



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:27 PM UTC

PDB ID : 2X6D / pdb_00002x6d
Title : Aurora-A bound to an inhibitor
Authors : Kosmopoulou, M.; Bayliss, R.
Deposited on : 2010-02-17
Resolution : 2.80 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

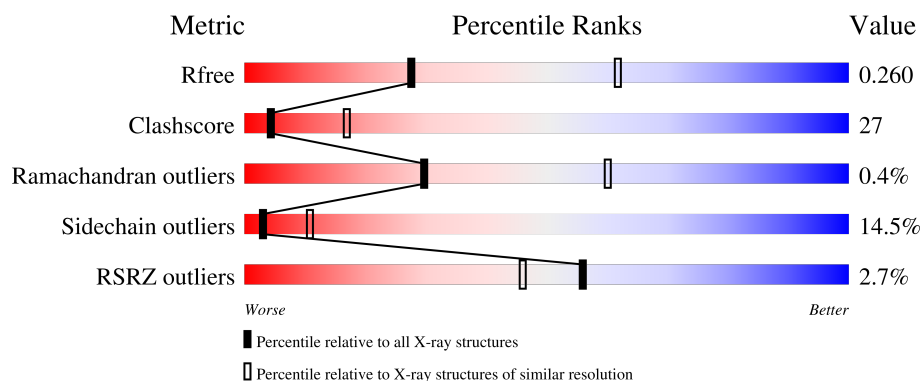
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	285	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2181 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 SERINE/THREONINE-PROTEIN KINASE 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	2107	1354	368	379	6	0	4	0

There are 3 discrepancies between the modelled and reference sequences:

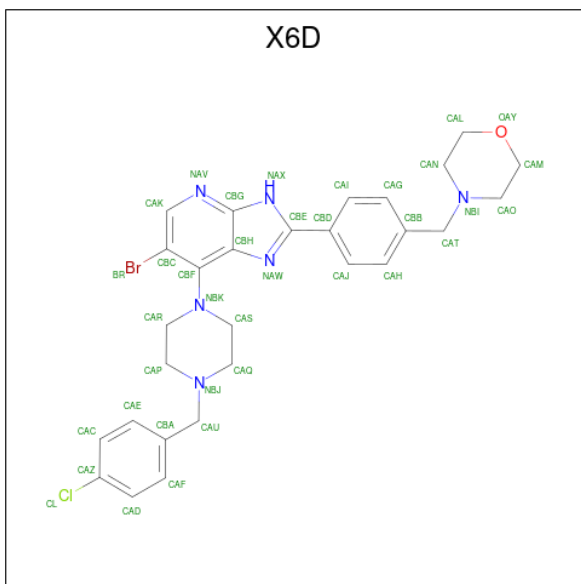
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP O14965
A	120	ALA	-	expression tag	UNP O14965
A	121	MET	-	expression tag	UNP O14965

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 6-BROMO-7-[4-(4-CHLOROBENZYL)PIPERAZIN-1-YL]-2-[4-(MORPHOLIN-4-YLMETHYL)PHENYL]-3H-IMIDAZO[4,5-B]PYRIDINE (CCD ID: X6D) (formula: $C_{28}H_{30}BrClN_6O$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	Br	C	Cl	N	O	0	0
			37	1	28	1	6	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	27	Total O 27 27	0	0

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.

Chain A:

47% 31% 10% 11%

GLY
ALA
MET
GLU
SER
LYS
LYS
L128
L130
L131
D132
F133
L134
I135
K143
F144
G145
M146
L149
E152
K153
Q154
S155
K156
F157
I158
L159
V162
V163
L164
F165
F166
L167
Q168
L169
E170
LYS
ALA
GLY
VAL
E175
H176
Q177
L178
R179
R180
E181
V182
E183
I184
Q185
S186
H187
L188
F189
H190
P191
M192
R195
L196
F200
H201
D202
A203
T204
R205
V206
Y207
L208
T209
L210
Y219
R220
E221
D223
K224
L225
S226
K227
R232
T238
E239
L240
L244
S245
Y246
L253
L254
R255
D256
L257
E260
A267
G268
E269
L272
A273
D274
V279
H280
R285
L286
L363
N367
P368
R371
L378
E379
H380
P381
W382
N386
S387
S388
LYS
PRO
SER
ASN
CYS
GLN
ASN
LYS
GLU
SER
ALA
SER
LYS
GLN
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	81.57Å 81.57Å 171.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 2.80 19.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.84-2.80) 99.4 (19.84-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.44 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.264 0.211 , 0.260	Depositor DCC
R_{free} test set	424 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2181	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: SO4, X6D

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	1.13	9/2160 (0.4%)	1.38	28/2922 (1.0%)

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 (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	SER	CA-C	15.74	1.74	1.52
1	A	225	LEU	CA-C	-7.20	1.43	1.52
1	A	177	GLN	CA-CB	-6.85	1.43	1.53
1	A	386	ASN	C-N	6.70	1.41	1.33
1	A	179	ARG	NE-CZ	-6.11	1.26	1.33
1	A	327	PRO	CA-C	5.29	1.55	1.52
1	A	224	LYS	C-O	-5.26	1.18	1.24
1	A	225	LEU	C-N	-5.20	1.26	1.33
1	A	343	ARG	CA-C	5.02	1.59	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ARG	NE-CZ-NH1	-14.82	106.68	121.50
1	A	176	HIS	N-CA-C	9.70	127.38	111.37
1	A	179	ARG	NH1-CZ-NH2	8.63	130.52	119.30
1	A	227	LYS	N-CA-C	-7.88	96.28	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LEU	CA-C-N	7.83	128.45	120.38
1	A	296	LEU	C-N-CA	7.83	128.45	120.38
1	A	225	LEU	N-CA-C	-7.64	96.77	109.46
1	A	175	GLU	CG-CD-OE1	-7.43	101.31	118.40
1	A	204	THR	N-CA-C	-7.43	94.98	110.80
1	A	179	ARG	N-CA-C	-6.81	103.79	111.07
1	A	386	ASN	CA-C-N	-6.77	111.04	121.74
1	A	386	ASN	C-N-CA	-6.77	111.04	121.74
1	A	177	GLN	N-CA-CB	-6.12	101.53	110.47
1	A	294	ASP	N-CA-C	6.08	117.90	111.28
1	A	190	HIS	CA-C-N	6.06	125.74	119.56
1	A	190	HIS	C-N-CA	6.06	125.74	119.56
1	A	209	ILE	CB-CA-C	-6.02	105.42	111.80
1	A	327	PRO	CA-C-N	5.70	125.41	119.82
1	A	327	PRO	C-N-CA	5.70	125.41	119.82
1	A	202	ASP	N-CA-C	-5.59	107.46	114.56
1	A	291	GLY	CA-C-O	-5.57	117.81	122.33
1	A	371	ARG	CA-C-N	5.43	125.37	119.78
1	A	371	ARG	C-N-CA	5.43	125.37	119.78
1	A	133	PHE	N-CA-C	5.37	117.65	108.90
1	A	175	GLU	OE1-CD-OE2	5.26	135.53	122.90
1	A	210	LEU	N-CA-C	5.14	118.11	110.14
1	A	387	SER	N-CA-CB	-5.11	102.67	110.39
1	A	345	GLU	N-CA-C	5.04	117.56	107.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	SER	Mainchain

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	2107	0	2069	111	9
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	37	0	30	5	0
4	A	27	0	0	6	0
All	All	2181	0	2099	114	9

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 (114) 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:168:GLN:O	1:A:170:GLU:HG3	1.44	1.15
1:A:180:ARG:HH21	1:A:279:VAL:HG23	1.10	1.14
1:A:302:GLU:OE2	1:A:304:ARG:NH2	1.83	1.09
1:A:180:ARG:NH2	1:A:279:VAL:HG23	1.69	1.06
1:A:178:LEU:O	1:A:178:LEU:HD12	1.55	1.05
1:A:190:HIS:HD2	1:A:192:ASN:H	1.03	1.00
1:A:178:LEU:HD12	1:A:178:LEU:C	1.91	0.95
1:A:333:THR:HG22	1:A:336:GLU:H	1.35	0.89
1:A:335:GLN:HE21	1:A:335:GLN:H	1.17	0.88
1:A:190:HIS:CD2	1:A:192:ASN:H	1.91	0.88
1:A:202:ASP:O	1:A:203:ALA:HB3	1.73	0.88
1:A:175:GLU:O	1:A:179:ARG:HG3	1.74	0.86
1:A:330:GLU:HG3	4:A:2022:HOH:O	1.79	0.81
1:A:200:PHE:CE1	1:A:207:TYR:CD2	2.68	0.80
1:A:166:LYS:HE3	1:A:206:VAL:HG23	1.65	0.79
1:A:180:ARG:NH2	1:A:279:VAL:CG2	2.45	0.79
1:A:221:GLU:OE2	1:A:232:ARG:NH1	2.15	0.78
1:A:182:VAL:O	1:A:186:SER:OG	2.04	0.76
1:A:333:THR:HG22	1:A:336:GLU:N	2.01	0.76
3:A:1391:X6D:NAW	3:A:1391:X6D:HAS1	2.02	0.73
1:A:175:GLU:O	1:A:179:ARG:CG	2.36	0.73
1:A:309:LYS:NZ	1:A:371:ARG:O	2.24	0.71
1:A:202:ASP:O	1:A:202:ASP:OD2	2.09	0.70
1:A:202:ASP:O	1:A:203:ALA:CB	2.41	0.69
1:A:359:LEU:HD22	1:A:363:LEU:HD22	1.74	0.69
1:A:290:CYS:N	4:A:2018:HOH:O	2.25	0.68
1:A:359:LEU:HD22	1:A:363:LEU:CD2	2.23	0.68
1:A:307:ASP:O	1:A:310:VAL:HG23	1.94	0.67
1:A:358:ASP:OD2	1:A:380:HIS:HE1	1.78	0.67
1:A:333:THR:HG23	1:A:335:GLN:HE21	1.60	0.67
1:A:181:GLU:O	1:A:181:GLU:HG3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLN:HB3	1:A:196:LEU:HD12	1.79	0.65
1:A:346:PHE:HA	4:A:2025:HOH:O	1.95	0.65
1:A:190:HIS:HD2	1:A:192:ASN:N	1.85	0.65
1:A:333:THR:HG23	1:A:335:GLN:NE2	2.13	0.64
1:A:166:LYS:HZ3	1:A:203:ALA:HA	1.62	0.64
1:A:253:ILE:HG22	1:A:308:GLU:HA	1.80	0.63
1:A:202:ASP:HB2	1:A:207:TYR:HE2	1.64	0.63
1:A:177:GLN:O	1:A:181:GLU:N	2.21	0.62
1:A:354:GLU:HA	1:A:354:GLU:OE1	1.99	0.61
1:A:327:PRO:HB2	4:A:2020:HOH:O	2.00	0.61
1:A:157:PHE:HD2	1:A:159:LEU:HD23	1.65	0.61
1:A:181:GLU:O	1:A:181:GLU:CG	2.50	0.60
1:A:220[A]:ARG:NH2	3:A:1391:X6D:HAO1	2.16	0.60
1:A:227:LYS:HG2	1:A:323:LEU:O	2.02	0.59
1:A:318:LEU:HD22	1:A:322:PHE:CZ	2.37	0.58
1:A:175:GLU:O	1:A:179:ARG:CD	2.52	0.58
1:A:343:ARG:HH11	1:A:343:ARG:CG	2.18	0.57
1:A:162:LYS:HD3	1:A:164:LEU:HD11	1.87	0.57
1:A:166:LYS:NZ	1:A:203:ALA:HA	2.20	0.57
1:A:335:GLN:HE21	1:A:335:GLN:N	1.96	0.57
1:A:168:GLN:O	1:A:170:GLU:CG	2.36	0.57
1:A:201:HIS:HB3	1:A:206:VAL:HG22	1.87	0.56
1:A:202:ASP:OD2	1:A:202:ASP:C	2.50	0.55
1:A:254:HIS:CG	1:A:257:ILE:HD12	2.41	0.55
1:A:253:ILE:CG2	1:A:308:GLU:HA	2.36	0.54
1:A:331:ALA:HB1	1:A:336:GLU:CD	2.33	0.54
1:A:240:LEU:HD23	1:A:272:ILE:HD11	1.90	0.54
1:A:346:PHE:CA	4:A:2025:HOH:O	2.54	0.53
1:A:317:VAL:HG13	1:A:328:PRO:HD2	1.91	0.53
1:A:224:LYS:HE2	1:A:225:LEU:HD21	1.92	0.52
1:A:190:HIS:CD2	1:A:192:ASN:HB2	2.45	0.52
1:A:254:HIS:HB3	1:A:257:ILE:HD12	1.91	0.52
1:A:343:ARG:HH11	1:A:343:ARG:HG3	1.75	0.51
1:A:387:SER:OG	1:A:388:SER:N	2.42	0.51
3:A:1391:X6D:HAN2	3:A:1391:X6D:CAH	2.41	0.50
1:A:208:LEU:HD12	1:A:208:LEU:N	2.27	0.50
1:A:279:VAL:HG22	1:A:280[B]:HIS:CD2	2.47	0.50
1:A:313:TRP:O	1:A:317:VAL:HG23	2.12	0.50
1:A:253:ILE:HG22	1:A:308:GLU:HG3	1.93	0.50
1:A:380:HIS:HD2	1:A:382:TRP:H	1.60	0.50
1:A:180:ARG:HD3	1:A:280[B]:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LYS:O	1:A:168:GLN:OE1	2.32	0.48
1:A:333:THR:HG23	1:A:335:GLN:H	1.79	0.48
1:A:180:ARG:HG2	1:A:184:ILE:HD12	1.96	0.47
1:A:166:LYS:HE3	1:A:206:VAL:CG2	2.39	0.47
1:A:220[A]:ARG:CZ	3:A:1391:X6D:HAO1	2.45	0.46
1:A:296:LEU:HD22	1:A:300:MET:HE2	1.97	0.46
1:A:253:ILE:HG13	1:A:255:ARG:HG3	1.97	0.46
1:A:222:LEU:O	1:A:225:LEU:O	2.33	0.46
1:A:169:LEU:C	1:A:170:GLU:HG3	2.41	0.46
1:A:279:VAL:CG2	1:A:280[B]:HIS:CD2	2.99	0.45
1:A:380:HIS:CD2	1:A:382:TRP:H	2.35	0.45
1:A:145:GLY:O	1:A:146:ASN:ND2	2.50	0.45
1:A:274:ASP:HA	4:A:2004:HOH:O	2.16	0.45
1:A:296:LEU:HA	1:A:297:PRO:HD3	1.61	0.45
1:A:169:LEU:C	1:A:170:GLU:CG	2.90	0.44
1:A:201:HIS:CB	1:A:206:VAL:HG22	2.48	0.44
1:A:254:HIS:ND1	1:A:257:ILE:HD12	2.33	0.44
1:A:176:HIS:O	1:A:176:HIS:CD2	2.71	0.42
1:A:178:LEU:HD13	1:A:178:LEU:HA	1.67	0.42
1:A:238:THR:HG23	1:A:378:LEU:CD2	2.49	0.42
1:A:255:ARG:HB3	1:A:300:MET:HE1	2.01	0.42
1:A:279:VAL:HG22	1:A:280[B]:HIS:N	2.33	0.42
1:A:144:PHE:CD1	1:A:169:LEU:HD23	2.55	0.42
1:A:315:LEU:HA	1:A:315:LEU:HD12	1.76	0.42
1:A:163:VAL:HG13	1:A:207:TYR:CE1	2.55	0.42
1:A:179:ARG:HG3	1:A:179:ARG:H	1.26	0.42
1:A:254:HIS:CG	1:A:257:ILE:CD1	3.03	0.42
1:A:331:ALA:HB1	1:A:336:GLU:OE1	2.20	0.41
1:A:244:LEU:HA	1:A:244:LEU:HD23	1.62	0.41
1:A:293:LEU:O	1:A:341:ILE:HD11	2.19	0.41
1:A:257:ILE:CG2	1:A:318:LEU:HD11	2.50	0.41
1:A:367:ASN:HA	1:A:368:PRO:HD2	1.82	0.41
1:A:267:ALA:HB3	1:A:269:GLU:OE1	2.21	0.41
3:A:1391:X6D:BR	3:A:1391:X6D:HAR1	2.75	0.41
1:A:224:LYS:HE2	1:A:225:LEU:CD2	2.50	0.41
1:A:166:LYS:HZ2	1:A:203:ALA:H	1.67	0.41
1:A:219:TYR:C	1:A:219:TYR:CD2	2.98	0.41
1:A:254:HIS:CB	1:A:257:ILE:HD12	2.51	0.41
1:A:297:PRO:HG2	1:A:310:VAL:HG13	2.02	0.41
1:A:152[B]:GLU:HG2	1:A:155:SER:OG	2.21	0.40
1:A:188:LEU:HD22	1:A:246:TYR:HE2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:VAL:CG1	1:A:207:TYR:N	2.80	0.40

All (9) 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)
1:A:175:GLU:OE2	1:A:179:ARG:NH1[10_555]	1.12	1.08
1:A:175:GLU:CD	1:A:179:ARG:NH1[10_555]	1.15	1.05
1:A:175:GLU:OE1	1:A:179:ARG:NH2[10_555]	1.23	0.97
1:A:175:GLU:OE1	1:A:179:ARG:CZ[10_555]	1.33	0.87
1:A:175:GLU:OE1	1:A:179:ARG:NH1[10_555]	1.61	0.59
1:A:175:GLU:CD	1:A:179:ARG:CZ[10_555]	1.89	0.31
1:A:153:LYS:NZ	1:A:350:ASP:OD2[8_666]	2.08	0.12
1:A:336:GLU:OE1	1:A:336:GLU:OE1[12_566]	2.08	0.12
1:A:336:GLU:OE1	1:A:336:GLU:OE2[12_566]	2.08	0.12

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	253/285 (89%)	235 (93%)	17 (7%)	1 (0%)	30 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	LEU

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	224/251 (89%)	192 (86%)	32 (14%)	3 11

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LEU
1	A	131	GLU
1	A	135	ILE
1	A	149	LEU
1	A	155	SER
1	A	159	LEU
1	A	162	LYS
1	A	170	GLU
1	A	175	GLU
1	A	178	LEU
1	A	180	ARG
1	A	186	SER
1	A	195	ARG
1	A	196	LEU
1	A	202	ASP
1	A	204	THR
1	A	205	ARG
1	A	226	SER
1	A	239	GLU
1	A	240	LEU
1	A	257	ILE
1	A	260	GLU
1	A	293	LEU
1	A	299	GLU
1	A	326	LYS
1	A	333	THR
1	A	335	GLN
1	A	343	ARG
1	A	359	LEU
1	A	360	ILE
1	A	363	LEU
1	A	379	GLU

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	146	ASN
1	A	185	GLN
1	A	187	HIS
1	A	190	HIS
1	A	192	ASN
1	A	201	HIS
1	A	261	ASN
1	A	335	GLN
1	A	370	GLN
1	A	380	HIS

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](#)

3 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	SO4	A	1390	-	4,4,4	1.09	0	6,6,6	0.99	0
2	SO4	A	1389	-	4,4,4	0.24	0	6,6,6	0.18	0
3	X6D	A	1391	-	42,42,42	1.77	6 (14%)	54,59,59	3.34	20 (37%)

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
3	X6D	A	1391	-	-	2/16/34/34	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1391	X6D	CAR-NBK	-6.20	1.36	1.46
3	A	1391	X6D	CBD-CBE	-4.24	1.39	1.47
3	A	1391	X6D	CBH-NAW	-4.10	1.32	1.39
3	A	1391	X6D	CBG-NAX	-3.81	1.32	1.37
3	A	1391	X6D	CAQ-CAS	3.22	1.63	1.51
3	A	1391	X6D	CAS-NBK	2.82	1.51	1.46

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1391	X6D	CAU-NBJ-CAQ	16.94	147.50	111.07
3	A	1391	X6D	CAU-NBJ-CAP	-8.55	92.67	111.07
3	A	1391	X6D	CAS-NBK-CAR	-6.47	97.01	111.57
3	A	1391	X6D	CAP-CAR-NBK	6.14	123.71	110.78
3	A	1391	X6D	CBG-CBH-NAW	-3.80	105.39	110.64
3	A	1391	X6D	CBH-NAW-CBE	3.46	110.76	105.09
3	A	1391	X6D	CBD-CBE-NAX	3.44	128.84	123.23
3	A	1391	X6D	NAX-CBE-NAW	-3.05	107.25	112.44
3	A	1391	X6D	CAQ-NBJ-CAP	-2.99	102.41	108.84
3	A	1391	X6D	NAX-CBG-NAV	2.82	131.03	125.32
3	A	1391	X6D	CBH-CBG-NAV	-2.79	121.67	126.75
3	A	1391	X6D	CAT-CBB-CAG	-2.76	115.66	120.75
3	A	1391	X6D	CAC-CAE-CBA	-2.68	117.48	121.00
3	A	1391	X6D	CAI-CBD-CBE	-2.33	116.68	120.83
3	A	1391	X6D	CAU-CBA-CAF	-2.25	116.61	120.75
3	A	1391	X6D	CAF-CBA-CAE	2.16	121.45	118.23
3	A	1391	X6D	CAS-CAQ-NBJ	-2.08	106.46	110.65
3	A	1391	X6D	CAE-CAC-CAZ	2.05	121.30	119.24
3	A	1391	X6D	CBA-CAU-NBJ	2.04	117.32	113.15
3	A	1391	X6D	BR-CBC-CAK	-2.02	114.68	118.48

There are no chirality outliers.

All (2) torsion outliers are listed below:

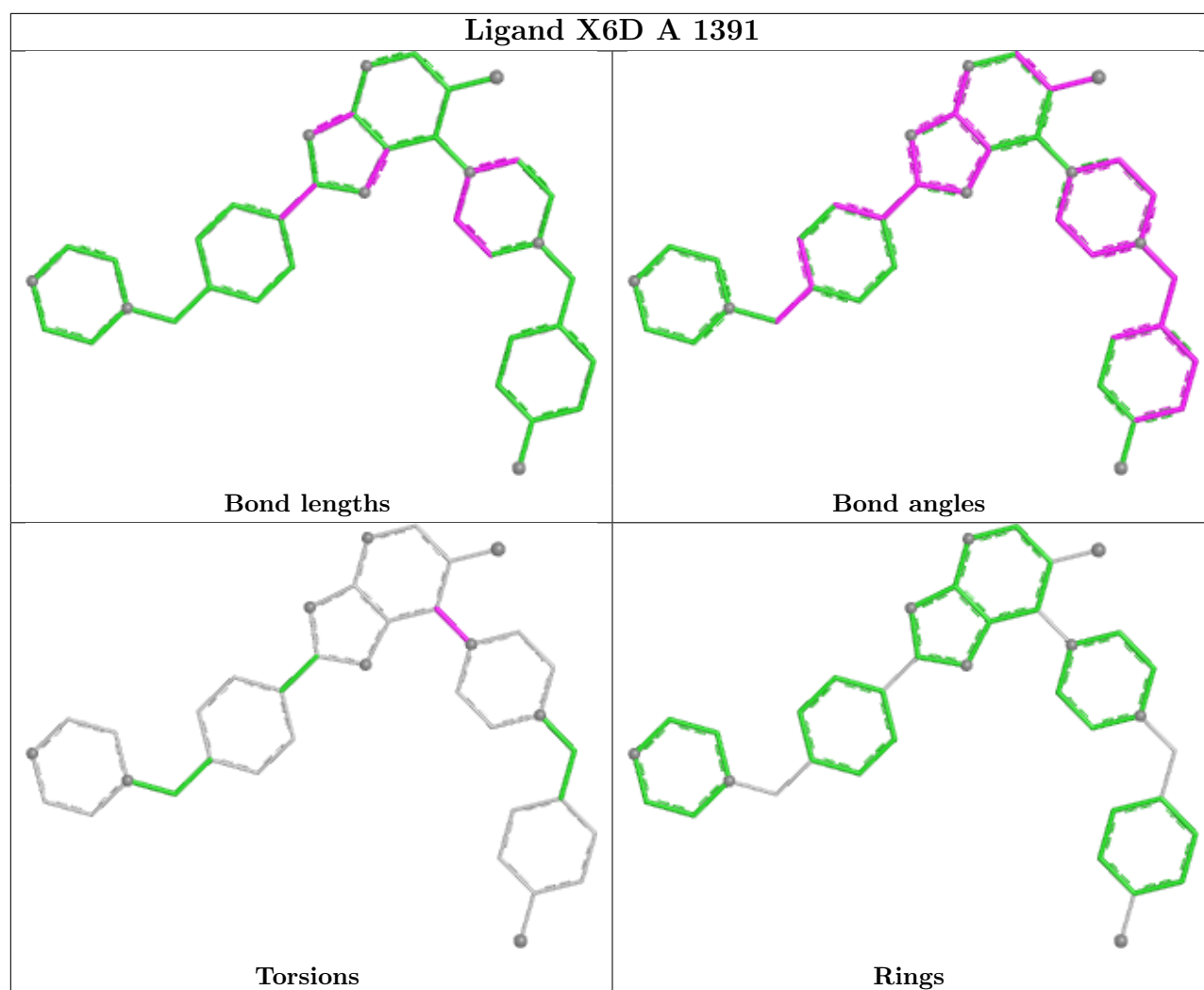
Mol	Chain	Res	Type	Atoms
3	A	1391	X6D	CBC-CBF-NBK-CAS
3	A	1391	X6D	CBH-CBF-NBK-CAS

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1391	X6D	5	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 [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	255/285 (89%)	-0.26	7 (2%) 56 46	21, 53, 114, 140	4 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280[A]	HIS	5.6
1	A	167	ALA	4.4
1	A	169	LEU	4.0
1	A	170	GLU	2.4
1	A	176	HIS	2.2
1	A	175	GLU	2.2
1	A	220[A]	ARG	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.

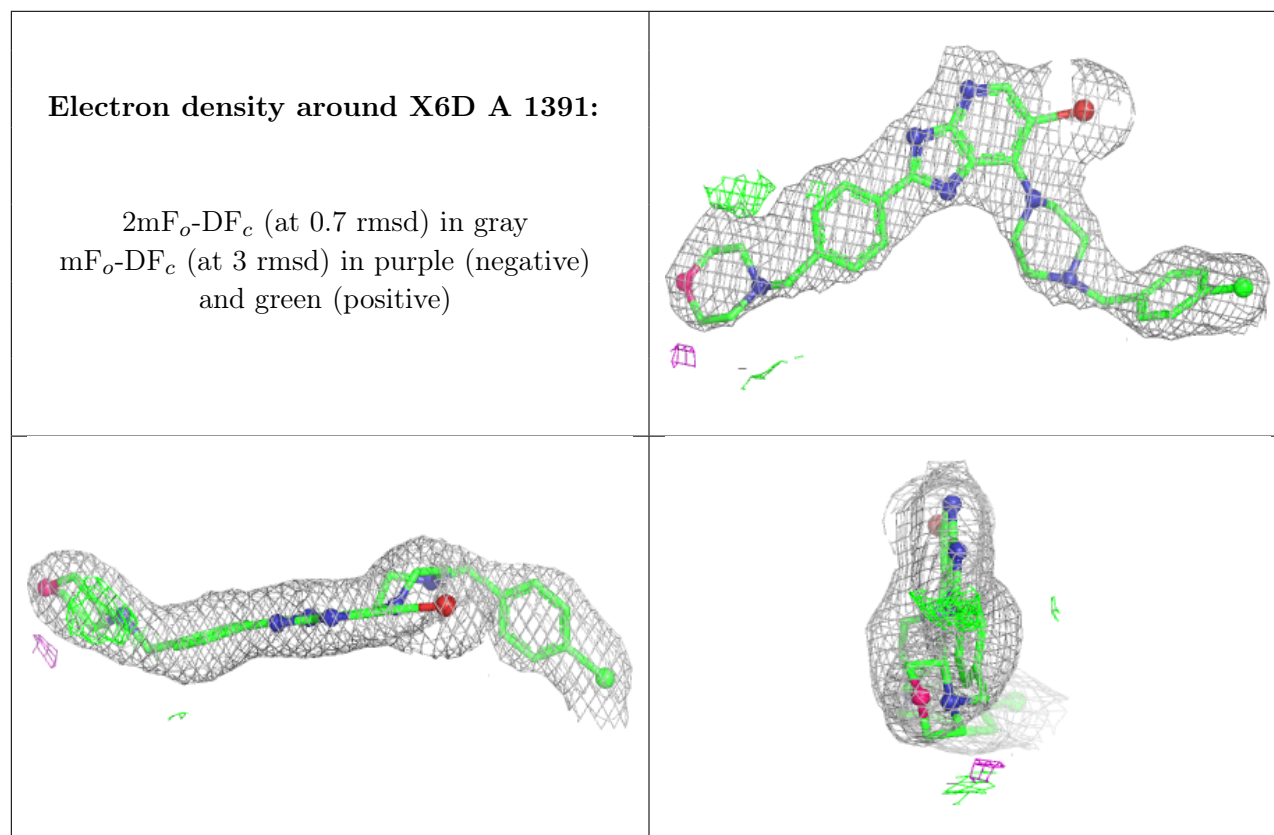
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	1389	5/5	0.77	0.28	59,69,88,122	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1390	5/5	0.81	0.19	20,50,62,65	5
3	X6D	A	1391	37/37	0.94	0.09	44,61,79,88	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 ⓘ

There are no such residues in this entry.