



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:48 AM UTC

PDB ID : 8A1Q / pdb_00008a1q
Title : HIV-1 Integrase Catalytic Core Domain and C-Terminal Domain in Complex with Allosteric Integrase Inhibitor STP0404 (Pirmitegravir)
Authors : Singer, M.R.; Pye, V.E.; Cook, N.J.; Cherepanov, P.
Deposited on : 2022-06-01
Resolution : 2.06 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

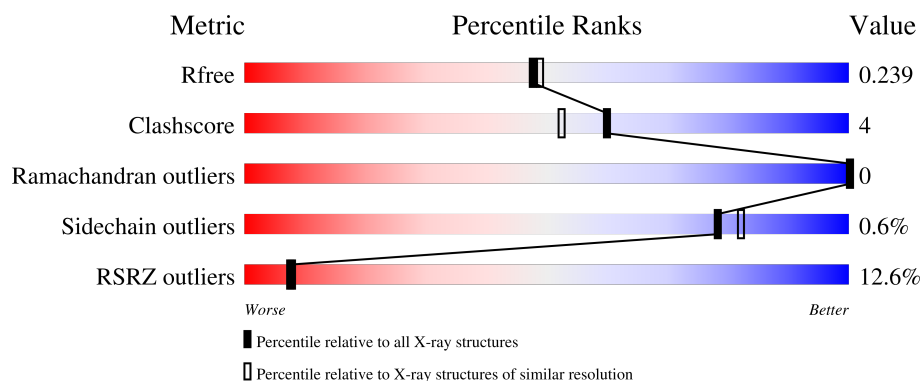
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	233	5% 21% 76%
1	B	233	6% 56% 8% 35%
1	C	233	8% 18% 6% 75%
1	D	233	4% 61% 37%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3498 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 Integrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	57	Total	C	N	O	S	0	1	0
			470	297	91	81	1			
1	B	151	Total	C	N	O	S	0	1	0
			1176	752	205	215	4			
1	C	58	Total	C	N	O	S	0	0	0
			469	295	88	85	1			
1	D	147	Total	C	N	O	S	0	1	0
			1141	728	200	209	4			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	SER	-	expression tag	UNP P12497
A	243	GLU	TRP	engineered mutation	UNP P12497
A	424	LYS	PHE	engineered mutation	UNP P12497
B	-20	SER	-	expression tag	UNP P12497
B	4	GLU	TRP	engineered mutation	UNP P12497
B	185	LYS	PHE	engineered mutation	UNP P12497
C	219	SER	-	expression tag	UNP P12497
C	243	GLU	TRP	engineered mutation	UNP P12497
C	424	LYS	PHE	engineered mutation	UNP P12497
D	-20	SER	-	expression tag	UNP P12497
D	4	GLU	TRP	engineered mutation	UNP P12497
D	185	LYS	PHE	engineered mutation	UNP P12497

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



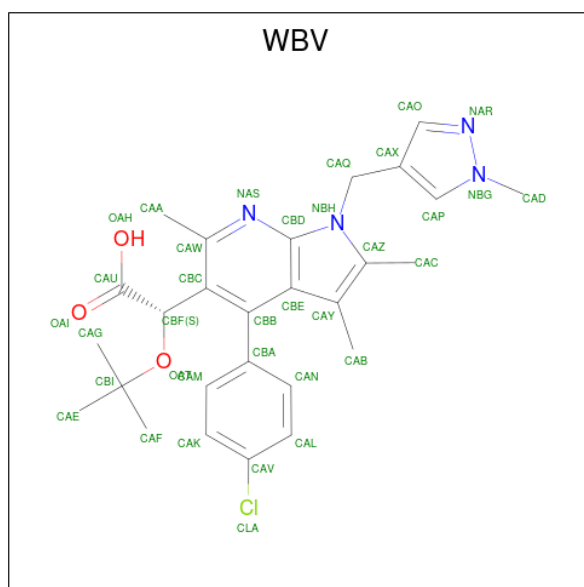
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is (2S)-tert-butoxy{4-(4-chlorophenyl)-2,3,6-trimethyl-1-[(1-methyl-1H-pyrazol-4-yl)methyl]-1H-pyrrolo[2,3-b]pyridin-5-yl}acetic acid (CCD ID: WBV) (formula: C₂₇H₃₁ClN₄O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	0	0
			35	27	1	4	3		
3	D	1	Total	C	Cl	N	O	0	0
			35	27	1	4	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	8	Total	O	0	0
			8	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	42	Total 42	O 42	0	0
5	C	6	Total 6	O 6	0	0
5	D	54	Total 54	O 54	0	0

GLY SER
SER
ALA
ASN
VAL
PHE
THR
ILE
SER
THR
THR
THR
VAL
LYS
ARG
LYS
ALA
ALA
CYS
TRP
TRP
ALA
GLY
TYR
ILE
LYS
LYS
GLN
GLY
GLN
GLY
VAL
ILE
ILE
GLY
SER
PRO
TYR
ASN
PRO
GLN
SER
SER
GLN
GLY
VAL
ILE
ILE
GLY
SER
MET
ASN
LYS
GLY
LEU
LYS
LYS
LYS
ILE
ILE
GLY
VAL
ARG
ASP
GLN
ALA
GLY
HIS
LYS
THR
VAL
ALA
GLN

MET
ALA
VAL
PHE
HIS
ASN
LYS
ARG
LYS
GLY
GLY
ILE
GLY
TRP
GLY
ALA
TYR
SER
ILE
ALA
GLY
GLY
ARG
PHE
ILE
ILE
VAL
ASP
PRO
ILE
ILE
ALA
THR
ASP
SER
ILE
GLN
THR
LYS
GLY

● Molecule 1: Integrase



SER
ILE
GLN
ASN
PHE
SER
ARG
VAL
THR
TYR
ARG
ASP
SER
SER
ARG
ASP
PRO
VAL
ASP
VAL
TRP
LYS
GLY
PRO
ALA
LYS
LEU
LEU
GLY
LYS
GLY
GLY
ALA
VAL
VAL
ILE
GLN
ASP
ASN
SER
SER
ASN
ASP
ILE
LYS
LYS
VAL
VAL
PRO
ARG
ARG
LYS
ALA
LYS
ILE
ILE
ARG
ASP
TYR
GLY
LYS
GLN
MET
ALA
GLY
ASP

ASP
CYS
VAL
ALA
SER
ARG
GLN
ASP
ASP
ASP
MET
HIS
GLY
GLN
VAL
ASP
ASP
CYS
S57
V77
A80
I84
T93
H134
T124
W131
G140
ILE
PRO
TYR
ASN
ASN
PRO
GLN
SER
GLN
G149
V150
I161
K173
R187
Y201
T210
K211
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.26Å 69.26Å 64.11Å 90.00° 102.38° 90.00°	Depositor
Resolution (Å)	62.61 – 2.06 62.61 – 2.06	Depositor EDS
% Data completeness (in resolution range)	99.7 (62.61-2.06) 99.8 (62.61-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 2.07Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.219 , 0.235 0.227 , 0.239	Depositor DCC
R_{free} test set	1635 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.095 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3498	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, WBV, MG

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	0.06	0/481	0.23	0/643
1	B	0.07	0/1200	0.22	0/1623
1	C	0.08	0/477	0.22	0/639
1	D	0.07	0/1163	0.24	0/1571
All	All	0.07	0/3321	0.23	0/4476

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 [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	470	0	490	5	0
1	B	1176	0	1186	12	0
1	C	469	0	477	10	0
1	D	1141	0	1153	6	0
2	A	8	0	12	1	0
2	B	28	0	42	2	0
2	C	8	0	12	0	0
2	D	16	0	24	1	0
3	B	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	35	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	8	0	0	0	0
5	B	42	0	0	0	0
5	C	6	0	0	0	0
5	D	54	0	0	0	0
All	All	3498	0	3396	29	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 4.

All (29) 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:C:244:LYS:HE2	1:C:267:ILE:HD13	1.71	0.72
1:B:95:GLN:HG2	2:B:302:EDO:H11	1.76	0.66
1:B:185:LYS:HD3	1:C:276:ALA:HB2	1.83	0.61
1:B:77:VAL:HG22	1:B:84:ILE:HG22	1.86	0.57
1:D:77:VAL:HG22	1:D:84:ILE:HG22	1.88	0.56
1:C:227:TYR:HB2	1:C:260:VAL:HG11	1.89	0.53
1:C:244:LYS:HG2	1:C:249:VAL:HG12	1.91	0.52
1:C:224:ARG:HG2	1:D:131:TRP:CE2	2.45	0.52
2:B:302:EDO:H21	1:D:173:LYS:HZ1	1.74	0.50
1:C:241:LEU:HA	1:C:251:ILE:HG22	1.94	0.50
1:B:211:LYS:HE2	1:D:187:ARG:HH22	1.78	0.49
1:B:152:GLU:HG2	1:B:156:LYS:HE3	1.94	0.49
1:C:268:ILE:HG22	1:D:131:TRP:HD1	1.79	0.47
1:A:266:LYS:HB3	2:A:502:EDO:H22	1.98	0.45
1:C:270:ASP:HB2	1:C:273:LYS:HB3	1.97	0.45
1:B:103:LYS:O	1:B:107:ARG:HG2	2.16	0.45
1:C:225:VAL:HG22	1:C:267:ILE:HG12	1.99	0.44
1:D:93:THR:HA	2:D:1305:EDO:H22	1.99	0.44
1:A:226:TYR:HD1	1:A:268:ILE:HD13	1.83	0.43
1:B:66:THR:HG23	1:B:73:ILE:HB	2.01	0.42
1:B:57:SER:HB3	1:B:58:PRO:HD3	2.03	0.41
1:B:167:ASP:OD1	1:B:167:ASP:N	2.54	0.41
1:B:62:GLN:HG2	1:B:114:HIS:HB2	2.03	0.41
1:A:270:ASP:HB2	1:A:273:LYS:HE2	2.02	0.41
1:B:101:LEU:HD23	1:B:101:LEU:HA	1.88	0.41
1:C:278:ASP:OD1	1:C:279:ASP:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:HD11	1:B:159:LYS:HD2	2.03	0.40
1:A:224[B]:ARG:HD2	1:A:238:PRO:HB2	2.02	0.40
1:A:240:LYS:HA	1:A:240:LYS:HD3	1.94	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	56/233 (24%)	52 (93%)	4 (7%)	0	100	100
1	B	148/233 (64%)	146 (99%)	2 (1%)	0	100	100
1	C	56/233 (24%)	53 (95%)	3 (5%)	0	100	100
1	D	144/233 (62%)	139 (96%)	5 (4%)	0	100	100
All	All	404/932 (43%)	390 (96%)	14 (4%)	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	49/193 (25%)	49 (100%)	0	100	100
1	B	123/193 (64%)	121 (98%)	2 (2%)	55	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	49/193 (25%)	49 (100%)	0	100	100
1	D	119/193 (62%)	119 (100%)	0	100	100
All	All	340/772 (44%)	338 (99%)	2 (1%)	78	82

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	144	ASN
1	B	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	155	ASN
1	C	274	GLN
1	D	155	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](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 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	$\# Z > 2$
2	EDO	A	502	-	3,3,3	0.43	0	2,2,2	0.39	0
2	EDO	B	302	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	B	307	-	3,3,3	0.42	0	2,2,2	0.37	0
2	EDO	D	1302	-	3,3,3	0.43	0	2,2,2	0.42	0
2	EDO	B	301	-	3,3,3	0.43	0	2,2,2	0.37	0
2	EDO	D	1303	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	D	1305	-	3,3,3	0.43	0	2,2,2	0.39	0
2	EDO	A	501	-	3,3,3	0.42	0	2,2,2	0.38	0
3	WBV	D	1301	-	36,38,38	1.57	6 (16%)	42,58,58	3.35	10 (23%)
2	EDO	C	501	-	3,3,3	0.41	0	2,2,2	0.41	0
2	EDO	C	502	-	3,3,3	0.43	0	2,2,2	0.40	0
2	EDO	D	1304	-	3,3,3	0.42	0	2,2,2	0.40	0
2	EDO	B	306	-	3,3,3	0.44	0	2,2,2	0.35	0
2	EDO	B	303	-	3,3,3	0.43	0	2,2,2	0.38	0
2	EDO	B	304	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	B	305	-	3,3,3	0.43	0	2,2,2	0.39	0
3	WBV	B	308	-	36,38,38	1.57	6 (16%)	42,58,58	3.38	10 (23%)

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	EDO	A	502	-	-	0/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	B	307	-	-	0/1/1/1	-
2	EDO	D	1302	-	-	0/1/1/1	-
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	D	1303	-	-	0/1/1/1	-
2	EDO	D	1305	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
3	WBV	D	1301	-	-	2/21/21/21	0/4/4/4
2	EDO	C	501	-	-	0/1/1/1	-
2	EDO	C	502	-	-	0/1/1/1	-
2	EDO	D	1304	-	-	0/1/1/1	-
2	EDO	B	306	-	-	0/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	B	304	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	305	-	-	0/1/1/1	-
3	WBV	B	308	-	-	3/21/21/21	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	308	WBV	CAZ-NBH	-4.07	1.32	1.38
3	D	1301	WBV	CAZ-NBH	-4.03	1.32	1.38
3	D	1301	WBV	CBB-CBA	3.71	1.56	1.50
3	B	308	WBV	CBB-CBA	3.58	1.56	1.50
3	B	308	WBV	CAC-CAZ	2.81	1.53	1.49
3	D	1301	WBV	CAC-CAZ	2.80	1.53	1.49
3	D	1301	WBV	CAP-NBG	-2.73	1.31	1.34
3	B	308	WBV	CAP-NBG	-2.67	1.31	1.34
3	B	308	WBV	CAA-CAW	2.18	1.53	1.50
3	D	1301	WBV	CAZ-CAY	2.17	1.40	1.37
3	D	1301	WBV	CAA-CAW	2.11	1.53	1.50
3	B	308	WBV	CAZ-CAY	2.10	1.40	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1301	WBV	CAX-CAO-NAR	-12.59	106.91	113.14
3	B	308	WBV	CAX-CAO-NAR	-12.50	106.96	113.14
3	B	308	WBV	CAO-NAR-NBG	10.56	110.21	104.41
3	D	1301	WBV	CAO-NAR-NBG	10.52	110.19	104.41
3	B	308	WBV	CBE-CBD-NAS	-7.20	121.39	127.31
3	D	1301	WBV	CBE-CBD-NAS	-7.12	121.46	127.31
3	B	308	WBV	CAX-CAQ-NBH	-6.26	104.05	113.32
3	D	1301	WBV	CAD-NBG-NAR	5.79	124.67	120.03
3	D	1301	WBV	CAX-CAQ-NBH	-5.61	105.02	113.32
3	B	308	WBV	CAD-NBG-NAR	5.60	124.52	120.03
3	B	308	WBV	CAC-CAZ-NBH	5.18	125.79	120.29
3	D	1301	WBV	CAC-CAZ-NBH	4.95	125.55	120.29
3	B	308	WBV	CBD-NAS-CAW	3.87	121.99	117.17
3	D	1301	WBV	CBD-NAS-CAW	3.77	121.87	117.17
3	D	1301	WBV	CAD-NBG-CAP	-3.43	124.50	127.94
3	B	308	WBV	CAD-NBG-CAP	-3.25	124.67	127.94
3	B	308	WBV	CAP-NBG-NAR	-2.25	110.80	112.08
3	D	1301	WBV	CAP-NBG-NAR	-2.21	110.83	112.08
3	B	308	WBV	NAS-CBD-NBH	2.20	129.36	125.67
3	D	1301	WBV	NAS-CBD-NBH	2.06	129.13	125.67

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	308	WBV	OAH-CAU-CBF-CBC
3	B	308	WBV	OAI-CAU-CBF-CBC
3	D	1301	WBV	OAH-CAU-CBF-CBC
3	D	1301	WBV	OAI-CAU-CBF-CBC
3	B	308	WBV	OAI-CAU-CBF-OAT

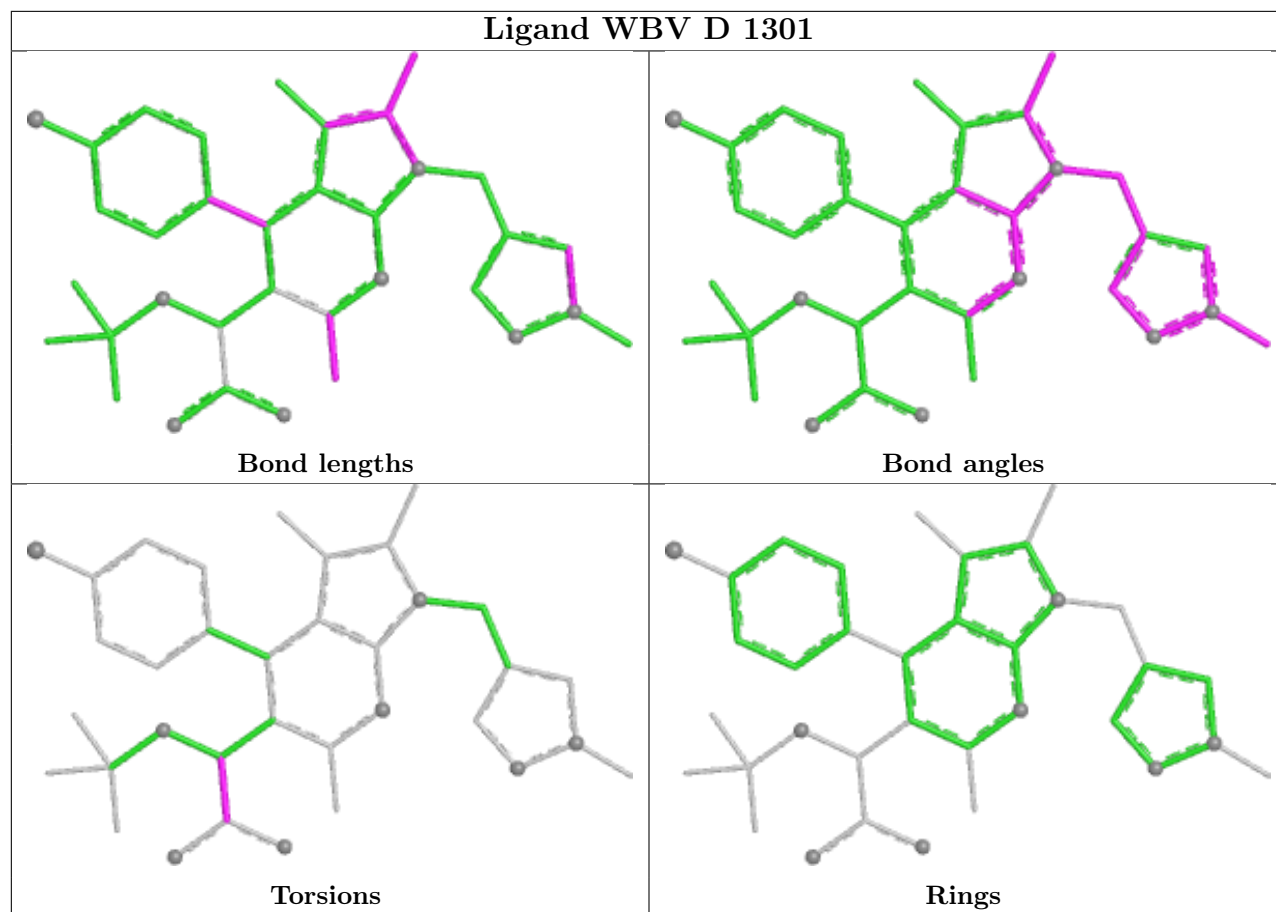
There are no ring outliers.

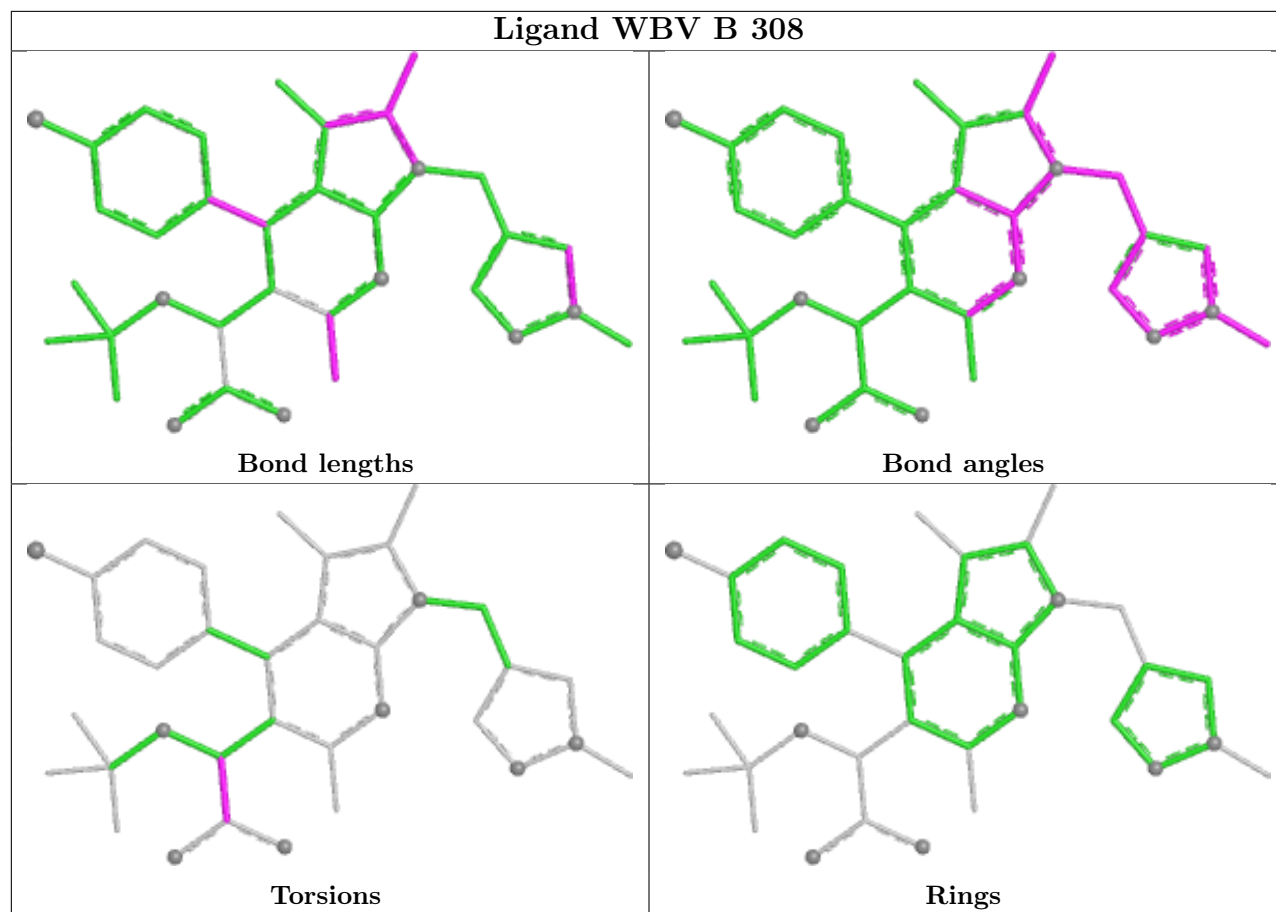
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	EDO	1	0
2	B	302	EDO	2	0
2	D	1305	EDO	1	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.

Ligand WBV D 1301





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	57/233 (24%)	1.48	11 (19%) 3 3	51, 98, 123, 139	1 (1%)
1	B	151/233 (64%)	0.74	13 (8%) 16 17	35, 65, 119, 134	1 (0%)
1	C	58/233 (24%)	1.47	18 (31%) 1 0	77, 108, 151, 164	0
1	D	147/233 (63%)	0.60	10 (6%) 23 23	32, 65, 95, 117	1 (0%)
All	All	413/932 (44%)	0.89	52 (12%) 8 7	32, 75, 123, 164	3 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	259	VAL	5.9
1	B	191	ILE	3.8
1	B	150	VAL	3.8
1	A	257	ILE	3.5
1	C	249	VAL	3.5
1	C	238	PRO	3.4
1	A	250	VAL	3.2
1	C	259	VAL	3.2
1	A	241	LEU	3.2
1	A	242	LEU	2.9
1	C	260	VAL	2.9
1	C	244	LYS	2.9
1	C	250	VAL	2.9
1	B	211	LYS	2.8
1	D	210	THR	2.8
1	B	141	ILE	2.8
1	B	143	TYR	2.7
1	B	142	PRO	2.7
1	A	251	ILE	2.7
1	A	249	VAL	2.6
1	D	149	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	242	LEU	2.5
1	C	276	ALA	2.5
1	C	241	LEU	2.5
1	D	211	LYS	2.4
1	B	202	ASP	2.4
1	C	251	ILE	2.4
1	C	262	ARG	2.4
1	D	151	ILE	2.4
1	C	261	PRO	2.3
1	D	124	THR	2.3
1	A	277	GLY	2.3
1	D	57	SER	2.2
1	A	260	VAL	2.2
1	B	208	ILE	2.2
1	C	225	VAL	2.2
1	D	201	VAL	2.2
1	C	248	ALA	2.2
1	B	182	ILE	2.1
1	D	80	ALA	2.1
1	B	149	GLY	2.1
1	C	264	LYS	2.1
1	A	255	SER	2.1
1	B	194	TYR	2.1
1	A	267	ILE	2.1
1	B	151	ILE	2.1
1	C	257	ILE	2.1
1	D	140	GLY	2.1
1	C	243	GLU	2.1
1	B	206	THR	2.1
1	C	239	ALA	2.1
1	D	114	HIS	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 ⓘ

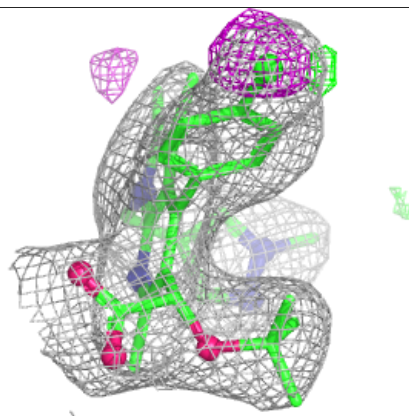
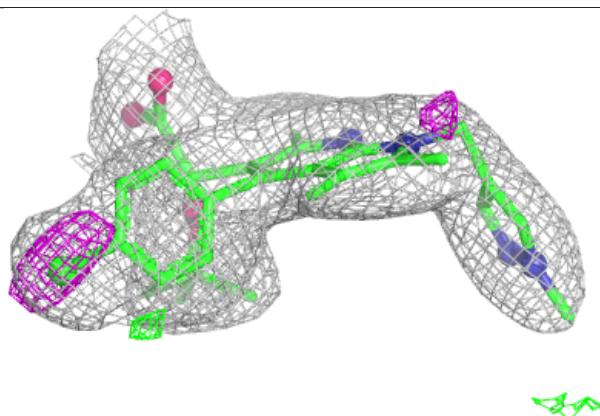
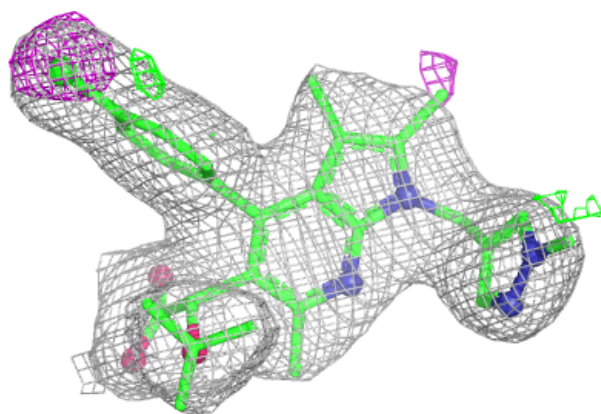
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	A	501	4/4	0.74	0.13	110,111,114,115	0
2	EDO	D	1305	4/4	0.75	0.16	75,76,80,82	0
2	EDO	A	502	4/4	0.83	0.18	66,72,73,78	0
2	EDO	C	502	4/4	0.85	0.15	75,80,83,85	0
2	EDO	B	304	4/4	0.86	0.16	65,69,72,74	0
2	EDO	B	301	4/4	0.86	0.12	79,80,82,83	0
2	EDO	D	1303	4/4	0.86	0.15	69,72,73,75	0
2	EDO	B	303	4/4	0.86	0.19	64,65,70,75	0
2	EDO	B	305	4/4	0.88	0.13	68,69,74,79	0
2	EDO	D	1304	4/4	0.89	0.12	72,76,79,80	0
2	EDO	D	1302	4/4	0.90	0.19	65,68,73,74	0
2	EDO	B	302	4/4	0.90	0.12	70,73,79,86	0
2	EDO	C	501	4/4	0.91	0.14	80,81,82,83	0
2	EDO	B	307	4/4	0.91	0.14	63,63,67,71	0
3	WBV	B	308	35/35	0.94	0.10	57,65,72,75	0
3	WBV	D	1301	35/35	0.94	0.11	54,61,72,73	0
2	EDO	B	306	4/4	0.95	0.09	70,77,78,83	0
4	MG	B	309	1/1	0.97	0.04	57,57,57,57	0
4	MG	D	1306	1/1	0.97	0.06	69,69,69,69	0

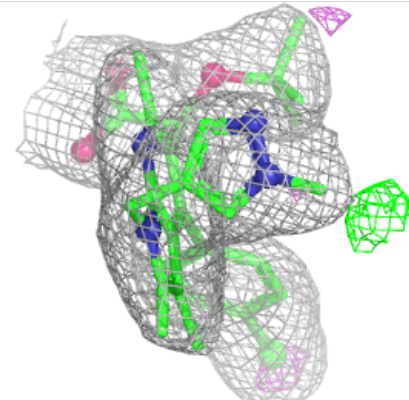
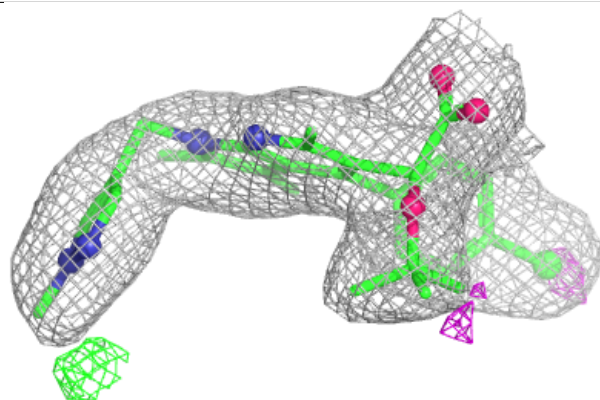
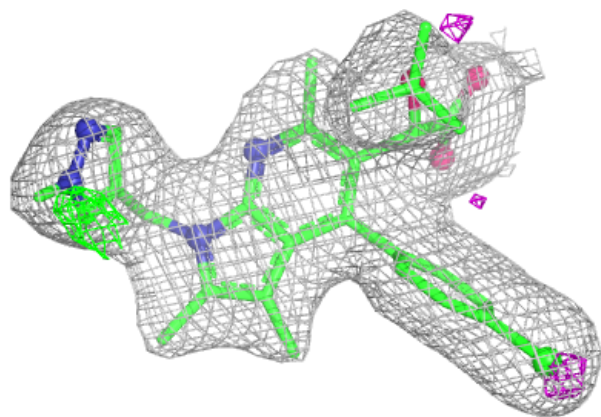
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around WBV B 308:

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

**Electron density around WBV D 1301:**

$2mF_o-DF_c$ (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.