



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:39 AM EDT

PDB ID : 2REX / pdb_00002rex
Title : Crystal structure of the effector domain of PLXNB1 bound with Rnd1 GTPase
Authors : Tong, Y.; Tempel, W.; Shen, L.; Arrowsmith, C.H.; Edwards, A.M.; Sundstrom, M.; Weigelt, J.; Bochkarev, A.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2007-09-27
Resolution : 2.30 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

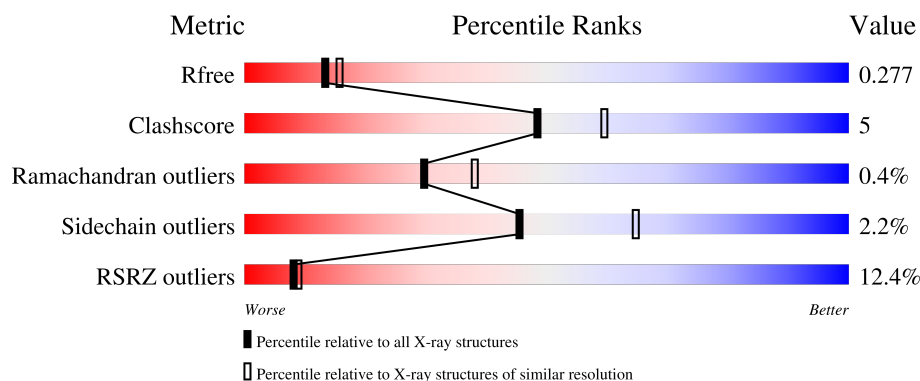
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	121	
1	C	121	
2	B	197	
2	D	197	

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	UNX	A	1	-	-	-	X
3	UNX	A	11	-	-	-	X
3	UNX	A	30	-	-	-	X
3	UNX	A	5	-	-	-	X
3	UNX	B	552	-	-	-	X
3	UNX	B	553	-	-	-	X
3	UNX	B	554	-	-	-	X
3	UNX	B	555	-	-	-	X
3	UNX	B	556	-	-	-	X
3	UNX	B	557	-	-	-	X
3	UNX	B	558	-	-	-	X
3	UNX	B	559	-	-	-	X
3	UNX	B	560	-	-	-	X
3	UNX	B	561	-	-	-	X
3	UNX	B	562	-	-	-	X
3	UNX	C	2	-	-	-	X
3	UNX	C	20	-	-	-	X
3	UNX	C	28	-	-	-	X
3	UNX	C	3	-	-	-	X
3	UNX	C	9	-	-	-	X
3	UNX	D	552	-	-	-	X
3	UNX	D	553	-	-	-	X
3	UNX	D	554	-	-	-	X
3	UNX	D	555	-	-	-	X
3	UNX	D	556	-	-	-	X
3	UNX	D	557	-	-	-	X
3	UNX	D	558	-	-	-	X
3	UNX	D	559	-	-	-	X
3	UNX	D	560	-	-	-	X
3	UNX	D	561	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4464 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 Plexin-B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	107	Total	C	N	O	S	0	0	0
			808	512	139	154	3			
1	C	107	Total	C	N	O	S	0	0	0
			806	511	139	153	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1742	GLY	-	expression tag	UNP O43157
C	1742	GLY	-	expression tag	UNP O43157

- Molecule 2 is a protein called Rho-related GTP-binding protein Rho6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	171	Total	C	N	O	S	0	2	0
			1310	834	209	252	15			
2	D	180	Total	C	N	O	S	0	2	0
			1367	876	217	259	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLY	-	expression tag	UNP Q92730
D	4	GLY	-	expression tag	UNP Q92730

- Molecule 3 is UNKNOWN ATOM OR ION (CCD ID: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	X	0	0
			4	4		
3	B	11	Total	X	0	0
			11	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	5	Total X 5 5	0	0
3	D	10	Total X 10 10	0	0

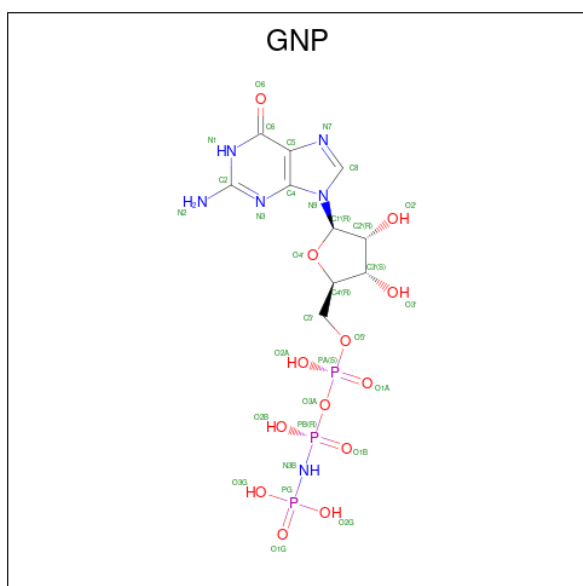
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
6	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

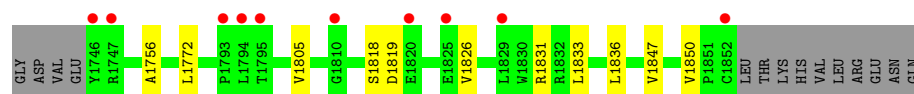
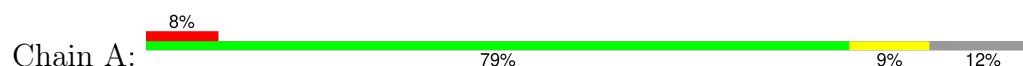
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	11	Total	O	0	0
			11	11		
7	B	24	Total	O	0	0
			24	24		
7	C	11	Total	O	0	0
			11	11		
7	D	29	Total	O	0	0
			29	29		

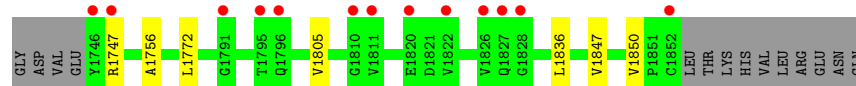
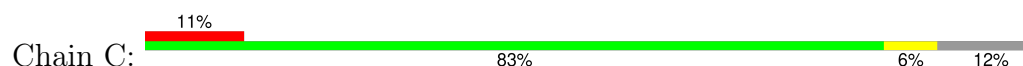
3 Residue-property plots

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.

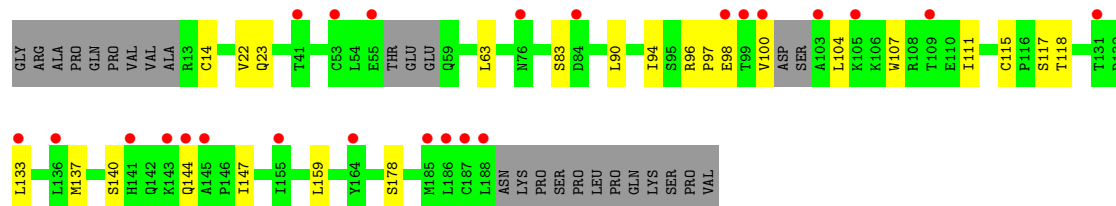
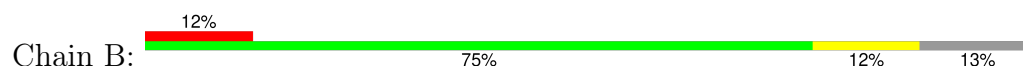
• Molecule 1: Plexin-B1



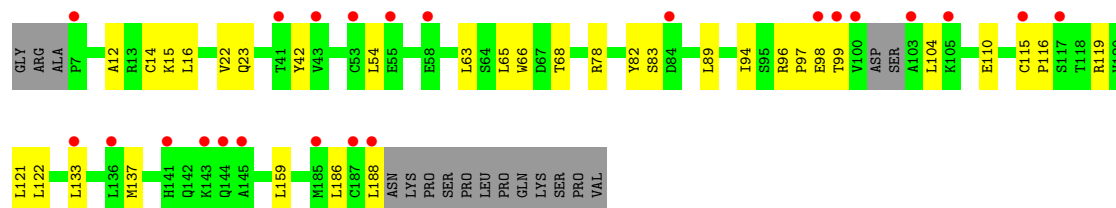
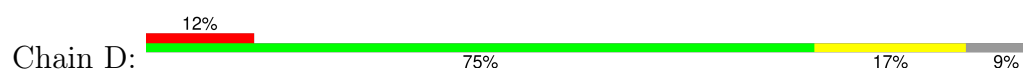
• Molecule 1: Plexin-B1



• Molecule 2: Rho-related GTP-binding protein Rho6



• Molecule 2: Rho-related GTP-binding protein Rho6



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.14Å 71.65Å 101.89Å 90.00° 128.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.30) 97.3 (20.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.248 0.258 , 0.277	Depositor DCC
R_{free} test set	999 reflections (2.64%)	wwPDB-VP
Wilson B-factor (Å ²)	37.9	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 77.6	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	0.91	EDS
Total number of atoms	4464	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% 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: UNX, MG, CA, GNP

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	0.92	0/824	0.83	0/1127
1	C	1.06	0/822	0.94	1/1125 (0.1%)
2	B	1.02	1/1338 (0.1%)	0.90	0/1818
2	D	1.07	1/1398 (0.1%)	0.90	0/1903
All	All	1.03	2/4382 (0.0%)	0.90	1/5973 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	22	VAL	CA-CB	7.52	1.61	1.54
2	B	22	VAL	CA-CB	5.63	1.59	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1747	ARG	N-CA-C	6.67	116.71	108.11

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	808	0	809	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	806	0	804	3	0
2	B	1310	0	1277	19	0
2	D	1367	0	1346	20	0
3	A	4	0	0	0	0
3	B	11	0	0	0	0
3	C	5	0	0	0	0
3	D	10	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	32	0	13	1	0
6	D	32	0	12	2	0
7	A	11	0	0	0	0
7	B	24	0	0	0	0
7	C	11	0	0	0	0
7	D	29	0	0	0	0
All	All	4464	0	4261	47	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 (47) 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)
2:B:133:LEU:HG	2:B:137:MET:HE2	1.61	0.82
2:B:115:CYS:SG	2:B:118:THR:HG21	2.24	0.77
2:D:104:LEU:HB3	2:D:159:LEU:HD11	1.66	0.76
2:D:23:GLN:H	6:D:500:GNP:HNB3	1.35	0.74
2:D:99:THR:O	2:D:104:LEU:HD13	1.97	0.64
2:B:115:CYS:SG	2:B:118:THR:CG2	2.85	0.64
2:B:90:LEU:HD11	2:B:104:LEU:CD2	2.27	0.63
2:D:54:LEU:HD13	2:D:63:LEU:HD12	1.82	0.62
2:D:96:ARG:C	2:D:98:GLU:H	2.09	0.61
1:A:1826:VAL:HG22	1:A:1831:ARG:HG2	1.85	0.58
2:B:23:GLN:H	6:B:500:GNP:HNB3	1.50	0.58
2:D:96:ARG:O	2:D:98:GLU:N	2.39	0.56
2:B:96:ARG:C	2:B:98:GLU:H	2.16	0.53
2:B:115:CYS:O	2:B:118:THR:HG22	2.11	0.51
1:C:1805:VAL:HG13	1:C:1847:VAL:CG1	2.40	0.51
2:B:90:LEU:HD11	2:B:104:LEU:HD23	1.91	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ARG:O	2:B:98:GLU:N	2.44	0.50
2:B:90:LEU:HD11	2:B:104:LEU:HD22	1.95	0.48
2:B:104:LEU:HB3	2:B:159:LEU:HD11	1.95	0.48
2:D:14[B]:CYS:HB3	2:D:63:LEU:HD23	1.96	0.47
2:B:14[B]:CYS:HB3	2:B:63:LEU:HD23	1.95	0.47
1:A:1819:ASP:HB3	1:A:1833:LEU:HD22	1.97	0.46
2:D:16:LEU:HB2	2:D:65:LEU:HD23	1.98	0.46
2:D:68:THR:HB	2:D:78:ARG:HG3	1.98	0.45
2:B:90:LEU:HG	2:B:104:LEU:HD22	1.98	0.45
2:D:133:LEU:HG	2:D:137:MET:HE2	1.99	0.45
1:A:1772:LEU:O	1:A:1836:LEU:HD12	2.16	0.45
2:B:96:ARG:C	2:B:98:GLU:N	2.76	0.44
2:D:104:LEU:HB3	2:D:159:LEU:CD1	2.42	0.43
2:D:15:LYS:HE3	2:D:66:TRP:CD1	2.54	0.43
2:B:90:LEU:HD13	2:B:107:TRP:HB3	2.01	0.43
1:A:1756:ALA:HB3	1:A:1850:VAL:HG12	2.01	0.42
1:C:1756:ALA:HB3	1:C:1850:VAL:HG12	2.01	0.42
2:D:42:TYR:OH	6:D:500:GNP:O2G	2.30	0.42
2:B:90:LEU:CG	2:B:104:LEU:HD22	2.50	0.42
1:C:1772:LEU:O	1:C:1836:LEU:HD12	2.20	0.42
2:D:96:ARG:C	2:D:98:GLU:N	2.73	0.42
1:A:1805:VAL:HG13	1:A:1847:VAL:CG1	2.51	0.41
2:D:121:LEU:HD23	2:D:121:LEU:N	2.36	0.41
2:B:100:VAL:HG21	2:B:147:ILE:HG13	2.03	0.41
2:D:12:ALA:HB3	2:D:188:LEU:HD11	2.02	0.41
2:D:82:TYR:OH	2:D:110:GLU:OE2	2.33	0.41
2:D:119:ARG:NH2	2:D:186:LEU:O	2.54	0.41
2:B:90:LEU:CD1	2:B:104:LEU:HD22	2.51	0.40
2:D:104:LEU:HD21	2:D:122:LEU:HD11	2.04	0.40
2:D:115:CYS:N	2:D:116:PRO:CD	2.84	0.40
2:B:111:ILE:O	2:B:115:CYS:HB3	2.21	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	105/121 (87%)	104 (99%)	1 (1%)	0	100	100
1	C	105/121 (87%)	103 (98%)	2 (2%)	0	100	100
2	B	167/197 (85%)	160 (96%)	6 (4%)	1 (1%)	21	27
2	D	178/197 (90%)	169 (95%)	8 (4%)	1 (1%)	21	27
All	All	555/636 (87%)	536 (97%)	17 (3%)	2 (0%)	30	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	97	PRO
2	B	97	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	87/103 (84%)	86 (99%)	1 (1%)	65	81
1	C	86/103 (84%)	86 (100%)	0	100	100
2	B	144/176 (82%)	138 (96%)	6 (4%)	26	40
2	D	149/176 (85%)	146 (98%)	3 (2%)	48	67
All	All	466/558 (84%)	456 (98%)	10 (2%)	45	66

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1818	SER
2	B	83	SER
2	B	94	ILE
2	B	117	SER
2	B	140	SER
2	B	144	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	178	SER
2	D	83	SER
2	D	89	LEU
2	D	94	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1796	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 36 ligands modelled in this entry, 30 are unknown and 4 are monoatomic - leaving 2 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
6	GNP	B	500	4	34,34,34	1.53	5 (14%)	47,54,54	1.44	4 (8%)
6	GNP	D	500	4	34,34,34	1.71	6 (17%)	47,54,54	1.06	3 (6%)

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
6	GNP	B	500	4	-	2/18/38/38	0/3/3/3
6	GNP	D	500	4	-	3/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	500	GNP	PB-O2B	-4.35	1.45	1.56
6	B	500	GNP	PG-O1G	4.12	1.52	1.46
6	D	500	GNP	PG-O1G	3.96	1.52	1.46
6	D	500	GNP	PB-O2B	-3.92	1.46	1.56
6	D	500	GNP	PB-O3A	-3.79	1.54	1.59
6	D	500	GNP	PA-O3A	-3.53	1.55	1.59
6	D	500	GNP	O3'-C3'	-3.51	1.34	1.43
6	B	500	GNP	PG-O2G	-3.38	1.47	1.56
6	D	500	GNP	PG-O3G	-3.24	1.48	1.56
6	B	500	GNP	PB-N3B	-2.94	1.55	1.63
6	B	500	GNP	PB-O3A	-2.08	1.56	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	500	GNP	O1G-PG-N3B	-7.41	100.86	111.77
6	D	500	GNP	O2B-PB-O1B	3.24	116.82	109.87
6	D	500	GNP	O3G-PG-O1G	-3.21	105.39	113.45
6	D	500	GNP	O2A-PA-O3A	2.99	115.34	107.27
6	B	500	GNP	O3G-PG-O1G	-2.83	106.36	113.45
6	B	500	GNP	O2G-PG-O3G	2.70	114.85	107.59
6	B	500	GNP	O2A-PA-O3A	2.65	114.43	107.27

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	500	GNP	PA-O3A-PB-O2B
6	D	500	GNP	PB-N3B-PG-O1G
6	D	500	GNP	PA-O3A-PB-O2B
6	B	500	GNP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

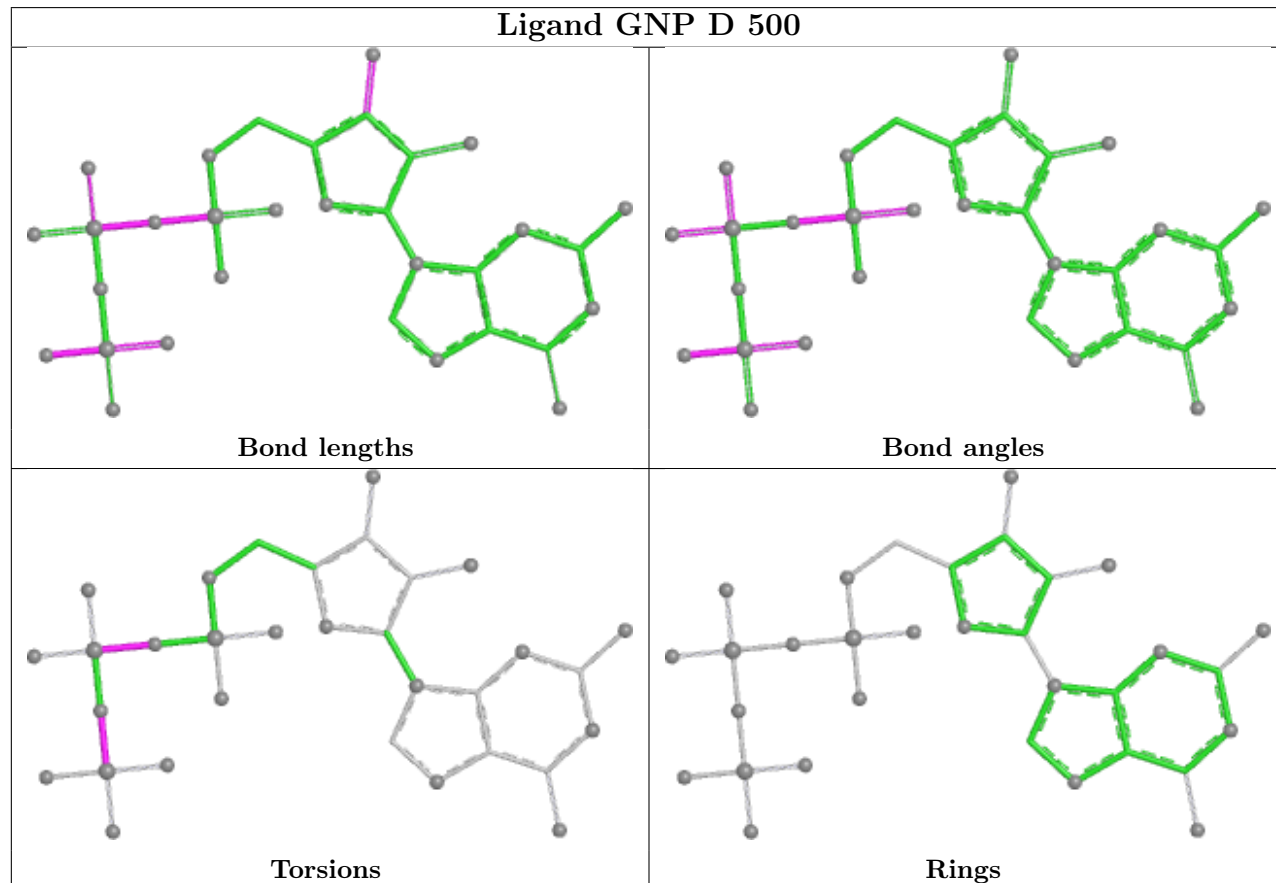
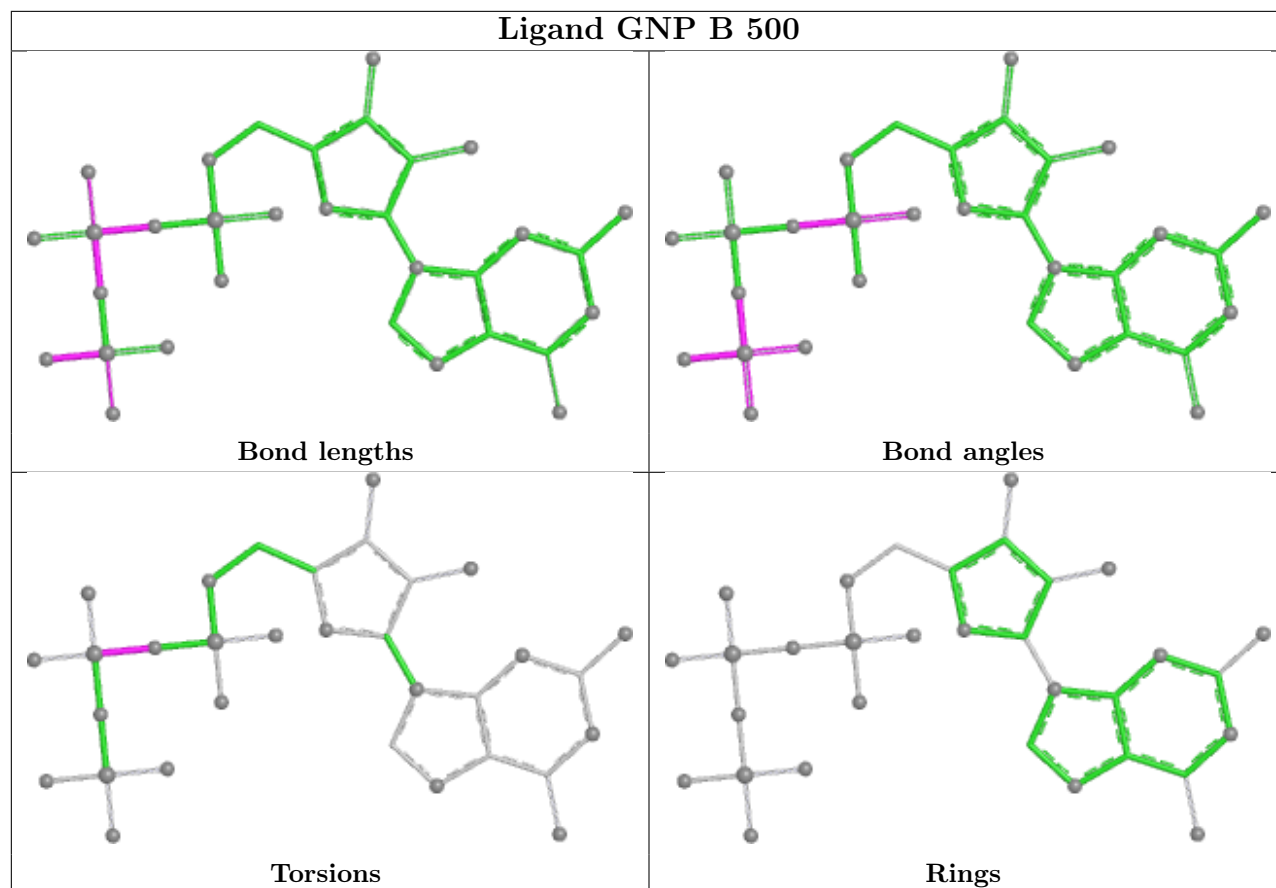
Mol	Chain	Res	Type	Atoms
6	D	500	GNP	PA-O3A-PB-O1B

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	500	GNP	1	0
6	D	500	GNP	2	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	107/121 (88%)	0.83	10 (9%) 14 16	28, 35, 41, 47	0
1	C	107/121 (88%)	0.95	13 (12%) 8 9	30, 34, 40, 48	0
2	B	171/197 (86%)	0.91	24 (14%) 6 7	26, 35, 42, 45	2 (1%)
2	D	180/197 (91%)	0.81	23 (12%) 7 8	23, 34, 44, 46	2 (1%)
All	All	565/636 (88%)	0.87	70 (12%) 8 9	23, 34, 42, 48	4 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	99	THR	5.0
2	B	145	ALA	4.4
2	B	99	THR	4.3
2	D	7	PRO	4.2
2	B	187[A]	CYS	3.9
2	B	105	LYS	3.9
2	D	133	LEU	3.8
1	C	1747	ARG	3.8
2	B	185	MET	3.7
2	D	105	LYS	3.7
2	B	188	LEU	3.4
1	C	1746	TYR	3.3
2	D	100	VAL	3.3
2	D	141	HIS	3.2
2	B	84	ASP	3.1
2	D	115	CYS	3.0
1	A	1820	GLU	3.0
2	D	98	GLU	3.0
1	C	1852	CYS	2.9
2	D	145	ALA	2.9
1	A	1747	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	84	ASP	2.8
2	D	117	SER	2.7
2	B	98	GLU	2.7
1	A	1852	CYS	2.7
1	A	1746	TYR	2.6
2	D	188	LEU	2.6
2	D	187[A]	CYS	2.6
2	D	144	GLN	2.5
2	B	186	LEU	2.5
1	C	1828	GLY	2.5
2	D	58	GLU	2.4
1	C	1826	VAL	2.4
1	C	1796	GLN	2.4
1	C	1791	GLY	2.4
1	C	1822	VAL	2.4
2	B	133	LEU	2.4
2	D	136	LEU	2.4
1	C	1810	GLY	2.3
2	B	131	THR	2.3
2	B	55	GLU	2.3
2	D	185	MET	2.3
1	C	1820	GLU	2.3
1	A	1794	LEU	2.3
2	B	164	TYR	2.3
2	D	41	THR	2.3
2	B	141	HIS	2.3
1	C	1811	VAL	2.3
2	B	136	LEU	2.3
2	B	109	THR	2.3
2	D	143	LYS	2.3
2	B	100	VAL	2.3
2	B	53	CYS	2.2
1	A	1810	GLY	2.2
2	B	41	THR	2.2
2	B	144	GLN	2.2
2	D	55	GLU	2.2
2	D	103	ALA	2.2
1	A	1829	LEU	2.2
2	B	76	ASN	2.2
1	A	1793	PRO	2.2
2	D	43	VAL	2.1
1	C	1827	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1825	GLU	2.1
2	B	155	ILE	2.1
2	D	53	CYS	2.1
2	B	143	LYS	2.0
1	A	1795	THR	2.0
2	B	103	ALA	2.0
1	C	1795	THR	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	UNX	B	562	1/1	-0.66	1.14	2,2,2,2	1
3	UNX	B	559	1/1	-0.59	1.89	2,2,2,2	1
3	UNX	B	555	1/1	-0.04	1.73	2,2,2,2	1
3	UNX	D	553	1/1	0.04	1.79	2,2,2,2	1
3	UNX	C	28	1/1	0.06	1.81	2,2,2,2	1
3	UNX	D	552	1/1	0.15	1.42	2,2,2,2	1
3	UNX	B	556	1/1	0.17	2.37	38,38,38,38	1
3	UNX	C	3	1/1	0.27	1.34	2,2,2,2	1
3	UNX	D	554	1/1	0.35	1.41	2,2,2,2	1
3	UNX	D	556	1/1	0.42	1.71	2,2,2,2	1
3	UNX	B	561	1/1	0.43	3.02	2,2,2,2	1
3	UNX	B	553	1/1	0.45	1.48	2,2,2,2	1
3	UNX	B	557	1/1	0.46	1.83	2,2,2,2	1
3	UNX	A	1	1/1	0.46	1.58	2,2,2,2	1
3	UNX	C	20	1/1	0.47	1.94	2,2,2,2	1

Continued on next page...

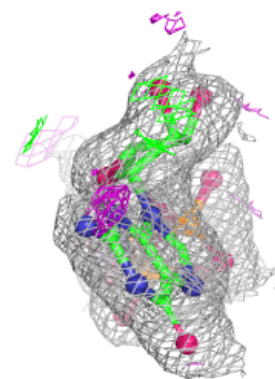
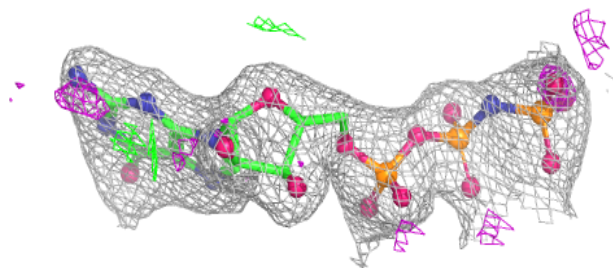
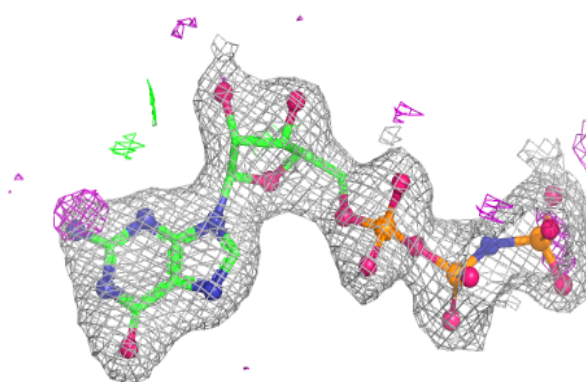
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UNX	D	559	1/1	0.47	1.93	2,2,2,2	1
3	UNX	B	554	1/1	0.52	2.33	2,2,2,2	1
3	UNX	D	558	1/1	0.53	1.13	2,2,2,2	1
3	UNX	D	561	1/1	0.53	2.27	2,2,2,2	1
3	UNX	C	9	1/1	0.55	2.21	2,2,2,2	1
3	UNX	D	560	1/1	0.56	1.68	2,2,2,2	1
3	UNX	A	30	1/1	0.59	2.17	2,2,2,2	1
3	UNX	B	558	1/1	0.60	1.26	2,2,2,2	1
3	UNX	C	2	1/1	0.60	1.97	2,2,2,2	1
3	UNX	B	552	1/1	0.61	1.62	2,2,2,2	1
3	UNX	B	560	1/1	0.63	1.68	13,13,13,13	1
3	UNX	D	557	1/1	0.65	1.18	15,15,15,15	1
3	UNX	A	11	1/1	0.66	2.16	2,2,2,2	1
3	UNX	A	5	1/1	0.70	1.57	2,2,2,2	1
3	UNX	D	555	1/1	0.71	1.90	2,2,2,2	1
4	MG	D	550	1/1	0.91	0.07	36,36,36,36	0
5	CA	D	551	1/1	0.97	0.10	32,32,32,32	0
6	GNP	D	500	32/32	0.97	0.07	28,31,33,34	0
4	MG	B	550	1/1	0.98	0.04	36,36,36,36	0
6	GNP	B	500	32/32	0.98	0.07	29,31,35,39	0
5	CA	B	551	1/1	0.98	0.08	30,30,30,30	0

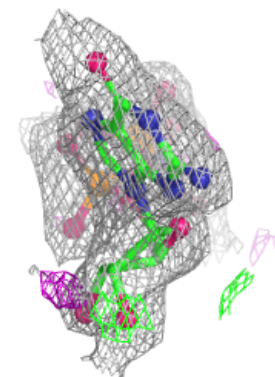
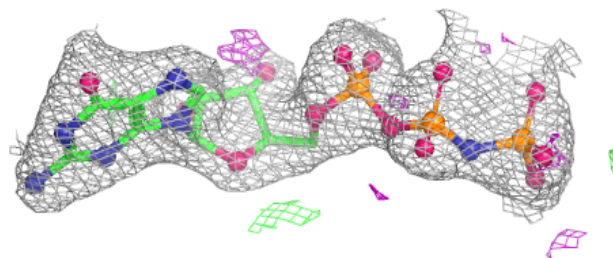
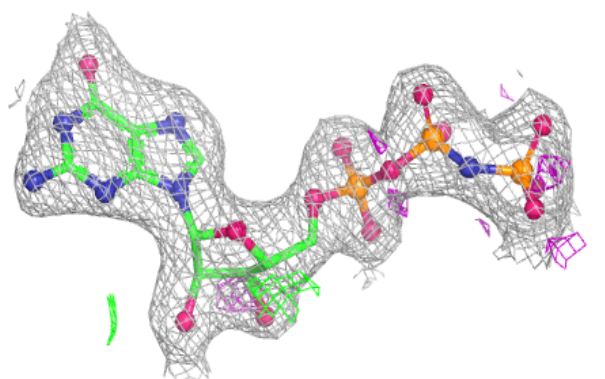
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP D 500:

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

**Electron density around GNP B 500:**

$2mF_o-DF_c$ (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.