



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:52 PM UTC

PDB ID : 3NEW / pdb_00003new
Title : p38-alpha complexed with Compound 10
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Deposited on : 2010-06-09
Resolution : 2.51 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

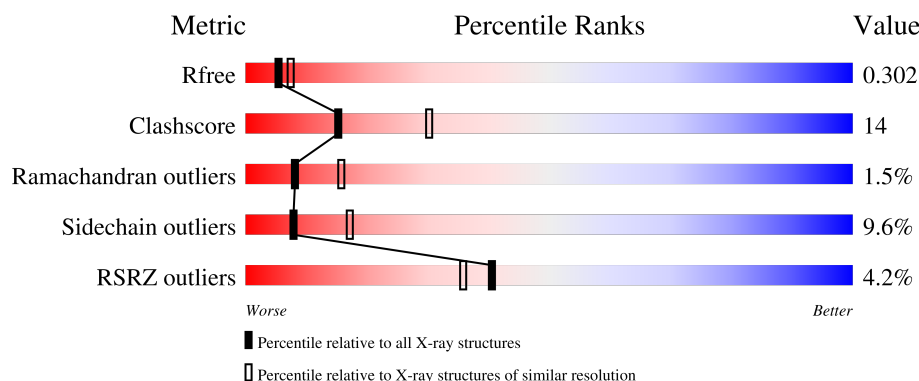
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	366	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2738 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.

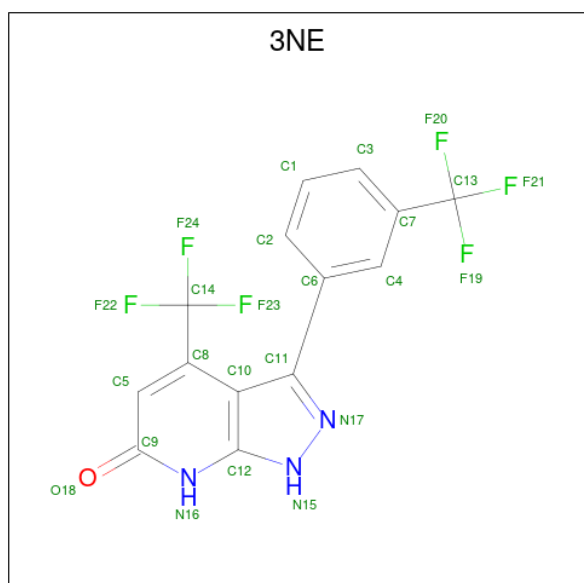
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	6	0
			2714	1741	459	503	11			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q16539
A	-4	SER	-	expression tag	UNP Q16539
A	-3	HIS	-	expression tag	UNP Q16539
A	-2	MET	-	expression tag	UNP Q16539
A	-1	LEU	-	expression tag	UNP Q16539
A	0	GLU	-	expression tag	UNP Q16539
A	162	SER	CYS	engineered mutation	UNP Q16539

- Molecule 2 is 4-(trifluoromethyl)-3-[3-(trifluoromethyl)phenyl]-1,7-dihydro-6H-pyrazolo[3,4-b]pyridin-6-one (CCD ID: 3NE) (formula: C₁₄H₇F₆N₃O).

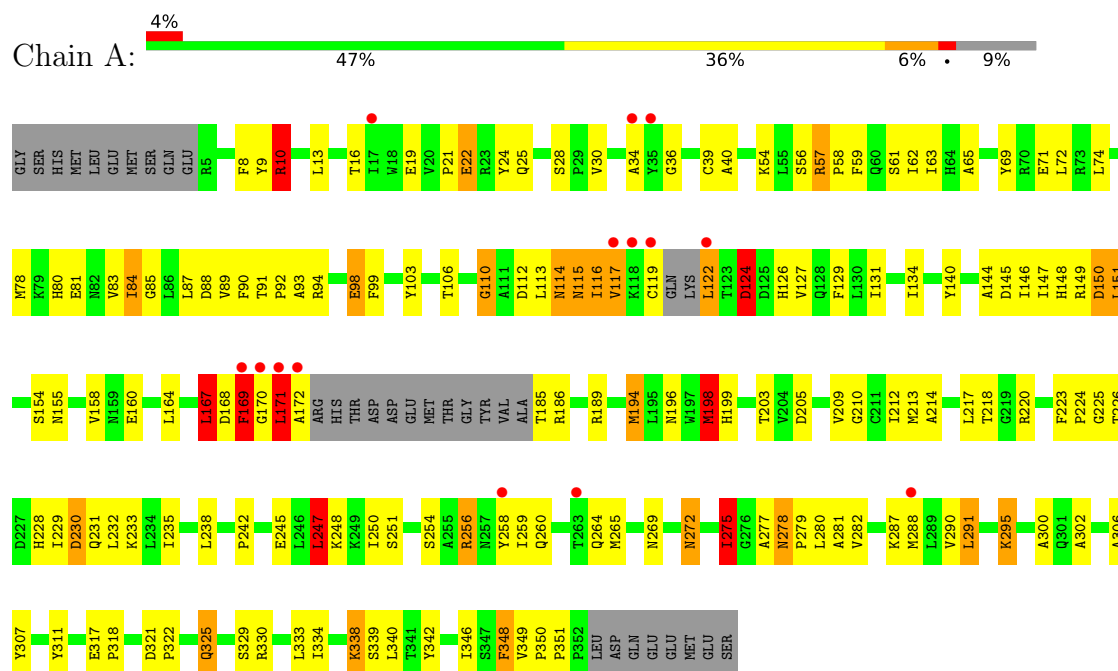


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	14	6	3	1		

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: Mitogen-activated protein kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.91Å 74.48Å 77.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 2.51 49.88 – 2.51	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.88-2.51) 99.1 (49.88-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.306 0.212 , 0.302	Depositor DCC
R_{free} test set	657 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2738	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3NE

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	2.03	65/2775 (2.3%)	1.69	41/3767 (1.1%)

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	1

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	57	ARG	C-O	-9.32	1.19	1.24
1	A	349	VAL	CA-CB	9.29	1.63	1.53
1	A	218	THR	CA-CB	9.16	1.67	1.54
1	A	57	ARG	N-CA	8.80	1.52	1.46
1	A	322	PRO	N-CA	8.76	1.57	1.47
1	A	351	PRO	CA-C	8.61	1.60	1.52
1	A	306	ALA	N-CA	8.31	1.56	1.46
1	A	278	ASN	CA-C	8.02	1.62	1.53
1	A	325	GLN	CD-NE2	8.01	1.50	1.33
1	A	168	ASP	CA-C	7.49	1.62	1.52
1	A	302	ALA	CA-CB	-7.31	1.41	1.53
1	A	169	PHE	N-CA	7.28	1.55	1.46
1	A	116	ILE	CA-CB	7.22	1.61	1.55
1	A	65	ALA	CA-CB	-7.03	1.42	1.53
1	A	40	ALA	CA-CB	-7.00	1.42	1.53
1	A	220	ARG	N-CA	6.82	1.53	1.45
1	A	114	ASN	CA-C	6.65	1.61	1.52
1	A	87	LEU	N-CA	6.46	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	ILE	C-O	-6.31	1.17	1.24
1	A	106	THR	C-O	6.21	1.31	1.23
1	A	34	ALA	CA-C	6.16	1.61	1.52
1	A	214	ALA	CA-C	6.03	1.60	1.52
1	A	348	PHE	N-CA	-6.02	1.38	1.46
1	A	57	ARG	NE-CZ	6.01	1.39	1.33
1	A	57	ARG	CA-CB	5.97	1.57	1.53
1	A	69	TYR	CA-C	5.97	1.60	1.52
1	A	24	TYR	CB-CG	5.97	1.64	1.51
1	A	84	ILE	CA-CB	5.96	1.60	1.54
1	A	212	ILE	CA-C	5.90	1.60	1.52
1	A	300	ALA	N-CA	5.88	1.53	1.46
1	A	84	ILE	CG1-CD1	5.86	1.74	1.51
1	A	72	LEU	C-O	5.79	1.30	1.24
1	A	85	GLY	CA-C	-5.76	1.45	1.51
1	A	250	ILE	CA-C	5.70	1.58	1.53
1	A	30	VAL	CA-CB	5.70	1.62	1.54
1	A	71	GLU	N-CA	-5.65	1.39	1.46
1	A	272	ASN	C-O	-5.65	1.17	1.24
1	A	282	VAL	CA-CB	-5.65	1.47	1.54
1	A	275	ILE	CA-CB	5.64	1.61	1.54
1	A	58	PRO	CA-C	5.62	1.61	1.52
1	A	80	HIS	CA-C	-5.62	1.45	1.52
1	A	291	LEU	N-CA	5.62	1.53	1.46
1	A	333	LEU	CA-C	5.59	1.59	1.52
1	A	198	MET	CG-SD	5.58	1.94	1.80
1	A	229	ILE	CA-CB	5.57	1.61	1.54
1	A	146	ILE	N-CA	-5.57	1.39	1.46
1	A	10	ARG	CG-CD	5.54	1.69	1.52
1	A	189	ARG	CB-CG	5.49	1.69	1.52
1	A	245	GLU	CG-CD	5.48	1.65	1.52
1	A	90	PHE	CA-C	5.46	1.59	1.52
1	A	167	LEU	N-CA	5.38	1.52	1.45
1	A	140	TYR	N-CA	5.37	1.52	1.46
1	A	230	ASP	N-CA	-5.36	1.40	1.46
1	A	134	ILE	N-CA	-5.33	1.40	1.46
1	A	349	VAL	CB-CG2	5.25	1.69	1.52
1	A	258	TYR	CE2-CZ	5.20	1.50	1.38
1	A	218	THR	C-O	-5.20	1.17	1.23
1	A	203	THR	CA-CB	5.19	1.62	1.53
1	A	24	TYR	CA-CB	5.17	1.61	1.53
1	A	224	PRO	CA-C	5.17	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	LEU	N-CA	5.14	1.52	1.46
1	A	9	TYR	C-O	-5.13	1.17	1.23
1	A	238	LEU	N-CA	5.06	1.52	1.46
1	A	342	TYR	N-CA	-5.06	1.40	1.46
1	A	116	ILE	CA-C	5.02	1.60	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	MET	CG-SD-CE	-8.88	81.35	100.90
1	A	57	ARG	CB-CA-C	-8.37	103.72	111.00
1	A	129	PHE	N-CA-C	-8.22	101.87	112.23
1	A	225	GLY	N-CA-C	-7.55	103.25	111.93
1	A	256	ARG	N-CA-C	-7.53	103.01	111.07
1	A	317	GLU	CA-C-N	7.12	127.08	120.03
1	A	317	GLU	C-N-CA	7.12	127.08	120.03
1	A	287	LYS	N-CA-C	7.00	121.08	112.54
1	A	350	PRO	CA-C-N	-6.97	113.20	120.38
1	A	350	PRO	C-N-CA	-6.97	113.20	120.38
1	A	116	ILE	CB-CA-C	6.92	117.59	111.71
1	A	277	ALA	CA-C-N	-6.85	111.33	120.65
1	A	277	ALA	C-N-CA	-6.85	111.33	120.65
1	A	280	LEU	N-CA-C	-6.83	103.91	111.36
1	A	340	LEU	N-CA-C	-6.66	104.10	111.36
1	A	124	ASP	N-CA-C	6.57	124.79	110.80
1	A	346	ILE	N-CA-C	6.54	117.23	110.36
1	A	154	SER	CA-C-N	-6.40	113.07	122.86
1	A	154	SER	C-N-CA	-6.40	113.07	122.86
1	A	155	ASN	CB-CA-C	6.24	121.18	111.13
1	A	22	GLU	N-CA-C	-6.22	105.17	112.89
1	A	98	GLU	N-CA-C	6.05	120.28	113.02
1	A	16	THR	CB-CA-C	6.04	119.74	109.53
1	A	232	LEU	N-CA-C	6.03	117.86	111.28
1	A	339	SER	N-CA-C	-5.88	105.20	112.90
1	A	321	ASP	CA-C-N	-5.87	113.90	119.89
1	A	321	ASP	C-N-CA	-5.87	113.90	119.89
1	A	85	GLY	N-CA-C	-5.78	99.75	110.73
1	A	160	GLU	CA-C-N	-5.67	114.19	122.86
1	A	160	GLU	C-N-CA	-5.67	114.19	122.86
1	A	318	PRO	CA-C-O	-5.60	114.92	122.08
1	A	233	LYS	N-CA-C	-5.57	105.11	111.07
1	A	87	LEU	N-CA-C	5.56	117.42	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	311	TYR	N-CA-C	-5.41	108.45	114.62
1	A	151	LEU	N-CA-C	-5.40	101.18	109.76
1	A	333	LEU	N-CA-C	5.34	117.97	110.23
1	A	247	LEU	N-CA-C	-5.29	105.69	111.82
1	A	150	ASP	N-CA-CB	-5.19	103.57	111.19
1	A	235	ILE	N-CA-C	5.17	115.39	110.42
1	A	39	CYS	N-CA-C	5.10	118.06	109.95
1	A	83	VAL	CA-C-O	-5.00	114.98	120.43

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	110	GLY	Peptide

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	A	2714	0	2697	74	0
2	A	24	0	7	0	0
All	All	2738	0	2704	74	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 14.

All (74) 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:84:ILE:CD1	1:A:84:ILE:CG1	1.74	1.57
1:A:10:ARG:HB2	1:A:10:ARG:NH1	1.73	1.01
1:A:10:ARG:HB2	1:A:10:ARG:CZ	2.00	0.92
1:A:210:GLY:HA2	1:A:288[A]:MET:HE3	1.55	0.88
1:A:210:GLY:HA2	1:A:288[A]:MET:CE	2.09	0.81
1:A:84:ILE:CD1	1:A:84:ILE:CB	2.60	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HG13	1:A:334:ILE:HG13	1.67	0.77
1:A:210:GLY:CA	1:A:288[A]:MET:HE3	2.15	0.76
1:A:22:GLU:O	1:A:25:GLN:NE2	2.19	0.75
1:A:194:MET:HE2	1:A:231:GLN:HB3	1.69	0.74
1:A:116:ILE:CD1	1:A:158:VAL:HG21	2.22	0.70
1:A:116:ILE:HD12	1:A:158:VAL:HG21	1.74	0.70
1:A:194:MET:HE1	1:A:228:HIS:HA	1.76	0.68
1:A:205:ASP:O	1:A:209:VAL:HG23	1.94	0.68
1:A:148:HIS:CD2	1:A:169:PHE:HA	2.34	0.63
1:A:116:ILE:O	1:A:119:CYS:N	2.33	0.61
1:A:114:ASN:O	1:A:116:ILE:N	2.33	0.61
1:A:19[B]:GLU:HB2	1:A:92:PRO:HG3	1.82	0.60
1:A:278:ASN:OD1	1:A:278:ASN:C	2.45	0.60
1:A:281:ALA:HB2	1:A:307:TYR:CE1	2.38	0.59
1:A:127:VAL:HG21	1:A:217:LEU:HD23	1.86	0.57
1:A:148:HIS:O	1:A:149:ARG:HB2	2.04	0.57
1:A:114:ASN:C	1:A:116:ILE:H	2.12	0.57
1:A:59:PHE:CE2	1:A:338:LYS:HA	2.40	0.56
1:A:114:ASN:C	1:A:116:ILE:N	2.65	0.55
1:A:265:MET:HA	1:A:265:MET:HE2	1.87	0.54
1:A:10:ARG:CZ	1:A:10:ARG:CB	2.83	0.54
1:A:226:THR:HG23	1:A:230:ASP:OD1	2.07	0.53
1:A:112:ASP:OD1	1:A:112:ASP:C	2.52	0.53
1:A:194:MET:HE1	1:A:228:HIS:CA	2.40	0.52
1:A:194:MET:CE	1:A:231:GLN:HB3	2.38	0.52
1:A:242:PRO:HG2	1:A:259[A]:ILE:CG2	2.41	0.51
1:A:74:LEU:O	1:A:78:MET:HG2	2.10	0.50
1:A:198:MET:HG2	1:A:199:HIS:CE1	2.47	0.50
1:A:223:PHE:HB2	1:A:231:GLN:HE22	1.77	0.50
1:A:242:PRO:HG2	1:A:259[A]:ILE:HG21	1.93	0.50
1:A:54:LYS:HG3	1:A:103:TYR:CE2	2.48	0.49
1:A:272:ASN:O	1:A:275:ILE:HG23	2.13	0.49
1:A:8:PHE:HA	1:A:21:PRO:HA	1.95	0.48
1:A:164:LEU:C	1:A:164:LEU:HD23	2.39	0.48
1:A:198:MET:HG2	1:A:199:HIS:ND1	2.28	0.47
1:A:112:ASP:O	1:A:115:ASN:HB2	2.14	0.47
1:A:93:ALA:HB2	1:A:99:PHE:HA	1.97	0.46
1:A:94:ARG:HG2	1:A:98:GLU:OE1	2.16	0.46
1:A:290:VAL:HG11	1:A:295:LYS:HB2	1.98	0.46
1:A:116:ILE:O	1:A:117:VAL:C	2.59	0.45
1:A:278:ASN:OD1	1:A:279:PRO:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ILE:HD11	1:A:158:VAL:HG21	1.97	0.45
1:A:223:PHE:CB	1:A:231:GLN:HE22	2.29	0.44
1:A:194:MET:HE3	1:A:194:MET:HB3	1.63	0.44
1:A:144:ALA:O	1:A:145:ASP:HB3	2.18	0.44
1:A:150:ASP:HB2	1:A:172:ALA:HB3	1.99	0.44
1:A:36:GLY:HA2	1:A:56[B]:SER:OG	2.18	0.43
1:A:144:ALA:O	1:A:145:ASP:CB	2.66	0.43
1:A:56[B]:SER:O	1:A:57:ARG:C	2.61	0.43
1:A:88:ASP:HA	1:A:348:PHE:CE2	2.54	0.43
1:A:10:ARG:HB2	1:A:10:ARG:HH11	1.74	0.43
1:A:148:HIS:CG	1:A:151:LEU:HD13	2.53	0.43
1:A:116:ILE:HD11	1:A:158:VAL:CG2	2.49	0.42
1:A:167:LEU:H	1:A:167:LEU:HG	1.72	0.42
1:A:74:LEU:HD12	1:A:171:LEU:HD23	2.01	0.42
1:A:84:ILE:HD13	1:A:84:ILE:HG21	2.00	0.42
1:A:334:ILE:HG21	1:A:334:ILE:HD13	1.77	0.42
1:A:57:ARG:HH11	1:A:57:ARG:HG3	1.83	0.42
1:A:57:ARG:HG3	1:A:57:ARG:NH1	2.36	0.41
1:A:275:ILE:HD12	1:A:275:ILE:H	1.84	0.41
1:A:149:ARG:HH11	1:A:149:ARG:HD2	1.73	0.41
1:A:122:LEU:HD23	1:A:126:HIS:HD2	1.86	0.41
1:A:185:THR:HG23	1:A:186:ARG:H	1.86	0.40
1:A:131:ILE:HG13	1:A:213:MET:HB2	2.03	0.40
1:A:247:LEU:HD11	1:A:260:GLN:HG3	2.03	0.40
1:A:91:THR:OG1	1:A:92:PRO:HD2	2.22	0.40
1:A:210:GLY:HA2	1:A:288[A]:MET:HE1	1.96	0.40
1:A:269:ASN:HB3	1:A:272:ASN:ND2	2.36	0.40

There are no symmetry-related clashes.

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	333/366 (91%)	301 (90%)	27 (8%)	5 (2%)	8	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLY
1	A	115	ASN
1	A	124	ASP
1	A	170	GLY
1	A	117	VAL

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	298/325 (92%)	269 (90%)	29 (10%)	8	17

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	13	LEU
1	A	28	SER
1	A	61	SER
1	A	63	ILE
1	A	81	GLU
1	A	89	VAL
1	A	113	LEU
1	A	122	LEU
1	A	124	ASP
1	A	167	LEU
1	A	169	PHE
1	A	171	LEU
1	A	196	ASN
1	A	198	MET
1	A	247	LEU

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Mol	Chain	Res	Type
1	A	248	LYS
1	A	251	SER
1	A	254	SER
1	A	256	ARG
1	A	264	GLN
1	A	275	ILE
1	A	291	LEU
1	A	295	LYS
1	A	325	GLN
1	A	329[A]	SER
1	A	329[B]	SER
1	A	330	ARG
1	A	338	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	196	ASN
1	A	257	ASN
1	A	269	ASN
1	A	272	ASN
1	A	325	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](#)

1 ligand is modelled in this entry.

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$
2	3NE	A	361	-	26,26,26	1.88	5 (19%)	34,41,41	3.49	17 (50%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	3NE	A	361	-	-	1/16/16/16	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	361	3NE	O18-C9	6.07	1.36	1.24
2	A	361	3NE	C12-N15	4.52	1.38	1.34
2	A	361	3NE	C9-N16	-2.99	1.33	1.38
2	A	361	3NE	N15-N17	-2.14	1.32	1.36
2	A	361	3NE	C1-C3	-2.07	1.35	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	3NE	C5-C9-N16	11.29	129.28	115.24
2	A	361	3NE	C10-C12-N16	9.77	131.34	123.46
2	A	361	3NE	O18-C9-C5	-7.09	115.67	125.46
2	A	361	3NE	F21-C13-C7	5.52	124.71	112.90
2	A	361	3NE	C6-C11-N17	-3.91	114.08	119.84
2	A	361	3NE	C3-C7-C4	3.31	124.22	117.86
2	A	361	3NE	C3-C7-C13	-3.04	115.07	119.96
2	A	361	3NE	O18-C9-N16	-2.92	115.05	119.27
2	A	361	3NE	C1-C3-C7	-2.83	117.88	120.75
2	A	361	3NE	C1-C2-C6	2.64	122.97	120.36
2	A	361	3NE	C6-C4-C7	-2.52	117.77	121.04
2	A	361	3NE	F22-C14-C8	2.51	117.51	112.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	3NE	C5-C8-C10	-2.38	115.28	118.48
2	A	361	3NE	F19-C13-C7	-2.34	107.89	112.90
2	A	361	3NE	C6-C11-C10	2.31	134.66	130.08
2	A	361	3NE	F23-C14-C8	2.25	117.03	112.68
2	A	361	3NE	F20-C13-C7	-2.16	108.27	112.90

There are no chirality outliers.

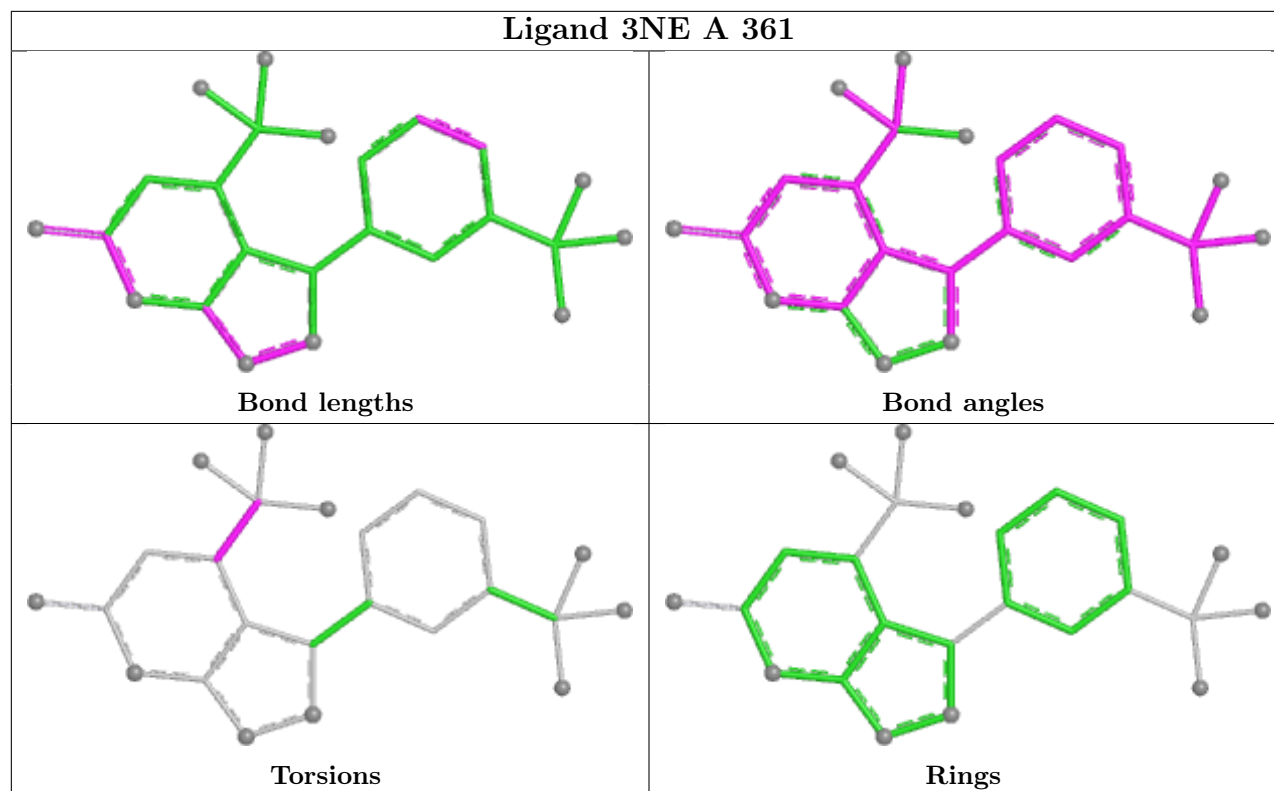
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	361	3NE	F23-C14-C8-C5

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 [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	334/366 (91%)	0.01	14 (4%)	40 36	11, 41, 67, 93	6 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	169	PHE	5.4
1	A	170	GLY	4.9
1	A	172	ALA	4.1
1	A	288[A]	MET	3.8
1	A	171	LEU	3.8
1	A	119	CYS	3.1
1	A	118	LYS	2.8
1	A	117	VAL	2.8
1	A	34	ALA	2.6
1	A	35	TYR	2.5
1	A	122	LEU	2.5
1	A	17	ILE	2.5
1	A	258	TYR	2.3
1	A	263	THR	2.2

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

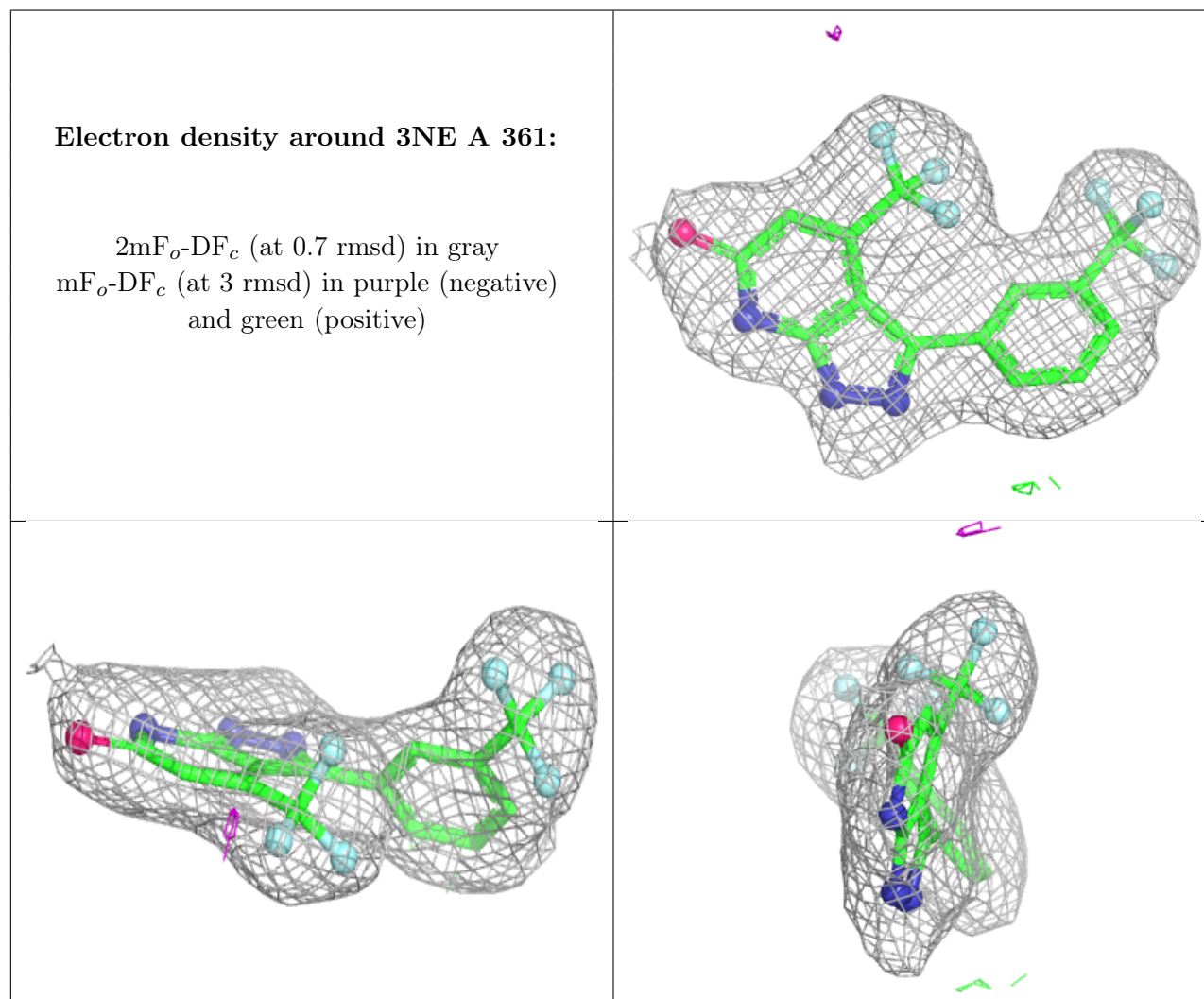
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3NE	A	361	24/24	0.94	0.08	39,50,56,58	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.