Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 01:40 pm GMT

PDB ID	:	4BE2
Title	:	PFV intasome with inhibitor XZ-259
Authors	:	Hare, S.; Cherepanov, P.
Deposited on	:	2012-10-08
Resolution	:	2.38 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 (i) 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 (i)) were used in the production of this report:

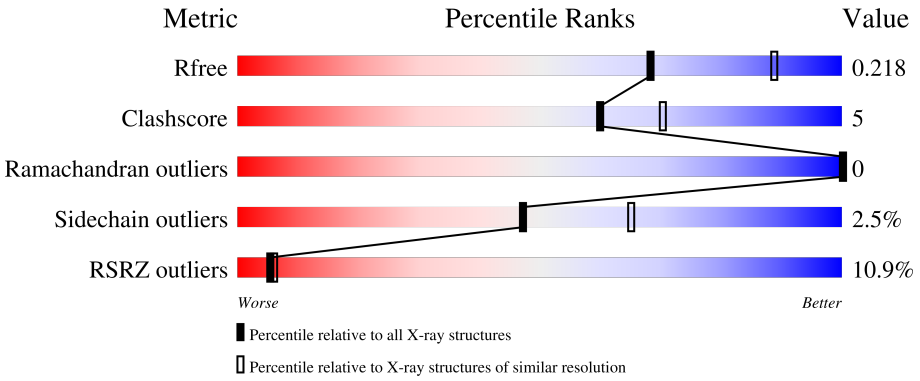
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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 <=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	395	10% 81% 12% • 7%
1	B	395	6% 41% 5% 53%
2	C	19	5% 68% 26% 5%
3	D	17	6% 76% 12% 12%

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
6	GOL	A	1383	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5489 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 PFV INTEGRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	0	1	0
			2928	1877	515	532	4			
1	B	184	Total	C	N	O	S	0	0	0
			1433	930	233	269	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P14350
A	-1	PRO	-	expression tag	UNP P14350
A	0	GLY	-	expression tag	UNP P14350
A	217	SER	GLY	variant	UNP P14350
A	218	GLY	SER	variant	UNP P14350
B	-2	GLY	-	expression tag	UNP P14350
B	-1	PRO	-	expression tag	UNP P14350
B	0	GLY	-	expression tag	UNP P14350
B	217	SER	GLY	variant	UNP P14350
B	218	GLY	SER	variant	UNP P14350

- Molecule 2 is a DNA chain called 19 NUCLEOTIDE PREPROCESSED PFV DONOR DNA (NON-TRANSFERRED STRAND).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	P	0	0	0
			387	187	68	114	18			

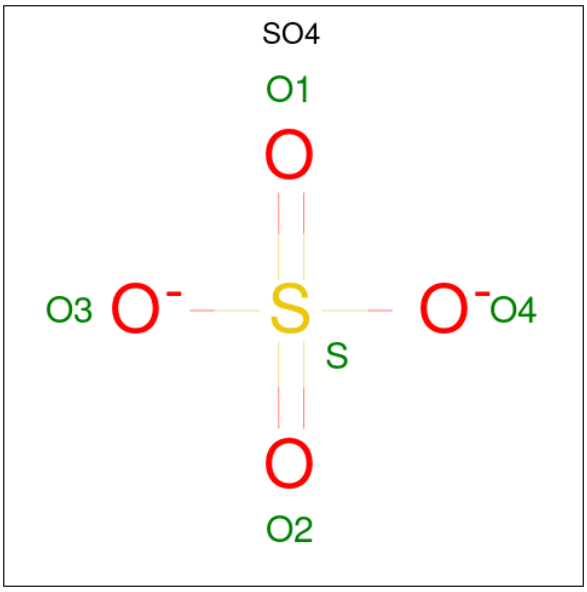
- Molecule 3 is a DNA chain called 17 NUCLEOTIDE PREPROCESSED PFV DONOR DNA (TRANSFERRED STRAND) *AP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	17	Total	C	N	O	P	0	0	0
			345	166	65	98	16			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

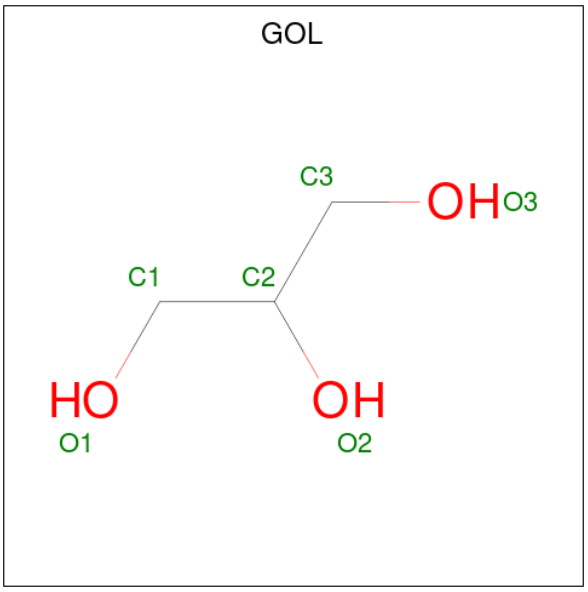
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Zn 1 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

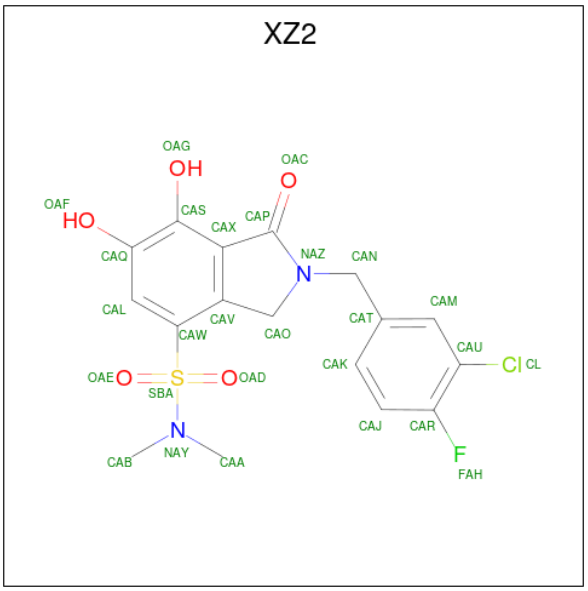


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Mg 2 2	0	0
7	B	1	Total Mg 1 1	0	0

- Molecule 8 is 2-(3-chloro-4-fluorobenzyl)-6,7-dihydroxy-N,N-dimethyl-1-oxo-2,3-dihydro-1H-isoindole-4-sulfonamide (three-letter code: XZ2) (formula: $C_{17}H_{16}ClFN_2O_5S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	D	1	Total	C	Cl	F	N	O	S	0	0
			27	17	1	1	2	5	1		

- Molecule 9 is water.

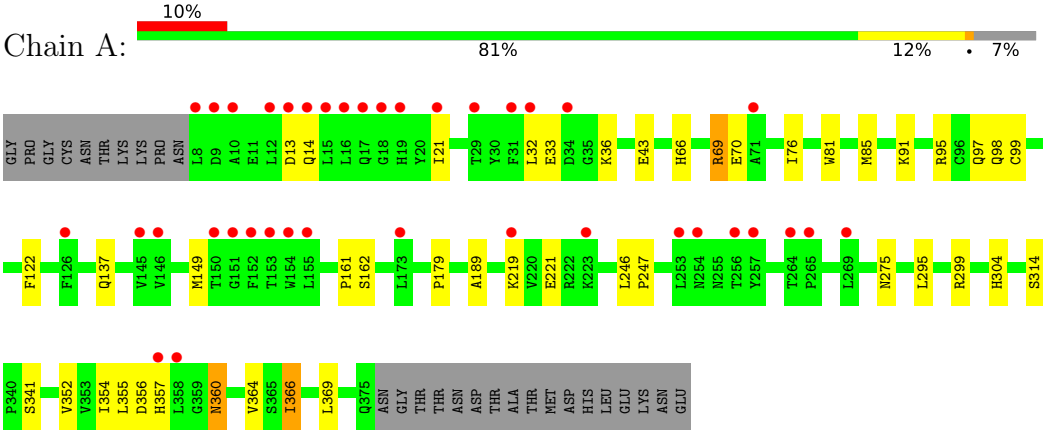
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	207	Total	O	0	0
			207	207		
9	B	54	Total	O	0	0
			54	54		
9	C	31	Total	O	0	0
			31	31		
9	D	28	Total	O	0	0
			28	28		

3 Residue-property plots (i)

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

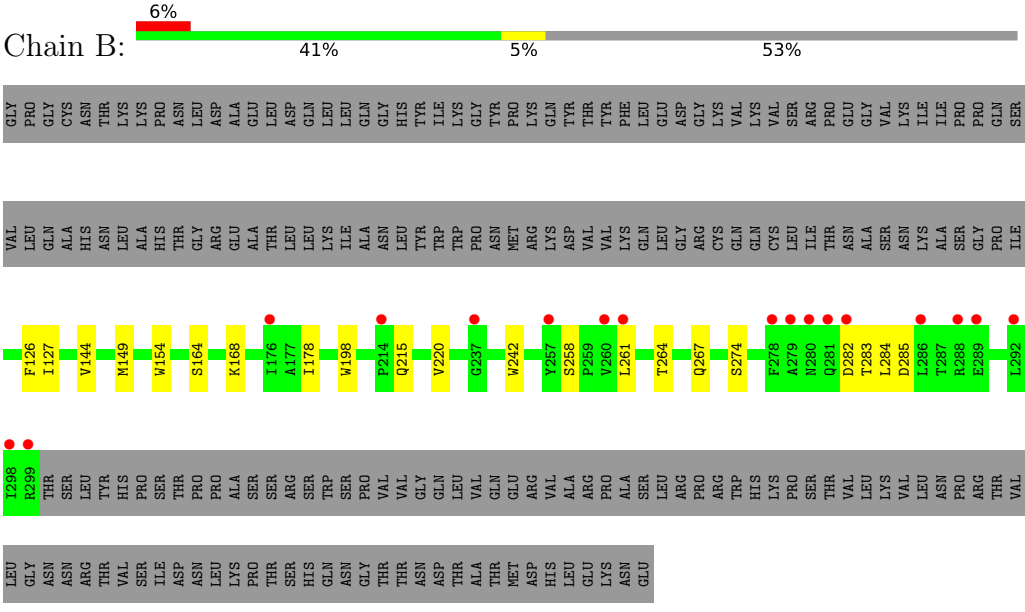
• Molecule 1: PFV INTEGRASE

Chain A:



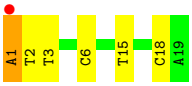
• Molecule 1: PFV INTEGRASE

Chain B:



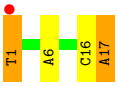
• Molecule 2: 19 NUCLEOTIDE PREPROCESSED PFV DONOR DNA (NON-TRANSFERRED STRAND)

Chain C:



• Molecule 3: 17 NUCLEOTIDE PREPROCESSED PFV DONOR DNA (TRANSFERRED STRAND) *AP*CP*A)-3'

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.42Å 159.42Å 123.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.72 – 2.38 38.67 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.72-2.38) 99.1 (38.67-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.195 , 0.223 0.191 , 0.218	Depositor DCC
R_{free} test set	3233 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	5489	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, GOL, SO4, XZ2, 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	0.64	1/3010 (0.0%)	0.71	2/4108 (0.0%)
1	B	0.64	3/1473 (0.2%)	0.65	0/2016
2	C	0.49	0/433	1.09	4/667 (0.6%)
3	D	0.47	0/387	1.16	4/595 (0.7%)
All	All	0.62	4/5303 (0.1%)	0.78	10/7386 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	154	TRP	CD2-CE2	6.58	1.49	1.41
1	B	198	TRP	CD2-CE2	5.26	1.47	1.41
1	A	81	TRP	CD2-CE2	5.22	1.47	1.41
1	B	242	TRP	CD2-CE2	5.18	1.47	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	DA	P-O3'-C3'	10.47	132.27	119.70
3	D	1	DT	P-O3'-C3'	10.12	131.84	119.70
1	A	69	ARG	NE-CZ-NH2	-8.16	116.22	120.30
3	D	17	DA	O5'-P-OP2	-7.12	99.29	105.70
1	A	69	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	C	15	DT	P-O3'-C3'	5.71	126.55	119.70
3	D	16	DC	P-O3'-C3'	5.48	126.28	119.70
3	D	6	DA	P-O3'-C3'	5.39	126.17	119.70
2	C	18	DC	P-O3'-C3'	5.26	126.01	119.70
2	C	1	DA	OP1-P-O3'	5.12	116.45	105.20

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	2928	0	2958	31	0
1	B	1433	0	1406	7	0
2	C	387	0	218	6	0
3	D	345	0	193	3	0
4	A	1	0	0	0	0
5	A	10	0	0	0	0
5	B	5	0	0	0	0
6	A	24	0	32	7	0
6	B	6	0	8	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
8	D	27	0	14	3	0
9	A	207	0	0	3	1
9	B	54	0	0	0	0
9	C	31	0	0	0	0
9	D	28	0	0	0	0
All	All	5489	0	4829	46	1

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 (46) 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)
6:A:1383:GOL:C3	2:C:3:DT:H3	1.55	1.19
6:A:1383:GOL:H32	2:C:3:DT:N3	1.66	1.10
6:A:1383:GOL:H32	2:C:3:DT:H3	0.81	0.97
1:A:137:GLN:H	6:A:1378:GOL:H2	1.35	0.90
1:B:258:SER:O	1:B:261:LEU:O	2.01	0.78
1:A:219:LYS:HE3	2:C:6:DC:OP1	1.84	0.77
6:A:1383:GOL:C3	2:C:3:DT:N3	2.36	0.76
3:D:17:DA:C2	8:D:1018:XZ2:HAAA	2.25	0.72
1:A:98:GLN:OE1	9:A:2032:HOH:O	2.15	0.65
1:A:69:ARG:HD2	1:A:70:GLU:OE2	2.00	0.61
1:A:91:LYS:HE3	1:A:95:ARG:HH21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:PRO:HB3	6:A:1383:GOL:H31	1.88	0.55
1:A:32:LEU:HD23	1:A:33:GLU:N	2.24	0.54
1:A:108:ALA:O	1:A:314:SER:HA	2.09	0.53
3:D:1:DT:O4'	3:D:1:DT:O2	2.26	0.53
1:A:162:SER:HB2	6:A:1377:GOL:H2	1.92	0.52
1:A:357:HIS:CD2	9:A:2183:HOH:O	2.62	0.51
1:A:97:GLN:HE21	1:A:339:LYS:HG2	1.76	0.50
1:A:295:LEU:HD21	1:A:299:ARG:NH2	2.26	0.50
1:A:91:LYS:HE3	1:A:95:ARG:NH2	2.26	0.50
2:C:1:DA:H2"	2:C:2:DT:H5'	1.93	0.49
1:A:357:HIS:HD2	9:A:2183:HOH:O	1.95	0.49
1:A:161:PRO:O	1:A:189:ALA:HB2	2.13	0.49
1:A:325:GLU:HA	1:A:369:LEU:HD23	1.95	0.48
1:B:264:THR:OG1	1:B:267:GLN:HG3	2.13	0.48
1:A:122:PHE:O	1:A:179:PRO:HA	2.13	0.48
1:A:360:ASN:N	1:A:360:ASN:OD1	2.48	0.47
1:A:341:SER:HB2	1:A:355:LEU:O	2.16	0.46
1:A:14:GLN:HB3	1:A:21:ILE:HD11	1.98	0.46
1:B:127:ILE:HA	1:B:144:VAL:O	2.15	0.46
1:A:97:GLN:NE2	1:A:339:LYS:HG2	2.31	0.45
8:D:1018:XZ2:HAB	8:D:1018:XZ2:HAOA	1.98	0.45
1:B:283:THR:C	1:B:285:ASP:H	2.19	0.44
1:A:275:ASN:HB3	1:B:178:ILE:HG22	2.00	0.44
1:A:114:ARG:O	1:A:304:HIS:HE1	2.02	0.43
1:A:356:ASP:C	1:A:356:ASP:OD1	2.58	0.42
1:A:221:GLU:HA	1:A:221:GLU:OE1	2.20	0.42
3:D:17:DA:H3'	8:D:1018:XZ2:HANA	2.01	0.42
1:A:246:LEU:HB2	1:A:247:PRO:HD3	2.00	0.41
1:A:43:GLU:H	1:A:43:GLU:CD	2.23	0.41
1:A:76:ILE:HG22	1:A:85:MET:CE	2.50	0.41
1:A:66:HIS:HB3	1:A:99:CYS:SG	2.62	0.40
1:A:352:VAL:HG23	1:A:354:ILE:HG23	2.02	0.40
1:A:366:ILE:HD13	1:A:366:ILE:HG21	1.64	0.40
1:B:284:LEU:HD12	1:B:284:LEU:HA	1.92	0.40
1:B:126:PHE:CD1	1:B:220:VAL:HG21	2.56	0.40

All (1) 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)
9:A:2014:HOH:O	9:A:2135:HOH:O[8_554]	2.05	0.15

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	367/395 (93%)	356 (97%)	11 (3%)	0	100	100
1	B	182/395 (46%)	169 (93%)	13 (7%)	0	100	100
All	All	549/790 (70%)	525 (96%)	24 (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	328/354 (93%)	322 (98%)	6 (2%)	59	75
1	B	157/354 (44%)	151 (96%)	6 (4%)	33	49
All	All	485/708 (68%)	473 (98%)	12 (2%)	47	65

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	36	LYS
1	A	149	MET
1	A	360	ASN
1	A	364	VAL
1	A	366	ILE
1	B	149	MET
1	B	164	SER

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Mol	Chain	Res	Type
1	B	168	LYS
1	B	215	GLN
1	B	274	SER
1	B	282	ASP

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

Mol	Chain	Res	Type
1	A	97	GLN
1	A	357	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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
5	SO4	A	1376	-	4,4,4	0.38	0	6,6,6	0.29	0
5	SO4	A	1382	-	4,4,4	0.40	0	6,6,6	0.46	0
6	GOL	A	1378	-	5,5,5	0.38	0	5,5,5	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	A	1377	-	5,5,5	0.42	0	5,5,5	0.89	0
5	SO4	B	1300	-	4,4,4	0.34	0	6,6,6	0.20	0
6	GOL	A	1379	-	5,5,5	0.24	0	5,5,5	0.42	0
6	GOL	B	1301	-	5,5,5	0.35	0	5,5,5	0.41	0
8	XZ2	D	1018	7	29,29,29	2.34	6 (20%)	39,45,45	2.84	12 (30%)
6	GOL	A	1383	-	5,5,5	0.37	0	5,5,5	1.05	0

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
6	GOL	A	1378	-	-	0/4/4/4	-
6	GOL	A	1377	-	-	3/4/4/4	-
6	GOL	A	1379	-	-	2/4/4/4	-
6	GOL	B	1301	-	-	0/4/4/4	-
8	XZ2	D	1018	7	-	2/16/28/28	0/3/3/3
6	GOL	A	1383	-	-	3/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	1018	XZ2	CAX-CAP	-5.94	1.38	1.49
8	D	1018	XZ2	OAE-SBA	5.93	1.50	1.43
8	D	1018	XZ2	OAD-SBA	5.76	1.49	1.43
8	D	1018	XZ2	SBA-NAY	-4.47	1.48	1.62
8	D	1018	XZ2	CAW-SBA	3.98	1.83	1.78
8	D	1018	XZ2	CAO-CAV	2.46	1.53	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	1018	XZ2	OAE-SBA-OAD	-9.20	104.62	119.52
8	D	1018	XZ2	CAX-CAP-NAZ	7.53	112.09	106.41
8	D	1018	XZ2	OAC-CAP-CAX	-5.34	121.48	129.09
8	D	1018	XZ2	CAL-CAW-CAV	-5.19	118.33	121.80
8	D	1018	XZ2	CAB-NAY-CAA	4.69	124.28	114.79
8	D	1018	XZ2	OAD-SBA-NAY	4.68	116.77	106.85
8	D	1018	XZ2	CAL-CAW-SBA	3.73	122.23	117.57
8	D	1018	XZ2	OAE-SBA-CAW	2.98	113.14	107.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	1018	XZ2	CAU-CAM-CAT	-2.94	118.45	120.46
8	D	1018	XZ2	CAN-NAZ-CAO	2.54	125.03	122.36
8	D	1018	XZ2	CAK-CAT-CAM	2.23	121.66	118.54
8	D	1018	XZ2	CAV-CAW-SBA	-2.16	119.44	123.00

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1377	GOL	O1-C1-C2-C3
6	A	1379	GOL	O1-C1-C2-C3
6	A	1383	GOL	C1-C2-C3-O3
6	A	1377	GOL	O1-C1-C2-O2
6	A	1383	GOL	O2-C2-C3-O3
6	A	1379	GOL	O1-C1-C2-O2
6	A	1377	GOL	O2-C2-C3-O3
8	D	1018	XZ2	CAA-NAY-SBA-OAD
6	A	1383	GOL	O1-C1-C2-O2
8	D	1018	XZ2	CAB-NAY-SBA-OAE

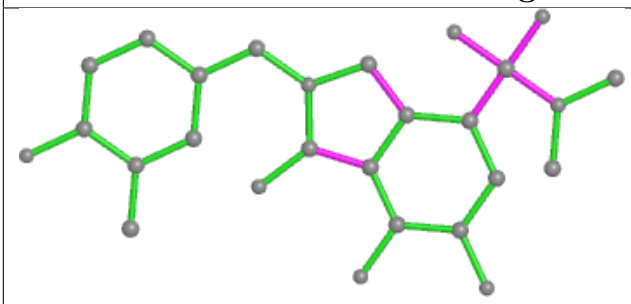
There are no ring outliers.

4 monomers are involved in 10 short contacts:

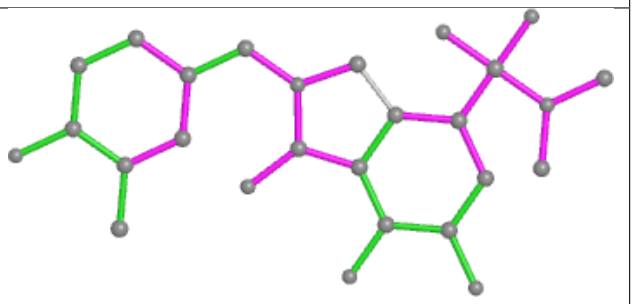
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1378	GOL	1	0
6	A	1377	GOL	1	0
8	D	1018	XZ2	3	0
6	A	1383	GOL	5	0

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 then 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.

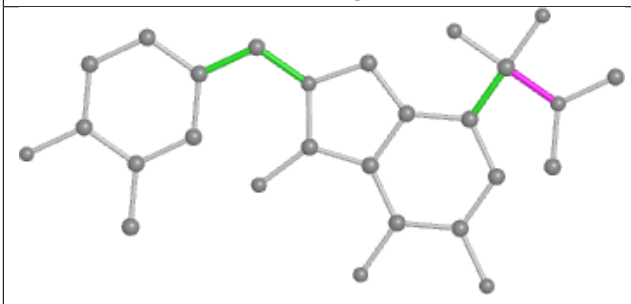
Ligand XZ2 D 1018



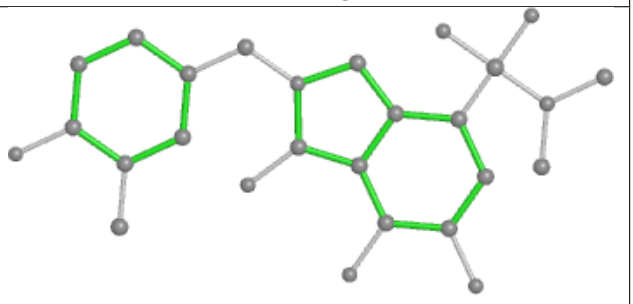
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	368/395 (93%)	0.44	38 (10%)	6	7	34, 48, 90, 130	0
1	B	184/395 (46%)	0.44	24 (13%)	3	3	39, 54, 121, 145	0
2	C	19/19 (100%)	-0.08	1 (5%)	26	29	38, 56, 80, 108	0
3	D	17/17 (100%)	-0.17	1 (5%)	22	24	40, 49, 73, 115	1 (5%)
All	All	588/826 (71%)	0.40	64 (10%)	5	6	34, 49, 101, 145	1 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	LEU	6.0
1	B	280	ASN	5.1
1	B	279	ALA	5.0
1	B	292	LEU	4.7
1	B	116	ASP	4.6
1	B	299	ARG	4.6
1	A	9	ASP	4.3
1	A	16	LEU	4.1
1	B	298	ILE	4.1
1	B	281	GLN	3.9
1	A	17	GLN	3.8
1	A	15	LEU	3.7
1	B	296	GLN	3.7
1	B	295	LEU	3.7
1	A	154	TRP	3.6
1	B	260	VAL	3.6
1	A	358	LEU	3.6
1	B	214	PRO	3.5
1	A	14	GLN	3.5
1	A	32	LEU	3.4
1	A	146	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	10	ALA	3.3
1	B	237	GLY	3.3
1	B	257	TYR	3.2
1	A	19	HIS	3.1
1	A	13	ASP	3.0
1	A	265	PRO	3.0
1	A	357	HIS	2.9
1	B	297	GLU	2.9
1	A	253	LEU	2.9
1	B	282	ASP	2.8
1	A	152	PHE	2.8
1	A	153	THR	2.8
1	A	145	VAL	2.8
1	B	278	PHE	2.7
1	A	269	LEU	2.7
1	B	176	ILE	2.6
1	A	71	ALA	2.6
1	B	289	GLU	2.6
1	A	256	THR	2.5
3	D	1	DT	2.5
1	A	173	LEU	2.5
1	B	294	LEU	2.5
1	A	254	ASN	2.5
1	B	117	ARG	2.5
1	A	257	TYR	2.5
1	B	286	LEU	2.5
1	A	29	THR	2.4
1	B	293	SER	2.4
1	A	264	THR	2.4
1	A	31	PHE	2.4
1	B	288	ARG	2.4
1	A	219	LYS	2.4
1	A	150	THR	2.4
1	A	151	GLY	2.3
2	C	1	DA	2.3
1	A	21	ILE	2.3
1	A	126	PHE	2.3
1	A	18	GLY	2.2
1	B	261	LEU	2.2
1	A	12	LEU	2.2
1	A	155	LEU	2.1
1	A	34	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	223	LYS	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)

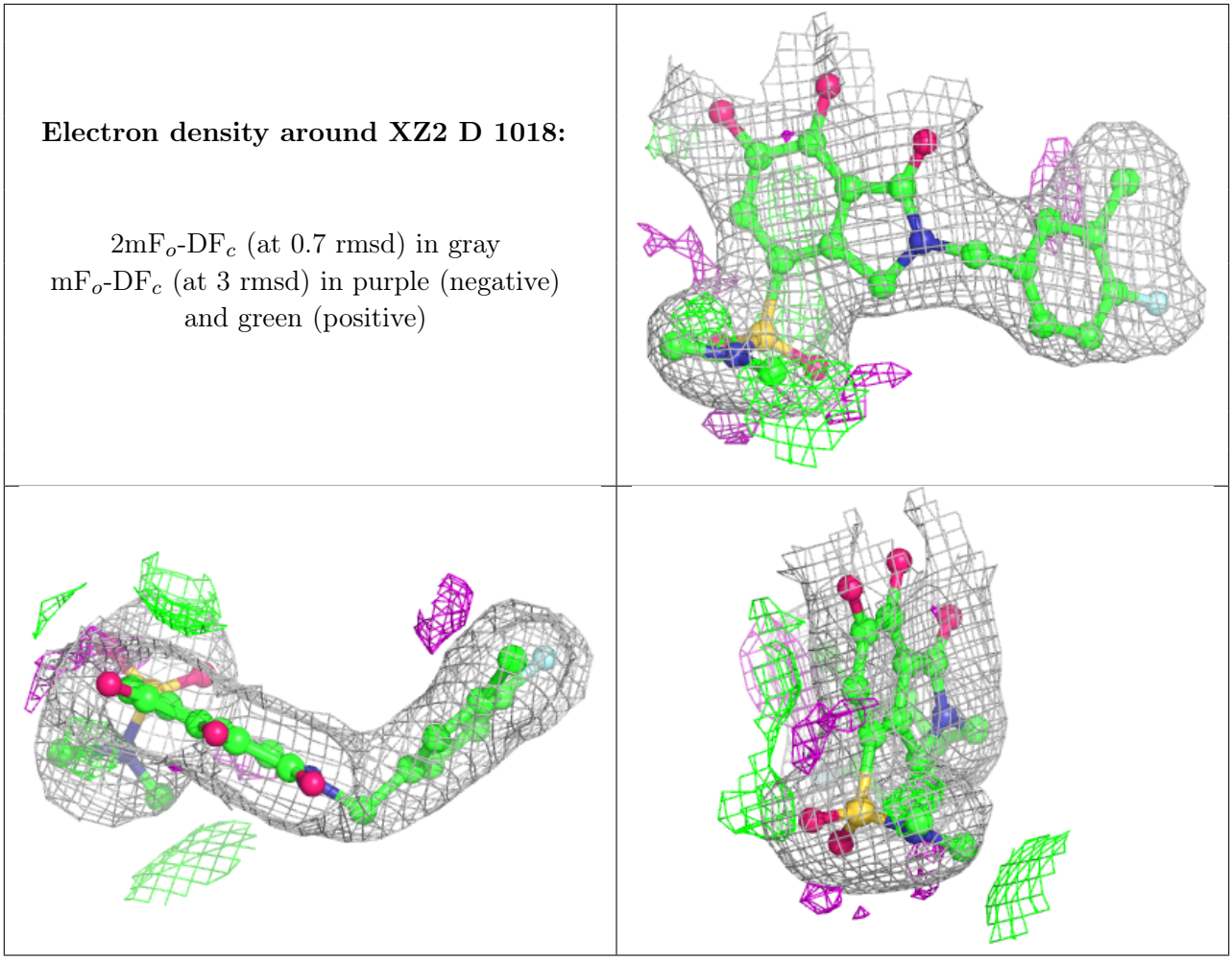
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
6	GOL	A	1378	6/6	0.71	0.28	63,74,81,89	0
6	GOL	A	1377	6/6	0.76	0.23	71,78,84,85	0
6	GOL	A	1383	6/6	0.89	0.29	58,61,71,73	0
5	SO4	A	1382	5/5	0.90	0.25	42,43,50,53	5
6	GOL	B	1301	6/6	0.91	0.27	68,72,74,82	0
6	GOL	A	1379	6/6	0.95	0.18	68,76,78,86	0
8	XZ2	D	1018	27/27	0.96	0.12	36,45,63,67	0
5	SO4	A	1376	5/5	0.97	0.16	81,84,92,94	0
7	MG	B	1302	1/1	0.97	0.26	97,97,97,97	0
5	SO4	B	1300	5/5	0.97	0.17	72,79,90,93	0
7	MG	A	1381	1/1	0.98	0.08	39,39,39,39	0
7	MG	A	1380	1/1	0.99	0.06	43,43,43,43	0
4	ZN	A	393	1/1	1.00	0.12	44,44,44,44	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 XZ2 D 1018:

$2mF_o$-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.