



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:30 AM UTC

PDB ID : 3L1C / pdb_00003l1c
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

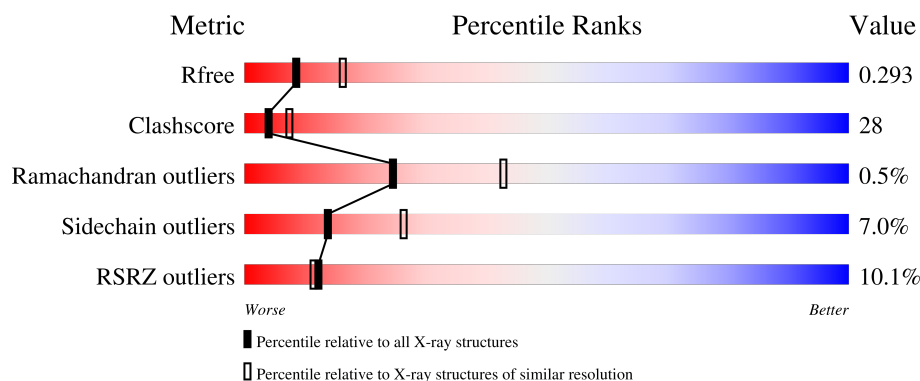
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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

Mol	Chain	Length	Quality of chain
1	A	383	
1	B	383	

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 Protein claret segregational.

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 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	MET	-	initiating methionine	UNP P20480
A	436	SER	THR	engineered mutation	UNP P20480
B	292	MET	-	initiating methionine	UNP P20480
B	436	SER	THR	engineered mutation	UNP P20480

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

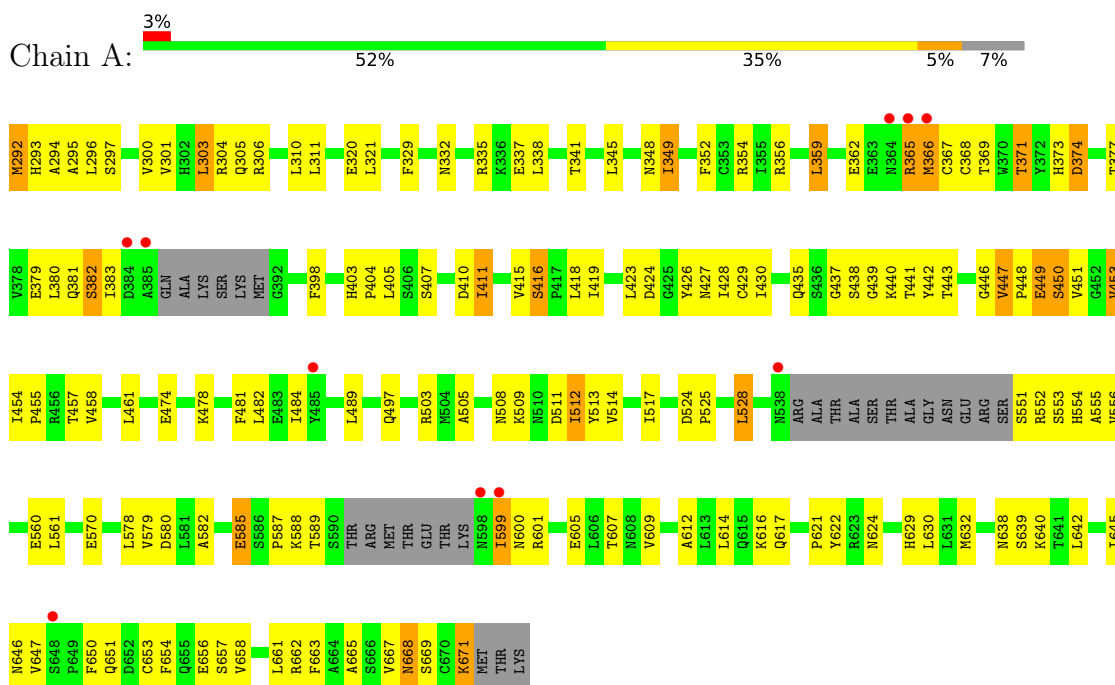
- Molecule 4 is water.

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

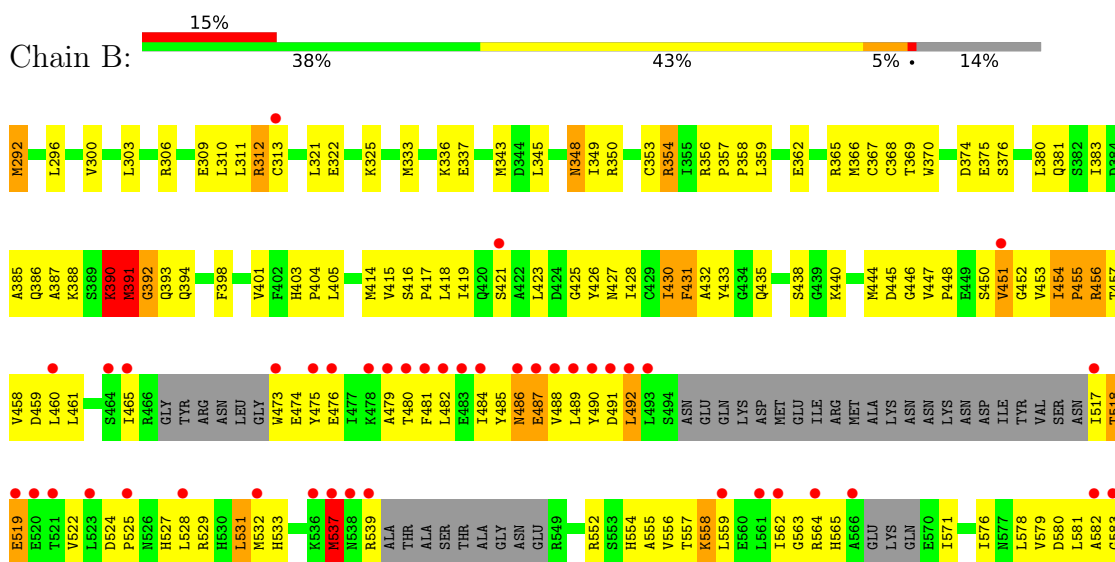
3 Residue-property plots

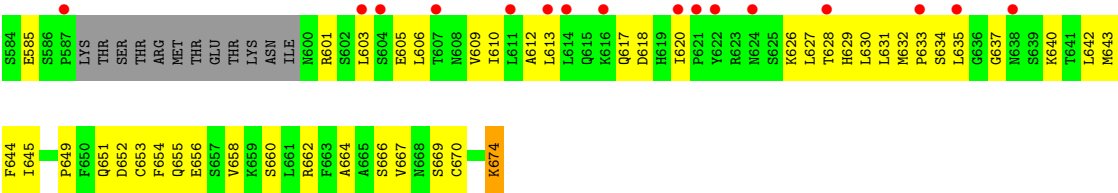
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Protein claret segregational



• Molecule 1: Protein claret segregational





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	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) 86.1 (19.34-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	47.7	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5768	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.74	5/2879 (0.2%)	1.05	10/3884 (0.3%)
1	B	0.86	11/2678 (0.4%)	1.10	20/3609 (0.6%)
All	All	0.80	16/5557 (0.3%)	1.07	30/7493 (0.4%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	MET	CA-C	-18.64	1.29	1.52
1	B	455	PRO	C-N	-17.55	1.06	1.33
1	A	367	CYS	C-O	-15.93	1.03	1.23
1	B	390	LYS	C-O	-12.48	1.08	1.23
1	A	292	MET	C-N	-11.29	1.19	1.33
1	A	367	CYS	CA-C	-11.27	1.39	1.52
1	B	454	ILE	C-N	-10.98	1.20	1.34
1	B	391	MET	C-O	-9.20	1.12	1.23
1	A	367	CYS	C-N	-8.72	1.20	1.33
1	B	390	LYS	CG-CD	-7.27	1.30	1.52
1	B	390	LYS	CA-C	-6.87	1.43	1.52
1	A	367	CYS	N-CA	-5.99	1.38	1.45
1	B	392	GLY	C-O	-5.74	1.16	1.23
1	B	390	LYS	CB-CG	-5.52	1.35	1.52
1	B	292	MET	C-N	5.35	1.40	1.33
1	B	392	GLY	CA-C	-5.26	1.44	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	N-CA-C	-20.93	76.78	109.23
1	A	366	MET	N-CA-CB	-19.58	80.52	110.29
1	B	486	ASN	N-CA-C	-19.05	80.08	109.79
1	B	618	ASP	N-CA-C	13.89	126.44	111.03
1	B	392	GLY	CA-C-N	10.72	138.74	122.23
1	B	392	GLY	C-N-CA	10.72	138.74	122.23
1	B	487	GLU	N-CA-CB	-9.58	92.49	109.93
1	B	456	ARG	N-CA-C	-9.39	101.59	113.23
1	B	618	ASP	CB-CA-C	-8.98	97.03	110.95
1	B	454	ILE	CA-C-N	8.55	128.28	119.64
1	B	454	ILE	C-N-CA	8.55	128.28	119.64
1	B	391	MET	CB-CG-SD	-8.51	87.18	112.70
1	A	366	MET	N-CA-C	8.30	122.77	110.48
1	A	367	CYS	N-CA-CB	8.30	125.28	111.08
1	B	454	ILE	O-C-N	-8.27	111.67	121.10
1	A	639	SER	N-CA-C	8.19	121.78	110.24
1	B	348	ASN	CB-CA-C	-7.53	99.25	109.71
1	B	391	MET	CB-CA-C	-7.20	98.23	109.61
1	B	487	GLU	N-CA-C	6.98	122.70	113.20
1	B	375	GLU	N-CA-C	6.87	121.11	112.87
1	A	639	SER	CB-CA-C	-6.76	98.82	109.70
1	B	390	LYS	CA-C-N	6.59	131.12	121.31
1	B	390	LYS	C-N-CA	6.59	131.12	121.31
1	B	518	THR	N-CA-C	5.93	123.44	110.80
1	A	453	VAL	N-CA-C	5.57	116.03	110.23
1	B	390	LYS	N-CA-CB	-5.51	101.73	110.06
1	A	367	CYS	N-CA-C	-5.46	100.98	109.72
1	A	587	PRO	CB-CA-C	-5.27	103.28	111.40
1	B	537	MET	N-CA-C	-5.27	102.19	110.36
1	A	367	CYS	O-C-N	-5.02	116.66	123.19

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	152	1
1	B	2636	0	2608	162	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	5422	307	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 28.

All (307) 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:455:PRO:HG3	1:B:532:MET:HE1	1.15	1.13
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:A:359:LEU:HD13	1:A:359:LEU:H	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:CE	2.03	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:455:PRO:CG	1:B:532:MET:HE1	2.07	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:TYR:C	1:B:486:ASN:O	2.11	0.77
1:B:431:PHE:HE2	1:B:643:MET:HE3	1.50	0.77
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: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:A:585:GLU:HA	1:A:656:GLU:CD	2.18	0.69
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:B:292:MET:HE2	1:B:296:LEU:HG	1.73	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:B:431:PHE:CE2	1:B:643:MET:HE3	2.28	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
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: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:B:391:MET:O	1:B:391:MET:HG2	1.91	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:TYR:HB2	1:A:632:MET:HE2	1.82	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:HE3	1:B:674:LYS:HA	1.83	0.61
1:B:343:MET:SD	1:B:350:ARG:HG2	2.40	0.61
1:B:393:GLN:HA	1:B:393:GLN:HE21	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:336:LYS:HG2	1:B:414:MET:HE1	1.83	0.60
1:B:473:TRP:HE1	1:B:563:GLY:C	2.10	0.59
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:306:ARG:HA	1:B:309:GLU:HG2	1.84	0.58
1:A:359:LEU:HD13	1:A:359:LEU:N	2.16	0.58
1:B:476:GLU:HB3	1:B:562:ILE:HB	1.84	0.58
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:HD11	1:B:444:MET:HE1	1.87	0.57
1:B:430:ILE:HA	1:B:642:LEU:O	2.04	0.57
1:B:444:MET:HE2	1:B:444:MET:HA	1.85	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:N	1:A:428:ILE:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:HH11	1:A:304:ARG:HG3	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: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:B:632:MET:C	1:B:634:SER:H	2.16	0.54
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:A:621:PRO:HB2	1:A:624:ASN:CG	2.33	0.54
1:B:393:GLN:HA	1:B:393:GLN:NE2	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:292:MET:HE3	1:B:292:MET:HA	1.90	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:356:ARG:NE	1:A:437:GLY:O	2.42	0.53
1:B:585:GLU:HA	1:B:656:GLU:CD	2.34	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
1:A:512:ILE:HG23	1:A:513:TYR:N	2.24	0.52
1:B:365:ARG:HH21	1:B:652:ASP:CG	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:GLU:OE2	1:A:474:GLU:HA	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:A:553:SER:C	1:A:582:ALA:HB2	2.36	0.51
1:A:671:LYS:HD2	1:A:671:LYS:N	2.25	0.51
1:B:428:ILE:HD12	1:B:428:ILE:N	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:HD13	1:A:599:ILE:N	2.27	0.50
1:B:479:ALA:HA	1:B:559:LEU:HD23	1.93	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:349:ILE:HG23	1:A:349:ILE:O	2.11	0.50
1:A:366:MET:SD	1:A:383:ILE:HD12	2.52	0.50
1:B:423:LEU:C	1:B:425:GLY:H	2.19	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ILE:HD13	1:A:349:ILE:C	2.39	0.47
1:A:514:VAL:HG12	1:A:517:ILE:HB	1.96	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:292:MET:HE2	1:A:294:ALA:H	1.79	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: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:A:427:ASN:C	1:A:428:ILE:HD12	2.41	0.46
1:B:380:LEU:HD23	1:B:380:LEU:H	1.80	0.45
1:A:614:LEU:C	1:A:616:LYS:H	2.24	0.45
1:A:668:ASN:HD22	1:A:668:ASN:N	2.13	0.45
1:A:629:HIS:HD2	1:A:632:MET:HE3	1.81	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:473:TRP:HE1	1:B:563:GLY:CA	2.30	0.45
1:B:527:HIS:O	1:B:531:LEU:HB2	2.15	0.45
1:B:453:VAL:O	1:B:454:ILE:C	2.60	0.45
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:HG2	1:A:503:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:SER:C	1:A:552:ARG:HD3	2.42	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:533:HIS:HE1	1:B:537:MET:HE1	1.84	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:556:VAL:HG22	1:A:579:VAL:HG13	2.01	0.43
1:B:370:TRP:CZ2	1:B:649:PRO:HA	2.54	0.43
1:A:304:ARG:HH12	1:B:303:LEU:HD11	1.79	0.43
1:A:668:ASN:N	1:A:668:ASN:ND2	2.67	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:438:SER:OG	1:A:646:ASN:HB2	2.19	0.42
1:A:454:ILE:HB	1:A:455:PRO:CD	2.40	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: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:398:PHE:HE2	1:A:645:ILE:HD12	1.85	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: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:292:MET:HE2	1:B:296:LEU:CG	2.45	0.42
1:B:322:GLU:HB3	4:B:274:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:TRP:CD1	1:B:565:HIS:HB2	2.55	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: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:433:TYR:HA	1:B:581:LEU:HD12	2.02	0.41
1:B:529:ARG:O	1:B:529:ARG:HD3	2.20	0.41
1:A:380:LEU:HD23	1:A:380:LEU:N	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:A:599:ILE:C	1:A:601:ARG:H	2.28	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:B:654:PHE:O	1:B:655:GLN:C	2.61	0.41
1:A:304:ARG:HH11	1:A:304:ARG:CG	2.31	0.41
1:B:488:VAL:HG22	1:B:489:LEU:N	2.34	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:A:438:SER:HB2	1:A:646:ASN:C	2.46	0.41
1:B:524:ASP:CG	1:B:525:PRO:HD2	2.46	0.41
1:B:667:VAL:C	1:B:669:SER:H	2.29	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:668:ASN:ND2	1:A:668:ASN:H	2.18	0.41
1:B:522:VAL:HG13	1:B:528:LEU:HB2	2.01	0.41
1:A:415:VAL:O	1:A:416:SER:C	2.64	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: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
1:B:416:SER:O	1:B:417:PRO:C	2.65	0.40
1:A:415:VAL:O	1:A:418:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	56
1	B	319/383 (83%)	266 (83%)	51 (16%)	2 (1%)	21	38
All	All	666/766 (87%)	586 (88%)	77 (12%)	3 (0%)	24	43

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%)	302 (93%)	22 (7%)	14	27
1	B	302/347 (87%)	280 (93%)	22 (7%)	13	24
All	All	626/694 (90%)	582 (93%)	44 (7%)	14	26

All (44) 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	449	GLU
1	A	450	SER
1	A	497	GLN
1	A	512	ILE
1	A	528	LEU
1	A	578	LEU
1	A	599	ILE
1	A	600	ASN
1	A	668	ASN
1	A	671	LYS
1	B	311	LEU
1	B	312	ARG
1	B	345	LEU
1	B	349	ILE
1	B	354	ARG
1	B	359	LEU
1	B	369	THR
1	B	391	MET
1	B	427	ASN
1	B	430	ILE
1	B	431	PHE
1	B	492	LEU

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Mol	Chain	Res	Type
1	B	519	GLU
1	B	531	LEU
1	B	537	MET
1	B	558	LYS
1	B	601	ARG
1	B	617	GLN
1	B	629	HIS
1	B	660	SER
1	B	666	SER
1	B	674	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	293	HIS
1	A	317	GLN
1	A	348	ASN
1	A	420	GLN
1	A	435	GLN
1	A	486	ASN
1	A	497	GLN
1	A	508	ASN
1	A	510	ASN
1	A	516	ASN
1	A	530	HIS
1	A	538	ASN
1	A	554	HIS
1	A	600	ASN
1	A	608	ASN
1	A	615	GLN
1	A	617	GLN
1	A	624	ASN
1	A	668	ASN
1	B	305	GLN
1	B	314	ASN
1	B	317	GLN
1	B	327	GLN
1	B	348	ASN
1	B	373	HIS
1	B	393	GLN
1	B	403	HIS
1	B	538	ASN

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Mol	Chain	Res	Type
1	B	600	ASN
1	B	655	GLN
1	B	668	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 oligosaccharides 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	28,29,29	1.31	4 (14%)	43,45,45	2.47	17 (39%)
3	ADP	A	998	2	28,29,29	1.42	5 (17%)	43,45,45	1.96	7 (16%)

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	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	998	2	-	4/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	998	ADP	C5-N7	-3.76	1.32	1.39
3	B	999	ADP	C5-C4	3.20	1.44	1.39
3	B	999	ADP	C5-N7	-2.95	1.33	1.39
3	B	999	ADP	C5-C6	2.54	1.48	1.41
3	A	998	ADP	PB-O2B	2.43	1.63	1.54
3	A	998	ADP	C4-N9	-2.33	1.32	1.37
3	A	998	ADP	PA-O2A	-2.20	1.45	1.55
3	A	998	ADP	PA-O3A	-2.15	1.57	1.59
3	B	999	ADP	PA-O3A	2.12	1.61	1.59

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	ADP	C5-C4-N3	-6.88	117.25	126.72
3	A	998	ADP	N3-C2-N1	-6.57	118.64	128.58
3	A	998	ADP	C5-C4-N3	-5.50	119.14	126.72
3	B	999	ADP	N3-C4-N9	5.43	136.41	127.17
3	B	999	ADP	C2-N3-C4	5.06	124.19	111.83
3	B	999	ADP	N3-C2-N1	-4.96	121.08	128.58
3	B	999	ADP	O4'-C1'-N9	-4.60	99.25	108.09
3	A	998	ADP	C2-N3-C4	4.59	123.04	111.83
3	A	998	ADP	N3-C4-N9	3.96	133.90	127.17
3	B	999	ADP	O3'-C3'-C4'	-3.15	102.04	111.08
3	A	998	ADP	C5-N7-C8	3.11	108.33	103.45
3	A	998	ADP	C4-C5-N7	-3.02	107.13	110.58
3	B	999	ADP	O3A-PA-O1A	-2.89	102.01	110.70
3	B	999	ADP	O3B-PB-O2B	2.81	118.33	107.80
3	A	998	ADP	N9-C8-N7	-2.76	110.02	113.94
3	B	999	ADP	O4'-C1'-C2'	-2.66	100.93	106.62
3	B	999	ADP	C4-C5-N7	-2.58	107.63	110.58
3	B	999	ADP	C4'-O4'-C1'	2.43	114.83	109.47
3	B	999	ADP	O4'-C4'-C5'	2.36	116.90	109.33
3	B	999	ADP	C5-N7-C8	2.31	107.07	103.45
3	B	999	ADP	O2A-PA-O3A	2.26	113.39	107.27
3	B	999	ADP	O3A-PB-O1B	-2.16	99.66	111.04
3	B	999	ADP	N6-C6-N1	2.08	123.00	118.38
3	B	999	ADP	C5-C6-N6	-2.06	118.18	123.29

There are no chirality outliers.

All (7) torsion outliers are listed below:

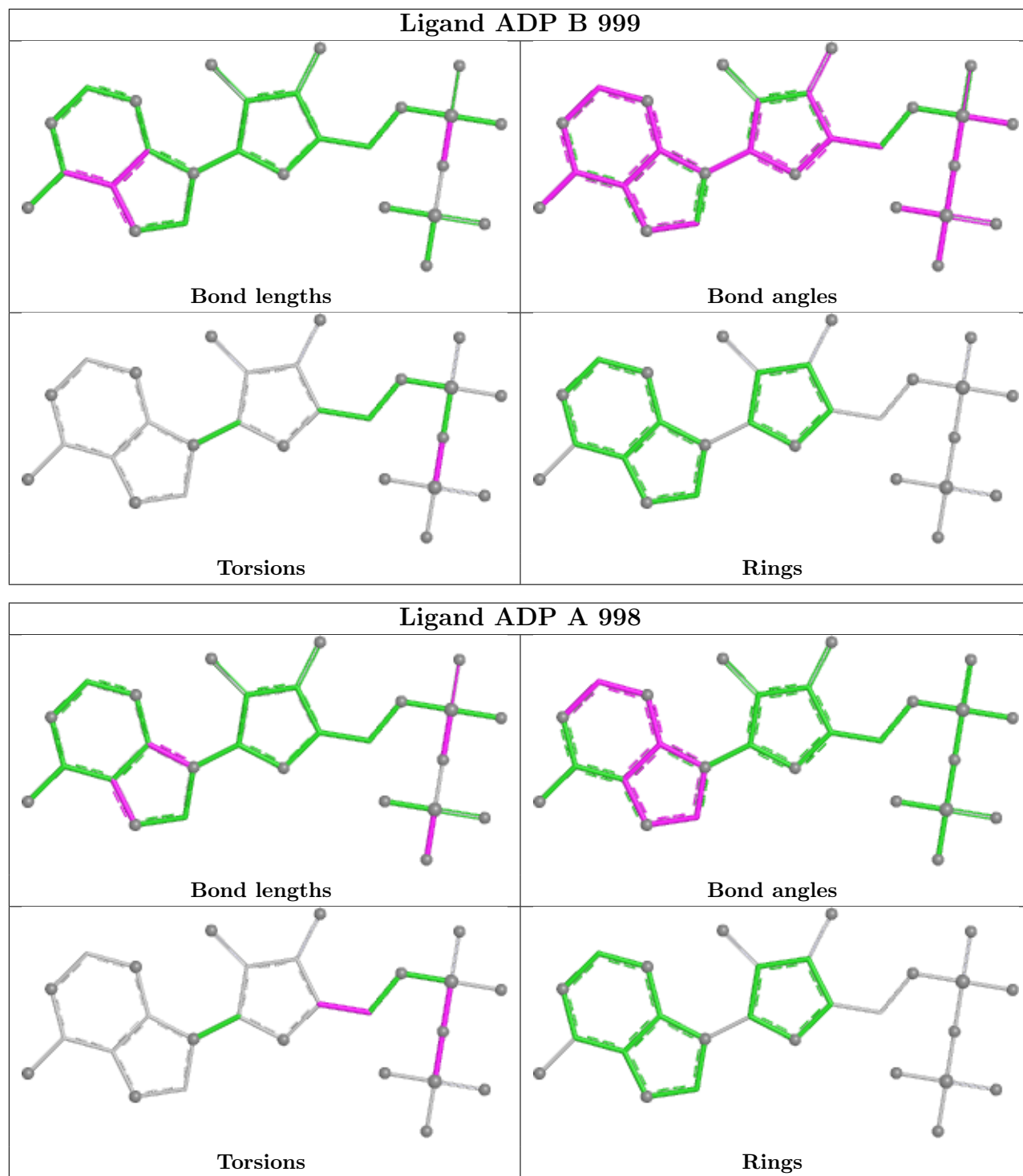
Mol	Chain	Res	Type	Atoms
3	A	998	ADP	O4'-C4'-C5'-O5'
3	B	999	ADP	PA-O3A-PB-O2B
3	A	998	ADP	C3'-C4'-C5'-O5'
3	B	999	ADP	PA-O3A-PB-O1B
3	A	998	ADP	PA-O3A-PB-O2B
3	B	999	ADP	PA-O3A-PB-O3B
3	A	998	ADP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 6 short contacts:

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



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	A	1
1	B	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, 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	355/383 (92%)	-0.02	10 (2%) 55 53	21, 46, 96, 135	0
1	B	331/383 (86%)	0.82	59 (17%) 4 3	23, 76, 162, 174	0
All	All	686/766 (89%)	0.38	69 (10%) 12 11	21, 55, 142, 174	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	536	LYS	4.5
1	B	532	MET	4.2
1	A	366	MET	3.9
1	B	635	LEU	3.7
1	B	493	LEU	3.6
1	B	561	LEU	3.5
1	B	525	PRO	3.4
1	B	486	ASN	3.4
1	B	464	SER	3.2
1	B	604	SER	3.2
1	B	451	VAL	3.1
1	B	539	ARG	3.1
1	B	480	THR	3.1
1	B	481	PHE	3.0
1	B	538	ASN	3.0
1	B	613	LEU	2.9
1	B	482	LEU	2.9
1	B	564	ARG	2.9
1	A	599	ILE	2.9
1	B	622	TYR	2.8
1	B	475	TYR	2.8
1	B	487	GLU	2.8
1	B	562	ILE	2.8
1	B	488	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	465	ILE	2.7
1	B	489	LEU	2.7
1	B	460	LEU	2.7
1	B	484	ILE	2.7
1	B	611	LEU	2.7
1	A	364	ASN	2.7
1	A	384	ASP	2.7
1	B	587	PRO	2.7
1	B	473	TRP	2.6
1	B	491	ASP	2.6
1	B	633	PRO	2.6
1	B	476	GLU	2.5
1	B	537	MET	2.5
1	B	519	GLU	2.5
1	B	492	LEU	2.5
1	B	559	LEU	2.5
1	B	520	GLU	2.5
1	B	583	GLY	2.5
1	B	479	ALA	2.4
1	A	648	SER	2.4
1	B	483	GLU	2.4
1	A	385	ALA	2.4
1	B	620	ILE	2.3
1	B	478	LYS	2.3
1	B	614	LEU	2.3
1	B	517	ILE	2.3
1	B	521	THR	2.3
1	A	598	ASN	2.3
1	B	624	ASN	2.3
1	B	638	ASN	2.3
1	B	523	LEU	2.3
1	B	603	LEU	2.3
1	B	616	LYS	2.2
1	B	607	THR	2.2
1	A	485	TYR	2.2
1	B	421	SER	2.2
1	B	566	ALA	2.2
1	A	365	ARG	2.2
1	B	528	LEU	2.2
1	B	621	PRO	2.1
1	B	582	ALA	2.1
1	A	538	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	490	TYR	2.1
1	B	313	CYS	2.0
1	B	628	THR	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

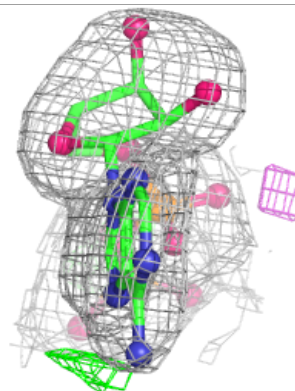
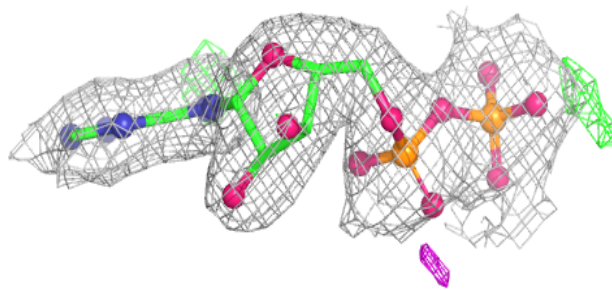
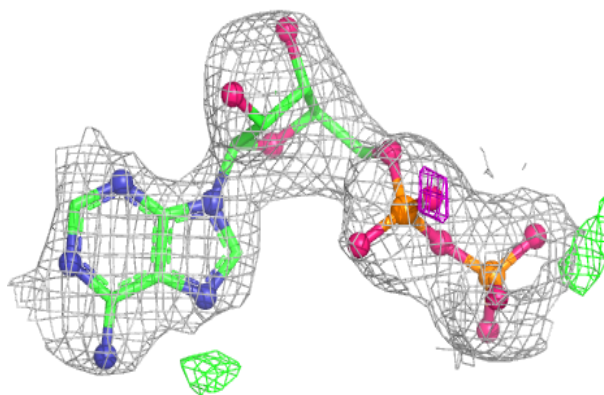
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.78	0.21	49,49,49,49	0
3	ADP	A	998	27/27	0.92	0.12	48,56,58,59	0
3	ADP	B	999	27/27	0.93	0.10	45,55,61,63	0
2	MG	A	996	1/1	0.98	0.16	35,35,35,35	0

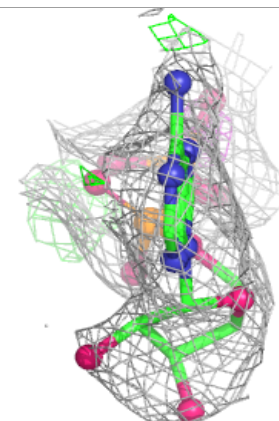
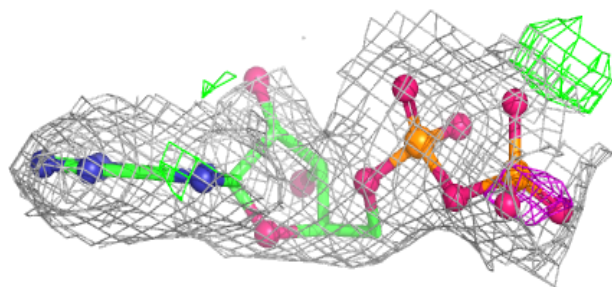
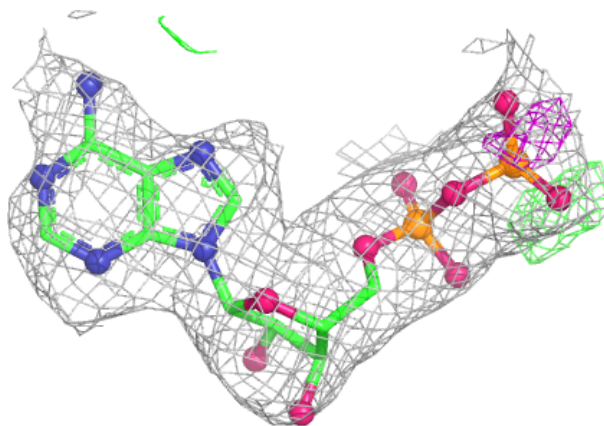
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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