1.82	0.45
1:B:390:LYS:HE3	4:B:690:HOH:O	2.17	0.45
1:B:447:VAL:HB	1:B:448:PRO:HD2	1.99	0.45
1:B:447:VAL:O	1:B:450:SER:O	2.35	0.45
1:A:621:PRO:HB2	1:A:624:ASN:OD1	2.17	0.44
1:A:607:THR:HB	1:A:663:PHE:CE1	2.52	0.44
1:A:612:ALA:HA	1:A:617:GLN:NE2	2.31	0.44
1:A:512:ILE:HD12	1:A:512:ILE:HA	1.83	0.44
1:B:356:ARG:HH21	1:B:358:PRO:HA	1.83	0.44
1:A:362:GLU:HG3	1:A:365:ARG:CB	2.44	0.44
1:B:451:VAL:HG12	1:B:452:GLY:N	2.34	0.43
1:B:583:GLY:H	1:B:603:LEU:HD11	1.83	0.43
1:A:292:MET:HG3	1:A:294:ALA:N	2.34	0.43
1:A:359:LEU:CD2	1:A:362:GLU:HB3	2.47	0.43
1:B:380:LEU:CD2	1:B:394:GLN:HB3	2.49	0.43
1:B:445:ASP:OD2	1:B:454:ILE:HD12	2.19	0.43
1:A:303:LEU:HD23	1:B:303:LEU:CB	2.49	0.43
1:B:539:ARG:HH12	1:B:555:ALA:CB	2.31	0.43
1:A:366:MET:HG2	4:A:725:HOH:O	2.19	0.43
1:A:380:LEU:H	1:A:380:LEU:HD23	1.82	0.43
1:A:349:ILE:HD13	1:A:349:ILE:C	2.39	0.43
1:A:556:VAL:HG22	1:A:579:VAL:HG13	2.01	0.43
1:B:431:PHE:HE2	1:B:643:MET:HE3	1.83	0.43
1:B:370:TRP:CZ2	1:B:649:PRO:HA	2.54	0.43
1:A:668:ASN:N	1:A:668:ASN:ND2	2.67	0.43
1:A:304:ARG:HH12	1:B:303:LEU:HD11	1.79	0.43
1:A:320:GLU:HG2	1:B:321:LEU:HD21	2.01	0.42
1:A:407:SER:O	1:A:410:ASP:HB2	2.19	0.42
1:A:454:ILE:HB	1:A:455:PRO:CD	2.40	0.42
1:A:438:SER:OG	1:A:646:ASN:HB2	2.19	0.42
1:A:368:CYS:HB2	1:A:381:GLN:O	2.19	0.42
1:A:588:LYS:HB3	1:A:589:THR:H	1.59	0.42
1:B:419:ILE:HB	1:B:460:LEU:HD23	2.02	0.42
1:B:488:VAL:HG22	1:B:489:LEU:N	2.34	0.42
1:B:643:MET:SD	1:B:645:ILE:CD1	3.07	0.42
1:B:321:LEU:O	1:B:325:LYS:HG2	2.19	0.42
1:A:447:VAL:HG12	1:A:450:SER:H	1.84	0.42
1:A:585:GLU:HA	1:A:656:GLU:OE1	2.20	0.42
1:A:398:PHE:HE2	1:A:645:ILE:HD12	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:MET:O	1:B:337:GLU:HG3	2.19	0.42
1:B:380:LEU:HD21	1:B:394:GLN:HB3	2.01	0.42
1:B:606:LEU:O	1:B:609:VAL:HB	2.19	0.42
1:A:657:SER:O	1:A:661:LEU:HG	2.19	0.42
1:B:451:VAL:HB	1:B:456:ARG:NH2	2.35	0.42
1:A:423:LEU:CD2	1:A:561:LEU:HD13	2.50	0.42
1:B:322:GLU:HB3	4:B:274:HOH:O	2.18	0.42
1:B:481:PHE:CE2	1:B:532:MET:HG3	2.55	0.42
1:B:558:LYS:NZ	1:B:558:LYS:HB3	2.35	0.42
1:B:473:TRP:CD1	1:B:565:HIS:HB2	2.55	0.42
1:B:609:VAL:HG21	1:B:628:THR:CG2	2.50	0.41
1:A:658:VAL:O	1:A:662:ARG:HB2	2.19	0.41
1:B:529:ARG:O	1:B:529:ARG:HD3	2.20	0.41
1:B:433:TYR:HA	1:B:581:LEU:HD12	2.02	0.41
1:A:380:LEU:N	1:A:380:LEU:HD23	2.35	0.41
1:A:423:LEU:HD23	1:A:561:LEU:HD13	2.02	0.41
1:A:440:LYS:HB2	3:A:998:ADP:O3B	2.20	0.41
1:B:474:GLU:HB2	1:B:564:ARG:HB2	2.01	0.41
1:A:428:ILE:CG2	1:A:429:CYS:N	2.84	0.41
1:A:430:ILE:HD12	1:A:642:LEU:HD12	2.03	0.41
1:B:368:CYS:HB2	1:B:381:GLN:O	2.20	0.41
1:B:490:TYR:HB3	1:B:491:ASP:H	1.57	0.41
1:A:304:ARG:CG	1:A:304:ARG:HH11	2.31	0.41
1:B:517:ILE:HG22	1:B:518:THR:N	2.36	0.41
1:A:403:HIS:HB2	1:A:404:PRO:HD2	2.03	0.41
1:B:458:VAL:HG23	1:B:459:ASP:N	2.35	0.41
1:A:362:GLU:CG	1:A:365:ARG:CB	2.75	0.41
1:A:427:ASN:C	1:A:428:ILE:HD12	2.41	0.41
1:A:668:ASN:H	1:A:668:ASN:ND2	2.18	0.41
1:B:522:VAL:HG13	1:B:528:LEU:HB2	2.01	0.41
1:B:454:ILE:HG12	1:B:578:LEU:HD13	2.01	0.41
1:B:552:ARG:HA	1:B:582:ALA:HB1	2.02	0.41
1:A:341:THR:O	1:A:345:LEU:HD13	2.21	0.41
1:A:366:MET:O	1:A:650:PHE:CD1	2.71	0.41
1:B:640:LYS:NZ	1:B:674:LYS:HD3	2.36	0.41
1:A:614:LEU:C	1:A:616:LYS:H	2.24	0.40
1:B:380:LEU:HD23	1:B:380:LEU:N	2.36	0.40
1:A:665:ALA:HA	1:A:668:ASN:HD21	1.86	0.40
1:B:362:GLU:H	1:B:362:GLU:HG2	1.67	0.40
1:A:359:LEU:HA	4:A:689:HOH:O	2.20	0.40
1:A:448:PRO:HG2	1:A:449:GLU:OE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:VAL:O	1:B:454:ILE:C	2.60	0.40
1:A:415:VAL:O	1:A:418:LEU:N	2.54	0.40
1:B:391:MET:HG3	1:B:392:GLY:N	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2:HOH:O	4:B:706:HOH:O[4_447]	2.17	0.03
1:A:373:HIS:O	1:A:373:HIS:O[2_556]	2.18	0.02

## 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	347/383 (91%)	320 (92%)	26 (8%)	1 (0%)	43	65
1	B	319/383 (83%)	266 (83%)	51 (16%)	2 (1%)	27	47
All	All	666/766 (87%)	586 (88%)	77 (12%)	3 (0%)	31	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	451	VAL
1	A	585	GLU
1	B	637	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	324/347 (93%)	298 (92%)	26 (8%)	13	24
1	B	302/347 (87%)	274 (91%)	28 (9%)	10	18
All	All	626/694 (90%)	572 (91%)	54 (9%)	11	21

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	LEU
1	A	311	LEU
1	A	321	LEU
1	A	338	LEU
1	A	349	ILE
1	A	359	LEU
1	A	371	THR
1	A	374	ASP
1	A	382	SER
1	A	411	ILE
1	A	416	SER
1	A	447	VAL
1	A	450	SER
1	A	497	GLN
1	A	508	ASN
1	A	512	ILE
1	A	528	LEU
1	A	552	ARG
1	A	578	LEU
1	A	588	LYS
1	A	599	ILE
1	A	600	ASN
1	A	626	LYS
1	A	640	LYS
1	A	668	ASN
1	A	671	LYS
1	B	297	SER
1	B	311	LEU
1	B	312	ARG
1	B	324	CYS
1	B	345	LEU
1	B	349	ILE
1	B	350	ARG

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Mol	Chain	Res	Type
1	B	354	ARG
1	B	359	LEU
1	B	369	THR
1	B	391	MET
1	B	414	MET
1	B	427	ASN
1	B	430	ILE
1	B	431	PHE
1	B	519	GLU
1	B	531	LEU
1	B	537	MET
1	B	558	LYS
1	B	601	ARG
1	B	616	LYS
1	B	617	GLN
1	B	629	HIS
1	B	639	SER
1	B	660	SER
1	B	666	SER
1	B	671	LYS
1	B	674	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	GLN
1	A	420	GLN
1	A	435	GLN
1	A	497	GLN
1	A	508	ASN
1	A	510	ASN
1	A	516	ASN
1	A	554	HIS
1	A	600	ASN
1	A	608	ASN
1	A	617	GLN
1	A	624	ASN
1	A	629	HIS
1	A	668	ASN
1	B	305	GLN
1	B	317	GLN
1	B	327	GLN

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Mol	Chain	Res	Type
1	B	348	ASN
1	B	393	GLN
1	B	403	HIS
1	B	486	ASN
1	B	600	ASN
1	B	655	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

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	A	998	2	25,29,29	1.26	4 (16%)	25,45,45	2.53	2 (8%)
3	ADP	B	999	2	25,29,29	1.07	2 (8%)	25,45,45	2.73	7 (28%)

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	ADP	PB-O3A	-2.31	1.56	1.60
3	A	998	ADP	C5-N7	-2.12	1.32	1.39
3	A	998	ADP	PA-O2A	-2.05	1.45	1.55
3	B	999	ADP	C2-N3	2.22	1.35	1.32
3	A	998	ADP	PB-O2B	2.23	1.63	1.54
3	B	999	ADP	PB-O3A	2.57	1.64	1.60

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	998	ADP	N3-C2-N1	-11.94	118.64	128.86
3	B	999	ADP	N3-C2-N1	-9.10	121.08	128.86
3	B	999	ADP	PA-O3A-PB	-5.42	114.42	132.63
3	B	999	ADP	O3'-C3'-C4'	-3.11	102.04	111.06
3	A	998	ADP	C4-C5-N7	-2.36	107.13	109.41
3	B	999	ADP	N6-C6-N1	2.14	123.00	118.57
3	B	999	ADP	O4'-C4'-C5'	2.26	116.90	109.39
3	B	999	ADP	O3B-PB-O2B	2.71	118.33	107.59
3	B	999	ADP	C4'-O4'-C1'	4.79	114.83	109.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	998	ADP	5	0
3	B	999	ADP	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	292:MET	C	293:HIS	N	1.19
1	B	455:PRO	C	456:ARG	N	1.06

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	355/383 (92%)	-0.14	13 (3%) 41 36	21, 46, 96, 135	0
1	B	331/383 (86%)	0.52	42 (12%) 3 2	23, 76, 162, 174	0
All	All	686/766 (89%)	0.18	55 (8%) 12 9	21, 55, 142, 174	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	385	ALA	5.7
1	B	538	ASN	5.7
1	A	384	ASP	5.3
1	B	466	ARG	4.9
1	B	549	ARG	4.7
1	A	587	PRO	4.7
1	B	566	ALA	4.5
1	B	486	ASN	4.1
1	B	484	ILE	4.0
1	A	589	THR	3.8
1	B	475	TYR	3.7
1	B	493	LEU	3.7
1	B	550	SER	3.7
1	A	366	MET	3.5
1	B	623	ARG	3.5
1	B	571	ILE	3.2
1	B	586	SER	3.2
1	B	619	HIS	3.1
1	A	590	SER	3.1
1	B	464	SER	3.0
1	B	563	GLY	3.0
1	B	517	ILE	2.9
1	B	534	THR	2.8
1	A	319	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	619	HIS	2.7
1	B	600	ASN	2.6
1	B	632	MET	2.6
1	B	520	GLU	2.6
1	B	488	VAL	2.5
1	B	638	ASN	2.5
1	A	485	TYR	2.5
1	B	366	MET	2.5
1	A	364	ASN	2.4
1	B	451	VAL	2.4
1	B	564	ARG	2.4
1	A	588	LYS	2.4
1	B	473	TRP	2.4
1	A	383	ILE	2.3
1	B	482	LEU	2.3
1	B	633	PRO	2.3
1	B	537	MET	2.3
1	B	561	LEU	2.3
1	B	562	ILE	2.2
1	B	613	LEU	2.2
1	B	477	ILE	2.2
1	B	485	TYR	2.2
1	B	521	THR	2.2
1	B	312	ARG	2.1
1	A	392	GLY	2.1
1	B	532	MET	2.1
1	B	539	ARG	2.1
1	B	362	GLU	2.1
1	B	489	LEU	2.0
1	B	622	TYR	2.0
1	B	616	LYS	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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	B	997	1/1	0.94	0.27	49,49,49,49	0
2	MG	A	996	1/1	0.97	0.15	35,35,35,35	0
3	ADP	A	998	27/27	0.97	0.16	48,56,58,59	0
3	ADP	B	999	27/27	0.97	0.11	45,55,61,63	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.