

Full wwPDB X-ray Structure Validation Report (i)

Sep 25, 2023 – 07:25 AM EDT

PDB ID : 5WFP

Title : Ligand-bound Ras:SOS:Ras complex

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Deposited on : 2017-07-12

Resolution : 2.08 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 (i) 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 (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : 2.35.1

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

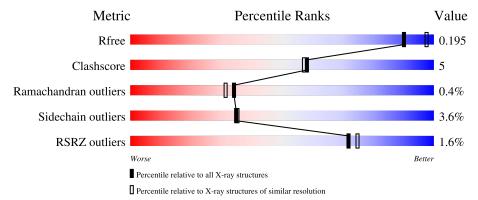
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	Similar resolution
Metric	$(\# ext{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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 <=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	0	1.05	%		_				
1	Q	167	87%	10%	••				
			4%						
1	\mathbf{R}	167	87%	11%	••				
			<u>%</u>						
2	N	482	86%	9% ••	•				



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7380 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 GTPase HRas.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Q	166	Total 1340			O 266	S 7	0	3	0
1	R	167	Total 1327	C 826		O 265	S 7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	0	GLY	-	expression tag	UNP P01112
R	0	GLY	-	expression tag	UNP P01112

• Molecule 2 is a protein called Son of sevenless homolog 1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	N	468	Total 3884	C 2493	N 670	O 708	S 13	0	0	0

There is a discrepancy between the modelled and reference sequences:

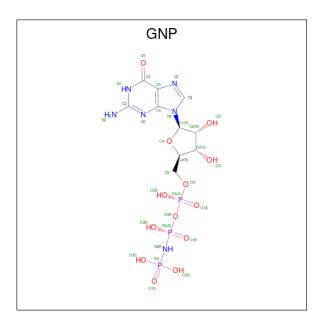
Chain	Residue	Modelled	Actual	Comment	Reference
N	565	GLY	-	expression tag	UNP Q07889

• Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	Q	1	Total Mg	0	0

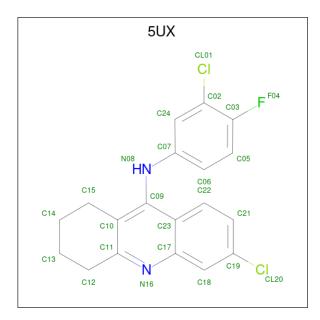
• Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).





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

• Molecule 5 is 6-chloranyl- $\{N\}$ -(3-chloranyl-4-fluoranyl-phenyl)-1,2,3,4-tetrahydroacridin-9-amine (three-letter code: 5UX) (formula: $C_{19}H_{15}Cl_2FN_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
5	N	1	Total 24	C 19	Cl 2	F 1	N 2	0	0

• Molecule 6 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Q	132	Total O 132 132	0	0
6	R	159	Total O 159 159	0	0
6	N	481	Total O 481 481	0	0



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.



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants	182.53Å 182.53Å 177.31Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 - 2.08	Depositor
Resolution (A)	48.68 - 2.08	EDS
% Data completeness	99.9 (48.68-2.08)	Depositor
(in resolution range)	99.9 (48.68-2.08)	EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.03 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
D.D.	0.162 , 0.203	Depositor
R, R_{free}	0.174 , 0.195	DCC
R_{free} test set	1988 reflections (2.22%)	wwPDB-VP
Wilson B-factor (Å ²)	26.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.37, 53.0	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.33$	Xtriage
Estimated twinning fraction	0.008 for l,-k,h	Xtriage
Estimated twinning fraction	0.011 for -h,-l,-k	Alliage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7380	wwPDB-VP
Average B, all atoms (\mathring{A}^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.

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



¹Intensities estimated from amplitudes.

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: GNP, MG, 5UX

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		
IVIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	Q	0.42	0/1364	0.54	0/1838	
1	R	0.44	0/1346	0.56	1/1815 (0.1%)	
2	N	0.42	0/3977	0.55	3/5378 (0.1%)	
All	All	0.42	0/6687	0.55	4/9031 (0.0%)	

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$Observed(^o)$	$Ideal(^{o})$
2	N	647	ARG	NE-CZ-NH2	-8.28	116.16	120.30
2	N	647	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	R	26	ASN	N-CA-C	-5.98	94.86	111.00
2	N	754	PHE	C-N-CA	5.51	135.47	121.70

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	Q	1340	0	1316	14	0
1	R	1327	0	1299	16	0
2	N	3884	0	3908	36	0
3	Q	1	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Q	32	0	13	0	0
5	N	24	0	0	1	0
6	N	481	0	0	9	4
6	Q	132	0	0	4	2
6	R	159	0	0	4	0
All	All	7380	0	6536	63	4

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 (63) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
1:R:26:ASN:HD21	1:R:29:VAL:HB	1.00	1.17
2:N:755:GLN:O	2:N:756:SER:OG	1.79	0.98
1:R:26:ASN:ND2	1:R:29:VAL:HB	1.78	0.97
1:R:26:ASN:HD21	1:R:29:VAL:CB	1.82	0.93
1:Q:51:CYS:SG	1:Q:164:ARG:NH2	2.43	0.92
1:R:27:HIS:CE1	1:R:149:ARG:NH2	2.42	0.88
1:R:27:HIS:CE1	1:R:149:ARG:HH21	1.92	0.86
2:N:1041:ARG:HD2	6:N:1207:HOH:O	1.83	0.78
2:N:988:LYS:NZ	6:N:1202:HOH:O	2.21	0.72
1:R:21:ILE:O	1:R:25:GLN:HB2	1.91	0.70
2:N:751:ASN:N	6:N:1204:HOH:O	2.24	0.70
2:N:620:ASP:OD1	6:N:1201:HOH:O	2.09	0.70
2:N:899:LYS:NZ	6:N:1208:HOH:O	2.26	0.68
2:N:751:ASN:ND2	6:N:1209:HOH:O	2.28	0.67
1:Q:67:MET:HE2	6:Q:301:HOH:O	1.95	0.65
2:N:576:ARG:HD3	2:N:646:GLU:OE2	1.96	0.65
1:R:166:HIS:HD2	6:R:334:HOH:O	1.78	0.64
1:R:147:LYS:HG3	6:R:269:HOH:O	2.01	0.61
2:N:920:ARG:NH2	6:N:1214:HOH:O	2.33	0.61
1:R:28:PHE:O	6:R:201:HOH:O	2.16	0.60
2:N:755:GLN:O	2:N:756:SER:CB	2.50	0.60
2:N:614:THR:OG1	2:N:647:ARG:HD3	2.01	0.60
2:N:606:VAL:HG22	2:N:956:ILE:HD11	1.83	0.60
2:N:831:LEU:HD12	2:N:873:GLU:OE1	2.02	0.60
2:N:847:GLU:HG2	2:N:1035:LEU:HD11	1.87	0.56
2:N:912:TYR:CG	2:N:932:ILE:HD11	2.41	0.55
2:N:755:GLN:C	2:N:756:SER:OG	2.45	0.53
2:N:587:ILE:HD11	2:N:950:ARG:HG3	1.92	0.52

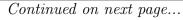


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A toma 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${\rm distance}({\rm \AA})$	overlap (Å)
1:Q:37:GLU:OE1	6:Q:301:HOH:O	2.19	0.51
2:N:615:TYR:CE2	2:N:617:MET:HG3	2.46	0.50
1:R:38:ASP:N	6:R:202:HOH:O	2.28	0.50
1:Q:37:GLU:HG3	2:N:621:PRO:HG3	1.92	0.49
1:R:85:ASN:ND2	1:R:119:ASP:OD1	2.45	0.49
1:R:33:ASP:OD1	1:R:35:THR:HB	2.12	0.49
2:N:831:LEU:HD13	2:N:835:PHE:CE2	2.47	0.49
2:N:755:GLN:HE21	2:N:755:GLN:HA	1.78	0.48
1:Q:70:GLN:O	6:Q:302:HOH:O	2.20	0.48
1:Q:31:GLU:H	1:Q:31:GLU:CD	2.17	0.47
1:R:37:GLU:O	1:R:38:ASP:HB3	2.13	0.47
1:Q:68:ARG:HA	1:Q:71:TYR:CE2	2.50	0.46
1:R:105:ASP:OD1	2:N:1019:ARG:NH2	2.42	0.46
2:N:859:LEU:HD11	2:N:871:VAL:HG13	1.97	0.46
1:Q:29:VAL:HG13	1:Q:31:GLU:OE1	2.16	0.46
1:Q:37:GLU:HG2	2:N:691:ASN:ND2	2.31	0.46
1:Q:148:THR:O	1:Q:149:ARG:HB2	2.15	0.46
1:Q:61:GLN:HG2	6:Q:332:HOH:O	2.16	0.45
2:N:577:PHE:HE2	2:N:646:GLU:HG2	1.82	0.45
2:N:788:LEU:HD13	2:N:831:LEU:HD11	1.98	0.44
2:N:647:ARG:NH2	2:N:681:TYR:OH	2.50	0.44
2:N:905:HIS:HB2	5:N:1101:5UX:CL20	2.55	0.43
1:R:26:ASN:HD21	1:R:29:VAL:CA	2.30	0.43
1:Q:56:LEU:HD23	1:Q:71:TYR:HB2	2.00	0.43
1:R:118:CYS:HA	1:R:146:ALA:HB3	2.01	0.43
2:N:764:HIS:CG	2:N:765:ILE:H	2.37	0.43
2:N:721:VAL:HB	2:N:730:VAL:HG21	2.01	0.42
2:N:906:GLU:OE1	6:N:1203:HOH:O	2.22	0.42
1:Q:94:HIS:O	1:Q:98:GLU:HG2	2.19	0.42
2:N:807:SER:HA	2:N:809:TRP:CZ3	2.55	0.41
2:N:754:PHE:HA	2:N:755:GLN:HB2	2.01	0.41
1:Q:97[A]:ARG:HG3	1:Q:137:TYR:CE2	2.56	0.41
2:N:764:HIS:CG	2:N:765:ILE:N	2.89	0.40
2:N:606:VAL:HG23	6:N:1511:HOH:O	2.21	0.40
2:N:941:GLU:HA	2:N:960:LYS:HE3	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
6:N:1601:HOH:O	6:N:1601:HOH:O[7_556]	1.91	0.29





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Atom-1	Atom-2	$egin{aligned} ext{Interatomic} \ ext{distance} & (ext{Å}) \end{aligned}$	Clash overlap (Å)
6:Q:390:HOH:O	6:N:1208:HOH:O[16_555]	2.01	0.19
6:Q:420:HOH:O	6:N:1590:HOH:O[16_555]	2.01	0.19
6:N:1630:HOH:O	6:N:1632:HOH:O[7_556]	2.09	0.11

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	Perce	ntiles
1	Q	167/167 (100%)	163 (98%)	4 (2%)	0	100	100
1	R	165/167 (99%)	158 (96%)	6 (4%)	1 (1%)	25	20
2	N	462/482 (96%)	454 (98%)	6 (1%)	2 (0%)	34	31
All	All	794/816 (97%)	775 (98%)	16 (2%)	3 (0%)	34	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	756	SER
2	N	755	GLN
1	R	38	ASP

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	Percei	ntiles
1	Q	146/144 (101%)	139 (95%)	7 (5%)	25	23



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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	R	144/144 (100%)	138 (96%)	6 (4%)	30 29
2	N	437/447 (98%)	423 (97%)	14 (3%)	39 40
All	All	727/735 (99%)	700 (96%)	27 (4%)	35 34

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Q	30	ASP TYR
1	Q	32	TYR
1	Q	79	LEU
1	Q	94	HIS
1	Q	97[A]	ARG
1	Q Q Q Q Q Q Q	97[B]	ARG
1	Q	164	ARG ASN
1	R	26	ASN
1	R	35	THR ASP
1	R	38	
1	R	53	LEU
1	R	68	ARG
1	R	76	GLU
2	N	571	SER
2	N	617	MET
2 2 2	N	647	ARG
2	N	716 722	GLU ARG
2	N	722	ARG
2	N	755	GLN
2	N	756	SER
2	N	772	GLU
2	N	831	LEU
2	N	895	SER
2 2 2 2	N	896	ARG
2	N	930	PHE
2	N	1006	THR

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	R	26	ASN
1	R	27	HIS



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Mol	Chain	Res	Type
2	N	751	ASN
2	N	755	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is 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	Trimo	Type Chain	Chain Res	Link	Bond lengths			Bond angles		
MIOI	Type		nes	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	$\mid \# Z > 2$
4	GNP	Q	202	3	29,34,34	1.63	6 (20%)	33,54,54	2.18	8 (24%)
5	5UX	N	1101	-	27,27,27	1.82	8 (29%)	35,39,39	1.53	7 (20%)

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.

\mathbf{Mol}	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GNP	Q	202	3	-	3/14/38/38	0/3/3/3
5	5UX	N	1101	-	-	0/4/11/11	0/4/4/4



All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
5	N	1101	5UX	C09-C23	-4.37	1.35	1.43
4	Q	202	GNP	PB-O3A	-4.16	1.53	1.59
4	Q	202	GNP	C6-N1	3.67	1.39	1.33
4	Q	202	GNP	PB-O2B	-3.41	1.47	1.56
4	Q	202	GNP	PG-O1G	3.19	1.51	1.46
5	N	1101	5UX	C02-C03	-3.09	1.34	1.38
5	N	1101	5UX	C22-C23	-2.90	1.36	1.42
5	N	1101	5UX	C23-C17	-2.78	1.37	1.42
5	N	1101	5UX	C18-C17	-2.49	1.38	1.41
4	Q	202	GNP	C8-N7	-2.42	1.30	1.34
5	N	1101	5UX	F04-C03	-2.32	1.29	1.35
4	Q	202	GNP	PG-O3G	-2.30	1.50	1.56
5	N	1101	5UX	C10-C11	-2.11	1.37	1.40
5	N	1101	5UX	C09-C10	-2.07	1.35	1.38

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
4	Q	202	GNP	C5-C6-N1	-8.26	112.14	123.43
5	N	1101	5UX	C10-C11-N16	-5.65	118.86	123.68
4	Q	202	GNP	C2-N1-C6	5.56	124.76	115.93
4	Q	202	GNP	O1G-PG-N3B	-3.14	107.14	111.77
4	Q	202	GNP	C2-N3-C4	-2.87	112.08	115.36
4	Q	202	GNP	O2B-PB-O1B	2.79	115.78	109.92
5	N	1101	5UX	C22-C23-C09	-2.69	119.94	124.78
4	Q	202	GNP	N3-C2-N1	-2.47	123.92	127.22
5	N	1101	5UX	C12-C11-N16	2.32	120.46	116.73
4	Q	202	GNP	C4-C5-C6	-2.30	118.60	120.80
4	Q	202	GNP	O1B-PB-N3B	-2.28	108.42	111.77
5	N	1101	5UX	C23-C17-N16	-2.16	120.52	122.81
5	N	1101	5UX	C24-C02-CL01	2.09	121.86	118.49
5	N	1101	5UX	C11-N16-C17	2.07	120.22	117.67
5	N	1101	5UX	C22-C23-C17	2.04	120.61	118.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	Q	202	GNP	PB-N3B-PG-O1G
4	Q	202	GNP	PG-N3B-PB-O1B
4	Q	202	GNP	PG-N3B-PB-O3A

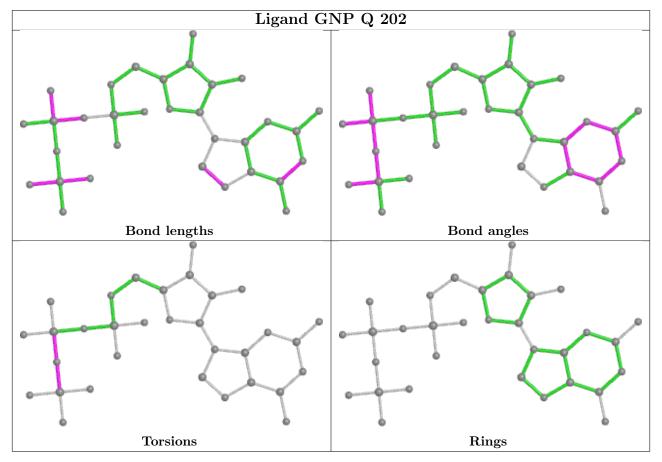


There are no ring outliers.

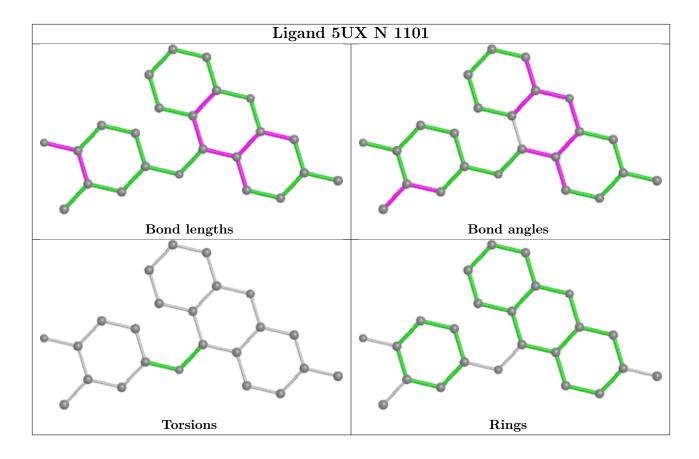
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	1101	5UX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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, 95^{th} 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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q<0.9
1	Q	166/167 (99%)	-0.48	2 (1%) 79 81	16, 23, 41, 51	0
1	R	167/167 (100%)	-0.20	6 (3%) 42 48	15, 27, 50, 67	0
2	N	468/482 (97%)	-0.48	5 (1%) 80 83	13, 23, 39, 58	0
All	All	801/816 (98%)	-0.42	13 (1%) 72 75	13, 23, 43, 67	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
1	R	0	GLY	7.4	
1	R	37	GLU	5.0	
1	R	38	ASP	4.1	
1	R	120	LEU	2.9	
1	Q	107	ASP	2.8	
2	N	724	LYS	2.8	
1	Q	71	TYR	2.7	
2	N	1021	PRO	2.6	
2	N	755	GLN	2.6	
2	N	751	ASN	2.4	
1	R	26	ASN	2.3	
2	N	743	ALA	2.0	
1	R	1	MET	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 monosaccharides in this entry.



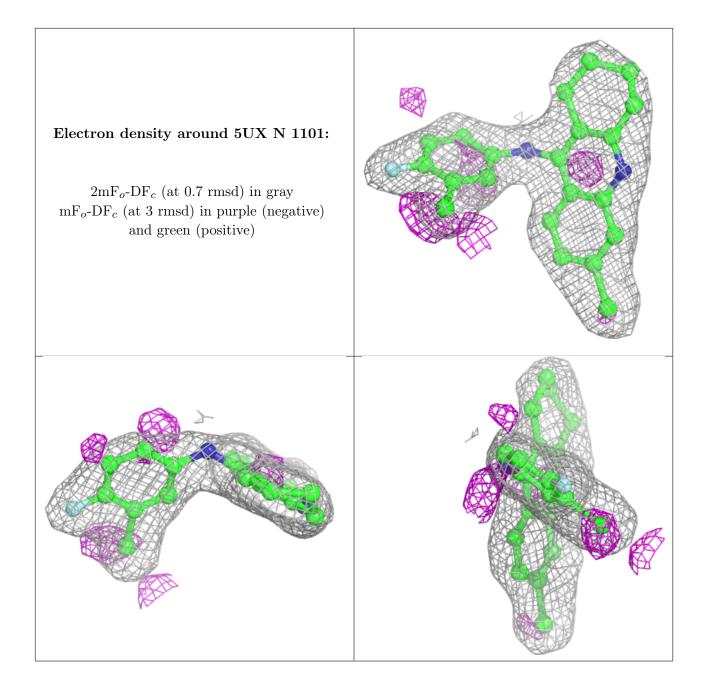
6.4 Ligands (i)

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, 95^{th} 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.

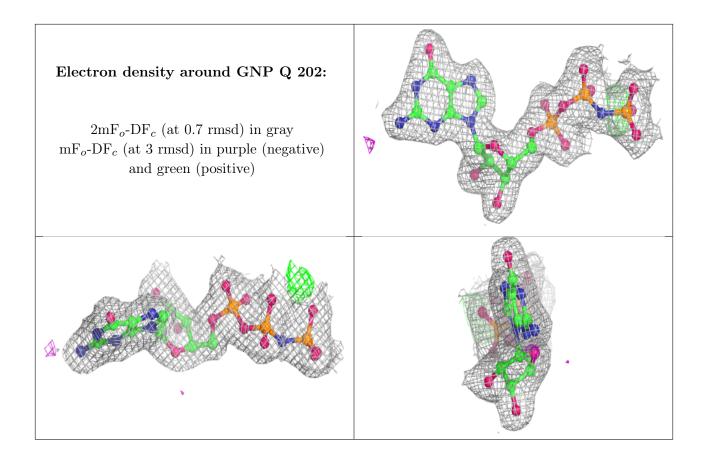
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	5UX	N	1101	24/24	0.96	0.14	25,32,39,48	0
4	GNP	Q	202	32/32	0.99	0.08	16,19,22,23	0
3	MG	Q	201	1/1	0.99	0.17	14,14,14,14	0

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









6.5 Other polymers (i)

There are no such residues in this entry.

