



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 02:29 PM UTC

PDB ID : 6UML / pdb_00006uml
Title : Structural Basis for Thalidomide Teratogenicity Revealed by the Cereblon-D
DB1-SALL4-Pomalidomide Complex
Authors : Clayton, T.L.; Matyskiela, M.E.; Pagarigan, B.E.; Tran, E.T.; Chamberlain,
P.P.
Deposited on : 2019-10-09
Resolution : 3.58 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

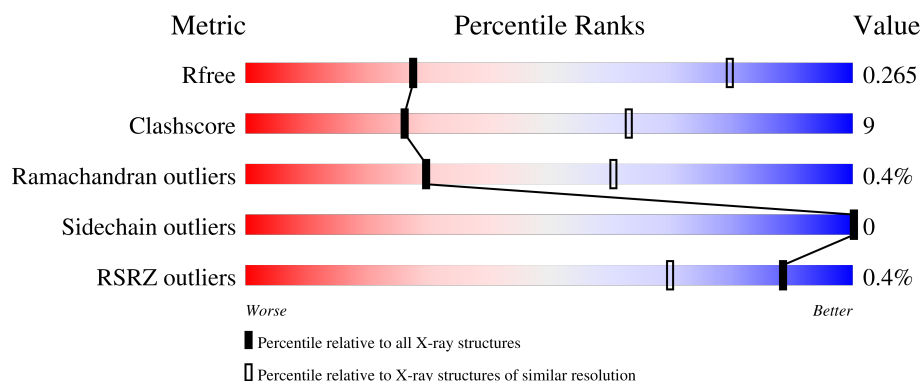
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.58 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	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

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	1140	 76% 19% .
2	C	406	 % 65% 18% 17%
3	E	28	 79% 11% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11104 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1089	Total	C	N	O	S	0	0	0
			8221	5239	1368	1568	46			

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	338	Total	C	N	O	S	0	0	0
			2668	1719	444	483	22			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	GLY	-	expression tag	UNP Q96SW2
C	38	SER	-	expression tag	UNP Q96SW2
C	39	MET	-	expression tag	UNP Q96SW2

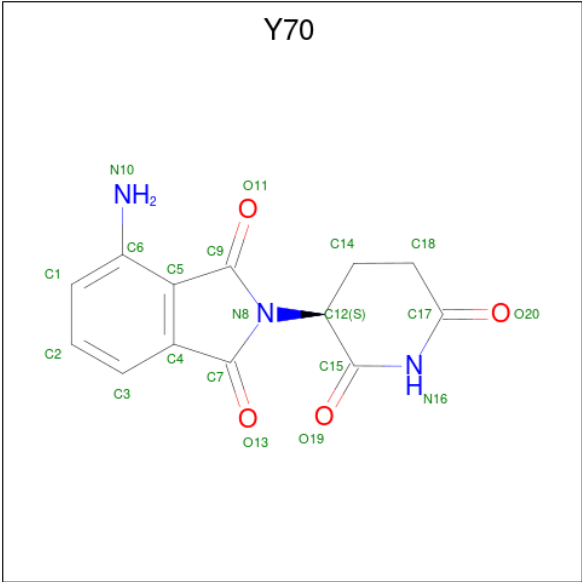
- Molecule 3 is a protein called Sal-like protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	25	Total	C	N	O	S	0	0	0
			193	123	39	29	2			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is S-Pomalidomide (CCD ID: Y70) (formula: C₁₃H₁₁N₃O₄) (labeled as "Ligand of Interest" by depositor).

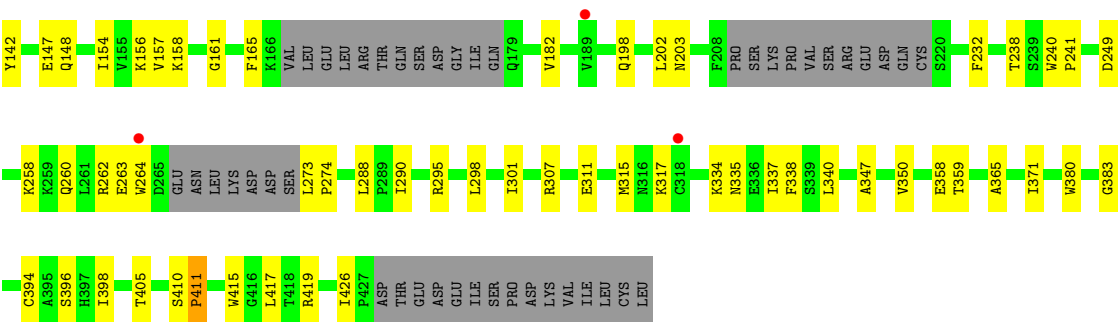


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			20	13	3	4		

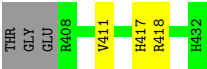
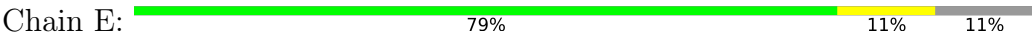
- Molecule 1: DNA damage-binding protein 1

L1051	R1057	V1061	V1065	W1073	W1078	GLU	ARG	K1081	I1089	S1101	R1102	P1103	K1104	M1105	Q1106	E1107	V1108	V1109	L1112	Q1113	Y1114	D1115	GLY	SER	GLY	GLY	MET	K1121	A1124	D1127	K1131	H1140											
R915	R917	G918	I921	L926	R928	L931	N941	F942	R947	W953	N970	D980	SER	ALA	ALA	THR	THR	THR	ASP	E987	E988	R989	E994	F998	E1002	V1013	MET	GLN	ASN	LEU	GLY	THR	THR	THR	P1024	T1032	V1033	N1034	V1040	Y1048			
SER	GLY	T749	T750	S768	K769	L770	F771	SER	SER	THR	ALA	PRO	HIS	GLU	THR	SER	PHE	GLY	E784	I793	Y812	A813	I830	Q845	Q846	R851	Q852	Y853	L858	K864	E865	R866	M873	M877	I884	L899	E902	C903	N904	L912	Y913	I914	
A566	R567	L571	P572	L576	LEU	H578	L582	I587	P483	T595	V487	H600	A605	L606	D625	ARG	K627	T636	F650	A651	C652	S653	T657	M670	V676	M679	D642	I643	T644	P645	GLY	ASP	SER	ASN	E718	S720	R722	L736	E741	V742	Q743	I744	S745
L448	F451	D454	Q455	L468	L478	E482	P483	V487	V500	N504	A511	R514	A515	Y517	Y518	L526	E533	M534	E535	H536	E537	V538	L541	D542	I543	T544	P545	L546	GLY	GLY	GLY	GLY	GLY	C556	A557	I558	C559	E560	M561	T562	D563	I564	S565
Q290	T294	K298	I310	L314	T315	Y316	L317	V322	L328	L333	V334	K335	L336	G344	S345	A349	F353	T354	N355	P358	I359	V360	R369	GLN	GLY	Q372	V376	G380	L387	R388	I389	L413	R414	E420	T424	L427	F429	A432					
L159	V164	I165	D166	V167	K168	T192	Y193	E194	L197	N203	P206	W207	E213	A214	P223	G227	F226	G227	I258	R263	GLY	V264	G268	S269	R270	Y271	L272	L273	G274	M276	E277	G278	R279	L284	T285	E286	A432						
MET	S2	Y3	Y5	V6	T113	V19	T20	K35	E40	A46	GLU	GLY	L49	V55	G56	M57	Y58	K60	I61	A62	V63	M64	F67	L80	T88	Q93	SER	GLY	GLY	S97	I100	I101	T102	T118	M130	R134	G138	I143	A154				

GLY	SER	MET	GLU	ALA	LYS	PRO	ASN	ILE	ILE	N48	F49	L60	GLY	ALA	ASP	MET	GLU	GLU	F67	H68	G69	D74	V53	L91	P98	L99	M109	V110	L113	T114	Q115	K116	D117	R118	T119	F120	A121	V122	L123	ALA	V125	S126	ASN	VAL	GLN	GLU	ARG	E132	E140	F141
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● Molecule 3: Sal-like protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.41Å 127.72Å 110.17Å 90.00° 109.69° 90.00°	Depositor
Resolution (Å)	38.70 – 3.58 38.70 – 3.58	Depositor EDS
% Data completeness (in resolution range)	98.5 (38.70-3.58) 92.8 (38.70-3.58)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.57Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.204 , 0.267 0.205 , 0.265	Depositor DCC
R_{free} test set	1092 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 73.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11104	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y70, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.17	0/8366	0.37	0/11371
2	C	0.21	0/2732	0.47	0/3714
3	E	0.08	0/199	0.28	0/268
All	All	0.18	0/11297	0.39	0/15353

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

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	8221	0	7916	149	0
2	C	2668	0	2605	60	0
3	E	193	0	176	2	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	C	20	0	11	0	0
All	All	11104	0	10708	206	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 9.

The worst 5 of 206 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:560:LEU:HB2	1:A:563:ASP:HB3	1.50	0.94
2:C:410:SER:HB3	2:C:411:PRO:HD2	1.51	0.93
1:A:504:ASN:HD22	1:A:545:PRO:HD3	1.39	0.88
1:A:482:GLU:HG3	1:A:483:PRO:HD2	1.61	0.83
1:A:851:PHE:HB3	1:A:858:LEU:HD11	1.63	0.81

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	1063/1140 (93%)	987 (93%)	72 (7%)	4 (0%)	30	60
2	C	324/406 (80%)	301 (93%)	22 (7%)	1 (0%)	36	65
3	E	23/28 (82%)	23 (100%)	0	0	100	100
All	All	1410/1574 (90%)	1311 (93%)	94 (7%)	5 (0%)	30	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	483	PRO
2	C	411	PRO
1	A	653	SER
1	A	213	GLU
1	A	359	ILE

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	870/999 (87%)	870 (100%)	0	100	100
2	C	291/368 (79%)	291 (100%)	0	100	100
3	E	20/25 (80%)	20 (100%)	0	100	100
All	All	1181/1392 (85%)	1181 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	970	ASN
1	A	1077	HIS
2	C	233	HIS
2	C	79	GLN
1	A	481	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 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	Y70	C	502	-	22,22,22	2.20	6 (27%)	31,33,33	1.76	10 (32%)

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	Y70	C	502	-	-	1/4/33/33	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	502	Y70	C5-C9	-5.71	1.39	1.49
5	C	502	Y70	C4-C7	-5.55	1.39	1.48
5	C	502	Y70	C9-N8	-3.37	1.33	1.40
5	C	502	Y70	C7-N8	-3.26	1.33	1.40
5	C	502	Y70	C5-C6	-2.09	1.39	1.42

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	502	Y70	C17-N16-C15	-4.07	121.33	126.69
5	C	502	Y70	C18-C17-N16	3.16	120.05	116.69
5	C	502	Y70	O11-C9-C5	-2.94	124.68	129.15
5	C	502	Y70	C3-C4-C7	2.65	134.03	129.59
5	C	502	Y70	C12-C15-N16	2.63	120.08	116.24

There are no chirality outliers.

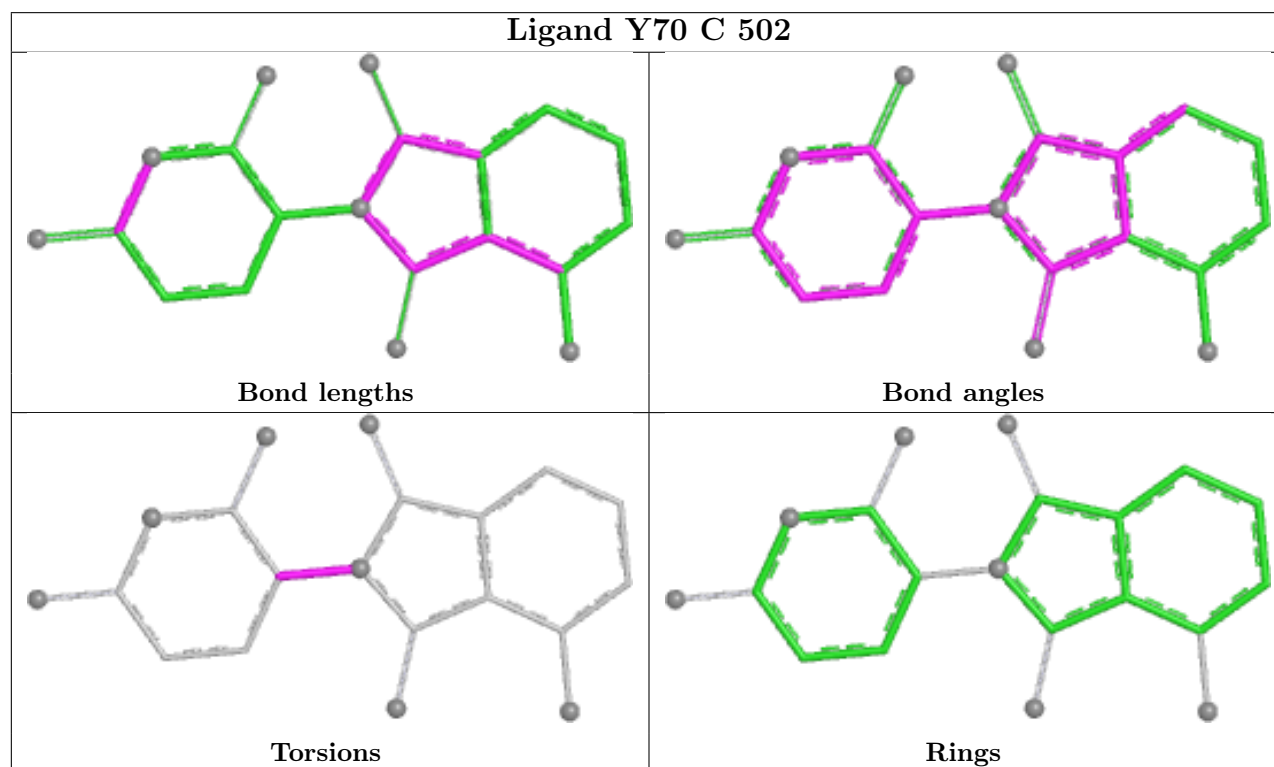
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	502	Y70	C15-C12-N8-C9

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1089/1140 (95%)	-0.07	2 (0%) 91 79	29, 78, 132, 202	1 (0%)
2	C	338/406 (83%)	0.13	4 (1%) 76 49	48, 83, 157, 237	0
3	E	25/28 (89%)	-0.03	0 100 100	77, 100, 125, 142	0
All	All	1452/1574 (92%)	-0.02	6 (0%) 88 70	29, 79, 138, 237	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	83	VAL	2.3
2	C	318	CYS	2.3
1	A	902	GLU	2.3
2	C	189	VAL	2.2
2	C	264	TRP	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

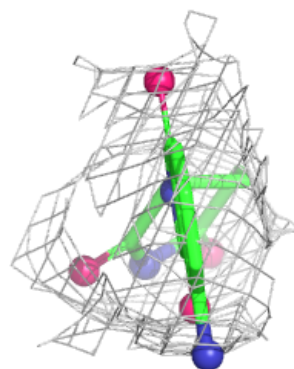
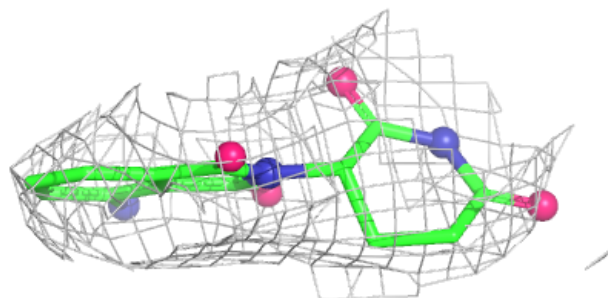
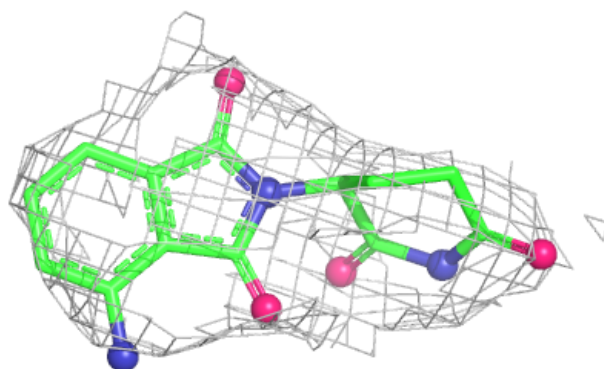
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	Y70	C	502	20/20	0.96	0.09	66,83,89,92	0
4	ZN	E	501	1/1	0.99	0.05	87,87,87,87	0
4	ZN	C	501	1/1	0.99	0.03	67,67,67,67	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 Y70 C 502:

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.