



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:02 PM UTC

PDB ID : 8OJH / pdb_00008ojh
Title : Crystal structure of human CRBN-DDB1 in complex with compound 4
Authors : Cabry, M.P.; Le Bihan, Y.-V.; van Montfort, R.L.M.
Deposited on : 2023-03-24
Resolution : 2.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

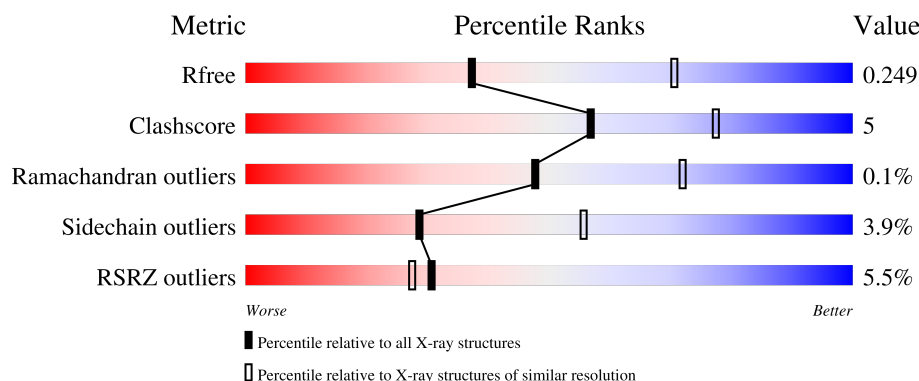
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	1148	
2	B	407	

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
3	EDO	A	1201	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11415 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	1112	Total	C	N	O	S	0	7	3
			8170	5190	1370	1563	47			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1141	TRP	-	expression tag	UNP Q16531
A	1142	SER	-	expression tag	UNP Q16531
A	1143	HIS	-	expression tag	UNP Q16531
A	1144	PRO	-	expression tag	UNP Q16531
A	1145	GLN	-	expression tag	UNP Q16531
A	1146	PHE	-	expression tag	UNP Q16531
A	1147	GLU	-	expression tag	UNP Q16531
A	1148	LYS	-	expression tag	UNP Q16531

- Molecule 2 is a protein called Protein cereblon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	0	4	0
			2837	1825	471	518	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	36	GLY	-	expression tag	UNP Q96SW2
B	37	PRO	-	expression tag	UNP Q96SW2
B	38	HIS	-	expression tag	UNP Q96SW2
B	39	MET	-	expression tag	UNP Q96SW2

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

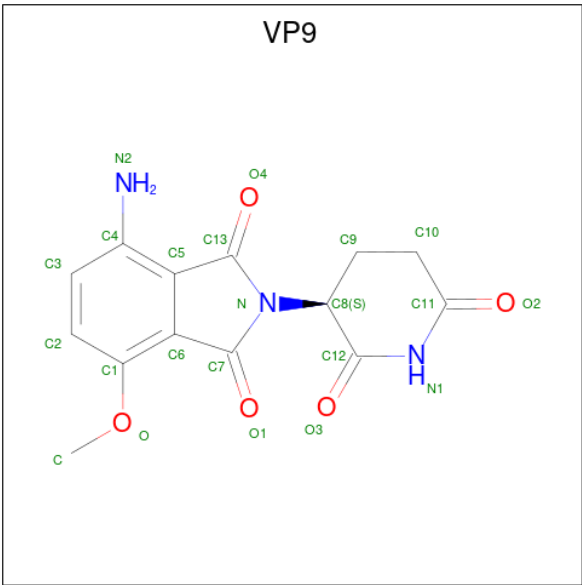


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	1
			8	4	4		
3	B	1	Total	C	O	0	0
			4	2	2		

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

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

- Molecule 5 is 4-azanyl-2-[(3 {S})-2,6-bis(oxidanylidene)piperidin-3-yl]-7-methoxy-isoin dolo-1,3-dione (CCD ID: VP9) (formula: C₁₄H₁₃N₃O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			22	14	3	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	282	Total	O	0	0
			282	282		
6	B	63	Total	O	0	0
			63	63		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.02Å 128.59Å 198.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.61 – 2.72 49.61 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.61-2.72) 99.9 (49.61-2.72)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.10.4 (21-NOV-2022)	Depositor
R, R_{free}	0.209 , 0.254 0.207 , 0.249	Depositor DCC
R_{free} test set	2535 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	56.5	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11415	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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, EDO, VP9

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	0.69	0/8318	0.99	9/11286 (0.1%)
2	B	0.65	0/2909	0.97	3/3966 (0.1%)
All	All	0.68	0/11227	0.98	12/15252 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	PRO	CA-C-N	7.87	127.53	119.19
1	A	250	PRO	C-N-CA	7.87	127.53	119.19
2	B	317	LYS	N-CA-C	7.08	118.78	111.14
1	A	544	THR	CA-C-N	6.65	126.41	119.76
1	A	544	THR	C-N-CA	6.65	126.41	119.76
1	A	925	ASP	CA-CB-CG	5.94	118.54	112.60
1	A	453	ASP	CA-C-N	5.80	128.32	120.38
1	A	453	ASP	C-N-CA	5.80	128.32	120.38
2	B	182	VAL	N-CA-CB	-5.42	103.93	111.41
1	A	698	THR	N-CA-C	5.38	117.56	109.23
2	B	89	MET	N-CA-C	5.26	117.07	110.24
1	A	1077	HIS	N-CA-C	5.11	117.39	108.76

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	8170	0	7473	70	0
2	B	2837	0	2557	28	0
3	A	28	0	42	6	0
3	B	12	0	18	1	0
4	B	1	0	0	0	0
5	B	22	0	0	0	0
6	A	282	0	0	0	0
6	B	63	0	0	0	0
All	All	11415	0	10090	98	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 (98) 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:546:LEU:HD22	1:A:595:THR:HG23	1.33	1.09
1:A:161:GLU:HA	3:A:1207:EDO:H12	1.59	0.84
1:A:1057:ARG:NH1	1:A:1111:ASN:H	1.77	0.83
1:A:848:ILE:HG23	1:A:873:MET:HE1	1.62	0.80
1:A:69:PRO:HG2	1:A:72:GLU:HG3	1.67	0.77
1:A:596:PHE:HB3	1:A:661:SER:HB2	1.72	0.72
1:A:35:LYS:NZ	3:A:1201:EDO:H12	2.04	0.71
2:B:60:LEU:HD13	2:B:64:MET:HE1	1.76	0.66
1:A:883:SER:HB2	1:A:911:ALA:HB3	1.76	0.65
1:A:492:GLU:HG3	1:A:512:VAL:HG21	1.77	0.65
1:A:870:VAL:HG11	1:A:873:MET:HE3	1.79	0.65
1:A:883:SER:HB2	1:A:911:ALA:CB	2.28	0.64
1:A:239:TYR:HB3	1:A:246:LEU:HB2	1.81	0.63
1:A:595:THR:HG22	1:A:600:HIS:CD2	2.34	0.62
2:B:388:VAL:HG13	2:B:397:HIS:HD2	1.64	0.61
1:A:181:VAL:HG22	1:A:190:VAL:HG22	1.83	0.59
2:B:202:LEU:HD13	2:B:233:HIS:ND1	2.17	0.59
1:A:315:THR:HG22	1:A:323:PHE:HB3	1.85	0.59
2:B:61:GLY:HA3	2:B:145:ARG:NH2	2.17	0.59
1:A:1030:PHE:HE2	1:A:1040:VAL:HG23	1.69	0.57
2:B:202:LEU:HD13	2:B:233:HIS:CE1	2.40	0.57
2:B:60:LEU:CD1	2:B:64:MET:HE1	2.35	0.57
1:A:280:LEU:HD23	1:A:347:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:VAL:HG23	1:A:830:ILE:HB	1.89	0.55
2:B:143:ALA:HB3	2:B:158:LYS:HB2	1.88	0.55
1:A:250:PRO:HG2	1:A:253:ILE:HG12	1.89	0.55
1:A:35:LYS:HZ1	3:A:1201:EDO:H12	1.71	0.55
1:A:514:ARG:HB3	1:A:537:GLU:CA	2.37	0.55
2:B:61:GLY:HA3	2:B:145:ARG:HH21	1.72	0.55
1:A:35:LYS:HZ3	3:A:1201:EDO:H12	1.70	0.54
1:A:848:ILE:HG12	1:A:873:MET:CE	2.37	0.54
1:A:613:TYR:CE2	1:A:627:LYS:CB	2.91	0.53
1:A:161:GLU:HA	3:A:1207:EDO:C1	2.37	0.53
1:A:353:PHE:HB3	3:A:1201:EDO:H11	1.89	0.53
1:A:546:LEU:HD22	1:A:595:THR:CG2	2.22	0.53
1:A:928:ARG:HD3	1:A:950:ASN:HB3	1.92	0.52
1:A:11:LYS:HB3	1:A:38[B]:ARG:NE	2.24	0.52
2:B:356:VAL:HB	3:B:503[A]:EDO:H22	1.92	0.52
1:A:837:TYR:HB2	1:A:840:GLU:HG2	1.91	0.52
1:A:1147:GLU:H	1:A:1147:GLU:CD	2.16	0.51
2:B:388:VAL:HG13	2:B:397:HIS:CD2	2.45	0.50
2:B:83:VAL:HG22	2:B:121:ALA:HB3	1.93	0.49
2:B:281:SER:O	2:B:311:GLU:OE1	2.29	0.49
1:A:725[A]:CYS:SG	1:A:829:PHE:CE1	3.05	0.49
1:A:190:VAL:HG23	1:A:212:VAL:HG11	1.93	0.49
1:A:725[A]:CYS:SG	1:A:829:PHE:HE1	2.36	0.49
1:A:430:VAL:HA	1:A:456:GLN:HE21	1.77	0.48
1:A:332:GLN:HG2	1:A:352:THR:HG22	1.94	0.48
1:A:744:ASP:OD1	1:A:744:ASP:N	2.31	0.48
2:B:95:GLN:HE22	2:B:295:ARG:HH22	1.59	0.48
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.75	0.48
1:A:948:ASP:HB2	1:A:992:LEU:HB2	1.96	0.47
1:A:595:THR:CG2	1:A:600:HIS:CD2	2.97	0.47
2:B:60:LEU:HD23	2:B:60:LEU:HA	1.74	0.47
1:A:271:TYR:HB2	1:A:283:LEU:HB3	1.95	0.47
1:A:835:MET:HB2	1:A:845:GLN:HG3	1.97	0.47
1:A:744:ASP:OD1	1:A:749:THR:HA	2.15	0.46
2:B:423:LEU:HD12	2:B:424:PRO:HD2	1.97	0.46
2:B:287:CYS:HB3	2:B:345:PRO:HD2	1.96	0.46
1:A:11:LYS:HB3	1:A:38[B]:ARG:HE	1.81	0.45
1:A:1057:ARG:HH11	1:A:1111:ASN:H	1.60	0.45
2:B:202:LEU:CD1	2:B:233:HIS:CE1	3.00	0.45
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.99	0.45
1:A:613:TYR:CZ	1:A:627:LYS:CB	3.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:PHE:HB2	1:A:432:GLN:HB3	1.99	0.44
2:B:198:GLN:NE2	2:B:234:CYS:SG	2.89	0.44
1:A:218:MET:HE1	1:A:258:ILE:HG22	1.99	0.44
1:A:651:ALA:HB3	1:A:657:THR:HB	1.99	0.44
2:B:109:MET:HE2	2:B:177:ILE:HG23	1.99	0.44
1:A:1030:PHE:CE2	1:A:1040:VAL:HG23	2.50	0.44
2:B:257:ILE:HG23	2:B:315:MET:HE1	2.00	0.44
1:A:848:ILE:HG23	1:A:873:MET:CE	2.41	0.44
2:B:332:THR:HG21	2:B:362:VAL:HG11	1.99	0.44
1:A:544:THR:HA	1:A:545:PRO:HD3	1.76	0.43
1:A:455:GLN:NE2	1:A:473:SER:OG	2.51	0.43
2:B:165:PHE:HB2	2:B:182:VAL:HG13	2.01	0.43
1:A:762:SER:O	1:A:803:HIS:HA	2.19	0.42
1:A:230:ILE:HD11	1:A:285:LEU:HD11	2.01	0.42
1:A:449:MET:HG3	1:A:484:LYS:O	2.19	0.42
2:B:290:ILE:HA	2:B:424:PRO:HG3	2.02	0.42
1:A:427:LEU:HD11	1:A:436:LEU:HD11	2.01	0.42
1:A:710:LEU:HD21	1:A:1141:TRP:CD2	2.55	0.42
1:A:69:PRO:HG2	1:A:72:GLU:CG	2.45	0.42
1:A:698:THR:CG2	1:A:699:LEU:N	2.83	0.42
1:A:35:LYS:HB2	1:A:38[B]:ARG:HG3	2.01	0.42
1:A:741:GLU:HG2	1:A:751:ALA:HA	2.02	0.41
2:B:331:ILE:HD12	2:B:368:LEU:HD21	2.02	0.41
1:A:356:LEU:HD21	1:A:712:ILE:HD13	2.02	0.41
1:A:565:SER:HB2	1:A:581:MET:HA	2.02	0.41
2:B:365:ALA:HB3	2:B:415:TRP:CD2	2.55	0.41
1:A:248:ILE:HG12	1:A:300:LEU:HD12	2.03	0.41
1:A:515:ALA:HA	1:A:533:GLU:HA	2.02	0.41
1:A:389:ILE:HD12	1:A:389:ILE:N	2.36	0.41
2:B:67:PHE:HE2	2:B:144:TYR:HB3	1.86	0.41
1:A:385:GLY:HA3	1:A:719:GLU:O	2.20	0.40
1:A:131:ILE:HD11	1:A:145:LEU:HD21	2.03	0.40
2:B:103[A]:HIS:HA	2:B:104:PRO:HD3	1.95	0.40
2:B:109:MET:HE2	2:B:177:ILE:CG2	2.52	0.40

There are no symmetry-related clashes.

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	1101/1148 (96%)	1058 (96%)	42 (4%)	1 (0%)	48	72
2	B	373/407 (92%)	356 (95%)	17 (5%)	0	100	100
All	All	1474/1555 (95%)	1414 (96%)	59 (4%)	1 (0%)	48	72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	ASN

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	778/1007 (77%)	746 (96%)	32 (4%)	27	54
2	B	264/369 (72%)	255 (97%)	9 (3%)	32	60
All	All	1042/1376 (76%)	1001 (96%)	41 (4%)	28	56

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38[A]	ARG
1	A	38[B]	ARG
1	A	54	GLU
1	A	101	ILE
1	A	127	GLU

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Mol	Chain	Res	Type
1	A	159	LEU
1	A	198	ARG
1	A	253	ILE
1	A	265	ASP
1	A	269	SER
1	A	300	LEU
1	A	366	ASP
1	A	391	ARG
1	A	413	LEU
1	A	419	ARG
1	A	427	LEU
1	A	492	GLU
1	A	561	TRP
1	A	630	THR
1	A	646	THR
1	A	647	THR
1	A	672	ASN
1	A	677	ASN
1	A	744	ASP
1	A	787	GLU
1	A	817	VAL
1	A	842	GLU
1	A	896	GLU
1	A	994	GLU
1	A	1116	ASP
1	A	1129	LEU
1	A	1147	GLU
2	B	55	THR
2	B	86	GLN
2	B	183	GLN
2	B	190	LEU
2	B	193	THR
2	B	246	SER
2	B	313	ASP
2	B	373	ARG
2	B	403	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	203	ASN

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Mol	Chain	Res	Type
1	A	255	GLN
1	A	455	GLN
1	A	456	GLN
1	A	462	ASN
1	A	578	HIS
1	A	664	HIS
1	A	672	ASN
1	A	759	GLN
1	A	907	ASN
1	A	978	GLN
1	A	1056	ASN
2	B	353	HIS
2	B	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 [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	EDO	B	503[A]	-	3,3,3	0.27	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	1203	-	3,3,3	0.22	0	2,2,2	0.27	0
3	EDO	A	1207	-	3,3,3	0.27	0	2,2,2	0.27	0
3	EDO	A	1201	-	3,3,3	0.18	0	2,2,2	0.40	0
3	EDO	B	503[B]	-	3,3,3	0.27	0	2,2,2	0.27	0
3	EDO	A	1202	-	3,3,3	0.21	0	2,2,2	0.41	0
3	EDO	A	1206	-	3,3,3	0.44	0	2,2,2	0.16	0
3	EDO	B	504	-	3,3,3	0.33	0	2,2,2	0.13	0
3	EDO	A	1205	-	3,3,3	0.33	0	2,2,2	0.27	0
3	EDO	A	1204	-	3,3,3	0.31	0	2,2,2	0.25	0
5	VP9	B	502	-	24,24,24	0.38	0	35,36,36	0.55	1 (2%)

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	EDO	B	503[A]	-	-	0/1/1/1	-
3	EDO	A	1203	-	-	1/1/1/1	-
3	EDO	A	1207	-	-	0/1/1/1	-
3	EDO	A	1201	-	-	0/1/1/1	-
3	EDO	B	503[B]	-	-	1/1/1/1	-
3	EDO	A	1202	-	-	1/1/1/1	-
3	EDO	A	1206	-	-	0/1/1/1	-
3	EDO	B	504	-	-	1/1/1/1	-
3	EDO	A	1205	-	-	1/1/1/1	-
3	EDO	A	1204	-	-	1/1/1/1	-
5	VP9	B	502	-	-	0/6/35/35	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	502	VP9	C9-C8-N	-2.59	107.84	113.60

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	EDO	O1-C1-C2-O2
3	B	503[B]	EDO	O1-C1-C2-O2

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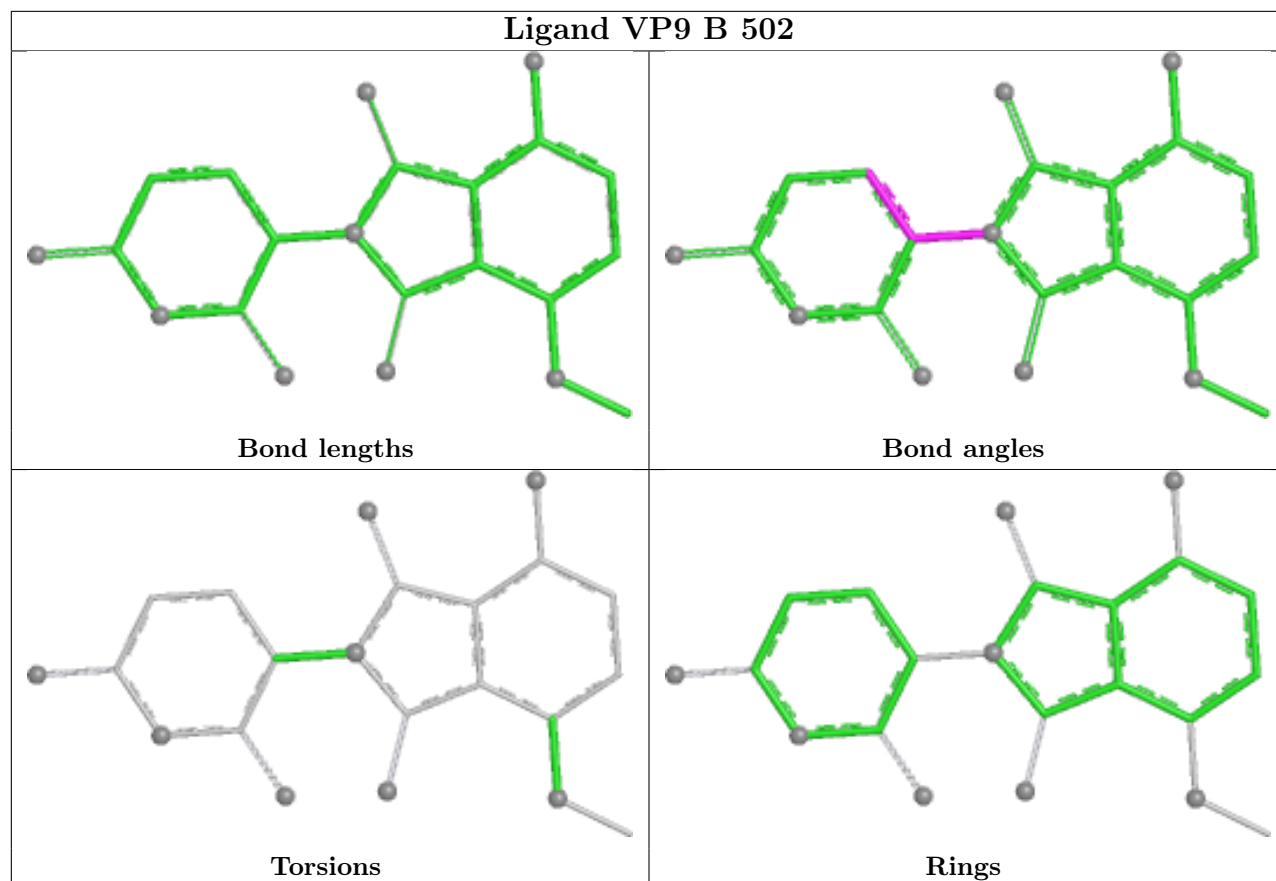
Mol	Chain	Res	Type	Atoms
3	B	504	EDO	O1-C1-C2-O2
3	A	1205	EDO	O1-C1-C2-O2
3	A	1204	EDO	O1-C1-C2-O2
3	A	1203	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503[A]	EDO	1	0
3	A	1207	EDO	2	0
3	A	1201	EDO	4	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	1112/1148 (96%)	0.30	49 (4%) 39 36	20, 56, 124, 146	9 (0%)
2	B	375/407 (92%)	0.44	33 (8%) 15 14	24, 68, 103, 137	4 (1%)
All	All	1487/1555 (95%)	0.34	82 (5%) 30 27	20, 60, 121, 146	13 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	SER	12.6
1	A	566	ALA	5.2
2	B	207	ILE	4.6
2	B	197	VAL	3.9
2	B	267	ASN	3.9
1	A	341	ASN	3.8
2	B	196	ALA	3.7
2	B	208	PHE	3.7
1	A	983	ALA	3.6
1	A	676	VAL	3.5
2	B	212	PRO	3.4
2	B	262	ARG	3.4
1	A	295	VAL	3.4
1	A	483	PRO	3.3
2	B	199	LEU	3.3
1	A	288	GLU	3.2
1	A	1014	MET	3.1
1	A	516	LEU	3.1
1	A	345	SER	3.1
1	A	338	VAL	3.1
2	B	178	GLN	3.0
2	B	46	ILE	3.0
1	A	497	ASN	2.9
2	B	210	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	202	LEU	2.8
2	B	200	GLU	2.8
1	A	561	TRP	2.7
1	A	601	TYR	2.7
2	B	205	CYS	2.7
2	B	271	ASP	2.6
1	A	225	PRO	2.6
1	A	707	ILE	2.6
1	A	367	LEU	2.6
1	A	536	HIS	2.5
1	A	668	PHE	2.5
2	B	206	GLN	2.5
1	A	782	PHE	2.5
2	B	329	THR	2.5
1	A	634	GLN	2.5
2	B	175	ASP	2.4
2	B	236[A]	ASN	2.4
2	B	428	ASP	2.4
1	A	535	GLU	2.4
1	A	650	PHE	2.4
2	B	203	ASN	2.3
2	B	153[A]	GLU	2.3
1	A	470	GLN	2.3
1	A	527	ARG	2.3
1	A	61	ILE	2.3
1	A	517	TYR	2.3
2	B	265	ASP	2.3
1	A	558	ILE	2.3
1	A	617	ASN	2.3
1	A	604	CYS	2.3
1	A	631	LEU	2.3
2	B	88	MET	2.2
1	A	271	TYR	2.2
1	A	662	SER	2.2
1	A	663	ASN	2.2
1	A	534	MET	2.2
1	A	482	GLU	2.2
1	A	528	GLN	2.2
1	A	559	GLY	2.2
1	A	538	VAL	2.1
1	A	557	ALA	2.1
1	A	709	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	204	LYS	2.1
1	A	420	GLU	2.1
1	A	1023	PRO	2.1
1	A	602	LEU	2.1
2	B	188	CYS	2.1
1	A	840	GLU	2.1
2	B	263	GLU	2.1
2	B	198	GLN	2.1
2	B	127	ASN	2.1
1	A	1123	GLU	2.0
1	A	603	LEU	2.0
2	B	103[A]	HIS	2.0
2	B	211	LYS	2.0
2	B	220	SER	2.0
1	A	618	ILE	2.0
2	B	177	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	B	504	4/4	0.64	0.17	68,68,69,69	0
3	EDO	B	503[B]	4/4	0.76	0.24	74,74,74,74	4
3	EDO	B	503[A]	4/4	0.76	0.24	78,78,78,78	4
3	EDO	A	1206	4/4	0.80	0.19	64,64,64,64	0
3	EDO	A	1204	4/4	0.85	0.16	70,70,70,70	0
3	EDO	A	1207	4/4	0.86	0.15	73,73,73,73	0
3	EDO	A	1205	4/4	0.86	0.11	60,61,61,61	0

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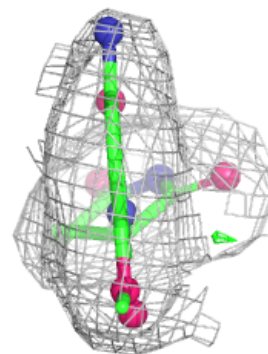
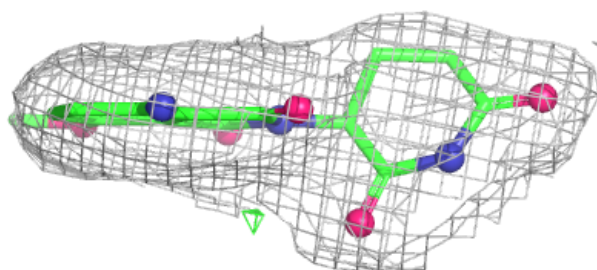
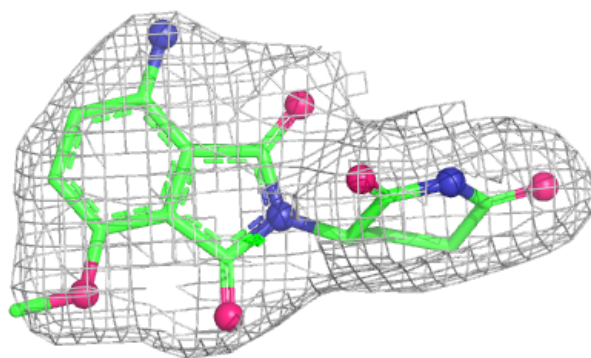
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	1202	4/4	0.92	0.15	56,57,57,57	0
3	EDO	A	1201	4/4	0.94	0.14	51,51,52,52	0
5	VP9	B	502	22/22	0.94	0.09	46,48,49,50	0
3	EDO	A	1203	4/4	0.96	0.09	55,55,55,55	0
4	ZN	B	501	1/1	0.99	0.04	66,66,66,66	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 VP9 B 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.