



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:41 PM UTC

PDB ID : 7SVP / pdb_00007svp
Title : Structure of compound 34 bound to human Phospholipase D2 catalytic domain
Authors : Metrick, C.M.; Chodaparambil, J.V.
Deposited on : 2021-11-19
Resolution : 2.90 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

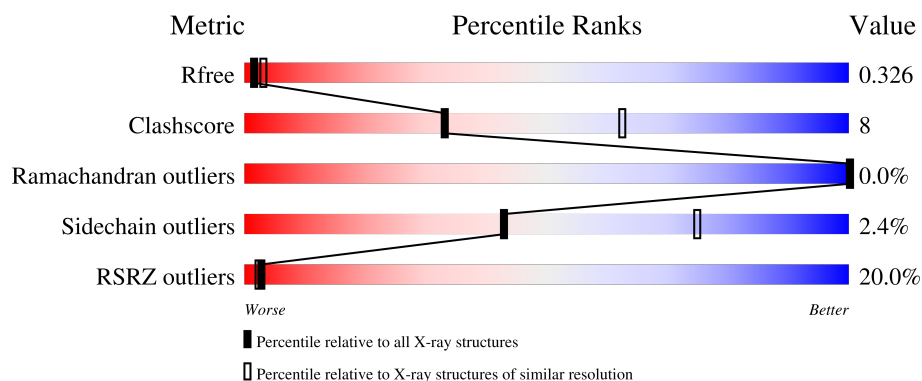
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	640	
1	B	640	
1	C	640	
1	D	640	

2 Entry composition [i](#)

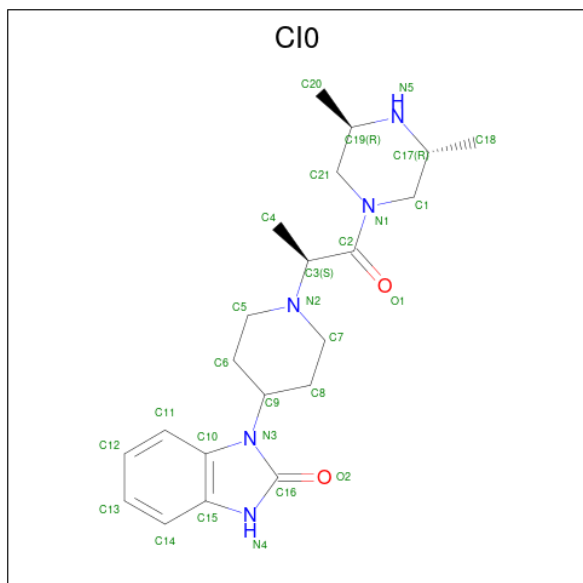
There are 3 unique types of molecules in this entry. The entry contains 17334 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospholipase D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	571	Total	C	N	O	S	0	0	0
			4453	2871	776	790	16			
1	A	555	Total	C	N	O	S	0	0	0
			4106	2626	724	740	16			
1	B	574	Total	C	N	O	S	0	1	0
			4412	2842	771	783	16			
1	D	550	Total	C	N	O	S	0	0	0
			4054	2606	712	723	13			

- Molecule 2 is 1-(1-{(2S)-1-[(3R,5R)-3,5-dimethylpiperazin-1-yl]-1-oxopropan-2-yl}piperidin-4-yl)-1,3-dihydro-2H-benzimidazol-2-one (CCD ID: C10) (formula: C₂₁H₃₁N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			28	21	5	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	21	5	2		
2	B	1	Total	C	N	O	0	0
			28	21	5	2		
2	D	1	Total	C	N	O	0	0
			28	21	5	2		

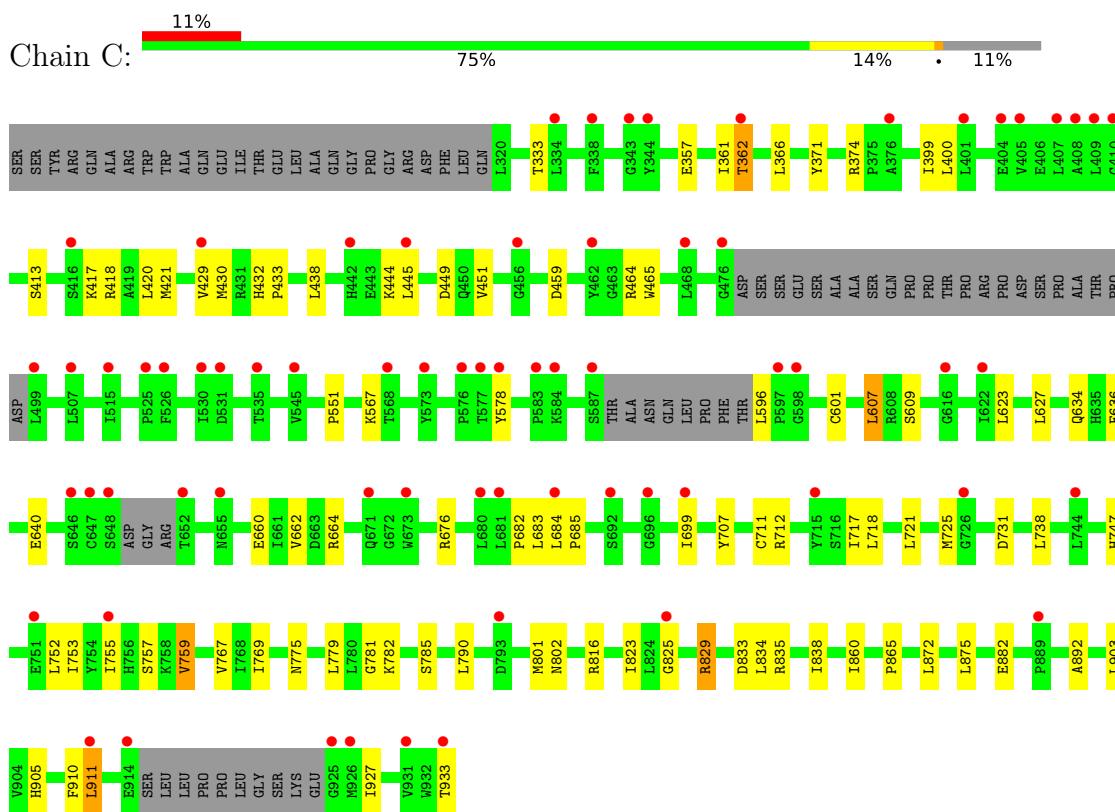
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	43	Total	O	0	0
			43	43		
3	A	45	Total	O	0	0
			45	45		
3	B	56	Total	O	0	0
			56	56		
3	D	53	Total	O	0	0
			53	53		

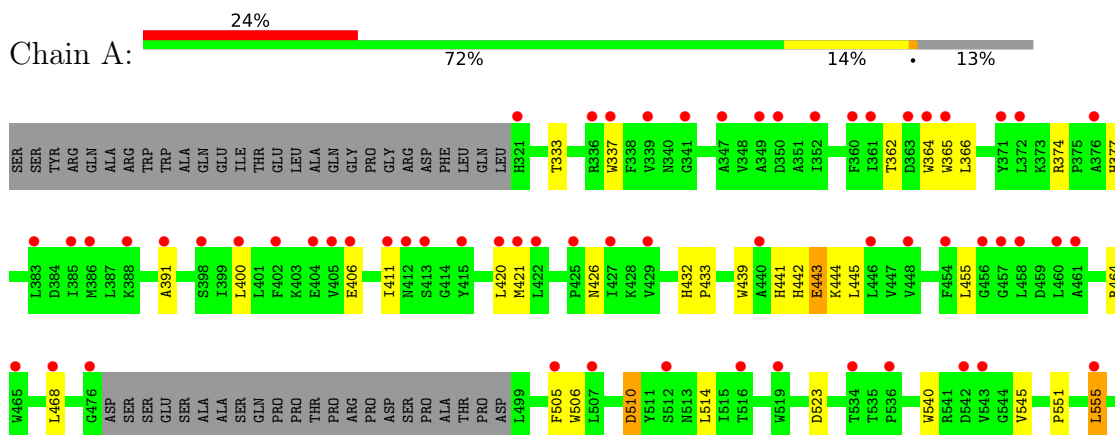
3 Residue-property plots

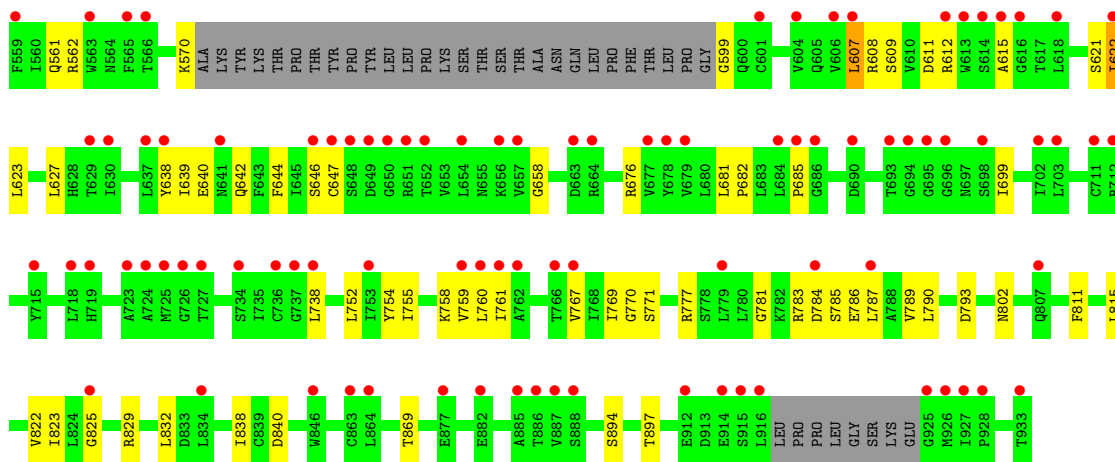
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phospholipase D2

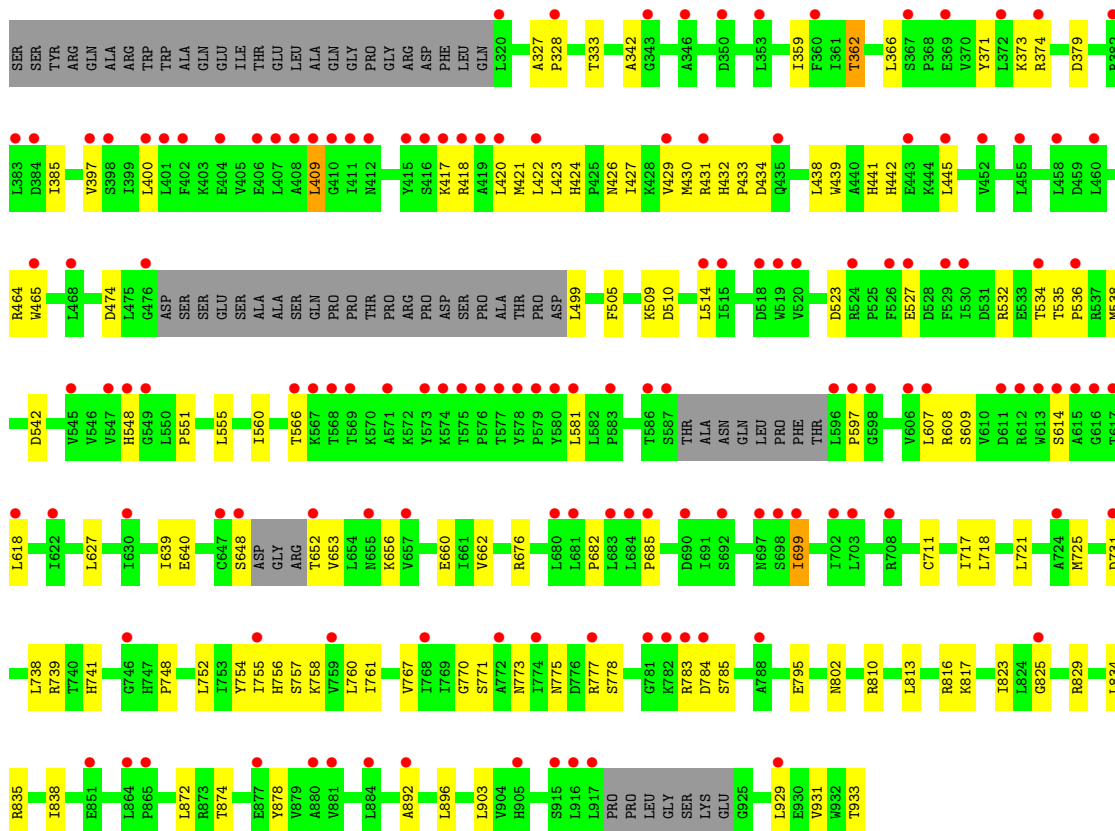


• Molecule 1: Phospholipase D2

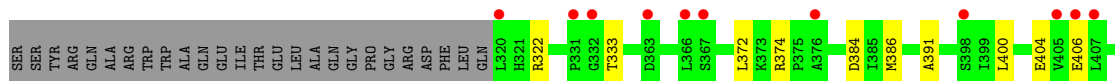


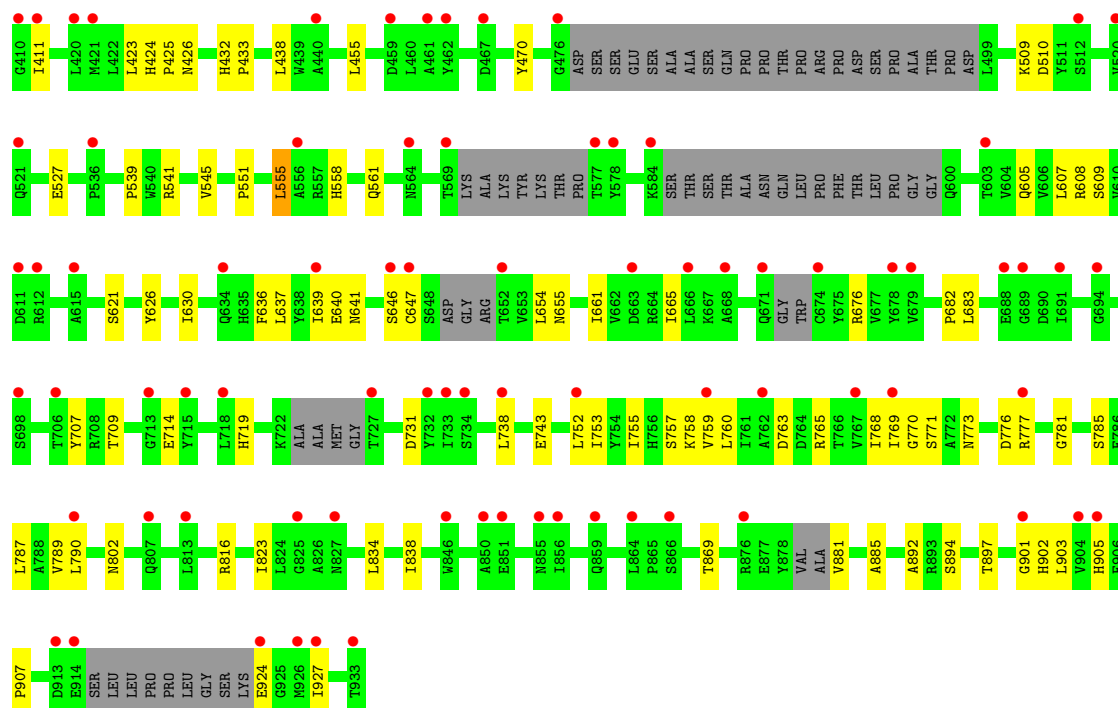


• Molecule 1: Phospholipase D2



• Molecule 1: Phospholipase D2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.72Å 132.24Å 113.86Å 90.00° 100.65° 90.00°	Depositor
Resolution (Å)	111.00 – 2.90 111.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (111.00-2.90) 99.2 (111.00-2.90)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.290 , 0.327 0.289 , 0.326	Depositor DCC
R_{free} test set	2853 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	60.8	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17334	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2774e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIO

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	0.09	0/4215	0.26	0/5770
1	B	0.09	0/4528	0.26	0/6179
1	C	0.11	0/4571	0.27	0/6232
1	D	0.09	0/4159	0.25	0/5693
All	All	0.10	0/17473	0.26	0/23874

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4106	0	3664	58	0
1	B	4412	0	4171	83	0
1	C	4453	0	4267	57	0
1	D	4054	0	3592	60	0
2	A	28	0	0	0	0
2	B	28	0	0	1	0
2	C	28	0	0	1	0
2	D	28	0	0	0	0
3	A	45	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	56	0	0	17	0
3	C	43	0	0	9	0
3	D	53	0	0	14	0
All	All	17334	0	15694	255	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 8.

All (255) 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:D:609:SER:O	1:D:785:SER:HA	1.60	1.00
1:C:361:ILE:O	3:C:1101:HOH:O	1.85	0.95
1:B:426:ASN:O	3:B:1101:HOH:O	1.84	0.94
1:B:609:SER:O	1:B:785:SER:HA	1.69	0.93
1:A:599:GLY:N	3:A:1101:HOH:O	2.04	0.89
1:D:470:TYR:O	3:D:1101:HOH:O	1.91	0.87
1:A:609:SER:O	1:A:785:SER:HA	1.77	0.84
1:D:881:VAL:N	3:D:1104:HOH:O	2.11	0.82
1:C:609:SER:O	1:C:785:SER:HA	1.79	0.82
1:B:608:ARG:O	3:B:1102:HOH:O	1.99	0.80
1:A:362:THR:HG22	1:A:400:LEU:HB2	1.64	0.80
1:C:707:TYR:HB3	1:C:712:ARG:HG3	1.65	0.78
1:D:630:ILE:HD12	1:D:637:LEU:HD21	1.66	0.77
1:D:777:ARG:NH1	3:D:1107:HOH:O	2.18	0.77
1:B:397:VAL:N	3:B:1101:HOH:O	2.17	0.76
1:B:371:TYR:HB2	1:B:374:ARG:HE	1.50	0.76
1:A:406:GLU:O	3:A:1102:HOH:O	2.05	0.75
1:C:429:VAL:O	3:C:1102:HOH:O	2.04	0.74
1:D:647:CYS:O	3:D:1102:HOH:O	2.07	0.71
1:B:777[B]:ARG:NH1	1:B:784:ASP:OD2	2.23	0.71
1:B:929:LEU:O	3:B:1103:HOH:O	2.10	0.70
1:D:759:VAL:HG22	1:D:769:ILE:HG12	1.74	0.70
1:A:738:LEU:HD21	1:A:823:ILE:HG13	1.74	0.69
1:A:570:LYS:O	3:A:1103:HOH:O	2.09	0.69
1:B:532:ARG:NH1	3:B:1105:HOH:O	2.23	0.69
1:B:474:ASP:O	3:B:1105:HOH:O	2.12	0.68
1:B:424:HIS:O	3:B:1104:HOH:O	2.12	0.68
1:B:652:THR:O	3:B:1106:HOH:O	2.13	0.67
1:A:642:GLN:NE2	1:A:754:TYR:OH	2.26	0.66
1:B:427:ILE:O	3:B:1104:HOH:O	2.13	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:THR:HA	3:C:1101:HOH:O	1.94	0.65
1:B:442:HIS:HB2	1:B:777[B]:ARG:HH12	1.62	0.65
1:A:443:GLU:HG2	3:A:1107:HOH:O	1.98	0.63
1:B:374:ARG:NH2	3:B:1108:HOH:O	2.22	0.63
1:B:442:HIS:NE2	3:B:1118:HOH:O	2.31	0.62
1:D:561:GLN:NE2	3:D:1113:HOH:O	2.32	0.62
1:B:711:CYS:HB3	1:B:718:LEU:HD12	1.82	0.61
1:D:404:GLU:HB3	1:D:411:ILE:HD11	1.82	0.61
1:A:676:ARG:NH2	1:A:840:ASP:OD1	2.31	0.61
1:C:609:SER:HB3	1:C:781:GLY:HA2	1.83	0.60
1:D:609:SER:HB3	1:D:781:GLY:HA2	1.84	0.60
1:C:438:LEU:HD21	1:D:438:LEU:HD21	1.84	0.60
1:A:627:LEU:O	3:A:1104:HOH:O	2.16	0.60
1:A:609:SER:HB3	1:A:781:GLY:HA2	1.83	0.60
1:B:777[B]:ARG:NH2	1:B:778:SER:OG	2.34	0.59
1:C:816:ARG:NH2	1:C:834:LEU:O	2.35	0.59
1:B:816:ARG:NH2	1:B:834:LEU:O	2.35	0.59
1:B:682:PRO:HD3	1:B:755:ILE:HB	1.84	0.58
1:D:709:THR:OG1	3:D:1103:HOH:O	2.10	0.58
1:C:627:LEU:HD22	1:C:660:GLU:HG3	1.84	0.58
1:C:640:GLU:HB3	1:C:759:VAL:HG13	1.86	0.58
1:C:374:ARG:NH2	3:C:1116:HOH:O	2.36	0.58
1:D:683:LEU:HB2	1:D:752:LEU:HD22	1.86	0.57
1:D:707:TYR:OH	3:D:1106:HOH:O	2.16	0.57
1:B:342:ALA:HA	1:B:465:TRP:NE1	2.20	0.57
1:C:361:ILE:HB	1:C:399:ILE:HG12	1.86	0.57
1:A:829:ARG:HB3	1:A:832:LEU:HD13	1.85	0.57
1:A:443:GLU:HB3	1:A:786:GLU:HA	1.86	0.57
1:D:802:ASN:HB2	1:D:838:ILE:HD11	1.85	0.57
1:D:626:TYR:O	1:D:630:ILE:HG12	2.05	0.57
1:D:455:LEU:HD11	1:D:789:VAL:HG13	1.87	0.56
1:B:648:SER:HA	1:B:653:VAL:HG23	1.87	0.56
1:B:685:PRO:HD2	1:B:699:ILE:HG13	1.86	0.56
1:B:795:GLU:OE1	1:B:810:ARG:NH1	2.38	0.56
1:A:442:HIS:O	1:A:444:LYS:NZ	2.38	0.56
1:B:509:LYS:NZ	1:B:527:GLU:O	2.37	0.56
1:D:641:ASN:HD21	1:D:773:ASN:HA	1.70	0.56
1:D:816:ARG:NH2	1:D:834:LEU:O	2.38	0.56
1:D:509:LYS:NZ	1:D:527:GLU:O	2.34	0.56
1:B:738:LEU:HD21	1:B:823:ILE:HG13	1.87	0.56
1:C:685:PRO:HD2	1:C:699:ILE:HG23	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:639:ILE:HG12	1:D:760:LEU:HD13	1.87	0.55
1:C:366:LEU:HD22	1:C:420:LEU:HD11	1.89	0.55
1:A:333:THR:HG21	1:A:551:PRO:HG2	1.89	0.55
1:C:738:LEU:HB3	1:C:753:ILE:HB	1.89	0.55
1:B:362:THR:HG23	1:B:445:LEU:HB3	1.89	0.54
1:B:532:ARG:NH2	3:B:1123:HOH:O	2.39	0.54
1:B:802:ASN:HB2	1:B:838:ILE:HD11	1.87	0.54
1:C:683:LEU:HB2	1:C:752:LEU:HD22	1.88	0.54
1:A:611:ASP:OD1	1:A:612:ARG:N	2.40	0.54
1:B:359:ILE:HB	1:B:397:VAL:HG22	1.90	0.54
1:D:541:ARG:NE	1:D:640:GLU:OE2	2.41	0.54
1:A:685:PRO:HD2	1:A:699:ILE:HG23	1.87	0.54
1:A:545:VAL:HG11	1:A:789:VAL:HG21	1.89	0.54
1:B:538:MET:HE2	1:B:754:TYR:HB2	1.89	0.54
1:D:391:ALA:HB1	1:D:426:ASN:HB2	1.90	0.54
1:A:607:LEU:HD11	1:A:790:LEU:HB2	1.88	0.54
1:B:627:LEU:HD22	1:B:660:GLU:HG3	1.90	0.54
1:D:545:VAL:HG11	1:D:789:VAL:HG21	1.90	0.54
1:A:464:ARG:HB2	3:A:1111:HOH:O	2.08	0.53
1:C:927:ILE:HD13	1:D:927:ILE:HD13	1.90	0.53
1:A:364:TRP:CZ2	1:A:411:ILE:HD11	2.43	0.53
1:B:823:ILE:HG23	1:B:903:LEU:HB2	1.90	0.53
1:C:802:ASN:HB2	1:C:838:ILE:HD11	1.90	0.53
1:D:760:LEU:HD23	1:D:768:ILE:HD12	1.91	0.53
1:D:621:SER:N	3:D:1108:HOH:O	2.41	0.52
1:C:711:CYS:HB3	1:C:718:LEU:HD12	1.92	0.52
1:B:379:ASP:HB3	1:B:385:ILE:HG13	1.90	0.52
1:D:322:ARG:NH1	1:D:605:GLN:OE1	2.43	0.52
1:D:743:GLU:O	3:D:1109:HOH:O	2.19	0.52
1:C:400:LEU:HD23	1:C:430:MET:HB2	1.89	0.52
1:C:418:ARG:NH2	3:C:1118:HOH:O	2.41	0.52
1:A:464:ARG:HG3	1:A:540:TRP:NE1	2.25	0.52
1:C:833:ASP:OD1	1:C:835:ARG:NH1	2.43	0.52
1:C:634:GLN:HA	1:C:664:ARG:HH21	1.75	0.52
1:C:636:PHE:HB3	1:C:838:ILE:HG22	1.92	0.52
1:A:646:SER:HG	1:A:658:GLY:H	1.57	0.52
1:B:464:ARG:NH2	2:B:1001:ClO:O1	2.42	0.52
1:C:676:ARG:NH1	1:C:731:ASP:O	2.40	0.51
1:A:640:GLU:HB2	1:A:759:VAL:HG12	1.93	0.51
1:B:676:ARG:NH1	1:B:731:ASP:O	2.44	0.51
1:C:823:ILE:HG23	1:C:903:LEU:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:THR:HG21	1:D:551:PRO:HG2	1.92	0.51
1:D:608:ARG:O	3:D:1108:HOH:O	2.19	0.51
1:A:365:TRP:CD1	1:A:411:ILE:HG23	2.46	0.51
1:B:773:ASN:HD22	1:B:777[B]:ARG:HH21	1.59	0.51
1:A:759:VAL:HG23	1:A:769:ILE:HG12	1.93	0.51
1:A:802:ASN:HB2	1:A:838:ILE:HD11	1.92	0.51
1:C:825:GLY:O	1:C:829:ARG:N	2.44	0.51
1:D:641:ASN:HA	1:D:757:SER:O	2.12	0.50
1:D:738:LEU:HD21	1:D:823:ILE:HG13	1.94	0.50
1:D:901:GLY:O	3:D:1105:HOH:O	2.20	0.50
1:C:721:LEU:O	1:C:725:MET:HG2	2.12	0.49
1:A:374:ARG:NH2	1:A:510:ASP:OD2	2.45	0.49
1:A:638:TYR:OH	1:A:640:GLU:OE2	2.20	0.49
1:B:761:ILE:HG12	1:B:767:VAL:HG22	1.95	0.49
1:A:639:ILE:HG12	1:A:760:LEU:HD12	1.94	0.48
1:B:560:ILE:HG12	1:B:581:LEU:HB3	1.95	0.48
1:B:366:LEU:HD22	1:B:420:LEU:HD11	1.94	0.48
1:B:523:ASP:OD1	1:B:523:ASP:N	2.45	0.48
1:D:384:ASP:HB2	1:D:423:LEU:HD21	1.95	0.48
1:D:432:HIS:CG	1:D:433:PRO:HA	2.48	0.48
1:A:793:ASP:OD2	1:A:811:PHE:N	2.43	0.48
1:A:825:GLY:O	1:A:829:ARG:N	2.46	0.48
1:B:499:LEU:N	3:B:1130:HOH:O	2.47	0.48
1:D:758:LYS:HD3	1:D:771:SER:HA	1.96	0.48
1:D:823:ILE:HG23	1:D:903:LEU:HB2	1.96	0.48
1:C:400:LEU:O	3:C:1101:HOH:O	2.20	0.48
1:C:432:HIS:CG	1:C:433:PRO:HA	2.49	0.48
1:A:682:PRO:HD3	1:A:755:ILE:HB	1.95	0.48
1:A:894:SER:O	1:A:897:THR:OG1	2.32	0.48
1:B:333:THR:HG21	1:B:551:PRO:HG2	1.96	0.48
1:B:430:MET:HE3	1:B:566:THR:HB	1.96	0.48
1:A:441:HIS:CE1	1:A:562:ARG:HH12	2.31	0.47
1:A:561:GLN:HE21	1:A:615:ALA:HB1	1.79	0.47
1:B:441:HIS:HE1	1:B:614:SER:HB2	1.80	0.47
1:D:676:ARG:NH1	1:D:731:ASP:O	2.46	0.47
1:C:464:ARG:NH2	2:C:1001:ClO:O1	2.45	0.47
1:C:684:LEU:HG	1:C:865:PRO:HD3	1.96	0.47
1:B:758:LYS:HB2	1:B:770:GLY:O	2.15	0.47
1:D:758:LYS:HB2	1:D:770:GLY:O	2.14	0.47
1:A:758:LYS:HB2	1:A:770:GLY:O	2.15	0.46
1:B:775:ASN:HB2	1:B:933:THR:C	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:LEU:HD12	1:D:386:MET:HE1	1.97	0.46
1:B:721:LEU:O	1:B:725:MET:HG2	2.16	0.46
1:A:391:ALA:HB1	1:A:426:ASN:HB2	1.98	0.46
1:A:758:LYS:HD3	1:A:771:SER:HA	1.98	0.46
1:B:656:LYS:NZ	3:B:1127:HOH:O	2.44	0.46
1:A:432:HIS:CG	1:A:433:PRO:HA	2.51	0.46
1:C:333:THR:HG21	1:C:551:PRO:HG2	1.98	0.46
1:C:711:CYS:HA	1:C:718:LEU:HB2	1.97	0.46
1:B:434:ASP:N	3:B:1120:HOH:O	2.36	0.46
1:B:359:ILE:O	1:B:397:VAL:HA	2.15	0.46
1:C:738:LEU:HD11	1:C:823:ILE:HG13	1.96	0.46
1:C:747:HIS:NE2	3:C:1115:HOH:O	2.36	0.46
1:D:894:SER:O	1:D:897:THR:OG1	2.34	0.46
1:B:418:ARG:O	1:B:421:MET:HG3	2.16	0.45
1:B:825:GLY:O	1:B:829:ARG:N	2.48	0.45
1:C:767:VAL:HG12	1:C:769:ILE:HG13	1.99	0.45
1:B:420:LEU:HB2	1:B:429:VAL:HG21	1.99	0.45
1:C:449:ASP:O	1:C:451:VAL:HG23	2.16	0.45
1:B:374:ARG:NH2	1:B:510:ASP:OD2	2.36	0.45
1:B:542:ASP:OD2	1:B:756:HIS:ND1	2.42	0.45
1:D:768:ILE:HG12	1:D:790:LEU:HD13	1.97	0.45
1:D:374:ARG:NH2	1:D:510:ASP:OD2	2.49	0.45
1:B:439:TRP:HB3	1:B:783:ARG:O	2.16	0.45
1:C:596:LEU:N	3:C:1123:HOH:O	2.50	0.45
1:B:874:THR:O	1:B:878:TYR:HB2	2.17	0.45
1:D:714:GLU:HA	1:D:719:HIS:ND1	2.32	0.45
1:D:885:ALA:HA	1:D:892:ALA:HB2	1.98	0.45
1:D:424:HIS:CG	1:D:425:PRO:HD2	2.51	0.45
1:C:910:PHE:CZ	1:C:911:LEU:HD23	2.52	0.45
1:C:444:LYS:NZ	1:C:459:ASP:OD2	2.48	0.44
1:D:682:PRO:HD3	1:D:755:ILE:HB	1.98	0.44
1:C:682:PRO:HB3	1:C:755:ILE:H	1.82	0.44
1:B:548:HIS:NE2	1:B:597:PRO:HD2	2.33	0.44
1:C:682:PRO:HD3	1:C:755:ILE:HB	1.99	0.44
1:B:639:ILE:HG12	1:B:760:LEU:HD12	2.00	0.44
1:D:902:HIS:HA	3:D:1105:HOH:O	2.16	0.44
1:A:506:TRP:HB3	1:A:510:ASP:HB3	2.00	0.44
1:B:417:LYS:HD3	1:B:431:ARG:HD3	2.00	0.44
1:D:924:GLU:N	3:D:1123:HOH:O	2.51	0.44
1:C:567:LYS:HE2	1:C:578:TYR:O	2.18	0.44
1:A:468:LEU:HD23	1:A:822:VAL:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:LYS:HD3	1:B:771:SER:HA	2.00	0.44
1:C:662:VAL:HG22	1:C:717:ILE:HG23	2.00	0.43
1:B:748:PRO:HG2	1:B:892:ALA:HB3	2.00	0.43
1:B:432:HIS:CG	1:B:433:PRO:HA	2.54	0.43
1:B:741:HIS:CD2	1:B:896:LEU:HD13	2.52	0.43
1:C:417:LYS:HG2	1:C:421:MET:HE2	2.01	0.43
1:C:371:TYR:O	1:C:374:ARG:NE	2.49	0.43
1:B:777[A]:ARG:HD2	1:B:931:VAL:O	2.19	0.43
1:D:646:SER:HA	1:D:655:ASN:HD21	1.84	0.43
1:C:775:ASN:HB2	1:C:933:THR:C	2.44	0.43
1:A:366:LEU:HD22	1:A:420:LEU:HD11	2.01	0.43
1:D:907:PRO:HG2	3:D:1106:HOH:O	2.18	0.43
1:C:640:GLU:HG2	1:C:757:SER:HB2	2.01	0.42
1:A:439:TRP:CD2	1:A:783:ARG:HB3	2.53	0.42
1:C:607:LEU:HD11	1:C:790:LEU:HB2	2.01	0.42
1:C:875:LEU:HD22	1:C:911:LEU:HD21	2.02	0.42
1:D:636:PHE:HB3	1:D:838:ILE:HG22	2.02	0.42
1:A:443:GLU:HA	1:A:771:SER:OG	2.19	0.42
1:A:608:ARG:H	1:A:621:SER:HG	1.67	0.42
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.74	0.42
1:A:644:PHE:HB3	1:A:681:LEU:HD21	2.02	0.42
1:C:623:LEU:HD13	1:C:779:LEU:HB3	2.01	0.42
1:D:763:ASP:O	1:D:765:ARG:HG3	2.20	0.42
1:C:374:ARG:HD3	1:C:465:TRP:CE2	2.54	0.42
1:D:400:LEU:HD12	1:D:400:LEU:HA	1.92	0.42
1:B:362:THR:CG2	1:B:445:LEU:HB3	2.48	0.42
1:B:441:HIS:CE1	1:B:614:SER:HB2	2.54	0.42
1:B:445:LEU:HD11	1:B:555:LEU:HD13	2.02	0.42
1:C:860:ILE:HG23	1:C:892:ALA:HB1	2.02	0.42
1:B:739:ARG:HA	1:B:752:LEU:HA	2.01	0.42
1:D:558:HIS:CD2	1:D:787:LEU:HD21	2.54	0.42
1:B:327:ALA:HA	1:B:328:PRO:HD3	1.94	0.42
1:A:337:TRP:HD1	1:A:811:PHE:CE1	2.38	0.41
1:C:664:ARG:HA	1:C:664:ARG:HD2	1.89	0.41
1:A:777:ARG:O	1:A:784:ASP:HB2	2.20	0.41
1:B:373:LYS:C	1:B:374:ARG:HD2	2.45	0.41
1:D:555:LEU:HD13	1:D:555:LEU:HA	1.90	0.41
1:D:654:LEU:N	1:D:776:ASP:OD2	2.48	0.41
1:C:362:THR:OG1	1:C:445:LEU:HB3	2.21	0.41
1:A:767:VAL:HG12	1:A:769:ILE:HG13	2.03	0.41
1:B:532:ARG:HD3	3:B:1105:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:ARG:HG2	1:B:505:PHE:O	2.21	0.41
1:B:400:LEU:HD23	1:B:430:MET:HB3	2.03	0.41
1:B:777[A]:ARG:HG3	1:B:933:THR:O	2.21	0.41
1:A:555:LEU:HD13	1:A:555:LEU:HA	1.90	0.41
1:A:607:LEU:HB2	1:A:622:ILE:HG22	2.02	0.41
1:B:662:VAL:HG22	1:B:717:ILE:HG23	2.02	0.41
1:A:443:GLU:HG3	1:A:787:LEU:HG	2.02	0.41
1:A:622:ILE:HG13	1:A:623:LEU:N	2.36	0.41
1:A:647:CYS:O	3:A:1105:HOH:O	2.22	0.41
1:A:761:ILE:HD11	1:A:815:LEU:HD23	2.01	0.41
1:B:933:THR:N	3:B:1103:HOH:O	2.45	0.41
1:D:661:ILE:O	1:D:665:ILE:HG12	2.21	0.41
1:B:738:LEU:HD12	1:B:755:ILE:HD11	2.02	0.41
1:B:813:LEU:HD11	1:B:817:LYS:HE3	2.02	0.41
1:B:640:GLU:HG2	1:B:757:SER:HB2	2.03	0.40
1:A:377:HIS:HB3	1:B:835:ARG:NH1	2.36	0.40
1:D:539:PRO:HB2	1:D:753:ILE:HG23	2.02	0.40
1:A:374:ARG:NH1	1:A:505:PHE:O	2.54	0.40
1:B:535:THR:HA	1:B:536:PRO:HD3	1.96	0.40
1:C:601:CYS:SG	3:C:1106:HOH:O	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	547/640 (86%)	529 (97%)	18 (3%)	0	100	100
1	B	565/640 (88%)	551 (98%)	14 (2%)	0	100	100
1	C	561/640 (88%)	546 (97%)	15 (3%)	0	100	100
1	D	532/640 (83%)	511 (96%)	20 (4%)	1 (0%)	43	72
All	All	2205/2560 (86%)	2137 (97%)	67 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	406	GLU

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	377/554 (68%)	365 (97%)	12 (3%)	34	68
1	B	436/554 (79%)	425 (98%)	11 (2%)	42	74
1	C	451/554 (81%)	439 (97%)	12 (3%)	39	73
1	D	365/554 (66%)	361 (99%)	4 (1%)	65	88
All	All	1629/2216 (74%)	1590 (98%)	39 (2%)	43	75

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	357	GLU
1	C	362	THR
1	C	413	SER
1	C	607	LEU
1	C	759	VAL
1	C	782	LYS
1	C	801	MET
1	C	829	ARG
1	C	872	LEU
1	C	882	GLU
1	C	905	HIS
1	C	911	LEU
1	A	421	MET
1	A	443	GLU
1	A	445	LEU
1	A	455	LEU
1	A	510	ASP
1	A	514	LEU
1	A	523	ASP

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Mol	Chain	Res	Type
1	A	555	LEU
1	A	607	LEU
1	A	622	ILE
1	A	752	LEU
1	A	869	THR
1	B	362	THR
1	B	409	LEU
1	B	422	LEU
1	B	423	LEU
1	B	438	LEU
1	B	514	LEU
1	B	534	THR
1	B	607	LEU
1	B	618	LEU
1	B	699	ILE
1	B	872	LEU
1	D	555	LEU
1	D	607	LEU
1	D	869	THR
1	D	905	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	624	ASN
1	C	628	HIS
1	A	321	HIS
1	A	377	HIS
1	A	513	ASN
1	A	902	HIS
1	B	635	HIS
1	B	642	GLN
1	B	773	ASN
1	D	426	ASN
1	D	561	GLN
1	D	635	HIS
1	D	655	ASN

5.3.3 RNA ⓘ

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](#)

4 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	CI0	D	1001	-	31,31,31	0.33	0	44,45,45	0.59	0
2	CI0	C	1001	-	31,31,31	0.33	0	44,45,45	0.48	0
2	CI0	A	1001	-	31,31,31	0.29	0	44,45,45	0.49	0
2	CI0	B	1001	-	31,31,31	0.28	0	44,45,45	0.47	0

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	CI0	D	1001	-	-	4/16/38/38	0/4/4/4
2	CI0	C	1001	-	-	4/16/38/38	0/4/4/4
2	CI0	A	1001	-	-	4/16/38/38	0/4/4/4
2	CI0	B	1001	-	-	5/16/38/38	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

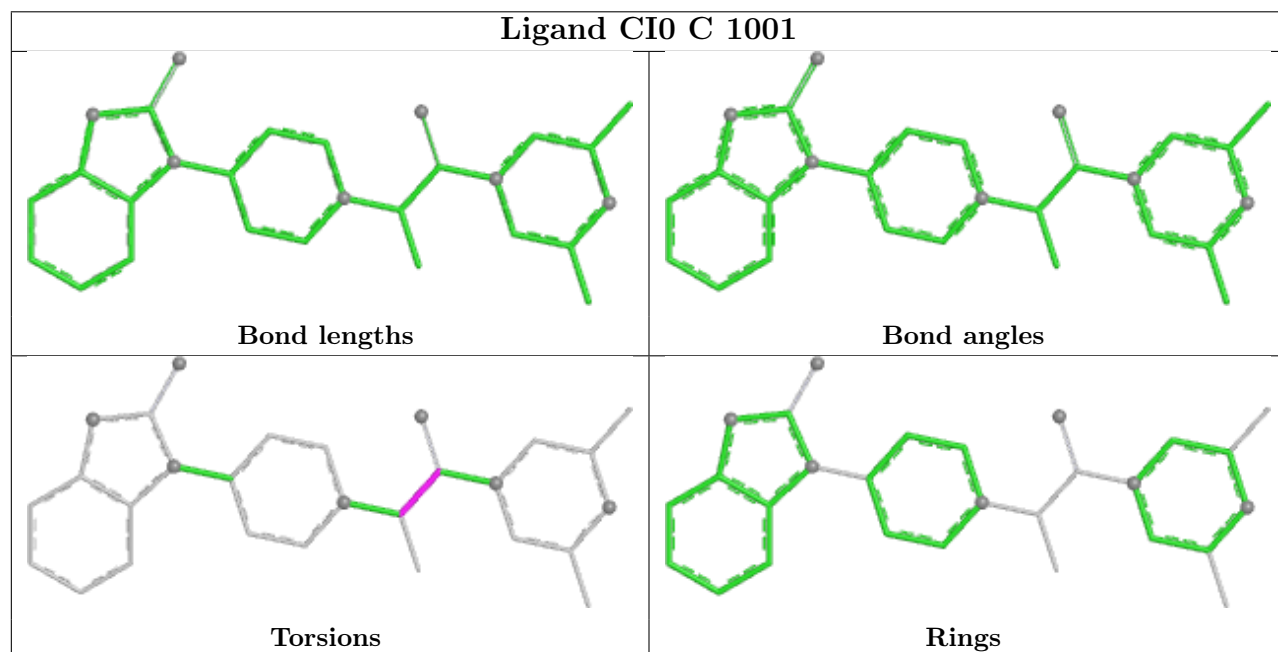
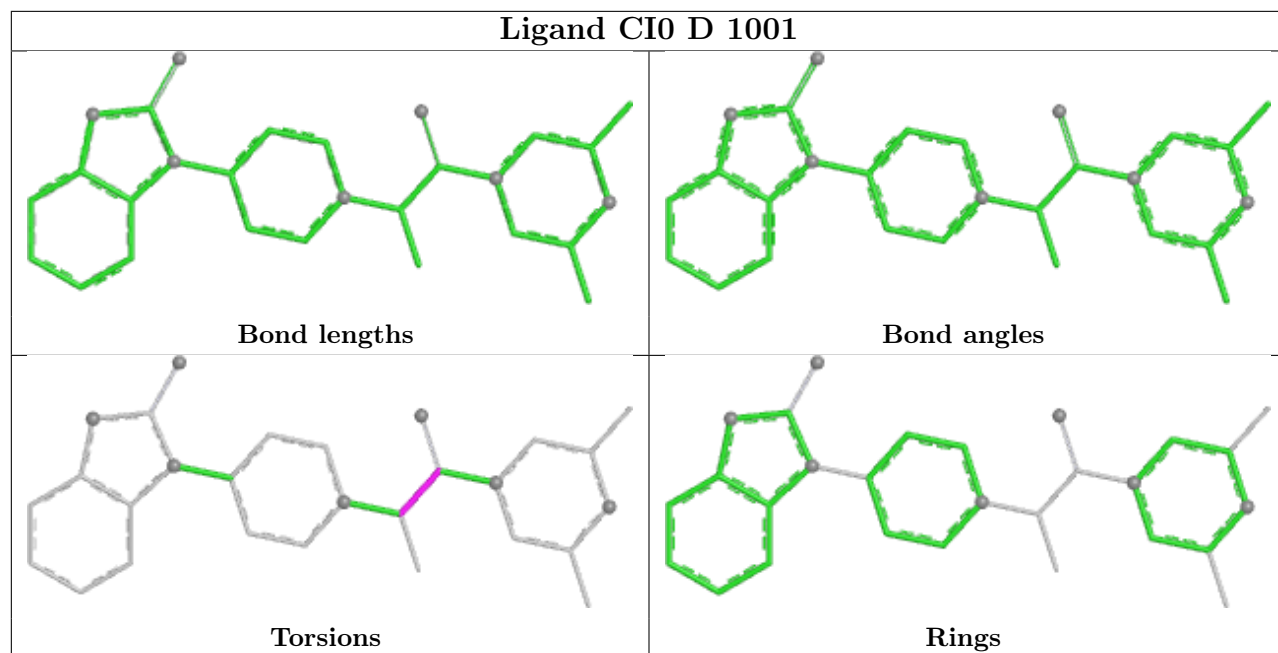
Mol	Chain	Res	Type	Atoms
2	B	1001	CI0	C3-C2-N1-C21
2	B	1001	CI0	O1-C2-N1-C21
2	B	1001	CI0	C3-C2-N1-C1
2	B	1001	CI0	O1-C2-N1-C1
2	C	1001	CI0	O1-C2-C3-C4
2	C	1001	CI0	N1-C2-C3-C4
2	A	1001	CI0	N1-C2-C3-C4
2	D	1001	CI0	N1-C2-C3-C4
2	D	1001	CI0	O1-C2-C3-N2
2	C	1001	CI0	N1-C2-C3-N2
2	A	1001	CI0	N1-C2-C3-N2
2	D	1001	CI0	N1-C2-C3-N2
2	A	1001	CI0	O1-C2-C3-C4
2	D	1001	CI0	O1-C2-C3-C4
2	C	1001	CI0	O1-C2-C3-N2
2	A	1001	CI0	O1-C2-C3-N2
2	B	1001	CI0	O1-C2-C3-C4

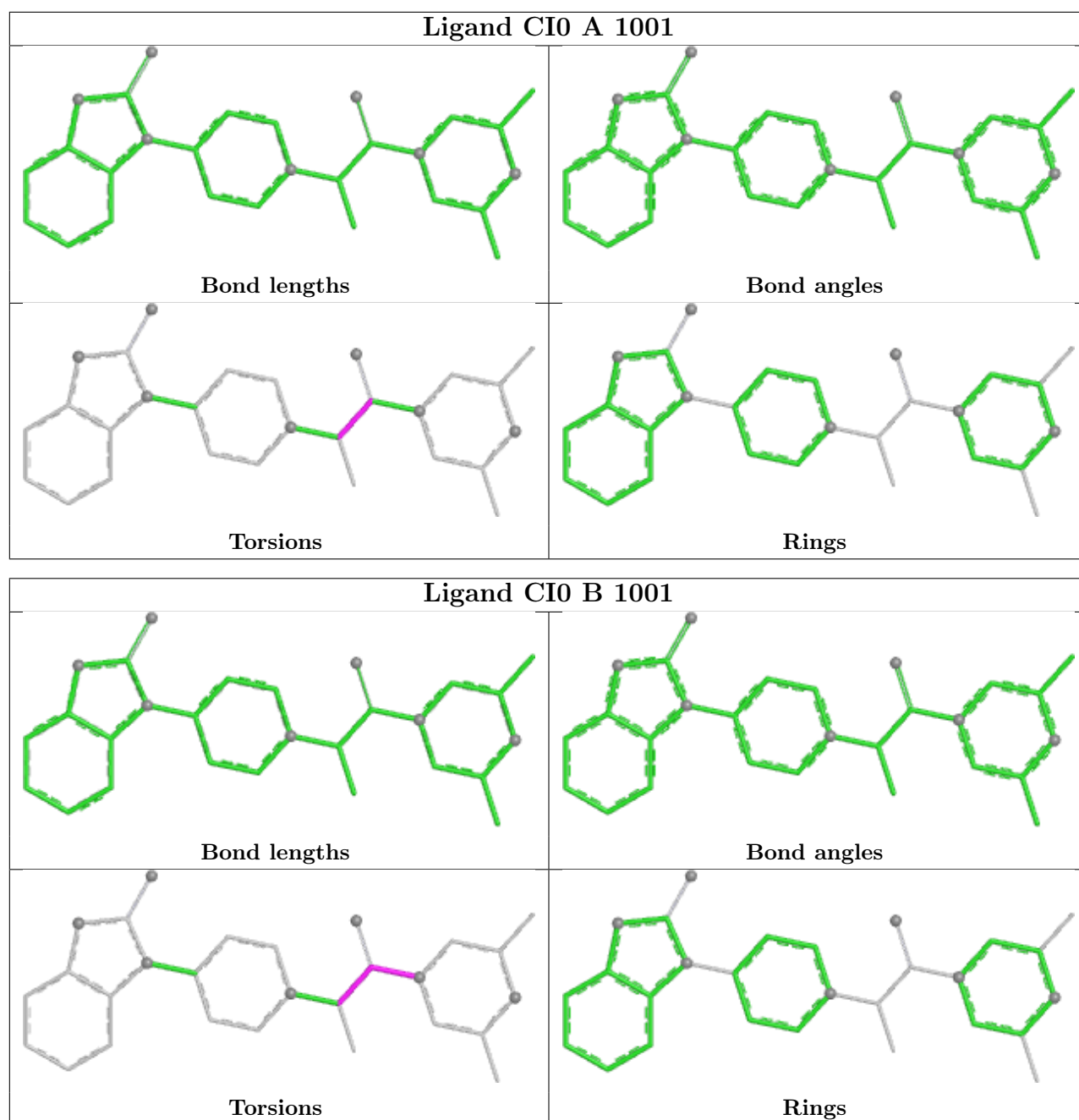
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	CI0	1	0
2	B	1001	CI0	1	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 [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 ⓘ

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	555/640 (86%)	1.54	151 (27%) 1 1	55, 75, 98, 116	0
1	B	574/640 (89%)	1.35	140 (24%) 2 1	35, 59, 78, 93	1 (0%)
1	C	571/640 (89%)	1.01	69 (12%) 8 7	31, 53, 76, 109	0
1	D	550/640 (85%)	1.25	90 (16%) 4 3	44, 68, 93, 117	0
All	All	2250/2560 (87%)	1.29	450 (20%) 3 2	31, 63, 91, 117	1 (0%)

All (450) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	616	GLY	6.4
1	B	777[A]	ARG	5.7
1	D	734	SER	5.3
1	A	440	ALA	4.9
1	D	924	GLU	4.8
1	A	863	CYS	4.7
1	A	726	GLY	4.7
1	C	647	CYS	4.6
1	B	384	ASP	4.5
1	A	762	ALA	4.3
1	B	647	CYS	4.3
1	A	505	PHE	4.3
1	B	568	THR	4.2
1	B	692	SER	4.2
1	D	674	CYS	4.2
1	D	678	TYR	4.2
1	B	529	PHE	4.2
1	B	681	LEU	4.2
1	A	678	TYR	4.1
1	B	410	GLY	4.1
1	A	916	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	618	LEU	4.0
1	A	406	GLU	4.0
1	B	884	LEU	4.0
1	D	440	ALA	3.8
1	B	684	LEU	3.8
1	B	545	VAL	3.8
1	C	409	LEU	3.8
1	A	456	GLY	3.8
1	C	598	GLY	3.8
1	C	692	SER	3.7
1	A	679	VAL	3.7
1	B	409	LEU	3.7
1	A	926	MET	3.7
1	C	715	TYR	3.7
1	A	360	PHE	3.6
1	A	736	CYS	3.6
1	C	577	THR	3.6
1	C	525	PRO	3.6
1	A	461	ALA	3.6
1	B	915	SER	3.6
1	C	573	TYR	3.6
1	A	915	SER	3.5
1	A	398	SER	3.5
1	B	597	PRO	3.5
1	D	577	THR	3.5
1	D	905	HIS	3.4
1	B	401	LEU	3.4
1	B	566	THR	3.4
1	A	337	TRP	3.4
1	A	476	GLY	3.4
1	B	418	ARG	3.4
1	D	926	MET	3.4
1	A	649	ASP	3.4
1	A	616	GLY	3.3
1	B	404	GLU	3.3
1	A	615	ALA	3.3
1	A	887	VAL	3.3
1	A	737	GLY	3.3
1	B	519	TRP	3.3
1	B	343	GLY	3.3
1	A	638	TYR	3.3
1	A	629	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	569	THR	3.3
1	A	420	LEU	3.2
1	B	534	THR	3.2
1	C	416	SER	3.2
1	B	788	ALA	3.2
1	A	385	ILE	3.2
1	B	455	LEU	3.2
1	A	657	VAL	3.2
1	A	677	VAL	3.2
1	D	671	GLN	3.2
1	B	577	THR	3.2
1	D	398	SER	3.2
1	D	461	ALA	3.2
1	C	568	THR	3.2
1	C	825	GLY	3.1
1	B	612	ARG	3.1
1	A	376	ALA	3.1
1	A	698	SER	3.1
1	D	646	SER	3.1
1	A	825	GLY	3.1
1	C	583	PRO	3.1
1	A	652	THR	3.1
1	A	715	TYR	3.1
1	B	578	TYR	3.1
1	D	866	SER	3.1
1	A	519	TRP	3.1
1	B	571	ALA	3.1
1	B	573	TYR	3.1
1	B	708	ARG	3.1
1	A	724	ALA	3.0
1	C	673	TRP	3.0
1	B	415	TYR	3.0
1	B	520	VAL	3.0
1	B	530	ILE	3.0
1	A	507	LEU	3.0
1	B	445	LEU	3.0
1	B	916	LEU	3.0
1	C	646	SER	3.0
1	B	549	GLY	3.0
1	A	727	THR	3.0
1	C	545	VAL	3.0
1	B	702	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	827	ASN	3.0
1	C	404	GLU	3.0
1	A	536	PRO	3.0
1	C	587	SER	3.0
1	A	363	ASP	3.0
1	B	905	HIS	3.0
1	D	864	LEU	2.9
1	C	531	ASP	2.9
1	A	734	SER	2.9
1	B	417	LYS	2.9
1	B	476	GLY	2.9
1	B	607	LEU	2.9
1	D	715	TYR	2.9
1	A	555	LEU	2.9
1	A	637	LEU	2.9
1	A	350	ASP	2.9
1	D	405	VAL	2.9
1	A	888	SER	2.9
1	B	929	LEU	2.9
1	D	694	GLY	2.8
1	D	759	VAL	2.8
1	C	530	ILE	2.8
1	A	415	TYR	2.8
1	B	431	ARG	2.8
1	B	783	ARG	2.8
1	A	766	THR	2.8
1	C	408	ALA	2.8
1	B	408	ALA	2.8
1	B	419	ALA	2.8
1	C	793	ASP	2.8
1	A	646	SER	2.8
1	A	767	VAL	2.8
1	B	617	THR	2.8
1	A	686	GLY	2.8
1	D	584	LYS	2.7
1	D	512	SER	2.7
1	D	679	VAL	2.7
1	B	346	ALA	2.7
1	B	680	LEU	2.7
1	D	738	LEU	2.7
1	B	574	LYS	2.7
1	D	825	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	576	PRO	2.7
1	A	648	SER	2.7
1	B	587	SER	2.7
1	B	759	VAL	2.7
1	C	526	PHE	2.7
1	B	411	ILE	2.7
1	D	718	LEU	2.7
1	B	613	TRP	2.7
1	A	341	GLY	2.7
1	D	536	PRO	2.7
1	C	744	LEU	2.7
1	B	652	THR	2.7
1	D	634	GLN	2.7
1	A	718	LEU	2.7
1	A	565	PHE	2.6
1	C	578	TYR	2.6
1	C	597	PRO	2.6
1	A	516	THR	2.6
1	D	420	LEU	2.6
1	D	913	ASP	2.6
1	B	416	SER	2.6
1	C	584	LYS	2.6
1	B	406	GLU	2.6
1	B	547	VAL	2.6
1	A	702	ILE	2.6
1	A	927	ILE	2.6
1	B	731	ASP	2.6
1	B	360	PHE	2.6
1	D	698	SER	2.6
1	D	462	TYR	2.6
1	B	576	PRO	2.6
1	A	711	CYS	2.6
1	A	446	LEU	2.6
1	A	352	ILE	2.6
1	A	912	GLU	2.6
1	A	349	ALA	2.6
1	B	548	HIS	2.6
1	A	563	TRP	2.6
1	C	726	GLY	2.6
1	C	684	LEU	2.6
1	C	933	THR	2.6
1	C	338	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	376	ALA	2.6
1	A	512	SER	2.5
1	A	429	VAL	2.5
1	C	671	GLN	2.5
1	D	569	THR	2.5
1	C	468	LEU	2.5
1	C	616	GLY	2.5
1	A	779	LEU	2.5
1	B	583	PRO	2.5
1	B	598	GLY	2.5
1	B	683	LEU	2.5
1	A	877	GLU	2.5
1	A	723	ALA	2.5
1	A	612	ARG	2.5
1	B	690	ASP	2.5
1	A	386	MET	2.5
1	B	596	LEU	2.5
1	D	666	LEU	2.5
1	B	526	PHE	2.5
1	B	611	ASP	2.5
1	A	760	LEU	2.5
1	A	694	GLY	2.5
1	A	925	GLY	2.5
1	A	388	LYS	2.5
1	B	412	ASN	2.5
1	B	697	ASN	2.5
1	A	685	PRO	2.4
1	D	733	ILE	2.4
1	C	343	GLY	2.4
1	C	914	GLU	2.4
1	A	559	PHE	2.4
1	C	462	TYR	2.4
1	D	615	ALA	2.4
1	B	383	LEU	2.4
1	B	422	LEU	2.4
1	B	864	LEU	2.4
1	C	410	GLY	2.4
1	A	448	VAL	2.4
1	B	367	SER	2.4
1	B	465	TRP	2.4
1	B	724	ALA	2.4
1	D	578	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	732	TYR	2.4
1	C	362	THR	2.4
1	C	652	THR	2.4
1	A	693	THR	2.4
1	D	706	THR	2.4
1	D	790	LEU	2.4
1	A	604	VAL	2.4
1	B	350	ASP	2.4
1	B	746	GLY	2.4
1	B	877	GLU	2.4
1	A	534	THR	2.4
1	C	926	MET	2.4
1	A	618	LEU	2.4
1	A	630	ILE	2.4
1	C	405	VAL	2.4
1	A	543	VAL	2.4
1	A	695	GLY	2.4
1	A	759	VAL	2.4
1	C	648	SER	2.4
1	C	401	LEU	2.4
1	A	321	HIS	2.4
1	A	372	LEU	2.4
1	A	607	LEU	2.4
1	A	864	LEU	2.4
1	C	622	ILE	2.4
1	B	630	ILE	2.4
1	D	769	ILE	2.4
1	A	606	VAL	2.3
1	A	656	LYS	2.3
1	D	410	GLY	2.3
1	B	892	ALA	2.3
1	A	807	GLN	2.3
1	B	614	SER	2.3
1	A	422	LEU	2.3
1	D	366	LEU	2.3
1	D	652	THR	2.3
1	B	536	PRO	2.3
1	A	336	ARG	2.3
1	B	772	ALA	2.3
1	D	688	GLU	2.3
1	C	334	LEU	2.3
1	D	752	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	622	ILE	2.3
1	B	774	ILE	2.3
1	C	476	GLY	2.3
1	A	391	ALA	2.3
1	D	762	ALA	2.3
1	A	690	ASP	2.3
1	A	647	CYS	2.3
1	A	684	LEU	2.3
1	B	420	LEU	2.3
1	A	411	ILE	2.3
1	A	614	SER	2.3
1	A	886	THR	2.3
1	B	575	THR	2.3
1	B	586	THR	2.3
1	B	579	PRO	2.3
1	A	412	ASN	2.3
1	B	443	GLU	2.3
1	C	445	LEU	2.3
1	A	703	LEU	2.3
1	A	787	LEU	2.3
1	B	353	LEU	2.3
1	C	755	ILE	2.3
1	B	648	SER	2.3
1	D	367	SER	2.3
1	A	339	VAL	2.3
1	A	402	PHE	2.2
1	A	347	ALA	2.2
1	A	882	GLU	2.2
1	B	527	GLU	2.2
1	D	914	GLU	2.2
1	B	458	LEU	2.2
1	D	407	LEU	2.2
1	B	518	ASP	2.2
1	D	856	ILE	2.2
1	C	889	PRO	2.2
1	D	767	VAL	2.2
1	B	580	TYR	2.2
1	D	476	GLY	2.2
1	A	885	ALA	2.2
1	B	400	LEU	2.2
1	B	407	LEU	2.2
1	B	581	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	515	ILE	2.2
1	D	663	ASP	2.2
1	A	365	TRP	2.2
1	D	904	VAL	2.2
1	C	344	TYR	2.2
1	A	725	MET	2.2
1	C	751	GLU	2.2
1	C	911	LEU	2.2
1	B	514	LEU	2.2
1	B	782	LYS	2.2
1	B	880	ALA	2.2
1	C	655	ASN	2.2
1	D	807	GLN	2.2
1	B	865	PRO	2.2
1	D	520	VAL	2.2
1	A	566	THR	2.2
1	D	603	THR	2.2
1	D	727	THR	2.2
1	A	457	GLY	2.2
1	A	696	GLY	2.2
1	A	454	PHE	2.2
1	C	680	LEU	2.2
1	C	681	LEU	2.2
1	A	383	LEU	2.2
1	A	404	GLU	2.2
1	D	521	GLN	2.2
1	C	442	HIS	2.2
1	B	784	ASP	2.2
1	B	881	VAL	2.2
1	D	331	PRO	2.2
1	D	363	ASP	2.2
1	C	925	GLY	2.2
1	A	364	TRP	2.2
1	B	825	GLY	2.2
1	A	413	SER	2.2
1	A	738	LEU	2.2
1	B	468	LEU	2.2
1	A	914	GLU	2.2
1	B	369	GLU	2.2
1	B	699	ILE	2.1
1	A	641	ASN	2.1
1	C	931	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	606	VAL	2.1
1	A	542	ASP	2.1
1	C	535	THR	2.1
1	B	781	GLY	2.1
1	A	846	TRP	2.1
1	A	458	LEU	2.1
1	A	468	LEU	2.1
1	A	834	LEU	2.1
1	B	402	PHE	2.1
1	B	460	LEU	2.1
1	B	917	LEU	2.1
1	B	698	SER	2.1
1	D	668	ALA	2.1
1	B	374	ARG	2.1
1	C	699	ILE	2.1
1	D	927	ILE	2.1
1	A	719	HIS	2.1
1	A	405	VAL	2.1
1	B	397	VAL	2.1
1	B	429	VAL	2.1
1	A	784	ASP	2.1
1	A	933	THR	2.1
1	D	332	GLY	2.1
1	D	713	GLY	2.1
1	D	901	GLY	2.1
1	C	507	LEU	2.1
1	A	613	TRP	2.1
1	A	712	ARG	2.1
1	D	376	ALA	2.1
1	D	556	ALA	2.1
1	D	777	ARG	2.1
1	D	850	ALA	2.1
1	D	876	ARG	2.1
1	A	601	CYS	2.1
1	A	622	ILE	2.1
1	B	755	ILE	2.1
1	B	768	ILE	2.1
1	C	429	VAL	2.1
1	A	421	MET	2.1
1	B	328	PRO	2.1
1	B	655	ASN	2.1
1	D	564	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	456	GLY	2.1
1	C	499	LEU	2.1
1	A	400	LEU	2.1
1	A	654	LEU	2.1
1	B	372	LEU	2.1
1	B	703	LEU	2.1
1	D	459	ASP	2.1
1	B	382	ARG	2.1
1	B	524	ARG	2.1
1	B	515	ILE	2.1
1	B	615	ALA	2.1
1	A	371	TYR	2.1
1	B	657	VAL	2.1
1	A	928	PRO	2.1
1	B	685	PRO	2.1
1	C	407	LEU	2.1
1	B	320	LEU	2.1
1	D	320	LEU	2.1
1	C	696	GLY	2.1
1	A	663	ASP	2.1
1	D	611	ASP	2.1
1	A	427	ILE	2.1
1	A	761	ILE	2.1
1	D	691	ILE	2.1
1	D	851	GLU	2.1
1	B	452	VAL	2.0
1	A	425	PRO	2.0
1	A	460	LEU	2.0
1	D	813	LEU	2.0
1	D	855	ASN	2.0
1	A	650	GLY	2.0
1	A	651	ARG	2.0
1	D	612	ARG	2.0
1	A	361	ILE	2.0
1	A	753	ILE	2.0
1	D	933	THR	2.0
1	D	467	ASP	2.0
1	D	846	TRP	2.0
1	D	421	MET	2.0
1	B	398	SER	2.0
1	B	435	GLN	2.0
1	D	859	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	647	CYS	2.0
1	A	664	ARG	2.0
1	D	689	GLY	2.0
1	D	411	ILE	2.0
1	D	639	ILE	2.0
1	B	567	LYS	2.0
1	B	851	GLU	2.0
1	D	406	GLU	2.0
1	A	465	TRP	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](#)

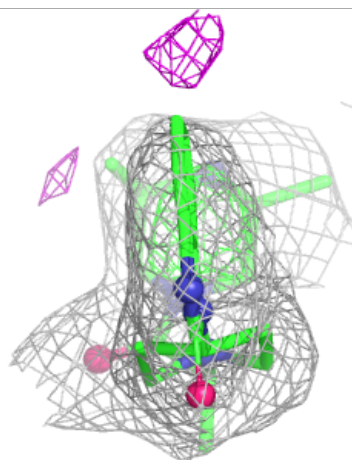
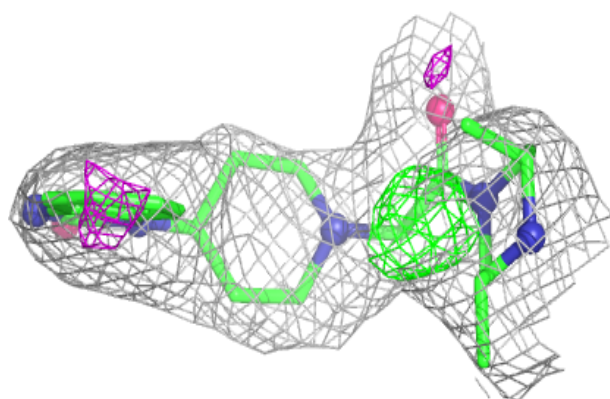
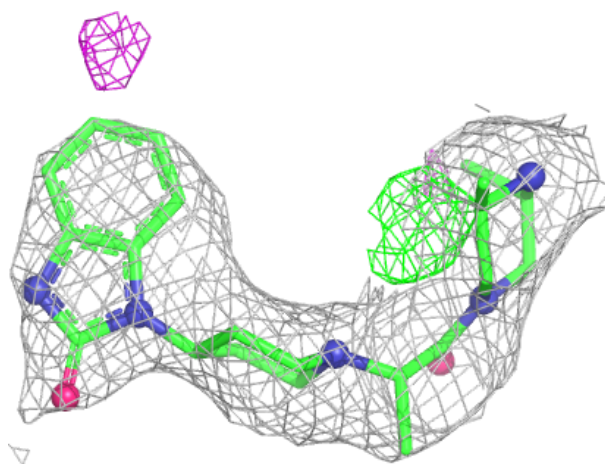
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CI0	C	1001	28/28	0.79	0.20	39,48,57,60	0
2	CI0	B	1001	28/28	0.81	0.20	39,55,68,72	0
2	CI0	D	1001	28/28	0.83	0.18	45,58,65,72	0
2	CI0	A	1001	28/28	0.84	0.17	47,58,69,72	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.

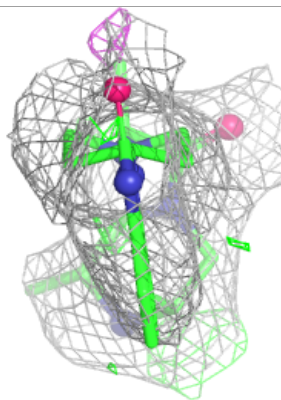
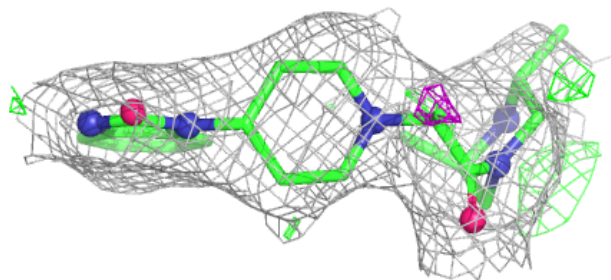
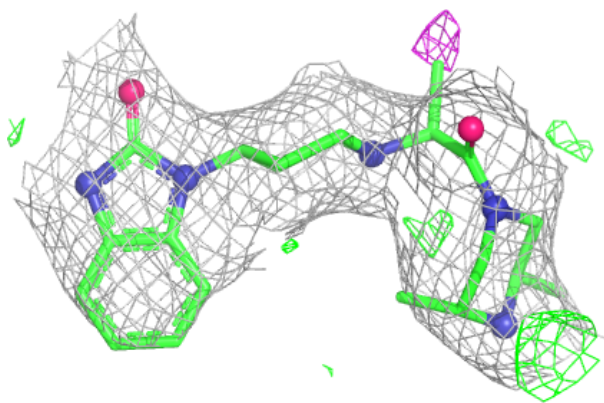
Electron density around CI0 C 1001:

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

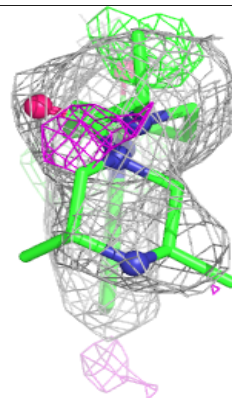
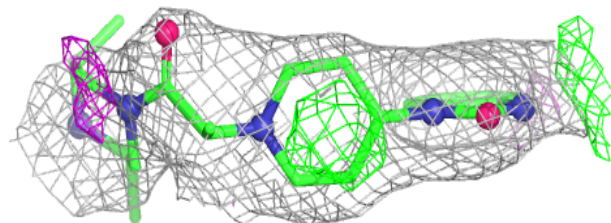
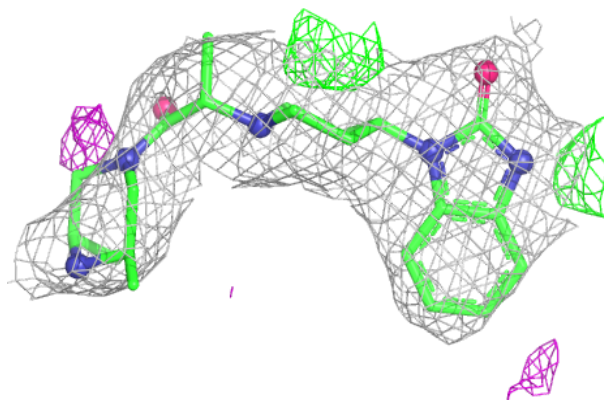


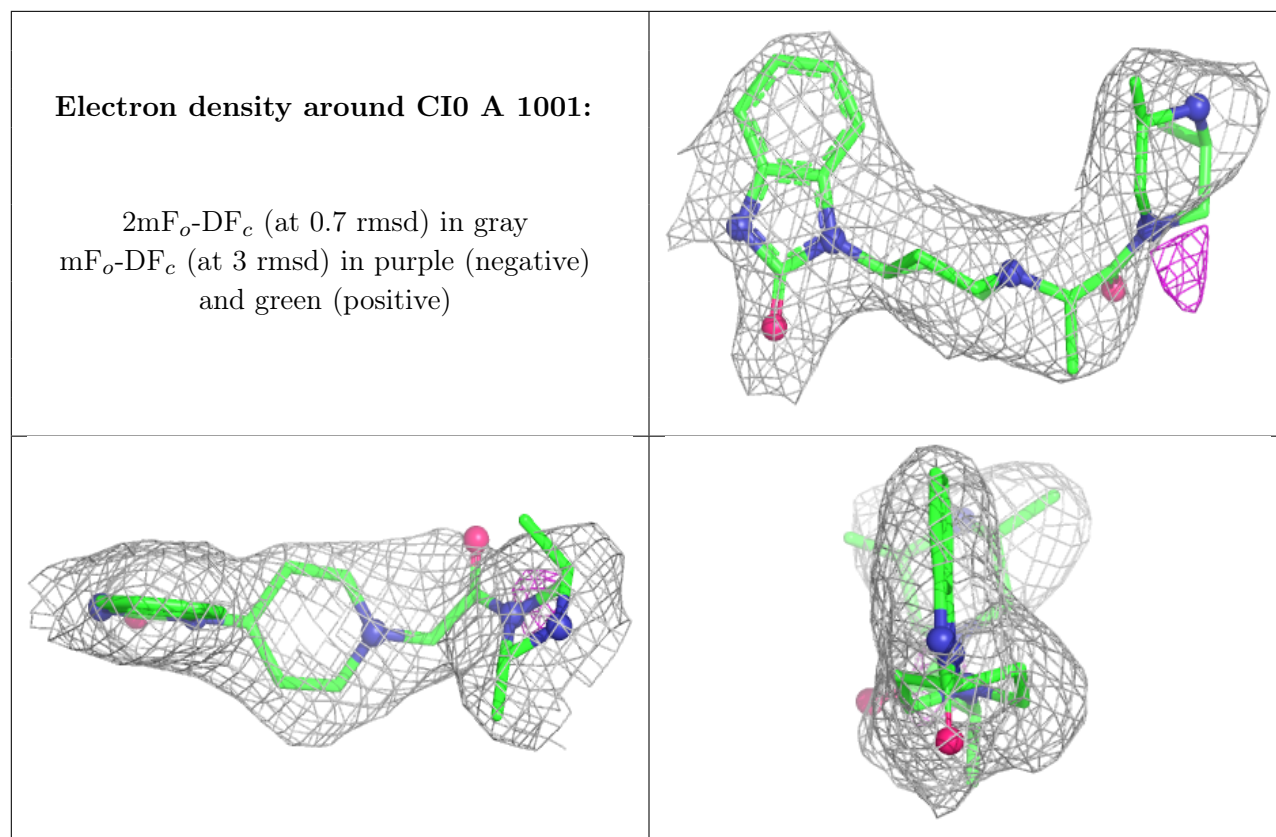
Electron density around CI0 B 1001:

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

**Electron density around CI0 D 1001:**

$2mF_o - DF_c$ (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.