



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:36 AM EDT

PDB ID : 7JV8 / pdb_00007jv8
Title : Human CD73 (ecto 5'-nucleotidase) in complex with compound 35
Authors : Gibbons, P.; Du, X.
Deposited on : 2020-08-20
Resolution : 2.46 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

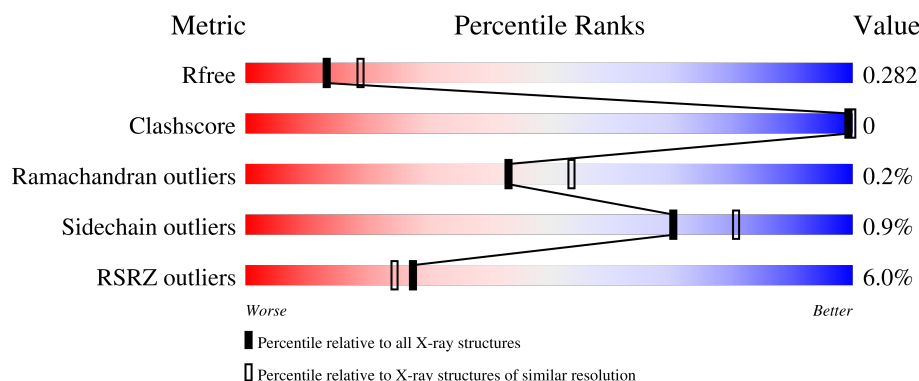
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	529	0% 97% ..
1	B	529	8% 96% ..
1	C	529	11% 99% .
1	D	529	3% 98% ..

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 16768 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 5'-nucleotidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	2	0
			4068	2594	681	773	20			
1	B	518	Total	C	N	O	S	0	1	0
			3948	2526	649	753	20			
1	C	529	Total	C	N	O	S	0	1	0
			4032	2575	681	758	18			
1	D	525	Total	C	N	O	S	0	2	0
			4066	2592	682	772	20			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	-	expression tag	UNP P21589
A	24	ALA	-	expression tag	UNP P21589
A	25	SER	-	expression tag	UNP P21589
A	26	MET	-	expression tag	UNP P21589
A	53	ASP	ASN	engineered mutation	UNP P21589
A	333	ASP	ASN	engineered mutation	UNP P21589
A	403	ASP	ASN	engineered mutation	UNP P21589
A	550	HIS	-	expression tag	UNP P21589
A	551	HIS	-	expression tag	UNP P21589
B	23	LEU	-	expression tag	UNP P21589
B	24	ALA	-	expression tag	UNP P21589
B	25	SER	-	expression tag	UNP P21589
B	26	MET	-	expression tag	UNP P21589
B	53	ASP	ASN	engineered mutation	UNP P21589
B	333	ASP	ASN	engineered mutation	UNP P21589
B	403	ASP	ASN	engineered mutation	UNP P21589
B	550	HIS	-	expression tag	UNP P21589
B	551	HIS	-	expression tag	UNP P21589
C	23	LEU	-	expression tag	UNP P21589
C	24	ALA	-	expression tag	UNP P21589
C	25	SER	-	expression tag	UNP P21589

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Chain	Residue	Modelled	Actual	Comment	Reference
C	26	MET	-	expression tag	UNP P21589
C	53	ASP	ASN	engineered mutation	UNP P21589
C	333	ASP	ASN	engineered mutation	UNP P21589
C	403	ASP	ASN	engineered mutation	UNP P21589
C	550	HIS	-	expression tag	UNP P21589
C	551	HIS	-	expression tag	UNP P21589
D	23	LEU	-	expression tag	UNP P21589
D	24	ALA	-	expression tag	UNP P21589
D	25	SER	-	expression tag	UNP P21589
D	26	MET	-	expression tag	UNP P21589
D	53	ASP	ASN	engineered mutation	UNP P21589
D	333	ASP	ASN	engineered mutation	UNP P21589
D	403	ASP	ASN	engineered mutation	UNP P21589
D	550	HIS	-	expression tag	UNP P21589
D	551	HIS	-	expression tag	UNP P21589

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

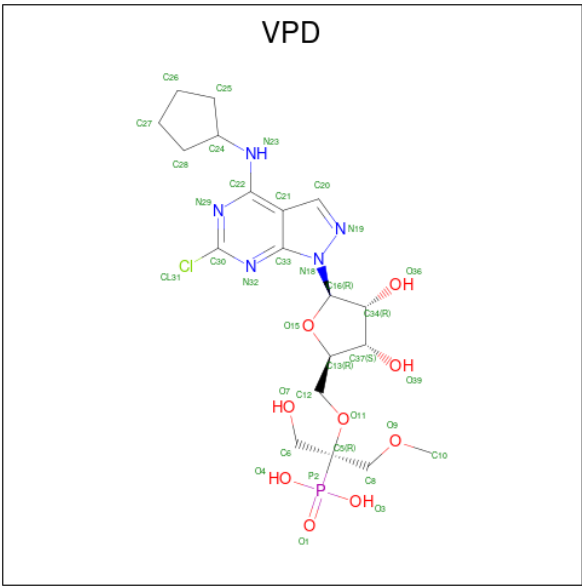
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0
2	C	2	Total Zn 2 2	0	0
2	D	2	Total Zn 2 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is 6-chloro-N-cyclopentyl-1-{5-O-[(2R)-1-hydroxy-3-methoxy-2-phosphonopropan-2-yl]-beta-D-ribofuranosyl}-1H-pyrazolo[3,4-d]pyrimidin-4-amine (CCD ID: VPD)

(formula: C₁₉H₂₉ClN₅O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	P	0	0
			35	19	1	5	9	1		
4	B	1	Total	C	Cl	N	O	P	0	0
			35	19	1	5	9	1		
4	C	1	Total	C	Cl	N	O	P	0	0
			35	19	1	5	9	1		
4	D	1	Total	C	Cl	N	O	P	0	0
			35	19	1	5	9	1		

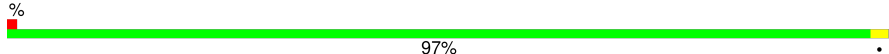
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	184	Total	O	0	1
			185	185		
5	B	67	Total	O	0	0
			67	67		
5	C	88	Total	O	0	0
			88	88		
5	D	162	Total	O	0	0
			162	162		

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.

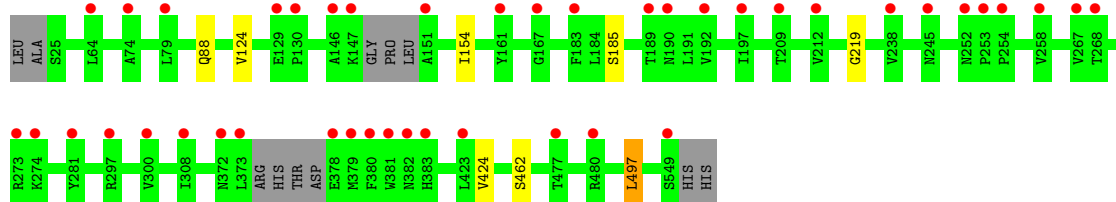
• Molecule 1: 5'-nucleotidase

Chain A: 

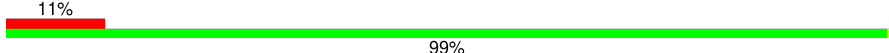


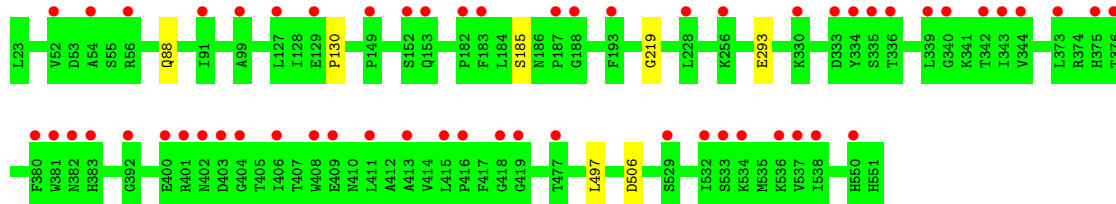
• Molecule 1: 5'-nucleotidase

Chain B: 

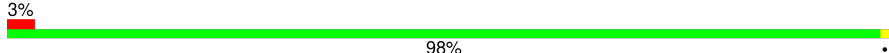


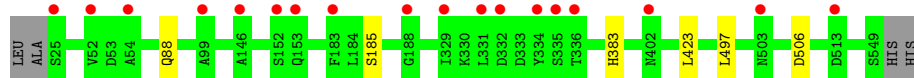
• Molecule 1: 5'-nucleotidase

Chain C: 



• Molecule 1: 5'-nucleotidase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.88Å 102.35Å 129.61Å 90.00° 103.22° 90.00°	Depositor
Resolution (Å)	126.17 – 2.46 126.17 – 2.46	Depositor EDS
% Data completeness (in resolution range)	94.7 (126.17-2.46) 94.7 (126.17-2.46)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.220 , 0.279 0.224 , 0.282	Depositor DCC
R_{free} test set	988 reflections (1.22%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 25.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16768	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: VPD, CA, 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	0.77	0/4154	1.00	3/5634 (0.1%)
1	B	0.77	0/4029	1.00	1/5472 (0.0%)
1	C	0.76	0/4120	0.99	1/5596 (0.0%)
1	D	0.75	0/4152	0.99	1/5633 (0.0%)
All	All	0.76	0/16455	0.99	6/22335 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	383	HIS	N-CA-C	6.06	118.85	111.82
1	A	336	THR	N-CA-C	5.71	118.24	111.33
1	A	337	GLN	N-CA-C	5.69	118.31	110.35
1	C	219	GLY	N-CA-C	5.43	119.46	110.55
1	A	219	GLY	N-CA-C	5.28	119.20	110.55
1	B	219	GLY	N-CA-C	5.24	119.14	110.55

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	4068	0	3980	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3948	0	3774	2	0
1	C	4032	0	3855	0	0
1	D	4066	0	3965	0	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	35	0	0	0	0
4	B	35	0	0	0	0
4	C	35	0	0	0	0
4	D	35	0	0	0	0
5	A	185	0	0	0	0
5	B	67	0	0	0	0
5	C	88	0	0	0	0
5	D	162	0	0	0	0
All	All	16768	0	15574	7	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 0.

All (7) 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:125[A]:GLU:H	1:A:125[A]:GLU:CD	1.92	0.75
1:A:125[A]:GLU:OE1	1:A:125[A]:GLU:N	2.23	0.72
1:B:424:VAL:HG22	1:B:497:LEU:HD22	2.00	0.42
1:A:124:VAL:HG11	1:A:150:LEU:HD11	2.00	0.42
1:A:88:GLN:HG2	1:A:417:PHE:CD1	2.56	0.41
1:B:124:VAL:HG13	1:B:154:ILE:HD12	2.02	0.41
1:A:88:GLN:HG2	1:A:417:PHE:CE1	2.56	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	525/529 (99%)	508 (97%)	16 (3%)	1 (0%)	43	54
1	B	513/529 (97%)	497 (97%)	15 (3%)	1 (0%)	43	54
1	C	528/529 (100%)	509 (96%)	17 (3%)	2 (0%)	30	37
1	D	525/529 (99%)	509 (97%)	15 (3%)	1 (0%)	43	54
All	All	2091/2116 (99%)	2023 (97%)	63 (3%)	5 (0%)	43	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	B	88	GLN
1	C	88	GLN
1	D	88	GLN
1	C	130	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	438/456 (96%)	433 (99%)	5 (1%)	65	76
1	B	406/456 (89%)	403 (99%)	3 (1%)	76	84
1	C	412/456 (90%)	408 (99%)	4 (1%)	68	77
1	D	434/456 (95%)	430 (99%)	4 (1%)	70	81
All	All	1690/1824 (93%)	1674 (99%)	16 (1%)	70	81

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	125[A]	GLU
1	A	125[B]	GLU
1	A	185	SER
1	A	402	ASN
1	A	497	LEU
1	B	185	SER
1	B	462	SER
1	B	497	LEU
1	C	185	SER
1	C	293	GLU
1	C	497	LEU
1	C	506	ASP
1	D	185	SER
1	D	423	LEU
1	D	497	LEU
1	D	506	ASP

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

Mol	Chain	Res	Type
1	A	370	ASN
1	A	425	GLN
1	B	304	HIS
1	B	370	ASN
1	C	279	GLN
1	C	370	ASN
1	C	503	ASN
1	D	69	GLN
1	D	311	ASN
1	D	370	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 16 ligands modelled in this entry, 12 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
4	VPD	D	604	2	35,38,38	0.85	1 (2%)	41,57,57	2.40	11 (26%)
4	VPD	C	604	2	35,38,38	1.01	3 (8%)	41,57,57	2.65	13 (31%)
4	VPD	A	604	2	35,38,38	0.91	2 (5%)	41,57,57	2.41	14 (34%)
4	VPD	B	604	2	35,38,38	1.01	3 (8%)	41,57,57	2.62	14 (34%)

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
4	VPD	D	604	2	-	8/18/53/53	0/4/4/4
4	VPD	C	604	2	-	8/18/53/53	0/4/4/4
4	VPD	A	604	2	-	6/18/53/53	0/4/4/4
4	VPD	B	604	2	-	8/18/53/53	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	VPD	C22-N23	2.79	1.39	1.35
4	B	604	VPD	P2-O3	2.59	1.61	1.54
4	C	604	VPD	P2-O3	2.47	1.61	1.54
4	B	604	VPD	C22-N23	2.43	1.38	1.35
4	D	604	VPD	C22-N23	2.36	1.38	1.35
4	A	604	VPD	C22-N23	2.26	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	604	VPD	P2-O4	2.03	1.60	1.54
4	B	604	VPD	N18-N19	2.01	1.39	1.37
4	A	604	VPD	P2-O4	2.01	1.60	1.54

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	604	VPD	C21-C33-N32	-10.64	119.80	126.56
4	C	604	VPD	C21-C33-N32	-10.37	119.97	126.56
4	D	604	VPD	C21-C33-N32	-9.19	120.72	126.56
4	A	604	VPD	C21-C33-N32	-9.12	120.77	126.56
4	D	604	VPD	N32-C30-N29	-4.64	121.03	129.52
4	C	604	VPD	O15-C16-N18	4.60	114.33	109.41
4	D	604	VPD	O7-C6-C5	-4.60	109.13	113.31
4	C	604	VPD	N32-C30-N29	-4.57	121.16	129.52
4	B	604	VPD	N32-C30-N29	-4.56	121.18	129.52
4	D	604	VPD	CL31-C30-N29	4.40	121.37	115.17
4	A	604	VPD	C34-C16-N18	-4.38	106.89	113.43
4	D	604	VPD	C30-N29-C22	4.35	122.74	116.60
4	B	604	VPD	O7-C6-C5	-4.26	109.44	113.31
4	C	604	VPD	C30-N29-C22	4.19	122.52	116.60
4	A	604	VPD	N32-C30-N29	-4.18	121.88	129.52
4	A	604	VPD	C30-N29-C22	4.16	122.47	116.60
4	B	604	VPD	N32-C33-N18	4.07	134.06	128.68
4	B	604	VPD	C20-N19-N18	4.06	108.72	105.95
4	C	604	VPD	C20-N19-N18	4.04	108.71	105.95
4	B	604	VPD	C30-N29-C22	4.01	122.27	116.60
4	D	604	VPD	C20-N19-N18	3.78	108.53	105.95
4	A	604	VPD	C20-N19-N18	3.71	108.48	105.95
4	C	604	VPD	C30-N32-C33	3.69	121.42	110.98
4	C	604	VPD	CL31-C30-N29	3.58	120.21	115.17
4	B	604	VPD	C30-N32-C33	3.57	121.10	110.98
4	D	604	VPD	C30-N32-C33	3.55	121.02	110.98
4	C	604	VPD	C33-N18-N19	-3.35	108.93	110.94
4	A	604	VPD	C30-N32-C33	3.29	120.30	110.98
4	C	604	VPD	C34-C16-N18	-3.26	108.56	113.43
4	B	604	VPD	CL31-C30-N32	3.22	119.70	115.17
4	C	604	VPD	N32-C33-N18	3.16	132.85	128.68
4	A	604	VPD	N32-C33-N18	3.08	132.75	128.68
4	A	604	VPD	CL31-C30-N29	2.89	119.24	115.17
4	B	604	VPD	CL31-C30-N29	2.80	119.12	115.17
4	D	604	VPD	N32-C33-N18	2.75	132.31	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	604	VPD	C33-N18-N19	-2.73	109.31	110.94
4	A	604	VPD	CL31-C30-N32	2.62	118.86	115.17
4	B	604	VPD	C33-N18-N19	-2.56	109.41	110.94
4	C	604	VPD	CL31-C30-N32	2.46	118.63	115.17
4	A	604	VPD	C12-C13-C37	-2.46	106.37	115.21
4	B	604	VPD	C21-C20-N19	-2.33	109.61	111.38
4	A	604	VPD	O7-C6-C5	-2.22	111.30	113.31
4	A	604	VPD	C21-C20-N19	-2.20	109.71	111.38
4	A	604	VPD	C13-O15-C16	-2.17	104.68	109.47
4	C	604	VPD	O3-P2-O1	-2.14	107.72	112.96
4	D	604	VPD	C21-C22-N29	-2.14	118.02	121.92
4	C	604	VPD	C21-C22-N29	-2.13	118.03	121.92
4	B	604	VPD	C34-C16-N18	-2.08	110.32	113.43
4	D	604	VPD	C34-C16-N18	-2.05	110.36	113.43
4	B	604	VPD	C12-C13-C37	-2.04	107.88	115.21
4	A	604	VPD	C21-C22-N29	-2.01	118.26	121.92
4	B	604	VPD	C33-C21-C20	2.00	106.12	104.42

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	604	VPD	O15-C16-N18-N19
4	A	604	VPD	C21-C22-N23-C24
4	B	604	VPD	O15-C16-N18-N19
4	B	604	VPD	C21-C22-N23-C24
4	B	604	VPD	N29-C22-N23-C24
4	C	604	VPD	O15-C16-N18-N19
4	C	604	VPD	C21-C22-N23-C24
4	D	604	VPD	O15-C16-N18-N19
4	D	604	VPD	C21-C22-N23-C24
4	D	604	VPD	O11-C12-C13-O15
4	B	604	VPD	O11-C12-C13-O15
4	D	604	VPD	O11-C12-C13-C37
4	B	604	VPD	O11-C12-C13-C37
4	C	604	VPD	O11-C12-C13-C37
4	A	604	VPD	N29-C22-N23-C24
4	C	604	VPD	N29-C22-N23-C24
4	D	604	VPD	N29-C22-N23-C24
4	C	604	VPD	O11-C12-C13-O15
4	A	604	VPD	C34-C16-N18-C33
4	A	604	VPD	O15-C16-N18-C33

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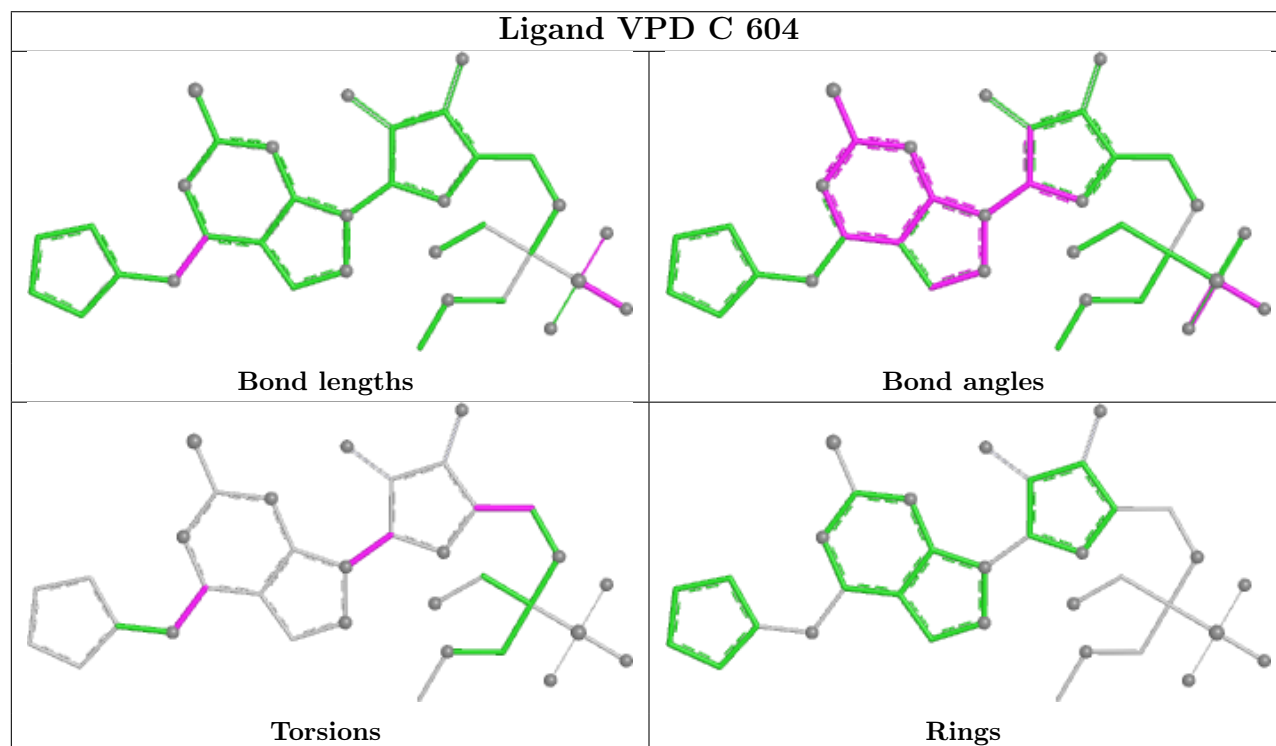
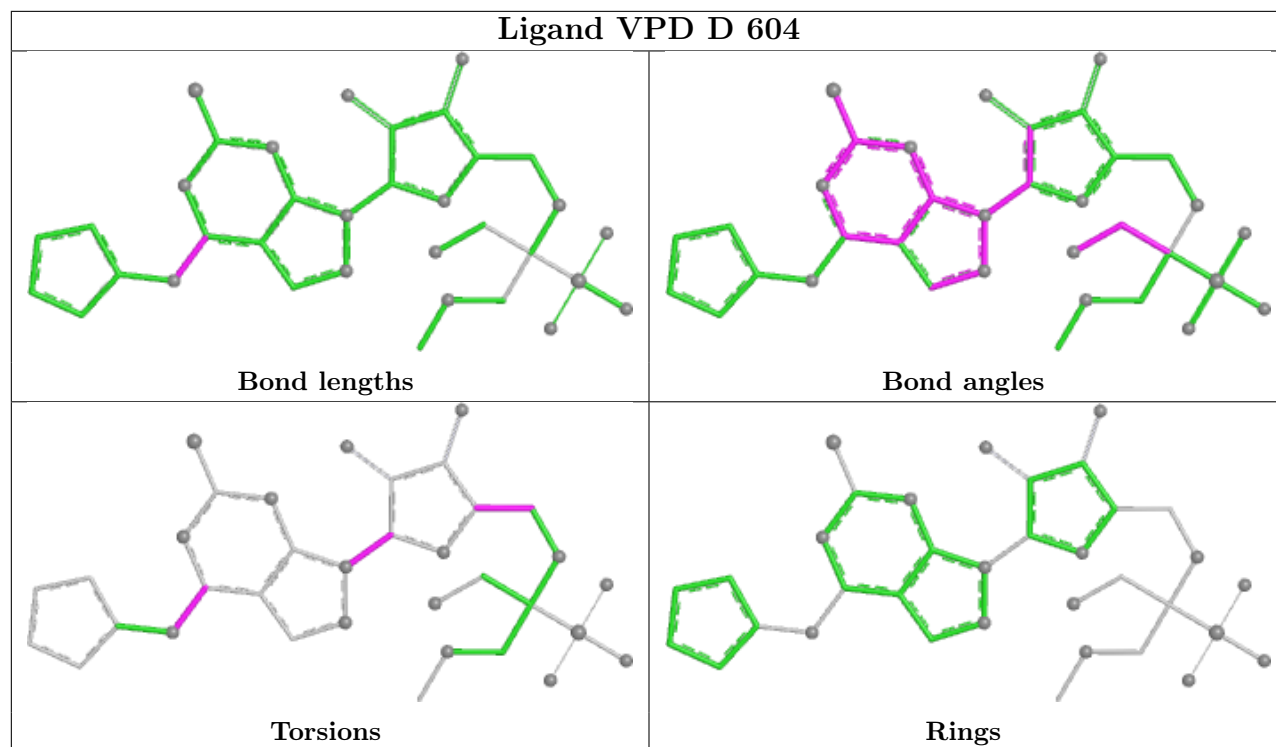
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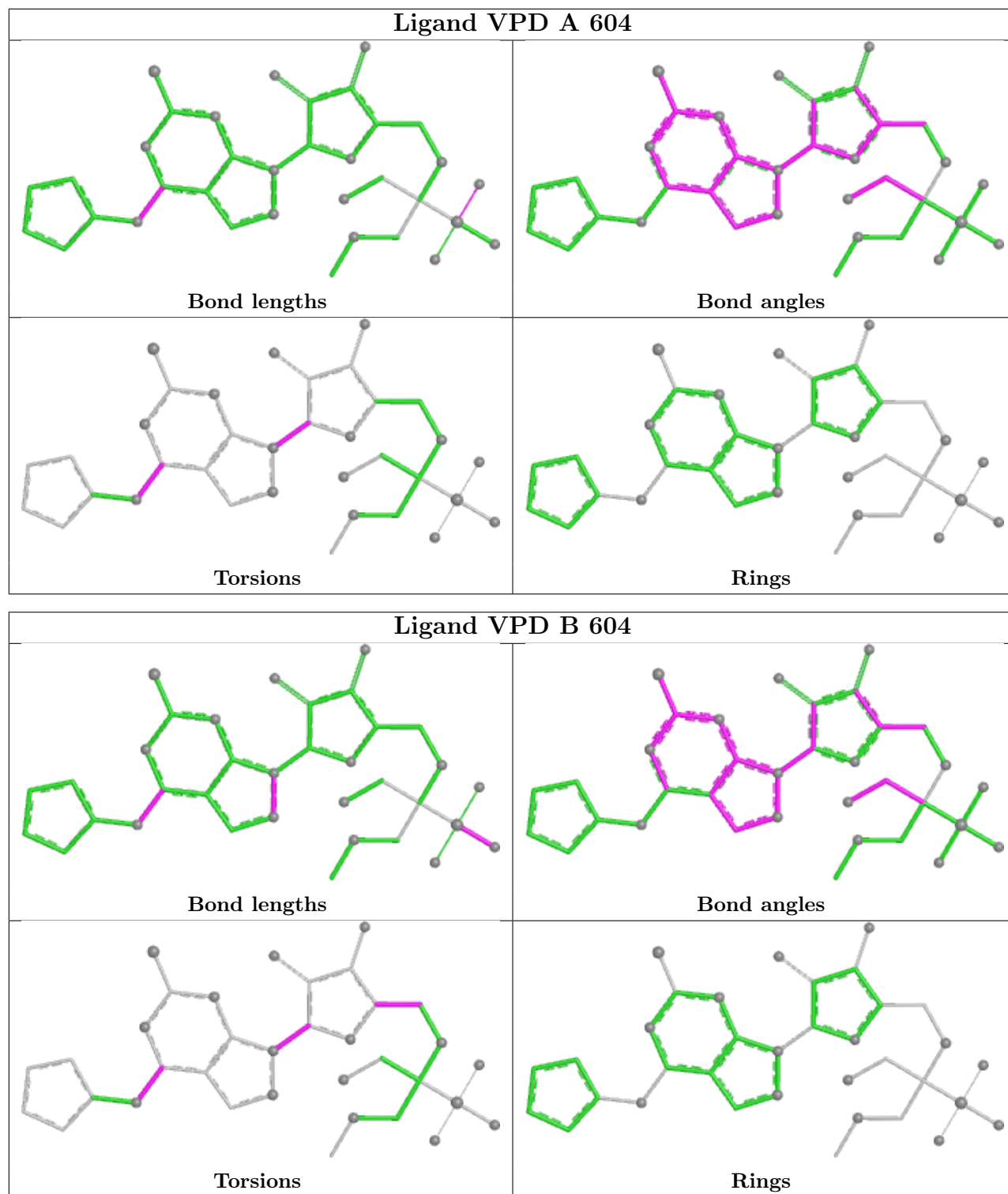
Mol	Chain	Res	Type	Atoms
4	B	604	VPD	C34-C16-N18-C33
4	B	604	VPD	O15-C16-N18-C33
4	C	604	VPD	C34-C16-N18-C33
4	D	604	VPD	C34-C16-N18-C33
4	D	604	VPD	O15-C16-N18-C33
4	C	604	VPD	C34-C16-N18-N19
4	C	604	VPD	O15-C16-N18-C33
4	A	604	VPD	C34-C16-N18-N19
4	B	604	VPD	C34-C16-N18-N19
4	D	604	VPD	C34-C16-N18-N19

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 ⓘ

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	525/529 (99%)	-0.02	7 (1%) 75 77	18, 35, 59, 103	2 (0%)
1	B	518/529 (97%)	0.74	43 (8%) 17 15	23, 52, 88, 130	1 (0%)
1	C	529/529 (100%)	0.74	58 (10%) 10 8	21, 50, 96, 143	1 (0%)
1	D	525/529 (99%)	0.19	18 (3%) 48 48	15, 37, 67, 100	2 (0%)
All	All	2097/2116 (99%)	0.41	126 (6%) 27 24	15, 43, 82, 143	6 (0%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	LEU	5.2
1	C	533	SER	4.8
1	B	380	PHE	4.5
1	C	415	LEU	4.5
1	C	149	PRO	4.2
1	B	383	HIS	4.2
1	C	403	ASP	4.0
1	C	333	ASP	3.8
1	B	373	LEU	3.6
1	C	419	GLY	3.6
1	D	329	ILE	3.6
1	B	382	ASN	3.6
1	C	408	TRP	3.5
1	B	146	ALA	3.4
1	C	183	PHE	3.3
1	C	336	THR	3.3
1	C	411	LEU	3.2
1	A	124	VAL	3.2
1	C	343	ILE	3.2
1	B	381	TRP	3.2
1	D	503	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	538	ILE	3.1
1	C	409	GLU	3.1
1	C	342	THR	3.0
1	B	379	MET	3.0
1	D	335	SER	3.0
1	B	209	THR	2.9
1	C	335	SER	2.9
1	C	402	ASN	2.9
1	C	401	ARG	2.9
1	C	536	LYS	2.8
1	B	254	PRO	2.8
1	B	151	ALA	2.8
1	C	404	GLY	2.8
1	B	281	TYR	2.8
1	C	537	VAL	2.8
1	D	334	TYR	2.8
1	C	99	ALA	2.8
1	B	297	ARG	2.8
1	D	332	ASP	2.8
1	B	258	VAL	2.7
1	C	373	LEU	2.7
1	B	197	ILE	2.7
1	B	189	THR	2.7
1	D	336	THR	2.7
1	B	147	LYS	2.7
1	A	336	THR	2.7
1	C	532	ILE	2.7
1	C	529	SER	2.7
1	C	376	THR	2.7
1	C	256	LYS	2.6
1	C	381	TRP	2.6
1	B	74	ALA	2.6
1	C	550	HIS	2.6
1	C	534	LYS	2.6
1	B	252	ASN	2.6
1	A	312	SER	2.6
1	B	477	THR	2.6
1	C	477	THR	2.6
1	D	188	GLY	2.5
1	C	406	ILE	2.5
1	C	382	ASN	2.5
1	B	238	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	152	SER	2.5
1	C	188	GLY	2.5
1	C	153	GLN	2.5
1	B	274	LYS	2.5
1	C	187	PRO	2.4
1	B	378	GLU	2.4
1	C	54	ALA	2.4
1	C	413	ALA	2.4
1	C	392	GLY	2.4
1	B	308	ILE	2.4
1	B	212	VAL	2.4
1	C	344	VAL	2.4
1	B	161	TYR	2.4
1	D	183	PHE	2.4
1	D	402	ASN	2.4
1	B	129	GLU	2.4
1	B	268	THR	2.3
1	C	380	PHE	2.3
1	B	267	VAL	2.3
1	B	253	PRO	2.3
1	D	152	SER	2.3
1	D	513	ASP	2.3
1	B	64	LEU	2.3
1	C	228	LEU	2.3
1	C	52	VAL	2.3
1	C	56	ARG	2.3
1	B	167	GLY	2.3
1	C	91	ILE	2.3
1	B	183	PHE	2.3
1	B	273	ARG	2.3
1	C	182	PRO	2.3
1	D	99	ALA	2.2
1	C	330	LYS	2.2
1	D	153	GLN	2.2
1	B	192	VAL	2.1
1	C	334	TYR	2.1
1	D	25	SER	2.1
1	B	300	VAL	2.1
1	C	375	HIS	2.1
1	A	146	ALA	2.1
1	B	245	ASN	2.1
1	A	376	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	418	GLY	2.1
1	C	129	GLU	2.1
1	C	416	PRO	2.1
1	C	383	HIS	2.1
1	B	423	LEU	2.1
1	C	340	GLY	2.1
1	A	108	LEU	2.1
1	B	190	ASN	2.1
1	D	331	LEU	2.1
1	C	193	PHE	2.0
1	D	52	VAL	2.0
1	A	109	ARG	2.0
1	B	480	ARG	2.0
1	C	400	GLU	2.0
1	B	130	PRO	2.0
1	B	549	SER	2.0
1	B	79	LEU	2.0
1	C	127	LEU	2.0
1	D	54	ALA	2.0
1	D	146	ALA	2.0
1	B	372	ASN	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.

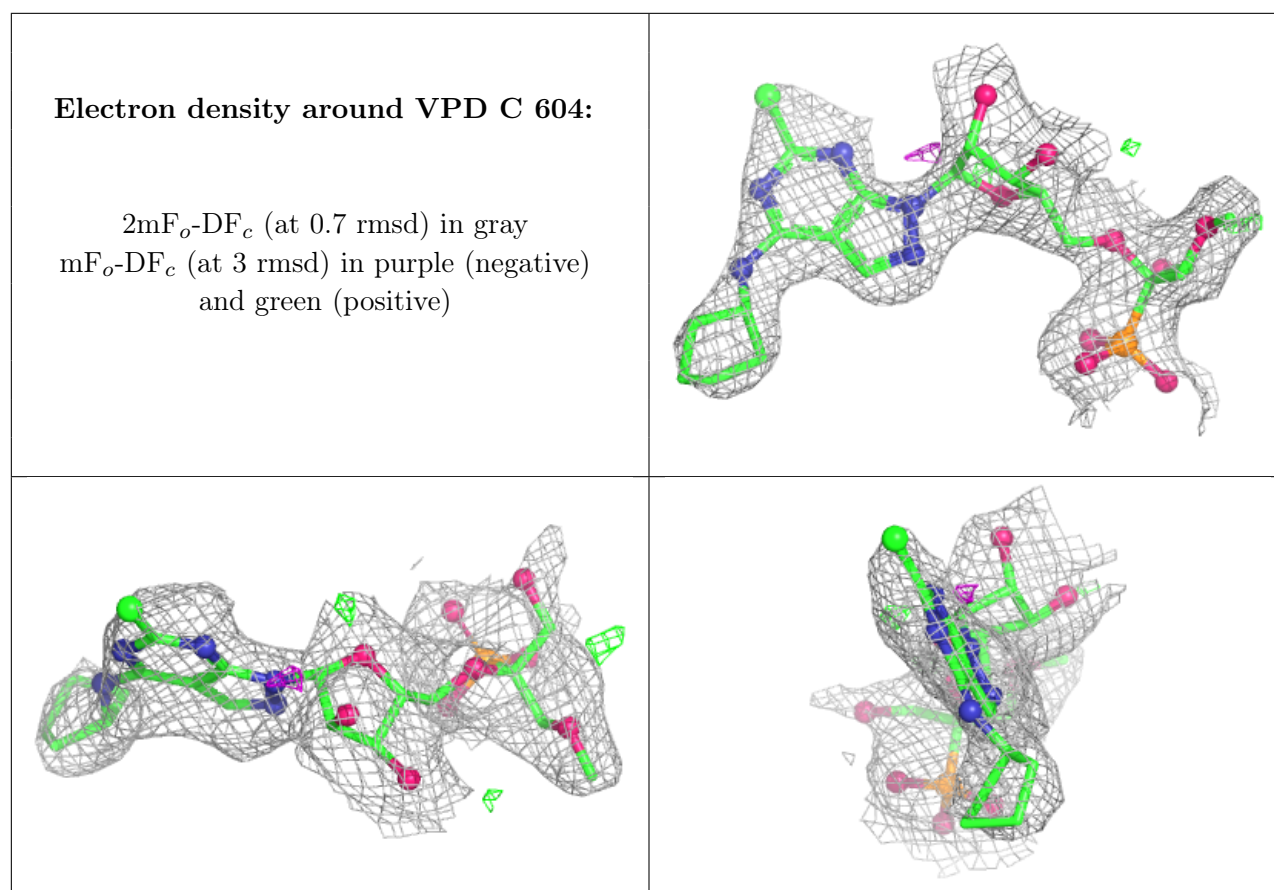
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	B	603	1/1	0.78	0.16	64,64,64,64	1
4	VPD	C	604	35/35	0.91	0.13	28,48,76,120	0

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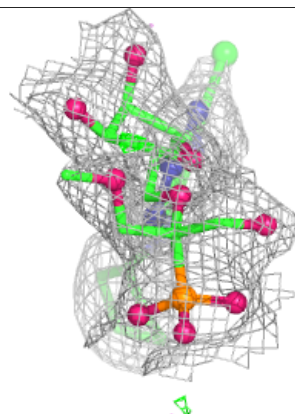
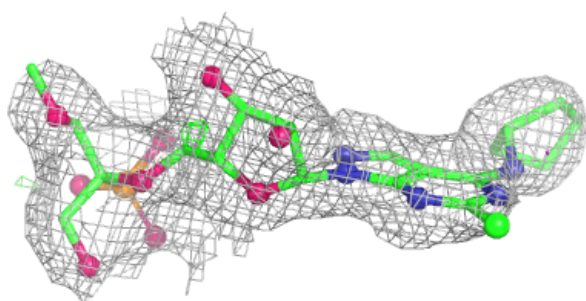
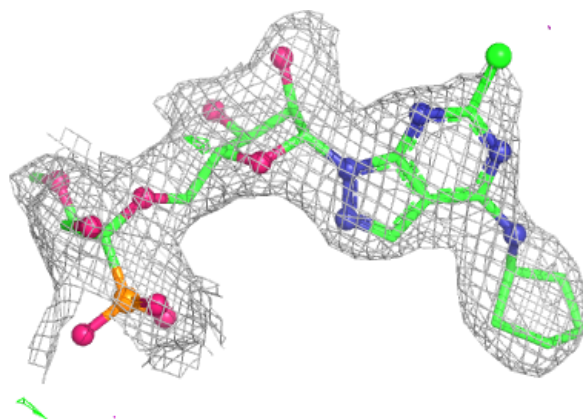
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	VPD	B	604	35/35	0.93	0.11	34,45,62,102	0
3	CA	D	603	1/1	0.94	0.08	36,36,36,36	1
4	VPD	D	604	35/35	0.94	0.08	21,29,45,71	0
4	VPD	A	604	35/35	0.96	0.08	15,26,35,73	0
2	ZN	B	601	1/1	0.96	0.04	47,47,47,47	0
2	ZN	B	602	1/1	0.97	0.04	41,41,41,41	0
2	ZN	C	601	1/1	0.98	0.04	52,52,52,52	0
2	ZN	C	602	1/1	0.98	0.03	38,38,38,38	0
3	CA	A	603	1/1	0.98	0.05	31,31,31,31	1
2	ZN	A	601	1/1	0.98	0.03	34,34,34,34	0
3	CA	C	603	1/1	0.98	0.03	28,28,28,28	1
2	ZN	D	602	1/1	0.99	0.02	29,29,29,29	0
2	ZN	A	602	1/1	0.99	0.02	25,25,25,25	0
2	ZN	D	601	1/1	0.99	0.04	36,36,36,36	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.

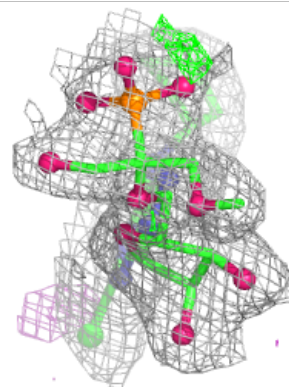
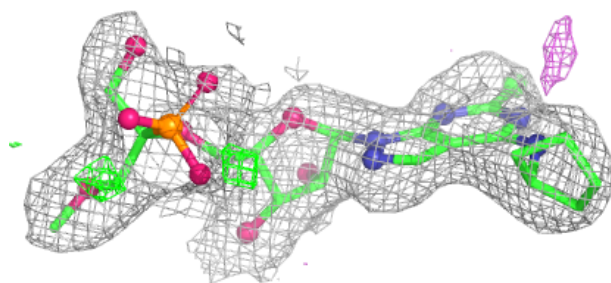
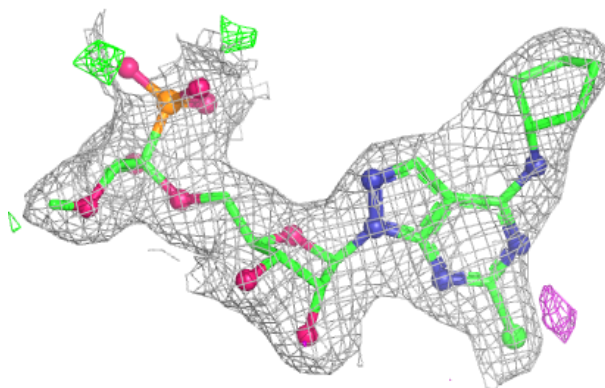


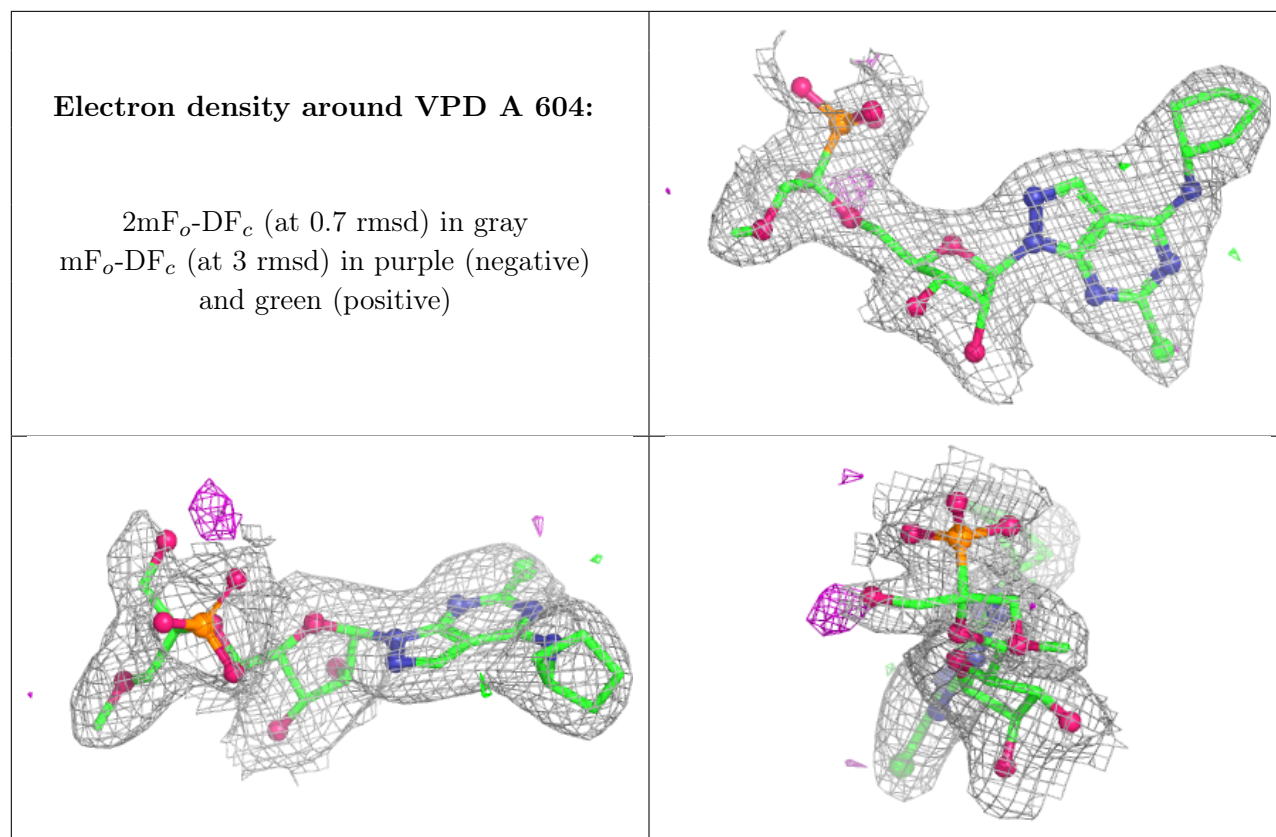
Electron density around VPD B 604:

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

**Electron density around VPD D 604:**

$2mF_o-DF_c$ (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.