



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2024 – 05:00 pm BST

PDB ID : 8RQ9
Title : Crystal structure of PROTAC CFT-1297 in complex with CRBN-midi and BRD4(BD2)
Authors : Darren, D.; Ramachandran, S.; Kroupova, A.; Zollman, D.; Ciulli, A.
Deposited on : 2024-01-17
Resolution : 2.91 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

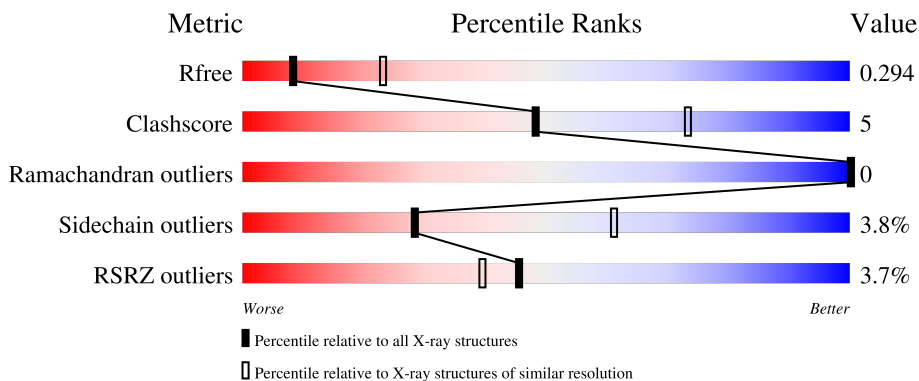
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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}	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

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	329	 3% 85% 10% .
1	C	329	 3% 79% 16% 5%
2	B	130	 5% 81% 12% 8%
2	D	130	 5% 87% 5% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6384 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	2345	1490	399	441	15	0	0	0
1	C	312	2279	1452	385	429	13	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	40	SER	-	expression tag	UNP Q96SW2
A	78	ILE	CYS	engineered mutation	UNP Q96SW2
A	92	VAL	ILE	engineered mutation	UNP Q96SW2
A	116	ASN	LYS	engineered mutation	UNP Q96SW2
A	134	GLU	GLN	engineered mutation	UNP Q96SW2
A	188	GLY	-	linker	UNP Q96SW2
A	189	SER	-	linker	UNP Q96SW2
A	190	GLY	-	linker	UNP Q96SW2
A	283	TRP	ARG	engineered mutation	UNP Q96SW2
A	287	ASN	CYS	engineered mutation	UNP Q96SW2
A	293	SER	VAL	engineered mutation	UNP Q96SW2
A	302	ASP	GLY	engineered mutation	UNP Q96SW2
A	342	ARG	LEU	engineered mutation	UNP Q96SW2
A	343	GLU	CYS	engineered mutation	UNP Q96SW2
A	359	ILE	THR	engineered mutation	UNP Q96SW2
A	423	ILE	LEU	engineered mutation	UNP Q96SW2
C	40	SER	-	expression tag	UNP Q96SW2
C	78	ILE	CYS	engineered mutation	UNP Q96SW2
C	92	VAL	ILE	engineered mutation	UNP Q96SW2
C	116	ASN	LYS	engineered mutation	UNP Q96SW2
C	134	GLU	GLN	engineered mutation	UNP Q96SW2
C	246	GLY	-	linker	UNP Q96SW2
C	247	SER	-	linker	UNP Q96SW2
C	248	GLY	-	linker	UNP Q96SW2
C	283	TRP	ARG	engineered mutation	UNP Q96SW2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	287	ASN	CYS	engineered mutation	UNP Q96SW2
C	293	SER	VAL	engineered mutation	UNP Q96SW2
C	302	ASP	GLY	engineered mutation	UNP Q96SW2
C	342	ARG	LEU	engineered mutation	UNP Q96SW2
C	343	GLU	CYS	engineered mutation	UNP Q96SW2
C	359	ILE	THR	engineered mutation	UNP Q96SW2
C	423	ILE	LEU	engineered mutation	UNP Q96SW2

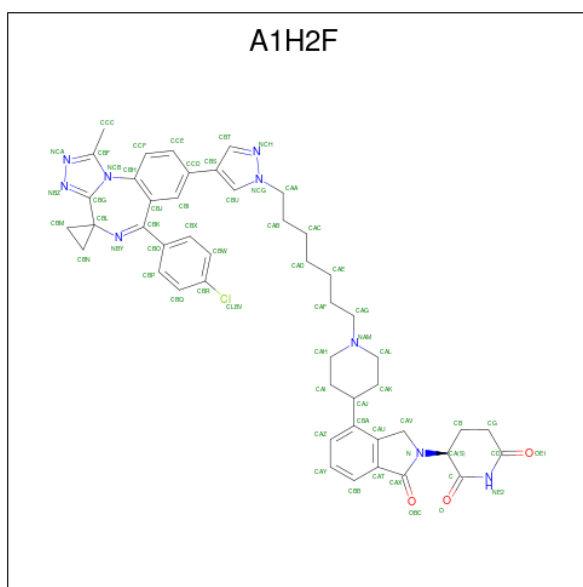
- Molecule 2 is a protein called Bromodomain-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	120	Total	C	N	O	S	0	0	0
			819	519	137	156	7			
2	D	120	Total	C	N	O	S	0	0	0
			788	500	134	148	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	331	SER	-	expression tag	UNP O60885
B	332	MET	-	expression tag	UNP O60885
D	331	SER	-	expression tag	UNP O60885
D	332	MET	-	expression tag	UNP O60885

- Molecule 3 is (3 {S})-3-[7-[1-[7-[4-[6-(4-chlorophenyl)-1-methyl-spiro[[1,2,4]triazolo[4,3-a][1,4]benzodiazepine-4,1'-cyclopropane]-8-yl]pyrazol-1-yl]heptyl]piperidin-4-yl]-3-oxidanylidene-1 {H}-isoindol-2-yl]piperidine-2,6-dione (three-letter code: A1H2F) (formula: C₄₇H₅₀ClN₉O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	Cl	N	O	0	0
			60	47	1	9	3		
3	C	1	Total	C	Cl	N	O	0	0
			60	47	1	9	3		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

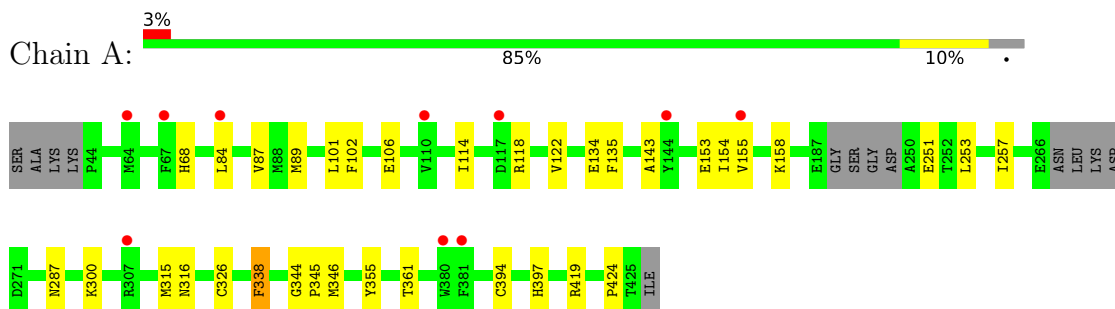
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	6	Total	O	0	0
			6	6		
5	D	6	Total	O	0	0
			6	6		
5	C	9	Total	O	0	0
			9	9		

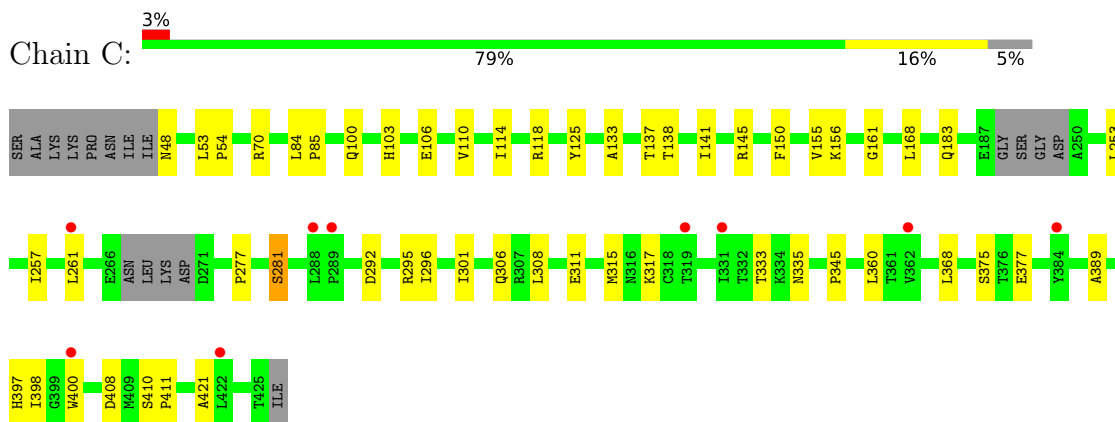
3 Residue-property plots [i](#)

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.

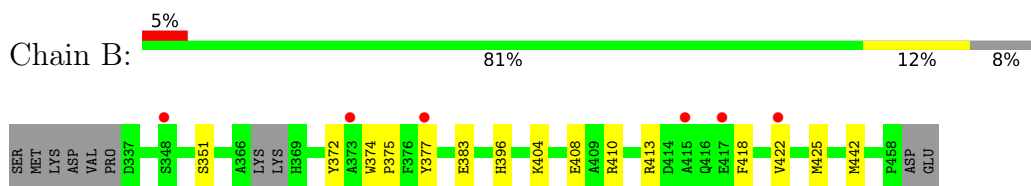
- Molecule 1: Protein cereblon



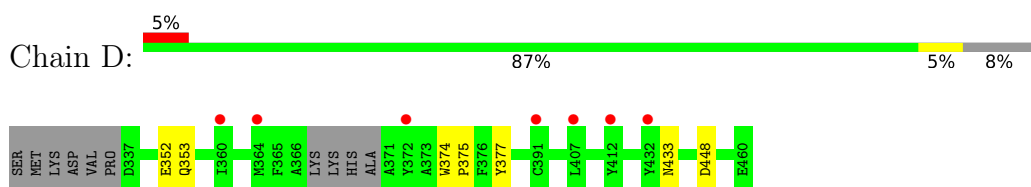
- Molecule 1: Protein cereblon



- Molecule 2: Bromodomain-containing protein 4



- Molecule 2: Bromodomain-containing protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.88Å 52.64Å 130.35Å 96.44° 91.49° 99.22°	Depositor
Resolution (Å)	43.27 – 2.91 43.27 – 2.91	Depositor EDS
% Data completeness (in resolution range)	81.0 (43.27-2.91) 78.5 (43.27-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.249 , 0.293 0.252 , 0.294	Depositor DCC
R_{free} test set	1951 reflections (8.02%)	wwPDB-VP
Wilson B-factor (Å ²)	90.5	Xtrriage
Anisotropy	0.125	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 95.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6384	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% 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: ZN, A1H2F

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	0.35	0/2398	0.51	0/3281
1	C	0.35	0/2331	0.50	0/3191
2	B	0.36	0/838	0.46	0/1148
2	D	0.35	0/807	0.46	0/1110
All	All	0.35	0/6374	0.49	0/8730

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	2345	0	2124	21	0
1	C	2279	0	2038	29	0
2	B	819	0	660	6	0
2	D	788	0	601	4	0
3	A	60	0	0	1	0
3	C	60	0	0	5	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
5	A	10	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	6	0	0	0	0
5	C	9	0	0	0	0
5	D	6	0	0	0	0
All	All	6384	0	5423	63	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 5.

All (63) 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)
3:C:501:A1H2F:CCF	3:C:501:A1H2F:CCC	2.64	0.75
2:B:372:TYR:HB3	2:B:442:MET:HB3	1.72	0.70
1:A:419:ARG:HH22	1:A:424:PRO:HD3	1.59	0.68
1:C:333:THR:HG23	1:C:335:ASN:H	1.59	0.67
1:A:257:ILE:HG23	1:A:315:MET:HE1	1.76	0.67
1:A:326:CYS:HB3	1:A:394:CYS:HB3	1.77	0.66
1:C:48:ASN:HB2	1:C:410:SER:H	1.62	0.64
3:C:501:A1H2F:CAH	3:C:501:A1H2F:CAZ	2.75	0.63
1:C:368:LEU:HD13	1:C:389:ALA:HB1	1.82	0.61
1:A:287:ASN:HD22	1:A:345:PRO:HD2	1.66	0.60
1:C:125:TYR:HA	1:C:133:ALA:HB2	1.84	0.59
2:D:374:TRP:HZ3	3:C:501:A1H2F:CBT	2.16	0.58
1:C:253:LEU:HD23	1:C:308:LEU:HB3	1.85	0.58
1:C:103:HIS:HB2	1:C:106:GLU:HG3	1.85	0.58
2:B:374:TRP:CD2	2:B:375:PRO:HD3	2.41	0.56
1:C:168:LEU:HD21	1:C:183:GLN:HB2	1.88	0.55
1:C:114:ILE:HA	1:C:118:ARG:HG2	1.89	0.54
1:C:311:GLU:O	1:C:315:MET:HG3	2.07	0.54
1:A:338:PHE:O	1:A:361:THR:OG1	2.25	0.54
2:B:351:SER:HA	2:B:410:ARG:HH21	1.72	0.54
1:C:145:ARG:HE	1:C:156:LYS:HD2	1.74	0.53
1:C:398:ILE:HD13	1:C:421:ALA:HB1	1.90	0.52
1:A:102:PHE:CD1	1:A:154:ILE:HD12	2.44	0.52
2:B:374:TRP:CG	2:B:375:PRO:HD3	2.45	0.52
1:A:287:ASN:ND2	1:A:344:GLY:HA3	2.27	0.49
1:C:397:HIS:HE1	1:C:400:TRP:CZ2	2.30	0.49
1:A:101:LEU:HD23	1:A:106:GLU:HB3	1.95	0.49
2:D:374:TRP:CZ3	3:C:501:A1H2F:CBT	2.97	0.47
2:D:374:TRP:CG	2:D:375:PRO:HD3	2.50	0.46
1:C:277:PRO:O	1:C:281:SER:OG	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:VAL:HG11	1:A:122:VAL:HG12	1.97	0.46
1:C:110:VAL:HG11	1:C:155:VAL:HG11	1.98	0.46
1:A:300:LYS:HB3	1:A:300:LYS:HE3	1.60	0.46
1:A:251:GLU:H	1:A:251:GLU:CD	2.19	0.45
1:A:143:ALA:HB3	1:A:158:LYS:HB2	1.98	0.44
1:C:292:ASP:O	1:C:296:ILE:HD12	2.16	0.44
1:C:410:SER:HB2	1:C:411:PRO:HD3	1.98	0.44
1:C:292:ASP:O	1:C:295:ARG:N	2.47	0.44
1:A:134:GLU:HG3	1:A:135:PHE:HD1	1.82	0.44
1:C:257:ILE:O	1:C:261:LEU:HD12	2.17	0.44
1:C:100:GLN:HG3	1:C:156:LYS:HG2	2.00	0.44
2:D:374:TRP:HZ3	3:C:501:A1H2F:NCH	2.15	0.44
3:A:501:A1H2F:CBX	3:A:501:A1H2F:CBI	2.93	0.43
1:C:317:LYS:HB3	1:C:317:LYS:HE3	1.83	0.43
1:A:84:LEU:HD23	1:A:87:VAL:HB	1.99	0.43
1:A:114:ILE:HA	1:A:118:ARG:HG2	2.01	0.43
2:B:404:LYS:O	2:B:408:GLU:HG3	2.18	0.43
1:C:375:SER:OG	1:C:377:GLU:HG3	2.17	0.43
1:C:301:ILE:HD12	1:C:301:ILE:H	1.84	0.43
1:A:253:LEU:O	1:A:257:ILE:HG13	2.19	0.42
2:B:418:PHE:O	2:B:422:VAL:HG23	2.19	0.42
1:C:345:PRO:HB2	1:C:360:LEU:HD21	2.00	0.42
1:A:101:LEU:HB2	1:A:155:VAL:HG22	2.01	0.42
1:C:53:LEU:HB3	1:C:54:PRO:HD3	2.01	0.42
1:A:397:HIS:CD2	1:A:397:HIS:N	2.87	0.42
1:A:287:ASN:HB3	1:A:345:PRO:HG2	2.02	0.41
1:C:118:ARG:HB3	1:C:141:ILE:HB	2.02	0.41
1:C:345:PRO:HB2	1:C:360:LEU:CD2	2.50	0.41
1:C:138:THR:O	1:C:161:GLY:HA2	2.20	0.41
1:A:287:ASN:ND2	1:A:345:PRO:HD2	2.34	0.41
1:C:84:LEU:HA	1:C:85:PRO:HD3	1.96	0.41
1:A:153:GLU:O	1:A:154:ILE:HD13	2.20	0.41
1:C:301:ILE:HG21	1:C:306:GLN:HB2	2.02	0.41

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	310/329 (94%)	301 (97%)	9 (3%)	0	100	100
1	C	306/329 (93%)	296 (97%)	10 (3%)	0	100	100
2	B	116/130 (89%)	109 (94%)	7 (6%)	0	100	100
2	D	116/130 (89%)	113 (97%)	3 (3%)	0	100	100
All	All	848/918 (92%)	819 (97%)	29 (3%)	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	227/293 (78%)	221 (97%)	6 (3%)	41	72
1	C	214/293 (73%)	209 (98%)	5 (2%)	45	75
2	B	64/115 (56%)	59 (92%)	5 (8%)	10	29
2	D	55/115 (48%)	50 (91%)	5 (9%)	7	23
All	All	560/816 (69%)	539 (96%)	21 (4%)	28	61

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	HIS
1	A	89	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	316	ASN
1	A	338	PHE
1	A	346	MET
1	A	355	TYR
2	B	377	TYR
2	B	383	GLU
2	B	396	HIS
2	B	413	ARG
2	B	425	MET
2	D	352	GLU
2	D	353	GLN
2	D	377	TYR
2	D	433	ASN
2	D	448	ASP
1	C	70	ARG
1	C	137	THR
1	C	150	PHE
1	C	281	SER
1	C	408	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	316	ASN
1	A	397	HIS
1	C	397	HIS

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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A1H2F	C	501	-	64,69,69	2.97	16 (25%)	78,102,102	2.78	21 (26%)
3	A1H2F	A	501	-	64,69,69	2.91	15 (23%)	78,102,102	2.89	21 (26%)

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	A1H2F	C	501	-	-	8/26/84/84	0/9/10/10
3	A1H2F	A	501	-	-	3/26/84/84	0/9/10/10

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	501	A1H2F	CAT-CAX	-9.68	1.33	1.48
3	A	501	A1H2F	CAT-CAX	-9.64	1.33	1.48
3	C	501	A1H2F	CAV-CAU	-9.24	1.39	1.50
3	A	501	A1H2F	CAV-CAU	-9.18	1.39	1.50
3	C	501	A1H2F	CBA-CAJ	-7.53	1.39	1.52
3	A	501	A1H2F	CBO-CBK	-7.09	1.39	1.49
3	A	501	A1H2F	CBA-CAJ	-7.08	1.39	1.52
3	C	501	A1H2F	CBO-CBK	-7.02	1.39	1.49
3	C	501	A1H2F	CBJ-CBK	-6.92	1.39	1.49
3	A	501	A1H2F	CBJ-CBK	-6.88	1.39	1.49
3	C	501	A1H2F	CA-C	-6.43	1.38	1.51
3	A	501	A1H2F	CA-C	-6.38	1.38	1.51
3	A	501	A1H2F	CCD-CBS	-6.34	1.33	1.49
3	C	501	A1H2F	CCD-CBS	-6.33	1.33	1.49
3	C	501	A1H2F	CG-CD	-5.03	1.38	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	A1H2F	CG-CD	-4.96	1.38	1.50
3	C	501	A1H2F	CAU-CBA	-4.63	1.33	1.40
3	C	501	A1H2F	CBK-NBY	4.53	1.34	1.28
3	A	501	A1H2F	CAU-CBA	-4.50	1.33	1.40
3	A	501	A1H2F	CBB-CAT	-4.13	1.33	1.39
3	C	501	A1H2F	CBB-CAT	-4.11	1.33	1.39
3	A	501	A1H2F	CBK-NBY	4.10	1.33	1.28
3	A	501	A1H2F	CAX-N	-3.86	1.32	1.36
3	C	501	A1H2F	CAX-N	-3.80	1.32	1.36
3	C	501	A1H2F	CBU-CBS	-2.94	1.33	1.38
3	A	501	A1H2F	CBU-CBS	-2.83	1.33	1.38
3	C	501	A1H2F	CBF-NCB	-2.77	1.33	1.37
3	C	501	A1H2F	CBG-NCB	-2.45	1.33	1.37
3	C	501	A1H2F	CAT-CAU	-2.19	1.34	1.39
3	A	501	A1H2F	CAT-CAU	-2.17	1.34	1.39
3	A	501	A1H2F	NCA-NBZ	-2.14	1.33	1.37

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	A1H2F	CAV-N-CAX	-16.60	106.29	113.12
3	C	501	A1H2F	CAV-N-CAX	-16.03	106.53	113.12
3	A	501	A1H2F	CAT-CAX-N	8.62	111.53	106.44
3	C	501	A1H2F	CAT-CAX-N	8.40	111.40	106.44
3	A	501	A1H2F	CAU-CAV-N	7.47	104.18	101.79
3	C	501	A1H2F	CAU-CAV-N	6.72	103.94	101.79
3	C	501	A1H2F	CCF-CBH-NCB	-5.55	112.17	119.47
3	A	501	A1H2F	CCF-CBH-CBJ	-5.54	117.90	122.95
3	A	501	A1H2F	CBI-CBJ-CBK	-4.54	112.29	118.88
3	C	501	A1H2F	CBI-CBJ-CBK	-3.93	113.19	118.88
3	A	501	A1H2F	CB-CA-N	-3.90	109.90	114.11
3	A	501	A1H2F	CBT-NCH-NCG	3.84	108.23	104.23
3	C	501	A1H2F	CBT-NCH-NCG	3.75	108.14	104.23
3	C	501	A1H2F	CBU-NCG-NCH	-3.49	108.52	111.56
3	A	501	A1H2F	CBU-NCG-NCH	-3.49	108.52	111.56
3	A	501	A1H2F	CD-NE2-C	-3.35	121.94	126.61
3	C	501	A1H2F	CAV-N-CA	3.32	126.87	123.69
3	A	501	A1H2F	CBI-CBJ-CBH	3.27	121.03	117.40
3	C	501	A1H2F	CD-NE2-C	-3.21	122.15	126.61
3	C	501	A1H2F	CB-CG-CD	-3.19	108.47	114.12
3	A	501	A1H2F	CAV-N-CA	3.15	126.70	123.69
3	A	501	A1H2F	CA-N-CAX	3.05	126.67	121.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	A1H2F	CBT-CBS-CCD	-2.97	123.86	127.74
3	A	501	A1H2F	CA-C-NE2	2.92	120.17	116.25
3	C	501	A1H2F	CA-N-CAX	2.88	126.39	121.81
3	A	501	A1H2F	CBH-CBJ-CBK	2.85	126.68	122.74
3	C	501	A1H2F	CCF-CBH-CBJ	-2.81	120.39	122.95
3	A	501	A1H2F	CB-CG-CD	-2.77	109.21	114.12
3	C	501	A1H2F	CBH-CBJ-CBK	2.77	126.57	122.74
3	C	501	A1H2F	CA-C-NE2	2.58	119.72	116.25
3	C	501	A1H2F	CBI-CBJ-CBH	2.56	120.24	117.40
3	C	501	A1H2F	CBT-CBS-CCD	-2.47	124.51	127.74
3	C	501	A1H2F	CG-CD-NE2	2.44	119.39	116.65
3	C	501	A1H2F	CB-CA-N	-2.42	111.50	114.11
3	A	501	A1H2F	CG-CD-NE2	2.39	119.33	116.65
3	A	501	A1H2F	CCF-CBH-NCB	-2.34	116.39	119.47
3	A	501	A1H2F	CAU-CBA-CAJ	-2.34	119.40	122.09
3	C	501	A1H2F	OBC-CAX-CAT	-2.34	124.13	128.68
3	A	501	A1H2F	OBC-CAX-CAT	-2.30	124.21	128.68
3	C	501	A1H2F	CAL-CAK-CAJ	-2.22	108.42	111.04
3	A	501	A1H2F	CAL-CAK-CAJ	-2.09	108.56	111.04
3	C	501	A1H2F	CBU-CBS-CCD	-2.06	125.05	127.74

There are no chirality outliers.

All (11) torsion outliers are listed below:

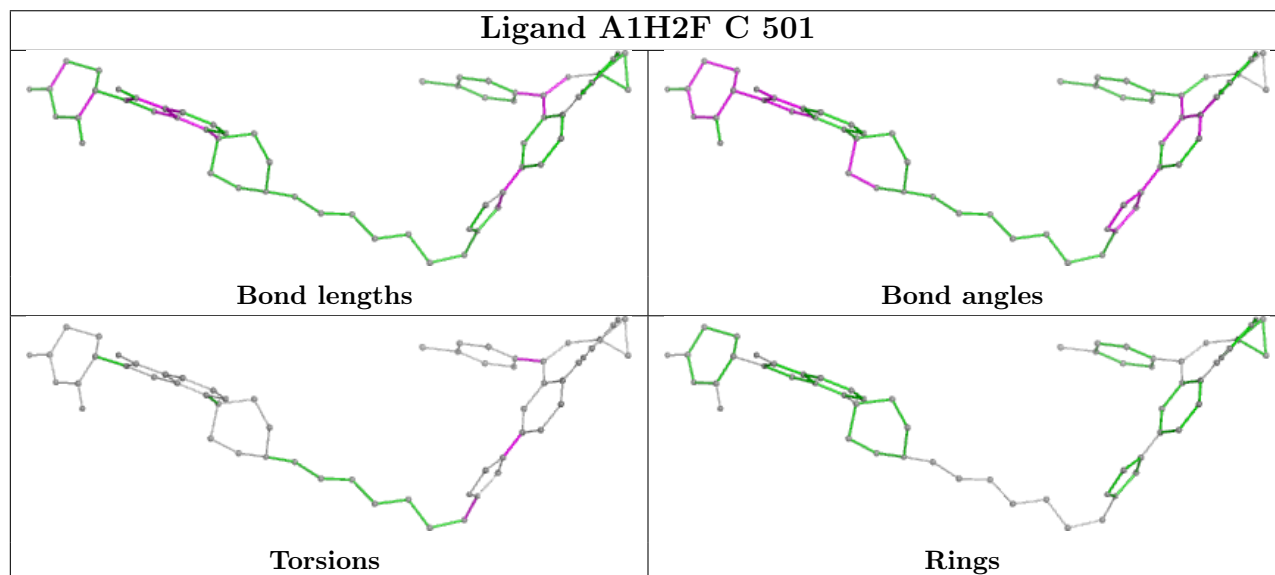
Mol	Chain	Res	Type	Atoms
3	A	501	A1H2F	CAB-CAA-NCG-CBU
3	A	501	A1H2F	CAB-CAA-NCG-NCH
3	C	501	A1H2F	CAB-CAA-NCG-CBU
3	C	501	A1H2F	CAB-CAA-NCG-NCH
3	C	501	A1H2F	NBY-CBK-CBO-CBP
3	A	501	A1H2F	NCG-CAA-CAB-CAC
3	C	501	A1H2F	NBY-CBK-CBO-CBX
3	C	501	A1H2F	CBJ-CBK-CBO-CBP
3	C	501	A1H2F	CBJ-CBK-CBO-CBX
3	C	501	A1H2F	CBT-CBS-CCD-CBI
3	C	501	A1H2F	CBU-CBS-CCD-CBI

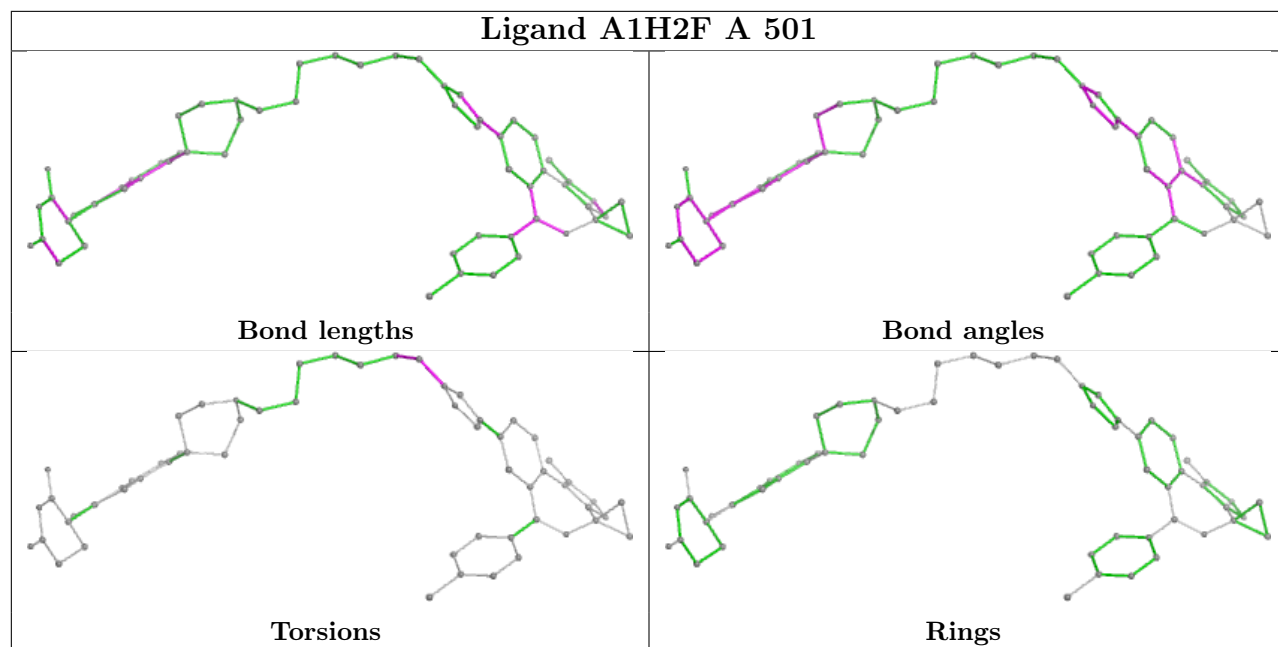
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	A1H2F	5	0
3	A	501	A1H2F	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	316/329 (96%)	0.16	10 (3%) 50 44	33, 73, 106, 138	0
1	C	312/329 (94%)	0.35	9 (2%) 54 48	45, 78, 111, 135	0
2	B	120/130 (92%)	0.16	6 (5%) 35 30	46, 66, 91, 122	0
2	D	120/130 (92%)	0.39	7 (5%) 30 26	46, 66, 89, 112	0
All	All	868/918 (94%)	0.26	32 (3%) 45 39	33, 73, 106, 138	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	372	TYR	6.5
2	B	415	ALA	5.5
1	C	422	LEU	4.0
2	D	364	MET	3.3
1	A	307	ARG	3.3
1	C	400	TRP	3.3
1	A	144	TYR	2.9
1	C	289	PRO	2.8
2	B	377	TYR	2.8
2	D	432	TYR	2.6
2	B	373	ALA	2.6
1	A	380	TRP	2.6
1	A	155	VAL	2.5
2	D	412	TYR	2.4
1	A	84	LEU	2.4
1	A	117	ASP	2.4
1	C	384	TYR	2.3
2	B	348	SER	2.3
2	B	422	VAL	2.3
1	C	261	LEU	2.2
1	C	288	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	362	VAL	2.2
1	A	381	PHE	2.2
1	A	64	MET	2.2
2	D	407	LEU	2.1
2	B	417	GLU	2.1
1	C	331	ILE	2.1
2	D	360	ILE	2.1
1	A	110	VAL	2.1
2	D	391	CYS	2.0
1	A	67	PHE	2.0
1	C	319	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

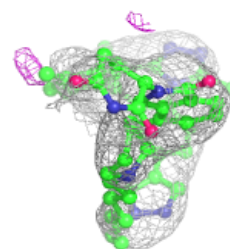
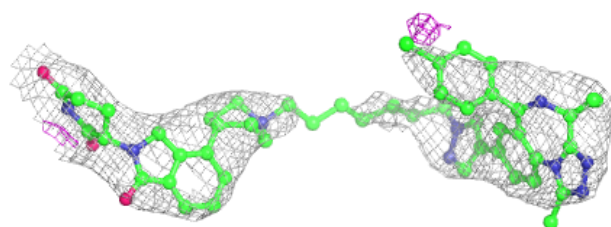
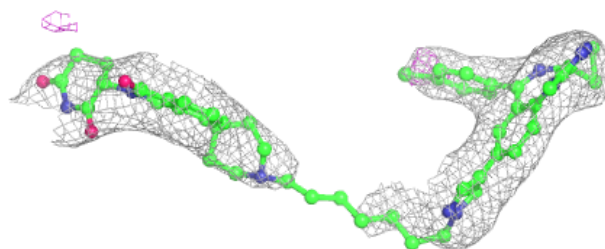
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1H2F	C	501	60/60	0.87	0.12	52,75,97,110	0
3	A1H2F	A	501	60/60	0.88	0.12	40,67,93,127	0
4	ZN	A	502	1/1	0.97	0.04	70,70,70,70	0
4	ZN	C	502	1/1	0.99	0.04	57,57,57,57	0

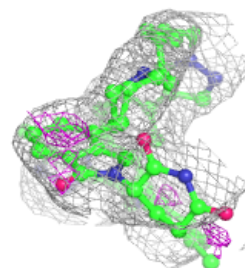
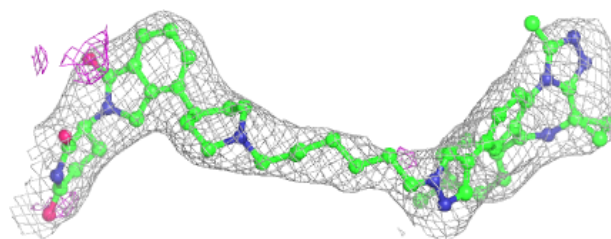
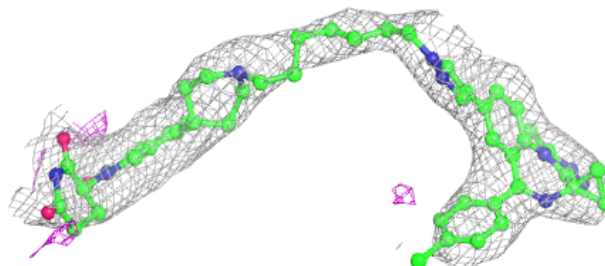
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H2F C 501:

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

**Electron density around A1H2F A 501:**

$2mF_o-DF_c$ (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.