



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:46 AM UTC

PDB ID : 3G4I / pdb_00003g4i
Title : Crystal structure of human phosphodiesterase 4d with d155871
Authors : Staker, B.L.
Deposited on : 2009-02-03
Resolution : 1.90 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

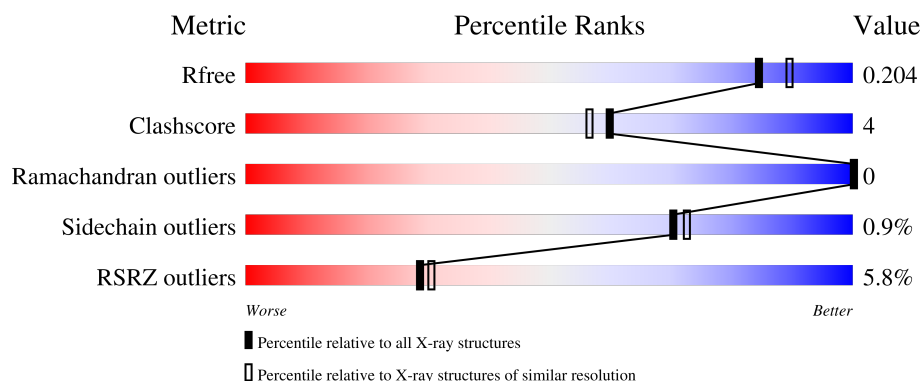
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

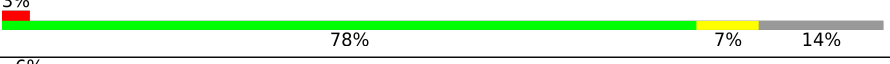
The reported resolution of this entry is 1.90 Å.

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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	381	
1	B	381	
1	C	381	
1	D	381	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	B	4	-	-	X	-
5	D71	B	902	-	X	-	-
6	EOH	A	5	-	-	X	-
6	EOH	B	11	-	-	X	-
6	EOH	D	7	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12017 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2678	1695	457	512	14			
1	B	326	Total	C	N	O	S	0	0	0
			2626	1660	446	506	14			
1	C	327	Total	C	N	O	S	0	0	0
			2647	1673	452	508	14			
1	D	334	Total	C	N	O	S	0	0	0
			2704	1712	463	515	14			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MET	-	expression tag	UNP Q08499
A	579	ALA	SER	engineered mutation	UNP Q08499
A	581	ALA	SER	engineered mutation	UNP Q08499
A	618	HIS	-	expression tag	UNP Q08499
A	619	HIS	-	expression tag	UNP Q08499
A	620	HIS	-	expression tag	UNP Q08499
A	621	HIS	-	expression tag	UNP Q08499
A	622	HIS	-	expression tag	UNP Q08499
A	623	HIS	-	expression tag	UNP Q08499
B	243	MET	-	expression tag	UNP Q08499
B	579	ALA	SER	engineered mutation	UNP Q08499
B	581	ALA	SER	engineered mutation	UNP Q08499
B	618	HIS	-	expression tag	UNP Q08499
B	619	HIS	-	expression tag	UNP Q08499
B	620	HIS	-	expression tag	UNP Q08499
B	621	HIS	-	expression tag	UNP Q08499
B	622	HIS	-	expression tag	UNP Q08499
B	623	HIS	-	expression tag	UNP Q08499
C	243	MET	-	expression tag	UNP Q08499
C	579	ALA	SER	engineered mutation	UNP Q08499
C	581	ALA	SER	engineered mutation	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
C	618	HIS	-	expression tag	UNP Q08499
C	619	HIS	-	expression tag	UNP Q08499
C	620	HIS	-	expression tag	UNP Q08499
C	621	HIS	-	expression tag	UNP Q08499
C	622	HIS	-	expression tag	UNP Q08499
C	623	HIS	-	expression tag	UNP Q08499
D	243	MET	-	expression tag	UNP Q08499
D	579	ALA	SER	engineered mutation	UNP Q08499
D	581	ALA	SER	engineered mutation	UNP Q08499
D	618	HIS	-	expression tag	UNP Q08499
D	619	HIS	-	expression tag	UNP Q08499
D	620	HIS	-	expression tag	UNP Q08499
D	621	HIS	-	expression tag	UNP Q08499
D	622	HIS	-	expression tag	UNP Q08499
D	623	HIS	-	expression tag	UNP Q08499

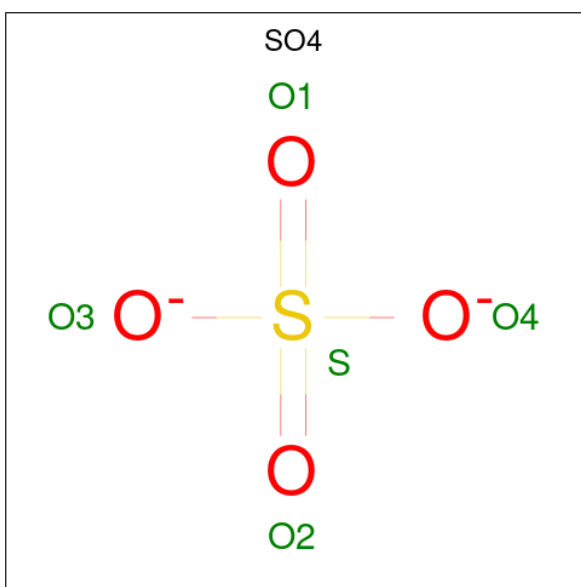
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

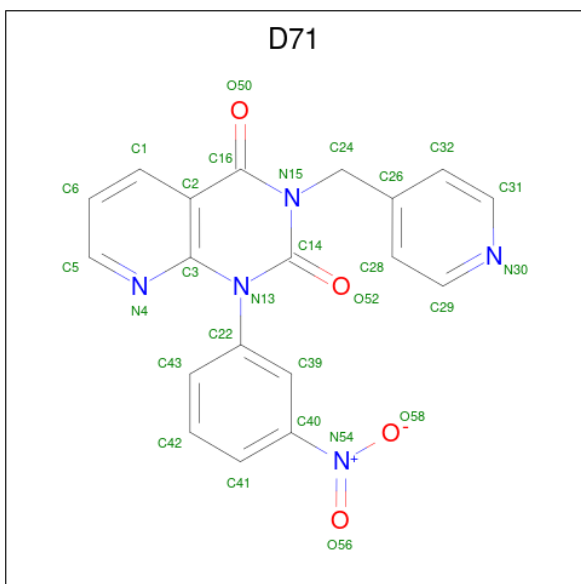
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



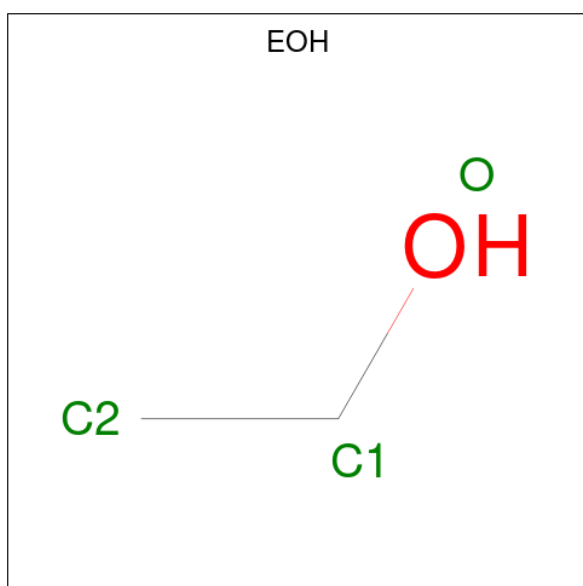
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1-(3-nitrophenyl)-3-(pyridin-4-ylmethyl)pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione (CCD ID: D71) (formula: C₁₉H₁₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			28	19	5	4		
5	B	1	Total	C	N	O	0	0
			28	19	5	4		
5	C	1	Total	C	N	O	0	0
			28	19	5	4		
5	D	1	Total	C	N	O	0	0
			28	19	5	4		

- Molecule 6 is ETHANOL (CCD ID: EOH) (formula: C_2H_6O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	2	1		
6	A	1	Total	C	O	0	0
			3	2	1		
6	A	1	Total	C	O	0	0
			3	2	1		
6	B	1	Total	C	O	0	0
			3	2	1		
6	B	1	Total	C	O	0	0
			3	2	1		
6	B	1	Total	C	O	0	0
			3	2	1		
6	C	1	Total	C	O	0	0
			3	2	1		
6	D	1	Total	C	O	0	0
			3	2	1		

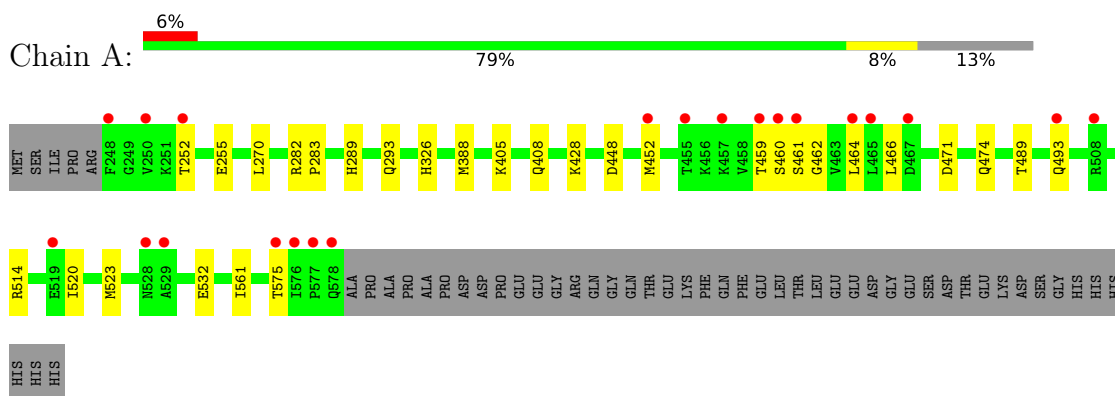
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	302	Total 302	O 302	0	0
7	B	286	Total 286	O 286	0	0
7	C	287	Total 287	O 287	0	0
7	D	328	Total 328	O 328	0	0

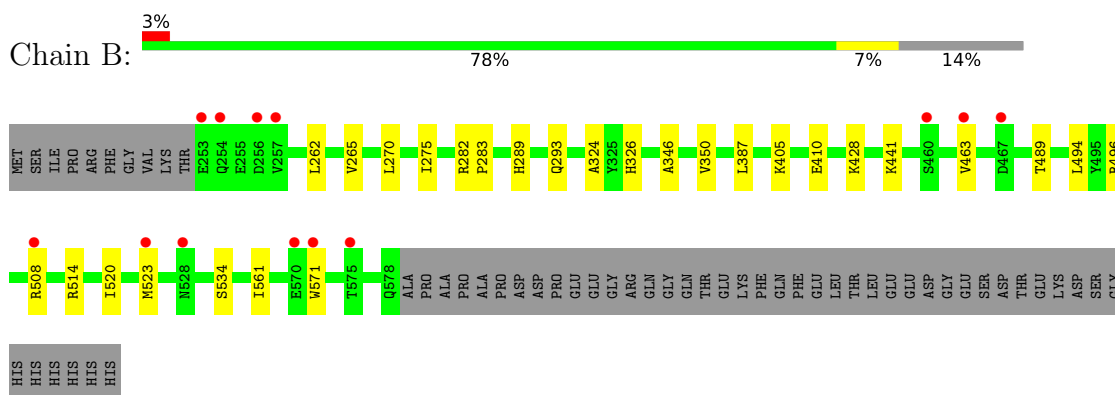
3 Residue-property plots [i](#)

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

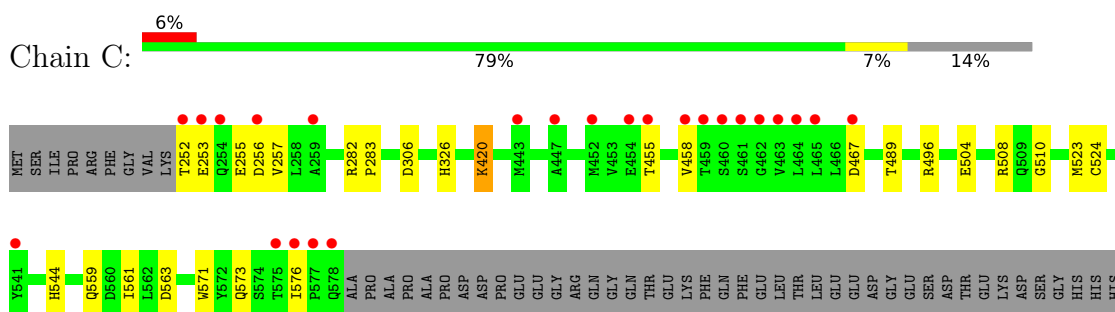
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D

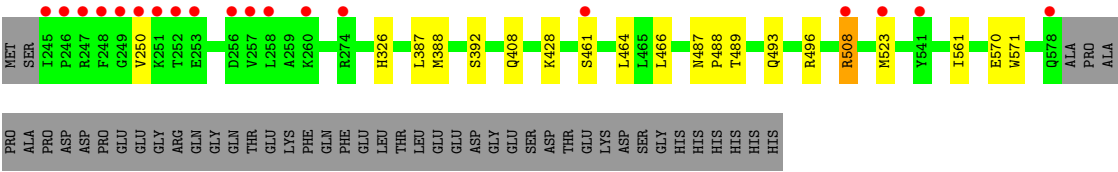
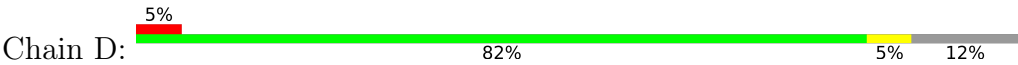


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



HIS
HIS
HIS

● Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.86Å 113.24Å 161.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.90) 92.9 (50.00-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.181 , 0.215 (Not available) , 0.204	Depositor DCC
R_{free} test set	6596 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12017	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MG, EOH, D71, ZN

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	0/2733	0.78	0/3712
1	B	0.63	0/2680	0.78	0/3645
1	C	0.68	0/2701	0.79	0/3670
1	D	0.72	0/2760	0.80	0/3749
All	All	0.68	0/10874	0.79	0/14776

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	SER	Peptide

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	2678	0	2633	31	0
1	B	2626	0	2559	27	0
1	C	2647	0	2599	18	0
1	D	2704	0	2664	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	2	0
4	C	5	0	0	0	0
5	A	28	0	13	3	0
5	B	28	0	13	6	0
5	C	28	0	13	2	0
5	D	28	0	13	1	0
6	A	9	0	18	2	0
6	B	9	0	18	3	0
6	C	3	0	6	0	0
6	D	3	0	6	2	0
7	A	302	0	0	5	0
7	B	286	0	0	6	0
7	C	287	0	0	7	0
7	D	328	0	0	3	0
All	All	12017	0	10555	91	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 4.

All (91) 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:523:MET:SD	5:B:902:D71:C41	2.57	0.92
1:B:387:LEU:HG	7:B:1212:HOH:O	1.74	0.87
6:B:10:EOH:H23	7:B:111:HOH:O	1.81	0.79
1:B:494:LEU:HD21	4:B:4:SO4:O4	1.84	0.77
1:A:405:LYS:NZ	1:A:408:GLN:OE1	2.21	0.74
1:C:252:THR:N	7:C:641:HOH:O	2.24	0.70
7:C:1068:HOH:O	1:D:387:LEU:HG	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:ARG:NH1	7:D:925:HOH:O	2.26	0.68
1:B:508:ARG:HG3	7:B:729:HOH:O	1.94	0.66
1:D:392:SER:HB2	7:D:702:HOH:O	1.96	0.65
1:B:534:SER:HB3	5:B:902:D71:H41	1.78	0.64
1:A:428:LYS:HG3	6:A:5:EOH:H23	1.81	0.63
1:D:523:MET:HG2	7:D:933:HOH:O	2.01	0.61
1:A:408:GLN:OE1	1:D:408:GLN:OE1	2.18	0.61
1:C:496:ARG:HD3	1:C:571:TRP:CH2	2.35	0.60
1:C:504:GLU:OE2	1:C:508:ARG:NH2	2.34	0.60
1:C:573:GLN:HE21	1:C:576:ILE:HD12	1.67	0.60
1:A:523:MET:SD	5:A:901:D71:C41	2.91	0.59
1:B:346:ALA:O	1:B:463:VAL:HG13	2.03	0.59
1:C:523:MET:HG2	7:C:717:HOH:O	2.02	0.58
1:C:326:HIS:CE1	5:C:903:D71:H29	2.39	0.57
1:B:523:MET:SD	5:B:902:D71:C40	2.93	0.57
1:A:252:THR:CG2	1:A:255:GLU:H	2.17	0.57
1:A:532:GLU:HG2	1:A:575:THR:HG22	1.86	0.56
1:A:252:THR:HG22	1:A:255:GLU:CG	2.37	0.55
6:A:5:EOH:H22	7:B:704:HOH:O	2.06	0.55
1:A:252:THR:HG23	1:A:255:GLU:H	1.71	0.55
1:B:350:VAL:CG2	1:B:463:VAL:CG1	2.85	0.54
1:D:496:ARG:HD3	1:D:571:TRP:CH2	2.42	0.54
1:A:514:ARG:HD3	1:A:520:ILE:HD11	1.91	0.53
1:D:428:LYS:HG3	6:D:7:EOH:H23	1.90	0.53
1:C:489:THR:HB	1:C:561:ILE:HG23	1.91	0.52
1:B:428:LYS:HG3	6:B:11:EOH:H23	1.92	0.52
1:D:508:ARG:HB2	1:D:508:ARG:HH11	1.74	0.52
1:B:489:THR:HB	1:B:561:ILE:HG23	1.92	0.52
1:A:388:MET:HA	1:A:388:MET:HE2	1.93	0.51
1:B:350:VAL:HG23	1:B:463:VAL:HG11	1.92	0.51
1:D:388:MET:HA	1:D:388:MET:HE2	1.92	0.51
1:A:448:ASP:HB3	1:A:474:GLN:NE2	2.25	0.51
1:C:306:ASP:HB3	7:C:729:HOH:O	2.11	0.51
1:A:575:THR:HG22	1:A:575:THR:O	2.11	0.50
1:A:448:ASP:C	1:A:474:GLN:NE2	2.69	0.50
1:C:326:HIS:NE2	5:C:903:D71:H29	2.26	0.50
7:C:137:HOH:O	6:D:7:EOH:H22	2.11	0.50
1:A:326:HIS:CE1	5:A:901:D71:H29	2.47	0.49
1:B:326:HIS:CE1	5:B:902:D71:H29	2.47	0.49
1:B:494:LEU:CD2	4:B:4:SO4:O4	2.58	0.49
1:B:514:ARG:HD3	1:B:520:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:HD11	1:B:275:ILE:HD11	1.95	0.49
1:A:464:LEU:HD21	1:A:466:LEU:HD21	1.95	0.49
1:B:262:LEU:O	1:B:265:VAL:HG23	2.13	0.49
1:A:452:MET:HE1	1:A:471:ASP:HA	1.94	0.48
1:A:489:THR:HB	1:A:561:ILE:HG23	1.95	0.48
1:B:289:HIS:CE1	1:B:293:GLN:HE21	2.32	0.48
1:A:523:MET:SD	5:A:901:D71:C40	3.03	0.47
1:D:326:HIS:CE1	5:D:904:D71:H29	2.50	0.47
1:B:326:HIS:NE2	5:B:902:D71:H29	2.29	0.47
1:B:350:VAL:HG23	1:B:463:VAL:CG1	2.44	0.46
1:A:289:HIS:CE1	1:A:293:GLN:HE21	2.34	0.46
1:D:489:THR:HB	1:D:561:ILE:HG23	1.97	0.46
1:C:573:GLN:NE2	1:C:576:ILE:HD12	2.29	0.46
7:A:633:HOH:O	6:B:11:EOH:H22	2.15	0.46
1:B:496:ARG:HD3	1:B:571:TRP:CH2	2.50	0.45
1:B:410:GLU:OE2	1:C:420:LYS:NZ	2.45	0.45
1:A:428:LYS:NZ	7:A:958:HOH:O	2.49	0.45
1:C:253:GLU:O	1:C:257:VAL:HG23	2.16	0.45
1:B:387:LEU:HD12	7:B:1194:HOH:O	2.15	0.45
1:A:575:THR:HG21	7:A:642:HOH:O	2.16	0.45
1:C:282:ARG:N	1:C:283:PRO:CD	2.81	0.44
1:B:324:ALA:H	1:B:508:ARG:HH22	1.65	0.43
1:D:464:LEU:HD21	1:D:466:LEU:HD21	1.99	0.43
1:C:420:LYS:HB2	1:C:420:LYS:HE2	1.68	0.42
1:B:523:MET:SD	5:B:902:D71:H41	2.55	0.42
1:A:459:THR:O	1:A:460:SER:C	2.63	0.41
1:A:493:GLN:NE2	7:A:942:HOH:O	2.48	0.41
1:A:282:ARG:N	1:A:283:PRO:CD	2.83	0.41
1:B:282:ARG:N	1:B:283:PRO:CD	2.83	0.41
1:C:508:ARG:NH1	7:C:692:HOH:O	2.53	0.41
1:D:487:ASN:HB2	1:D:488:PRO:HD3	2.02	0.41
1:A:252:THR:HG22	1:A:255:GLU:CB	2.50	0.41
1:D:496:ARG:HD3	1:D:571:TRP:CZ3	2.55	0.41
1:A:448:ASP:CB	1:A:474:GLN:NE2	2.83	0.41
1:A:575:THR:O	1:A:575:THR:CG2	2.69	0.41
1:A:459:THR:O	1:A:462:GLY:HA2	2.20	0.41
1:B:441:LYS:NZ	7:B:875:HOH:O	2.43	0.41
1:C:510:GLY:HA3	1:C:524:CYS:O	2.21	0.40
1:C:544:HIS:ND1	7:C:672:HOH:O	2.37	0.40
1:A:388:MET:HE1	1:B:405:LYS:NZ	2.37	0.40
1:A:448:ASP:C	1:A:474:GLN:HE22	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:559:GLN:NE2	1:C:563:ASP:OD1	2.51	0.40
1:A:270:LEU:HD12	7:A:710:HOH:O	2.21	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	329/381 (86%)	321 (98%)	8 (2%)	0	100	100
1	B	324/381 (85%)	319 (98%)	5 (2%)	0	100	100
1	C	325/381 (85%)	317 (98%)	8 (2%)	0	100	100
1	D	332/381 (87%)	325 (98%)	7 (2%)	0	100	100
All	All	1310/1524 (86%)	1282 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	302/345 (88%)	302 (100%)	0	100	100
1	B	295/345 (86%)	295 (100%)	0	100	100
1	C	299/345 (87%)	293 (98%)	6 (2%)	48	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	305/345 (88%)	300 (98%)	5 (2%)	55	54
All	All	1201/1380 (87%)	1190 (99%)	11 (1%)	70	73

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	255	GLU
1	C	256	ASP
1	C	420	LYS
1	C	455	THR
1	C	458	VAL
1	C	467	ASP
1	D	250	VAL
1	D	461	SER
1	D	493	GLN
1	D	508	ARG
1	D	570	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	A	289	HIS
1	A	318	HIS
1	A	535	GLN
1	B	289	HIS
1	B	376	GLN
1	B	528	ASN
1	B	555	HIS
1	B	573	GLN
1	C	254	GLN
1	C	376	GLN
1	C	535	GLN
1	C	573	GLN
1	C	578	GLN
1	D	289	HIS
1	D	293	GLN
1	D	535	GLN
1	D	573	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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	$\# Z > 2$
5	D71	B	902	-	31,31,31	3.60	16 (51%)	40,44,44	2.34	19 (47%)
6	EOH	B	10	-	2,2,2	0.52	0	1,1,1	0.09	0
6	EOH	A	5	-	2,2,2	0.62	0	1,1,1	0.11	0
6	EOH	A	12	-	2,2,2	0.50	0	1,1,1	0.07	0
4	SO4	A	3	-	4,4,4	0.23	0	6,6,6	0.52	0
6	EOH	D	7	-	2,2,2	0.64	0	1,1,1	0.17	0
4	SO4	B	4	-	4,4,4	0.28	0	6,6,6	0.26	0
6	EOH	B	8	-	2,2,2	0.51	0	1,1,1	0.10	0
6	EOH	A	9	-	2,2,2	0.51	0	1,1,1	0.12	0
6	EOH	B	11	-	2,2,2	0.56	0	1,1,1	0.13	0
5	D71	A	901	-	31,31,31	3.59	16 (51%)	40,44,44	2.16	15 (37%)
4	SO4	C	2	-	4,4,4	0.21	0	6,6,6	0.35	0
6	EOH	C	6	-	2,2,2	0.60	0	1,1,1	0.08	0
5	D71	C	903	-	31,31,31	3.49	15 (48%)	40,44,44	2.06	12 (30%)
5	D71	D	904	-	31,31,31	3.48	16 (51%)	40,44,44	2.33	19 (47%)

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
5	D71	B	902	-	-	4/10/12/12	0/4/4/4
5	D71	C	903	-	-	0/10/12/12	0/4/4/4
5	D71	D	904	-	-	0/10/12/12	0/4/4/4
5	D71	A	901	-	-	0/10/12/12	0/4/4/4

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	901	D71	C2-C3	8.16	1.51	1.40
5	C	903	D71	C2-C3	7.92	1.51	1.40
5	B	902	D71	C2-C3	7.80	1.51	1.40
5	D	904	D71	C2-C3	7.63	1.50	1.40
5	B	902	D71	C41-C40	6.61	1.51	1.38
5	A	901	D71	C42-C43	6.58	1.50	1.38
5	C	903	D71	C42-C43	6.49	1.50	1.38
5	A	901	D71	C41-C40	6.48	1.50	1.38
5	D	904	D71	C41-C40	6.37	1.50	1.38
5	C	903	D71	C41-C40	6.32	1.50	1.38
5	B	902	D71	C42-C43	6.32	1.49	1.38
5	D	904	D71	C42-C43	6.19	1.49	1.38
5	B	902	D71	C14-N13	5.75	1.49	1.39
5	B	902	D71	C6-C1	5.59	1.48	1.38
5	A	901	D71	C39-C22	5.54	1.49	1.39
5	A	901	D71	C14-N13	5.54	1.48	1.39
5	D	904	D71	C6-C1	5.43	1.48	1.38
5	C	903	D71	C14-N13	5.41	1.48	1.39
5	A	901	D71	C6-C1	5.41	1.48	1.38
5	B	902	D71	C32-C31	5.39	1.49	1.38
5	C	903	D71	C32-C31	5.35	1.48	1.38
5	A	901	D71	C32-C31	5.26	1.48	1.38
5	D	904	D71	C39-C22	5.25	1.48	1.39
5	B	902	D71	C39-C22	5.24	1.48	1.39
5	D	904	D71	C14-N13	5.19	1.48	1.39
5	D	904	D71	C32-C31	5.16	1.48	1.38
5	C	903	D71	C6-C1	5.14	1.47	1.38
5	C	903	D71	C39-C22	5.11	1.48	1.39
5	D	904	D71	C28-C26	5.06	1.48	1.38
5	B	902	D71	C14-N15	4.96	1.47	1.38
5	A	901	D71	C28-C26	4.84	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	902	D71	C28-C26	4.81	1.48	1.38
5	A	901	D71	C14-N15	4.76	1.47	1.38
5	D	904	D71	C14-N15	4.58	1.46	1.38
5	C	903	D71	C14-N15	4.41	1.46	1.38
5	B	902	D71	C3-N13	4.26	1.46	1.40
5	C	903	D71	C28-C26	4.20	1.47	1.38
5	C	903	D71	C3-N13	4.12	1.46	1.40
5	A	901	D71	C5-N4	4.06	1.43	1.34
5	D	904	D71	C3-N13	3.98	1.46	1.40
5	B	902	D71	C5-N4	3.94	1.42	1.34
5	C	903	D71	C5-N4	3.82	1.42	1.34
5	A	901	D71	C3-N13	3.71	1.45	1.40
5	D	904	D71	C5-N4	3.69	1.42	1.34
5	D	904	D71	C29-N30	3.68	1.44	1.33
5	A	901	D71	C29-N30	3.45	1.43	1.33
5	B	902	D71	C29-N30	3.41	1.43	1.33
5	C	903	D71	C29-N30	3.32	1.43	1.33
5	C	903	D71	C22-N13	2.74	1.48	1.44
5	C	903	D71	C1-C2	-2.63	1.36	1.39
5	D	904	D71	C1-C2	-2.63	1.36	1.39
5	D	904	D71	C22-N13	2.54	1.47	1.44
5	B	902	D71	C22-N13	2.44	1.47	1.44
5	B	902	D71	C28-C29	-2.42	1.33	1.38
5	C	903	D71	C28-C29	-2.41	1.33	1.38
5	A	901	D71	O50-C16	2.41	1.27	1.22
5	B	902	D71	C1-C2	-2.35	1.36	1.39
5	A	901	D71	C28-C29	-2.30	1.34	1.38
5	A	901	D71	C1-C2	-2.25	1.36	1.39
5	B	902	D71	C42-C41	-2.23	1.35	1.38
5	D	904	D71	C28-C29	-2.20	1.34	1.38
5	A	901	D71	C22-N13	2.18	1.47	1.44
5	D	904	D71	C42-C41	-2.02	1.35	1.38

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	902	D71	C16-N15-C14	-7.14	120.11	125.33
5	D	904	D71	C16-N15-C14	-6.80	120.36	125.33
5	A	901	D71	C16-N15-C14	-6.49	120.59	125.33
5	C	903	D71	C16-N15-C14	-6.16	120.83	125.33
5	B	902	D71	C41-C40-N54	4.01	122.84	119.34
5	D	904	D71	N13-C14-N15	3.80	121.78	115.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	903	D71	N13-C14-N15	3.78	121.74	115.61
5	D	904	D71	C24-C26-C28	-3.75	113.84	120.75
5	A	901	D71	C24-C26-C28	-3.62	114.07	120.75
5	B	902	D71	C24-C26-C28	-3.60	114.11	120.75
5	A	901	D71	N13-C14-N15	3.60	121.46	115.61
5	B	902	D71	N13-C14-N15	3.45	121.21	115.61
5	D	904	D71	C43-C22-N13	3.45	123.68	119.72
5	C	903	D71	C24-C26-C28	-3.44	114.42	120.75
5	B	902	D71	C2-C16-N15	3.40	120.24	115.26
5	B	902	D71	C5-N4-C3	3.38	122.69	115.05
5	A	901	D71	C43-C22-N13	3.24	123.44	119.72
5	C	903	D71	O52-C14-N15	-3.22	117.64	121.98
5	D	904	D71	C5-N4-C3	3.22	122.34	115.05
5	B	902	D71	C43-C22-N13	3.20	123.39	119.72
5	D	904	D71	C2-C16-N15	3.14	119.86	115.26
5	D	904	D71	C41-C40-N54	3.06	122.01	119.34
5	A	901	D71	C39-C22-N13	-3.04	116.27	119.42
5	A	901	D71	C5-N4-C3	3.00	121.84	115.05
5	C	903	D71	C5-N4-C3	2.99	121.83	115.05
5	D	904	D71	N4-C3-N13	2.90	121.45	117.52
5	C	903	D71	C41-C40-N54	2.89	121.87	119.34
5	D	904	D71	C39-C22-N13	-2.83	116.49	119.42
5	C	903	D71	C2-C16-N15	2.82	119.40	115.26
5	A	901	D71	C2-C16-N15	2.81	119.38	115.26
5	B	902	D71	N4-C3-N13	2.80	121.30	117.52
5	D	904	D71	C29-N30-C31	2.71	123.06	116.86
5	D	904	D71	C26-C24-N15	-2.71	108.56	113.09
5	C	903	D71	C32-C31-N30	-2.63	119.11	123.60
5	B	902	D71	C29-N30-C31	2.59	122.79	116.86
5	C	903	D71	O56-N54-C40	2.54	122.31	118.82
5	C	903	D71	N4-C3-N13	2.52	120.93	117.52
5	A	901	D71	C41-C40-N54	2.52	121.54	119.34
5	D	904	D71	O56-N54-C40	2.47	122.22	118.82
5	C	903	D71	C29-N30-C31	2.40	122.36	116.86
5	A	901	D71	C29-N30-C31	2.39	122.33	116.86
5	B	902	D71	C41-C40-C39	-2.38	117.05	120.11
5	A	901	D71	C24-C26-C32	2.35	125.08	120.75
5	B	902	D71	C39-C22-N13	-2.35	116.99	119.42
5	B	902	D71	C32-C31-N30	-2.31	119.65	123.60
5	D	904	D71	C32-C31-N30	-2.31	119.67	123.60
5	A	901	D71	N4-C3-N13	2.30	120.63	117.52
5	A	901	D71	C32-C31-N30	-2.30	119.68	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	901	D71	O52-C14-N15	-2.26	118.93	121.98
5	A	901	D71	C39-C40-N54	2.26	120.69	118.74
5	D	904	D71	C28-C29-N30	-2.23	119.80	123.60
5	A	901	D71	O56-N54-C40	2.23	121.88	118.82
5	B	902	D71	O56-N54-C40	2.21	121.86	118.82
5	B	902	D71	C6-C5-N4	-2.21	119.93	123.42
5	D	904	D71	C28-C26-C32	2.20	121.50	118.23
5	B	902	D71	C24-C26-C32	2.19	124.79	120.75
5	D	904	D71	C24-N15-C14	2.18	119.97	116.92
5	D	904	D71	O52-C14-N13	-2.16	118.80	121.86
5	B	902	D71	C26-C24-N15	-2.11	109.56	113.09
5	D	904	D71	C24-C26-C32	2.09	124.60	120.75
5	B	902	D71	O52-C14-N15	-2.09	119.17	121.98
5	D	904	D71	C6-C5-N4	-2.08	120.12	123.42
5	B	902	D71	C24-N15-C14	2.04	119.78	116.92
5	C	903	D71	C43-C22-N13	2.03	122.06	119.72
5	B	902	D71	C28-C29-N30	-2.02	120.16	123.60

There are no chirality outliers.

All (4) torsion outliers are listed below:

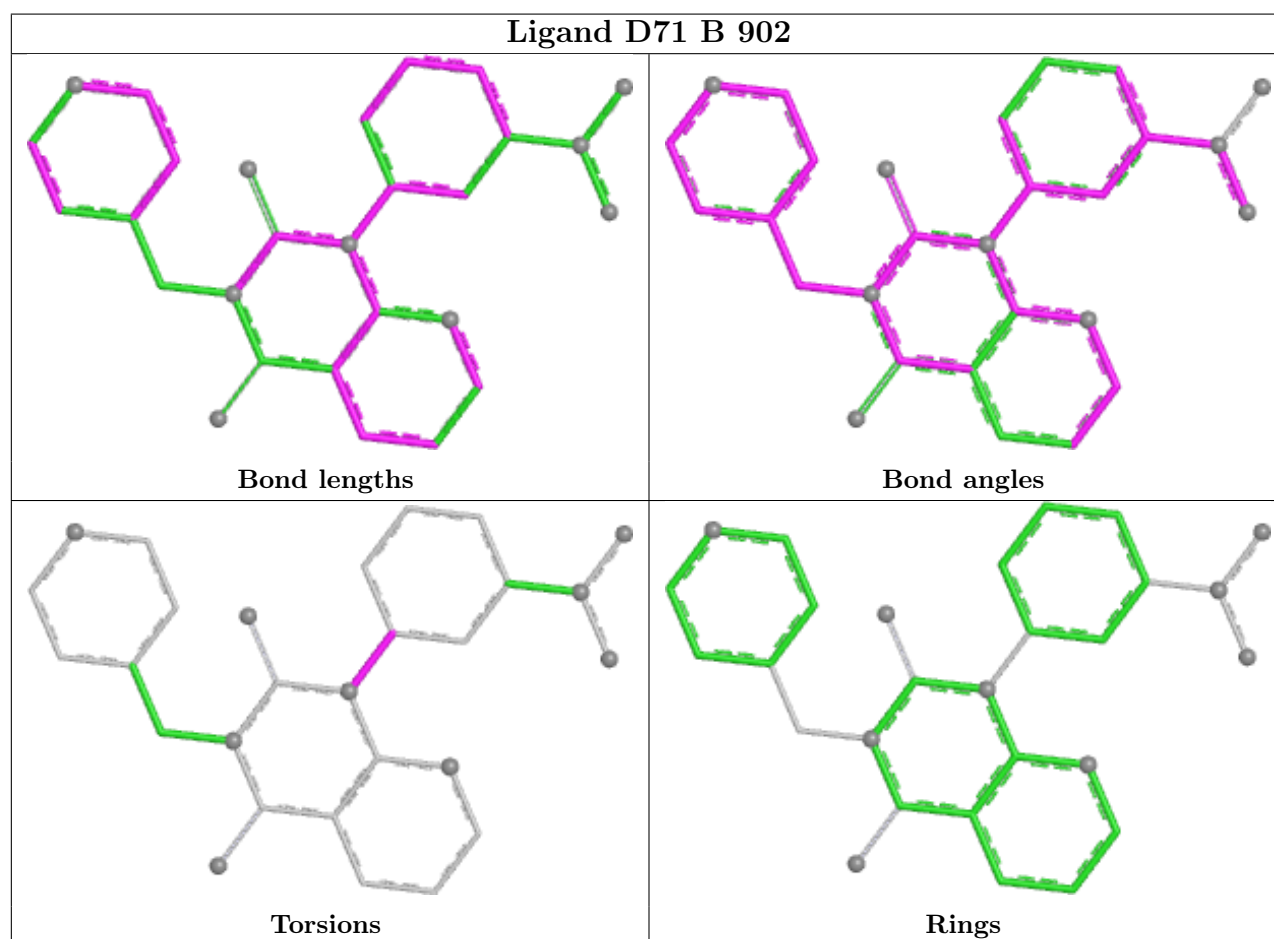
Mol	Chain	Res	Type	Atoms
5	B	902	D71	C39-C22-N13-C14
5	B	902	D71	C43-C22-N13-C14
5	B	902	D71	C43-C22-N13-C3
5	B	902	D71	C39-C22-N13-C3

There are no ring outliers.

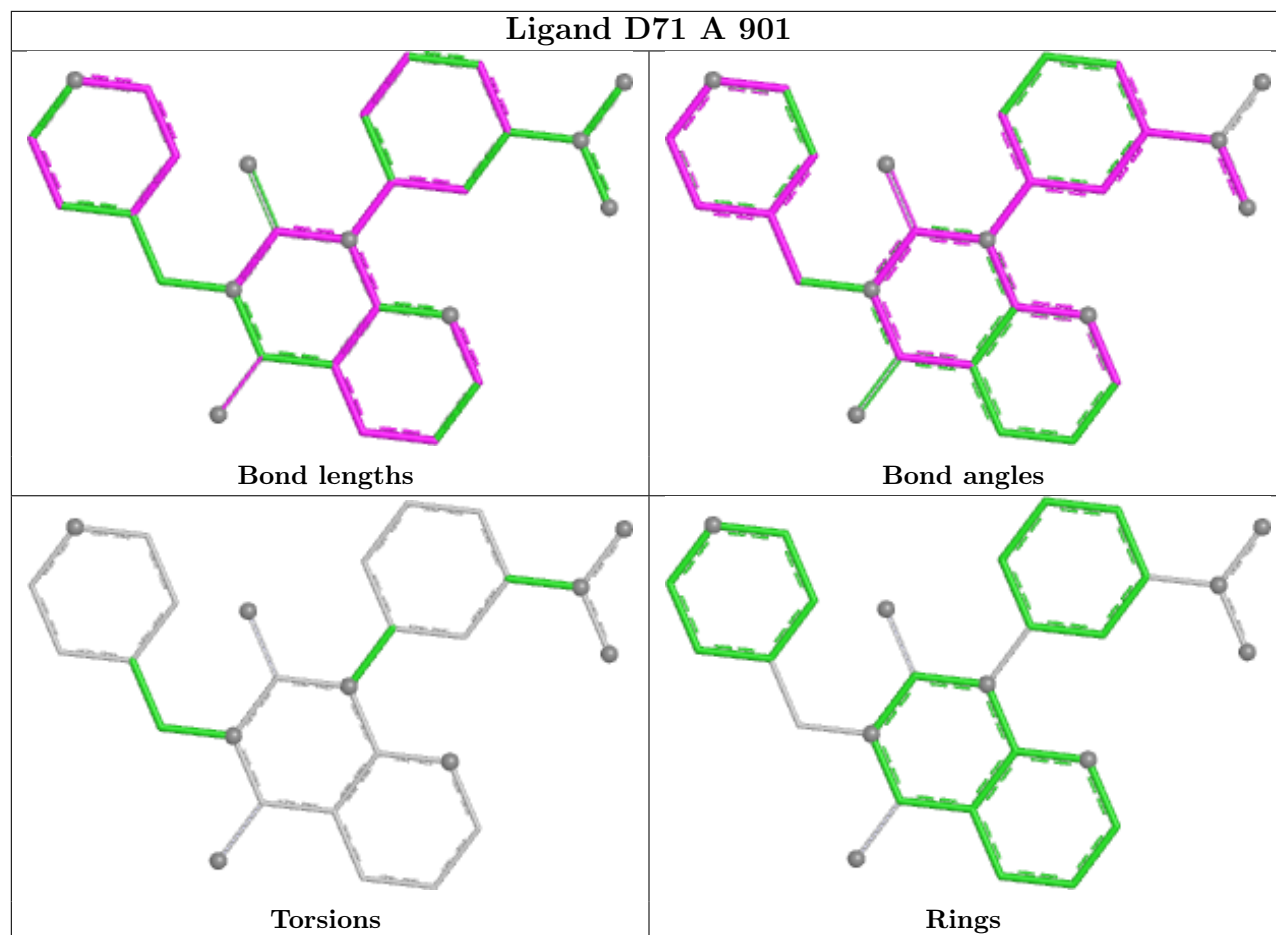
9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	902	D71	6	0
6	B	10	EOH	1	0
6	A	5	EOH	2	0
6	D	7	EOH	2	0
4	B	4	SO4	2	0
6	B	11	EOH	2	0
5	A	901	D71	3	0
5	C	903	D71	2	0
5	D	904	D71	1	0

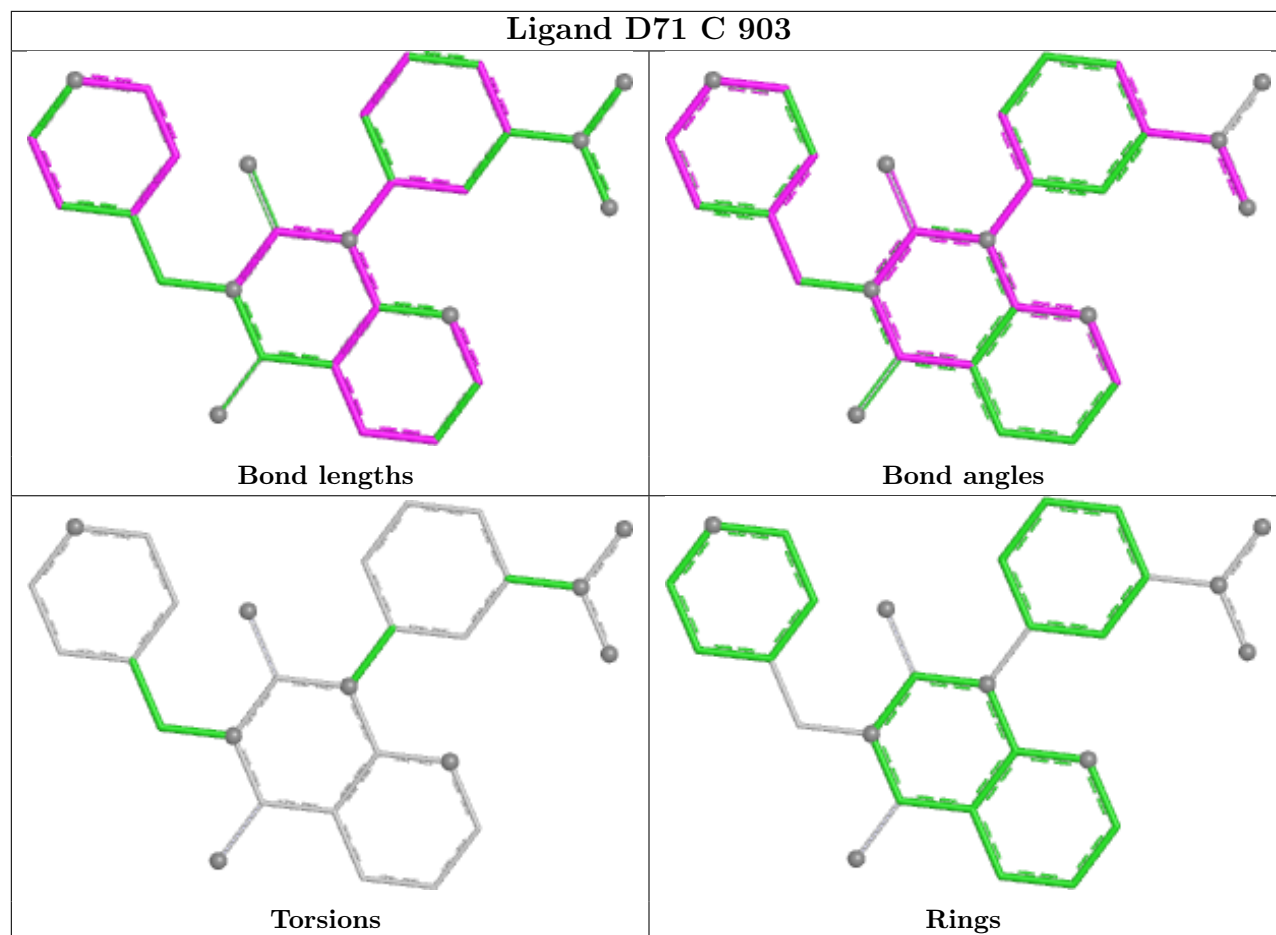
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

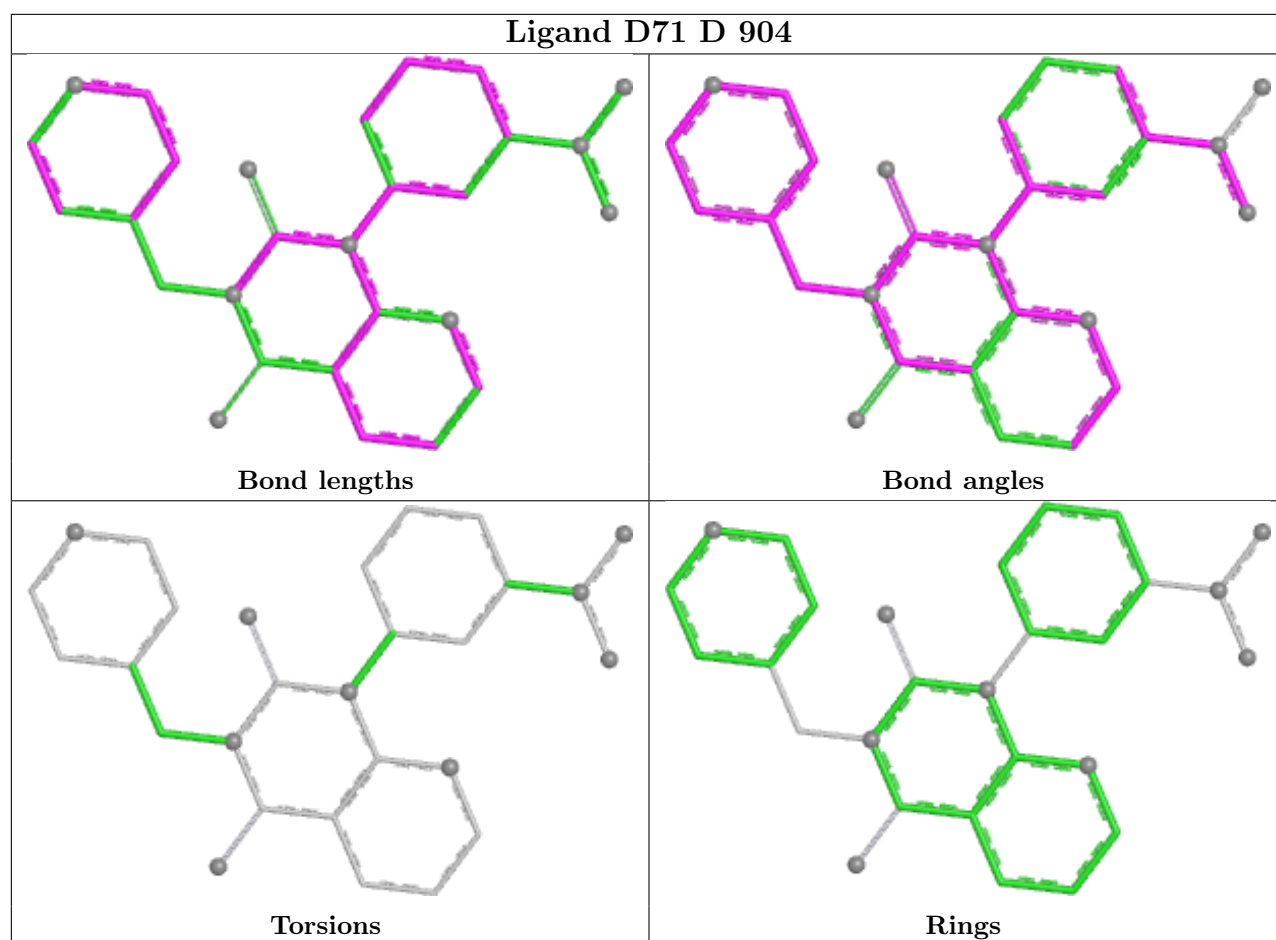


Ligand D71 A 901



Ligand D71 C 903





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	331/381 (86%)	0.15	21 (6%) 26 27	13, 22, 48, 61	0
1	B	326/381 (85%)	0.28	13 (3%) 42 45	14, 26, 41, 65	0
1	C	327/381 (85%)	0.33	24 (7%) 21 22	13, 24, 53, 67	0
1	D	334/381 (87%)	0.09	19 (5%) 29 31	13, 22, 41, 65	0
All	All	1318/1524 (86%)	0.21	77 (5%) 29 30	13, 23, 46, 67	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	577	PRO	6.2
1	D	245	ILE	6.0
1	C	459	THR	4.6
1	A	248	PHE	4.2
1	D	248	PHE	4.2
1	C	252	THR	4.2
1	A	465	LEU	3.9
1	A	578	GLN	3.9
1	B	254	GLN	3.8
1	D	578	GLN	3.8
1	B	467	ASP	3.7
1	D	250	VAL	3.7
1	A	460	SER	3.4
1	B	575	THR	3.4
1	C	462	GLY	3.3
1	D	246	PRO	3.3
1	C	575	THR	3.2
1	C	460	SER	3.2
1	A	452	MET	3.2
1	C	254	GLN	3.1
1	D	253	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	576	ILE	3.0
1	C	465	LEU	3.0
1	C	452	MET	3.0
1	D	251	LYS	2.9
1	A	467	ASP	2.9
1	D	249	GLY	2.9
1	B	508	ARG	2.9
1	C	447	ALA	2.9
1	A	461	SER	2.9
1	D	541	TYR	2.8
1	B	256	ASP	2.8
1	D	256	ASP	2.8
1	C	463	VAL	2.8
1	B	523	MET	2.8
1	B	253	GLU	2.8
1	D	461	SER	2.7
1	B	528	ASN	2.7
1	A	252	THR	2.7
1	A	519	GLU	2.7
1	D	257	VAL	2.7
1	D	252	THR	2.6
1	C	461	SER	2.6
1	C	455	THR	2.6
1	A	250	VAL	2.6
1	A	575	THR	2.5
1	A	529	ALA	2.5
1	C	256	ASP	2.5
1	C	458	VAL	2.5
1	A	464	LEU	2.4
1	C	443	MET	2.4
1	A	455	THR	2.4
1	C	259	ALA	2.4
1	C	467	ASP	2.4
1	B	571	TRP	2.4
1	A	508	ARG	2.4
1	B	257	VAL	2.4
1	B	570	GLU	2.3
1	C	577	PRO	2.3
1	A	457	LYS	2.3
1	D	247	ARG	2.3
1	A	459	THR	2.3
1	D	260	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	508	ARG	2.2
1	B	463	VAL	2.2
1	B	460	SER	2.2
1	C	541	TYR	2.1
1	C	464	LEU	2.1
1	C	454	GLU	2.1
1	D	523	MET	2.1
1	C	253	GLU	2.1
1	C	578	GLN	2.1
1	A	576	ILE	2.1
1	D	274	ARG	2.1
1	A	493	GLN	2.1
1	D	258	LEU	2.1
1	A	528	ASN	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
6	EOH	A	5	3/3	0.76	0.18	19,19,23,23	0
6	EOH	B	11	3/3	0.78	0.17	24,24,26,26	0
6	EOH	D	7	3/3	0.78	0.20	19,19,21,21	0
6	EOH	C	6	3/3	0.82	0.17	25,25,26,26	0
6	EOH	B	8	3/3	0.85	0.16	30,30,31,31	0
6	EOH	A	12	3/3	0.85	0.17	31,31,31,32	0
4	SO4	C	2	5/5	0.86	0.16	46,52,54,54	0
6	EOH	B	10	3/3	0.87	0.14	24,24,26,27	0
5	D71	B	902	28/28	0.87	0.13	41,42,45,47	0

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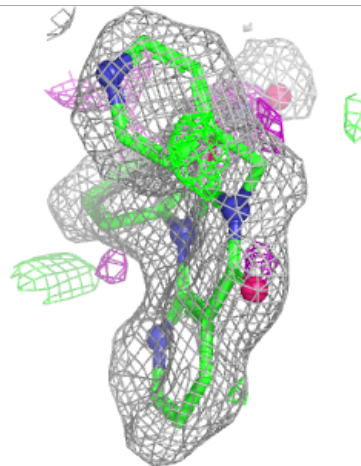
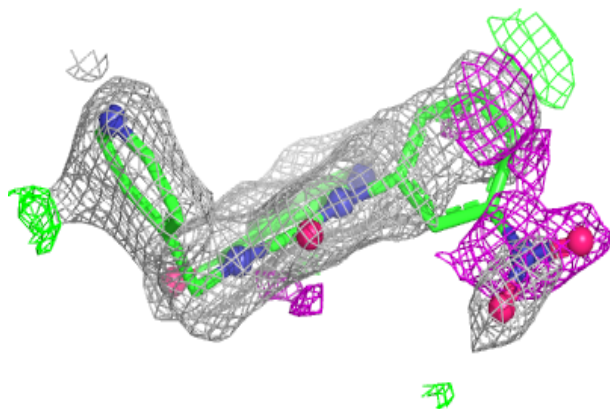
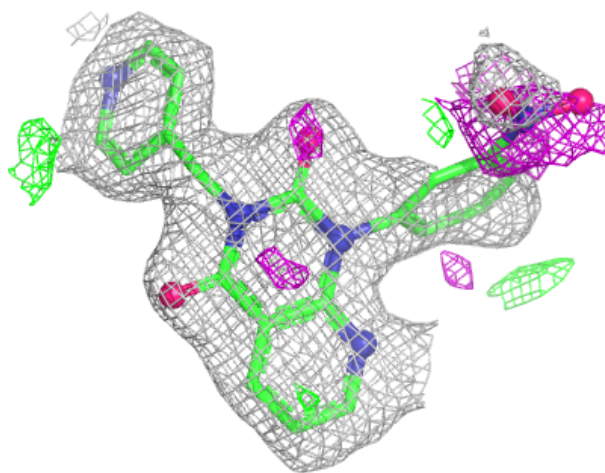
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	4	5/5	0.88	0.14	56,56,59,59	0
5	D71	A	901	28/28	0.88	0.12	35,37,40,44	0
6	EOH	A	9	3/3	0.89	0.12	24,24,25,25	0
5	D71	C	903	28/28	0.90	0.10	30,31,34,40	0
4	SO4	A	3	5/5	0.92	0.14	34,39,42,42	0
5	D71	D	904	28/28	0.92	0.10	27,28,32,36	0
3	MG	D	808	1/1	0.98	0.03	22,22,22,22	0
3	MG	A	802	1/1	0.98	0.06	25,25,25,25	0
3	MG	B	804	1/1	0.99	0.02	25,25,25,25	0
3	MG	C	806	1/1	0.99	0.02	23,23,23,23	0
2	ZN	B	803	1/1	0.99	0.06	26,26,26,26	0
2	ZN	C	805	1/1	1.00	0.04	24,24,24,24	0
2	ZN	D	807	1/1	1.00	0.04	23,23,23,23	0
2	ZN	A	801	1/1	1.00	0.05	24,24,24,24	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.

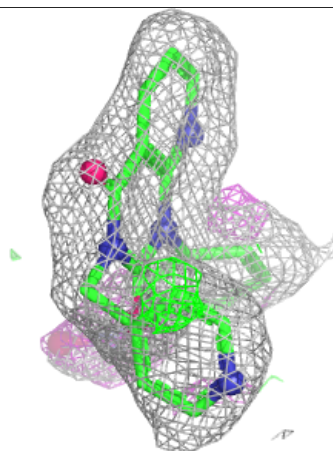
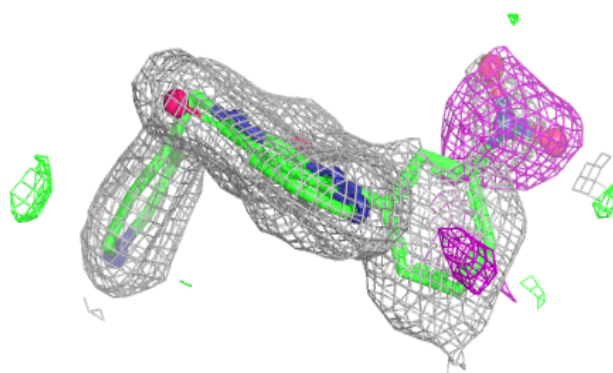
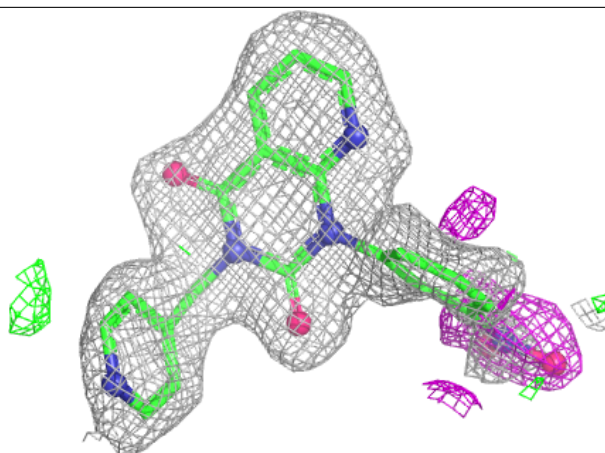
Electron density around D71 B 902:

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



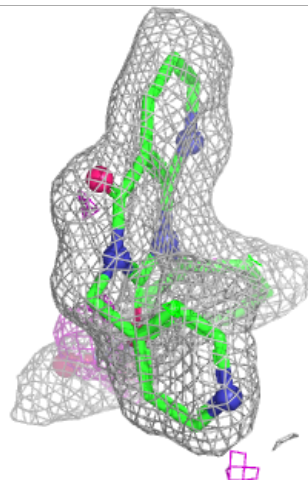
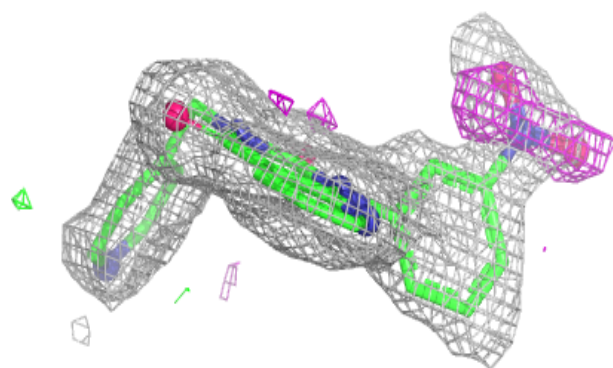
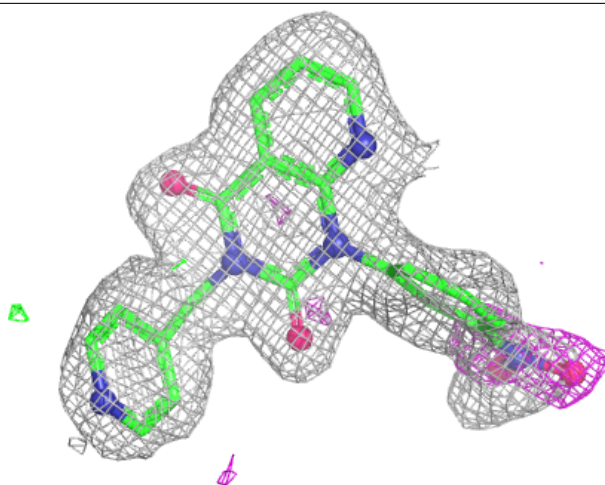
Electron density around D71 A 901:

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



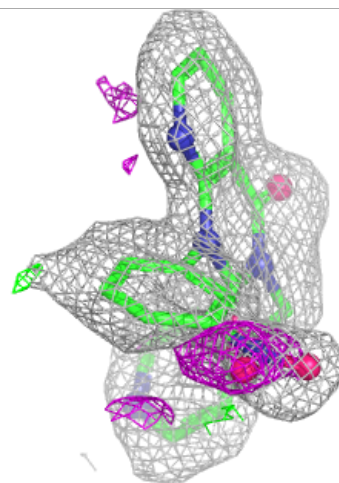
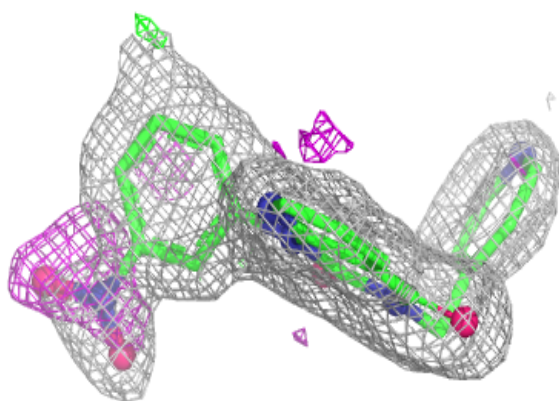
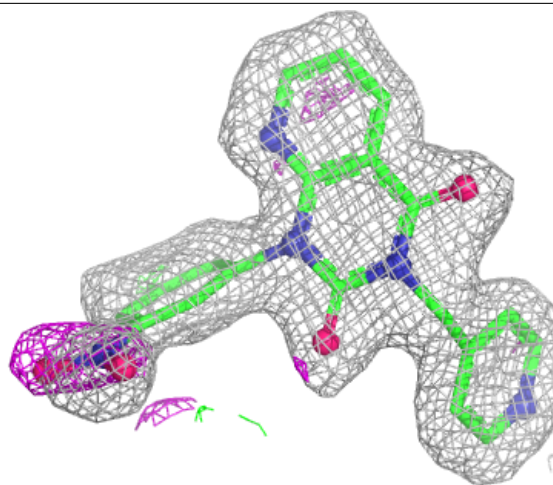
Electron density around D71 C 903:

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



Electron density around D71 D 904:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.