



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:46 AM UTC

PDB ID : 3Q3B / pdb_00003q3b
Title : 6-Amino-4-(pyrimidin-4-yl)pyridones: Novel Glycogen Synthase Kinase-3 Inhibitors
Authors : Pandit, J.
Deposited on : 2010-12-21
Resolution : 2.70 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

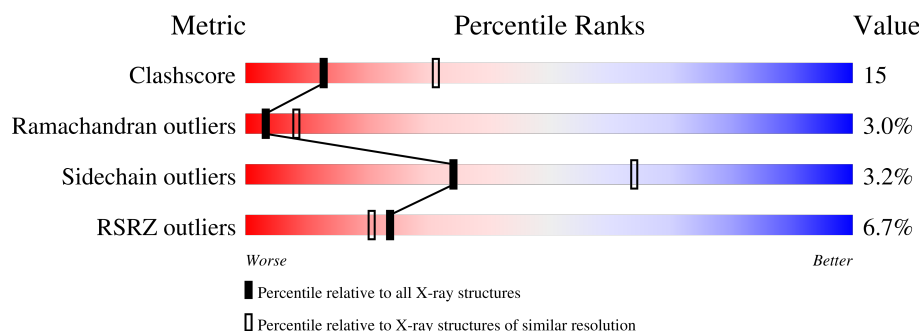
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	424	7% 55% 23% • 19%
1	B	424	4% 56% 21% • • 20%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5521 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.

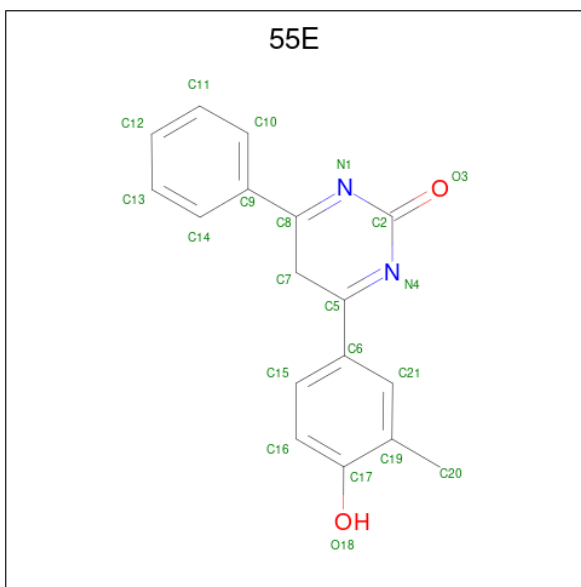
- Molecule 1 is a protein called Glycogen synthase kinase-3 beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2730	1756	470	493	11			
1	B	341	Total	C	N	O	S	0	0	0
			2708	1742	465	490	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P49841
A	-2	PRO	-	expression tag	UNP P49841
A	-1	LEU	-	expression tag	UNP P49841
A	0	GLY	-	expression tag	UNP P49841
A	1	SER	-	expression tag	UNP P49841
B	-3	GLY	-	expression tag	UNP P49841
B	-2	PRO	-	expression tag	UNP P49841
B	-1	LEU	-	expression tag	UNP P49841
B	0	GLY	-	expression tag	UNP P49841
B	1	SER	-	expression tag	UNP P49841

- Molecule 2 is 4-(4-hydroxy-3-methylphenyl)-6-phenylpyrimidin-2(5H)-one (CCD ID: 55E) (formula: C₁₇H₁₄N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	17	2	2		
2	B	1	Total	C	N	O	0	0
			21	17	2	2		

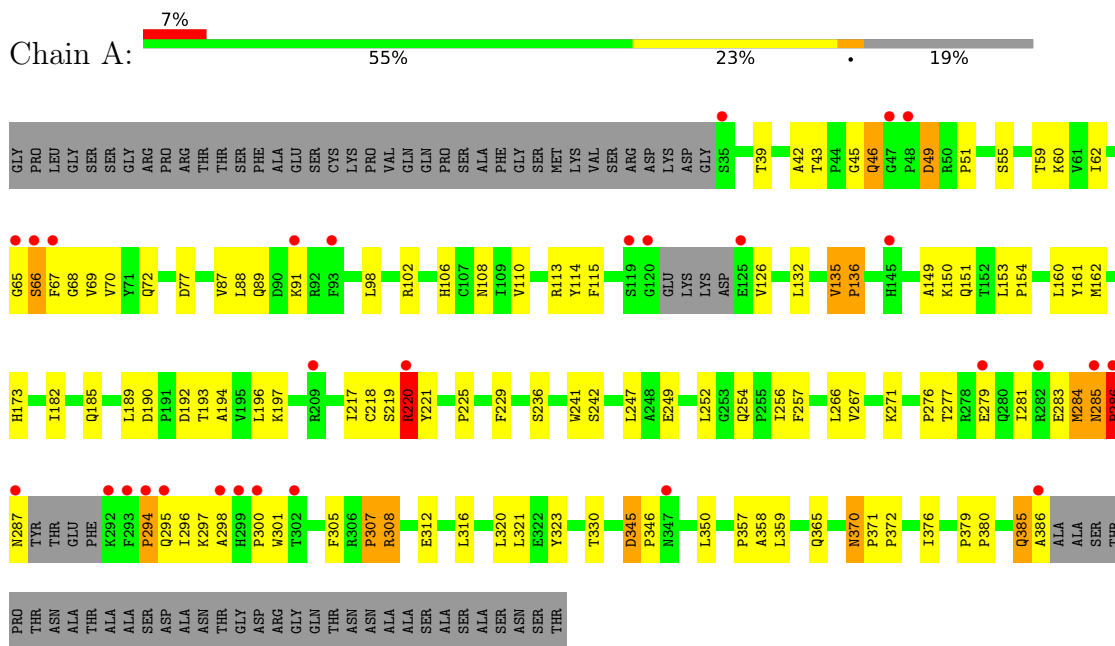
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	25	Total	O	0	0
			25	25		

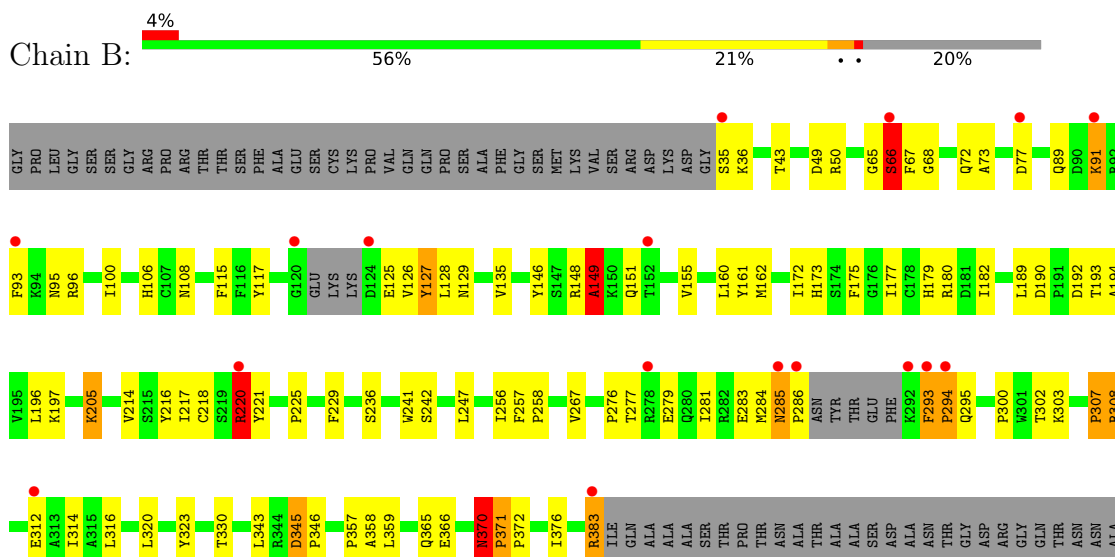
3 Residue-property plots [i](#)

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: Glycogen synthase kinase-3 beta



• Molecule 1: Glycogen synthase kinase-3 beta



ALA
SER
ALA
SER
ALA
SER
ASN
SER
THR

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.45Å 85.65Å 178.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 30.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.70) 88.8 (30.00-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.68Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.228 , 0.259 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.8	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5521	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: 55E

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/2797	1.09	14/3806 (0.4%)
1	B	0.68	0/2775	1.13	21/3776 (0.6%)
All	All	0.65	0/5572	1.11	35/7582 (0.5%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	VAL	CA-C-N	10.02	132.37	119.84
1	B	135	VAL	C-N-CA	10.02	132.37	119.84
1	A	135	VAL	CA-C-N	8.59	130.58	119.84
1	A	135	VAL	C-N-CA	8.59	130.58	119.84
1	B	66	SER	N-CA-C	-8.56	101.92	111.07
1	B	50	ARG	CA-C-N	6.88	127.26	119.83
1	B	50	ARG	C-N-CA	6.88	127.26	119.83
1	A	284	MET	N-CA-C	-6.47	105.38	113.28
1	B	127	TYR	N-CA-C	6.36	119.82	109.59
1	B	330	THR	N-CA-C	-6.16	102.33	110.40
1	A	190	ASP	N-CA-C	-6.08	97.48	109.10
1	B	345	ASP	CA-C-N	6.06	126.50	119.47
1	B	345	ASP	C-N-CA	6.06	126.50	119.47
1	A	330	THR	N-CA-C	-5.97	102.57	110.40
1	B	307	PRO	N-CA-C	-5.90	101.99	111.38
1	B	126	VAL	N-CA-C	5.89	116.41	108.17
1	B	220	ARG	N-CA-C	5.82	123.20	110.80
1	A	307	PRO	N-CA-C	-5.80	102.16	111.38
1	B	376	ILE	CB-CA-C	-5.75	105.78	111.30
1	B	149	ALA	N-CA-C	-5.67	98.73	110.80
1	A	345	ASP	CA-C-N	5.65	125.49	119.28
1	A	345	ASP	C-N-CA	5.65	125.49	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	THR	N-CA-C	5.55	117.78	108.23
1	B	190	ASP	N-CA-C	-5.55	98.50	109.10
1	A	219	SER	N-CA-C	5.41	118.92	110.32
1	A	192	ASP	N-CA-C	5.40	116.84	111.07
1	A	297	LYS	N-CA-C	5.39	118.40	109.94
1	A	376	ILE	CB-CA-C	-5.29	105.73	110.91
1	B	192	ASP	N-CA-C	5.23	116.67	111.07
1	B	205	LYS	N-CA-C	5.20	116.98	108.55
1	B	371	PRO	N-CA-C	5.16	117.00	110.70
1	B	370	ASN	CA-C-N	5.15	125.68	120.38
1	B	370	ASN	C-N-CA	5.15	125.68	120.38
1	B	175	PHE	N-CA-C	-5.14	106.85	113.02
1	A	42	ALA	N-CA-C	5.07	117.57	109.81

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2730	0	2752	84	0
1	B	2708	0	2726	86	0
2	A	21	0	14	0	0
2	B	21	0	13	0	0
3	A	16	0	0	0	0
3	B	25	0	0	0	0
All	All	5521	0	5505	166	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 15.

All (166) 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:385:GLN:HG3	1:A:386:ALA:H	1.17	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ASN:HB3	1:B:286:PRO:HD3	1.38	1.02
1:A:220:ARG:HD2	1:A:221:TYR:H	1.24	1.01
1:A:220:ARG:CD	1:A:221:TYR:H	1.74	0.99
1:A:307:PRO:O	1:A:308:ARG:HB2	1.69	0.92
1:A:89:GLN:HB3	1:A:126:VAL:HG12	1.52	0.90
1:A:220:ARG:HD2	1:A:221:TYR:N	1.87	0.88
1:A:66:SER:HB2	1:B:267:VAL:HG11	1.54	0.88
1:B:106:HIS:HD2	1:B:108:ASN:H	1.21	0.87
1:A:106:HIS:HD2	1:A:108:ASN:H	1.23	0.86
1:A:162:MET:HE2	1:A:247:LEU:HB2	1.58	0.85
1:A:60:LYS:HE2	1:A:72:GLN:NE2	1.92	0.84
1:A:385:GLN:HG3	1:A:386:ALA:N	1.91	0.84
1:B:106:HIS:CD2	1:B:108:ASN:H	1.98	0.82
1:A:285:ASN:HB3	1:A:286:PRO:HD3	1.62	0.81
1:A:284:MET:O	1:A:286:PRO:HD2	1.82	0.80
1:B:162:MET:HE2	1:B:247:LEU:HB2	1.64	0.79
1:B:285:ASN:CB	1:B:286:PRO:HD3	2.13	0.77
1:A:162:MET:HG3	1:A:247:LEU:HD13	1.69	0.75
1:B:281:ILE:HA	1:B:284:MET:HE3	1.69	0.75
1:B:220:ARG:HD3	1:B:221:TYR:H	1.54	0.72
1:B:285:ASN:HB3	1:B:286:PRO:CD	2.19	0.72
1:B:100:ILE:HG23	1:B:177:ILE:HD13	1.72	0.71
1:A:276:PRO:HG3	1:A:323:TYR:CZ	2.26	0.71
1:B:383:ARG:HA	1:B:383:ARG:HH11	1.53	0.70
1:A:385:GLN:CG	1:A:386:ALA:H	2.00	0.69
1:A:267:VAL:HG11	1:B:66:SER:HB2	1.75	0.69
1:A:308:ARG:HG3	1:A:308:ARG:HH11	1.57	0.69
1:A:49:ASP:O	1:A:51:PRO:HD3	1.93	0.68
1:B:149:ALA:O	1:B:151:GLN:HG3	1.96	0.66
1:B:220:ARG:HG2	1:B:220:ARG:HH11	1.60	0.65
1:A:106:HIS:CD2	1:A:108:ASN:H	2.09	0.65
1:A:308:ARG:HG3	1:A:308:ARG:NH1	2.10	0.65
1:B:220:ARG:CD	1:B:221:TYR:H	2.10	0.65
1:B:370:ASN:HD22	1:B:370:ASN:C	2.06	0.64
1:A:365:GLN:HE21	1:A:365:GLN:HA	1.63	0.63
1:B:229:PHE:O	1:B:286:PRO:HG2	1.97	0.63
1:B:148:ARG:HG3	1:B:148:ARG:O	1.98	0.63
1:A:285:ASN:HB3	1:A:286:PRO:CD	2.28	0.63
1:A:43:THR:HB	1:A:115:PHE:CE2	2.34	0.62
1:B:65:GLY:HA3	1:B:67:PHE:CE2	2.34	0.62
1:B:89:GLN:HE22	1:B:95:ASN:HB2	1.64	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PRO:HG3	1:B:323:TYR:CZ	2.36	0.61
1:B:196:LEU:C	1:B:196:LEU:HD23	2.26	0.60
1:B:293:PHE:H	1:B:293:PHE:HD1	1.45	0.60
1:A:196:LEU:C	1:A:196:LEU:HD23	2.27	0.60
1:A:284:MET:O	1:A:286:PRO:CD	2.50	0.60
1:A:370:ASN:HD22	1:A:370:ASN:C	2.11	0.59
1:B:357:PRO:O	1:B:359:LEU:HG	2.04	0.58
1:A:279:GLU:O	1:A:283:GLU:HG3	2.03	0.58
1:B:146:TYR:HB3	1:B:151:GLN:O	2.03	0.58
1:A:98:LEU:O	1:A:102:ARG:HG3	2.04	0.58
1:B:96:ARG:HH11	1:B:205:LYS:HG3	1.69	0.57
1:B:307:PRO:O	1:B:308:ARG:CB	2.53	0.57
1:B:162:MET:HG3	1:B:247:LEU:HD13	1.87	0.56
1:A:220:ARG:CD	1:A:221:TYR:N	2.54	0.56
1:B:358:ALA:O	1:B:359:LEU:HD23	2.05	0.56
1:B:365:GLN:HE21	1:B:365:GLN:HA	1.70	0.56
1:B:284:MET:O	1:B:285:ASN:CB	2.54	0.56
1:B:383:ARG:HA	1:B:383:ARG:NH1	2.18	0.56
1:A:220:ARG:HD3	1:A:221:TYR:H	1.64	0.56
1:B:106:HIS:HD2	1:B:108:ASN:N	1.97	0.55
1:B:293:PHE:CD1	1:B:293:PHE:N	2.59	0.55
1:B:279:GLU:O	1:B:283:GLU:HG3	2.05	0.55
1:B:370:ASN:HD22	1:B:372:PRO:HD2	1.71	0.55
1:B:371:PRO:HB2	1:B:372:PRO:HD3	1.88	0.55
1:B:370:ASN:C	1:B:370:ASN:ND2	2.65	0.55
1:B:89:GLN:HG3	1:B:91:LYS:H	1.73	0.54
1:A:149:ALA:O	1:A:151:GLN:HG3	2.07	0.54
1:B:96:ARG:NH1	1:B:205:LYS:HG3	2.23	0.54
1:A:45:GLY:N	1:A:113:ARG:O	2.39	0.54
1:A:312:GLU:H	1:A:312:GLU:CD	2.15	0.54
1:B:65:GLY:HA3	1:B:67:PHE:CD2	2.42	0.54
1:A:277:THR:O	1:A:281:ILE:HG13	2.08	0.54
1:A:281:ILE:HA	1:A:284:MET:HE3	1.90	0.54
1:A:365:GLN:HA	1:A:365:GLN:NE2	2.22	0.54
1:A:285:ASN:O	1:A:286:PRO:C	2.51	0.53
1:A:67:PHE:CD1	1:A:68:GLY:N	2.76	0.53
1:A:173:HIS:CE1	1:A:236:SER:HB3	2.44	0.53
1:A:371:PRO:HB2	1:A:372:PRO:HD3	1.91	0.53
1:B:221:TYR:CD2	1:B:258:PRO:HA	2.44	0.52
1:A:308:ARG:HH11	1:A:308:ARG:CG	2.22	0.52
1:B:300:PRO:HG2	1:B:303:LYS:CB	2.39	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:HE2	1:A:72:GLN:HE22	1.73	0.51
1:B:220:ARG:HG2	1:B:220:ARG:NH1	2.25	0.51
1:B:89:GLN:HA	1:B:89:GLN:OE1	2.11	0.51
1:B:284:MET:O	1:B:285:ASN:HB3	2.11	0.51
1:B:307:PRO:O	1:B:308:ARG:HB2	2.09	0.51
1:A:301:TRP:HH2	1:A:321:LEU:HD12	1.75	0.51
1:A:161:TYR:CE1	1:A:189:LEU:HD22	2.46	0.51
1:A:271:LYS:NZ	1:B:66:SER:HA	2.26	0.50
1:B:173:HIS:CE1	1:B:236:SER:HB3	2.46	0.50
1:A:69:VAL:HG12	1:A:70:VAL:N	2.27	0.50
1:B:312:GLU:H	1:B:312:GLU:CD	2.18	0.50
1:A:252:LEU:HG	1:A:305:PHE:CE1	2.47	0.50
1:A:301:TRP:CH2	1:A:321:LEU:HD12	2.46	0.50
1:A:39:THR:HG23	1:A:55:SER:OG	2.11	0.50
1:B:300:PRO:HG2	1:B:303:LYS:HB3	1.93	0.49
1:B:307:PRO:O	1:B:308:ARG:HG2	2.12	0.49
1:B:193:THR:O	1:B:194:ALA:HB3	2.12	0.49
1:A:67:PHE:CG	1:A:68:GLY:N	2.80	0.49
1:A:217:ILE:O	1:A:218:CYS:CB	2.60	0.49
1:B:35:SER:OG	1:B:36:LYS:N	2.44	0.49
1:A:62:ILE:HG12	1:A:70:VAL:O	2.12	0.49
1:A:357:PRO:O	1:A:359:LEU:HG	2.13	0.49
1:A:370:ASN:C	1:A:370:ASN:ND2	2.70	0.49
1:B:160:LEU:CD2	1:B:343:LEU:HD22	2.43	0.49
1:A:285:ASN:CB	1:A:286:PRO:CD	2.92	0.48
1:B:95:ASN:ND2	1:B:128:LEU:HD23	2.28	0.48
1:B:277:THR:O	1:B:281:ILE:HG13	2.14	0.48
1:B:365:GLN:HA	1:B:365:GLN:NE2	2.28	0.48
1:B:160:LEU:HD23	1:B:343:LEU:HD22	1.94	0.48
1:A:153:LEU:HD12	1:A:154:PRO:HD2	1.96	0.48
1:A:271:LYS:HZ1	1:B:66:SER:HA	1.79	0.48
1:A:370:ASN:HD22	1:A:372:PRO:HD2	1.80	0.47
1:B:43:THR:HB	1:B:115:PHE:CE2	2.50	0.47
1:A:294:PRO:O	1:A:296:ILE:HG13	2.15	0.47
1:B:161:TYR:CE1	1:B:189:LEU:HD22	2.49	0.47
1:B:115:PHE:HA	1:B:129:ASN:O	2.15	0.46
1:A:87:VAL:CG1	1:A:88:LEU:N	2.78	0.46
1:A:196:LEU:HD23	1:A:197:LYS:N	2.31	0.46
1:B:106:HIS:CD2	1:B:108:ASN:HB2	2.51	0.46
1:B:196:LEU:HD23	1:B:197:LYS:N	2.31	0.46
1:A:193:THR:O	1:A:194:ALA:HB3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ILE:HB	1:A:242:SER:CB	2.47	0.45
1:B:307:PRO:O	1:B:308:ARG:CG	2.65	0.45
1:B:182:ILE:HB	1:B:242:SER:CB	2.47	0.45
1:A:87:VAL:HG12	1:A:88:LEU:N	2.31	0.45
1:A:135:VAL:HA	1:A:136:PRO:HD3	1.83	0.45
1:A:284:MET:O	1:A:285:ASN:HB3	2.17	0.45
1:B:172:ILE:HG13	1:B:173:HIS:N	2.32	0.45
1:A:266:LEU:HD23	1:A:266:LEU:HA	1.80	0.44
1:B:193:THR:O	1:B:357:PRO:HG3	2.17	0.44
1:B:256:ILE:HG23	1:B:257:PHE:CG	2.51	0.44
1:A:217:ILE:O	1:A:218:CYS:HB3	2.18	0.44
1:A:256:ILE:HG23	1:A:257:PHE:CG	2.52	0.44
1:A:345:ASP:HA	1:A:346:PRO:HD3	1.85	0.44
1:B:217:ILE:O	1:B:218:CYS:CB	2.64	0.44
1:A:106:HIS:HD2	1:A:108:ASN:N	2.04	0.44
1:B:67:PHE:CD1	1:B:68:GLY:N	2.86	0.43
1:A:229:PHE:O	1:A:286:PRO:HG2	2.18	0.43
1:A:358:ALA:O	1:A:359:LEU:HD23	2.17	0.43
1:B:148:ARG:O	1:B:148:ARG:CG	2.66	0.43
1:B:302:THR:HA	1:B:314:ILE:HD13	2.01	0.43
1:A:379:PRO:HA	1:A:380:PRO:HD3	1.93	0.42
1:B:316:LEU:O	1:B:320:LEU:HG	2.18	0.42
1:B:285:ASN:HD22	1:B:286:PRO:HD3	1.84	0.42
1:B:345:ASP:HA	1:B:346:PRO:HD3	1.84	0.42
1:A:316:LEU:O	1:A:320:LEU:HG	2.20	0.42
1:B:285:ASN:CB	1:B:286:PRO:CD	2.80	0.42
1:A:249:GLU:HG3	1:A:254:GLN:C	2.45	0.42
1:B:72:GLN:HG2	1:B:73:ALA:N	2.35	0.41
1:B:225:PRO:HD3	1:B:241:TRP:CE2	2.55	0.41
1:B:117:TYR:HA	1:B:127:TYR:O	2.21	0.41
1:A:160:LEU:HD11	1:A:350:LEU:CD2	2.50	0.41
1:A:298:ALA:O	1:A:300:PRO:HD3	2.21	0.41
1:A:185:GLN:NE2	1:A:220:ARG:NH2	2.69	0.41
1:B:214:VAL:HB	1:B:216:TYR:CE2	2.56	0.41
1:A:229:PHE:O	1:A:286:PRO:CG	2.69	0.41
1:A:65:GLY:O	1:A:66:SER:C	2.64	0.40
1:B:106:HIS:HE1	1:B:366:GLU:OE1	2.04	0.40
1:B:179:HIS:O	1:B:180:ARG:HB2	2.21	0.40
1:A:46:GLN:HE21	1:A:46:GLN:HB3	1.50	0.40
1:B:89:GLN:C	1:B:91:LYS:N	2.79	0.40
1:B:67:PHE:CG	1:B:68:GLY:N	2.90	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:HD3	1:A:241:TRP:CE2	2.56	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	338/424 (80%)	310 (92%)	17 (5%)	11 (3%)	3	7
1	B	335/424 (79%)	314 (94%)	12 (4%)	9 (3%)	4	10
All	All	673/848 (79%)	624 (93%)	29 (4%)	20 (3%)	3	8

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	220	ARG
1	A	285	ASN
1	B	77	ASP
1	B	149	ALA
1	B	220	ARG
1	B	285	ASN
1	A	49	ASP
1	A	77	ASP
1	A	91	LYS
1	A	294	PRO
1	A	295	GLN
1	B	308	ARG
1	A	286	PRO
1	B	49	ASP
1	B	91	LYS
1	B	155	VAL
1	B	294	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	150	LYS
1	A	385	GLN
1	A	136	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/366 (82%)	292 (97%)	10 (3%)	33	63
1	B	300/366 (82%)	291 (97%)	9 (3%)	36	66
All	All	602/732 (82%)	583 (97%)	19 (3%)	34	64

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	66	SER
1	A	110	VAL
1	A	114	TYR
1	A	132	LEU
1	A	220	ARG
1	A	286	PRO
1	A	287	ASN
1	A	308	ARG
1	A	370	ASN
1	B	66	SER
1	B	93	PHE
1	B	125	GLU
1	B	220	ARG
1	B	293	PHE
1	B	294	PRO
1	B	295	GLN
1	B	370	ASN
1	B	383	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	72	GLN
1	A	106	HIS
1	A	108	ASN
1	A	185	GLN
1	A	299	HIS
1	A	365	GLN
1	A	370	ASN
1	B	72	GLN
1	B	106	HIS
1	B	108	ASN
1	B	145	HIS
1	B	285	ASN
1	B	365	GLN
1	B	370	ASN

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](#)

2 ligands are 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	55E	B	421	-	21,23,23	2.84	12 (57%)	27,32,32	1.04	3 (11%)
2	55E	A	421	-	21,23,23	2.52	9 (42%)	27,32,32	1.05	2 (7%)

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
2	55E	B	421	-	-	0/8/20/20	0/2/3/3
2	55E	A	421	-	-	0/8/20/20	0/2/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	421	55E	C2-N4	6.95	1.48	1.38
2	B	421	55E	C8-N1	6.38	1.51	1.33
2	A	421	55E	C8-N1	5.87	1.50	1.33
2	A	421	55E	C2-N4	5.82	1.47	1.38
2	B	421	55E	C14-C9	3.56	1.44	1.39
2	B	421	55E	C9-C8	3.16	1.53	1.47
2	B	421	55E	C6-C5	2.97	1.53	1.47
2	B	421	55E	C10-C9	2.91	1.43	1.39
2	A	421	55E	C13-C14	2.77	1.43	1.38
2	B	421	55E	C13-C14	2.76	1.43	1.38
2	A	421	55E	C14-C9	2.75	1.43	1.39
2	B	421	55E	C11-C12	2.67	1.44	1.38
2	A	421	55E	C10-C9	2.61	1.43	1.39
2	A	421	55E	C11-C10	2.49	1.43	1.38
2	A	421	55E	C17-C19	2.46	1.43	1.40
2	A	421	55E	C12-C13	2.32	1.43	1.38
2	B	421	55E	C21-C6	2.16	1.42	1.39
2	B	421	55E	C12-C13	2.16	1.43	1.38
2	B	421	55E	C17-C19	2.11	1.42	1.40
2	A	421	55E	C6-C5	2.06	1.51	1.47
2	B	421	55E	C11-C10	2.05	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	421	55E	O3-C2-N4	2.39	122.76	118.72
2	B	421	55E	O18-C17-C19	2.29	122.01	117.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	421	55E	O18-C17-C19	2.19	121.82	117.60
2	B	421	55E	N1-C2-N4	-2.11	117.51	122.56
2	A	421	55E	O3-C2-N4	2.06	122.20	118.72

There are no chirality outliers.

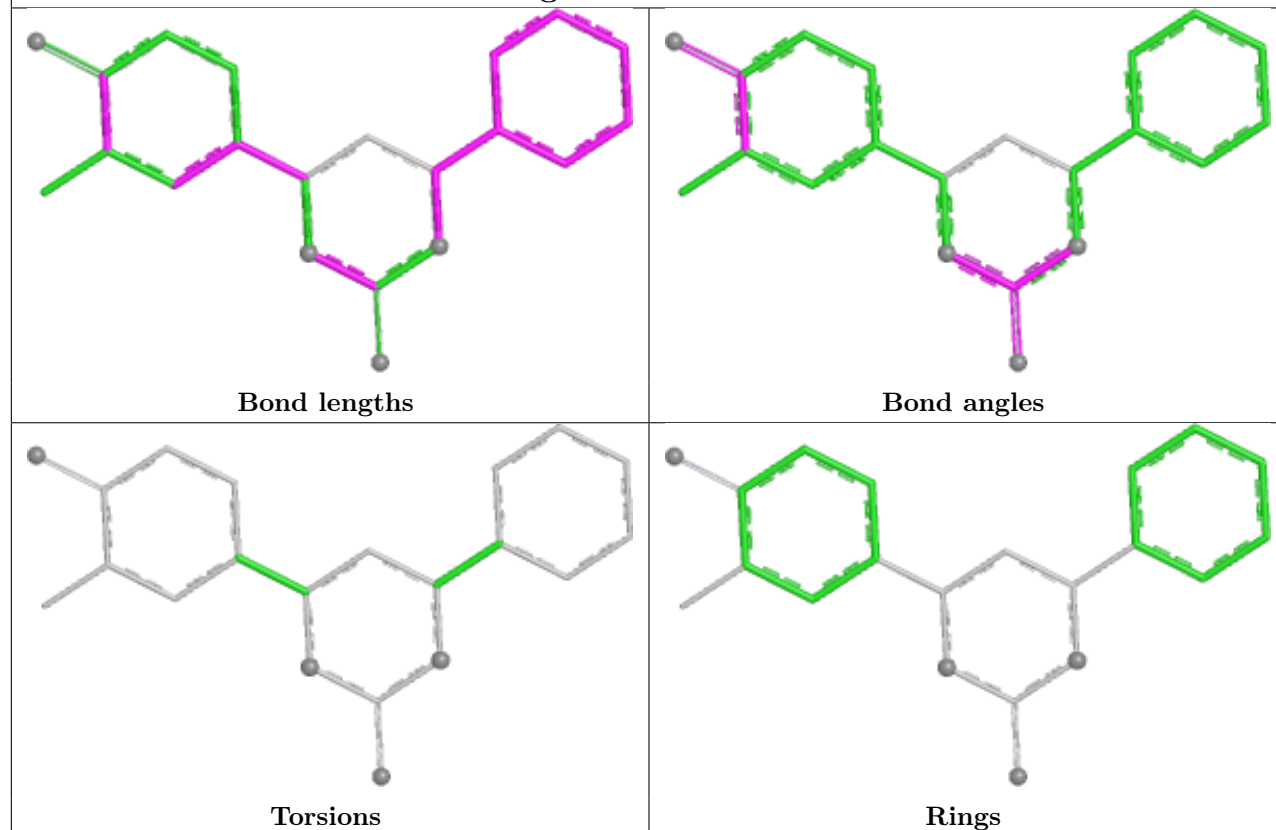
There are no torsion outliers.

There are no ring outliers.

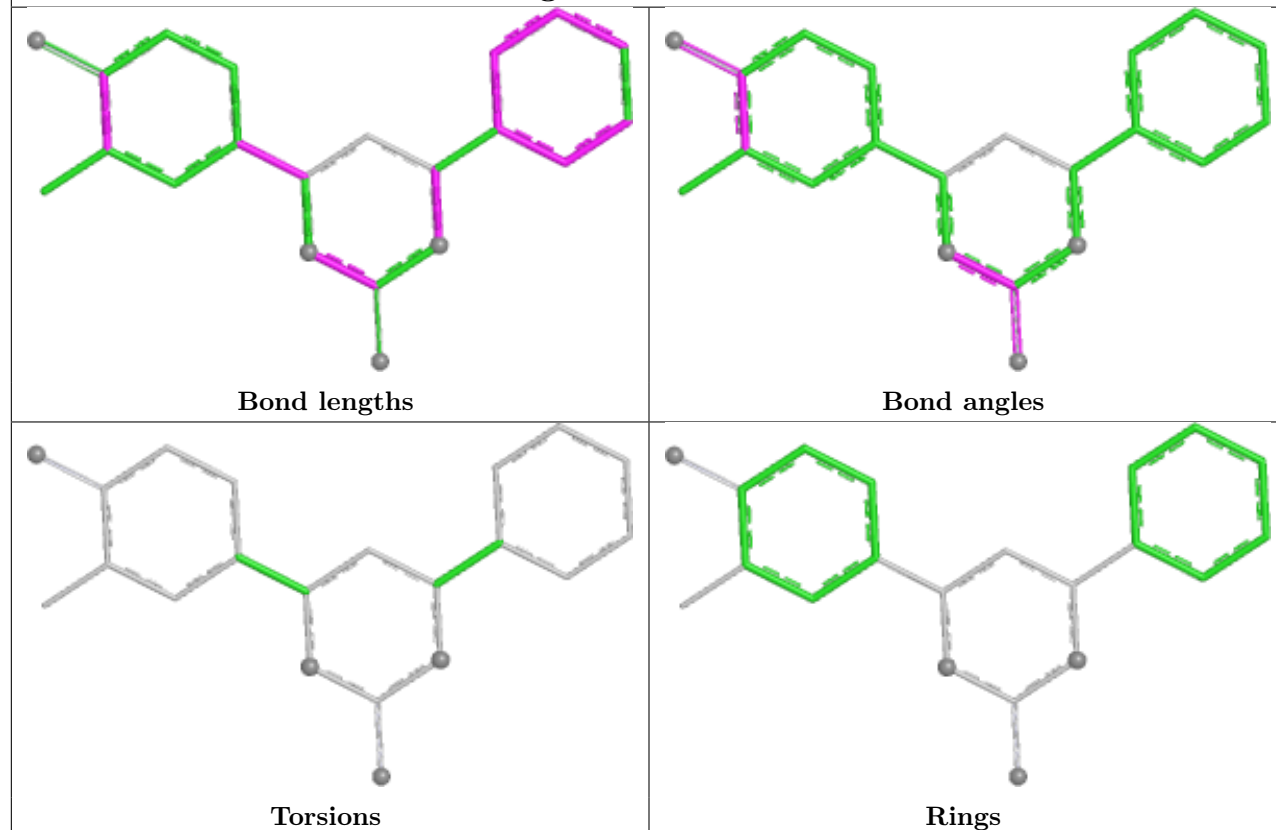
No monomer is involved in short contacts.

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.

Ligand 55E B 421



Ligand 55E A 421



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	344/424 (81%)	0.43	29 (8%) 17 14	26, 51, 111, 164	0
1	B	341/424 (80%)	0.26	17 (4%) 34 30	25, 45, 99, 156	0
All	All	685/848 (80%)	0.34	46 (6%) 24 21	25, 47, 107, 164	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	ALA	7.5
1	B	286	PRO	6.2
1	A	285	ASN	6.1
1	A	286	PRO	5.9
1	B	120	GLY	5.8
1	A	120	GLY	5.8
1	B	91	LYS	4.9
1	B	292	LYS	4.4
1	A	93	PHE	4.3
1	B	220	ARG	4.2
1	B	93	PHE	4.2
1	A	287	ASN	3.8
1	A	125	GLU	3.8
1	B	293	PHE	3.8
1	B	383	ARG	3.7
1	A	35	SER	3.6
1	B	124	ASP	3.3
1	A	295	GLN	3.3
1	B	77	ASP	3.3
1	A	302	THR	3.2
1	A	298	ALA	3.1
1	B	294	PRO	2.9
1	B	66	SER	2.9
1	A	66	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	285	ASN	2.7
1	A	220	ARG	2.7
1	A	48	PRO	2.6
1	A	294	PRO	2.6
1	A	300	PRO	2.6
1	A	293	PHE	2.6
1	B	35	SER	2.5
1	B	152	THR	2.4
1	A	299	HIS	2.4
1	A	67	PHE	2.4
1	A	292	LYS	2.4
1	A	65	GLY	2.4
1	A	119	SER	2.3
1	A	347	ASN	2.3
1	A	47	GLY	2.3
1	A	209	ARG	2.1
1	A	279	GLU	2.1
1	A	145	HIS	2.1
1	A	282	ARG	2.1
1	B	312	GLU	2.1
1	A	91	LYS	2.1
1	B	278	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	55E	A	421	21/21	0.91	0.12	48,48,48,48	0

Continued on next page...

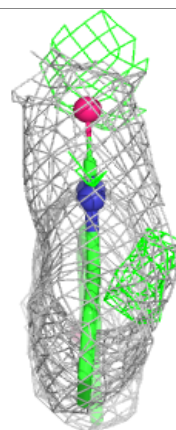
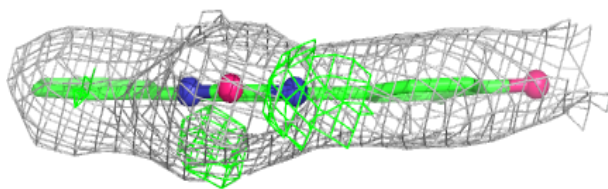
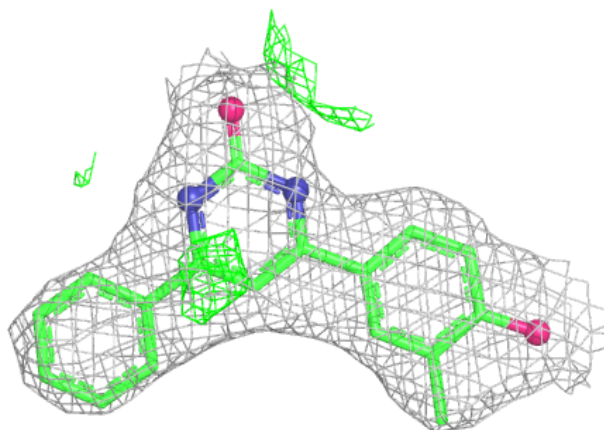
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	55E	B	421	21/21	0.94	0.11	45,45,45,45	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.

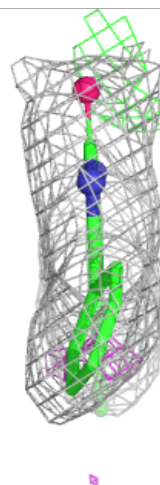
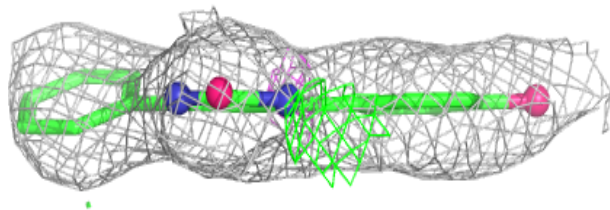
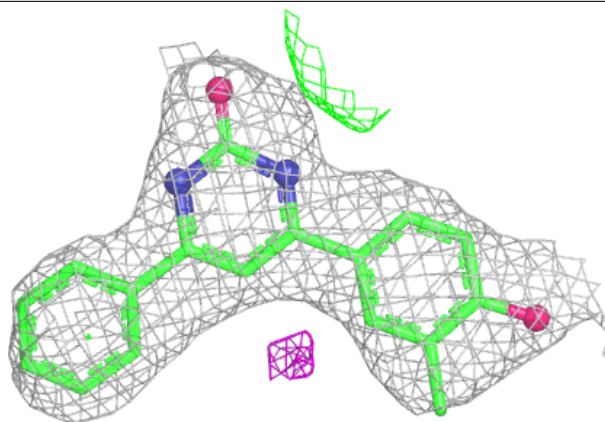
Electron density around 55E A 421:

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



Electron density around 55E B 421:

$2mF_o-DF_c$ (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.