



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:29 PM UTC

PDB ID : 7QH1 / pdb_00007qh1
Title : Discovery and development of a novel inhaled antivirulence therapy for the treatment of *Pseudomonas aeruginosa* infections in patients with chronic respiratory disease
Authors : Leonard, P.M.; Davies, D.; Pallin, T.D.
Deposited on : 2021-12-10
Resolution : 2.74 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

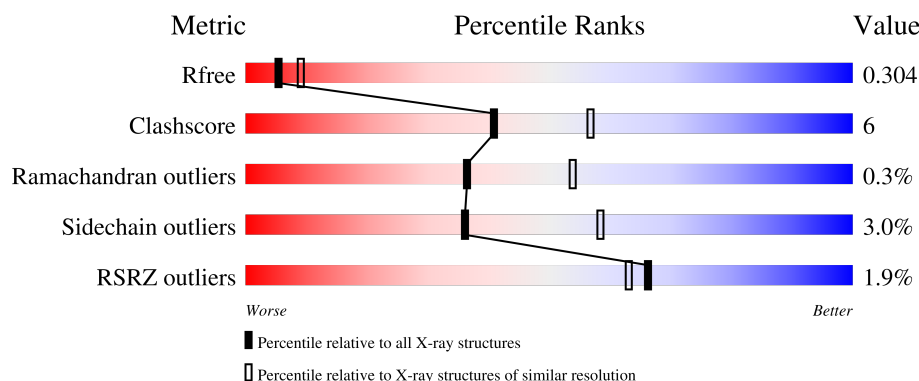
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	301	3% 85% 13% ..
1	B	301	2% 85% 13% ..
1	C	301	2% 82% 16% ..
1	D	301	2% 85% 13% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9562 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.

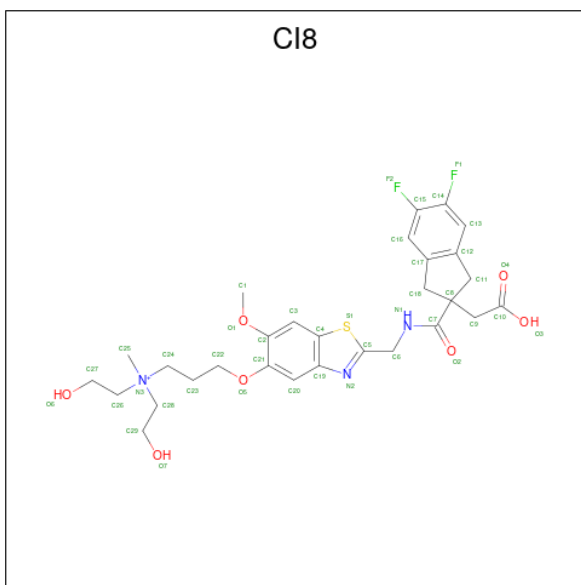
- Molecule 1 is a protein called Keratinase KP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	3	0
			2340	1466	405	456	13			
1	B	298	Total	C	N	O	S	0	2	0
			2334	1463	404	454	13			
1	C	298	Total	C	N	O	S	0	3	0
			2340	1466	405	456	13			
1	D	298	Total	C	N	O	S	0	3	0
			2340	1466	405	456	13			

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

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

- Molecule 3 is 2-[2-[[5-[3-bis(2-hydroxyethyl)-methyl- $\text{S}^{\{4\}}$ -azanyl]propoxy]-6-methoxy-1,3-benzothiazol-2-yl]methylcarbamoyl]-5,6-bis(fluoranyl)-1,3-dihydroinden-2-yl]ethanoic acid (CCD ID: CI8) (formula: $\text{C}_{29}\text{H}_{36}\text{F}_2\text{N}_3\text{O}_7\text{S}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 42	C 29	F 2	N 3	O 7	S 1	0	0
3	B	1	Total 42	C 29	F 2	N 3	O 7	S 1	0	0
3	C	1	Total 42	C 29	F 2	N 3	O 7	S 1	0	0
3	D	1	Total 42	C 29	F 2	N 3	O 7	S 1	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Ca 2 2	0	0
4	B	2	Total Ca 2 2	0	0
4	C	2	Total Ca 2 2	0	0
4	D	2	Total Ca 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0

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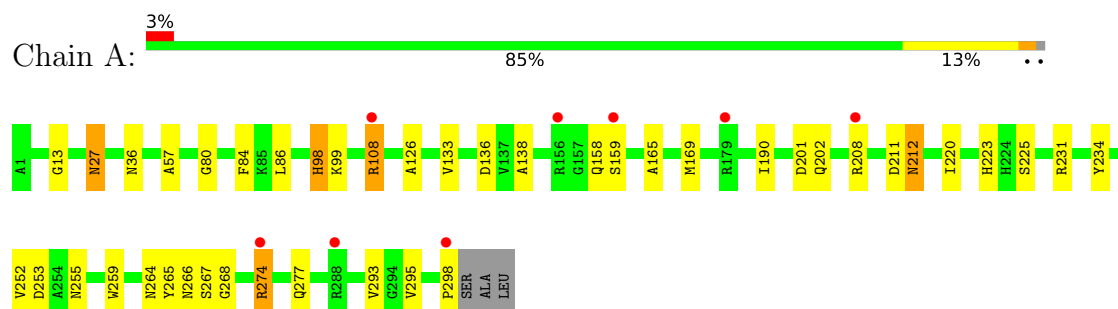
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	7	Total	O	0	0
			7	7		
5	C	7	Total	O	0	0
			7	7		
5	D	7	Total	O	0	0
			7	7		

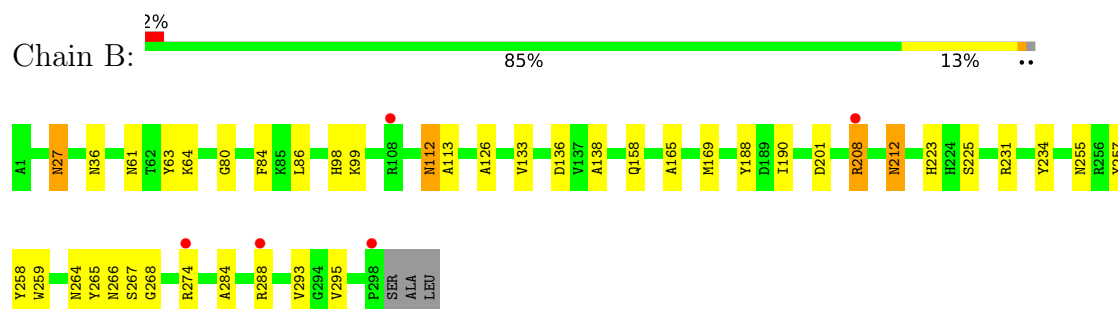
3 Residue-property plots [i](#)

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.

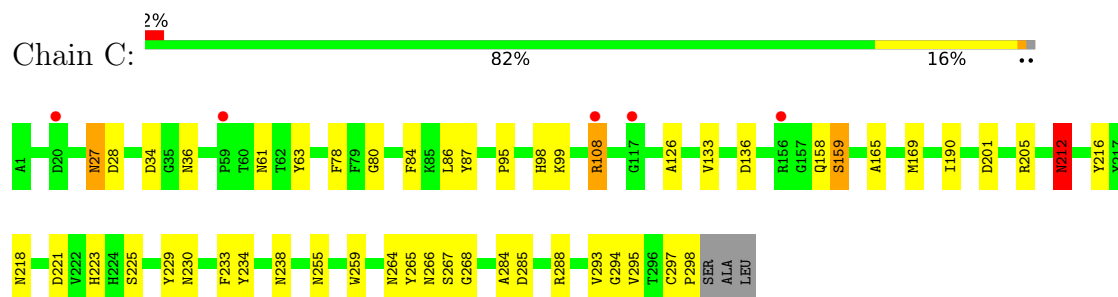
• Molecule 1: Keratinase KP2



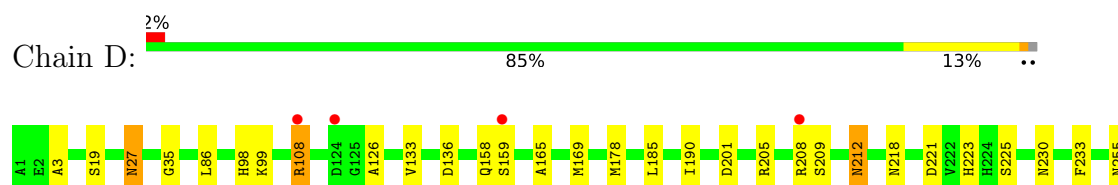
• Molecule 1: Keratinase KP2

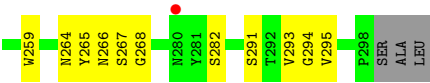


• Molecule 1: Keratinase KP2



• Molecule 1: Keratinase KP2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.98Å 44.52Å 161.71Å 90.00° 100.61° 90.00°	Depositor
Resolution (Å)	41.73 – 2.74 41.73 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.1 (41.73-2.74) 97.1 (41.73-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.256 , 0.301 0.261 , 0.304	Depositor DCC
R_{free} test set	2143 reflections (4.70%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.6	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	0.87	EDS
Total number of atoms	9562	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 23.72 % 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 4.4065e-03. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CI8, CA, 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	1.06	1/2402 (0.0%)	1.51	9/3254 (0.3%)
1	B	1.03	0/2396	1.51	5/3246 (0.2%)
1	C	1.05	0/2402	1.51	9/3254 (0.3%)
1	D	1.08	0/2402	1.52	5/3254 (0.2%)
All	All	1.06	1/9602 (0.0%)	1.51	28/13008 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	HIS	C-O	5.21	1.27	1.24

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136	ASP	CA-CB-CG	6.66	119.26	112.60
1	C	80	GLY	CA-C-N	6.07	126.72	119.98
1	C	80	GLY	C-N-CA	6.07	126.72	119.98
1	A	274	ARG	CB-CG-CD	6.05	125.22	111.30
1	D	136	ASP	CA-CB-CG	6.01	118.61	112.60
1	B	136	ASP	CA-CB-CG	5.96	118.56	112.60
1	A	13	GLY	CA-C-O	-5.95	118.35	122.22
1	B	138	ALA	CA-C-N	5.78	128.02	120.28
1	B	138	ALA	C-N-CA	5.78	128.02	120.28
1	B	80	GLY	CA-C-N	5.77	126.38	119.98
1	B	80	GLY	C-N-CA	5.77	126.38	119.98
1	C	34	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	216	TYR	CA-C-O	-5.49	114.49	120.81
1	D	201	ASP	N-CA-C	-5.32	105.65	111.82
1	A	138	ALA	CA-C-N	5.23	127.29	120.28
1	A	138	ALA	C-N-CA	5.23	127.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	GLY	CA-C-N	5.20	125.72	120.00
1	A	80	GLY	C-N-CA	5.20	125.72	120.00
1	D	3	ALA	CA-C-N	5.15	126.01	121.58
1	D	3	ALA	C-N-CA	5.15	126.01	121.58
1	C	78	PHE	CA-C-N	5.14	127.17	120.28
1	C	78	PHE	C-N-CA	5.14	127.17	120.28
1	A	298	PRO	CA-C-O	5.13	134.40	119.00
1	D	218	ASN	CB-CA-C	-5.07	101.53	109.70
1	C	136	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	220	ILE	CA-C-O	-5.01	115.85	121.36
1	C	212	ASN	CA-C-N	5.01	127.25	120.38
1	C	212	ASN	C-N-CA	5.01	127.25	120.38

There are no chirality outliers.

There are no planarity outliers.

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	2340	0	2163	25	0
1	B	2334	0	2160	36	0
1	C	2340	0	2164	33	1
1	D	2340	0	2164	29	1
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	42	0	0	0	0
3	B	42	0	0	2	0
3	C	42	0	0	1	0
3	D	42	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	7	0	0	1	0
5	C	7	0	0	1	0
5	D	7	0	0	5	0
All	All	9562	0	8651	118	1

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 6.

All (118) 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:288:ARG:HD3	1:D:178:MET:O	1.23	1.25
1:C:159[A]:SER:OG	5:C:501:HOH:O	1.85	0.90
1:D:223:HIS:ND1	5:D:501:HOH:O	2.04	0.89
1:B:288:ARG:CD	1:D:178:MET:O	2.18	0.86
1:D:27:ASN:C	1:D:27:ASN:HD22	1.94	0.76
1:A:27:ASN:C	1:A:27:ASN:HD22	1.94	0.75
1:D:223:HIS:CE1	5:D:501:HOH:O	2.40	0.74
1:C:27:ASN:C	1:C:27:ASN:HD22	1.94	0.74
1:B:27:ASN:HD22	1:B:27:ASN:C	1.96	0.74
1:D:209:SER:OG	5:D:502:HOH:O	2.06	0.73
1:A:223:HIS:CE1	5:A:501:HOH:O	2.43	0.72
1:D:221:ASP:OD2	5:D:501:HOH:O	2.10	0.69
1:C:234:TYR:CE1	1:C:238:ASN:ND2	2.63	0.66
1:A:158:GLN:HE21	1:A:265:TYR:H	1.44	0.65
1:D:158:GLN:HE21	1:D:265:TYR:H	1.45	0.65
1:B:190:ILE:HD11	3:B:402:CI8:F1	1.87	0.65
1:C:212:ASN:HB2	1:C:293:VAL:HA	1.80	0.64
1:B:201:ASP:HB3	1:B:234:TYR:CE2	2.33	0.64
1:A:201:ASP:HB3	1:A:234:TYR:CE2	2.33	0.63
1:C:158:GLN:HE21	1:C:265:TYR:H	1.47	0.63
1:B:201:ASP:O	1:B:231:ARG:HD2	1.99	0.62
1:A:108[B]:ARG:HG3	1:A:108[B]:ARG:HH11	1.64	0.62
1:D:264:ASN:HD22	1:D:266:ASN:H	1.48	0.61
1:B:212:ASN:HB2	1:B:293:VAL:HA	1.82	0.61
1:B:158:GLN:HE21	1:B:265:TYR:H	1.49	0.60
1:A:212:ASN:HB2	1:A:293:VAL:HA	1.83	0.59
1:B:223:HIS:CE1	5:B:502:HOH:O	2.55	0.58
1:C:133:VAL:HG12	1:C:133:VAL:O	2.03	0.58
1:B:258:TYR:CE2	1:B:274:ARG:HG2	2.38	0.58
1:A:86:LEU:C	1:A:86:LEU:HD23	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:LEU:C	1:B:86:LEU:HD23	2.29	0.58
1:D:212:ASN:HB2	1:D:293:VAL:HA	1.85	0.58
1:B:133:VAL:HG12	1:B:133:VAL:O	2.05	0.57
1:D:133:VAL:HG12	1:D:133:VAL:O	2.04	0.57
1:B:264:ASN:HD22	1:B:266:ASN:H	1.54	0.56
1:B:112:ASN:HD22	1:B:113:ALA:N	2.03	0.56
1:A:266:ASN:HD22	1:A:295:VAL:HG13	1.71	0.55
1:A:255:ASN:C	1:A:255:ASN:HD22	2.14	0.55
1:C:234:TYR:CD1	1:C:238:ASN:ND2	2.75	0.55
1:C:86:LEU:C	1:C:86:LEU:HD23	2.33	0.54
1:D:86:LEU:C	1:D:86:LEU:HD23	2.32	0.54
1:B:27:ASN:C	1:B:27:ASN:ND2	2.65	0.54
1:C:264:ASN:HD22	1:C:266:ASN:H	1.56	0.53
1:A:264:ASN:HD22	1:A:266:ASN:H	1.57	0.52
1:A:133:VAL:O	1:A:133:VAL:HG12	2.09	0.52
1:B:255:ASN:HD22	1:B:255:ASN:C	2.16	0.52
1:A:274:ARG:HA	1:A:277:GLN:HE21	1.74	0.51
1:B:112:ASN:ND2	1:B:113:ALA:O	2.43	0.51
1:D:264:ASN:HD22	1:D:266:ASN:N	2.08	0.50
1:D:266:ASN:HD22	1:D:295:VAL:HG13	1.76	0.50
1:C:288:ARG:NH1	1:D:185:LEU:HD21	2.27	0.50
1:A:27:ASN:C	1:A:27:ASN:ND2	2.64	0.50
1:D:264:ASN:ND2	1:D:267:SER:H	2.10	0.49
1:C:108[B]:ARG:HH11	1:C:108[B]:ARG:HG3	1.77	0.49
3:C:402:CI8:C18	3:C:402:CI8:O4	2.60	0.49
1:D:158:GLN:NE2	1:D:264:ASN:HB2	2.28	0.49
1:C:285:ASP:CG	1:D:205:ARG:HH12	2.18	0.48
1:B:112:ASN:ND2	1:B:113:ALA:H	2.11	0.48
1:B:284:ALA:O	1:B:288:ARG:HG3	2.13	0.48
1:C:285:ASP:OD2	1:D:205:ARG:NH1	2.32	0.48
1:A:158:GLN:NE2	1:A:264:ASN:HB2	2.28	0.48
1:C:264:ASN:ND2	1:C:267:SER:H	2.12	0.48
1:A:264:ASN:ND2	1:A:267:SER:H	2.11	0.47
1:C:27:ASN:C	1:C:27:ASN:ND2	2.65	0.47
1:D:255:ASN:C	1:D:255:ASN:HD22	2.18	0.47
1:C:259:TRP:CD1	1:C:268:GLY:HA2	2.49	0.47
1:B:266:ASN:HD22	1:B:295:VAL:HG13	1.80	0.47
1:B:264:ASN:ND2	1:B:267:SER:H	2.12	0.47
1:A:202:GLN:HG2	1:A:202:GLN:O	2.15	0.47
1:B:165:ALA:O	1:B:169:MET:HG3	2.16	0.46
1:C:266:ASN:HD22	1:C:295:VAL:HG13	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:ASN:HD22	1:B:266:ASN:N	2.13	0.46
1:B:112:ASN:HD22	1:B:113:ALA:H	1.62	0.46
1:C:28:ASP:OD1	1:C:28:ASP:N	2.35	0.46
1:C:264:ASN:HD22	1:C:266:ASN:N	2.13	0.46
1:B:201:ASP:HB3	1:B:234:TYR:CZ	2.52	0.45
1:D:212:ASN:ND2	1:D:294:GLY:HA3	2.31	0.45
1:C:212:ASN:ND2	1:C:294:GLY:HA3	2.31	0.45
1:C:255:ASN:C	1:C:255:ASN:HD22	2.20	0.45
1:B:259:TRP:CD1	1:B:268:GLY:HA2	2.51	0.45
1:A:264:ASN:HD22	1:A:266:ASN:N	2.15	0.45
1:B:158:GLN:NE2	1:B:264:ASN:HB2	2.32	0.45
1:A:108[B]:ARG:HH11	1:A:108[B]:ARG:CG	2.30	0.45
1:C:165:ALA:O	1:C:169:MET:HG3	2.17	0.45
1:B:188:TYR:CD1	1:B:188:TYR:C	2.95	0.45
1:D:27:ASN:C	1:D:27:ASN:ND2	2.65	0.44
1:D:259:TRP:CD1	1:D:268:GLY:HA2	2.53	0.44
1:A:98:HIS:HD2	1:A:99:LYS:O	2.01	0.44
1:B:208:ARG:HH22	3:B:402:CI8:C25	2.29	0.44
1:D:108[B]:ARG:H	1:D:108[B]:ARG:HG2	1.64	0.43
1:B:98:HIS:HD2	1:B:99:LYS:O	2.01	0.43
1:C:36:ASN:HB3	1:C:84:PHE:CE2	2.53	0.43
1:A:36:ASN:HB3	1:A:84:PHE:CE2	2.53	0.43
1:A:165:ALA:O	1:A:169:MET:HG3	2.19	0.43
1:C:87:TYR:CD2	1:C:95:PRO:HB3	2.53	0.43
1:B:63:TYR:HA	1:B:64:LYS:HA	1.81	0.43
1:C:61:ASN:HD21	1:C:63:TYR:HB3	1.84	0.43
1:A:57:ALA:HB2	1:B:98:HIS:CE1	2.53	0.42
1:A:259:TRP:CD1	1:A:268:GLY:HA2	2.54	0.42
1:B:257:TYR:HB2	1:B:258:TYR:CE1	2.54	0.42
1:C:229:TYR:OH	1:C:265:TYR:O	2.31	0.42
1:D:230:ASN:O	1:D:233:PHE:HB3	2.19	0.42
1:D:165:ALA:O	1:D:169:MET:HG3	2.19	0.42
1:C:98:HIS:HD2	1:C:99:LYS:O	2.02	0.42
1:B:61:ASN:HD21	1:B:63:TYR:HB3	1.85	0.42
1:A:211:ASP:HB3	1:A:231:ARG:HH21	1.84	0.41
1:C:230:ASN:O	1:C:233:PHE:HB3	2.20	0.41
1:C:297:CYS:HA	1:C:298:PRO:HD3	1.95	0.41
1:A:252:VAL:O	1:A:253:ASP:C	2.63	0.41
1:C:221:ASP:OD2	1:C:223:HIS:ND1	2.34	0.41
1:C:284:ALA:HA	5:D:505:HOH:O	2.21	0.41
1:D:169:MET:HG2	1:D:233:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:HIS:HD2	1:D:99:LYS:O	2.04	0.41
1:B:36:ASN:HB3	1:B:84:PHE:CE2	2.56	0.40
1:C:108[B]:ARG:HH11	1:C:108[B]:ARG:CG	2.34	0.40
1:D:35:GLY:O	1:D:99:LYS:NZ	2.54	0.40
1:B:158:GLN:NE2	1:B:265:TYR:H	2.17	0.40
1:C:158:GLN:NE2	1:C:264:ASN:HB2	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ASP:OD2	1:D:282:SER:OG[1_565]	2.07	0.13

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	299/301 (99%)	281 (94%)	17 (6%)	1 (0%)	36	54
1	B	298/301 (99%)	281 (94%)	16 (5%)	1 (0%)	36	54
1	C	299/301 (99%)	278 (93%)	20 (7%)	1 (0%)	36	54
1	D	299/301 (99%)	281 (94%)	17 (6%)	1 (0%)	36	54
All	All	1195/1204 (99%)	1121 (94%)	70 (6%)	4 (0%)	36	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	ALA
1	B	126	ALA
1	C	126	ALA
1	D	126	ALA

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	242/241 (100%)	233 (96%)	9 (4%)	30	52
1	B	241/241 (100%)	236 (98%)	5 (2%)	47	66
1	C	242/241 (100%)	232 (96%)	10 (4%)	27	48
1	D	242/241 (100%)	231 (96%)	11 (4%)	24	44
All	All	967/964 (100%)	932 (96%)	35 (4%)	36	53

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	108[A]	ARG
1	A	108[B]	ARG
1	A	159[A]	SER
1	A	159[B]	SER
1	A	190	ILE
1	A	208	ARG
1	A	212	ASN
1	A	225	SER
1	B	27	ASN
1	B	112	ASN
1	B	208	ARG
1	B	212	ASN
1	B	225	SER
1	C	27	ASN
1	C	108[A]	ARG
1	C	108[B]	ARG
1	C	159[A]	SER
1	C	159[B]	SER
1	C	190	ILE
1	C	205	ARG
1	C	212	ASN
1	C	218	ASN
1	C	225	SER

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Mol	Chain	Res	Type
1	D	19	SER
1	D	27	ASN
1	D	108[A]	ARG
1	D	108[B]	ARG
1	D	159[A]	SER
1	D	159[B]	SER
1	D	190	ILE
1	D	208	ARG
1	D	212	ASN
1	D	225	SER
1	D	291	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	43	ASN
1	A	61	ASN
1	A	74	ASN
1	A	98	HIS
1	A	158	GLN
1	A	182	ASN
1	A	202	GLN
1	A	255	ASN
1	A	264	ASN
1	A	266	ASN
1	A	277	GLN
1	B	27	ASN
1	B	61	ASN
1	B	74	ASN
1	B	98	HIS
1	B	112	ASN
1	B	158	GLN
1	B	182	ASN
1	B	202	GLN
1	B	255	ASN
1	B	264	ASN
1	B	266	ASN
1	C	27	ASN
1	C	61	ASN
1	C	74	ASN
1	C	98	HIS

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Mol	Chain	Res	Type
1	C	158	GLN
1	C	182	ASN
1	C	255	ASN
1	C	264	ASN
1	C	266	ASN
1	D	27	ASN
1	D	43	ASN
1	D	61	ASN
1	D	74	ASN
1	D	98	HIS
1	D	158	GLN
1	D	182	ASN
1	D	202	GLN
1	D	255	ASN
1	D	264	ASN
1	D	266	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CI8	B	402	2	43,45,45	0.47	0	57,65,65	1.03	3 (5%)
3	CI8	C	402	2	43,45,45	0.45	0	57,65,65	0.81	1 (1%)
3	CI8	D	402	2	43,45,45	0.45	0	57,65,65	0.80	1 (1%)
3	CI8	A	402	2	43,45,45	0.44	0	57,65,65	0.88	2 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CI8	B	402	2	-	6/34/44/44	0/4/4/4
3	CI8	C	402	2	-	4/34/44/44	0/4/4/4
3	CI8	D	402	2	-	3/34/44/44	0/4/4/4
3	CI8	A	402	2	-	5/34/44/44	0/4/4/4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	CI8	C6-C5-S1	-4.02	116.95	121.32
3	B	402	CI8	C6-C5-N2	3.75	126.77	124.00
3	C	402	CI8	C8-C7-N1	-3.03	114.58	117.54
3	A	402	CI8	C11-C8-C7	-2.36	103.77	110.83
3	A	402	CI8	C6-C5-S1	-2.36	118.76	121.32
3	D	402	CI8	O4-C10-C9	-2.06	117.12	122.95
3	B	402	CI8	C18-C17-C12	-2.05	108.52	110.50

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	CI8	C7-C8-C9-C10
3	B	402	CI8	C7-C8-C9-C10
3	C	402	CI8	N3-C28-C29-O7
3	D	402	CI8	C3-C2-O1-C1
3	A	402	CI8	C3-C2-O1-C1
3	B	402	CI8	C3-C2-O1-C1
3	C	402	CI8	C3-C2-O1-C1

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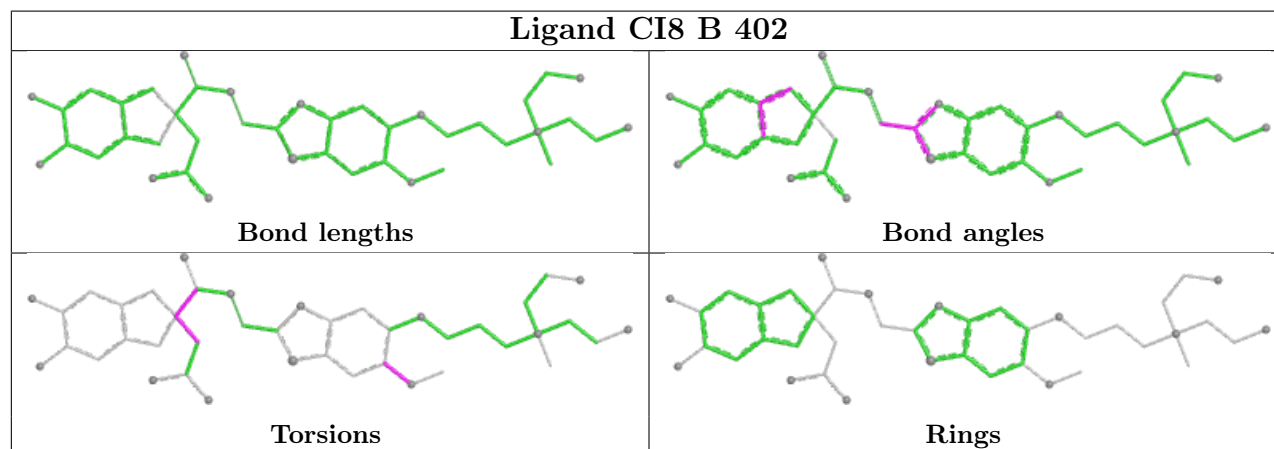
Mol	Chain	Res	Type	Atoms
3	D	402	CI8	C21-C2-O1-C1
3	A	402	CI8	C21-C2-O1-C1
3	B	402	CI8	C21-C2-O1-C1
3	C	402	CI8	C21-C2-O1-C1
3	B	402	CI8	O2-C7-C8-C11
3	C	402	CI8	C5-C6-N1-C7
3	B	402	CI8	C11-C8-C9-C10
3	A	402	CI8	N1-C7-C8-C11
3	A	402	CI8	O2-C7-C8-C11
3	B	402	CI8	N1-C7-C8-C11
3	D	402	CI8	C5-C6-N1-C7

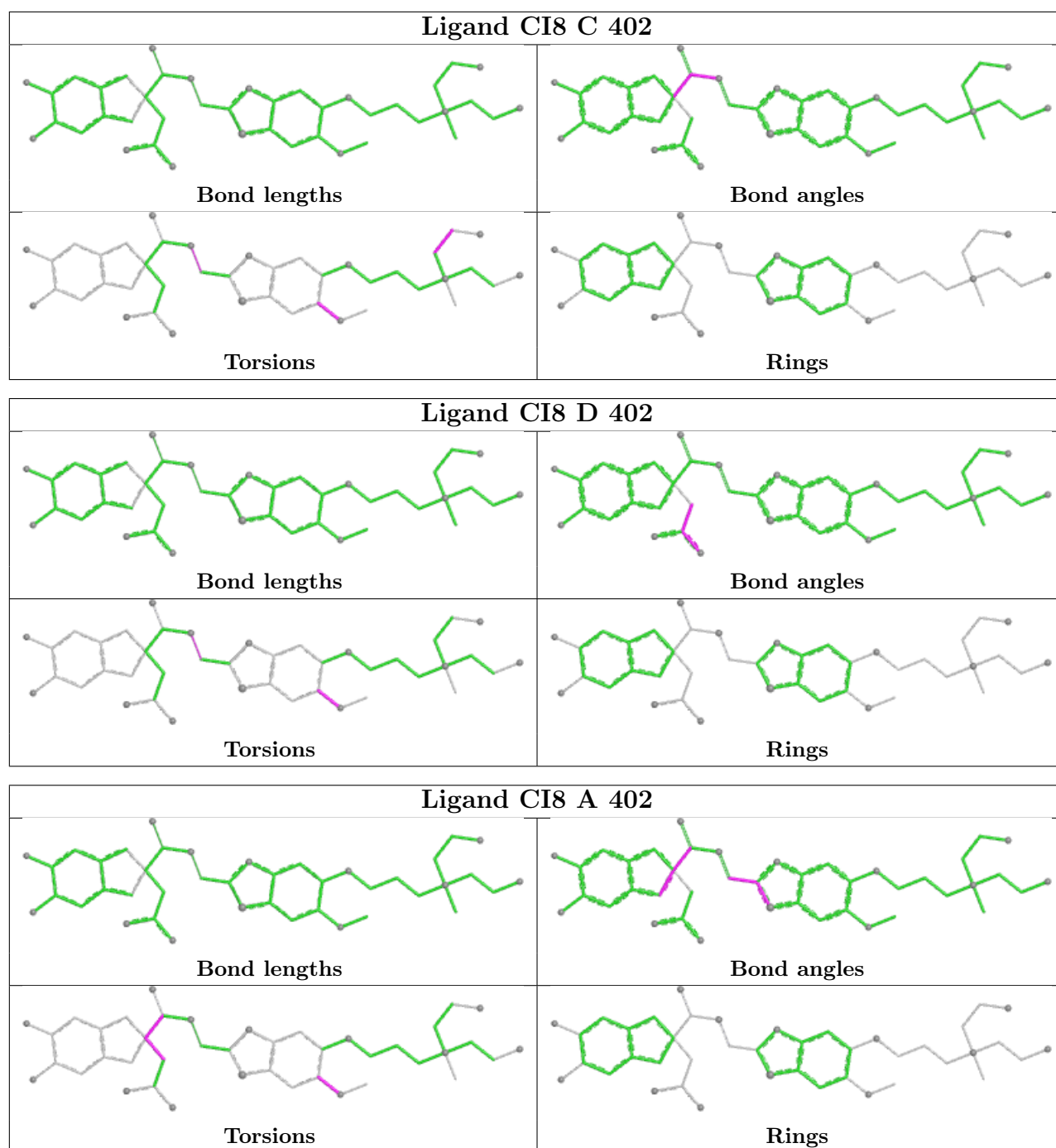
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	CI8	2	0
3	C	402	CI8	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	298/301 (99%)	0.55	8 (2%) 56 53	14, 40, 54, 71	3 (1%)
1	B	298/301 (99%)	0.55	5 (1%) 69 66	17, 41, 53, 91	2 (0%)
1	C	298/301 (99%)	0.41	5 (1%) 69 66	15, 34, 49, 69	3 (1%)
1	D	298/301 (99%)	0.43	5 (1%) 69 66	17, 35, 47, 60	3 (1%)
All	All	1192/1204 (99%)	0.49	23 (1%) 66 63	14, 37, 51, 91	11 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	108[A]	ARG	6.4
1	A	108[A]	ARG	5.9
1	C	108[A]	ARG	4.7
1	B	288	ARG	4.6
1	D	108[A]	ARG	3.5
1	A	288	ARG	2.9
1	A	156	ARG	2.9
1	C	20	ASP	2.9
1	C	156	ARG	2.8
1	A	159[A]	SER	2.8
1	B	298	PRO	2.6
1	C	117	GLY	2.6
1	A	298	PRO	2.6
1	B	208	ARG	2.5
1	D	280	ASN	2.5
1	B	274	ARG	2.5
1	A	179	ARG	2.4
1	C	59	PRO	2.3
1	D	124	ASP	2.3
1	D	159[A]	SER	2.3
1	A	208	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	208	ARG	2.1
1	A	274	ARG	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](#)

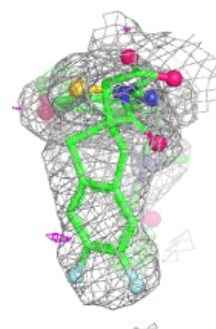
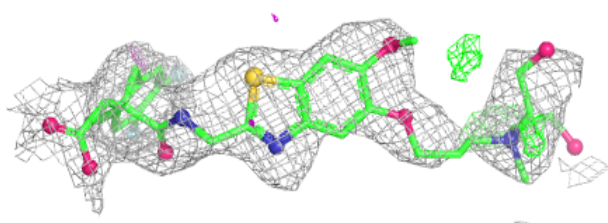
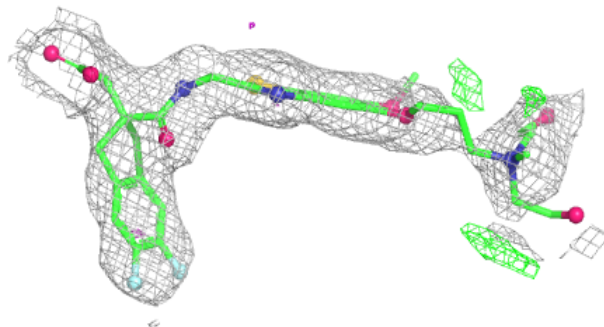
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
3	CI8	A	402	42/42	0.88	0.17	25,40,98,105	0
3	CI8	B	402	42/42	0.88	0.16	31,45,78,79	0
3	CI8	D	402	42/42	0.88	0.18	24,34,97,103	0
3	CI8	C	402	42/42	0.89	0.16	24,35,86,89	0
4	CA	B	403	1/1	0.92	0.06	81,81,81,81	0
4	CA	A	404	1/1	0.98	0.06	31,31,31,31	0
4	CA	B	404	1/1	0.98	0.05	37,37,37,37	0
4	CA	C	403	1/1	0.98	0.05	35,35,35,35	0
4	CA	C	404	1/1	0.98	0.05	33,33,33,33	0
4	CA	D	404	1/1	0.98	0.04	35,35,35,35	0
2	ZN	C	401	1/1	0.99	0.04	25,25,25,25	0
4	CA	D	403	1/1	0.99	0.04	29,29,29,29	0
4	CA	A	403	1/1	0.99	0.02	40,40,40,40	0
2	ZN	B	401	1/1	1.00	0.01	30,30,30,30	0
2	ZN	A	401	1/1	1.00	0.01	29,29,29,29	0
2	ZN	D	401	1/1	1.00	0.02	23,23,23,23	0

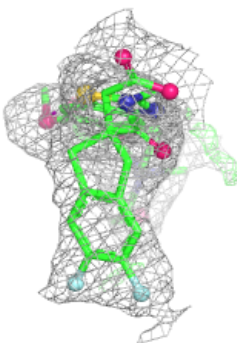
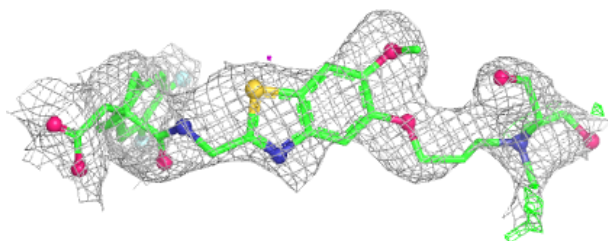
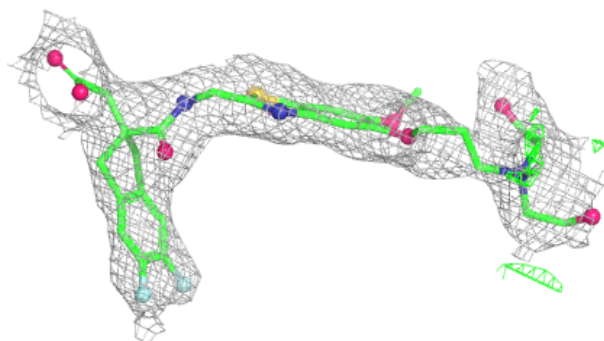
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CI8 A 402:

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

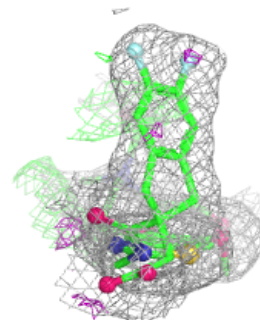
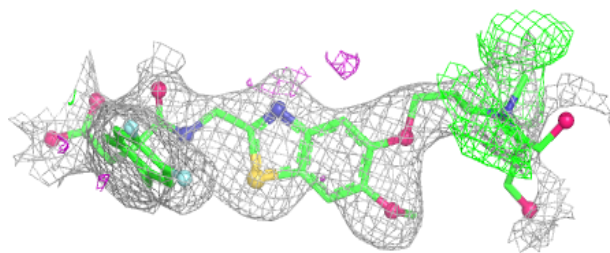
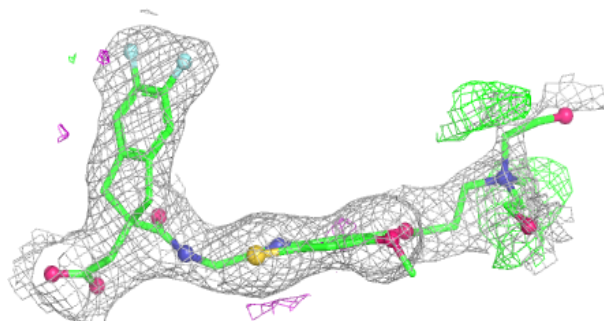
**Electron density around CI8 B 402:**

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

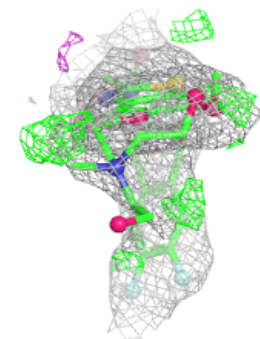
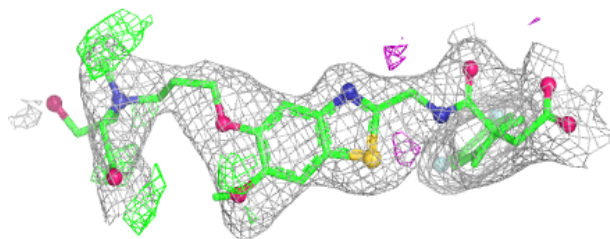
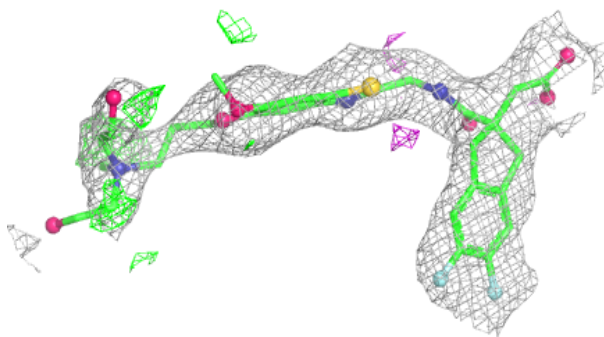


Electron density around CI8 D 402:

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

**Electron density around CI8 C 402:**

$2mF_o-DF_c$ (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.