



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2018 – 12:22 AM EST

PDB ID : 2X6D  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

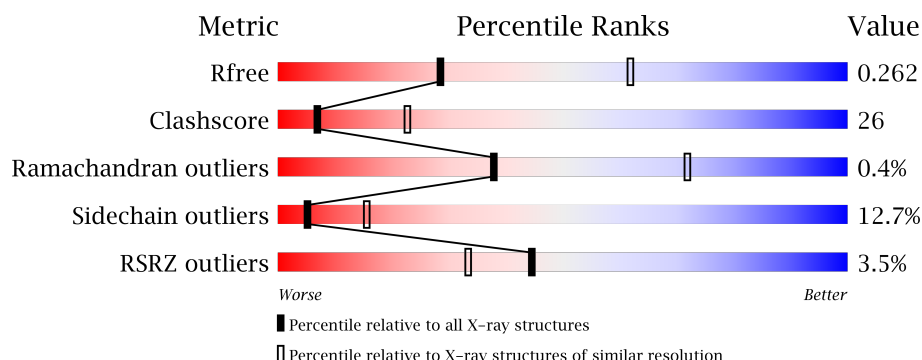
# 1 Overall quality at a glance

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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	

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	SO4	A	1389	-	-	-	X

## 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
1	A	255	Total	C	N	O	S	0	4	0
			2107	1354	368	379	6			

There are 3 discrepancies between the modelled and reference sequences:

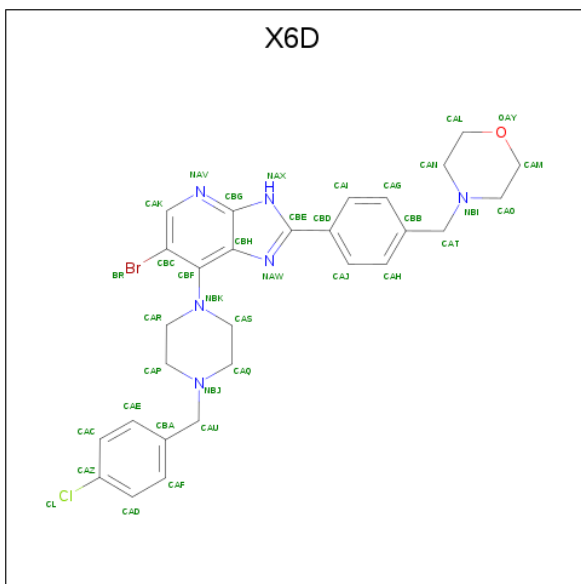
Chain	Residue	Modelled	Actual	Comment	Reference
A	119	GLY	-	expression tag	UNP O14965
A	120	ALA	-	expression tag	UNP O14965
A	121	MET	-	expression tag	UNP O14965

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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 (three-letter code: 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		

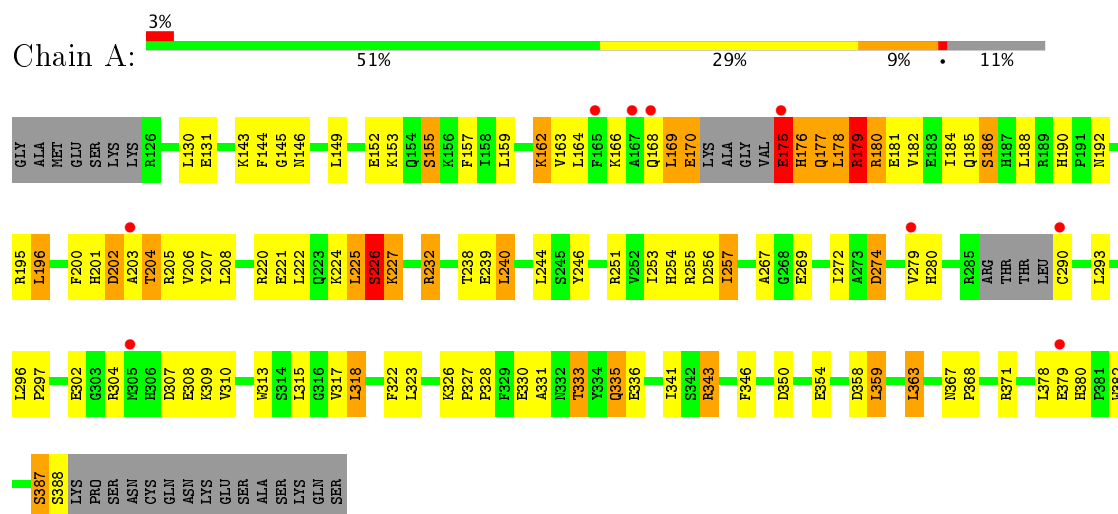
- Molecule 4 is water.

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

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: SERINE/THREONINE-PROTEIN KINASE 6



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.57Å 81.57Å 171.99Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.84 – 2.80 36.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.84-2.80) 99.8 (36.85-2.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.44 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.217 , 0.264 0.210 , 0.262	Depositor DCC
$R_{free}$ test set	424 reflections (4.75%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.7	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	2181	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.87	2/2160 (0.1%)	1.12	14/2922 (0.5%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	226	SER	CA-C	8.25	1.74	1.52
1	A	179	ARG	NE-CZ	-5.17	1.26	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	ARG	NE-CZ-NH1	-27.24	106.68	120.30
1	A	175	GLU	OE1-CD-OE2	10.20	135.53	123.30
1	A	179	ARG	NH1-CZ-NH2	10.11	130.52	119.40
1	A	175	GLU	CG-CD-OE1	-8.49	101.31	118.30
1	A	176	HIS	N-CA-C	6.07	127.38	111.00
1	A	274	ASP	CB-CG-OD1	-6.00	112.91	118.30
1	A	204	THR	N-CA-C	-5.93	94.98	111.00
1	A	232	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	318	LEU	CB-CG-CD1	-5.79	101.15	111.00
1	A	227	LYS	N-CA-C	-5.45	96.28	111.00
1	A	256	ASP	CB-CG-OD2	-5.42	113.42	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	LEU	N-CA-C	-5.27	96.77	111.00
1	A	387	SER	N-CA-CB	-5.22	102.67	110.50
1	A	177	GLN	N-CA-CB	-5.04	101.53	110.60

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	106	7
2	A	10	0	0	0	0
3	A	37	0	30	5	0
4	A	27	0	0	6	0
All	All	2181	0	2099	109	7

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 26.

All (109) 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: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

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:178:LEU:HD12	1:A:178:LEU:C	1.91	0.80
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
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:253:ILE:HG22	1:A:308:GLU:HA	1.80	0.63
1:A:166:LYS:HZ3	1:A:203:ALA:HA	1.63	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:GLN:N	1:A:335:GLN:HE21	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: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: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
1:A:202:ASP:OD2	1:A:202:ASP:C	2.50	0.50
3:A:1391:X6D:CAH	3:A:1391:X6D:HAN2	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:331:ALA:HB1	1:A:336:GLU:CD	2.33	0.49
1:A:180:ARG:HD3	1:A:280[B]:HIS:CE1	2.48	0.49
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: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: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:206:VAL:CG1	1:A:207:TYR:N	2.80	0.45
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:CD2	1:A:176:HIS:O	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:279:VAL:HG22	1:A:280[B]:HIS:N	2.33	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:A:179:ARG:HG3	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:166:LYS:HZ2	1:A:203:ALA:H	1.66	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
3:A:1391:X6D:BR	3:A:1391:X6D:HAR1	2.75	0.41
1:A:267:ALA:HB3	1:A:269:GLU:OE1	2.21	0.41
1:A:224:LYS:HE2	1:A:225:LEU:CD2	2.50	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

All (7) 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:OE1	1:A:179:ARG:NH2[10_555]	1.23	0.97
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: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
1:A:153:LYS:NZ	1:A:350:ASP:OD2[8_666]	2.08	0.12

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	253/285 (89%)	235 (93%)	17 (7%)	1 (0%)	38 72

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	LEU

### 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	224/251 (89%)	196 (88%)	28 (12%)	5 16

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	LEU
1	A	131	GLU
1	A	149	LEU
1	A	155	SER
1	A	162	LYS
1	A	170	GLU
1	A	175	GLU
1	A	178	LEU
1	A	179	ARG
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	251	ARG
1	A	257	ILE
1	A	326	LYS
1	A	333	THR
1	A	335	GLN
1	A	343	ARG
1	A	359	LEU
1	A	363	LEU
1	A	379	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) 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	380	HIS

### 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 carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

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	1389	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	A	1390	-	4,4,4	1.12	0	6,6,6	1.04	1 (16%)
3	X6D	A	1391	-	42,42,42	1.86	8 (19%)	47,59,59	3.57	17 (36%)

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	SO4	A	1389	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1390	-	-	0/0/0/0	0/0/0/0
3	X6D	A	1391	-	-	0/16/34/34	1/6/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1391	X6D	CAR-NBK	-6.93	1.36	1.46
3	A	1391	X6D	CBH-NAW	-4.99	1.32	1.38
3	A	1391	X6D	CBD-CBE	-3.57	1.39	1.48
3	A	1391	X6D	CBE-NAX	-2.24	1.33	1.35
3	A	1391	X6D	CBF-CBH	-2.07	1.41	1.44
3	A	1391	X6D	CBE-NAW	-2.00	1.33	1.35
3	A	1391	X6D	CAQ-CAS	3.03	1.63	1.51
3	A	1391	X6D	CAS-NBK	3.15	1.51	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1391	X6D	CAU-NBJ-CAP	-8.69	92.67	111.08
3	A	1391	X6D	CAS-NBK-CAR	-6.87	97.01	111.57
3	A	1391	X6D	CBG-CBH-NAW	-4.35	105.39	109.47
3	A	1391	X6D	CAQ-NBJ-CAP	-2.85	102.41	108.87
3	A	1391	X6D	CAT-CBB-CAG	-2.69	115.66	120.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1391	X6D	CAC-CAE-CBA	-2.56	117.48	121.02
3	A	1391	X6D	CAI-CBD-CBE	-2.49	116.68	120.79
3	A	1391	X6D	CAU-CBA-CAF	-2.19	116.61	120.78
3	A	1391	X6D	CAS-CAQ-NBJ	-2.06	106.46	110.63
3	A	1391	X6D	BR-CBC-CAK	-2.06	114.68	118.63
2	A	1390	SO4	O4-S-O3	2.04	118.13	108.96
3	A	1391	X6D	CAF-CBA-CAE	2.07	121.45	118.16
3	A	1391	X6D	CAQ-CAS-NBK	2.13	114.86	110.68
3	A	1391	X6D	CBA-CAU-NBJ	2.16	117.32	113.17
3	A	1391	X6D	BR-CBC-CBF	3.38	126.14	121.59
3	A	1391	X6D	CBD-CBE-NAX	3.98	128.84	123.51
3	A	1391	X6D	CAP-CAR-NBK	6.62	123.71	110.68
3	A	1391	X6D	CAU-NBJ-CAQ	17.20	147.50	111.08

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1391	X6D	CAP-CAQ-CAR-CAS-NBJ-NBK

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1391	X6D	5	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	255/285 (89%)	0.25	9 (3%) 44 33	36, 53, 114, 140	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	167	ALA	8.5
1	A	305	MET	3.9
1	A	203	ALA	3.8
1	A	279	VAL	3.6
1	A	168	GLN	3.5
1	A	379	GLU	2.9
1	A	175	GLU	2.5
1	A	165	PHE	2.3
1	A	290	CYS	2.1

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	1389	5/5	0.84	0.34	2.63	59,69,88,122	5
3	X6D	A	1391	37/37	0.94	0.18	-0.34	44,61,79,88	0
2	SO4	A	1390	5/5	0.76	0.66	-	20,50,62,65	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.