



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 03:48 PM JST

PDB ID : 7VI0
Title : Crystal structure of EP300 HAT domain in complex with compound 11
Authors : Takahashi, M.; Hanzawa, H.
Deposited on : 2021-09-24
Resolution : 2.10 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

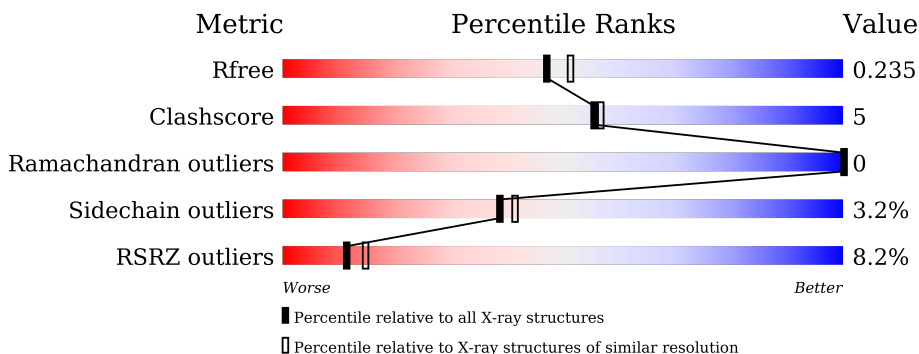
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	454	 8% 86% 10% ..
1	B	454	 8% 81% 13% . 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7551 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 Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	441	3505	2231	597	649	28	0	0	0
1	B	433	3465	2205	597	635	28	0	0	0

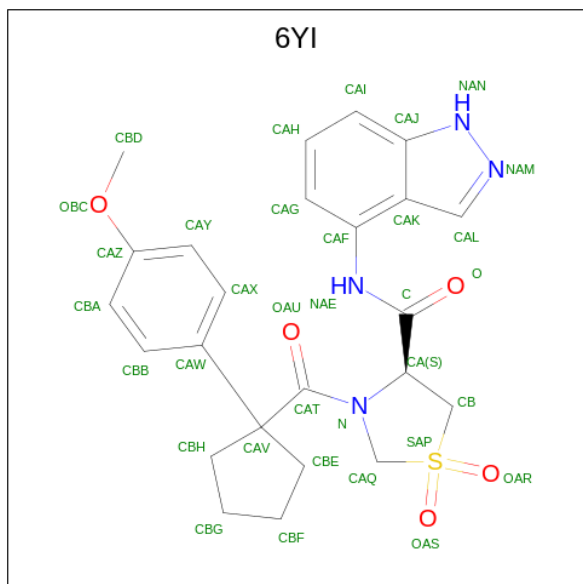
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1157	GLY	-	expression tag	UNP Q09472
A	1158	PRO	-	expression tag	UNP Q09472
A	1467	PHE	TYR	engineered mutation	UNP Q09472
A	1520	SER	-	linker	UNP Q09472
A	1521	GLY	-	linker	UNP Q09472
A	1578	GLY	-	linker	UNP Q09472
A	1579	SER	-	linker	UNP Q09472
A	1580	GLY	-	linker	UNP Q09472
B	1157	GLY	-	expression tag	UNP Q09472
B	1158	PRO	-	expression tag	UNP Q09472
B	1467	PHE	TYR	engineered mutation	UNP Q09472
B	1520	SER	-	linker	UNP Q09472
B	1521	GLY	-	linker	UNP Q09472
B	1578	GLY	-	linker	UNP Q09472
B	1579	SER	-	linker	UNP Q09472
B	1580	GLY	-	linker	UNP Q09472

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

- Molecule 3 is (4S)-N-(3H-indazol-4-yl)-3-[1-(4-methoxyphenyl)cyclopentyl]carbonyl-1,1-bis(oxidanylidene)-1,3-thiazolidine-4-carboxamide (three-letter code: 6YI) (formula: C₂₄H₂₆N₄O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			34	24	4	5	1		
3	B	1	Total	C	N	O	S	0	0
			34	24	4	5	1		

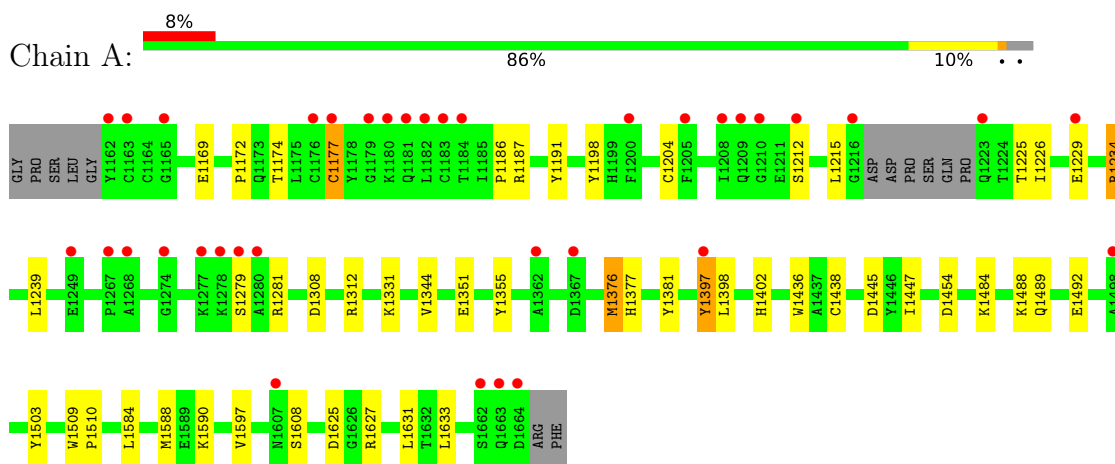
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	277	Total	O	0	0
			277	277		
4	B	230	Total	O	0	0
			230	230		

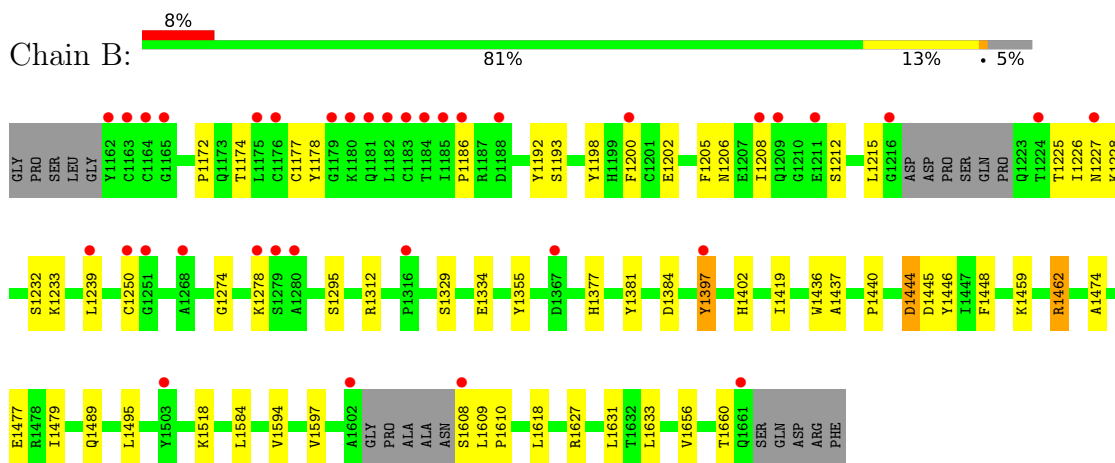
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Histone acetyltransferase p300



- Molecule 1: Histone acetyltransferase p300



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.55Å 88.36Å 90.66Å 116.52° 94.38° 91.36°	Depositor
Resolution (Å)	19.72 – 2.10 19.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.3 (19.72-2.10) 95.4 (19.72-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 2.11Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.199 , 0.235 0.199 , 0.235	Depositor DCC
R_{free} test set	3323 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	35.0	Xtrriage
Anisotropy	0.088	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.011 for -h,-l,-k	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7551	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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: 6YI, ZN

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	0.27	0/3598	0.51	0/4871
1	B	0.27	0/3556	0.53	0/4810
All	All	0.27	0/7154	0.52	0/9681

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3505	0	3336	28	0
1	B	3465	0	3315	42	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	34	0	0	0	0
3	B	34	0	0	0	0
4	A	277	0	0	0	0
4	B	230	0	0	1	0
All	All	7551	0	6651	70	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 5.

All (70) 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:1174:THR:HG22	1:A:1186:PRO:HA	1.55	0.88
1:A:1279:SER:HB3	1:A:1281:ARG:HE	1.47	0.80
1:B:1459:LYS:HG2	1:B:1462:ARG:HH21	1.56	0.71
1:A:1376:MET:HG3	1:A:1398:LEU:HD23	1.75	0.67
1:B:1274:GLY:O	1:B:1278:LYS:HD3	1.96	0.66
1:A:1177:CYS:SG	1:A:1204:CYS:CB	2.87	0.62
1:B:1215:LEU:HD22	1:B:1226:ILE:HD13	1.82	0.61
1:B:1205:PHE:O	1:B:1208:ILE:HG12	2.01	0.60
1:B:1440:PRO:HB2	1:B:1444:ASP:OD1	2.01	0.60
1:A:1397:TYR:HD1	1:A:1447:ILE:HD11	1.66	0.59
1:A:1198:TYR:CD1	1:A:1215:LEU:HD22	2.40	0.56
1:B:1440:PRO:HB3	1:B:1446:TYR:CE1	2.40	0.56
1:B:1397:TYR:CE1	1:B:1627:ARG:HB3	2.40	0.56
1:B:1172:PRO:HD3	1:B:1239:LEU:HD23	1.87	0.56
1:B:1200:PHE:HB3	1:B:1205:PHE:HB2	1.88	0.55
1:A:1397:TYR:CE1	1:A:1627:ARG:HB3	2.42	0.55
1:B:1212:SER:HB2	1:B:1225:THR:HG23	1.91	0.53
1:B:1477:GLU:HB3	1:B:1479:ILE:HD12	1.91	0.52
1:A:1172:PRO:HG2	1:A:1187:ARG:HG3	1.91	0.52
1:B:1377:HIS:CD2	1:B:1397:TYR:HE1	2.27	0.51
1:B:1445:ASP:HB3	1:B:1448:PHE:O	2.11	0.51
1:B:1397:TYR:OH	1:B:1627:ARG:N	2.43	0.51
1:A:1445:ASP:HB3	1:A:1631:LEU:HD11	1.92	0.50
1:B:1227:ASN:OD1	1:B:1228:LYS:N	2.44	0.50
1:B:1446:TYR:O	1:B:1627:ARG:HD2	2.11	0.50
1:B:1489:GLN:HG2	1:B:1597:VAL:HG11	1.95	0.49
1:B:1609:LEU:HD13	1:B:1610:PRO:HD2	1.94	0.49
1:B:1495:LEU:HD21	1:B:1584:LEU:HD21	1.95	0.49
1:A:1454:ASP:OD1	1:A:1454:ASP:N	2.47	0.47
1:A:1584:LEU:O	1:A:1588:MET:HG3	2.14	0.47
1:A:1225:THR:O	1:A:1226:ILE:HD13	2.14	0.47
1:B:1377:HIS:CG	1:B:1397:TYR:CE1	3.03	0.47
1:B:1174:THR:HG22	1:B:1186:PRO:HA	1.97	0.47
1:A:1355:TYR:HB3	1:A:1381:TYR:CE2	2.50	0.46
1:B:1445:ASP:O	1:B:1631:LEU:HD11	2.15	0.46
1:A:1377:HIS:CD2	1:A:1397:TYR:HE1	2.34	0.46
1:A:1484:LYS:HE3	1:A:1492:GLU:OE1	2.16	0.46
1:B:1212:SER:HB2	1:B:1225:THR:CG2	2.46	0.45
1:B:1312:ARG:NH1	4:B:1810:HOH:O	2.41	0.45
1:A:1198:TYR:CD2	1:A:1215:LEU:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1192:TYR:HA	1:B:1232:SER:O	2.17	0.45
1:B:1444:ASP:OD1	1:B:1444:ASP:C	2.55	0.45
1:B:1178:TYR:HB3	1:B:1200:PHE:CZ	2.51	0.45
1:B:1437:ALA:O	1:B:1594:VAL:HG13	2.16	0.45
1:B:1656:VAL:O	1:B:1660:THR:HG23	2.16	0.45
1:B:1192:TYR:OH	1:B:1233:LYS:HD2	2.17	0.45
1:A:1344:VAL:HG11	1:A:1351:GLU:HG3	1.98	0.45
1:B:1202:GLU:HG3	1:B:1206:ASN:ND2	2.32	0.45
1:A:1172:PRO:HD3	1:A:1239:LEU:HD23	1.99	0.44
1:B:1397:TYR:CZ	1:B:1627:ARG:HB3	2.52	0.44
1:A:1397:TYR:OH	1:A:1627:ARG:N	2.50	0.44
1:A:1331:LYS:NZ	1:A:1625:ASP:OD1	2.49	0.44
1:A:1355:TYR:HB3	1:A:1381:TYR:CD2	2.52	0.44
1:B:1329:SER:HA	1:B:1618:LEU:HD22	1.98	0.44
1:B:1202:GLU:HG3	1:B:1206:ASN:HD22	1.82	0.43
1:A:1509:TRP:CH2	1:A:1588:MET:HG2	2.53	0.43
1:B:1436:TRP:HD1	1:B:1594:VAL:HG12	1.83	0.43
1:A:1489:GLN:HG2	1:A:1597:VAL:HG11	2.00	0.43
1:B:1377:HIS:CD2	1:B:1397:TYR:CE1	3.05	0.43
1:B:1609:LEU:CD1	1:B:1610:PRO:HD2	2.49	0.43
1:A:1397:TYR:CD1	1:A:1447:ILE:HD11	2.50	0.42
1:B:1419:ILE:HG12	1:B:1474:ALA:HB2	2.00	0.42
1:B:1193:SER:HA	1:B:1198:TYR:O	2.19	0.42
1:B:1198:TYR:CD2	1:B:1215:LEU:HD23	2.54	0.42
1:B:1355:TYR:HB3	1:B:1381:TYR:CE2	2.55	0.42
1:A:1191:TYR:CZ	1:A:1234:ARG:HG3	2.55	0.41
1:A:1503:TYR:CZ	1:A:1510:PRO:HB3	2.56	0.41
1:A:1436:TRP:CE2	1:A:1438:CYS:HB2	2.55	0.41
1:A:1308:ASP:O	1:A:1312:ARG:HG3	2.21	0.40
1:B:1355:TYR:HB3	1:B:1381:TYR:CD2	2.55	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	437/454 (96%)	425 (97%)	12 (3%)	0	100	100
1	B	427/454 (94%)	418 (98%)	9 (2%)	0	100	100
All	All	864/908 (95%)	843 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	378/407 (93%)	366 (97%)	12 (3%)	39	41
1	B	376/407 (92%)	364 (97%)	12 (3%)	39	41
All	All	754/814 (93%)	730 (97%)	24 (3%)	39	41

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1169	GLU
1	A	1177	CYS
1	A	1212	SER
1	A	1229	GLU
1	A	1234	ARG
1	A	1376	MET
1	A	1397	TYR
1	A	1402	HIS
1	A	1488	LYS
1	A	1590	LYS
1	A	1608	SER
1	A	1633	LEU
1	B	1177	CYS
1	B	1250	CYS
1	B	1295	SER

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Mol	Chain	Res	Type
1	B	1334	GLU
1	B	1384	ASP
1	B	1397	TYR
1	B	1402	HIS
1	B	1444	ASP
1	B	1462	ARG
1	B	1518	LYS
1	B	1608	SER
1	B	1633	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1206	ASN
1	B	1415	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	6YI	A	1704	-	33,38,38	4.15	14 (42%)	43,57,57	1.54	7 (16%)
3	6YI	B	1704	-	33,38,38	3.90	14 (42%)	43,57,57	1.64	8 (18%)

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	6YI	A	1704	-	-	3/26/49/49	0/5/5/5
3	6YI	B	1704	-	-	3/26/49/49	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1704	6YI	NAM-NAN	-14.33	1.09	1.37
3	B	1704	6YI	NAM-NAN	-11.57	1.15	1.37
3	A	1704	6YI	CB-SAP	10.88	1.92	1.78
3	B	1704	6YI	CB-SAP	10.30	1.91	1.78
3	B	1704	6YI	CAV-CAW	-8.61	1.39	1.53
3	A	1704	6YI	CAV-CAW	-8.13	1.40	1.53
3	B	1704	6YI	CA-C	-5.88	1.39	1.52
3	A	1704	6YI	CA-C	-5.33	1.40	1.52
3	B	1704	6YI	CAF-CAK	-5.20	1.32	1.43
3	A	1704	6YI	CAF-CAK	-5.06	1.33	1.43
3	A	1704	6YI	CAI-CAJ	-5.03	1.33	1.41
3	B	1704	6YI	CAI-CAJ	-4.91	1.33	1.41
3	A	1704	6YI	CAL-CAK	-4.45	1.31	1.40
3	B	1704	6YI	OAR-SAP	4.27	1.52	1.44
3	B	1704	6YI	CAL-CAK	-4.10	1.32	1.40
3	A	1704	6YI	OAR-SAP	3.96	1.52	1.44
3	A	1704	6YI	CAK-CAJ	-3.91	1.32	1.42
3	B	1704	6YI	CAK-CAJ	-3.83	1.32	1.42
3	B	1704	6YI	OAS-SAP	3.80	1.51	1.44
3	A	1704	6YI	OAS-SAP	3.53	1.51	1.44
3	A	1704	6YI	CA-N	3.21	1.53	1.47
3	B	1704	6YI	CAF-NAE	-3.14	1.33	1.41
3	B	1704	6YI	CBE-CAV	-3.14	1.50	1.55
3	B	1704	6YI	CA-N	2.87	1.52	1.47
3	A	1704	6YI	CAF-NAE	-2.79	1.34	1.41
3	A	1704	6YI	CBE-CAV	-2.76	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1704	6YI	CBH-CAV	-2.30	1.51	1.55
3	A	1704	6YI	CBH-CAV	-2.29	1.51	1.55

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1704	6YI	CAF-NAE-C	-5.11	119.19	127.73
3	A	1704	6YI	CAF-NAE-C	-4.68	119.90	127.73
3	B	1704	6YI	OAS-SAP-OAR	-3.67	112.06	117.44
3	A	1704	6YI	OAR-SAP-CB	3.66	115.37	110.30
3	A	1704	6YI	OAS-SAP-OAR	-3.57	112.20	117.44
3	B	1704	6YI	CBE-CAV-CAW	-3.35	107.79	113.28
3	B	1704	6YI	CBD-OBC-CAZ	-3.31	110.33	117.51
3	B	1704	6YI	OAR-SAP-CB	3.09	114.59	110.30
3	A	1704	6YI	CBE-CAV-CAW	-3.08	108.25	113.28
3	B	1704	6YI	CA-N-CAT	-2.70	114.07	118.09
3	A	1704	6YI	OAS-SAP-CB	2.67	114.01	110.30
3	A	1704	6YI	CA-N-CAT	-2.51	114.35	118.09
3	A	1704	6YI	CBD-OBC-CAZ	-2.43	112.24	117.51
3	B	1704	6YI	OAS-SAP-CB	2.18	113.33	110.30
3	B	1704	6YI	CAK-CAL-NAM	-2.09	106.11	110.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

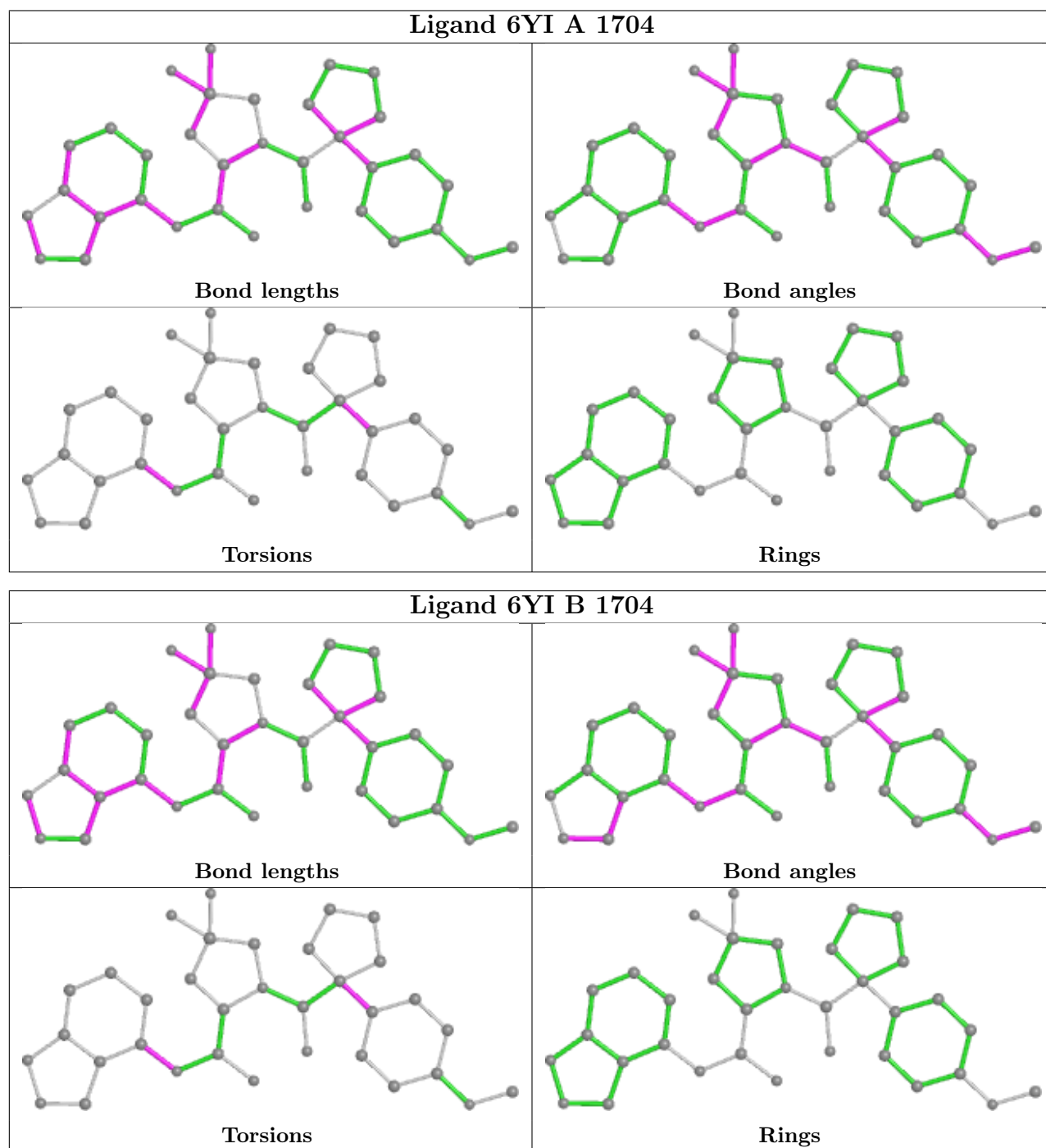
Mol	Chain	Res	Type	Atoms
3	B	1704	6YI	CAG-CAF-NAE-C
3	A	1704	6YI	CAG-CAF-NAE-C
3	A	1704	6YI	CBE-CAV-CAW-CAX
3	B	1704	6YI	CAK-CAF-NAE-C
3	A	1704	6YI	CBE-CAV-CAW-CBB
3	B	1704	6YI	CBE-CAV-CAW-CBB

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

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	441/454 (97%)	0.27	36 (8%) 11 15	24, 40, 89, 120	0
1	B	433/454 (95%)	0.31	36 (8%) 11 14	26, 43, 91, 123	0
All	All	874/908 (96%)	0.29	72 (8%) 11 15	24, 41, 90, 123	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1210	GLY	7.7
1	B	1162	TYR	7.3
1	A	1162	TYR	7.0
1	A	1183	CYS	6.6
1	B	1182	LEU	6.5
1	B	1181	GLN	6.1
1	A	1663	GLN	5.1
1	B	1183	CYS	5.1
1	B	1185	ILE	5.1
1	A	1280	ALA	5.0
1	B	1186	PRO	5.0
1	B	1280	ALA	4.9
1	B	1278	LYS	4.8
1	B	1211	GLU	4.7
1	A	1664	ASP	4.6
1	A	1209	GLN	4.4
1	B	1179	GLY	4.4
1	A	1180	LYS	4.4
1	B	1209	GLN	4.1
1	A	1163	CYS	4.0
1	A	1184	THR	3.9
1	A	1223	GLN	3.9
1	A	1181	GLN	3.9
1	B	1163	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1176	CYS	3.8
1	A	1212	SER	3.7
1	B	1176	CYS	3.7
1	B	1208	ILE	3.6
1	A	1267	PRO	3.6
1	B	1279	SER	3.6
1	A	1205	PHE	3.5
1	A	1182	LEU	3.5
1	A	1274	GLY	3.5
1	B	1184	THR	3.5
1	A	1279	SER	3.4
1	B	1175	LEU	3.4
1	A	1179	GLY	3.3
1	A	1249	GLU	3.2
1	A	1208	ILE	3.2
1	B	1608	SER	3.0
1	A	1662	SER	2.9
1	B	1367	ASP	2.9
1	A	1498	ALA	2.9
1	A	1277	LYS	2.9
1	B	1200	PHE	2.8
1	A	1278	LYS	2.8
1	B	1268	ALA	2.8
1	B	1316	PRO	2.8
1	B	1165	GLY	2.7
1	A	1268	ALA	2.6
1	A	1165	GLY	2.5
1	B	1602	ALA	2.5
1	A	1397	TYR	2.5
1	B	1180	LYS	2.5
1	B	1164	CYS	2.4
1	B	1250	CYS	2.4
1	A	1216	GLY	2.4
1	B	1397	TYR	2.4
1	A	1177	CYS	2.3
1	B	1188	ASP	2.3
1	B	1239	LEU	2.3
1	A	1200	PHE	2.3
1	A	1362	ALA	2.3
1	B	1224	THR	2.2
1	B	1503	TYR	2.2
1	A	1607	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1229	GLU	2.1
1	B	1661	GLN	2.1
1	B	1227	ASN	2.1
1	A	1367	ASP	2.0
1	B	1216	GLY	2.0
1	B	1251	GLY	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 monosaccharides in this entry.

6.4 Ligands [i](#)

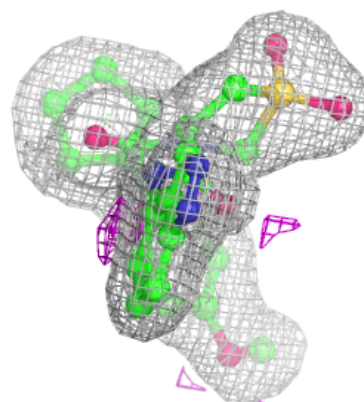
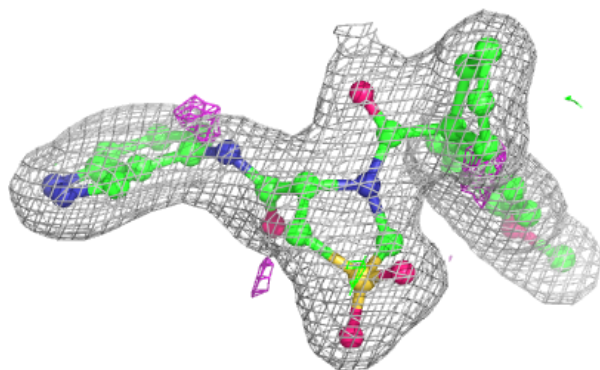
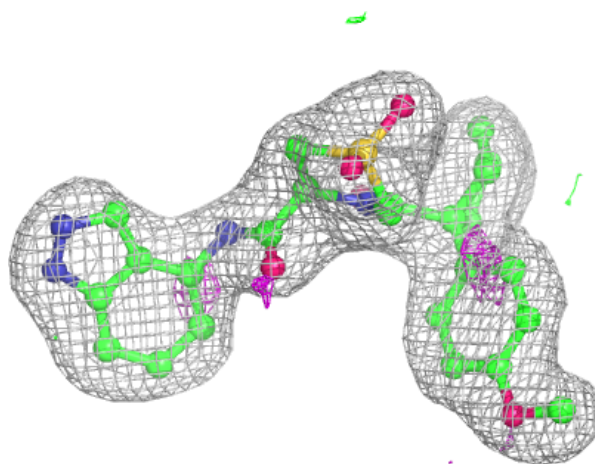
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

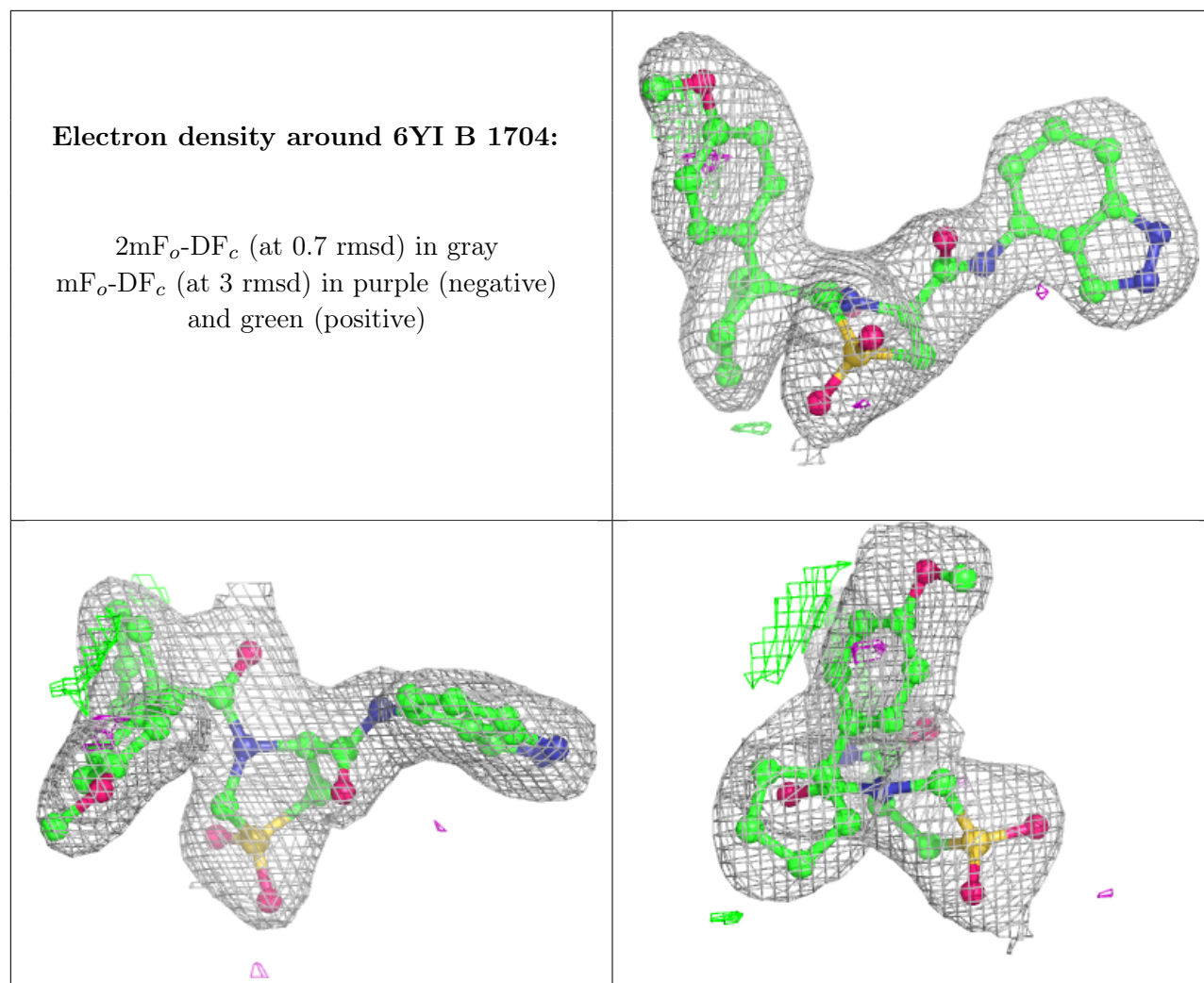
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	1703	1/1	0.40	0.07	108,108,108,108	0
2	ZN	A	1702	1/1	0.90	0.06	72,72,72,72	0
2	ZN	B	1703	1/1	0.92	0.14	112,112,112,112	0
3	6YI	A	1704	34/34	0.94	0.12	22,32,40,40	0
3	6YI	B	1704	34/34	0.94	0.11	35,46,52,58	0
2	ZN	B	1702	1/1	0.96	0.04	70,70,70,70	0
2	ZN	A	1701	1/1	0.99	0.05	51,51,51,51	0
2	ZN	B	1701	1/1	0.99	0.05	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 6YI A 1704:

$2mF_o-DF_c$ (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.