



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:12 PM UTC

PDB ID : 6R0Q / pdb_00006r0q
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

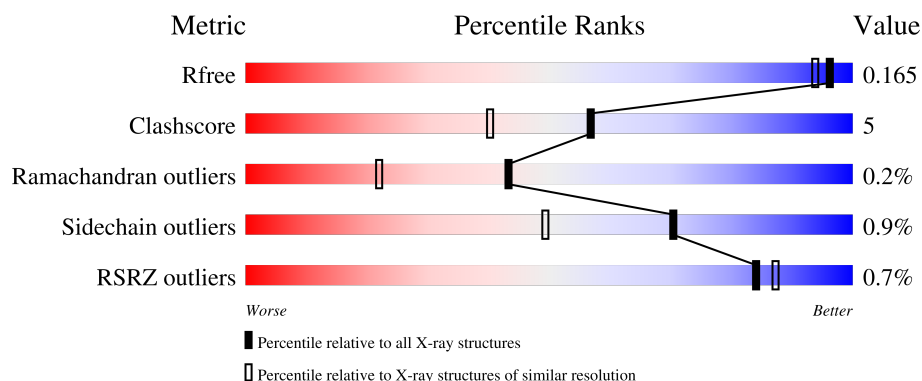
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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}	180053	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (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 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	124	
1	B	124	
1	C	124	
1	D	124	
2	E	3	

Continued on next page...

Continued from previous page...

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	JNW	B	202	-	X	-	-
5	JNW	D	202	-	X	-	-

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

Continued on next page...

Continued from previous page...

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			

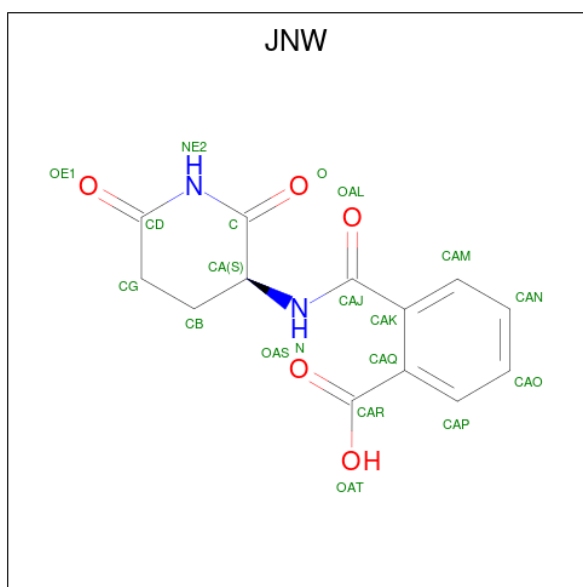
- Molecule 3 is a protein called ALA-ALA-ALA-ALA.

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is 2-[[[(3 {S})-2,6-bis(oxidanylidene)piperidin-3-yl]carbamoyl]benzoic acid (CCD ID: 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		

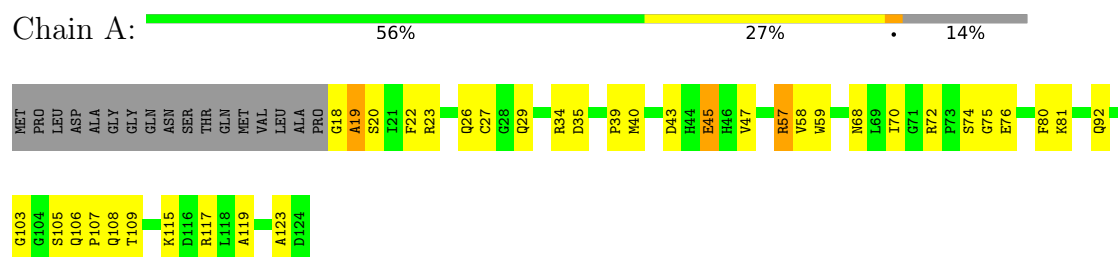
- Molecule 6 is water.

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		

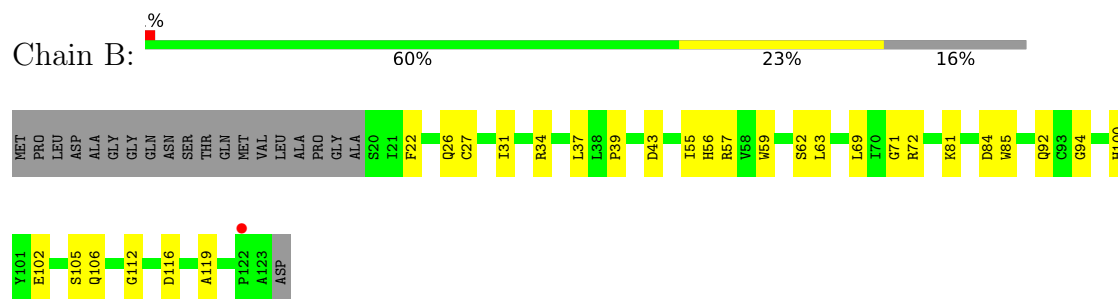
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

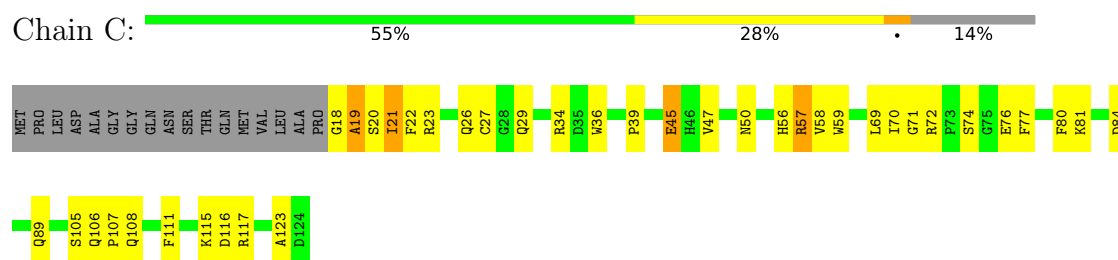
• Molecule 1: Cereblon isoform 4



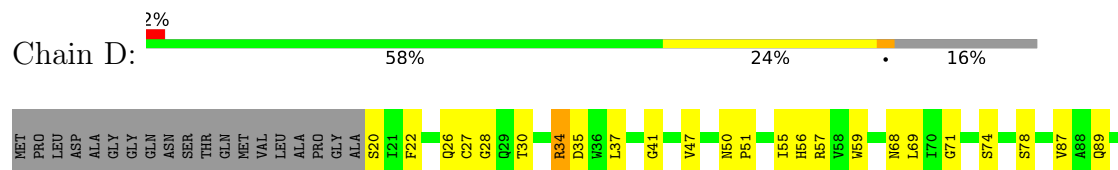
• Molecule 1: Cereblon isoform 4



• Molecule 1: Cereblon isoform 4



• Molecule 1: Cereblon isoform 4





- Molecule 2: ALA-ALA-ALA

Chain F: 67% 33%



- 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	61.73Å 59.16Å 61.75Å 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 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.158 , 0.190 (Not available) , 0.165	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)	0.40 , 30.2	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	0.98	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.*

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: JNW, 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	2.11	29/889 (3.3%)	1.58	8/1202 (0.7%)
1	B	2.07	25/875 (2.9%)	1.53	6/1184 (0.5%)
1	C	2.19	29/910 (3.2%)	1.66	13/1230 (1.1%)
1	D	2.14	25/891 (2.8%)	1.55	7/1204 (0.6%)
All	All	2.13	108/3565 (3.0%)	1.58	34/4820 (0.7%)

All (108) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	106	GLN	CA-CB	12.02	1.61	1.52
1	D	26	GLN	C-O	9.67	1.35	1.24
1	B	26	GLN	C-O	9.59	1.35	1.24
1	B	34	ARG	C-O	8.83	1.35	1.24
1	C	26	GLN	C-O	8.60	1.34	1.24
1	A	81	LYS	CA-C	-8.49	1.41	1.52
1	C	81	LYS	CA-C	-8.45	1.41	1.52
1	A	70	ILE	C-O	-8.38	1.15	1.24
1	B	105	SER	C-O	-8.26	1.12	1.23
1	A	105	SER	N-CA	7.92	1.55	1.46
1	D	105	SER	C-O	-7.91	1.13	1.23
1	C	47	VAL	C-O	7.81	1.32	1.24
1	B	27	CYS	CA-CB	-7.74	1.43	1.54
1	D	34	ARG	C-O	7.64	1.33	1.24
1	C	107	PRO	N-CA	-7.47	1.34	1.47
1	A	74	SER	C-O	-7.42	1.14	1.23
1	D	74[A]	SER	CA-C	7.42	1.61	1.52
1	D	74[B]	SER	CA-C	7.42	1.61	1.52
1	D	37	LEU	N-CA	7.40	1.55	1.46
1	B	57	ARG	CD-NE	7.32	1.56	1.46
1	D	102	GLU	CD-OE1	6.89	1.38	1.25
1	D	27	CYS	CA-CB	-6.85	1.44	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLN	CA-CB	6.69	1.64	1.53
1	A	23	ARG	CZ-NH1	6.61	1.42	1.32
1	C	58	VAL	C-O	6.58	1.31	1.24
1	B	56	HIS	ND1-CE1	6.57	1.39	1.32
1	B	69	LEU	C-O	6.54	1.31	1.24
1	C	27	CYS	CA-C	-6.53	1.43	1.52
1	A	47	VAL	N-CA	-6.52	1.38	1.46
1	A	92	GLN	CD-OE1	6.48	1.35	1.23
1	A	27	CYS	CA-CB	-6.38	1.45	1.54
1	A	80	PHE	CA-C	-6.31	1.45	1.52
1	C	117	ARG	CZ-NH2	6.30	1.41	1.33
1	A	72	ARG	C-O	-6.29	1.16	1.23
1	C	108	GLN	CA-C	6.23	1.60	1.52
1	B	39	PRO	CA-C	6.14	1.60	1.52
1	C	23	ARG	CZ-NH1	6.11	1.41	1.32
1	D	55	ILE	CA-CB	6.11	1.61	1.54
1	C	50	ASN	C-N	-6.09	1.28	1.34
1	A	108	GLN	CA-C	6.09	1.60	1.52
1	A	22	PHE	N-CA	-6.05	1.38	1.46
1	C	19	ALA	CA-C	6.03	1.60	1.52
1	C	89	GLN	CA-C	-6.00	1.45	1.52
1	D	78	SER	N-CA	-5.98	1.38	1.46
1	B	84	ASP	C-O	-5.95	1.16	1.23
1	D	35	ASP	N-CA	-5.94	1.38	1.46
1	B	37	LEU	N-CA	5.93	1.53	1.46
1	B	116	ASP	CA-C	-5.91	1.44	1.52
1	D	106	GLN	N-CA	-5.91	1.37	1.46
1	B	34	ARG	CA-C	-5.89	1.44	1.52
1	C	111	PHE	CA-C	-5.89	1.45	1.52
1	C	72	ARG	CZ-NH1	-5.88	1.24	1.32
1	B	106	GLN	N-CA	-5.81	1.37	1.46
1	D	102	GLU	CD-OE2	5.80	1.36	1.25
1	C	47	VAL	N-CA	-5.77	1.39	1.46
1	D	30	THR	C-O	5.74	1.30	1.23
1	D	109	THR	N-CA	5.74	1.53	1.45
1	D	56	HIS	ND1-CE1	5.72	1.38	1.32
1	A	107	PRO	N-CA	-5.71	1.37	1.47
1	B	62	SER	CA-CB	5.71	1.62	1.53
1	A	45	GLU	CA-C	-5.69	1.45	1.52
1	C	84	ASP	C-N	-5.67	1.25	1.33
1	C	36	TRP	N-CA	-5.67	1.39	1.46
1	C	21	ILE	CB-CG1	5.64	1.64	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	56	HIS	N-CA	-5.63	1.39	1.46
1	D	92	GLN	CA-CB	-5.62	1.45	1.53
1	D	87	VAL	N-CA	5.57	1.52	1.46
1	D	69	LEU	C-O	5.54	1.30	1.24
1	C	21	ILE	CA-CB	-5.53	1.47	1.54
1	A	26	GLN	C-O	5.52	1.30	1.24
1	C	80	PHE	CA-C	-5.50	1.46	1.52
1	A	117	ARG	NE-CZ	-5.50	1.26	1.33
1	A	40	MET	CA-CB	-5.50	1.45	1.53
1	D	28	GLY	C-O	5.49	1.31	1.24
1	A	29	GLN	C-O	-5.48	1.17	1.23
1	C	74	SER	C-O	-5.47	1.17	1.23
1	D	94	GLY	CA-C	5.46	1.58	1.51
1	D	71	GLY	CA-C	5.45	1.59	1.52
1	B	43	ASP	N-CA	-5.45	1.39	1.46
1	A	119	ALA	C-O	5.42	1.30	1.24
1	D	34	ARG	CA-C	-5.41	1.45	1.52
1	B	92	GLN	CA-CB	-5.38	1.45	1.53
1	C	70	ILE	C-O	-5.37	1.18	1.24
1	C	45	GLU	CA-C	-5.35	1.46	1.52
1	A	75	GLY	N-CA	-5.34	1.38	1.45
1	A	43	ASP	CG-OD2	5.30	1.35	1.25
1	A	75	GLY	C-N	-5.28	1.26	1.33
1	B	34	ARG	CZ-NH1	5.26	1.40	1.32
1	B	63	LEU	C-O	-5.26	1.17	1.23
1	A	19	ALA	CA-C	5.25	1.59	1.52
1	C	19	ALA	CA-CB	5.23	1.62	1.53
1	D	34	ARG	CZ-NH1	5.22	1.40	1.32
1	A	103	GLY	CA-C	-5.20	1.44	1.51
1	C	84	ASP	CG-OD1	-5.19	1.15	1.25
1	A	34	ARG	CA-C	-5.18	1.46	1.52
1	B	85	TRP	C-O	-5.18	1.17	1.23
1	B	119	ALA	N-CA	5.17	1.52	1.46
1	B	94	GLY	CA-C	5.17	1.58	1.51
1	B	112	GLY	CA-C	-5.15	1.44	1.51
1	A	109	THR	CB-OG1	-5.12	1.35	1.43
1	C	22	PHE	N-CA	-5.12	1.39	1.46
1	B	69	LEU	C-N	-5.10	1.27	1.33
1	A	123	ALA	N-CA	5.09	1.52	1.46
1	D	89	GLN	CD-OE1	5.08	1.33	1.23
1	B	72	ARG	CA-C	-5.08	1.45	1.52
1	C	69	LEU	CA-CB	-5.05	1.46	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	55	ILE	CA-CB	5.05	1.60	1.54
1	A	58	VAL	C-O	5.04	1.29	1.24

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	21	ILE	CB-CG1-CD1	-11.64	89.35	113.80
1	B	71	GLY	O-C-N	8.70	131.17	122.91
1	A	19	ALA	N-CA-C	-7.71	99.56	110.35
1	C	21	ILE	CA-CB-CG1	-6.91	98.66	110.40
1	A	20	SER	N-CA-CB	-6.89	100.51	110.36
1	C	106	GLN	CB-CA-C	6.74	116.86	111.00
1	C	19	ALA	N-CA-C	-6.61	101.10	110.35
1	D	74[A]	SER	CA-C-O	6.50	127.38	120.36
1	D	74[B]	SER	CA-C-O	6.50	127.38	120.36
1	B	81	LYS	CA-C-N	-6.46	110.36	122.05
1	B	81	LYS	C-N-CA	-6.46	110.36	122.05
1	A	57	ARG	CG-CD-NE	-6.32	98.09	112.00
1	C	71	GLY	O-C-N	6.08	130.16	122.68
1	A	26	GLN	CB-CG-CD	-6.03	102.36	112.60
1	C	20	SER	N-CA-CB	-6.01	101.77	110.36
1	C	19	ALA	N-CA-CB	5.95	119.37	109.56
1	B	57	ARG	CG-CD-NE	-5.92	98.98	112.00
1	A	23	ARG	NE-CZ-NH2	-5.87	113.92	119.20
1	C	72	ARG	CG-CD-NE	5.87	124.91	112.00
1	A	19	ALA	N-CA-CB	5.81	119.15	109.56
1	B	31	ILE	N-CA-C	5.68	116.45	111.56
1	D	41	GLY	O-C-N	-5.57	116.95	122.41
1	C	57	ARG	CG-CD-NE	-5.49	99.93	112.00
1	D	68	ASN	CA-CB-CG	5.42	118.03	112.60
1	B	116	ASP	N-CA-C	5.42	119.76	113.20
1	C	23	ARG	NE-CZ-NH2	-5.41	114.33	119.20
1	D	71	GLY	O-C-N	5.40	128.04	122.91
1	D	92	GLN	CG-CD-NE2	-5.32	108.42	116.40
1	D	30	THR	CA-CB-OG1	-5.14	101.89	109.60
1	C	80	PHE	CA-C-O	5.10	125.76	120.40
1	A	80	PHE	CA-C-O	5.07	125.81	120.33
1	C	57	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	C	116	ASP	N-CA-C	5.04	119.05	113.01
1	A	26	GLN	CA-C-O	-5.03	115.09	120.42

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	8	0
1	D	852	0	802	9	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
6	D	105	0	0	5	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:OAL	5:D:202:JNW:CAR	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:A:59:TRP:CH2	1:A:115:LYS:HE3	2.46	0.50
1:C:18:GLY:O	1:C:19:ALA:C	2.54	0.49
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:22:PHE:CZ	1:D:59:TRP:HZ3	2.30	0.49
1:D:57[A]:ARG:HD3	6:D:308:HOH:O	2.10	0.49
1:B:100:HIS:CE1	1:B:102:GLU:HG3	2.49	0.48
1:A:18:GLY:O	1:A:19:ALA:C	2.55	0.47
5:C:202:JNW:OAL	5:C:202:JNW:CAR	2.61	0.47
1:A:45:GLU:CD	1:A:57:ARG:HH11	2.25	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:C:45:GLU:CD	1:C:57:ARG:HH11	2.27	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

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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	12	2
All	All	424/496 (86%)	419 (99%)	4 (1%)	1 (0%)	43	22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	122	PRO

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	87/99 (88%)	86 (99%)	1 (1%)	65	41
1	B	85/99 (86%)	85 (100%)	0	100	100
1	C	90/99 (91%)	86 (96%)	4 (4%)	25	4
1	D	88/99 (89%)	88 (100%)	0	100	100
All	All	350/396 (88%)	345 (99%)	5 (1%)	70	33

All (5) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

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

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 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	C	202	-	21,21,21	3.18	9 (42%)	28,29,29	3.04	15 (53%)
5	JNW	B	202	-	21,21,21	3.49	14 (66%)	28,29,29	3.27	16 (57%)
5	JNW	A	202	-	21,21,21	3.41	10 (47%)	28,29,29	3.18	14 (50%)
5	JNW	D	202	-	21,21,21	3.04	14 (66%)	28,29,29	2.83	14 (50%)

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	C	202	-	-	4/12/25/25	0/2/2/2
5	JNW	B	202	-	-	5/12/25/25	0/2/2/2
5	JNW	A	202	-	-	4/12/25/25	0/2/2/2
5	JNW	D	202	-	-	5/12/25/25	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	202	JNW	CAP-CAQ	-10.19	1.24	1.39
5	D	202	JNW	CAP-CAQ	-8.10	1.27	1.39
5	C	202	JNW	CB-CG	-7.84	1.36	1.53
5	A	202	JNW	CB-CG	-7.61	1.36	1.53
5	C	202	JNW	CAN-CAO	-6.13	1.24	1.38
5	C	202	JNW	CAQ-CAR	-5.73	1.37	1.49
5	A	202	JNW	CAK-CAJ	-5.59	1.39	1.50
5	A	202	JNW	CAN-CAO	-5.27	1.26	1.38
5	A	202	JNW	CAQ-CAR	-5.08	1.38	1.49
5	A	202	JNW	CAN-CAM	-4.96	1.30	1.38
5	B	202	JNW	CB-CG	-4.91	1.42	1.53
5	A	202	JNW	CAP-CAQ	-4.91	1.32	1.39
5	C	202	JNW	CAK-CAJ	-4.69	1.40	1.50
5	B	202	JNW	CAM-CAK	-4.20	1.33	1.39
5	B	202	JNW	CAN-CAM	-3.88	1.32	1.38
5	B	202	JNW	CAK-CAJ	-3.72	1.42	1.50
5	B	202	JNW	CB-CA	-3.72	1.46	1.53
5	D	202	JNW	O-C	3.70	1.30	1.23
5	A	202	JNW	C-NE2	3.60	1.43	1.37
5	C	202	JNW	CAP-CAQ	-3.60	1.34	1.39
5	D	202	JNW	CB-CG	-3.53	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	202	JNW	CAO-CAP	-3.45	1.33	1.38
5	D	202	JNW	CAK-CAJ	-3.42	1.43	1.50
5	B	202	JNW	CAN-CAO	-3.36	1.30	1.38
5	D	202	JNW	CAN-CAO	-3.30	1.31	1.38
5	D	202	JNW	C-NE2	3.17	1.42	1.37
5	B	202	JNW	CAO-CAP	2.98	1.44	1.38
5	D	202	JNW	OE1-CD	-2.95	1.17	1.23
5	C	202	JNW	CAN-CAM	-2.86	1.34	1.38
5	D	202	JNW	CAO-CAP	2.84	1.43	1.38
5	A	202	JNW	OE1-CD	-2.72	1.17	1.23
5	D	202	JNW	CAJ-N	-2.71	1.28	1.34
5	D	202	JNW	OAL-CAJ	2.69	1.29	1.23
5	D	202	JNW	CAQ-CAR	-2.63	1.44	1.49
5	B	202	JNW	C-NE2	2.63	1.42	1.37
5	B	202	JNW	OAS-CAR	2.59	1.30	1.22
5	A	202	JNW	CB-CA	-2.56	1.48	1.53
5	C	202	JNW	OE1-CD	-2.53	1.18	1.23
5	B	202	JNW	CAK-CAQ	-2.33	1.36	1.40
5	D	202	JNW	CAM-CAK	-2.22	1.36	1.39
5	D	202	JNW	OAT-CAR	-2.20	1.24	1.30
5	C	202	JNW	CAO-CAP	-2.19	1.35	1.38
5	D	202	JNW	OAS-CAR	2.11	1.28	1.22
5	C	202	JNW	C-NE2	2.09	1.41	1.37
5	B	202	JNW	OAT-CAR	-2.05	1.24	1.30
5	B	202	JNW	CAJ-N	-2.04	1.29	1.34
5	B	202	JNW	CA-C	-2.01	1.47	1.52

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	202	JNW	CAN-CAO-CAP	-9.35	108.70	120.24
5	A	202	JNW	OAL-CAJ-N	-7.73	107.77	122.47
5	A	202	JNW	CAP-CAQ-CAK	-7.17	111.21	119.26
5	C	202	JNW	CAP-CAQ-CAK	-7.13	111.27	119.26
5	D	202	JNW	CAN-CAO-CAP	-6.64	112.05	120.24
5	C	202	JNW	OAL-CAJ-N	-6.64	109.85	122.47
5	B	202	JNW	CAO-CAP-CAQ	6.23	131.05	119.80
5	C	202	JNW	OAT-CAR-OAS	-6.01	110.43	123.35
5	A	202	JNW	OAT-CAR-OAS	-5.63	111.24	123.35
5	D	202	JNW	CB-CA-N	5.50	121.63	112.13
5	A	202	JNW	OAL-CAJ-CAK	5.04	130.28	121.03
5	B	202	JNW	CAP-CAQ-CAK	-4.86	113.81	119.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	202	JNW	CB-CA-N	4.67	120.19	112.13
5	A	202	JNW	CB-CA-N	4.59	120.05	112.13
5	D	202	JNW	CAO-CAP-CAQ	4.45	127.84	119.80
5	B	202	JNW	CB-CA-N	4.26	119.48	112.13
5	D	202	JNW	CD-NE2-C	-4.15	121.22	126.69
5	B	202	JNW	OAL-CAJ-N	-4.08	114.71	122.47
5	A	202	JNW	CA-N-CAJ	4.02	131.21	121.56
5	B	202	JNW	CAO-CAN-CAM	4.02	125.20	120.24
5	C	202	JNW	OAT-CAR-CAQ	3.79	126.06	115.28
5	B	202	JNW	OAT-CAR-OAS	-3.72	115.36	123.35
5	D	202	JNW	C-CA-N	3.71	116.71	110.23
5	D	202	JNW	CB-CA-C	-3.63	104.59	112.68
5	D	202	JNW	CAO-CAN-CAM	3.56	124.63	120.24
5	D	202	JNW	CAP-CAQ-CAK	-3.40	115.44	119.26
5	C	202	JNW	OAL-CAJ-CAK	3.39	127.25	121.03
5	B	202	JNW	OAL-CAJ-CAK	3.33	127.14	121.03
5	C	202	JNW	CAO-CAP-CAQ	3.26	125.68	119.80
5	C	202	JNW	CA-N-CAJ	3.24	129.34	121.56
5	C	202	JNW	CAP-CAQ-CAR	3.24	126.08	118.64
5	B	202	JNW	CD-NE2-C	-3.02	122.71	126.69
5	A	202	JNW	CAO-CAP-CAQ	2.99	125.20	119.80
5	D	202	JNW	OAT-CAR-OAS	-2.98	116.95	123.35
5	D	202	JNW	CAQ-CAK-CAJ	-2.98	113.54	122.06
5	A	202	JNW	CAQ-CAK-CAJ	-2.93	113.67	122.06
5	A	202	JNW	OAT-CAR-CAQ	2.90	123.52	115.28
5	C	202	JNW	CAK-CAJ-N	2.84	122.84	116.67
5	B	202	JNW	CA-N-CAJ	2.76	128.19	121.56
5	C	202	JNW	OE1-CD-CG	2.75	127.84	122.20
5	A	202	JNW	OE1-CD-NE2	-2.74	116.07	120.30
5	B	202	JNW	OAT-CAR-CAQ	2.72	123.01	115.28
5	B	202	JNW	CG-CD-NE2	2.69	119.55	116.69
5	B	202	JNW	CAQ-CAK-CAJ	-2.66	114.45	122.06
5	D	202	JNW	CG-CB-CA	2.65	118.75	110.77
5	B	202	JNW	C-CA-N	2.63	114.82	110.23
5	D	202	JNW	CAM-CAK-CAQ	2.62	122.20	119.26
5	A	202	JNW	CG-CB-CA	2.61	118.64	110.77
5	B	202	JNW	CG-CB-CA	2.61	118.63	110.77
5	D	202	JNW	OAL-CAJ-N	-2.61	117.51	122.47
5	D	202	JNW	O-C-NE2	-2.54	116.58	121.10
5	C	202	JNW	CAQ-CAK-CAJ	-2.54	114.80	122.06
5	A	202	JNW	CAK-CAJ-N	2.43	121.94	116.67
5	A	202	JNW	OE1-CD-CG	2.43	127.17	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	202	JNW	CG-CB-CA	2.42	118.06	110.77
5	C	202	JNW	CG-CD-NE2	-2.33	114.21	116.69
5	B	202	JNW	CB-CA-C	-2.30	107.54	112.68
5	A	202	JNW	CAP-CAQ-CAR	2.22	123.74	118.64
5	C	202	JNW	OE1-CD-NE2	-2.04	117.16	120.30

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

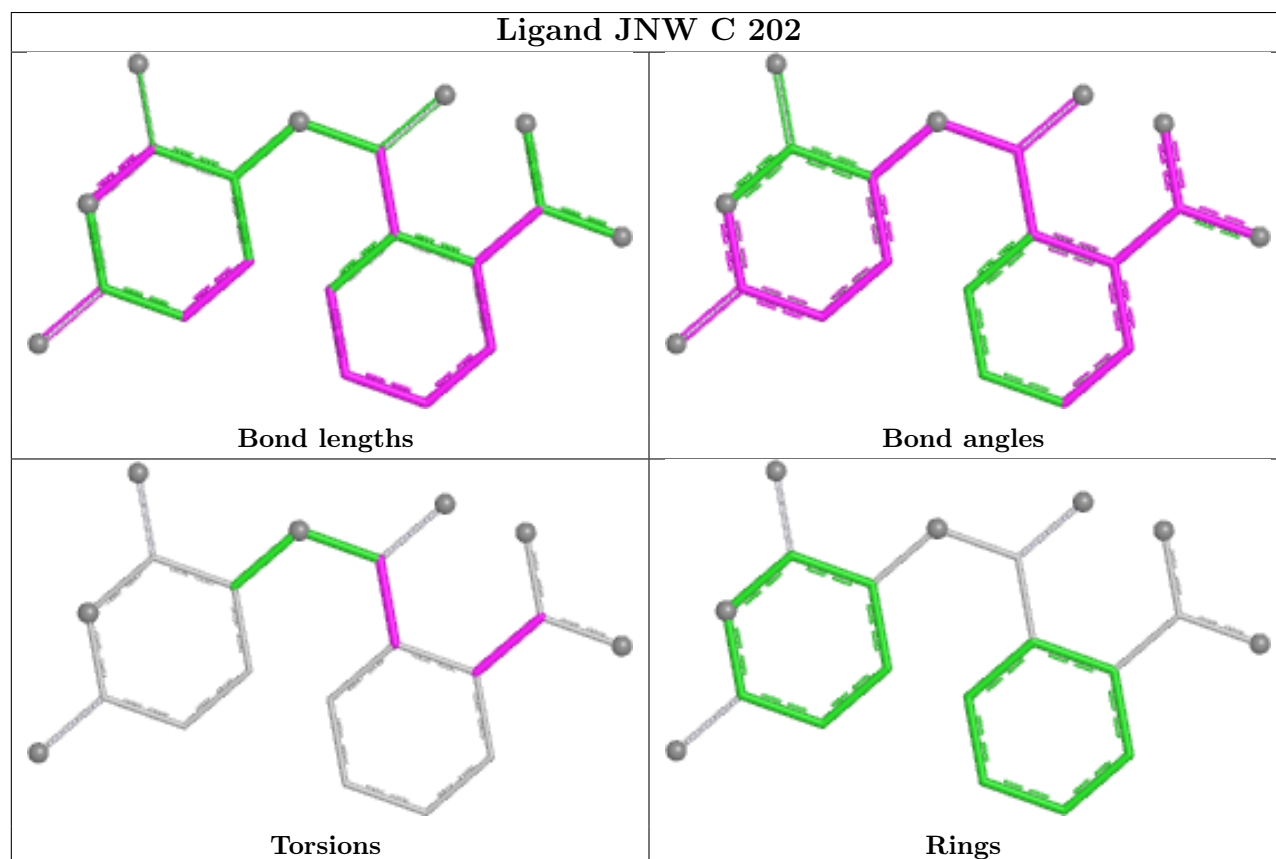
There are no ring outliers.

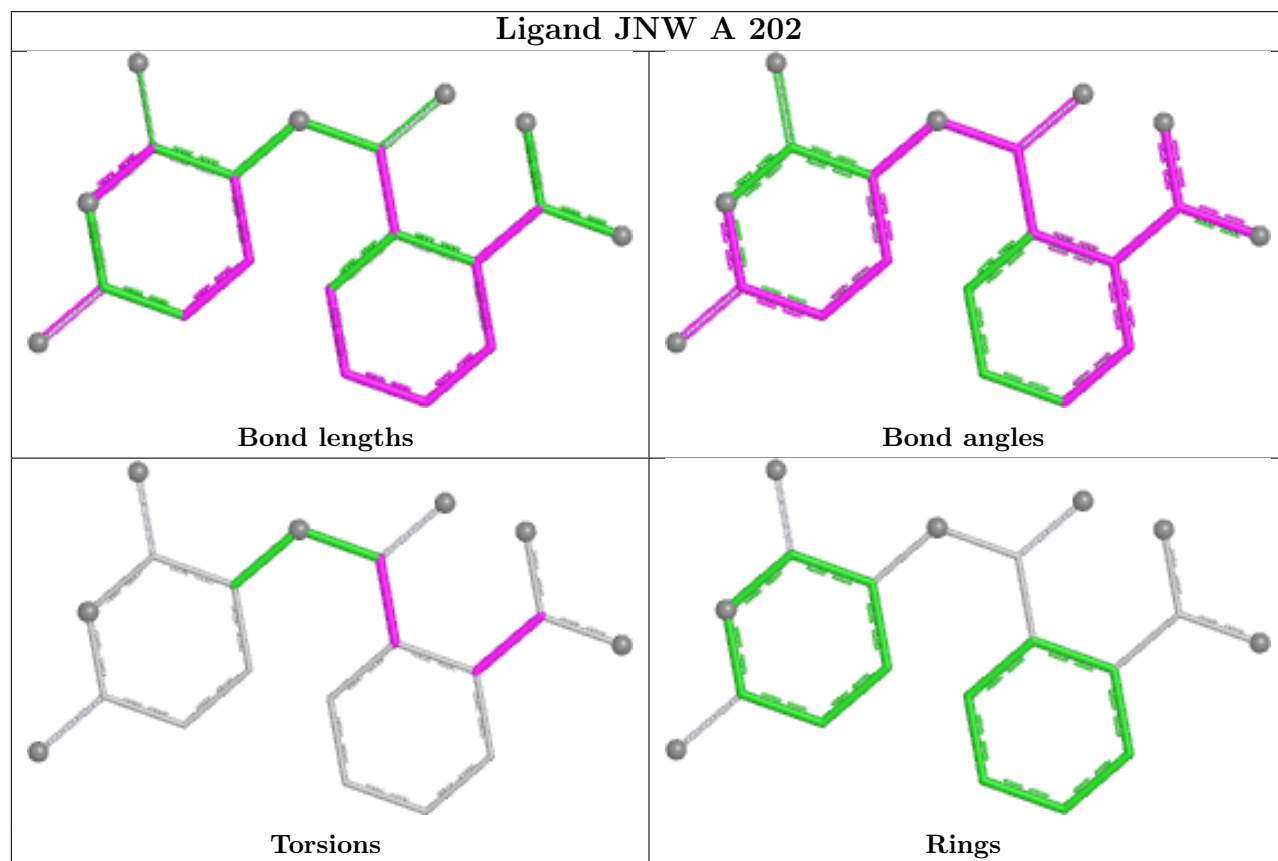
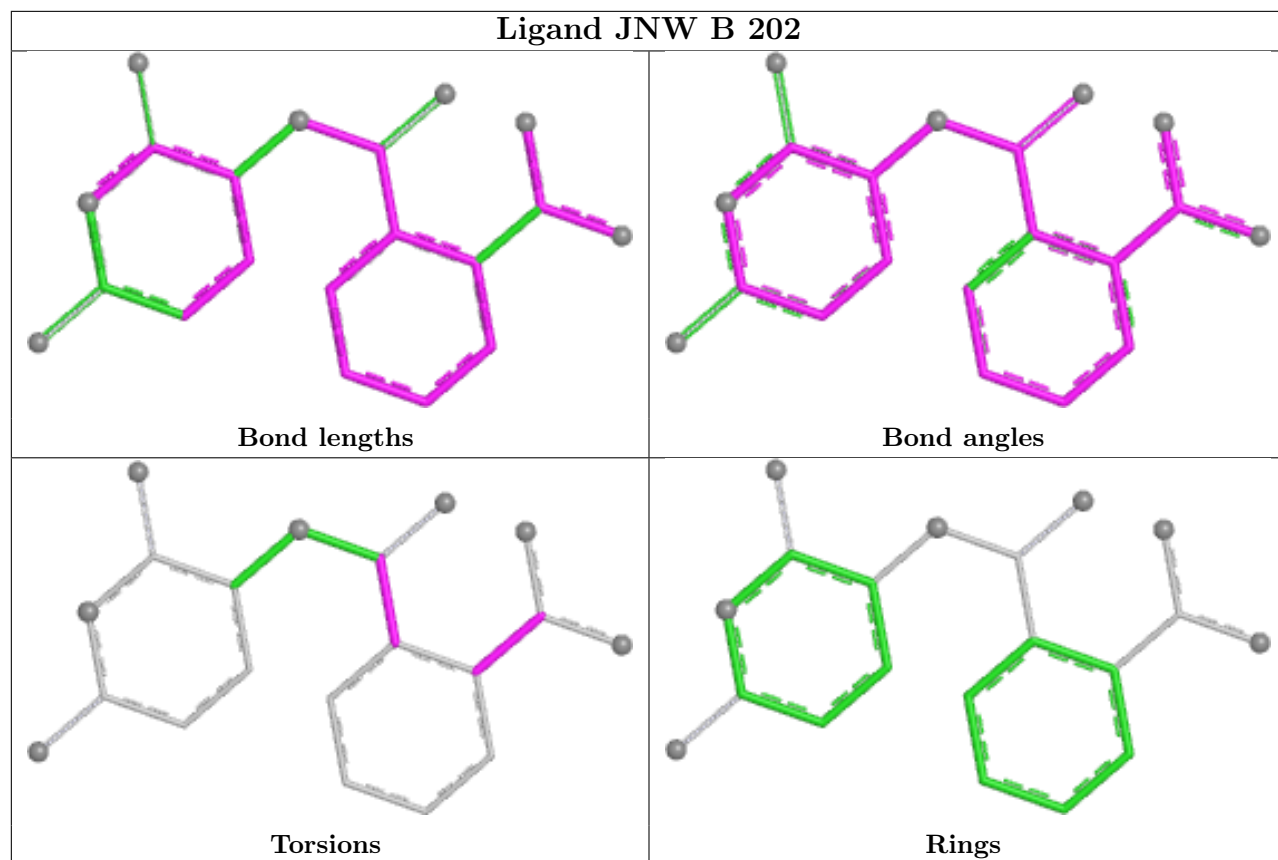
4 monomers are involved in 4 short contacts:

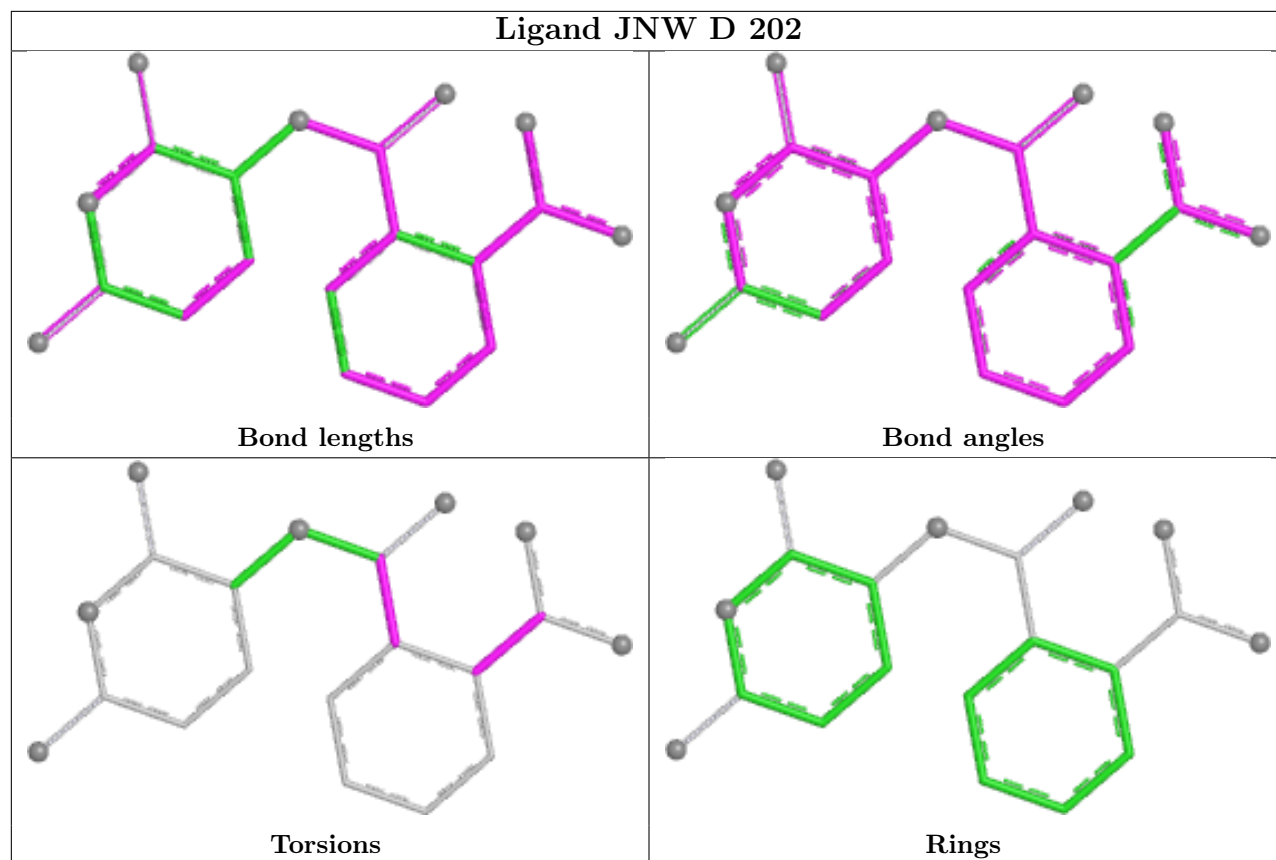
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	202	JNW	1	0
5	B	202	JNW	1	0
5	A	202	JNW	1	0
5	D	202	JNW	1	0

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.







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	107/124 (86%)	-1.15	0 100 100	11, 17, 35, 69	1 (0%)
1	B	104/124 (83%)	-1.09	1 (0%) 79 82	11, 19, 38, 78	2 (1%)
1	C	107/124 (86%)	-1.14	0 100 100	9, 18, 35, 70	4 (3%)
1	D	104/124 (83%)	-1.04	2 (1%) 66 70	10, 19, 38, 76	3 (2%)
2	E	0/3	-	-	-	-
2	F	0/3	-	-	-	-
2	G	0/3	-	-	-	-
3	H	0/4	-	-	-	-
All	All	422/509 (82%)	-1.10	3 (0%) 84 87	9, 18, 38, 78	10 (2%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	PRO	2.6
1	D	123	ALA	2.3
1	D	122	PRO	2.1

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 ⓘ

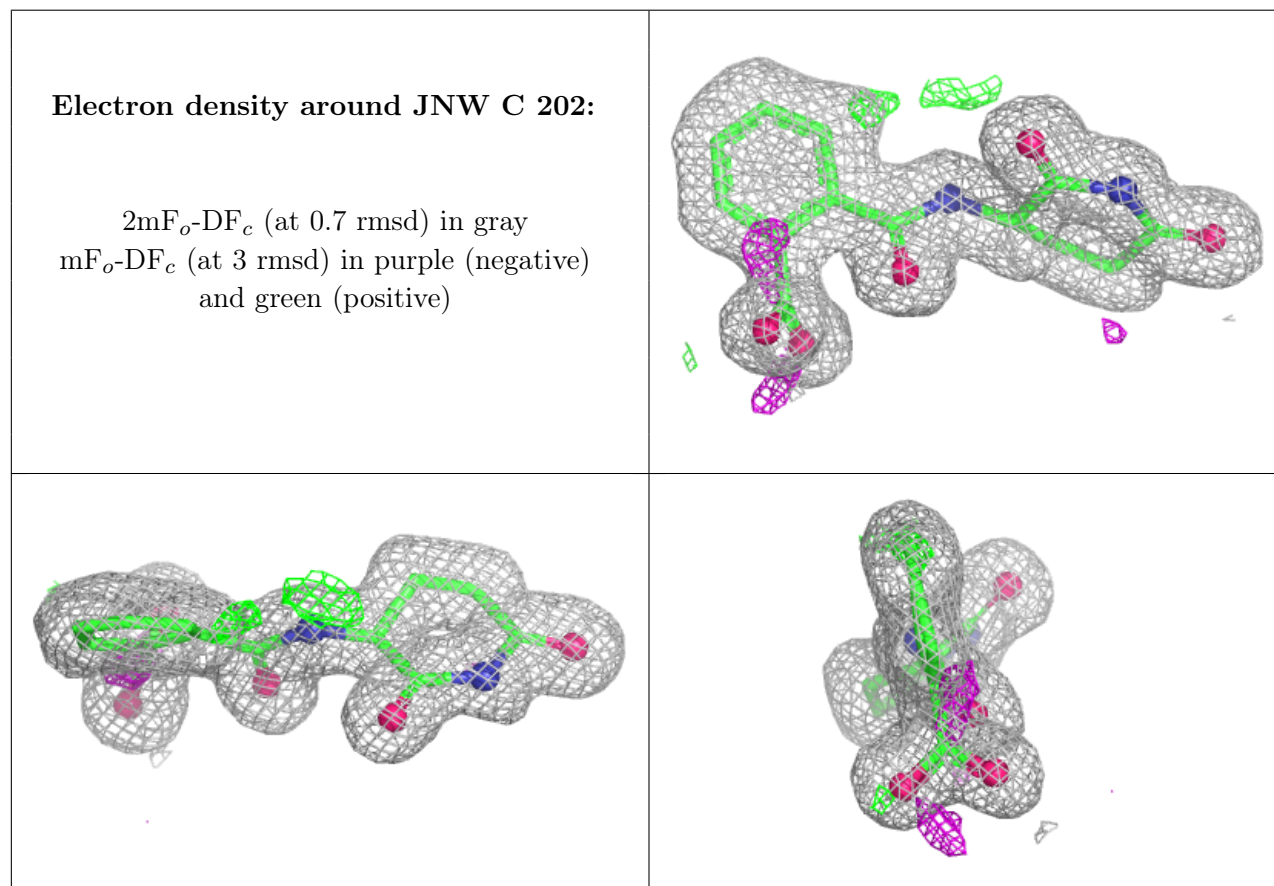
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

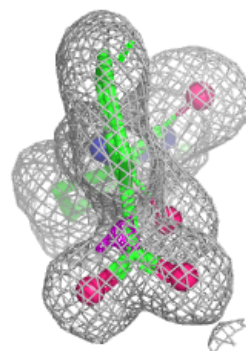
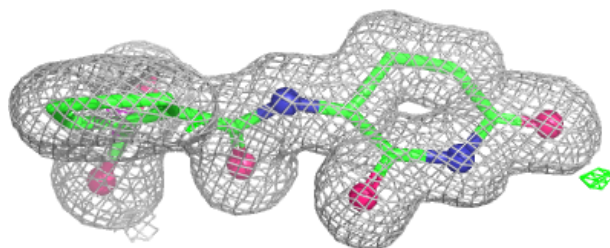
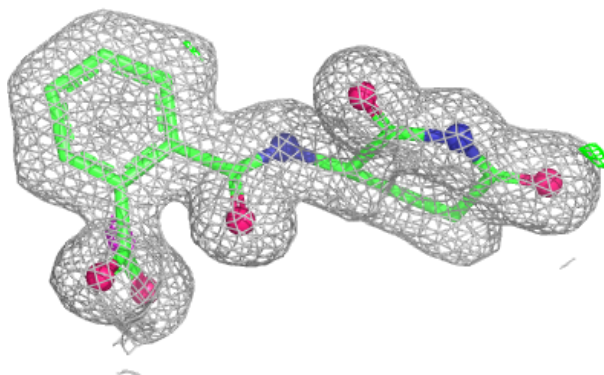
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	JNW	C	202	20/20	0.99	0.03	11,15,17,19	0
5	JNW	D	202	20/20	0.99	0.02	11,14,16,17	0
4	ZN	C	201	1/1	1.00	0.00	12,12,12,12	0
4	ZN	D	201	1/1	1.00	0.01	14,14,14,14	0
5	JNW	A	202	20/20	1.00	0.02	11,15,16,18	0
5	JNW	B	202	20/20	1.00	0.02	11,14,16,16	0
4	ZN	A	201	1/1	1.00	0.01	12,12,12,12	0
4	ZN	B	201	1/1	1.00	0.01	14,14,14,14	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.

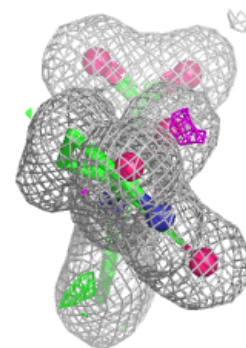
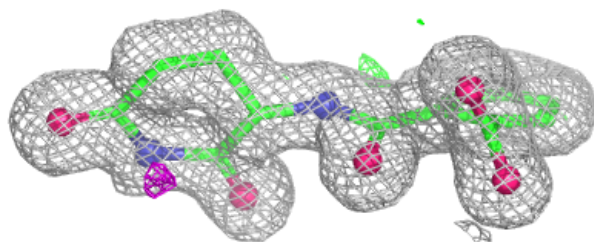
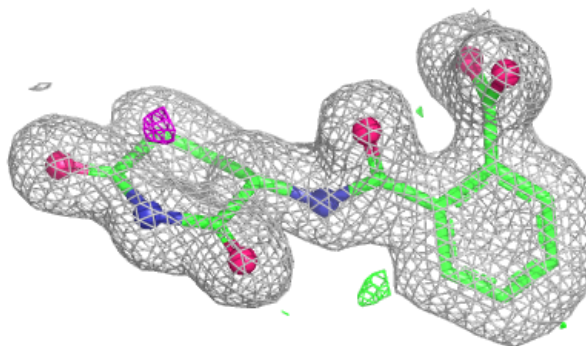


Electron density around JNW D 202:

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

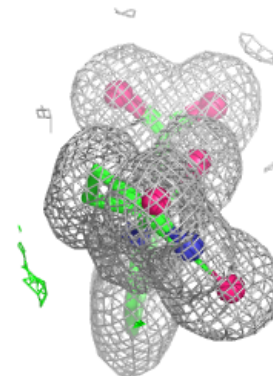
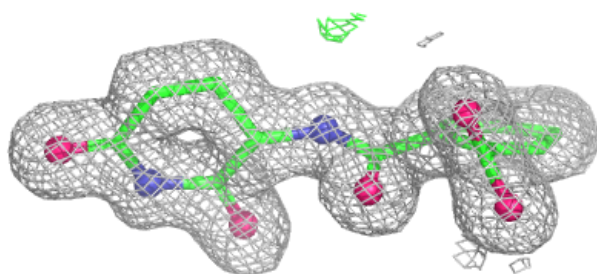
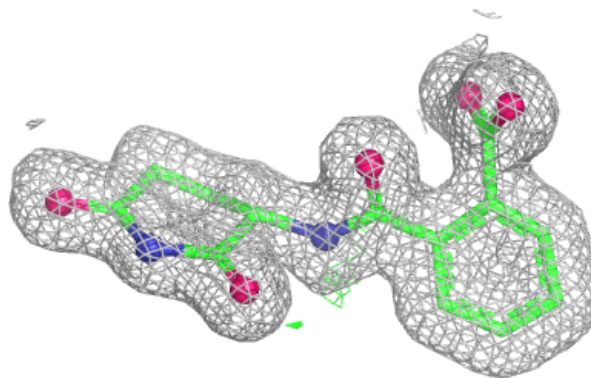
**Electron density around JNW A 202:**

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.