



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:57 AM UTC

PDB ID : 1NVV / pdb_00001nvv
Title : Structural evidence for feedback activation by RasGTP of the Ras-specific nucleotide exchange factor SOS
Authors : Margarit, S.M.; Sondermann, H.; Hall, B.E.; Nagar, B.; Hoelz, A.; Pirruccello, M.; Bar-Sagi, D.; Kuriyan, J.
Deposited on : 2003-02-04
Resolution : 2.18 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

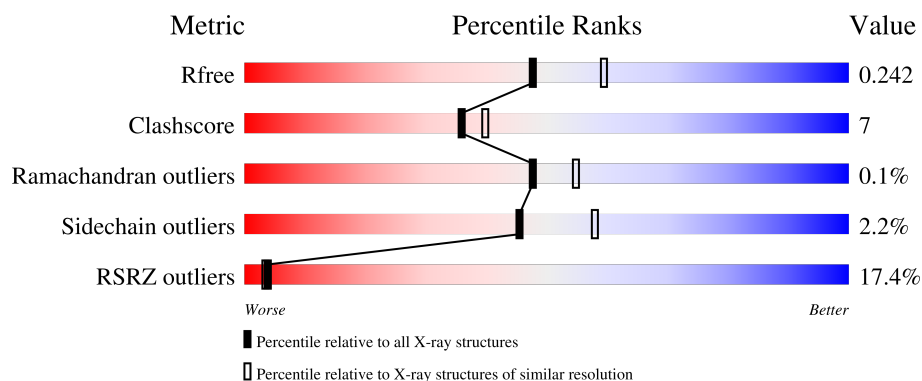
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	Q	166	23% 77% 22% .
2	R	166	17% 82% 17% .
3	S	481	15% 78% 18% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6908 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 Transforming protein p21/H-RAS-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	166	Total	C	N	O	S	0	0	0
			1316	818	228	263	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	64	ALA	TYR	engineered mutation	UNP P01112

- Molecule 2 is a protein called Transforming protein p21/H-RAS-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	166	Total	C	N	O	S	0	0	0
			1323	824	228	264	7			

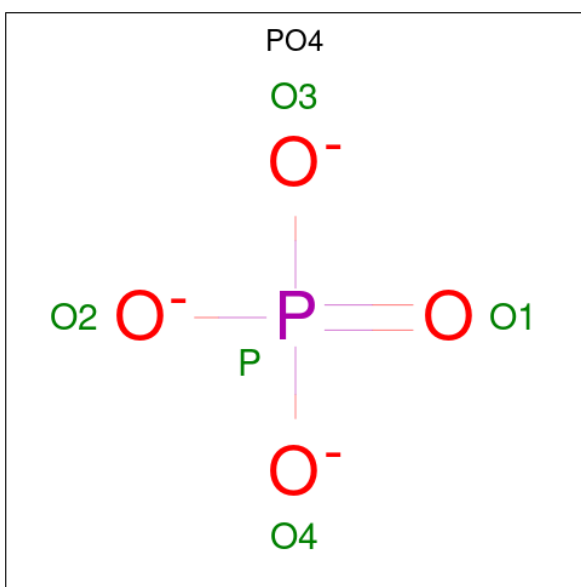
- Molecule 3 is a protein called Son of sevenless protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	469	Total	C	N	O	S	0	0	0
			3896	2499	673	711	13			

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

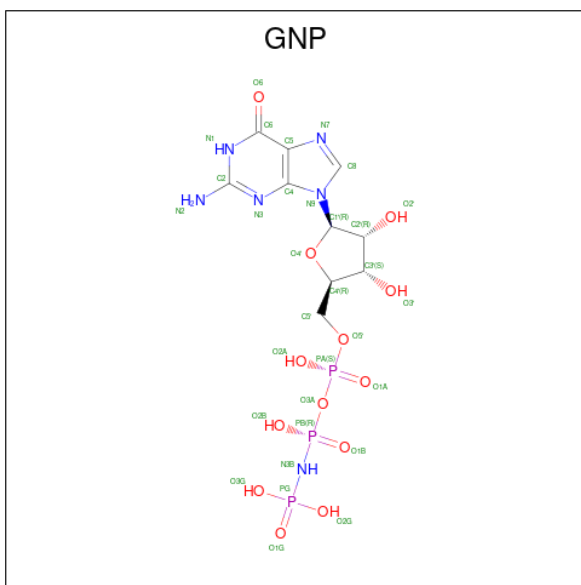
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	Q	1	Total	O	P	0	0
			5	4	1		
5	R	1	Total	O	P	0	0
			5	4	1		
5	S	1	Total	O	P	0	0
			5	4	1		
5	S	1	Total	O	P	0	0
			5	4	1		
5	S	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

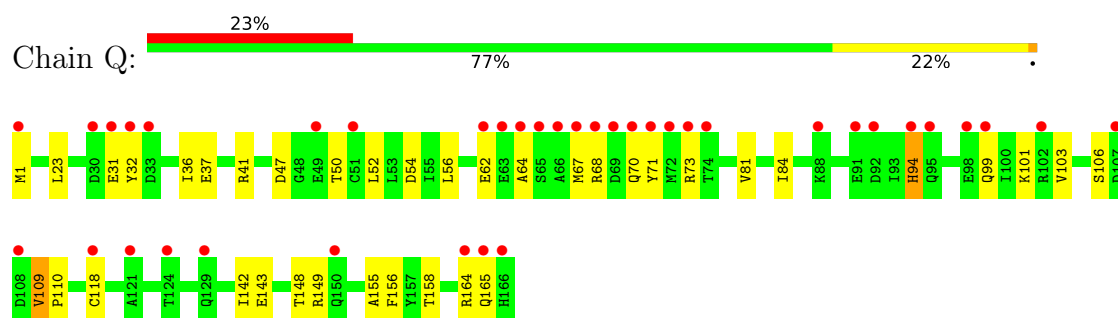
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	Q	38	Total O 38 38	0	0
7	R	54	Total O 54 54	0	0
7	S	223	Total O 223 223	0	0

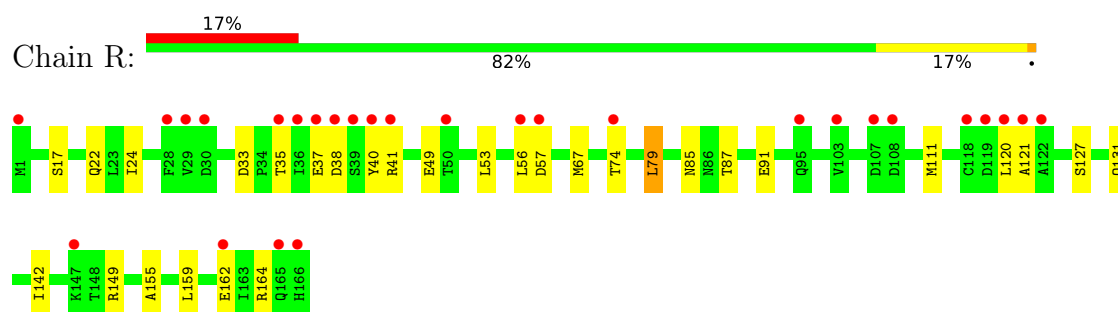
3 Residue-property plots [i](#)

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.

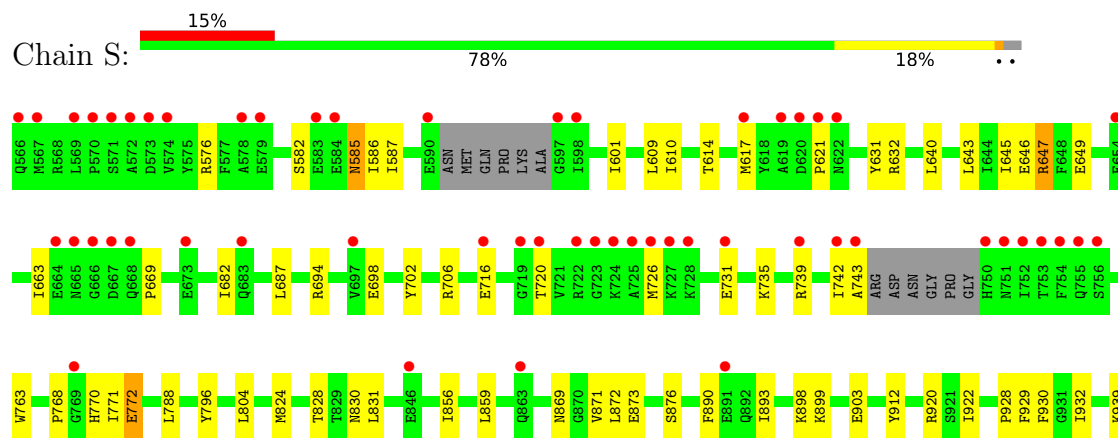
- Molecule 1: Transforming protein p21/H-RAS-1

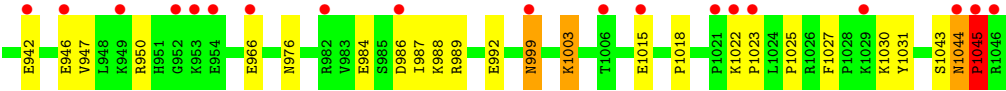


- Molecule 2: Transforming protein p21/H-RAS-1



- Molecule 3: Son of sevenless protein homolog 1





4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.16Å 184.16Å 179.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.19 – 2.18 64.19 – 2.18	Depositor EDS
% Data completeness (in resolution range)	90.8 (64.19-2.18) 90.8 (64.19-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.208 , 0.241 0.207 , 0.242	Depositor DCC
R_{free} test set	5164 reflections (6.63%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for l,-k,h 0.014 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6908	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GNP, PO4, MG

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	Q	0.51	0/1334	0.92	4/1799 (0.2%)
2	R	0.50	0/1342	0.90	1/1810 (0.1%)
3	S	0.53	0/3990	0.92	8/5397 (0.1%)
All	All	0.52	0/6666	0.91	13/9006 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	36	ILE	N-CA-C	-9.69	102.37	111.48
2	R	24	ILE	N-CA-C	8.56	119.42	111.45
3	S	1044	ASN	CA-C-N	6.59	128.08	119.84
3	S	1044	ASN	C-N-CA	6.59	128.08	119.84
3	S	631	TYR	N-CA-C	6.57	119.27	111.71
3	S	976	ASN	N-CA-C	6.52	119.71	111.69
1	Q	81	VAL	N-CA-C	6.51	118.42	108.71
3	S	682	ILE	N-CA-C	5.76	115.95	110.42
3	S	617	MET	N-CA-C	5.66	118.30	111.40
1	Q	109	VAL	N-CA-C	5.59	113.43	108.63
3	S	1044	ASN	N-CA-C	5.55	119.31	108.21
1	Q	158	THR	N-CA-C	-5.14	105.76	111.36
3	S	632	ARG	N-CA-C	5.05	118.55	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Q	1316	0	1290	25	0
2	R	1323	0	1296	19	0
3	S	3896	0	3915	59	0
4	Q	1	0	0	0	0
5	Q	5	0	0	0	0
5	R	5	0	0	0	0
5	S	15	0	0	0	0
6	Q	32	0	13	0	0
7	Q	38	0	0	0	0
7	R	54	0	0	0	0
7	S	223	0	0	1	0
All	All	6908	0	6514	96	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 7.

All (96) 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)
3:S:716:GLU:O	3:S:720:THR:HG23	1.72	0.89
1:Q:118:CYS:SG	1:Q:143:GLU:HB3	2.18	0.83
3:S:828:THR:HG23	3:S:873:GLU:HG2	1.60	0.82
3:S:576:ARG:HD3	3:S:646:GLU:OE2	1.78	0.82
3:S:587:ILE:HD11	3:S:950:ARG:HG3	1.63	0.80
3:S:824:MET:HE1	3:S:930:PHE:CD2	2.18	0.78
1:Q:31:GLU:HG3	3:S:739:ARG:NH1	2.00	0.75
3:S:946:GLU:HG3	3:S:947:VAL:HG13	1.66	0.75
3:S:1018:PRO:HB3	3:S:1022:LYS:HD3	1.69	0.74
3:S:831:LEU:HD23	3:S:873:GLU:OE1	1.87	0.73
2:R:142:ILE:HD12	2:R:155:ALA:HA	1.70	0.73
3:S:614:THR:OG1	3:S:647:ARG:HD3	1.90	0.71
3:S:912:TYR:CD2	3:S:932:ILE:HD11	2.28	0.68
1:Q:41:ARG:HE	1:Q:52:LEU:HD21	1.59	0.68
3:S:999:ASN:C	3:S:999:ASN:HD22	2.02	0.68
1:Q:31:GLU:HG3	3:S:739:ARG:HH12	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:859:LEU:HD11	3:S:871:VAL:HG13	1.74	0.67
1:Q:68:ARG:HA	1:Q:71:TYR:CE2	2.32	0.65
3:S:869:ASN:O	3:S:873:GLU:HG3	1.99	0.63
3:S:788:LEU:HD13	3:S:831:LEU:HD21	1.81	0.63
3:S:1044:ASN:N	3:S:1045:PRO:HD3	2.12	0.63
2:R:35:THR:HG22	2:R:35:THR:O	2.00	0.61
3:S:1003:LYS:HE3	3:S:1003:LYS:HA	1.82	0.61
3:S:645:ILE:O	3:S:649:GLU:HG2	2.01	0.59
2:R:17:SER:HB3	3:S:942:GLU:OE2	2.03	0.59
1:Q:41:ARG:HD2	1:Q:54:ASP:OD1	2.04	0.57
1:Q:67:MET:O	1:Q:70:GLN:HB2	2.04	0.57
1:Q:1:MET:HE3	1:Q:50:THR:HG22	1.85	0.57
3:S:890:PHE:O	3:S:898:LYS:HE2	2.04	0.57
1:Q:148:THR:O	1:Q:149:ARG:HB2	2.06	0.56
3:S:582:SER:H	3:S:585:ASN:HD21	1.54	0.56
2:R:120:LEU:HD22	2:R:120:LEU:N	2.21	0.55
2:R:41:ARG:HH11	2:R:41:ARG:HG2	1.72	0.54
1:Q:56:LEU:CD2	1:Q:71:TYR:HB2	2.38	0.54
2:R:79:LEU:HD13	2:R:159:LEU:HD22	1.90	0.54
3:S:771:ILE:HG22	3:S:986:ASP:HB2	1.89	0.54
3:S:694:ARG:O	3:S:698:GLU:HB2	2.07	0.53
1:Q:23:LEU:HD22	1:Q:156:PHE:CD2	2.44	0.53
2:R:127:SER:O	2:R:131:GLN:HG3	2.10	0.52
1:Q:47:ASP:HB2	1:Q:164:ARG:HH12	1.75	0.52
2:R:85:ASN:HD22	2:R:121:ALA:HB3	1.74	0.52
2:R:33:ASP:OD1	2:R:35:THR:HB	2.09	0.51
2:R:57:ASP:OD2	3:S:939:LYS:NZ	2.42	0.51
3:S:610:ILE:HD12	3:S:643:LEU:HD13	1.93	0.51
3:S:988:LYS:O	3:S:992:GLU:HG3	2.11	0.50
3:S:585:ASN:C	3:S:585:ASN:HD22	2.19	0.50
3:S:763:TRP:CE2	3:S:768:PRO:HG3	2.47	0.50
2:R:56:LEU:CD1	2:R:74:THR:HG23	2.43	0.49
3:S:899:LYS:O	3:S:903:GLU:HG2	2.11	0.49
1:Q:94:HIS:ND1	1:Q:94:HIS:N	2.59	0.49
1:Q:37:GLU:HG3	3:S:621:PRO:HG3	1.95	0.48
3:S:1030:LYS:HD2	3:S:1031:TYR:CZ	2.48	0.48
1:Q:23:LEU:HD22	1:Q:156:PHE:CG	2.49	0.47
3:S:999:ASN:C	3:S:999:ASN:ND2	2.72	0.47
3:S:770:HIS:HA	3:S:772:GLU:OE2	2.15	0.47
3:S:986:ASP:OD1	3:S:987:ILE:N	2.47	0.47
1:Q:73:ARG:HG2	1:Q:103:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:922:ILE:C	3:S:922:ILE:HD12	2.41	0.46
1:Q:62:GLU:C	1:Q:64:ALA:H	2.23	0.46
3:S:585:ASN:HD22	3:S:586:ILE:N	2.13	0.46
2:R:49:GLU:HB3	2:R:164:ARG:NH2	2.31	0.46
3:S:984:GLU:HG2	3:S:987:ILE:HD12	1.98	0.45
3:S:1043:SER:C	3:S:1045:PRO:HD3	2.41	0.45
3:S:1025:PRO:HG2	3:S:1027:PHE:CE1	2.51	0.45
2:R:111:MET:O	2:R:162:GLU:OE1	2.34	0.45
3:S:601:ILE:HD12	3:S:601:ILE:N	2.32	0.45
2:R:142:ILE:CD1	2:R:155:ALA:HA	2.45	0.45
1:Q:32:TYR:C	1:Q:32:TYR:CD1	2.95	0.44
3:S:872:LEU:HD12	3:S:929:PHE:HB2	1.99	0.44
3:S:663:ILE:HG13	3:S:669:PRO:HG3	2.00	0.44
3:S:984:GLU:HG3	3:S:986:ASP:OD1	2.17	0.44
1:Q:101:LYS:HG3	1:Q:106:SER:O	2.17	0.44
1:Q:84:ILE:HD11	1:Q:118:CYS:HA	2.00	0.44
1:Q:142:ILE:HD12	1:Q:155:ALA:HA	1.98	0.44
3:S:582:SER:H	3:S:585:ASN:ND2	2.16	0.43
3:S:828:THR:HA	3:S:873:GLU:OE2	2.19	0.43
3:S:856:ILE:O	3:S:859:LEU:HB3	2.18	0.43
3:S:859:LEU:CD1	3:S:871:VAL:HG13	2.46	0.43
3:S:1015:GLU:HG3	7:S:136:HOH:O	2.18	0.43
2:R:87:THR:O	2:R:91:GLU:HG3	2.18	0.43
3:S:702:TYR:O	3:S:706:ARG:HG3	2.19	0.43
3:S:742:ILE:HG13	3:S:743:ALA:N	2.34	0.42
3:S:1022:LYS:HG3	3:S:1023:PRO:HD2	2.01	0.42
3:S:893:ILE:O	3:S:898:LYS:HE3	2.20	0.42
2:R:67:MET:HG2	3:S:876:SER:OG	2.19	0.42
1:Q:50:THR:HG21	3:S:920:ARG:O	2.20	0.41
3:S:731:GLU:HG2	3:S:735:LYS:HE3	2.01	0.41
3:S:984:GLU:OE2	3:S:986:ASP:OD1	2.39	0.41
1:Q:109:VAL:HA	1:Q:110:PRO:HD3	1.97	0.41
2:R:22:GLN:OE1	2:R:149:ARG:HG2	2.21	0.41
3:S:687:LEU:HG	3:S:726:MET:HE1	2.03	0.41
1:Q:164:ARG:HE	1:Q:165:GLN:HE21	1.68	0.41
3:S:796:TYR:CZ	3:S:928:PRO:HG2	2.56	0.41
1:Q:68:ARG:HH11	1:Q:99:GLN:HE22	1.68	0.40
2:R:37:GLU:O	2:R:38:ASP:HB2	2.21	0.40
2:R:56:LEU:HD13	2:R:74:THR:HG23	2.03	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	Q	164/166 (99%)	156 (95%)	8 (5%)	0	100	100
2	R	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
3	S	463/481 (96%)	451 (97%)	11 (2%)	1 (0%)	43	49
All	All	791/813 (97%)	765 (97%)	25 (3%)	1 (0%)	48	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	S	1045	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	Q	143/143 (100%)	142 (99%)	1 (1%)	76	86
2	R	144/144 (100%)	141 (98%)	3 (2%)	47	59
3	S	438/447 (98%)	426 (97%)	12 (3%)	39	50
All	All	725/734 (99%)	709 (98%)	16 (2%)	45	58

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

Mol	Chain	Res	Type
1	Q	94	HIS
2	R	40	TYR

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Mol	Chain	Res	Type
2	R	53	LEU
2	R	79	LEU
3	S	585	ASN
3	S	609	LEU
3	S	640	LEU
3	S	647	ARG
3	S	772	GLU
3	S	804	LEU
3	S	830	ASN
3	S	966	GLU
3	S	989	ARG
3	S	999	ASN
3	S	1003	LYS
3	S	1045	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	Q	99	GLN
1	Q	150	GLN
1	Q	165	GLN
2	R	27	HIS
2	R	61	GLN
3	S	585	ASN
3	S	683	GLN
3	S	712	GLN
3	S	800	GLN
3	S	820	ASN
3	S	860	GLN
3	S	999	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

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	R	1003	-	4,4,4	1.74	1 (25%)	6,6,6	0.46	0
5	PO4	S	1049	-	4,4,4	1.70	1 (25%)	6,6,6	0.46	0
5	PO4	Q	1007	-	4,4,4	1.69	0	6,6,6	0.46	0
6	GNP	Q	1001	4	34,34,34	2.28	12 (35%)	47,54,54	1.80	6 (12%)
5	PO4	S	1048	-	4,4,4	1.70	0	6,6,6	0.48	0
5	PO4	S	1047	-	4,4,4	1.75	1 (25%)	6,6,6	0.45	0

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	Q	1001	4	-	4/18/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	1001	GNP	C5-N7	5.10	1.49	1.39
6	Q	1001	GNP	PA-O3A	-4.95	1.54	1.59
6	Q	1001	GNP	C8-N9	4.49	1.47	1.37
6	Q	1001	GNP	C2-N2	4.20	1.44	1.34
6	Q	1001	GNP	PG-O3G	-3.76	1.46	1.56
6	Q	1001	GNP	PG-N3B	3.49	1.72	1.63
6	Q	1001	GNP	PG-O1G	3.48	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	Q	1001	GNP	O6-C6	-3.06	1.17	1.23
6	Q	1001	GNP	PB-O2B	-2.83	1.49	1.56
6	Q	1001	GNP	PB-N3B	2.69	1.70	1.63
6	Q	1001	GNP	O4'-C4'	-2.56	1.39	1.45
6	Q	1001	GNP	PG-O2G	-2.12	1.51	1.56
5	S	1049	PO4	P-O3	-2.06	1.48	1.54
5	S	1047	PO4	P-O3	-2.05	1.48	1.54
5	R	1003	PO4	P-O3	-2.05	1.48	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	1001	GNP	O1G-PG-N3B	-6.14	102.73	111.77
6	Q	1001	GNP	N1-C2-N3	5.49	133.37	123.32
6	Q	1001	GNP	O2B-PB-O1B	4.11	118.69	109.87
6	Q	1001	GNP	N2-C2-N1	-3.57	109.24	116.76
6	Q	1001	GNP	C2-N1-C6	-3.25	119.21	125.11
6	Q	1001	GNP	C2-N3-C4	-2.94	107.24	112.30

There are no chirality outliers.

All (4) torsion outliers are listed below:

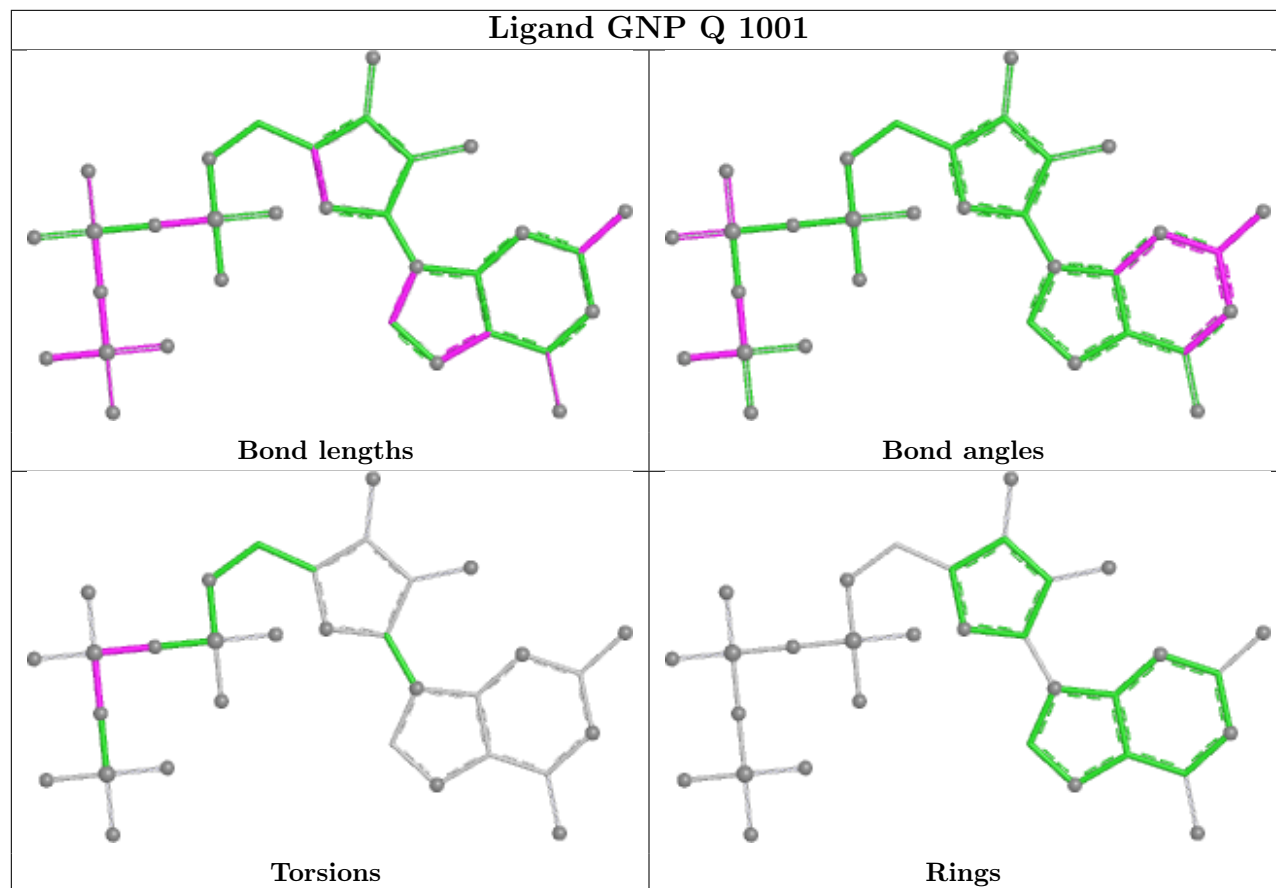
Mol	Chain	Res	Type	Atoms
6	Q	1001	GNP	PG-N3B-PB-O1B
6	Q	1001	GNP	PG-N3B-PB-O3A
6	Q	1001	GNP	PA-O3A-PB-O2B
6	Q	1001	GNP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	Q	166/166 (100%)	0.99	38 (22%) 2 2	18, 34, 70, 83	0
2	R	166/166 (100%)	0.91	28 (16%) 4 4	20, 34, 58, 80	0
3	S	469/481 (97%)	0.75	73 (15%) 5 4	18, 31, 57, 80	0
All	All	801/813 (98%)	0.83	139 (17%) 4 3	18, 32, 60, 83	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	S	743	ALA	10.7
3	S	1044	ASN	7.0
2	R	120	LEU	6.7
2	R	40	TYR	6.7
3	S	621	PRO	6.6
1	Q	71	TYR	6.4
3	S	1045	PRO	6.1
3	S	742	ILE	5.6
1	Q	66	ALA	5.6
1	Q	64	ALA	5.5
3	S	750	HIS	5.5
2	R	38	ASP	5.5
3	S	590	GLU	5.3
2	R	37	GLU	5.2
3	S	724	LYS	5.0
3	S	1046	ARG	4.9
2	R	36	ILE	4.9
3	S	986	ASP	4.8
3	S	755	GLN	4.8
3	S	620	ASP	4.7
1	Q	63	GLU	4.7
3	S	597	GLY	4.6
3	S	725	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
3	S	751	ASN	4.5
2	R	29	VAL	4.4
3	S	722	ARG	4.3
3	S	1023	PRO	4.2
3	S	1022	LYS	4.2
1	Q	118	CYS	4.2
3	S	756	SER	4.1
3	S	946	GLU	4.1
2	R	122	ALA	4.1
1	Q	62	GLU	4.1
1	Q	69	ASP	4.0
1	Q	165	GLN	4.0
1	Q	30	ASP	4.0
1	Q	68	ARG	4.0
3	S	769	GLY	3.8
2	R	108	ASP	3.7
3	S	723	GLY	3.7
2	R	121	ALA	3.7
3	S	619	ALA	3.7
3	S	752	ILE	3.7
3	S	720	THR	3.6
3	S	1021	PRO	3.6
2	R	162	GLU	3.6
3	S	667	ASP	3.5
1	Q	70	GLN	3.5
3	S	566	GLN	3.5
3	S	753	THR	3.5
3	S	673	GLU	3.4
2	R	147	LYS	3.4
1	Q	67	MET	3.4
3	S	583	GLU	3.4
2	R	166	HIS	3.4
2	R	165	GLN	3.4
1	Q	94	HIS	3.3
3	S	954	GLU	3.3
1	Q	108	ASP	3.3
3	S	654	GLU	3.3
2	R	57	ASP	3.2
3	S	668	GLN	3.2
2	R	35	THR	3.2
2	R	118	CYS	3.1
3	S	573	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
3	S	754	PHE	3.1
3	S	716	GLU	3.1
2	R	28	PHE	3.0
1	Q	49	GLU	3.0
1	Q	33	ASP	3.0
1	Q	73	ARG	3.0
3	S	574	VAL	3.0
2	R	30	ASP	3.0
1	Q	166	HIS	3.0
1	Q	65	SER	2.9
1	Q	121	ALA	2.9
2	R	39	SER	2.9
1	Q	95	GLN	2.9
2	R	56	LEU	2.8
3	S	739	ARG	2.8
3	S	584	GLU	2.8
3	S	942	GLU	2.8
3	S	570	PRO	2.8
3	S	982	ARG	2.8
3	S	617	MET	2.8
3	S	664	GLU	2.8
3	S	731	GLU	2.7
3	S	567	MET	2.7
2	R	74	THR	2.7
1	Q	91	GLU	2.7
1	Q	129	GLN	2.6
3	S	726	MET	2.6
3	S	683	GLN	2.6
1	Q	102	ARG	2.6
3	S	966	GLU	2.6
3	S	953	LYS	2.6
2	R	1	MET	2.5
3	S	999	ASN	2.5
3	S	863	GLN	2.5
1	Q	107	ASP	2.5
3	S	569	LEU	2.5
1	Q	72	MET	2.5
3	S	891	GLU	2.5
1	Q	124	THR	2.5
3	S	719	GLY	2.5
3	S	622	ASN	2.5
3	S	1015	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	Q	98	GLU	2.4
2	R	119	ASP	2.4
3	S	949	LYS	2.4
3	S	572	ALA	2.4
3	S	579	GLU	2.4
3	S	578	ALA	2.3
1	Q	74	THR	2.3
3	S	666	GLY	2.3
1	Q	99	GLN	2.2
3	S	571	SER	2.2
3	S	1029	LYS	2.2
1	Q	164	ARG	2.2
1	Q	88	LYS	2.2
2	R	41	ARG	2.2
2	R	50	THR	2.2
3	S	697	VAL	2.2
1	Q	32	TYR	2.2
3	S	727	LYS	2.2
3	S	728	LYS	2.2
1	Q	31	GLU	2.1
1	Q	150	GLN	2.1
1	Q	1	MET	2.1
1	Q	51	CYS	2.1
1	Q	92	ASP	2.1
2	R	103	VAL	2.1
3	S	846	GLU	2.0
2	R	95	GLN	2.0
3	S	1006	THR	2.0
3	S	952	GLY	2.0
3	S	598	ILE	2.0
3	S	665	ASN	2.0
2	R	107	ASP	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](#)

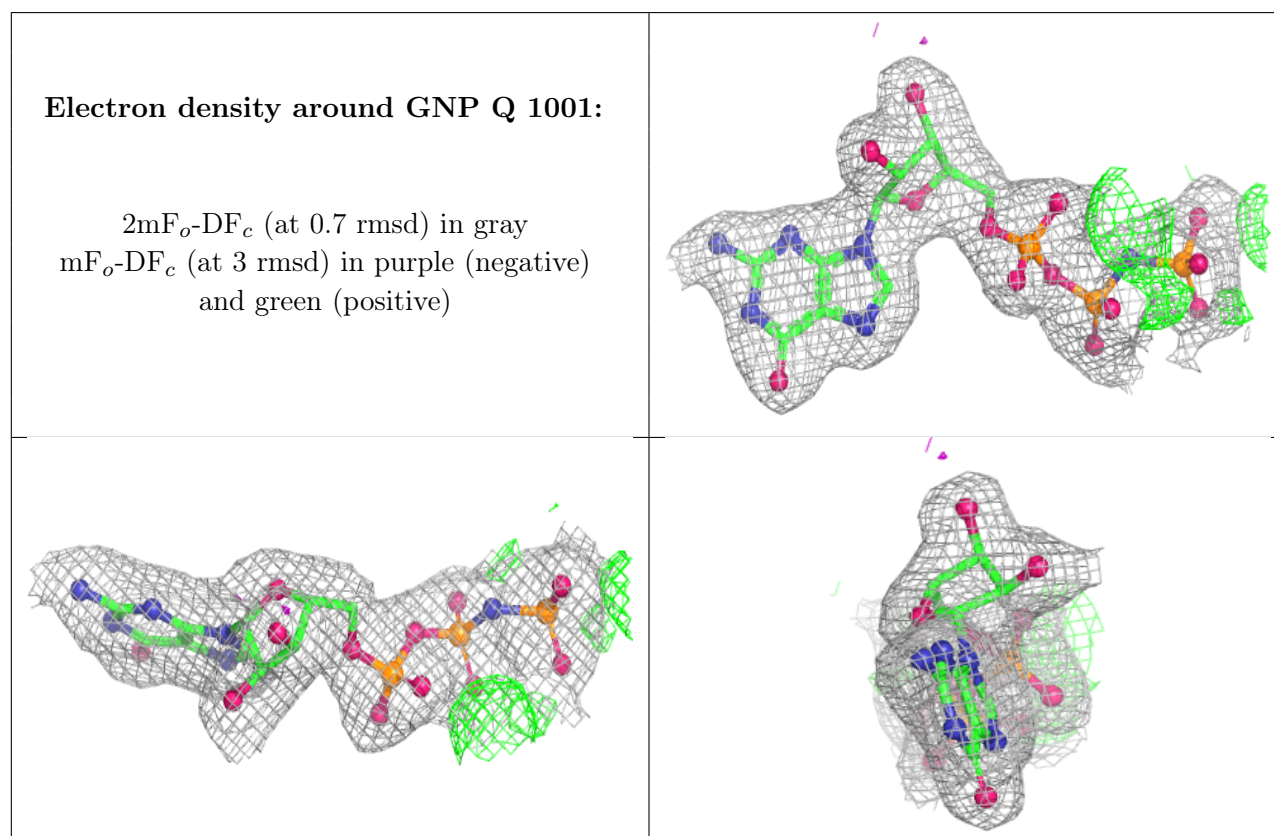
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PO4	S	1048	5/5	0.83	0.17	64,66,66,66	0
5	PO4	Q	1007	5/5	0.85	0.19	116,116,116,116	0
5	PO4	S	1047	5/5	0.93	0.15	62,62,63,63	0
5	PO4	S	1049	5/5	0.94	0.11	52,52,53,54	0
5	PO4	R	1003	5/5	0.95	0.09	40,41,44,45	0
4	MG	Q	1002	1/1	0.97	0.10	16,16,16,16	0
6	GNP	Q	1001	32/32	0.98	0.06	22,28,32,33	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.