



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:26 PM UTC

PDB ID : 3IW4 / pdb_00003iw4
Title : Crystal structure of PKC alpha in complex with NVP-AEB071
Authors : Stark, W.; Rummel, G.; Strauss, A.; Cowan-Jacob, S.W.
Deposited on : 2009-09-02
Resolution : 2.80 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

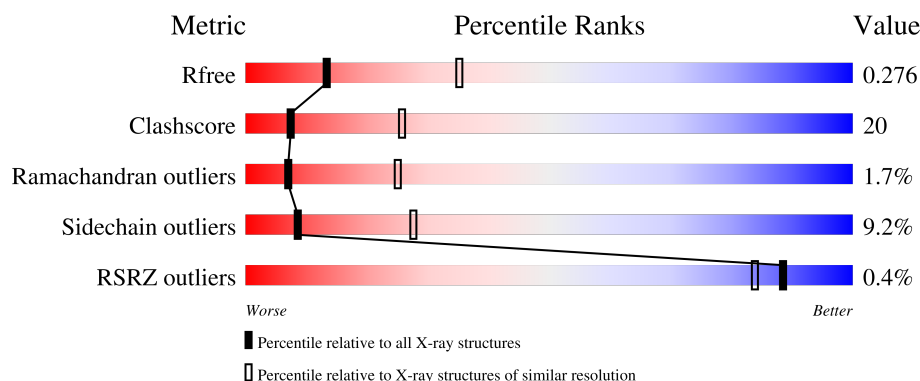
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	360	54% 34% • 8%
1	B	360	% 46% 38% 6% • 9%
1	C	360	% 56% 32% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8196 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 kinase C alpha type.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	P	S	0	0	0
			2686	1730	441	495	2	18			
1	B	327	Total	C	N	O	P	S	0	0	0
			2658	1714	436	488	2	18			
1	C	334	Total	C	N	O	P	S	0	0	0
			2707	1742	445	500	2	18			

There are 24 discrepancies between the modelled and reference sequences:

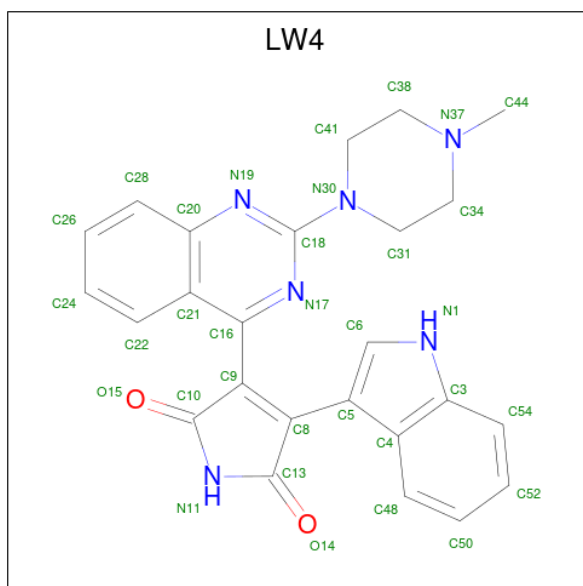
Chain	Residue	Modelled	Actual	Comment	Reference
A	319	MET	-	cloning artifact	UNP P17252
A	497	GLU	THR	engineered mutation	UNP P17252
A	673	HIS	-	expression tag	UNP P17252
A	674	HIS	-	expression tag	UNP P17252
A	675	HIS	-	expression tag	UNP P17252
A	676	HIS	-	expression tag	UNP P17252
A	677	HIS	-	expression tag	UNP P17252
A	678	HIS	-	expression tag	UNP P17252
B	319	MET	-	cloning artifact	UNP P17252
B	497	GLU	THR	engineered mutation	UNP P17252
B	673	HIS	-	expression tag	UNP P17252
B	674	HIS	-	expression tag	UNP P17252
B	675	HIS	-	expression tag	UNP P17252
B	676	HIS	-	expression tag	UNP P17252
B	677	HIS	-	expression tag	UNP P17252
B	678	HIS	-	expression tag	UNP P17252
C	319	MET	-	cloning artifact	UNP P17252
C	497	GLU	THR	engineered mutation	UNP P17252
C	673	HIS	-	expression tag	UNP P17252
C	674	HIS	-	expression tag	UNP P17252
C	675	HIS	-	expression tag	UNP P17252
C	676	HIS	-	expression tag	UNP P17252
C	677	HIS	-	expression tag	UNP P17252

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Chain	Residue	Modelled	Actual	Comment	Reference
C	678	HIS	-	expression tag	UNP P17252

- Molecule 2 is 3-(1H-indol-3-yl)-4-[2-(4-methylpiperazin-1-yl)quinazolin-4-yl]-1H-pyrrole-2,5-dione (CCD ID: LW4) (formula: C₂₅H₂₂N₆O₂).



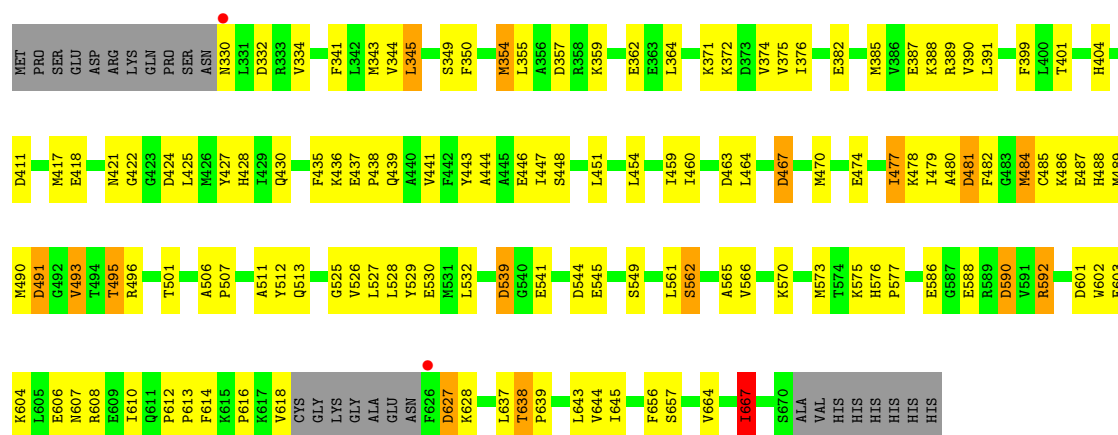
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	25	6	2		
2	B	1	Total	C	N	O	0	0
			33	25	6	2		
2	C	1	Total	C	N	O	0	0
			33	25	6	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	7	Total	O	0	0
			7	7		
3	C	20	Total	O	0	0
			20	20		

● Molecule 1: Protein kinase C alpha type

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.87Å 100.67Å 251.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.42 – 2.80 64.42 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (64.42-2.80) 99.5 (64.42-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.277 0.193 , 0.276	Depositor DCC
R_{free} test set	1417 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8196	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.06% 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: TPO, SEP, LW4

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	0.69	0/2730	0.98	1/3681 (0.0%)
1	B	0.65	0/2702	0.98	9/3640 (0.2%)
1	C	0.74	0/2751	1.02	9/3709 (0.2%)
All	All	0.69	0/8183	0.99	19/11030 (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	A	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	632	ARG	N-CA-C	-7.50	103.70	114.12
1	C	345	LEU	N-CA-C	-6.70	104.06	111.36
1	C	493	VAL	N-CA-C	-6.64	102.70	110.21
1	C	362	GLU	N-CA-C	-6.27	105.27	113.17
1	B	500	GLY	N-CA-C	-6.02	104.71	111.63
1	C	627	ASP	N-CA-C	5.93	118.61	109.07
1	C	506	ALA	CA-C-N	5.85	125.32	119.24
1	C	506	ALA	C-N-CA	5.85	125.32	119.24
1	C	628	LYS	N-CA-C	5.69	119.48	112.54
1	C	667	ILE	CB-CA-C	-5.67	105.35	111.59
1	B	506	ALA	CA-C-N	5.40	124.86	119.24
1	B	506	ALA	C-N-CA	5.40	124.86	119.24
1	B	421	ASN	N-CA-C	5.39	119.80	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	TYR	N-CA-C	5.32	116.38	109.72
1	B	499	CYS	N-CA-C	5.20	116.34	108.07
1	B	410	VAL	N-CA-CB	5.14	116.21	110.51
1	C	539	ASP	N-CA-C	5.08	116.79	109.07
1	B	396	LYS	CA-C-N	5.03	123.33	119.66
1	B	396	LYS	C-N-CA	5.03	123.33	119.66

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	VAL	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	2686	0	2635	95	0
1	B	2658	0	2611	132	0
1	C	2707	0	2661	99	0
2	A	33	0	22	5	0
2	B	33	0	22	3	0
2	C	33	0	22	6	0
3	A	19	0	0	1	0
3	B	7	0	0	0	0
3	C	20	0	0	2	0
All	All	8196	0	7973	329	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 20.

All (329) 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:C:436:LYS:HE2	1:C:438:PRO:HB2	1.28	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:GLU:O	1:C:441:VAL:HG23	1.62	0.97
1:A:460:ILE:HG22	1:A:462:ARG:HG3	1.48	0.94
1:A:644:VAL:HA	1:B:426:MET:HE1	1.51	0.92
1:A:350:PHE:O	1:A:368:LYS:HE3	1.72	0.90
1:B:486:LYS:CG	1:B:489:MET:HE3	2.05	0.85
1:C:501:THR:HG22	3:C:17:HOH:O	1.77	0.84
1:A:404:HIS:HD2	1:A:405:SER:OG	1.62	0.82
1:B:486:LYS:HG3	1:B:489:MET:HE3	1.60	0.82
1:B:428:HIS:CD2	1:B:471:LEU:HD12	2.15	0.81
1:B:510:ILE:HG21	1:B:551:MET:HE1	1.63	0.80
1:A:460:ILE:CG2	1:A:462:ARG:HG3	2.10	0.80
1:A:589:ARG:O	1:A:593:GLU:HG3	1.82	0.79
1:B:408:GLN:HG2	1:B:657:SEP:O2P	1.83	0.79
1:B:551:MET:HG2	1:C:667:ILE:CG2	2.12	0.79
1:C:401:THR:HG21	1:C:480:ALA:HB2	1.65	0.78
1:A:604:LYS:HG3	1:A:609:GLU:HB2	1.65	0.78
1:B:429:ILE:HD11	1:B:531:MET:HA	1.64	0.78
1:C:390:VAL:HG22	1:C:459:ILE:HD13	1.64	0.78
1:B:388:LYS:HE3	1:B:656:PHE:O	1.86	0.76
1:C:422:GLY:O	1:C:428:HIS:HE1	1.69	0.76
1:A:599:ARG:NH1	3:A:21:HOH:O	2.18	0.75
1:B:490:MET:O	1:B:493:VAL:HG23	1.86	0.75
1:B:593:GLU:O	1:B:594:HIS:O	2.06	0.74
1:C:487:GLU:O	1:C:489:MET:HG2	1.88	0.74
1:B:426:MET:HE3	1:B:430:GLN:HE21	1.54	0.73
1:B:581:LEU:HD12	1:B:590:ASP:HB3	1.71	0.72
1:C:388:LYS:HE3	1:C:656:PHE:O	1.90	0.71
1:C:447:ILE:HG13	1:C:477:ILE:HD13	1.72	0.71
1:C:525:GLY:C	1:C:573:MET:HE2	2.16	0.71
1:B:640:PRO:HB3	1:B:645:ILE:HD11	1.71	0.70
1:B:404:HIS:HB3	1:B:416:VAL:HG12	1.74	0.69
1:A:595:ALA:O	1:A:598:ARG:HG3	1.92	0.68
1:A:589:ARG:HG3	1:A:593:GLU:OE2	1.94	0.68
1:B:358:ARG:HB3	1:B:361:THR:HG23	1.76	0.68
1:B:510:ILE:CG2	1:B:551:MET:HE1	2.22	0.68
1:B:605:LEU:C	1:B:607:ASN:H	2.02	0.68
1:A:437:GLU:O	1:A:441:VAL:HG23	1.94	0.68
1:B:602:TRP:O	1:B:606:GLU:HG2	1.95	0.67
1:A:564:GLU:HG2	1:A:598:ARG:NH1	2.10	0.66
1:C:390:VAL:HG22	1:C:459:ILE:CD1	2.25	0.66
1:A:422:GLY:N	1:A:471:LEU:O	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:401:THR:CG2	1:C:480:ALA:HB2	2.25	0.66
1:C:627:ASP:OD1	1:C:627:ASP:C	2.39	0.65
1:B:486:LYS:HG2	1:B:489:MET:HE3	1.78	0.65
1:B:472:ASP:OD2	1:B:608:ARG:NH2	2.29	0.65
1:C:436:LYS:HG2	1:C:439:GLN:HG2	1.79	0.65
1:B:551:MET:HG2	1:C:667:ILE:HG23	1.77	0.65
1:B:664:VAL:HG12	1:B:666:PRO:HD2	1.78	0.65
1:B:368:LYS:NZ	1:B:387:GLU:OE1	2.28	0.64
1:B:422:GLY:O	1:B:428:HIS:NE2	2.30	0.64
1:B:661:PRO:HG2	1:B:662:GLN:HE21	1.62	0.64
1:C:435:PHE:HB3	1:C:439:GLN:HG3	1.77	0.64
1:C:588:GLU:O	1:C:592:ARG:HB2	1.98	0.64
1:C:345:LEU:HD21	1:C:355:LEU:HB2	1.80	0.63
1:C:436:LYS:HE2	1:C:438:PRO:CB	2.16	0.63
1:A:445:ALA:HB1	1:A:605:LEU:CD2	2.28	0.63
1:B:511:ALA:O	1:B:512:TYR:HB2	1.99	0.63
1:B:641:ASP:OD1	1:B:641:ASP:C	2.42	0.63
1:B:439:GLN:HG3	1:B:613:PRO:HB3	1.80	0.63
1:C:588:GLU:OE2	1:C:592:ARG:NH1	2.32	0.63
1:C:411:ASP:HB3	1:C:645:ILE:CD1	2.28	0.62
1:C:437:GLU:OE1	1:C:562:SER:HB3	1.99	0.62
1:A:528:LEU:HD23	1:A:531:MET:HE3	1.80	0.62
1:B:559:LYS:HE3	1:C:330:ASN:HB2	1.83	0.61
1:B:453:PHE:O	1:B:457:ARG:HG2	2.00	0.61
1:C:421:ASN:ND2	1:C:618:VAL:HG23	2.15	0.61
1:B:593:GLU:O	1:B:594:HIS:C	2.44	0.61
1:A:644:VAL:HA	1:B:426:MET:CE	2.30	0.60
1:B:541:GLU:H	1:B:545:GLU:HG2	1.66	0.60
1:B:382:GLU:CD	1:B:382:GLU:H	2.10	0.60
1:B:426:MET:HE3	1:B:430:GLN:NE2	2.17	0.60
1:C:490:MET:HE3	1:C:490:MET:HA	1.82	0.60
1:A:398:PRO:CB	1:A:608:ARG:HD2	2.31	0.60
1:C:590:ASP:N	1:C:590:ASP:OD1	2.34	0.60
1:A:476:HIS:CE1	1:A:612:PRO:HG3	2.36	0.60
1:C:486:LYS:HE2	1:C:495:THR:HG21	1.84	0.60
2:A:901:LW4:H48	2:A:901:LW4:C16	2.32	0.59
1:B:434:LYS:HD2	1:B:532:LEU:O	2.03	0.59
1:A:398:PRO:HB2	1:A:608:ARG:HD2	1.85	0.59
1:B:645:ILE:HA	1:B:648:ILE:HG13	1.84	0.59
1:B:487:GLU:O	1:B:489:MET:HE2	2.01	0.58
1:B:605:LEU:O	1:B:607:ASN:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:TPO:HG23	1:B:639:PRO:HD2	1.85	0.58
1:C:444:ALA:CB	1:C:528:LEU:HD11	2.34	0.58
1:C:422:GLY:O	1:C:428:HIS:CE1	2.54	0.58
1:B:460:ILE:CD1	1:B:489:MET:HG3	2.33	0.58
1:B:428:HIS:CD2	1:B:471:LEU:CD1	2.86	0.58
1:C:436:LYS:CE	1:C:438:PRO:HB2	2.19	0.58
1:C:481:ASP:HB2	2:C:901:LW4:N19	2.19	0.58
1:B:442:PHE:CZ	1:B:446:GLU:OE2	2.56	0.58
1:B:505:ILE:CG2	1:B:509:ILE:HB	2.34	0.57
1:C:527:LEU:O	1:C:528:LEU:C	2.44	0.57
1:A:445:ALA:HB1	1:A:605:LEU:HD21	1.86	0.57
1:B:424:ASP:HA	1:B:470:MET:HA	1.87	0.57
2:A:901:LW4:N17	2:A:901:LW4:C48	2.68	0.56
1:A:451:LEU:HD11	1:A:464:LEU:HD22	1.87	0.56
1:C:467:ASP:OD2	2:C:901:LW4:H44	2.04	0.56
1:B:397:PRO:HD3	1:B:453:PHE:CD1	2.41	0.56
1:A:557:TYR:HE2	1:A:569:CYS:HB3	1.71	0.56
1:B:589:ARG:O	1:B:590:ASP:C	2.48	0.56
1:B:524:TYR:O	1:B:528:LEU:HB2	2.07	0.55
1:C:350:PHE:CD2	1:C:350:PHE:C	2.83	0.55
1:A:382:GLU:OE1	1:A:382:GLU:HA	2.06	0.55
1:B:564:GLU:HB3	1:B:596:PHE:HA	1.89	0.55
1:A:510:ILE:HB	1:A:551:MET:HE1	1.89	0.55
1:B:496:ARG:HG2	1:B:514:PRO:HG3	1.87	0.55
1:C:486:LYS:CE	1:C:495:THR:HG21	2.37	0.55
1:C:463:ASP:CG	1:C:484:MET:HE3	2.32	0.55
1:C:529:TYR:HB2	1:C:573:MET:HE1	1.89	0.55
1:C:602:TRP:O	1:C:606:GLU:HG3	2.07	0.55
1:C:586:GLU:O	1:C:590:ASP:OD1	2.25	0.54
1:C:496:ARG:HH21	1:C:512:TYR:HB3	1.73	0.54
1:A:409:THR:HG22	1:A:412:ARG:HB2	1.89	0.54
1:B:471:LEU:HD23	1:B:477:ILE:HD13	1.90	0.54
1:B:540:GLY:CA	1:B:545:GLU:HG2	2.38	0.54
1:B:445:ALA:O	1:B:448:SER:OG	2.22	0.54
1:C:424:ASP:HA	1:C:470:MET:HA	1.89	0.53
2:C:901:LW4:H22	2:C:901:LW4:C10	2.38	0.53
1:A:368:LYS:NZ	1:A:387:GLU:OE1	2.41	0.53
1:B:452:PHE:CD1	1:B:588:GLU:HG3	2.44	0.53
1:C:372:LYS:O	1:C:376:ILE:HG13	2.09	0.53
1:A:340:ASN:HB2	1:A:357:ASP:OD1	2.09	0.53
1:C:401:THR:HG23	1:C:479:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:GLU:N	1:A:545:GLU:OE2	2.25	0.52
2:C:901:LW4:H22	2:C:901:LW4:O15	2.10	0.52
1:B:599:ARG:C	1:B:600:ILE:HD12	2.34	0.52
1:A:409:THR:CG2	1:A:412:ARG:HB2	2.40	0.52
1:A:638:TPO:O3P	1:A:638:TPO:N	2.24	0.52
1:A:376:ILE:O	1:A:377:GLN:C	2.53	0.52
1:A:528:LEU:HD23	1:A:531:MET:CE	2.39	0.52
1:B:601:ASP:HB3	1:B:604:LYS:HD2	1.92	0.52
1:B:398:PRO:HB2	1:B:608:ARG:HD2	1.91	0.52
1:B:439:GLN:HG3	1:B:613:PRO:CB	2.40	0.52
1:B:484:MET:CE	1:B:499:CYS:HB2	2.40	0.52
1:B:516:GLY:C	1:B:518:SER:H	2.17	0.52
1:C:371:LYS:NZ	1:C:638:TPO:O2P	2.33	0.52
1:C:566:VAL:CG1	1:C:570:LYS:HE3	2.40	0.52
1:A:637:LEU:O	1:A:638:TPO:C	2.58	0.51
1:B:587:GLY:O	1:B:590:ASP:HB2	2.11	0.51
1:C:345:LEU:CD2	1:C:355:LEU:HB2	2.40	0.51
1:C:350:PHE:C	1:C:350:PHE:HD2	2.19	0.51
1:A:465:LYS:HA	1:A:504:TYR:CE2	2.45	0.51
1:B:546:LEU:O	1:B:549:SER:HB3	2.11	0.50
1:B:638:TPO:O1P	1:B:638:TPO:N	2.35	0.50
1:B:505:ILE:HG22	1:B:506:ALA:O	2.11	0.50
1:C:460:ILE:CD1	1:C:489:MET:HG3	2.42	0.50
1:A:422:GLY:HA3	1:A:471:LEU:HB2	1.93	0.50
1:B:429:ILE:HG13	1:B:435:PHE:CE2	2.46	0.50
1:A:587:GLY:O	1:A:590:ASP:HB2	2.11	0.50
1:A:473:SER:O	1:A:616:PRO:HD2	2.11	0.50
1:A:599:ARG:HG2	1:A:599:ARG:HH11	1.78	0.49
1:B:665:HIS:O	1:B:666:PRO:C	2.54	0.49
1:C:490:MET:O	1:C:491:ASP:C	2.55	0.49
1:A:607:ASN:HB2	1:A:609:GLU:HG3	1.94	0.49
1:B:428:HIS:HD2	1:B:471:LEU:CD1	2.24	0.49
1:B:532:LEU:HD13	1:B:565:ALA:HB1	1.94	0.49
1:B:597:PHE:CD2	1:B:602:TRP:HZ2	2.31	0.49
1:A:524:TYR:O	1:A:528:LEU:HB2	2.12	0.49
1:B:429:ILE:HG22	1:B:430:GLN:N	2.26	0.49
1:B:541:GLU:N	1:B:545:GLU:HG2	2.28	0.49
1:B:535:GLN:OE1	1:B:535:GLN:HA	2.13	0.48
2:B:901:LW4:C10	2:B:901:LW4:H22	2.43	0.48
1:A:594:HIS:C	1:A:596:PHE:N	2.71	0.48
1:B:442:PHE:CD2	1:B:613:PRO:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:TYR:C	1:B:427:TYR:CD2	2.91	0.48
1:B:428:HIS:O	1:B:429:ILE:C	2.56	0.48
1:B:605:LEU:C	1:B:607:ASN:N	2.68	0.48
1:B:458:GLY:HA2	1:B:490:MET:HG3	1.95	0.48
1:B:601:ASP:OD2	1:B:604:LYS:HG3	2.13	0.48
1:C:421:ASN:ND2	1:C:618:VAL:CG2	2.77	0.48
1:A:374:VAL:O	1:A:375:VAL:C	2.55	0.47
1:B:394:LEU:CD2	1:B:662:GLN:HE22	2.27	0.47
1:C:343:MET:HE2	1:C:344:VAL:O	2.13	0.47
1:B:558:PRO:O	1:B:560:SER:N	2.47	0.47
1:B:398:PRO:CB	1:B:608:ARG:HD2	2.45	0.47
1:B:425:LEU:O	1:B:426:MET:C	2.58	0.47
1:C:341:PHE:CD2	1:C:354:MET:HE3	2.49	0.47
1:C:507:PRO:HG2	1:C:575:LYS:HA	1.97	0.47
1:C:618:VAL:O	1:C:618:VAL:HG13	2.14	0.47
1:A:343:MET:O	1:A:354:MET:HG3	2.15	0.47
1:A:402:GLN:HB2	1:A:418:GLU:CD	2.40	0.47
1:A:557:TYR:HE2	1:A:569:CYS:CB	2.28	0.47
1:B:551:MET:HG2	1:C:667:ILE:HG22	1.93	0.47
1:B:551:MET:C	1:B:575:LYS:HZ3	2.22	0.47
1:C:350:PHE:CE1	2:C:901:LW4:H38A	2.50	0.47
1:B:505:ILE:HG23	1:B:509:ILE:HD12	1.97	0.47
1:A:402:GLN:HB2	1:A:418:GLU:CG	2.45	0.46
1:A:420:VAL:HG12	1:A:421:ASN:N	2.30	0.46
1:A:428:HIS:CD2	1:A:471:LEU:HD12	2.50	0.46
1:C:332:ASP:OD2	1:C:404:HIS:HE1	1.98	0.46
1:C:607:ASN:O	1:C:608:ARG:HB2	2.14	0.46
1:B:415:PHE:N	1:B:415:PHE:CD1	2.84	0.46
1:B:665:HIS:N	1:B:666:PRO:HD2	2.31	0.46
1:C:425:LEU:HD12	1:C:425:LEU:HA	1.75	0.46
1:A:461:TYR:N	1:A:520:ASP:OD2	2.41	0.46
1:B:391:LEU:HD23	1:B:391:LEU:HA	1.73	0.46
1:C:359:LYS:HB2	1:C:359:LYS:HE3	1.35	0.46
1:C:447:ILE:O	1:C:448:SER:C	2.56	0.46
1:C:643:LEU:O	1:C:644:VAL:C	2.58	0.46
2:C:901:LW4:O15	2:C:901:LW4:C22	2.63	0.46
1:B:474:GLU:HB2	1:B:476:HIS:HD2	1.79	0.46
1:B:612:PRO:O	1:B:613:PRO:C	2.59	0.46
1:B:437:GLU:HB3	1:B:438:PRO:HD3	1.98	0.46
1:A:378:ASP:O	1:A:379:ASP:HB2	2.15	0.46
1:C:638:TPO:HG23	1:C:639:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:GLU:HG2	1:A:598:ARG:HH11	1.80	0.45
1:B:516:GLY:C	1:B:518:SER:N	2.71	0.45
1:A:526:VAL:HG22	1:A:537:PRO:HG2	1.98	0.45
1:A:647:ASN:ND2	1:B:504:TYR:OH	2.45	0.45
1:A:559:LYS:HE3	1:A:559:LYS:HB3	1.69	0.45
1:B:404:HIS:HB3	1:B:416:VAL:O	2.17	0.45
1:B:549:SER:O	1:B:553:HIS:HB3	2.16	0.45
1:C:443:TYR:O	1:C:444:ALA:C	2.57	0.45
1:A:475:GLY:O	1:A:612:PRO:HB3	2.17	0.45
1:B:461:TYR:O	1:B:462:ARG:HB2	2.17	0.45
2:B:901:LW4:C16	2:B:901:LW4:H48	2.47	0.45
1:A:537:PRO:HB2	1:A:538:PHE:CD2	2.52	0.45
1:B:540:GLY:HA2	1:B:545:GLU:HG2	1.98	0.45
1:C:526:VAL:O	1:C:530:GLU:HG3	2.17	0.45
1:B:358:ARG:HB3	1:B:361:THR:CG2	2.45	0.45
1:A:354:MET:HE2	1:A:354:MET:HB2	1.91	0.44
1:C:343:MET:HE3	1:C:343:MET:HB2	1.72	0.44
1:C:439:GLN:HB3	1:C:613:PRO:HB3	1.98	0.44
1:C:444:ALA:HB1	1:C:528:LEU:HD11	1.99	0.44
1:C:489:MET:HE1	1:C:493:VAL:CG1	2.47	0.44
1:B:429:ILE:CG2	1:B:430:GLN:N	2.79	0.44
1:B:447:ILE:O	1:B:448:SER:C	2.60	0.44
1:B:558:PRO:C	1:B:560:SER:H	2.25	0.44
1:B:565:ALA:O	1:B:568:ILE:HG22	2.17	0.44
1:C:511:ALA:O	1:C:512:TYR:C	2.60	0.44
1:B:627:ASP:C	1:B:627:ASP:OD1	2.59	0.44
2:B:901:LW4:H22	2:B:901:LW4:O15	2.17	0.44
1:A:398:PRO:O	1:A:478:LYS:NZ	2.41	0.44
1:C:391:LEU:HD22	1:C:417:MET:HE1	1.99	0.44
1:A:594:HIS:O	1:A:595:ALA:C	2.61	0.44
1:B:437:GLU:O	1:B:441:VAL:HG23	2.18	0.44
1:B:551:MET:HB2	1:B:551:MET:HE2	1.72	0.44
1:C:592:ARG:NH2	1:C:606:GLU:CD	2.76	0.44
1:A:513:GLN:HA	1:A:513:GLN:OE1	2.17	0.44
1:B:631:THR:OG1	1:B:632:ARG:N	2.50	0.44
1:A:396:LYS:HB2	1:A:396:LYS:HE2	1.89	0.44
1:C:614:PHE:HE1	1:C:616:PRO:HA	1.83	0.44
1:A:352:LYS:HD3	1:A:354:MET:HE1	2.00	0.43
1:A:368:LYS:HE2	1:A:370:LEU:HD11	2.00	0.43
1:B:628:LYS:H	1:B:628:LYS:HG3	1.38	0.43
1:C:385:MET:HB3	1:C:389:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:GLU:HG3	1:C:482:PHE:C	2.43	0.43
2:A:901:LW4:H22	2:A:901:LW4:C10	2.48	0.43
1:B:577:PRO:O	1:B:578:ALA:C	2.60	0.43
1:A:418:GLU:O	1:A:418:GLU:HG3	2.18	0.43
1:A:648:ILE:O	1:A:650:GLN:N	2.51	0.43
1:C:418:GLU:OE2	1:C:478:LYS:HE3	2.18	0.43
1:A:369:ILE:HG12	1:A:414:TYR:CD1	2.53	0.43
1:A:425:LEU:O	1:A:426:MET:C	2.60	0.43
1:B:665:HIS:N	1:B:666:PRO:CD	2.81	0.43
1:C:411:ASP:HB3	1:C:645:ILE:HD12	2.00	0.43
1:C:451:LEU:HD11	1:C:464:LEU:HD22	2.01	0.43
1:A:382:GLU:OE1	1:A:382:GLU:CA	2.66	0.43
1:B:530:GLU:O	1:B:531:MET:C	2.59	0.43
1:B:536:PRO:HA	1:B:537:PRO:HD3	1.88	0.43
1:A:369:ILE:HG12	1:A:414:TYR:HD1	1.83	0.43
1:B:612:PRO:HA	1:B:613:PRO:HD2	1.81	0.43
1:B:530:GLU:O	1:B:534:GLY:N	2.46	0.43
1:A:637:LEU:HD12	1:A:637:LEU:HA	1.89	0.43
1:B:465:LYS:HA	1:B:504:TYR:CE2	2.54	0.43
1:C:460:ILE:O	1:C:485:CYS:HA	2.18	0.43
1:A:368:LYS:HB3	1:A:415:PHE:HB2	2.00	0.42
1:B:464:LEU:HD12	1:B:464:LEU:HA	1.79	0.42
1:A:355:LEU:HD12	1:A:355:LEU:HA	1.75	0.42
2:A:901:LW4:H22	2:A:901:LW4:O15	2.19	0.42
1:C:489:MET:CE	1:C:493:VAL:HG11	2.48	0.42
1:A:453:PHE:CE1	1:A:457:ARG:CZ	3.03	0.42
1:A:502:PRO:HA	1:A:505:ILE:HG13	2.00	0.42
1:B:381:VAL:HG11	1:B:652:ASP:HB3	2.01	0.42
1:B:506:ALA:HB3	1:B:519:VAL:HG12	2.01	0.42
1:B:552:GLU:HB3	1:C:664:VAL:HG13	2.00	0.42
1:A:425:LEU:HG	1:A:469:VAL:HG12	2.00	0.42
1:A:634:GLN:HA	1:A:635:PRO:HD3	1.92	0.42
1:B:587:GLY:O	1:B:588:GLU:C	2.62	0.42
1:C:411:ASP:HB3	1:C:645:ILE:HD11	2.00	0.42
1:A:370:LEU:O	1:A:412:ARG:HA	2.20	0.42
2:A:901:LW4:C16	2:A:901:LW4:C48	2.96	0.42
1:B:477:ILE:HD13	1:B:477:ILE:HA	1.76	0.42
1:B:564:GLU:N	1:B:564:GLU:OE1	2.53	0.42
1:A:518:SER:HA	1:A:583:CYS:SG	2.60	0.42
1:B:476:HIS:CD2	1:B:612:PRO:HG3	2.55	0.42
1:C:474:GLU:O	1:C:612:PRO:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:LYS:HA	3:C:28:HOH:O	2.20	0.42
1:A:402:GLN:HB2	1:A:418:GLU:HB3	2.02	0.41
1:B:378:ASP:HB3	1:B:380:ASP:OD2	2.20	0.41
1:B:437:GLU:O	1:B:438:PRO:C	2.61	0.41
1:B:581:LEU:CD1	1:B:590:ASP:HB3	2.44	0.41
1:A:481:ASP:OD1	1:A:481:ASP:C	2.62	0.41
1:B:389:ARG:HE	1:B:487:GLU:CD	2.28	0.41
1:B:471:LEU:HA	1:B:476:HIS:O	2.20	0.41
1:A:564:GLU:CG	1:A:598:ARG:NH1	2.83	0.41
1:C:399:PHE:CE1	1:C:446:GLU:CD	2.98	0.41
1:C:511:ALA:HB3	1:C:513:GLN:HG2	2.01	0.41
1:A:484:MET:HE3	1:A:499:CYS:SG	2.61	0.41
1:A:528:LEU:HD23	1:A:528:LEU:HA	1.72	0.41
1:C:390:VAL:CG2	1:C:459:ILE:HD13	2.44	0.41
1:C:411:ASP:OD1	1:C:411:ASP:N	2.53	0.41
1:C:427:TYR:HA	1:C:430:GLN:HE21	1.84	0.41
1:A:445:ALA:HB1	1:A:605:LEU:HD22	2.03	0.41
1:A:486:LYS:HG3	1:A:489:MET:HE3	2.03	0.41
1:B:405:SER:HB2	1:B:658:TYR:O	2.21	0.41
1:C:436:LYS:O	1:C:437:GLU:C	2.64	0.41
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.95	0.41
1:C:489:MET:HE2	1:C:489:MET:HA	2.03	0.41
1:A:337:THR:C	1:A:339:PHE:H	2.29	0.41
1:C:601:ASP:OD2	1:C:604:LYS:HG3	2.20	0.41
1:A:349:SER:C	1:A:351:GLY:H	2.28	0.41
1:A:352:LYS:HD3	1:A:354:MET:CE	2.51	0.41
1:A:428:HIS:O	1:A:431:GLN:HB2	2.21	0.41
1:A:439:GLN:HG3	1:A:613:PRO:HG2	2.03	0.41
1:B:460:ILE:O	1:B:485:CYS:HA	2.21	0.41
1:C:541:GLU:HB2	1:C:545:GLU:OE1	2.21	0.41
1:C:576:HIS:O	1:C:577:PRO:C	2.64	0.41
1:A:442:PHE:CD2	1:A:613:PRO:HD3	2.56	0.41
1:B:405:SER:HB2	1:B:659:VAL:HA	2.03	0.41
1:A:541:GLU:HB2	1:A:545:GLU:OE2	2.21	0.40
1:C:532:LEU:HD13	1:C:565:ALA:HB1	2.03	0.40
1:A:406:CYS:HB3	1:A:656:PHE:CE2	2.56	0.40
1:C:489:MET:CE	1:C:493:VAL:CG1	2.99	0.40
1:A:627:ASP:OD1	1:A:628:LYS:N	2.54	0.40
1:A:600:ILE:HD13	1:A:600:ILE:HA	1.92	0.40
1:B:593:GLU:OE1	1:B:593:GLU:HA	2.21	0.40
1:C:374:VAL:O	1:C:375:VAL:C	2.64	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	326/360 (91%)	286 (88%)	37 (11%)	3 (1%)	14	41
1	B	319/360 (89%)	281 (88%)	27 (8%)	11 (3%)	3	11
1	C	328/360 (91%)	295 (90%)	30 (9%)	3 (1%)	14	41
All	All	973/1080 (90%)	862 (89%)	94 (10%)	17 (2%)	7	25

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	594	HIS
1	B	362	GLU
1	B	559	LYS
1	B	606	GLU
1	B	613	PRO
1	C	488	HIS
1	C	491	ASP
1	B	481	ASP
1	A	649	ASP
1	A	652	ASP
1	B	590	ASP
1	B	593	GLU
1	C	481	ASP
1	A	342	LEU
1	B	429	ILE
1	B	578	ALA
1	B	585	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/316 (92%)	261 (90%)	28 (10%)	8	25
1	B	287/316 (91%)	256 (89%)	31 (11%)	6	21
1	C	293/316 (93%)	272 (93%)	21 (7%)	13	39
All	All	869/948 (92%)	789 (91%)	80 (9%)	8	27

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	334	VAL
1	A	335	LYS
1	A	337	THR
1	A	338	ASP
1	A	340	ASN
1	A	343	MET
1	A	361	THR
1	A	364	LEU
1	A	375	VAL
1	A	394	LEU
1	A	396	LYS
1	A	424	ASP
1	A	436	LYS
1	A	456	LYS
1	A	467	ASP
1	A	474	GLU
1	A	491	ASP
1	A	527	LEU
1	A	528	LEU
1	A	539	ASP
1	A	559	LYS
1	A	561	LEU
1	A	589	ARG
1	A	603	GLU
1	A	617	LYS
1	A	618	VAL

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Mol	Chain	Res	Type
1	A	628	LYS
1	A	637	LEU
1	B	332	ASP
1	B	334	VAL
1	B	335	LYS
1	B	342	LEU
1	B	363	GLU
1	B	364	LEU
1	B	382	GLU
1	B	401	THR
1	B	410	VAL
1	B	412	ARG
1	B	415	PHE
1	B	421	ASN
1	B	425	LEU
1	B	429	ILE
1	B	473	SER
1	B	474	GLU
1	B	479	ILE
1	B	495	THR
1	B	544	ASP
1	B	548	GLN
1	B	551	MET
1	B	560	SER
1	B	561	LEU
1	B	563	LYS
1	B	588	GLU
1	B	593	GLU
1	B	626	PHE
1	B	628	LYS
1	B	634	GLN
1	B	648	ILE
1	B	665	HIS
1	C	334	VAL
1	C	349	SER
1	C	354	MET
1	C	357	ASP
1	C	364	LEU
1	C	382	GLU
1	C	467	ASP
1	C	477	ILE
1	C	484	MET

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Mol	Chain	Res	Type
1	C	495	THR
1	C	539	ASP
1	C	544	ASP
1	C	549	SER
1	C	561	LEU
1	C	562	SER
1	C	590	ASP
1	C	592	ARG
1	C	603	GLU
1	C	610	ILE
1	C	637	LEU
1	C	667	ILE

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	377	GLN
1	A	404	HIS
1	A	430	GLN
1	A	439	GLN
1	A	476	HIS
1	A	535	GLN
1	A	554	ASN
1	A	634	GLN
1	A	647	ASN
1	A	665	HIS
1	B	340	ASN
1	B	421	ASN
1	B	430	GLN
1	B	439	GLN
1	B	455	HIS
1	B	554	ASN
1	B	662	GLN
1	C	404	HIS
1	C	428	HIS
1	C	430	GLN
1	C	431	GLN
1	C	439	GLN
1	C	607	ASN
1	C	642	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
1	SEP	A	657	1	8,9,10	1.84	1 (12%)	7,12,14	0.58	0
1	TPO	B	638	1	8,10,11	1.00	1 (12%)	10,14,16	1.57	2 (20%)
1	SEP	B	657	1	8,9,10	1.68	1 (12%)	7,12,14	0.80	0
1	TPO	A	638	1	8,10,11	1.00	0	10,14,16	1.19	1 (10%)
1	SEP	C	657	1	8,9,10	1.72	1 (12%)	7,12,14	1.11	1 (14%)
1	TPO	C	638	1	8,10,11	0.86	0	10,14,16	1.52	1 (10%)

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
1	SEP	A	657	1	-	2/6/8/10	-
1	TPO	B	638	1	-	0/9/11/13	-
1	SEP	B	657	1	-	5/6/8/10	-
1	TPO	A	638	1	-	1/9/11/13	-
1	SEP	C	657	1	-	3/6/8/10	-
1	TPO	C	638	1	-	1/9/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	657	SEP	P-O1P	4.06	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	657	SEP	P-O1P	3.83	1.62	1.50
1	B	657	SEP	P-O1P	3.73	1.62	1.50
1	B	638	TPO	P-OG1	2.07	1.63	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	638	TPO	CG2-CB-CA	-3.50	106.44	113.26
1	C	638	TPO	CG2-CB-CA	-3.18	107.07	113.26
1	C	657	SEP	O2P-P-OG	2.35	112.80	106.67
1	B	638	TPO	O-C-CA	-2.33	118.79	124.77
1	A	638	TPO	O3P-P-O2P	2.14	115.83	107.80

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	657	SEP	N-CA-CB-OG
1	A	657	SEP	C-CA-CB-OG
1	B	657	SEP	N-CA-CB-OG
1	B	657	SEP	C-CA-CB-OG
1	B	657	SEP	CB-OG-P-O1P
1	B	657	SEP	CB-OG-P-O2P
1	B	657	SEP	CB-OG-P-O3P
1	C	638	TPO	O-C-CA-CB
1	C	657	SEP	CB-OG-P-O1P
1	C	657	SEP	CB-OG-P-O2P
1	C	657	SEP	CB-OG-P-O3P
1	A	638	TPO	CB-OG1-P-O2P

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	638	TPO	2	0
1	B	657	SEP	1	0
1	A	638	TPO	2	0
1	C	638	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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
2	LW4	C	901	-	38,38,38	1.44	7 (18%)	52,56,56	2.45	20 (38%)
2	LW4	A	901	-	38,38,38	1.41	5 (13%)	52,56,56	2.31	19 (36%)
2	LW4	B	901	-	38,38,38	1.46	7 (18%)	52,56,56	2.65	23 (44%)

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
2	LW4	C	901	-	-	2/12/38/38	0/6/6/6
2	LW4	A	901	-	-	2/12/38/38	0/6/6/6
2	LW4	B	901	-	-	2/12/38/38	0/6/6/6

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	LW4	C6-N1	-3.51	1.31	1.37
2	C	901	LW4	C16-C21	-3.34	1.39	1.43
2	B	901	LW4	C6-N1	-3.34	1.31	1.37
2	A	901	LW4	C6-N1	-3.20	1.32	1.37
2	A	901	LW4	C4-C5	3.15	1.51	1.45
2	B	901	LW4	C6-C5	-3.03	1.33	1.38
2	B	901	LW4	C16-C21	-2.98	1.40	1.43
2	B	901	LW4	C4-C5	2.81	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	LW4	C6-C5	-2.74	1.34	1.38
2	B	901	LW4	C16-N17	2.66	1.34	1.32
2	C	901	LW4	C4-C5	2.65	1.50	1.45
2	C	901	LW4	C3-N1	-2.62	1.33	1.37
2	A	901	LW4	C6-C5	-2.60	1.34	1.38
2	A	901	LW4	C3-N1	-2.33	1.34	1.37
2	A	901	LW4	C16-C21	-2.32	1.40	1.43
2	C	901	LW4	C24-C22	2.19	1.41	1.36
2	B	901	LW4	C26-C28	2.18	1.41	1.36
2	B	901	LW4	C3-N1	-2.06	1.34	1.37
2	C	901	LW4	C26-C28	2.05	1.41	1.36

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	LW4	C16-N17-C18	7.47	123.54	116.27
2	B	901	LW4	C3-C4-C5	-7.42	101.86	106.62
2	C	901	LW4	C16-N17-C18	6.48	122.58	116.27
2	C	901	LW4	C3-C4-C5	-6.21	102.64	106.62
2	A	901	LW4	C3-C4-C5	-5.99	102.78	106.62
2	A	901	LW4	C16-N17-C18	5.73	121.85	116.27
2	C	901	LW4	C31-C34-N37	-5.01	102.80	110.86
2	A	901	LW4	C16-C21-C20	4.83	117.70	115.57
2	B	901	LW4	N19-C18-N17	-4.71	118.90	127.35
2	C	901	LW4	C9-C10-N11	4.46	109.31	106.64
2	B	901	LW4	C21-C16-N17	-4.32	118.86	122.19
2	A	901	LW4	N19-C18-N17	-4.30	119.64	127.35
2	A	901	LW4	C18-N19-C20	4.15	121.47	115.23
2	B	901	LW4	C9-C10-N11	4.09	109.09	106.64
2	C	901	LW4	N19-C18-N17	-3.95	120.26	127.35
2	C	901	LW4	C13-N11-C10	-3.80	107.32	111.36
2	A	901	LW4	C34-C31-N30	-3.77	102.85	110.78
2	B	901	LW4	C41-N30-C31	3.77	120.04	111.57
2	C	901	LW4	C41-N30-C31	3.67	119.81	111.57
2	C	901	LW4	C16-C21-C20	3.65	117.18	115.57
2	C	901	LW4	C18-N19-C20	3.62	120.67	115.23
2	C	901	LW4	C21-C16-N17	-3.60	119.41	122.19
2	B	901	LW4	C16-C21-C20	3.58	117.15	115.57
2	A	901	LW4	C9-C10-N11	3.57	108.78	106.64
2	A	901	LW4	C38-N37-C34	3.54	115.18	109.54
2	B	901	LW4	C44-N37-C38	3.44	117.20	110.63
2	B	901	LW4	C18-N19-C20	3.37	120.30	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	LW4	C41-C38-N37	-3.33	105.51	110.86
2	A	901	LW4	C13-N11-C10	-3.31	107.85	111.36
2	A	901	LW4	C21-C16-N17	-3.26	119.67	122.19
2	B	901	LW4	C3-N1-C6	3.24	111.96	109.08
2	B	901	LW4	C48-C4-C3	3.22	122.18	118.84
2	B	901	LW4	C13-N11-C10	-3.21	107.96	111.36
2	B	901	LW4	N19-C18-N30	3.17	121.72	117.92
2	B	901	LW4	C4-C5-C6	3.08	107.85	106.15
2	C	901	LW4	C44-N37-C34	3.06	116.46	110.63
2	A	901	LW4	C21-C20-N19	-2.98	119.64	122.80
2	A	901	LW4	C38-C41-N30	-2.97	104.53	110.78
2	A	901	LW4	C41-N30-C31	2.89	118.07	111.57
2	C	901	LW4	C44-N37-C38	2.83	116.03	110.63
2	C	901	LW4	C38-N37-C34	2.79	113.99	109.54
2	B	901	LW4	C44-N37-C34	2.77	115.90	110.63
2	C	901	LW4	C4-C3-N1	2.75	109.81	107.52
2	C	901	LW4	C34-C31-N30	-2.75	104.99	110.78
2	C	901	LW4	C21-C20-N19	-2.75	119.89	122.80
2	B	901	LW4	C8-C9-C10	-2.72	106.43	107.78
2	B	901	LW4	O15-C10-C9	-2.63	123.39	128.25
2	A	901	LW4	C3-N1-C6	2.56	111.36	109.08
2	C	901	LW4	O15-C10-C9	-2.55	123.53	128.25
2	C	901	LW4	C48-C4-C3	2.49	121.42	118.84
2	B	901	LW4	C50-C48-C4	-2.43	115.40	119.80
2	A	901	LW4	C48-C4-C3	2.39	121.32	118.84
2	A	901	LW4	O15-C10-C9	-2.33	123.94	128.25
2	A	901	LW4	N19-C18-N30	2.30	120.68	117.92
2	B	901	LW4	C38-C41-N30	-2.25	106.05	110.78
2	A	901	LW4	C4-C3-N1	2.19	109.35	107.52
2	C	901	LW4	C54-C3-N1	-2.16	127.28	130.74
2	B	901	LW4	C38-N37-C34	2.14	112.95	109.54
2	B	901	LW4	C22-C21-C16	-2.11	122.53	124.39
2	B	901	LW4	C4-C3-N1	2.11	109.28	107.52
2	A	901	LW4	C28-C20-C21	2.08	121.38	119.13
2	C	901	LW4	N19-C18-N30	2.06	120.38	117.92

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	LW4	C21-C16-C9-C8
2	B	901	LW4	C21-C16-C9-C8

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Mol	Chain	Res	Type	Atoms
2	C	901	LW4	C21-C16-C9-C8
2	C	901	LW4	C21-C16-C9-C10
2	A	901	LW4	C21-C16-C9-C10
2	B	901	LW4	C21-C16-C9-C10

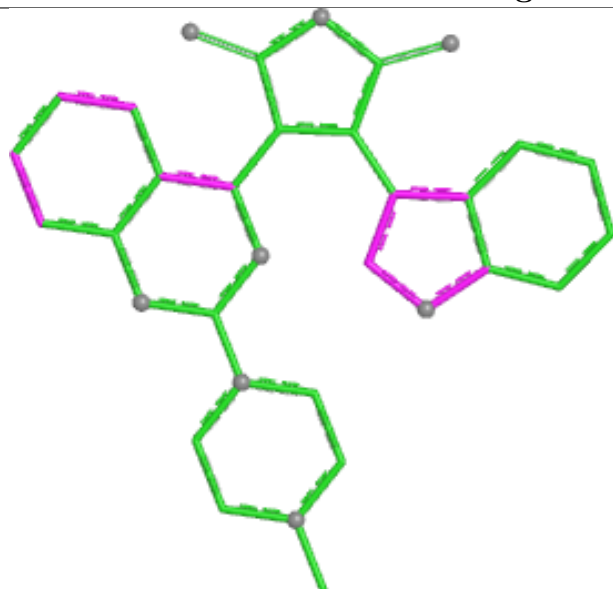
There are no ring outliers.

3 monomers are involved in 14 short contacts:

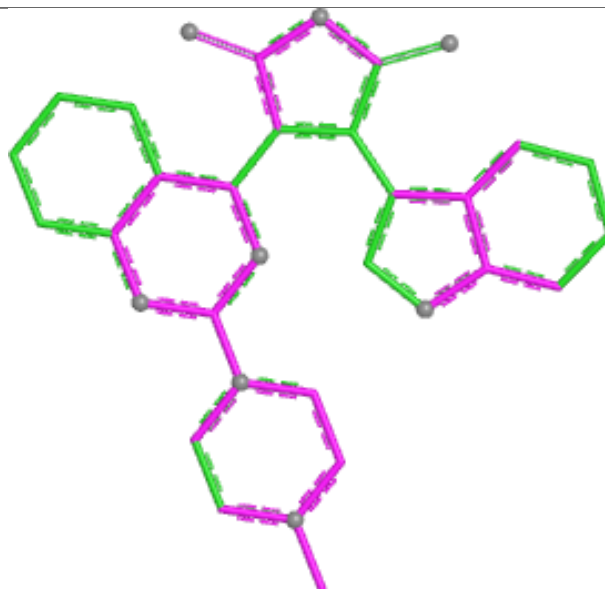
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	LW4	6	0
2	A	901	LW4	5	0
2	B	901	LW4	3	0

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 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.

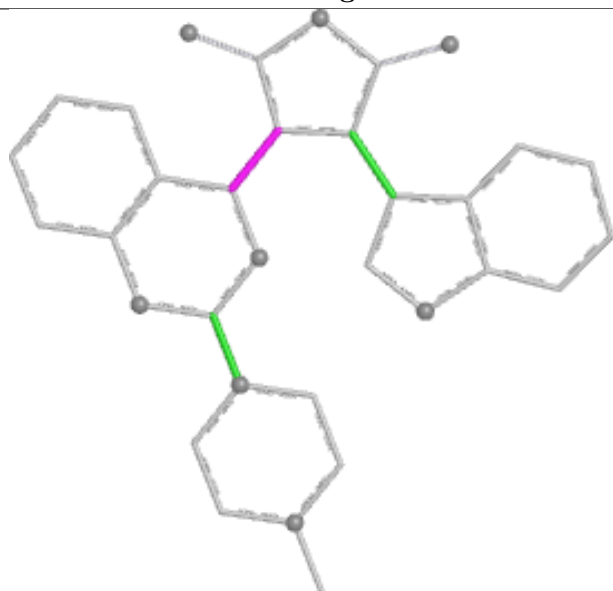
Ligand LW4 C 901



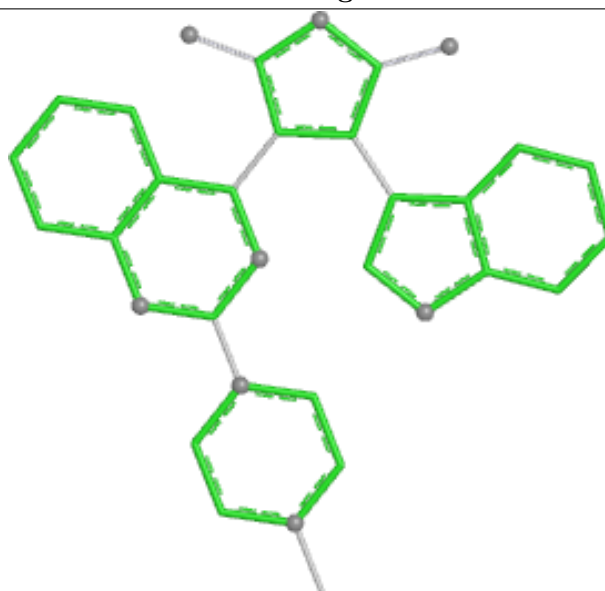
Bond lengths



Bond angles

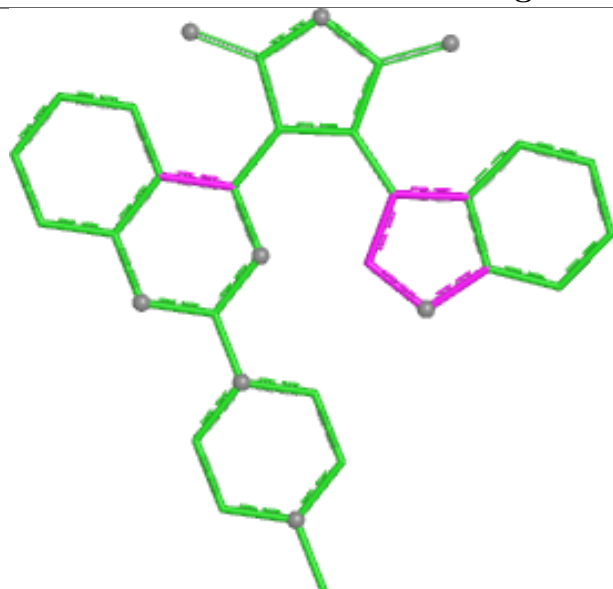


Torsions

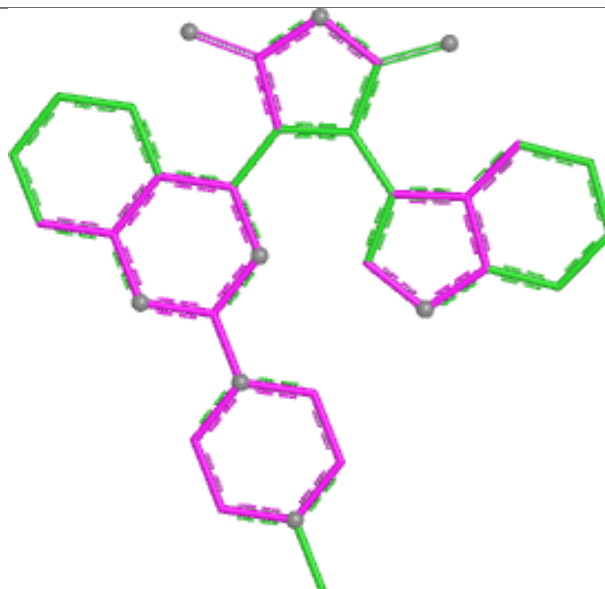


Rings

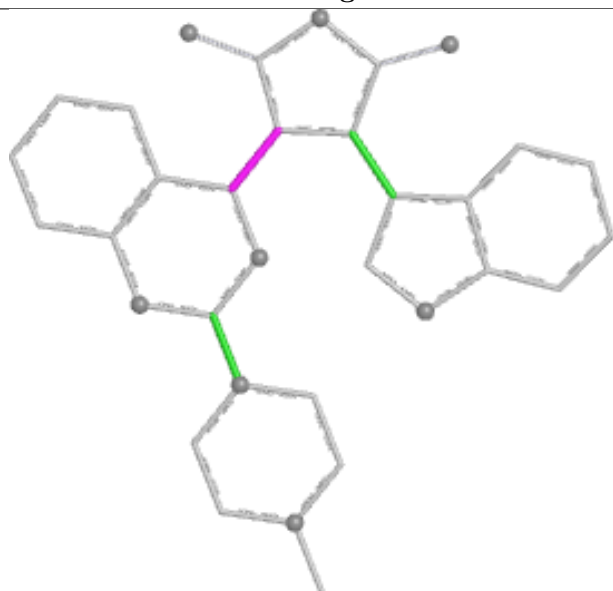
Ligand LW4 A 901



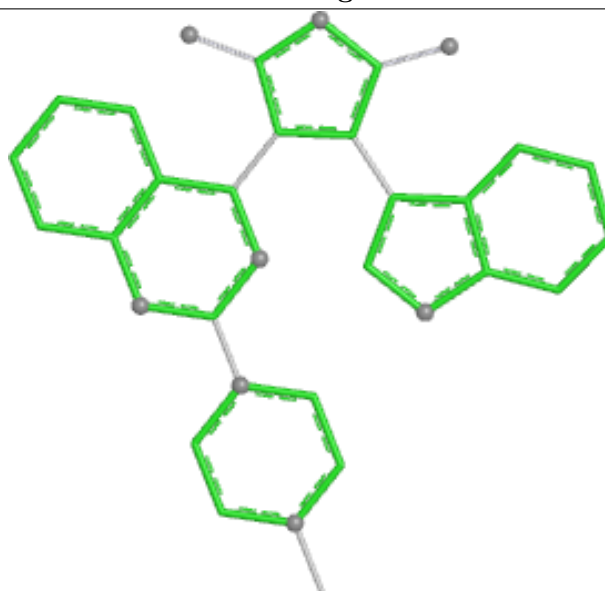
Bond lengths



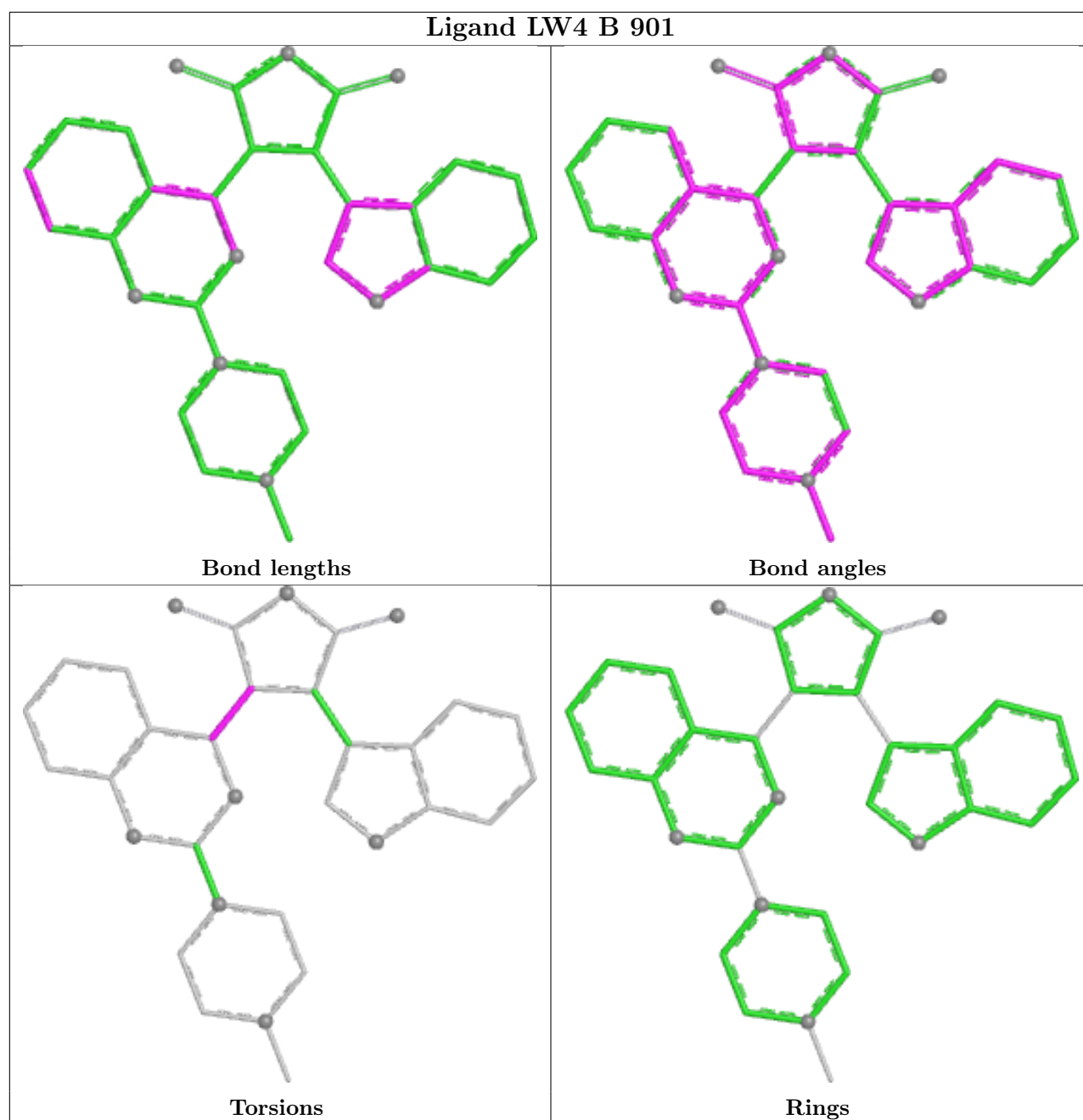
Bond angles



Torsions



Rings



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	330/360 (91%)	-0.28	0 100 100	18, 37, 61, 72	0
1	B	325/360 (90%)	-0.20	2 (0%) 85 80	21, 43, 70, 82	0
1	C	332/360 (92%)	-0.61	2 (0%) 85 80	16, 33, 53, 72	0
All	All	987/1080 (91%)	-0.36	4 (0%) 88 84	16, 38, 65, 82	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	666	PRO	2.5
1	B	490	MET	2.3
1	C	330	ASN	2.1
1	C	626	PHE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPO	C	638	11/12	0.79	0.11	50,52,74,75	0
1	TPO	B	638	11/12	0.81	0.12	50,53,71,72	0
1	TPO	A	638	11/12	0.89	0.09	63,65,69,70	0
1	SEP	A	657	10/11	0.94	0.07	33,34,44,46	0
1	SEP	B	657	10/11	0.95	0.06	30,32,49,50	0
1	SEP	C	657	10/11	0.95	0.07	27,28,40,41	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

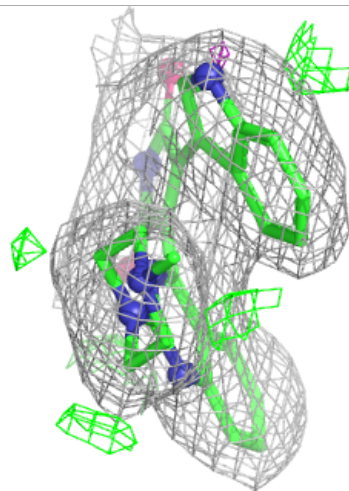
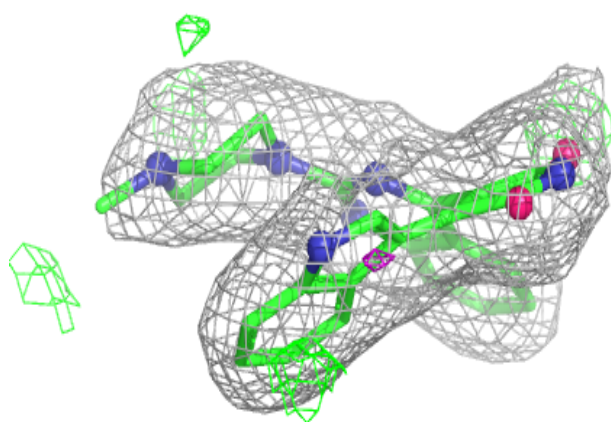
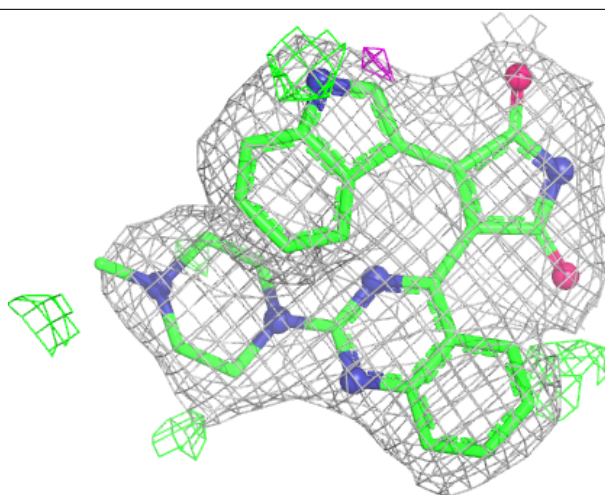
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LW4	A	901	33/33	0.94	0.07	26,32,36,38	0
2	LW4	B	901	33/33	0.94	0.07	23,30,33,39	0
2	LW4	C	901	33/33	0.97	0.06	20,28,35,38	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.

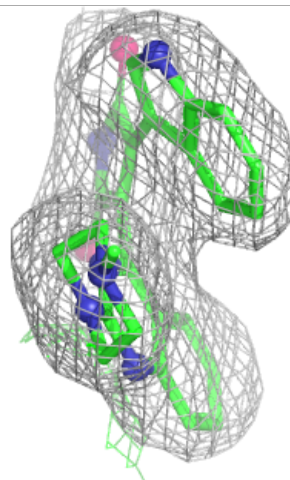
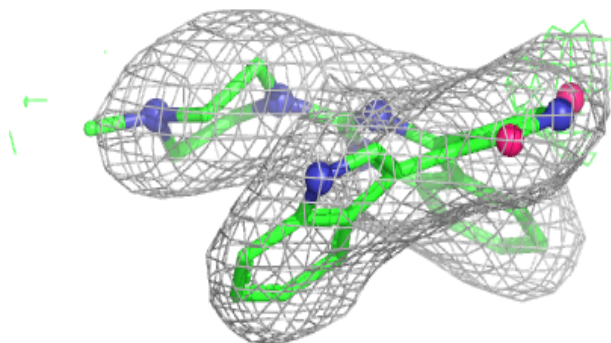
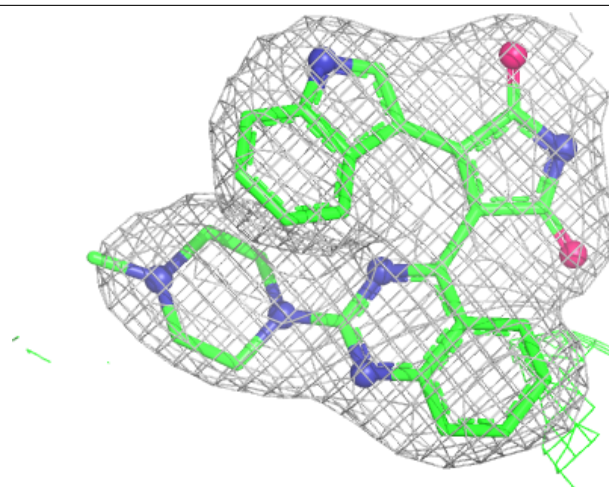
Electron density around LW4 A 901:

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



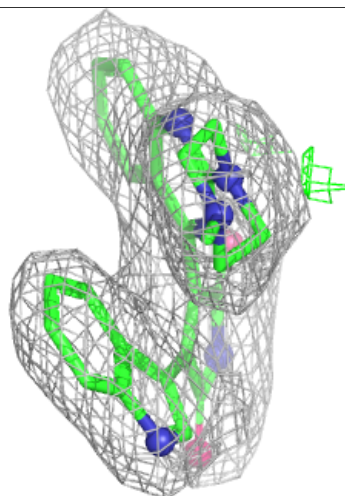
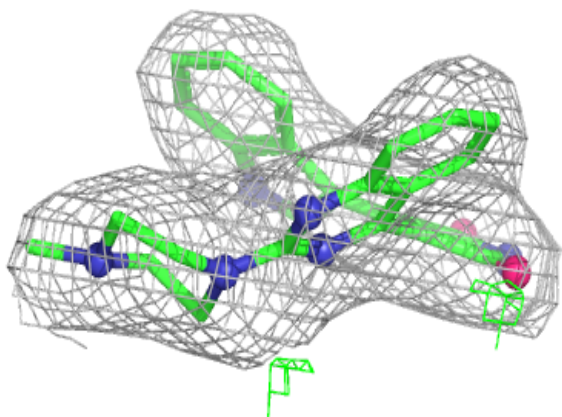
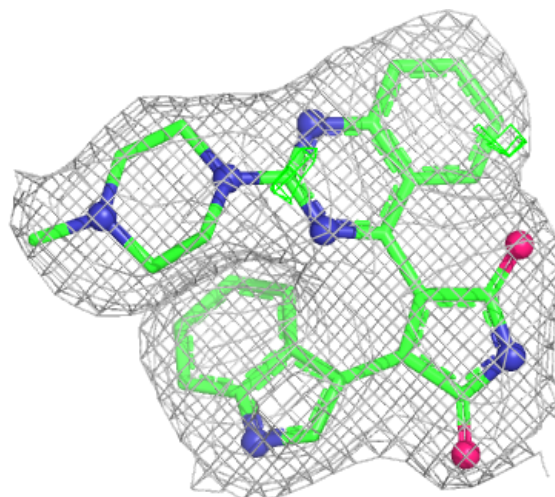
Electron density around LW4 B 901:

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



Electron density around LW4 C 901:

$2mF_o-DF_c$ (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.