



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:34 am BST

PDB ID : 6R0Q
Title : Mutant cereblon isoform 4 from *Magnetospirillum gryphiswaldense* in complex with thalidomide metabolite alpha-(o-carboxybenzamido)glutarimide
Authors : Heim, C.; Hartmann, M.D.
Deposited on : 2019-03-13
Resolution : 1.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

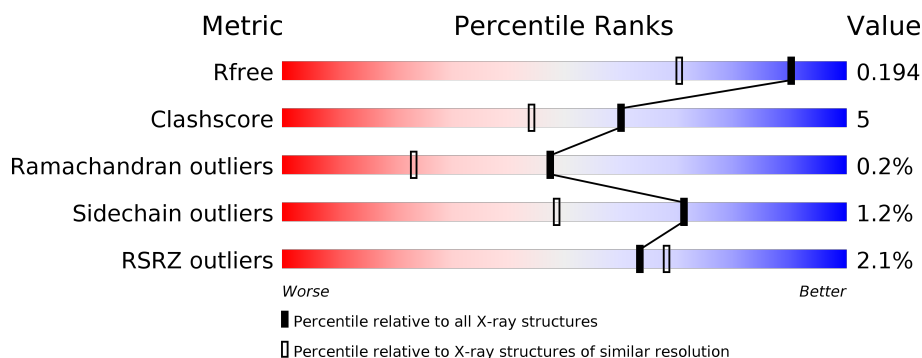
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on 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	124	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>17%</div> <div>•</div> <div>14%</div> </div> </div>
1	B	124	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>•</div> <div>16%</div> </div> </div>
1	C	124	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>20%</div> <div>•</div> <div>14%</div> </div> </div>
1	D	124	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>15%</div> <div>•</div> <div>16%</div> </div> </div>
2	E	3	<div> <div></div> <div>100%</div> </div>
2	F	3	<div> <div></div> <div>67%</div> <div>33%</div> </div>

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Mol	Chain	Length	Quality of chain
2	G	3	 67% 33%
3	H	4	 75% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3985 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 Cereblon isoform 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	1	0
			856	544	156	150	6			
1	B	104	Total	C	N	O	S	0	2	0
			839	537	157	139	6			
1	C	107	Total	C	N	O	S	0	4	0
			868	554	157	151	6			
1	D	104	Total	C	N	O	S	0	3	0
			852	544	159	143	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	HIS	ALA	engineered mutation	UNP A4TVL0
A	54	TYR	MET	engineered mutation	UNP A4TVL0
A	56	HIS	PHE	engineered mutation	UNP A4TVL0
A	68	ASN	ARG	engineered mutation	UNP A4TVL0
A	72	ARG	ALA	engineered mutation	UNP A4TVL0
A	87	VAL	ILE	engineered mutation	UNP A4TVL0
A	89	GLN	LEU	engineered mutation	UNP A4TVL0
B	52	HIS	ALA	engineered mutation	UNP A4TVL0
B	54	TYR	MET	engineered mutation	UNP A4TVL0
B	56	HIS	PHE	engineered mutation	UNP A4TVL0
B	68	ASN	ARG	engineered mutation	UNP A4TVL0
B	72	ARG	ALA	engineered mutation	UNP A4TVL0
B	87	VAL	ILE	engineered mutation	UNP A4TVL0
B	89	GLN	LEU	engineered mutation	UNP A4TVL0
C	52	HIS	ALA	engineered mutation	UNP A4TVL0
C	54	TYR	MET	engineered mutation	UNP A4TVL0
C	56	HIS	PHE	engineered mutation	UNP A4TVL0
C	68	ASN	ARG	engineered mutation	UNP A4TVL0
C	72	ARG	ALA	engineered mutation	UNP A4TVL0
C	87	VAL	ILE	engineered mutation	UNP A4TVL0
C	89	GLN	LEU	engineered mutation	UNP A4TVL0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	52	HIS	ALA	engineered mutation	UNP A4TVL0
D	54	TYR	MET	engineered mutation	UNP A4TVL0
D	56	HIS	PHE	engineered mutation	UNP A4TVL0
D	68	ASN	ARG	engineered mutation	UNP A4TVL0
D	72	ARG	ALA	engineered mutation	UNP A4TVL0
D	87	VAL	ILE	engineered mutation	UNP A4TVL0
D	89	GLN	LEU	engineered mutation	UNP A4TVL0

- Molecule 2 is a protein called ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	E	3	Total	C	N	O	0	0	0
			15	9	3	3			
2	G	3	Total	C	N	O	0	0	0
			15	9	3	3			

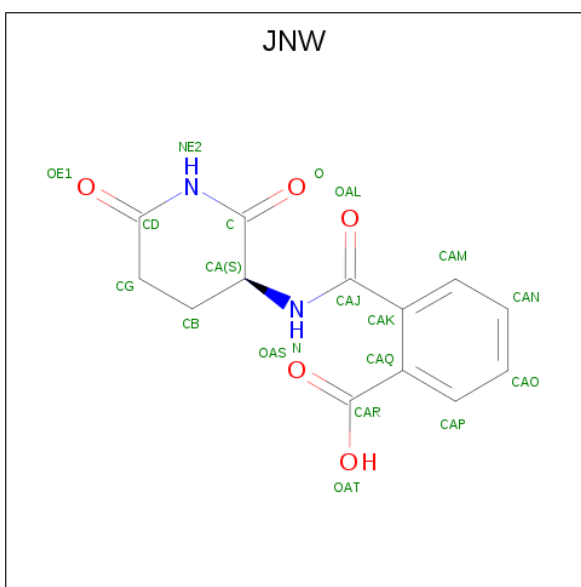
- Molecule 3 is a protein called ALA-ALA-ALA-ALA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	4	Total	C	N	O	0	0	0
			20	12	4	4			

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

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

- Molecule 5 is 2-[[[(3 {S})-2,6-bis(oxidanylidene)piperidin-3-yl]carbamoyl]benzoic acid (three-letter code: JNW) (formula: C₁₃H₁₂N₂O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			20	13	2	5		
5	B	1	Total	C	N	O	0	0
			20	13	2	5		
5	C	1	Total	C	N	O	0	0
			20	13	2	5		
5	D	1	Total	C	N	O	0	0
			20	13	2	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	107	Total	O	0	0
			107	107		
6	B	97	Total	O	0	0
			97	97		
6	C	104	Total	O	0	0
			104	104		
6	D	105	Total	O	0	0
			105	105		
6	E	3	Total	O	0	0
			3	3		
6	G	2	Total	O	0	0
			2	2		
6	H	3	Total	O	0	0
			3	3		

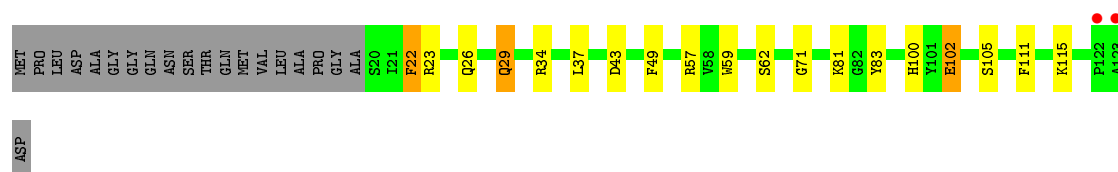
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

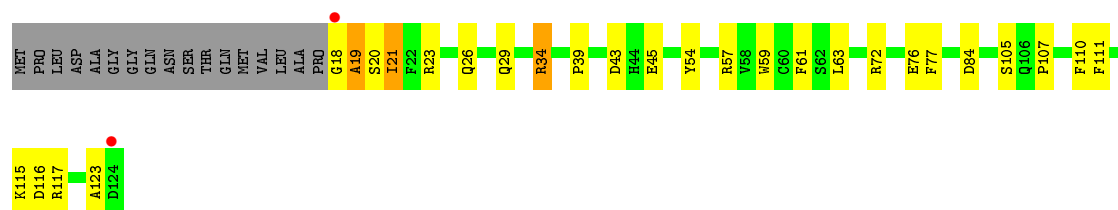
- Molecule 1: Cereblon isoform 4



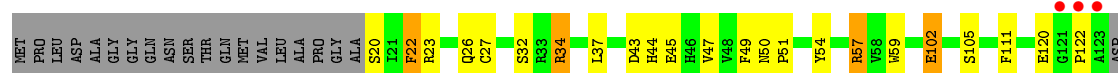
- Molecule 1: Cereblon isoform 4



- Molecule 1: Cereblon isoform 4



- Molecule 1: Cereblon isoform 4



- Molecule 2: ALA-ALA-ALA





- Molecule 2: ALA-ALA-ALA

Chain E:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: ALA-ALA-ALA

Chain G:  67% 33%



- Molecule 3: ALA-ALA-ALA-ALA

Chain H:  75% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.73 Å 59.16 Å 61.75 Å 90.00° 105.59° 90.00°	Depositor
Resolution (Å)	49.17 – 1.50 49.17 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.17-1.50) 99.6 (49.17-1.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.50 Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.158 , 0.190 0.164 , 0.194	Depositor DCC
R_{free} test set	3422 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.478 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3985	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 32.28 % 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 9.6459e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, JNW

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	1.73	10/889 (1.1%)	1.62	15/1202 (1.2%)
1	B	1.70	12/875 (1.4%)	1.54	17/1184 (1.4%)
1	C	1.75	6/910 (0.7%)	1.69	21/1230 (1.7%)
1	D	1.81	14/891 (1.6%)	1.63	17/1204 (1.4%)
All	All	1.75	42/3565 (1.2%)	1.62	70/4820 (1.5%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	GLU	CD-OE1	11.62	1.38	1.25
1	D	102	GLU	CD-OE2	9.74	1.36	1.25
1	D	102	GLU	CG-CD	7.49	1.63	1.51
1	C	107	PRO	N-CA	-7.47	1.34	1.47
1	B	102	GLU	CG-CD	7.32	1.62	1.51
1	A	76	GLU	CD-OE1	7.18	1.33	1.25
1	A	23	ARG	CZ-NH1	6.89	1.42	1.33
1	D	22	PHE	CG-CD2	-6.84	1.28	1.38
1	C	117	ARG	CZ-NH2	6.61	1.41	1.33
1	C	72	ARG	CZ-NH1	-6.56	1.24	1.33
1	B	62	SER	CA-CB	6.54	1.62	1.52
1	B	22	PHE	CG-CD2	-6.49	1.29	1.38
1	C	23	ARG	CZ-NH1	6.35	1.41	1.33
1	D	26	GLN	C-O	6.30	1.35	1.23
1	D	45	GLU	CD-OE1	6.30	1.32	1.25
1	B	26	GLN	C-O	6.25	1.35	1.23
1	B	34	ARG	C-O	6.15	1.35	1.23
1	C	45	GLU	CD-OE1	-6.11	1.19	1.25
1	A	22	PHE	CG-CD2	-6.11	1.29	1.38
1	A	45	GLU	CD-OE2	6.10	1.32	1.25
1	B	57	ARG	CD-NE	5.91	1.56	1.46
1	C	26	GLN	C-O	5.79	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	107	PRO	N-CA	-5.71	1.37	1.47
1	A	54	TYR	CE1-CZ	-5.66	1.31	1.38
1	A	76	GLU	CG-CD	5.63	1.60	1.51
1	D	57[A]	ARG	NE-CZ	5.55	1.40	1.33
1	D	57[B]	ARG	NE-CZ	5.55	1.40	1.33
1	B	105	SER	C-O	-5.52	1.12	1.23
1	B	34	ARG	CZ-NH1	5.44	1.40	1.33
1	A	92	GLN	CD-OE1	5.42	1.35	1.24
1	D	34	ARG	CZ-NH1	5.39	1.40	1.33
1	D	102	GLU	CB-CG	-5.34	1.42	1.52
1	B	29[A]	GLN	CD-NE2	-5.30	1.19	1.32
1	B	29[B]	GLN	CD-NE2	-5.30	1.19	1.32
1	D	32	SER	CB-OG	5.29	1.49	1.42
1	A	75	GLY	N-CA	-5.26	1.38	1.46
1	A	116	ASP	CB-CG	5.19	1.62	1.51
1	D	34	ARG	C-O	5.14	1.33	1.23
1	B	115	LYS	CB-CG	-5.10	1.38	1.52
1	B	62	SER	CB-OG	-5.05	1.35	1.42
1	D	105	SER	C-O	-5.02	1.13	1.23
1	D	27	CYS	CB-SG	5.01	1.90	1.82

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	23	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	C	23	ARG	NE-CZ-NH2	-11.94	114.33	120.30
1	D	34	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	C	43	ASP	CB-CG-OD1	10.72	127.95	118.30
1	C	23	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	A	43	ASP	CB-CG-OD1	10.45	127.70	118.30
1	D	57[A]	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	D	57[B]	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	B	34	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	D	43	ASP	CB-CG-OD1	9.80	127.12	118.30
1	B	43	ASP	CB-CG-OD1	9.77	127.09	118.30
1	B	23[A]	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	B	23[B]	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	A	23	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	D	34	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	C	21	ILE	CB-CG1-CD1	-8.77	89.35	113.90
1	D	23[A]	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	D	23[B]	ARG	NE-CZ-NH2	-8.37	116.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	LEU	CB-CG-CD1	-8.01	97.39	111.00
1	A	25	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	C	116	ASP	CB-CG-OD2	-7.76	111.32	118.30
1	D	22	PHE	CB-CG-CD1	-7.66	115.44	120.80
1	D	111	PHE	CB-CG-CD1	-7.46	115.58	120.80
1	C	84	ASP	CB-CG-OD2	-7.03	111.97	118.30
1	D	23[A]	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	D	23[B]	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	C	57	ARG	NE-CZ-NH2	6.87	123.73	120.30
1	C	61	PHE	CB-CG-CD2	6.81	125.57	120.80
1	D	54	TYR	CG-CD1-CE1	-6.79	115.86	121.30
1	C	110	PHE	CB-CG-CD2	6.76	125.53	120.80
1	B	22	PHE	CB-CG-CD1	-6.67	116.13	120.80
1	A	20	SER	N-CA-CB	-6.66	100.51	110.50
1	C	19	ALA	N-CA-CB	6.62	119.37	110.10
1	A	57	ARG	CG-CD-NE	-6.53	98.09	111.80
1	C	21	ILE	CA-CB-CG1	-6.50	98.66	111.00
1	A	19	ALA	N-CA-CB	6.47	119.15	110.10
1	A	84	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	B	111	PHE	CB-CG-CD1	-6.30	116.39	120.80
1	C	72	ARG	CG-CD-NE	6.24	124.91	111.80
1	C	72	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	B	57	ARG	CG-CD-NE	-6.11	98.98	111.80
1	A	34	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	34	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	20	SER	N-CA-CB	-5.82	101.77	110.50
1	D	102	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	C	63	LEU	CB-CG-CD1	-5.69	101.32	111.00
1	B	81	LYS	C-N-CA	-5.69	110.36	122.30
1	B	37	LEU	CB-CG-CD2	-5.68	101.34	111.00
1	A	110	PHE	CB-CG-CD2	5.66	124.77	120.80
1	C	57	ARG	CG-CD-NE	-5.65	99.93	111.80
1	D	37	LEU	CB-CG-CD2	-5.64	101.41	111.00
1	D	43	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	B	83	TYR	CG-CD2-CE2	5.62	125.80	121.30
1	B	83	TYR	CD1-CE1-CZ	5.62	124.86	119.80
1	C	111	PHE	CB-CG-CD1	-5.61	116.87	120.80
1	C	116	ASP	CB-CG-OD1	5.56	123.30	118.30
1	B	23[A]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	23[B]	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	34	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	D	49	PHE	CD1-CE1-CZ	-5.34	113.70	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	71	GLY	O-C-N	5.29	131.17	122.70
1	C	54	TYR	CZ-CE2-CD2	-5.25	115.07	119.80
1	D	54	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	54	TYR	CZ-CE2-CD2	-5.22	115.10	119.80
1	B	49	PHE	CD1-CE1-CZ	-5.20	113.86	120.10
1	A	54	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	124	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	72	ARG	NH1-CZ-NH2	-5.06	113.84	119.40
1	B	83	TYR	CG-CD1-CE1	-5.04	117.27	121.30
1	A	25	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	856	0	787	7	0
1	B	839	0	784	3	0
1	C	868	0	812	7	0
1	D	852	0	802	10	0
2	E	15	0	6	0	0
2	F	15	0	6	1	0
2	G	15	0	5	1	0
3	H	20	0	6	0	1
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	20	0	0	1	0
5	B	20	0	0	1	0
5	C	20	0	0	1	0
5	D	20	0	0	1	0
6	A	107	0	0	1	1
6	B	97	0	0	1	2
6	C	104	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	105	0	0	6	0
6	E	3	0	0	0	0
6	G	2	0	0	1	0
6	H	3	0	0	0	0
All	All	3985	0	3208	31	2

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 (31) 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:A:39:PRO:HG2	1:C:39:PRO:HG2	1.68	0.73
1:D:34:ARG:NH2	6:D:302:HOH:O	2.22	0.71
1:B:102:GLU:OE1	6:B:301:HOH:O	2.10	0.70
1:C:21:ILE:CD1	1:C:123:ALA:HA	2.31	0.61
1:D:102:GLU:HG3	6:D:322:HOH:O	2.03	0.58
1:C:34:ARG:HD2	6:C:369:HOH:O	2.05	0.57
1:C:59:TRP:CH2	1:C:115:LYS:HE3	2.44	0.52
5:D:202:JNW:CAR	5:D:202:JNW:OAL	2.57	0.51
1:D:57[A]:ARG:NH1	6:D:305:HOH:O	2.35	0.51
1:A:68:ASN:HD22	2:F:2:UNK:HA	1.75	0.50
1:D:44:HIS:ND1	6:D:304:HOH:O	2.35	0.50
1:A:59:TRP:CH2	1:A:115:LYS:HE3	2.46	0.50
5:B:202:JNW:OAL	5:B:202:JNW:CAR	2.59	0.49
1:B:22:PHE:CZ	1:B:59:TRP:HZ3	2.30	0.49
1:D:57[A]:ARG:HD3	6:D:308:HOH:O	2.10	0.49
1:D:22:PHE:CZ	1:D:59:TRP:HZ3	2.30	0.49
1:B:100:HIS:CE1	1:B:102:GLU:HG3	2.49	0.48
5:C:202:JNW:CAR	5:C:202:JNW:OAL	2.61	0.47
1:C:18:GLY:O	1:C:19:ALA:C	2.54	0.45
5:A:202:JNW:OAL	5:A:202:JNW:CAR	2.65	0.45
2:G:3:UNK:CB	6:G:102:HOH:O	2.66	0.43
1:C:76:GLU:HG2	1:C:77:PHE:CD2	2.54	0.43
1:D:22:PHE:CE1	1:D:120:GLU:HG3	2.54	0.43
1:A:18:GLY:O	1:A:19:ALA:C	2.55	0.42
1:D:20:SER:HB2	6:D:390:HOH:O	2.19	0.42
1:D:50:ASN:HB2	1:D:51:PRO:CD	2.50	0.42
1:D:47:VAL:HG22	1:D:57[A]:ARG:HG2	2.02	0.41
1:C:18:GLY:N	6:C:306:HOH:O	2.52	0.41
1:A:18:GLY:N	6:A:306:HOH:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLU:CD	1:A:57:ARG:HH11	2.25	0.40

All (2) 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)
3:H:1:UNK:CB	6:B:390:HOH:O[2_546]	1.77	0.43
6:A:304:HOH:O	6:B:308:HOH:O[2_556]	1.94	0.26

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	106/124 (86%)	104 (98%)	2 (2%)	0	100	100
1	B	104/124 (84%)	103 (99%)	1 (1%)	0	100	100
1	C	109/124 (88%)	108 (99%)	1 (1%)	0	100	100
1	D	105/124 (85%)	104 (99%)	0	1 (1%)	15	3
All	All	424/496 (86%)	419 (99%)	4 (1%)	1 (0%)	47	23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	122	PRO

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	87/99 (88%)	86 (99%)	1 (1%)	73	53
1	B	85/99 (86%)	83 (98%)	2 (2%)	49	19
1	C	90/99 (91%)	86 (96%)	4 (4%)	28	5
1	D	88/99 (89%)	88 (100%)	0	100	100
All	All	350/396 (88%)	343 (98%)	7 (2%)	71	25

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	GLU
1	B	29[A]	GLN
1	B	29[B]	GLN
1	C	29[A]	GLN
1	C	29[B]	GLN
1	C	105[A]	SER
1	C	105[B]	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	68	ASN
1	A	92	GLN
1	B	68	ASN
1	B	89	GLN
1	B	92	GLN
1	B	100	HIS
1	C	26	GLN
1	C	92	GLN
1	D	92	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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$
5	JNW	D	202	-	19,21,21	3.07	12 (63%)	23,29,29	2.92	12 (52%)
5	JNW	B	202	-	19,21,21	3.44	12 (63%)	23,29,29	3.23	14 (60%)
5	JNW	C	202	-	19,21,21	3.70	8 (42%)	23,29,29	3.01	12 (52%)
5	JNW	A	202	-	19,21,21	3.75	10 (52%)	23,29,29	3.22	11 (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	JNW	D	202	-	-	2/8/25/25	0/2/2/2
5	JNW	B	202	-	-	2/8/25/25	0/2/2/2
5	JNW	C	202	-	-	2/8/25/25	0/2/2/2
5	JNW	A	202	-	-	2/8/25/25	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	202	JNW	CAQ-CAR	-10.42	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	202	JNW	CAP-CAQ	-9.82	1.24	1.40
5	A	202	JNW	CAQ-CAR	-9.00	1.38	1.47
5	D	202	JNW	CAP-CAQ	-7.81	1.27	1.40
5	C	202	JNW	CB-CG	-7.46	1.36	1.52
5	A	202	JNW	CB-CG	-7.23	1.36	1.52
5	A	202	JNW	CAK-CAJ	-5.47	1.39	1.50
5	C	202	JNW	CAN-CAO	-4.99	1.24	1.38
5	A	202	JNW	CAP-CAQ	-4.73	1.32	1.40
5	B	202	JNW	CB-CG	-4.66	1.42	1.52
5	C	202	JNW	CAK-CAJ	-4.58	1.40	1.50
5	A	202	JNW	CAN-CAO	-4.27	1.26	1.38
5	A	202	JNW	CAN-CAM	-4.04	1.30	1.38
5	B	202	JNW	CAM-CAK	-3.96	1.33	1.39
5	B	202	JNW	CB-CA	-3.94	1.46	1.53
5	A	202	JNW	C-NE2	3.71	1.43	1.37
5	B	202	JNW	CAK-CAJ	-3.63	1.42	1.50
5	D	202	JNW	O-C	3.57	1.30	1.23
5	D	202	JNW	CAQ-CAR	-3.57	1.44	1.47
5	C	202	JNW	CAP-CAQ	-3.47	1.34	1.40
5	D	202	JNW	CB-CG	-3.35	1.45	1.52
5	D	202	JNW	CAK-CAJ	-3.34	1.43	1.50
5	D	202	JNW	C-NE2	3.26	1.42	1.37
5	B	202	JNW	CAN-CAM	-3.16	1.32	1.38
5	D	202	JNW	OAL-CAJ	3.11	1.29	1.23
5	D	202	JNW	OE1-CD	-2.88	1.17	1.23
5	D	202	JNW	CAJ-N	-2.85	1.28	1.34
5	A	202	JNW	CAO-CAP	-2.81	1.33	1.38
5	A	202	JNW	CB-CA	-2.72	1.48	1.53
5	B	202	JNW	C-NE2	2.70	1.42	1.37
5	B	202	JNW	CAN-CAO	-2.70	1.30	1.38
5	A	202	JNW	OE1-CD	-2.66	1.17	1.23
5	D	202	JNW	CAN-CAO	-2.64	1.31	1.38
5	B	202	JNW	CAK-CAQ	-2.58	1.36	1.40
5	C	202	JNW	OE1-CD	-2.47	1.18	1.23
5	B	202	JNW	CAO-CAP	2.41	1.44	1.38
5	C	202	JNW	CAN-CAM	-2.33	1.34	1.38
5	D	202	JNW	CAO-CAP	2.30	1.43	1.38
5	B	202	JNW	OAL-CAJ	2.26	1.27	1.23
5	B	202	JNW	CAJ-N	-2.14	1.29	1.34
5	C	202	JNW	C-NE2	2.14	1.41	1.37
5	D	202	JNW	CAM-CAK	-2.08	1.36	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	202	JNW	OAL-CAJ-N	-7.98	107.77	122.45
5	B	202	JNW	CAN-CAO-CAP	-7.54	108.70	120.19
5	C	202	JNW	OAL-CAJ-N	-6.85	109.85	122.45
5	B	202	JNW	CAO-CAP-CAQ	6.35	131.05	120.33
5	D	202	JNW	CB-CA-N	6.22	121.63	112.07
5	A	202	JNW	CAP-CAQ-CAK	-6.01	111.21	118.03
5	C	202	JNW	CAP-CAQ-CAK	-5.97	111.27	118.03
5	D	202	JNW	CAN-CAO-CAP	-5.34	112.05	120.19
5	C	202	JNW	CB-CA-N	5.28	120.19	112.07
5	A	202	JNW	CB-CA-N	5.19	120.05	112.07
5	A	202	JNW	OAL-CAJ-CAK	5.07	130.28	121.01
5	B	202	JNW	CB-CA-N	4.82	119.48	112.07
5	D	202	JNW	CAO-CAP-CAQ	4.45	127.84	120.33
5	D	202	JNW	CAQ-CAK-CAJ	-4.35	113.54	121.87
5	A	202	JNW	CAQ-CAK-CAJ	-4.28	113.67	121.87
5	B	202	JNW	OAL-CAJ-N	-4.20	114.71	122.45
5	D	202	JNW	C-CA-N	3.95	116.71	110.07
5	C	202	JNW	CAP-CAQ-CAR	3.95	126.08	120.20
5	A	202	JNW	CA-N-CAJ	3.93	131.21	121.60
5	D	202	JNW	CD-NE2-C	-3.87	121.22	126.61
5	B	202	JNW	CAQ-CAK-CAJ	-3.87	114.45	121.87
5	B	202	JNW	CAP-CAQ-CAK	-3.72	113.81	118.03
5	D	202	JNW	CB-CA-C	-3.69	104.59	112.57
5	C	202	JNW	CAQ-CAK-CAJ	-3.69	114.80	121.87
5	C	202	JNW	OAL-CAJ-CAK	3.41	127.25	121.01
5	B	202	JNW	OAL-CAJ-CAK	3.35	127.14	121.01
5	B	202	JNW	CAO-CAN-CAM	3.29	125.20	120.19
5	C	202	JNW	CAK-CAJ-N	3.26	122.84	116.80
5	C	202	JNW	CAO-CAP-CAQ	3.17	125.68	120.33
5	C	202	JNW	CA-N-CAJ	3.16	129.34	121.60
5	D	202	JNW	CAO-CAN-CAM	2.91	124.63	120.19
5	A	202	JNW	CAO-CAP-CAQ	2.88	125.20	120.33
5	B	202	JNW	C-CA-N	2.83	114.82	110.07
5	B	202	JNW	CD-NE2-C	-2.80	122.71	126.61
5	A	202	JNW	CAK-CAJ-N	2.78	121.94	116.80
5	B	202	JNW	CA-N-CAJ	2.69	128.19	121.60
5	D	202	JNW	OAL-CAJ-N	-2.69	117.51	122.45
5	C	202	JNW	OE1-CD-CG	2.65	127.84	122.17
5	A	202	JNW	OE1-CD-NE2	-2.65	116.07	120.28
5	B	202	JNW	CG-CD-NE2	2.59	119.55	116.65
5	D	202	JNW	O-C-NE2	-2.49	116.58	121.01
5	A	202	JNW	CAP-CAQ-CAR	2.38	123.74	120.20
5	A	202	JNW	OE1-CD-CG	2.34	127.17	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	202	JNW	CB-CA-C	-2.33	107.54	112.57
5	D	202	JNW	CAP-CAQ-CAK	-2.28	115.44	118.03
5	C	202	JNW	CG-CD-NE2	-2.17	114.21	116.65
5	D	202	JNW	CAM-CAK-CAQ	2.14	122.20	119.74
5	B	202	JNW	CB-CG-CD	-2.11	110.38	114.12
5	C	202	JNW	C-CA-N	2.10	113.60	110.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

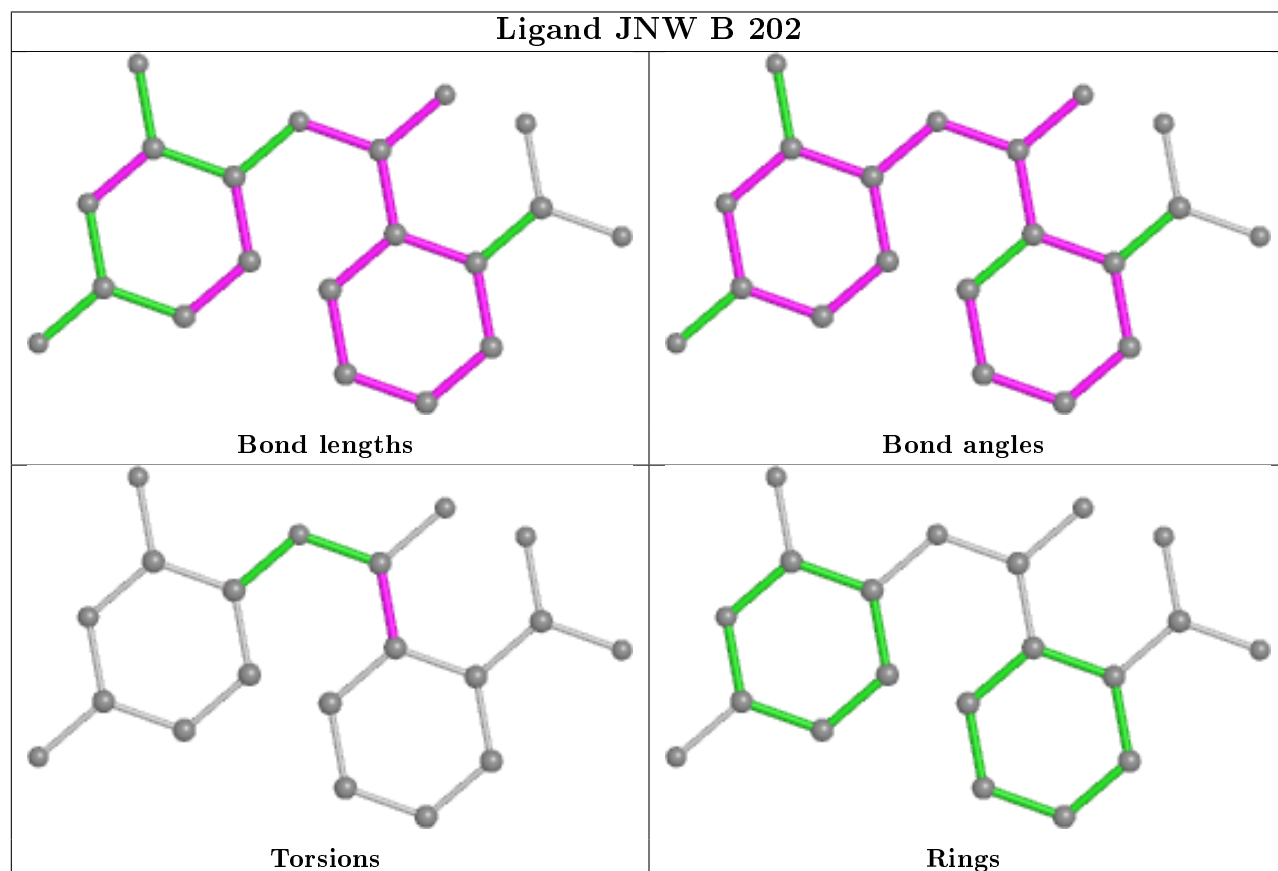
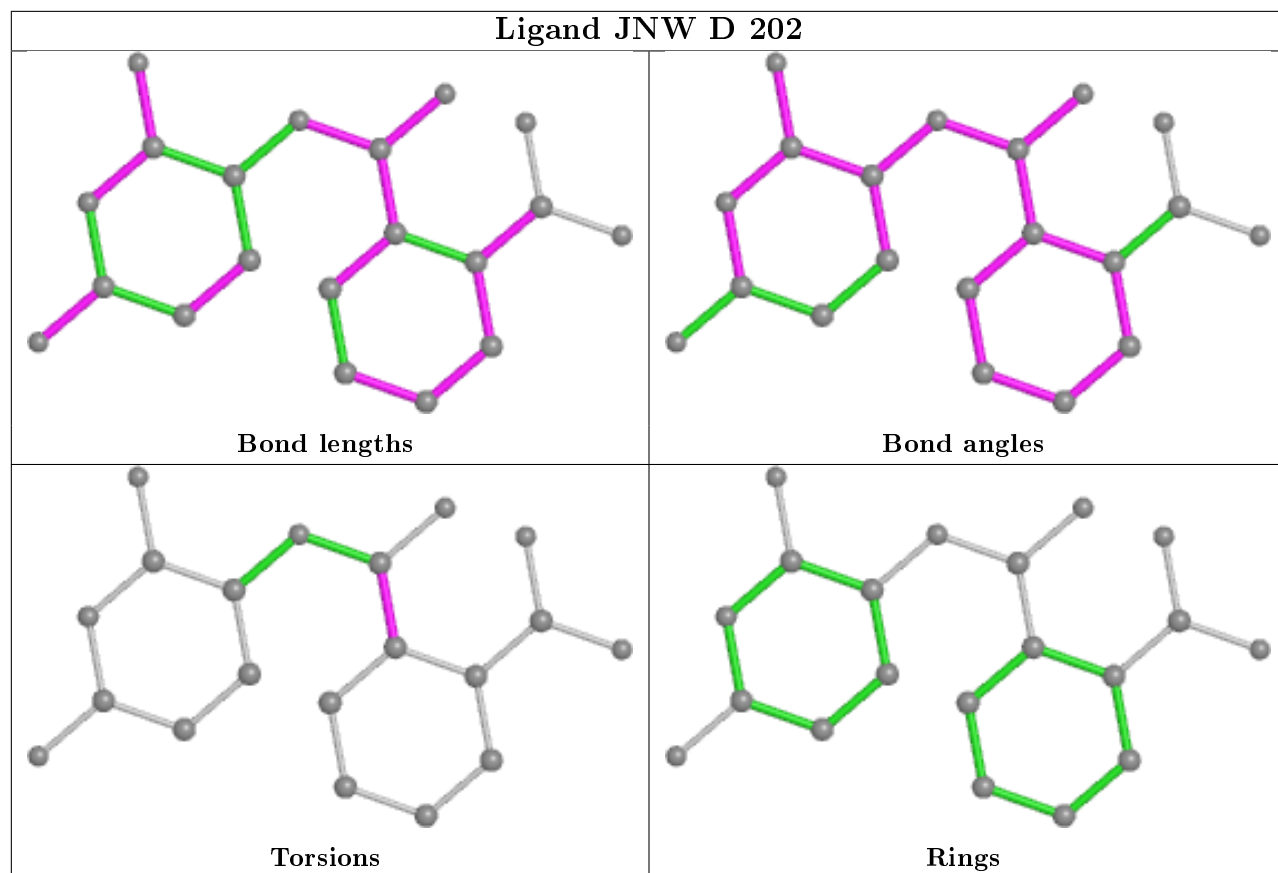
Mol	Chain	Res	Type	Atoms
5	B	202	JNW	OAL-CAJ-CAK-CAQ
5	D	202	JNW	OAL-CAJ-CAK-CAQ
5	C	202	JNW	N-CAJ-CAK-CAQ
5	A	202	JNW	OAL-CAJ-CAK-CAQ
5	C	202	JNW	OAL-CAJ-CAK-CAQ
5	A	202	JNW	N-CAJ-CAK-CAQ
5	B	202	JNW	N-CAJ-CAK-CAQ
5	D	202	JNW	N-CAJ-CAK-CAQ

There are no ring outliers.

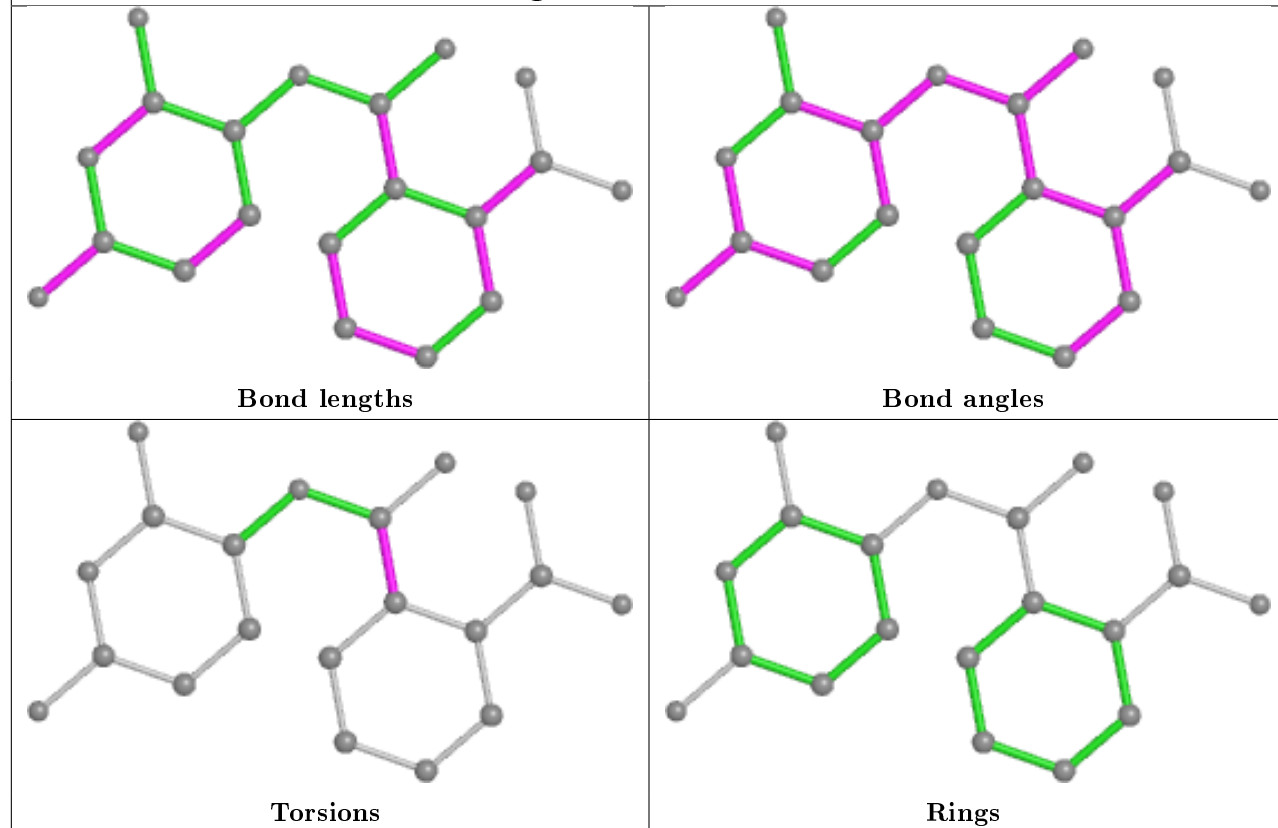
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	202	JNW	1	0
5	B	202	JNW	1	0
5	C	202	JNW	1	0
5	A	202	JNW	1	0

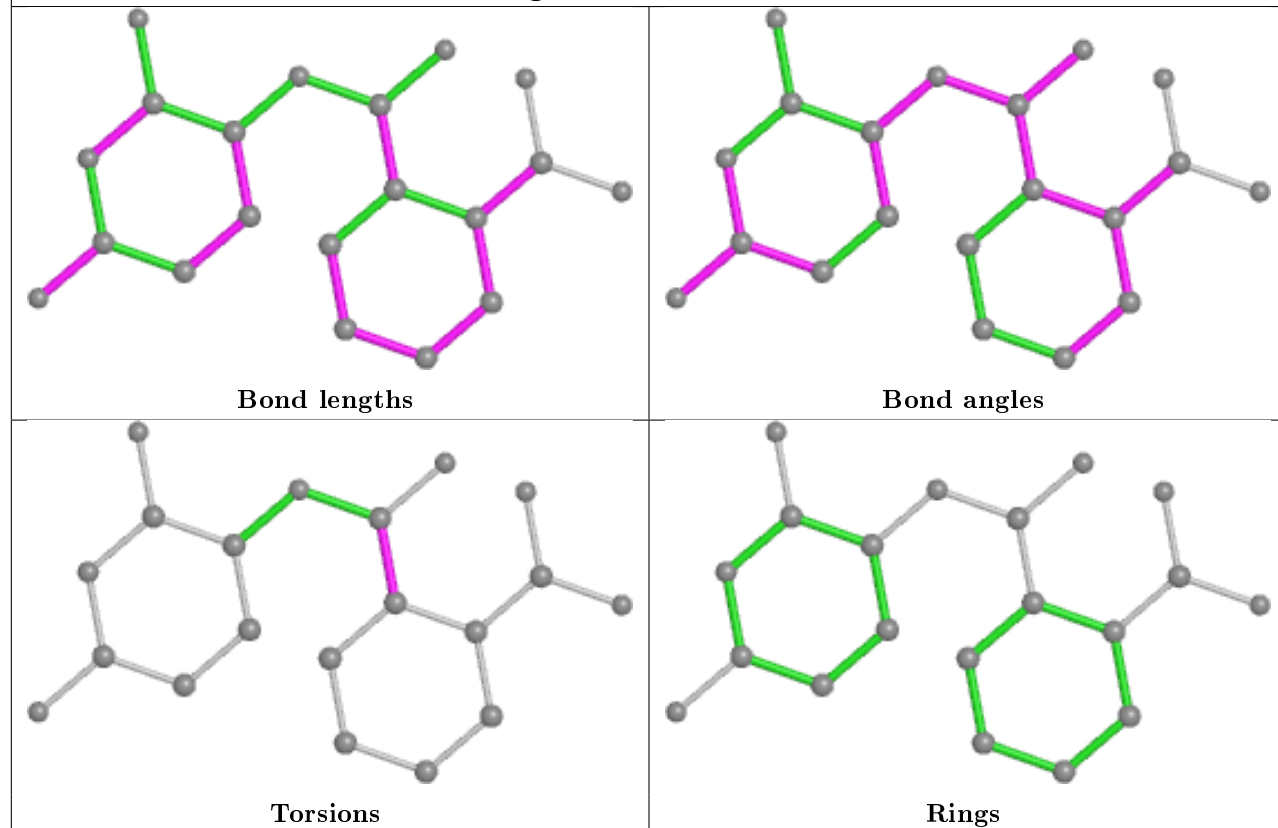
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 JNW C 202



Ligand JNW A 202



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	107/124 (86%)	-0.45	2 (1%) 66 71	11, 18, 35, 69	0
1	B	104/124 (83%)	-0.40	2 (1%) 66 71	11, 20, 38, 78	0
1	C	107/124 (86%)	-0.49	2 (1%) 66 71	10, 18, 35, 70	0
1	D	104/124 (83%)	-0.35	3 (2%) 51 56	11, 19, 38, 76	0
2	E	0/3	-	-	-	-
2	F	0/3	-	-	-	-
2	G	0/3	-	-	-	-
3	H	0/4	-	-	-	-
All	All	422/509 (82%)	-0.42	9 (2%) 63 68	10, 18, 38, 78	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	123	ALA	6.2
1	C	124	ASP	4.9
1	B	123	ALA	3.8
1	D	122	PRO	3.5
1	C	18	GLY	3.4
1	B	122	PRO	3.3
1	A	124	ASP	3.2
1	D	121	GLY	3.1
1	A	18	GLY	2.2

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

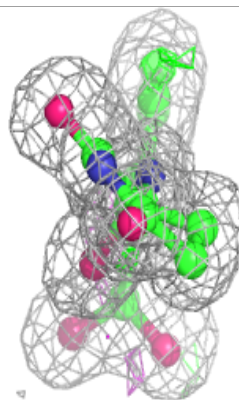
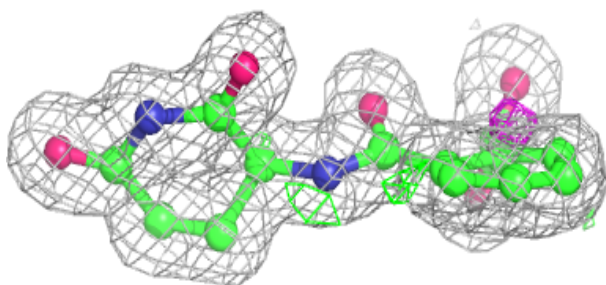
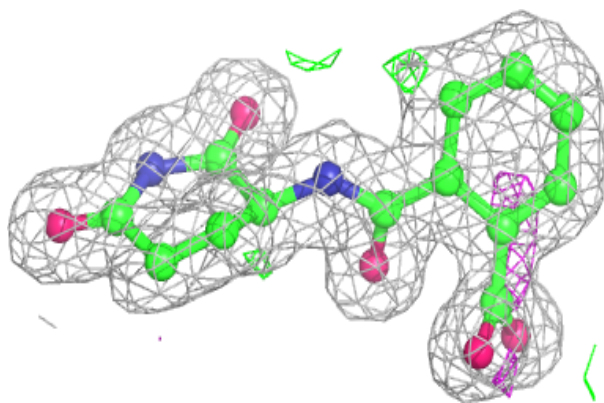
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	JNW	C	202	20/20	0.96	0.06	11,15,17,19	0
5	JNW	D	202	20/20	0.97	0.06	11,14,16,17	0
5	JNW	A	202	20/20	0.97	0.05	11,15,16,18	0
5	JNW	B	202	20/20	0.98	0.05	11,14,16,16	0
4	ZN	D	201	1/1	1.00	0.04	14,14,14,14	0
4	ZN	B	201	1/1	1.00	0.05	14,14,14,14	0
4	ZN	C	201	1/1	1.00	0.05	12,12,12,12	0
4	ZN	A	201	1/1	1.00	0.06	12,12,12,12	0

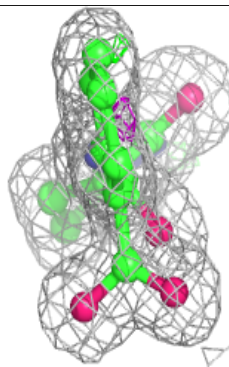
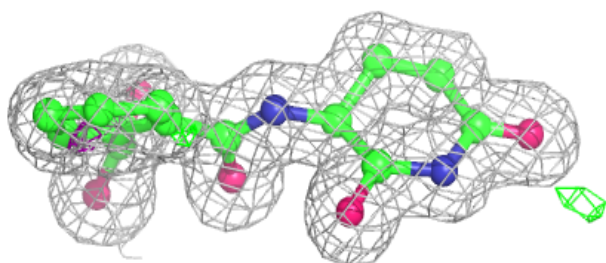
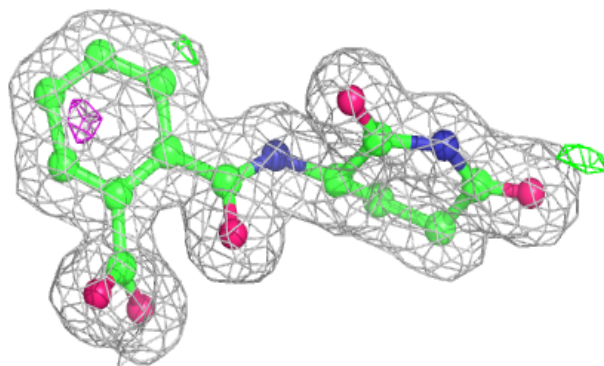
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JNW C 202:

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

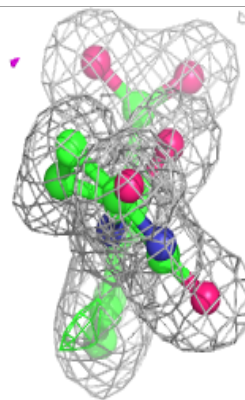
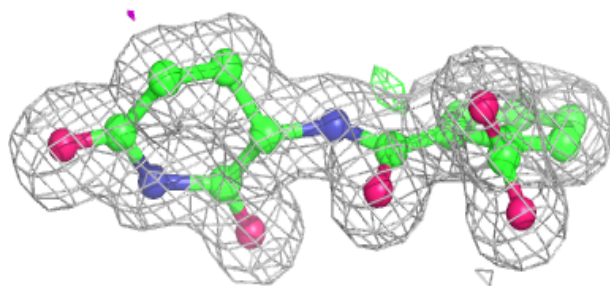
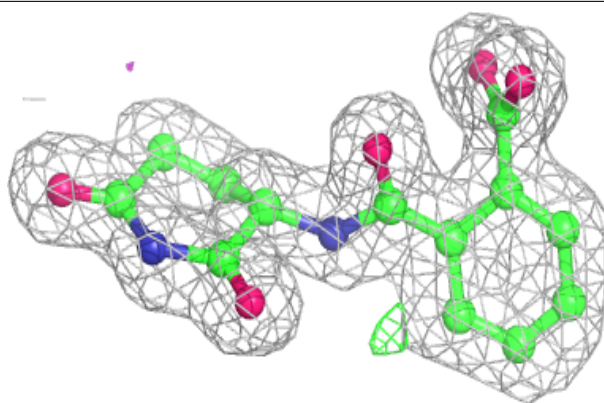
**Electron density around JNW D 202:**

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

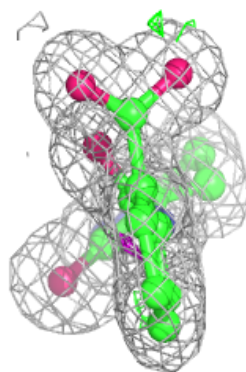
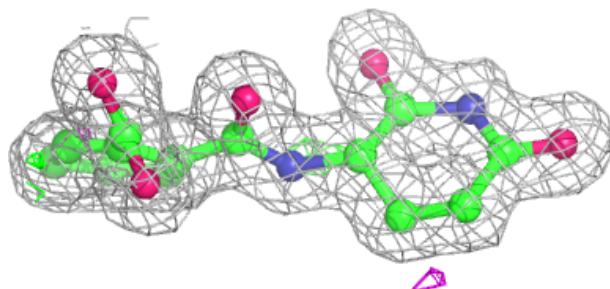
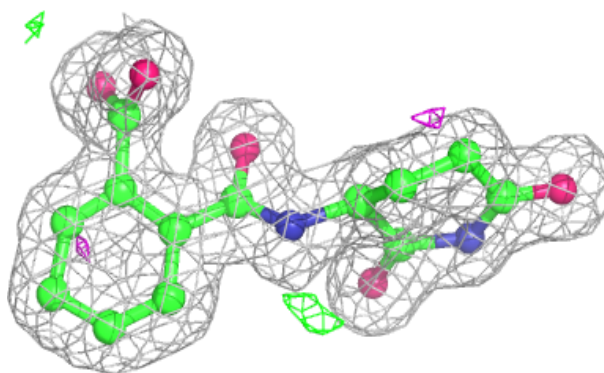


Electron density around JNW A 202:

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

**Electron density around JNW B 202:**

$2mF_o-DF_c$ (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.