



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:43 PM UTC

PDB ID : 3O9J / pdb_00003o9j
Title : Influenza NA in complex with compound 5
Authors : Russell, R.J.; Kerry, P.S.
Deposited on : 2010-08-04
Resolution : 2.00 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

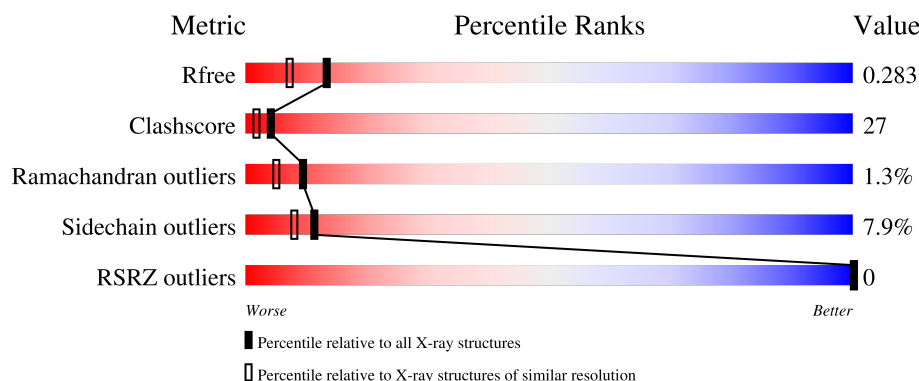
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	387	 61% 30% 7%

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
2	RP6	A	1	X	-	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3361 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.

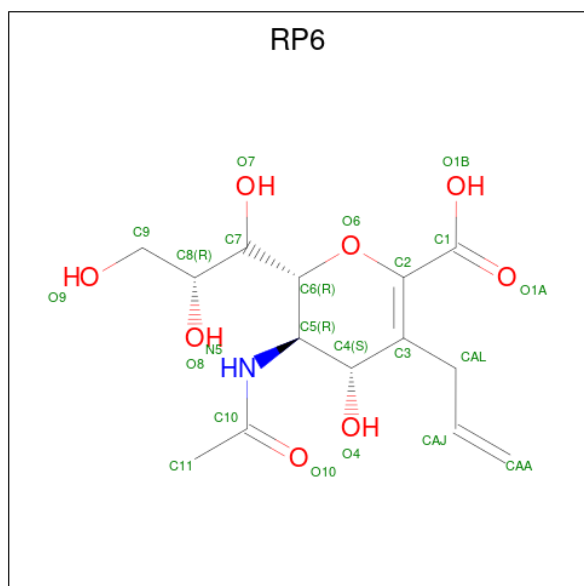
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	387	3002	1880	525	573	24	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	ASN	GLY	conflict	UNP Q07599

- Molecule 2 is 5-acetamido-2,6-anhydro-3,5-dideoxy-3-prop-2-en-1-yl-D-glycero-D-galacto-n-2-enonic acid (CCD ID: RP6) (formula: $C_{14}H_{21}NO_8$).

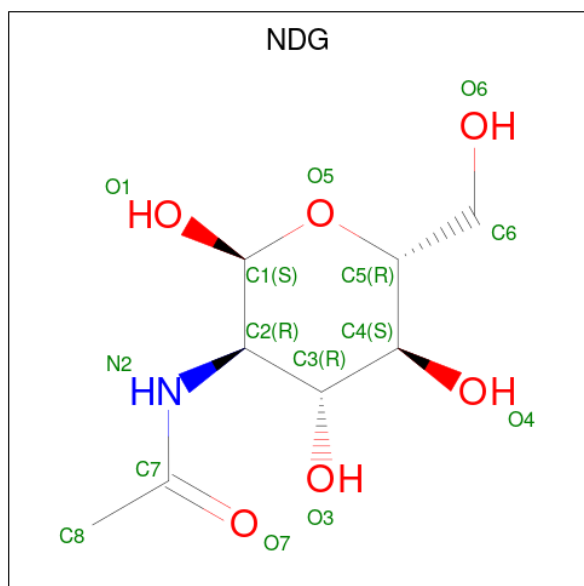


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	23	14	1	8	0	0

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

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

- Molecule 4 is 2-acetamido-2-deoxy- α -D-glucopyranose (CCD ID: NDG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	8	1	6		

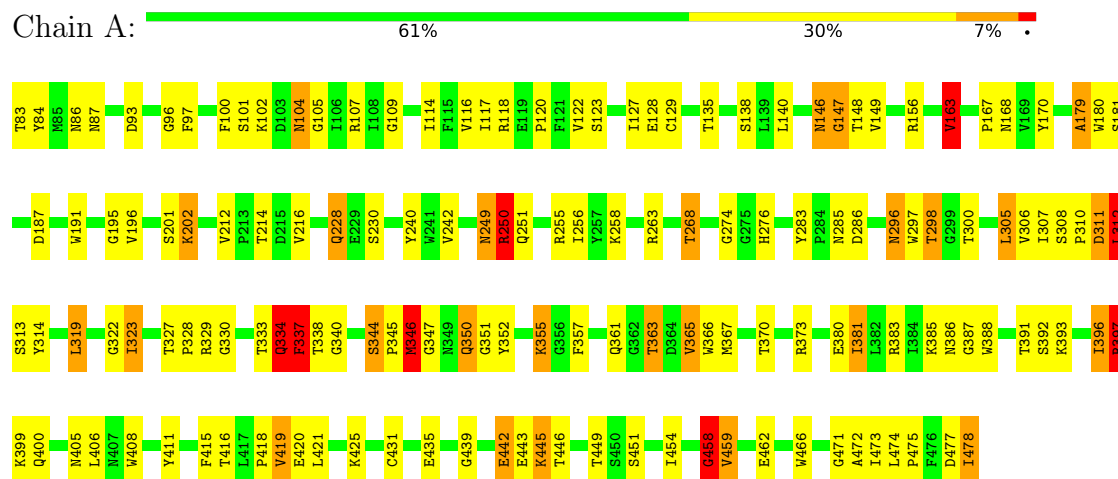
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	320	Total	O	0	0
			320	320		

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: Neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	90.58Å 90.58Å 109.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.64 – 2.00 28.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.64-2.00) 97.3 (28.64-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6_289)	Depositor
R, R_{free}	0.215 , 0.282 0.225 , 0.283	Depositor DCC
R_{free} test set	1465 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.983	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.289 for -h,k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3361	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% 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: NDG, CA, RP6

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	1.68	25/3077 (0.8%)	1.62	36/4177 (0.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	445	LYS	CB-CG	23.18	2.21	1.52
1	A	308	SER	C-N	22.99	1.66	1.33
1	A	421	LEU	C-N	18.74	1.59	1.34
1	A	170	TYR	C-N	17.33	1.56	1.33
1	A	310	PRO	N-CD	-14.46	1.27	1.47
1	A	445	LYS	C-N	-14.26	1.16	1.33
1	A	346	MET	C-N	-13.12	1.15	1.33
1	A	397	ARG	CA-C	12.41	1.68	1.52
1	A	350	GLN	C-N	-10.56	1.19	1.33
1	A	421	LEU	CA-C	10.33	1.66	1.53
1	A	397	ARG	C-N	9.89	1.47	1.33
1	A	310	PRO	N-CA	9.79	1.60	1.47
1	A	334	GLN	CB-CG	9.55	1.81	1.52
1	A	311	ASP	C-N	-9.14	1.20	1.33
1	A	181	SER	CA-C	5.66	1.59	1.52
1	A	323	ILE	CA-C	5.61	1.57	1.52
1	A	296	ASN	C-O	5.52	1.31	1.23
1	A	123	SER	N-CA	5.50	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	473	ILE	CA-CB	5.45	1.60	1.53
1	A	122	VAL	CA-CB	5.34	1.61	1.54
1	A	179	ALA	N-CA	5.33	1.52	1.46
1	A	333	THR	C-N	5.32	1.41	1.33
1	A	104	ASN	N-CA	5.29	1.54	1.46
1	A	420	GLU	C-N	-5.20	1.26	1.33
1	A	355	LYS	C-O	5.03	1.29	1.23

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	MET	CA-C-N	31.57	167.18	121.09
1	A	346	MET	C-N-CA	31.57	167.18	121.09
1	A	346	MET	O-C-N	-27.89	90.67	123.31
1	A	445	LYS	CA-CB-CG	-15.69	82.73	114.10
1	A	397	ARG	O-C-N	-9.34	109.58	122.94
1	A	350	GLN	O-C-N	-9.29	111.16	123.23
1	A	308	SER	CA-C-N	-9.06	108.96	119.47
1	A	308	SER	C-N-CA	-9.06	108.96	119.47
1	A	311	ASP	O-C-N	-8.69	113.12	122.07
1	A	421	LEU	O-C-N	-8.44	110.91	122.30
1	A	337	PHE	CA-C-N	8.10	134.08	122.09
1	A	337	PHE	C-N-CA	8.10	134.08	122.09
1	A	308	SER	O-C-N	7.65	131.28	121.34
1	A	310	PRO	N-CA-CB	-7.57	94.82	103.30
1	A	344	SER	N-CA-C	7.52	120.28	108.55
1	A	311	ASP	CA-C-N	7.19	135.28	121.54
1	A	311	ASP	C-N-CA	7.19	135.28	121.54
1	A	337	PHE	O-C-N	-7.00	114.97	123.30
1	A	323	ILE	CB-CA-C	6.94	117.17	110.16
1	A	283	TYR	N-CA-C	-6.27	102.49	108.13
1	A	396	ILE	CB-CA-C	-6.13	103.98	112.02
1	A	228	GLN	N-CA-C	6.02	117.93	111.36
1	A	311	ASP	N-CA-C	-5.99	104.66	111.07
1	A	459	VAL	N-CA-C	5.89	121.59	109.34
1	A	392	SER	N-CA-C	5.88	118.75	110.23
1	A	179	ALA	N-CA-C	5.78	117.19	108.46
1	A	163	VAL	CB-CA-C	-5.59	102.29	111.51
1	A	458	GLY	N-CA-C	5.56	126.36	113.18
1	A	87	ASN	N-CA-C	-5.48	99.13	110.80
1	A	101	SER	N-CA-C	5.26	117.25	108.99
1	A	163	VAL	N-CA-CB	5.24	118.58	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	GLY	N-CA-C	5.19	121.67	114.92
1	A	180	TRP	N-CA-C	-5.18	105.64	112.94
1	A	420	GLU	O-C-N	-5.09	116.27	122.22
1	A	323	ILE	N-CA-CB	-5.03	105.44	112.27
1	A	308	SER	N-CA-C	-5.01	103.65	110.36

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	GLY	Peptide
1	A	337	PHE	Mainchain,Peptide
1	A	346	MET	Mainchain,Peptide
1	A	397	ARG	Mainchain

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	3002	0	2861	161	0
2	A	23	0	3	4	0
3	A	1	0	0	0	0
4	A	15	0	12	1	0
5	A	320	0	0	38	1
All	All	3361	0	2876	162	1

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 27.

All (162) 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:334:GLN:CG	1:A:334:GLN:CB	1.81	1.56
1:A:298:THR:HB	5:A:40:HOH:O	1.23	1.34
1:A:329:ARG:C	1:A:350:GLN:HE22	1.39	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:GLU:OE1	1:A:474:LEU:HD12	1.29	1.30
1:A:445:LYS:CB	1:A:445:LYS:CG	2.22	1.18
1:A:329:ARG:CA	1:A:350:GLN:HE22	1.54	1.18
1:A:96:GLY:O	1:A:458:GLY:O	1.61	1.16
1:A:116:VAL:HB	5:A:591:HOH:O	1.54	1.06
1:A:365:VAL:HB	5:A:50:HOH:O	1.55	1.05
1:A:305:LEU:HB3	5:A:637:HOH:O	1.56	1.04
1:A:328:PRO:O	1:A:350:GLN:OE1	1.74	1.03
1:A:329:ARG:C	1:A:350:GLN:NE2	2.20	0.99
1:A:329:ARG:CA	1:A:350:GLN:NE2	2.28	0.96
1:A:329:ARG:HA	1:A:350:GLN:NE2	1.81	0.94
1:A:443:GLU:OE1	1:A:474:LEU:CD1	2.19	0.91
1:A:408:TRP:CH2	1:A:442:GLU:HG2	2.05	0.91
1:A:337:PHE:CZ	1:A:346:MET:HB2	2.05	0.90
1:A:147:GLY:C	1:A:149:VAL:H	1.81	0.88
1:A:445:LYS:CG	1:A:445:LYS:HA	2.04	0.88
1:A:86:ASN:ND2	5:A:667:HOH:O	2.03	0.88
1:A:329:ARG:HA	1:A:350:GLN:HE22	1.36	0.88
1:A:83:THR:N	5:A:58:HOH:O	2.06	0.88
1:A:445:LYS:CG	1:A:445:LYS:CA	2.52	0.87
1:A:298:THR:HG21	5:A:596:HOH:O	1.75	0.85
1:A:329:ARG:HA	1:A:350:GLN:CD	2.01	0.85
1:A:249:ASN:HB2	5:A:540:HOH:O	1.77	0.84
1:A:249:ASN:O	1:A:250:ARG:O	1.96	0.84
1:A:118:ARG:NH2	2:A:1:RP6:HAA	1.93	0.82
1:A:328:PRO:C	1:A:350:GLN:OE1	2.24	0.80
1:A:346:MET:HE3	5:A:500:HOH:O	1.82	0.79
1:A:276:HIS:HD2	1:A:296:ASN:H	1.28	0.79
1:A:201:SER:C	1:A:202:LYS:HG3	2.05	0.79
1:A:268:THR:HG23	5:A:558:HOH:O	1.80	0.79
1:A:298:THR:O	1:A:347:GLY:O	2.01	0.78
1:A:391:THR:HG22	5:A:23:HOH:O	1.83	0.78
1:A:263:ARG:HD2	5:A:541:HOH:O	1.84	0.78
1:A:445:LYS:O	1:A:446:THR:HG23	1.83	0.77
1:A:337:PHE:CE1	1:A:346:MET:HB2	2.19	0.77
1:A:380:GLU:OE1	1:A:399:LYS:NZ	2.18	0.76
1:A:311:ASP:O	1:A:312:LEU:HB2	1.85	0.76
1:A:397:ARG:NH1	1:A:462:GLU:OE1	2.19	0.76
1:A:365:VAL:CG1	1:A:388:TRP:HE3	1.99	0.75
1:A:329:ARG:HA	1:A:350:GLN:OE1	1.85	0.75
1:A:300:THR:HG21	1:A:350:GLN:CD	2.12	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLN:CG	1:A:334:GLN:CA	2.65	0.75
1:A:146:ASN:HD21	4:A:479:NDG:H8C3	1.53	0.73
1:A:477:ASP:O	1:A:478:ILE:HB	1.89	0.73
1:A:425:LYS:HE2	5:A:617:HOH:O	1.88	0.72
1:A:249:ASN:HD22	1:A:249:ASN:H	1.38	0.71
1:A:330:GLY:N	1:A:350:GLN:HE22	1.88	0.71
1:A:337:PHE:HE2	1:A:340:GLY:HA2	1.57	0.70
1:A:313:SER:HA	5:A:535:HOH:O	1.91	0.69
1:A:330:GLY:N	1:A:350:GLN:NE2	2.40	0.69
1:A:337:PHE:CE2	1:A:338:THR:O	2.46	0.69
1:A:251:GLN:HE22	1:A:274:GLY:H	1.41	0.68
1:A:337:PHE:CE2	1:A:340:GLY:HA2	2.28	0.68
1:A:128:GLU:HB2	5:A:692:HOH:O	1.92	0.68
1:A:373:ARG:NH1	5:A:650:HOH:O	2.28	0.67
1:A:408:TRP:CZ3	1:A:442:GLU:HG2	2.30	0.66
1:A:357:PHE:HZ	1:A:381:ILE:HD12	1.61	0.66
1:A:109:GLY:HA3	1:A:140:LEU:HD12	1.77	0.65
1:A:416:THR:HG23	5:A:52:HOH:O	1.97	0.64
1:A:214:THR:O	1:A:263:ARG:CZ	2.45	0.64
1:A:365:VAL:CG1	5:A:50:HOH:O	2.47	0.62
1:A:346:MET:CE	5:A:500:HOH:O	2.44	0.62
1:A:408:TRP:CH2	1:A:442:GLU:CG	2.81	0.61
1:A:419:VAL:HG22	1:A:425:LYS:O	2.00	0.61
1:A:319:LEU:HD21	1:A:365:VAL:HG11	1.82	0.61
1:A:214:THR:O	1:A:263:ARG:NH1	2.34	0.61
1:A:365:VAL:HG13	1:A:388:TRP:HB2	1.83	0.60
1:A:256:ILE:HD13	1:A:307:ILE:HG12	1.84	0.59
1:A:276:HIS:CD2	1:A:296:ASN:H	2.15	0.59
1:A:230:SER:HB3	1:A:355:LYS:HE2	1.84	0.59
1:A:116:VAL:HG12	1:A:138:SER:O	2.04	0.57
1:A:255:ARG:NH2	5:A:710:HOH:O	2.13	0.57
1:A:118:ARG:NH2	2:A:1:RP6:CAA	2.65	0.57
1:A:300:THR:HG22	1:A:350:GLN:OE1	2.04	0.57
1:A:365:VAL:HG12	1:A:388:TRP:HE3	1.69	0.57
1:A:97:PHE:H	1:A:400:GLN:HE22	1.53	0.57
1:A:365:VAL:HG22	1:A:387:GLY:HA3	1.87	0.57
1:A:249:ASN:HD22	1:A:249:ASN:N	2.03	0.57
1:A:118:ARG:CZ	2:A:1:RP6:HAA	2.35	0.56
1:A:300:THR:CG2	1:A:350:GLN:CD	2.77	0.56
1:A:415:PHE:CE2	1:A:431:CYS:HB2	2.41	0.56
1:A:329:ARG:CA	1:A:350:GLN:CD	2.75	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:CYS:O	1:A:163:VAL:HG22	2.06	0.55
1:A:251:GLN:NE2	1:A:274:GLY:H	2.05	0.55
1:A:147:GLY:C	1:A:149:VAL:N	2.51	0.55
1:A:116:VAL:HG13	5:A:63:HOH:O	2.07	0.54
1:A:329:ARG:CA	1:A:350:GLN:OE1	2.55	0.54
1:A:300:THR:CG2	1:A:350:GLN:OE1	2.56	0.54
1:A:445:LYS:O	1:A:446:THR:CG2	2.55	0.53
1:A:116:VAL:HG11	1:A:138:SER:OG	2.08	0.53
1:A:117:ILE:HD13	1:A:167:PRO:HG3	1.90	0.52
1:A:383:ARG:NH2	5:A:607:HOH:O	2.42	0.52
1:A:408:TRP:HH2	5:A:638:HOH:O	1.91	0.52
1:A:116:VAL:HG23	1:A:449:THR:O	2.10	0.52
1:A:357:PHE:CZ	1:A:381:ILE:HD12	2.42	0.52
1:A:116:VAL:CG1	1:A:138:SER:OG	2.57	0.51
1:A:201:SER:OG	1:A:202:LYS:HG3	2.10	0.51
1:A:411:TYR:HB2	1:A:435:GLU:OE1	2.10	0.51
1:A:107:ARG:HG2	1:A:472:ALA:HA	1.93	0.51
1:A:478:ILE:HD12	5:A:55:HOH:O	2.10	0.51
1:A:365:VAL:CB	5:A:50:HOH:O	2.33	0.50
1:A:116:VAL:CG1	5:A:63:HOH:O	2.60	0.50
1:A:322:GLY:O	1:A:393:LYS:HE2	2.11	0.50
1:A:228:GLN:HE21	1:A:242:VAL:H	1.59	0.50
1:A:418:PRO:HG3	5:A:683:HOH:O	2.13	0.49
1:A:334:GLN:CB	1:A:334:GLN:CD	2.76	0.49
1:A:346:MET:HE3	5:A:492:HOH:O	2.11	0.49
1:A:249:ASN:O	1:A:250:ARG:C	2.57	0.48
1:A:249:ASN:H	1:A:249:ASN:ND2	2.09	0.48
1:A:337:PHE:CE1	1:A:346:MET:CB	2.95	0.48
1:A:249:ASN:N	1:A:249:ASN:ND2	2.61	0.47
1:A:298:THR:HG23	1:A:345:PRO:HB2	1.95	0.47
1:A:474:LEU:HB3	1:A:475:PRO:HA	1.96	0.47
1:A:268:THR:OG1	1:A:312:LEU:HB3	2.14	0.47
1:A:298:THR:HA	1:A:350:GLN:O	2.16	0.46
1:A:298:THR:HG22	5:A:61:HOH:O	2.15	0.46
1:A:425:LYS:CE	5:A:617:HOH:O	2.54	0.46
1:A:363:THR:HG22	1:A:386:ASN:HA	1.97	0.46
1:A:439:GLY:HA2	1:A:446:THR:OG1	2.16	0.46
1:A:337:PHE:CD2	1:A:338:THR:O	2.69	0.45
1:A:350:GLN:NE2	5:A:671:HOH:O	2.49	0.45
1:A:297:TRP:O	1:A:351:GLY:HA2	2.17	0.45
1:A:323:ILE:HG22	1:A:367:MET:SD	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLN:HE22	1:A:274:GLY:N	2.10	0.44
1:A:381:ILE:HG22	1:A:400:GLN:HB3	1.99	0.44
1:A:435:GLU:HG3	1:A:451:SER:HB2	1.99	0.44
1:A:116:VAL:O	5:A:63:HOH:O	2.21	0.44
1:A:306:VAL:O	1:A:314:TYR:HA	2.17	0.44
1:A:105:GLY:O	1:A:114:ILE:HG21	2.17	0.44
1:A:337:PHE:HZ	1:A:346:MET:HB2	1.73	0.44
1:A:385:LYS:O	1:A:386:ASN:HB2	2.17	0.44
1:A:120:PRO:HD2	1:A:435:GLU:HB2	1.99	0.44
1:A:127:ILE:HG12	5:A:544:HOH:O	2.18	0.44
1:A:116:VAL:HG13	1:A:116:VAL:O	2.17	0.43
1:A:250:ARG:HA	1:A:297:TRP:CE2	2.53	0.43
1:A:285:ASN:O	1:A:286:ASP:HB2	2.18	0.43
1:A:352:TYR:HD1	5:A:483:HOH:O	2.01	0.43
1:A:86:ASN:HA	5:A:708:HOH:O	2.18	0.42
1:A:337:PHE:HB2	5:A:629:HOH:O	2.18	0.42
1:A:361:GLN:HG3	1:A:366:TRP:CD1	2.55	0.42
1:A:383:ARG:O	1:A:396:ILE:N	2.51	0.42
1:A:179:ALA:HB2	1:A:195:GLY:HA3	2.01	0.42
1:A:363:THR:CG2	1:A:386:ASN:OD1	2.68	0.42
1:A:240:TYR:CE2	1:A:258:LYS:HD2	2.54	0.42
1:A:93:ASP:OD2	5:A:78:HOH:O	2.22	0.42
1:A:334:GLN:CG	1:A:334:GLN:HA	2.49	0.42
1:A:102:LYS:NZ	1:A:104:ASN:ND2	2.68	0.41
1:A:357:PHE:HZ	1:A:381:ILE:CD1	2.32	0.41
1:A:114:ILE:HD13	1:A:168:ASN:HB3	2.02	0.41
1:A:327:THR:HG1	1:A:370:THR:HG1	1.59	0.41
1:A:116:VAL:CG2	1:A:449:THR:O	2.68	0.41
1:A:367:MET:HG3	1:A:367:MET:O	2.21	0.41
1:A:109:GLY:CA	1:A:114:ILE:HG13	2.51	0.41
1:A:346:MET:HE3	1:A:346:MET:HB3	1.94	0.41
2:A:1:RP6:CAJ	2:A:1:RP6:O4	2.69	0.41
1:A:84:TYR:HA	1:A:187:ASP:O	2.20	0.40
1:A:385:LYS:HG3	1:A:396:ILE:HD11	2.03	0.40
1:A:191:TRP:CD1	5:A:35:HOH:O	2.74	0.40
1:A:135:THR:O	1:A:156:ARG:HA	2.22	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
5:A:572:HOH:O	5:A:585:HOH:O[4_545]	2.15	0.05

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	Percentiles
1	A	385/387 (100%)	349 (91%)	31 (8%)	5 (1%)	9 5

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	ARG
1	A	148	THR
1	A	312	LEU
1	A	458	GLY
1	A	459	VAL

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	Percentiles
1	A	330/330 (100%)	304 (92%)	26 (8%)	11 8

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	PHE

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Mol	Chain	Res	Type
1	A	146	ASN
1	A	163	VAL
1	A	196	VAL
1	A	202	LYS
1	A	212	VAL
1	A	216	VAL
1	A	249	ASN
1	A	250	ARG
1	A	268	THR
1	A	298	THR
1	A	305	LEU
1	A	312	LEU
1	A	319	LEU
1	A	334	GLN
1	A	344	SER
1	A	363	THR
1	A	365	VAL
1	A	381	ILE
1	A	405	ASN
1	A	406	LEU
1	A	419	VAL
1	A	442	GLU
1	A	454	ILE
1	A	466	TRP
1	A	478	ILE

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	104	ASN
1	A	146	ASN
1	A	228	GLN
1	A	249	ASN
1	A	251	GLN
1	A	276	HIS
1	A	350	GLN
1	A	400	GLN
1	A	405	ASN
1	A	407	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 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NDG	A	479	-	15,15,15	0.61	0	21,21,21	1.54	2 (9%)
2	RP6	A	1	-	21,23,23	3.50	7 (33%)	20,32,32	3.52	11 (55%)

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	NDG	A	479	-	-	1/6/26/26	0/1/1/1
2	RP6	A	1	-	1/1/9/11	11/21/41/41	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	RP6	C8-C7	-11.50	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	RP6	O8-C8	-5.24	1.32	1.43
2	A	1	RP6	O6-C2	5.09	1.45	1.36
2	A	1	RP6	O7-C7	-4.37	1.32	1.43
2	A	1	RP6	C4-C5	4.09	1.57	1.53
2	A	1	RP6	CAL-CAJ	-3.45	1.33	1.49
2	A	1	RP6	C7-C6	-3.41	1.48	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	RP6	O6-C6-C7	-9.95	88.48	105.98
4	A	479	NDG	C1-C2-N2	-5.87	103.93	110.73
2	A	1	RP6	O7-C7-C6	5.31	120.92	109.44
2	A	1	RP6	O4-C4-C3	-5.12	100.08	109.90
2	A	1	RP6	O7-C7-C8	3.97	117.95	108.93
2	A	1	RP6	C8-C7-C6	3.95	120.48	113.05
2	A	1	RP6	O9-C9-C8	-3.67	103.45	111.16
2	A	1	RP6	O8-C8-C7	3.53	117.52	109.25
2	A	1	RP6	C6-C5-N5	2.85	115.46	110.91
2	A	1	RP6	O10-C10-C11	-2.81	117.05	122.05
2	A	1	RP6	O8-C8-C9	2.72	115.20	109.03
2	A	1	RP6	C5-N5-C10	-2.09	118.21	123.11
4	A	479	NDG	O5-C5-C6	2.06	111.54	106.44

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1	RP6	C7

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	RP6	C11-C10-N5-C5
2	A	1	RP6	O10-C10-N5-C5
2	A	1	RP6	O1B-C1-C2-O6
2	A	1	RP6	O7-C7-C8-C9
2	A	1	RP6	O6-C6-C7-O7
2	A	1	RP6	C5-C6-C7-O7
2	A	1	RP6	CAA-CAJ-CAL-C3
2	A	1	RP6	C6-C7-C8-O8
2	A	1	RP6	O7-C7-C8-O8
2	A	1	RP6	O1A-C1-C2-O6

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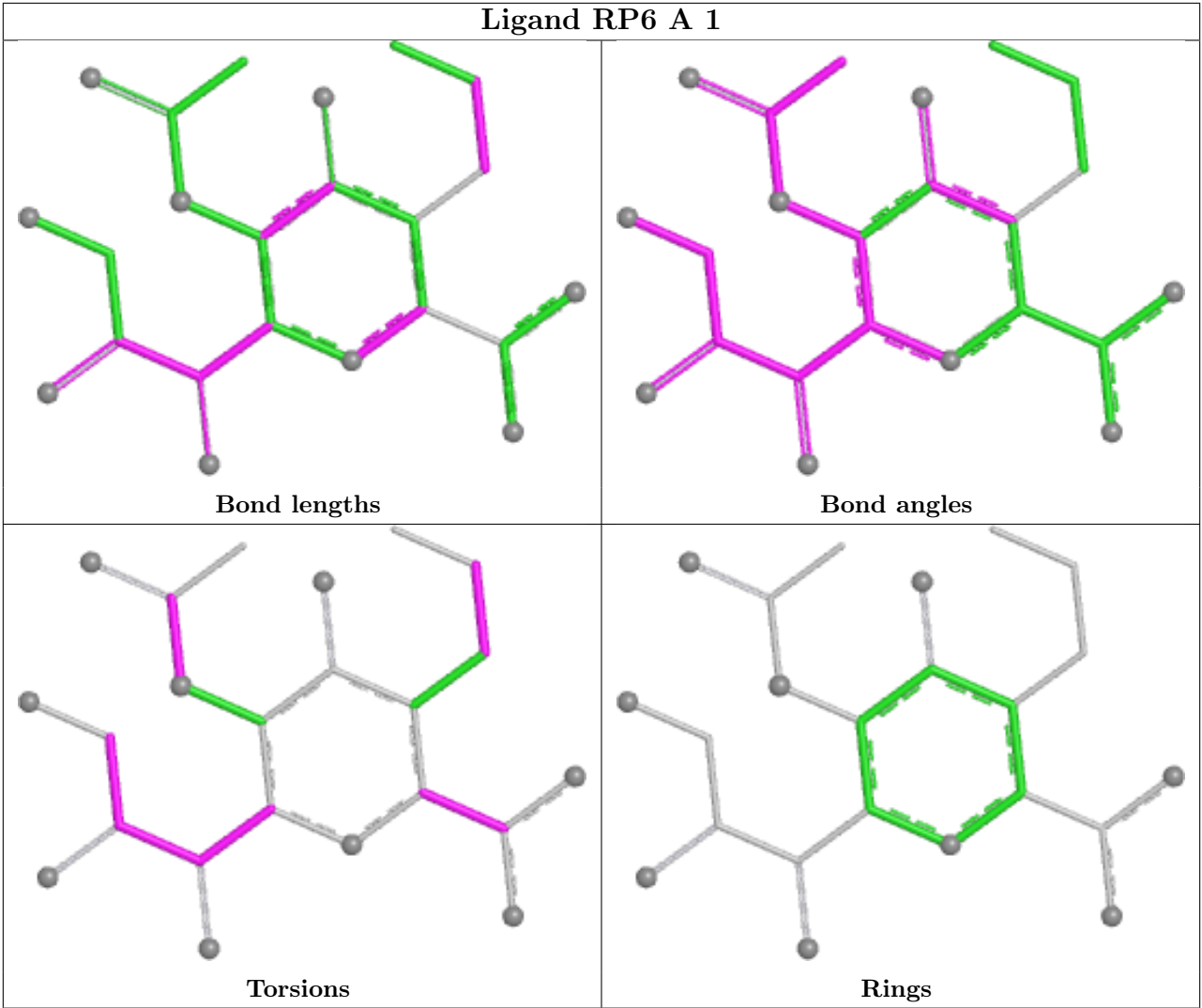
Mol	Chain	Res	Type	Atoms
2	A	1	RP6	C7-C8-C9-O9
4	A	479	NDG	O5-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	479	NDG	1	0
2	A	1	RP6	4	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	308:SER	C	310:PRO	N	1.66

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	350:GLN	C	351:GLY	N	1.19
1	A	445:LYS	C	446:THR	N	1.16
1	A	346:MET	C	347:GLY	N	1.15

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, 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	387/387 (100%)	-1.49	0 100 100	14, 24, 36, 43	0

There are no RSRZ outliers to report.

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](#)

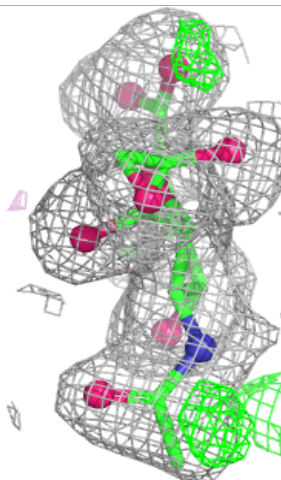
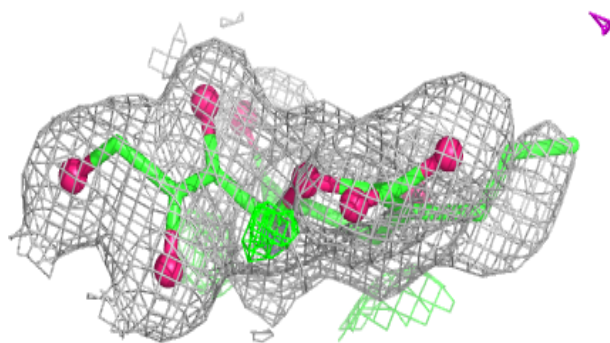
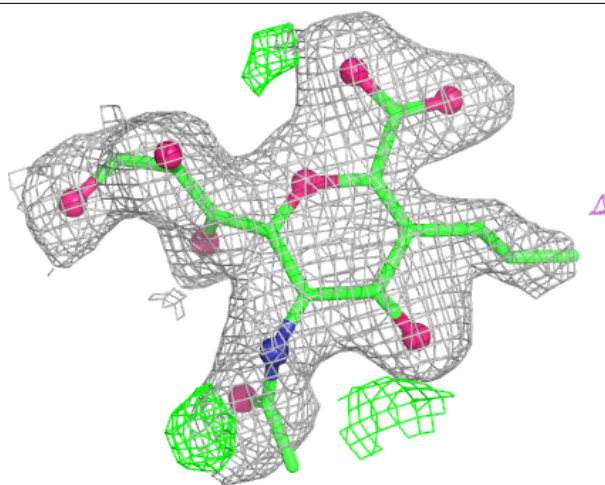
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NDG	A	479	15/15	0.95	0.06	93,94,95,95	0
3	CA	A	995	1/1	0.99	0.02	33,33,33,33	0
2	RP6	A	1	23/23	0.99	0.03	18,24,35,36	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 RP6 A 1:

$2mF_o-DF_c$ (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.