Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2024 – 11:55 AM EDT

PDB ID	:	1IGJ
Title	:	26-10 FAB:DIGOXIN COMPLEX-AFFINITY AND SPECIFICITY DUE TO SURFACE COMPLEMENTARITY
Authors	:	Jeffrey, P.D.; Sheriff, S.
Deposited on	:	1993-02-19
Resolution	:	2.50 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:

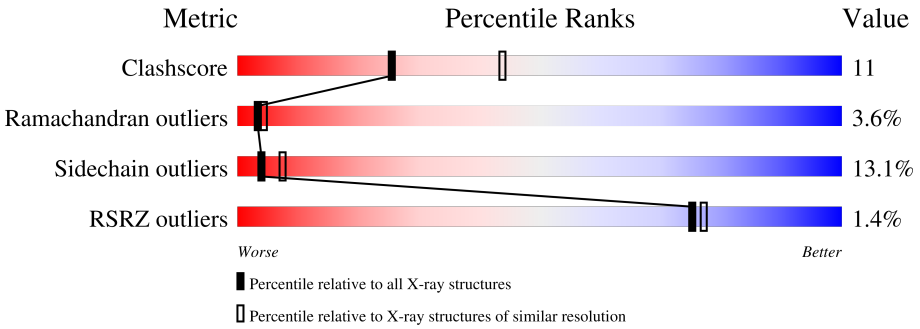
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	219	59% 34% 5% •
1	C	219	65% 28% 5% ••
2	B	218	3% 58% 33% 8%
2	D	218	2% 55% 36% 7% •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6650 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 IGG2A-KAPPA 26-10 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1666	1040	284	336	6			
1	C	216	Total	C	N	O	S	0	0	0
			1666	1040	284	336	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	THR	SER	conflict	PIR S52028
A	27B	LEU	ILE	conflict	PIR S52028
A	34	ASN	GLU	conflict	PIR S52028
A	40	ALA	PRO	conflict	PIR S52028
A	85	ILE	VAL	conflict	PIR S52028
A	87	PHE	TYR	conflict	PIR S52028
A	89	SER	PHE	conflict	PIR S52028
A	91	THR	GLY	conflict	PIR S52028
A	92	THR	SER	conflict	PIR S52028
A	103	LYS	ASN	conflict	PIR S52028
C	7	THR	SER	conflict	PIR S52028
C	27B	LEU	ILE	conflict	PIR S52028
C	34	ASN	GLU	conflict	PIR S52028
C	40	ALA	PRO	conflict	PIR S52028
C	85	ILE	VAL	conflict	PIR S52028
C	87	PHE	TYR	conflict	PIR S52028
C	89	SER	PHE	conflict	PIR S52028
C	91	THR	GLY	conflict	PIR S52028
C	92	THR	SER	conflict	PIR S52028
C	103	LYS	ASN	conflict	PIR S52028

- Molecule 2 is a protein called IGG2A-KAPPA 26-10 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1622	1024	264	325	9			
2	D	217	Total	C	N	O	S	0	0	0
			1622	1024	264	325	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	13	LYS	ARG	conflict	PIR S38950
B	19	ARG	LYS	conflict	PIR S38950
B	20	MET	ILE	conflict	PIR S38950
B	24	SER	ALA	conflict	PIR S38950
B	28	ILE	THR	conflict	PIR S38950
B	32	PHE	TYR	conflict	PIR S38950
B	34	MET	ILE	conflict	PIR S38950
B	35	ASN	HIS	conflict	PIR S38950
B	38	ARG	LYS	conflict	PIR S38950
B	40	SER	ARG	conflict	PIR S38950
B	41	HIS	PRO	conflict	PIR S38950
B	43	LYS	GLU	conflict	PIR S38950
B	44	SER	GLY	conflict	PIR S38950
B	46	ASP	GLU	conflict	PIR S38950
B	47	TYR	TRP	conflict	PIR S38950
B	50	TYR	TRP	conflict	PIR S38950
B	52	SER	TYR	conflict	PIR S38950
B	53	TYR	GLY	conflict	PIR S38950
B	56	VAL	ASN	conflict	PIR S38950
B	58	GLY	LYS	conflict	PIR S38950
B	61	GLN	GLU	conflict	PIR S38950
B	73	LYS	THR	conflict	PIR S38950
B	81	GLU	GLN	conflict	PIR S38950
B	82A	ARG	SER	conflict	PIR S38950
B	91	TYR	PHE	conflict	PIR S38950
B	94	GLY	-	insertion	PIR S38950
B	95	SER	-	insertion	PIR S38950
B	96	SER	ARG	conflict	PIR S38950
B	98	ASN	GLY	conflict	PIR S38950
B	100	TRP	PHE	conflict	PIR S38950
B	105	HIS	GLN	conflict	PIR S38950
B	107	ALA	THR	conflict	PIR S38950
D	13	LYS	ARG	conflict	PIR S38950
D	19	ARG	LYS	conflict	PIR S38950
D	20	MET	ILE	conflict	PIR S38950

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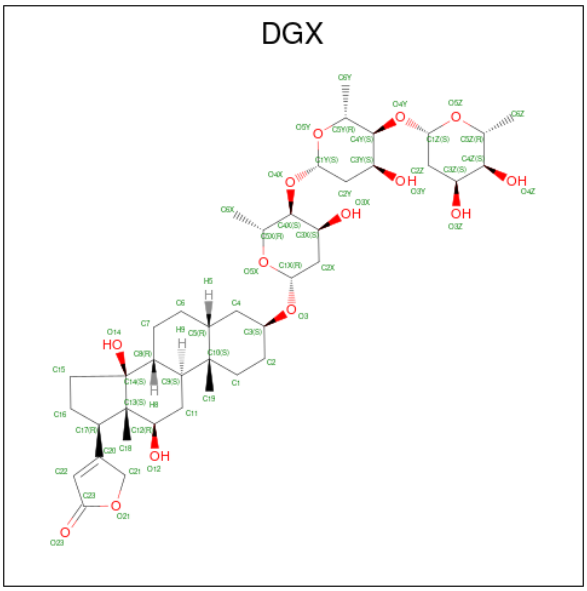
Chain	Residue	Modelled	Actual	Comment	Reference
D	24	SER	ALA	conflict	PIR S38950
D	28	ILE	THR	conflict	PIR S38950
D	32	PHE	TYR	conflict	PIR S38950
D	34	MET	ILE	conflict	PIR S38950
D	35	ASN	HIS	conflict	PIR S38950
D	38	ARG	LYS	conflict	PIR S38950
D	40	SER	ARG	conflict	PIR S38950
D	41	HIS	PRO	conflict	PIR S38950
D	43	LYS	GLU	conflict	PIR S38950
D	44	SER	GLY	conflict	PIR S38950
D	46	ASP	GLU	conflict	PIR S38950
D	47	TYR	TRP	conflict	PIR S38950
D	50	TYR	TRP	conflict	PIR S38950
D	52	SER	TYR	conflict	PIR S38950
D	53	TYR	GLY	conflict	PIR S38950
D	56	VAL	ASN	conflict	PIR S38950
D	58	GLY	LYS	conflict	PIR S38950
D	61	GLN	GLU	conflict	PIR S38950
D	73	LYS	THR	conflict	PIR S38950
D	81	GLU	GLN	conflict	PIR S38950
D	82A	ARG	SER	conflict	PIR S38950
D	91	TYR	PHE	conflict	PIR S38950
D	94	GLY	-	insertion	PIR S38950
D	95	SER	-	insertion	PIR S38950
D	96	SER	ARG	conflict	PIR S38950
D	98	ASN	GLY	conflict	PIR S38950
D	100	TRP	PHE	conflict	PIR S38950
D	105	HIS	GLN	conflict	PIR S38950
D	107	ALA	THR	conflict	PIR S38950

- Molecule 3 is DIGOXIN (three-letter code: DGX) (formula: $C_{41}H_{64}O_{14}$).



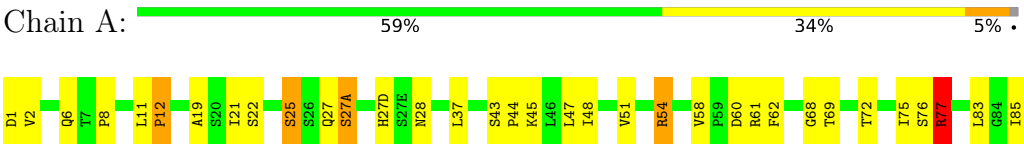
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 37 29 8	0	0
3	D	1	Total C O 37 29 8	0	0

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: IGG2A-KAPPA 26-10 FAB (LIGHT CHAIN)

Chain A:

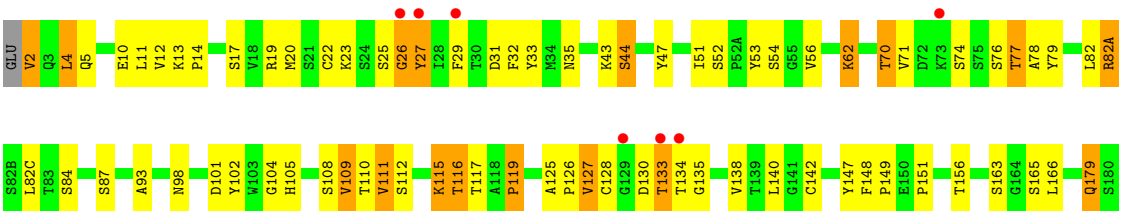


• Molecule 1: IGG2A-KAPPA 26-10 FAB (LIGHT CHAIN)

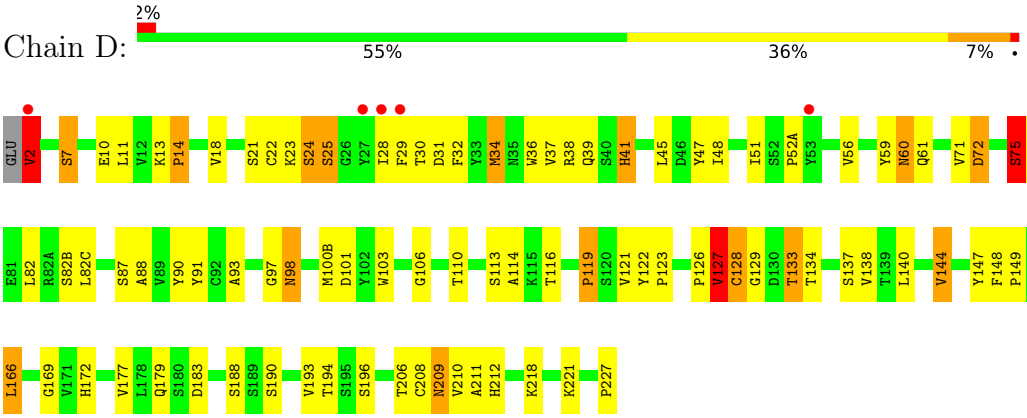
Chain C:

• Molecule 2: IGG2A-KAPPA 26-10 FAB (HEAVY CHAIN)

Chain B:



• Molecule 2: IGG2A-KAPPA 26-10 FAB (HEAVY CHAIN)



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.16Å 164.43Å 70.01Å 90.00° 108.37° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50 51.68 – 2.42	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.50) 75.4 (51.68-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.42Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.176 , (Not available) 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 36.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6650	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: DGX

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	0.65	0/1703	1.47	9/2312 (0.4%)
1	C	0.65	0/1703	1.57	20/2312 (0.9%)
2	B	0.67	0/1664	1.58	22/2268 (1.0%)
2	D	0.65	0/1664	1.56	15/2268 (0.7%)
All	All	0.65	0/6734	1.55	66/9160 (0.7%)

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	C	0	1

There are no bond length outliers.

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	211	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	A	88	CYS	CA-CB-SG	8.93	130.07	114.00
1	A	211	ARG	NE-CZ-NH1	8.73	124.66	120.30
1	C	190	ASN	CA-C-N	7.30	133.27	117.20
1	C	2	VAL	N-CA-C	-6.96	92.21	111.00
1	C	1	ASP	N-CA-C	-6.86	92.49	111.00
2	D	2	VAL	N-CA-C	-6.86	92.49	111.00
1	A	198	HIS	CA-CB-CG	6.83	125.21	113.60
1	A	90	GLN	CA-CB-CG	6.80	128.35	113.40
2	B	25	SER	CA-C-N	-6.79	102.63	116.20
2	D	133	THR	N-CA-C	-6.72	92.85	111.00
2	D	31	ASP	CA-C-N	-6.52	102.85	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	187	LEU	CA-CB-CG	6.42	130.08	115.30
2	B	20	MET	CG-SD-CE	-6.30	90.12	100.20
2	D	227	PRO	N-CA-CB	6.23	110.78	103.30
2	B	128	CYS	CA-CB-SG	-6.18	102.88	114.00
2	B	43	LYS	CA-CB-CG	6.17	126.98	113.40
2	B	128	CYS	N-CA-C	6.16	127.63	111.00
2	D	144	VAL	CG1-CB-CG2	-6.14	101.08	110.90
1	A	160	LEU	CA-CB-CG	6.08	129.29	115.30
1	C	211	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	77	ARG	CA-CB-CG	6.05	126.72	113.40
2	B	208	CYS	CA-CB-SG	-6.02	103.16	114.00
2	D	127	VAL	CA-CB-CG1	6.01	119.91	110.90
1	C	105	GLU	CA-CB-CG	6.00	126.60	113.40
2	D	98	ASN	N-CA-C	5.96	127.08	111.00
1	C	106	ILE	CA-CB-CG1	-5.95	99.70	111.00
1	C	68	GLY	O-C-N	5.93	132.18	122.70
2	D	82(B)	SER	CA-C-N	-5.89	104.25	117.20
2	B	19	ARG	NE-CZ-NH2	-5.79	117.41	120.30
2	D	37	VAL	CG1-CB-CG2	-5.75	101.69	110.90
2	B	31	ASP	CA-C-N	-5.72	104.61	117.20
1	C	105	GLU	N-CA-CB	-5.67	100.39	110.60
1	C	180	THR	CA-C-N	-5.65	104.78	117.20
2	D	59	TYR	CB-CG-CD1	-5.63	117.62	121.00
2	B	33	TYR	O-C-N	5.59	131.65	122.70
2	B	82(A)	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	D	31	ASP	O-C-N	5.53	131.56	122.70
1	A	54	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	A	160	LEU	N-CA-CB	-5.52	99.36	110.40
2	D	75	SER	O-C-N	5.50	131.50	122.70
2	B	142	CYS	CA-CB-SG	5.45	123.81	114.00
2	B	109	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	C	77	ARG	N-CA-C	-5.37	96.50	111.00
1	C	136	LEU	N-CA-C	-5.32	96.64	111.00
2	B	101	ASP	CA-CB-CG	5.31	125.08	113.40
1	C	75	ILE	N-CA-C	-5.29	96.71	111.00
2	B	156	THR	CA-CB-CG2	-5.25	105.05	112.40
2	B	208	CYS	CA-C-N	5.25	128.74	117.20
2	B	4	LEU	CA-CB-CG	5.23	127.33	115.30
1	C	140	TYR	CB-CG-CD2	-5.22	117.87	121.00
2	B	111	VAL	CG1-CB-CG2	-5.20	102.58	110.90
2	B	218	LYS	N-CA-C	-5.20	96.96	111.00
1	C	81	GLU	CA-CB-CG	5.20	124.84	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	22	SER	CB-CA-C	-5.17	100.28	110.10
1	C	94	VAL	CG1-CB-CG2	-5.17	102.63	110.90
2	B	2	VAL	N-CA-C	-5.14	97.11	111.00
2	D	60	ASN	N-CA-C	-5.12	97.17	111.00
1	C	47	LEU	CB-CG-CD1	-5.12	102.30	111.00
2	D	128	CYS	N-CA-C	5.12	124.81	111.00
1	C	185	GLU	CA-CB-CG	5.10	124.62	113.40
2	B	47	TYR	CB-CG-CD2	5.10	124.06	121.00
1	C	108	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	194	CYS	CA-CB-SG	-5.08	104.86	114.00
2	B	27	TYR	CB-CG-CD1	5.03	124.02	121.00
2	D	166	LEU	CB-CG-CD1	-5.03	102.45	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	140	TYR	Sidechain

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	1666	0	1617	40	0
1	C	1666	0	1617	27	0
2	B	1622	0	1566	35	0
2	D	1622	0	1566	43	0
3	B	37	0	43	0	0
3	D	37	0	43	0	0
All	All	6650	0	6452	139	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 11.

All (139) 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)
2:B:119:PRO:HB3	2:B:147:TYR:HB3	1.52	0.89
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.56	0.84
1:A:150:ILE:HD12	1:A:155:ARG:HD3	1.64	0.78
2:B:82:LEU:HB3	2:B:82(C):LEU:HD21	1.67	0.76
2:D:119:PRO:HB2	2:D:144:VAL:HG12	1.68	0.74
2:D:138:VAL:HG23	2:D:193:VAL:HG23	1.70	0.72
1:C:24:ARG:HA	1:C:69:THR:O	1.90	0.71
2:D:22:CYS:O	2:D:77:THR:HA	1.91	0.69
2:B:23:LYS:HB3	2:B:77:THR:HG23	1.75	0.67
1:A:12:PRO:HA	1:A:105:GLU:O	1.96	0.66
2:D:48:ILE:HD13	2:D:80:MET:SD	2.36	0.66
2:B:87:SER:HA	2:B:109:VAL:O	1.96	0.66
1:C:19:ALA:HB3	1:C:75:ILE:HD13	1.79	0.65
1:C:12:PRO:HA	1:C:105:GLU:O	1.96	0.65
1:A:54:ARG:HD2	1:A:62:PHE:O	1.98	0.64
2:B:35:ASN:HB2	2:B:93:ALA:HB3	1.81	0.63
2:B:11:LEU:HD23	2:B:110:THR:HB	1.81	0.62
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.82	0.61
2:B:51:ILE:HA	2:B:56:VAL:O	2.00	0.60
2:B:5:GLN:O	2:B:22:CYS:HA	2.02	0.59
1:C:189:HIS:O	1:C:211:ARG:HD3	2.03	0.58
2:B:119:PRO:HD2	2:B:217:THR:HG21	1.86	0.57
1:C:27(B):LEU:O	1:C:31:THR:HA	2.04	0.57
2:D:72:ASP:HB3	2:D:75:SER:OG	2.04	0.57
2:D:209:ASN:HB3	2:D:218:LYS:HE3	1.87	0.56
2:D:153:THR:HB	2:D:211:ALA:HB3	1.88	0.56
2:D:2:VAL:HA	2:D:25:SER:O	2.06	0.55
2:D:114:ALA:HB2	2:D:183:ASP:HB3	1.88	0.55
2:D:119:PRO:HB3	2:D:147:TYR:HB3	1.89	0.54
2:B:116:THR:HG22	2:B:215:SER:HB3	1.89	0.54
2:B:211:ALA:HB2	2:B:218:LYS:HE2	1.89	0.54
2:D:82:LEU:HB3	2:D:82(C):LEU:HD21	1.90	0.54
2:D:52(A):PRO:HB3	2:D:71:VAL:HG21	1.90	0.53
1:C:160:LEU:HD11	2:D:177:VAL:HG11	1.90	0.53
1:A:160:LEU:HD21	2:B:186:THR:HG21	1.91	0.53
2:B:133:THR:HB	2:B:135:GLY:H	1.73	0.52
1:C:140:TYR:HB2	1:C:172:THR:HG22	1.92	0.52
1:A:184:ASP:O	1:A:188:ARG:HB2	2.09	0.51
1:C:145:ASN:O	1:C:196:ALA:HA	2.09	0.51
1:C:115:VAL:HG22	1:C:136:LEU:HD23	1.91	0.51
1:A:150:ILE:HD11	1:A:179:LEU:CD2	2.35	0.51
1:A:186:TYR:O	1:A:211:ARG:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LYS:HD2	1:C:154:GLU:HG3	1.92	0.51
2:D:126:PRO:O	2:D:127:VAL:HG12	2.10	0.50
2:D:41:HIS:NE2	2:D:87:SER:O	2.44	0.50
2:D:39:GLN:O	2:D:88:ALA:HB1	2.12	0.50
1:C:17:ASP:O	1:C:78:VAL:HG23	2.11	0.50
1:C:189:HIS:HB2	1:C:192:TYR:OH	2.12	0.50
2:B:54:SER:HB2	2:B:56:VAL:HG23	1.94	0.49
1:C:13:VAL:HG21	1:C:78:VAL:HG11	1.94	0.49
2:B:10:GLU:HB2	2:B:109:VAL:HG22	1.94	0.49
2:D:206:THR:HA	2:D:221:LYS:O	2.13	0.49
1:A:27(D):HIS:ND1	1:A:28:ASN:OD1	2.46	0.49
1:A:37:LEU:HD12	1:A:85:ILE:O	2.13	0.48
1:A:85:ILE:HA	1:A:102:THR:O	2.13	0.48
2:D:90:TYR:O	2:D:106:GLY:HA2	2.13	0.48
2:D:7:SER:HB3	2:D:21:SER:OG	2.13	0.48
2:D:11:LEU:HD23	2:D:110:THR:HB	1.96	0.48
1:A:144:ILE:HD11	1:A:196:ALA:HB1	1.95	0.47
2:B:11:LEU:HD22	2:B:148:PHE:CZ	2.49	0.47
2:B:71:VAL:HA	2:B:78:ALA:HA	1.95	0.47
2:D:48:ILE:HG21	2:D:80:MET:SD	2.55	0.47
2:B:23:LYS:HA	2:B:76:SER:O	2.14	0.47
2:D:210:VAL:O	2:D:218:LYS:HA	2.15	0.47
2:D:28:ILE:O	2:D:30:THR:N	2.48	0.47
1:A:2:VAL:HG21	1:A:93:HIS:CG	2.49	0.46
1:A:37:LEU:O	1:A:44:PRO:HA	2.15	0.46
1:A:192:TYR:HE2	1:A:211:ARG:HG2	1.79	0.46
2:B:17:SER:HA	2:B:82(A):ARG:HA	1.98	0.46
2:D:127:VAL:O	2:D:127:VAL:HG13	2.15	0.46
2:D:23:LYS:HG3	2:D:77:THR:OG1	2.15	0.46
1:A:11:LEU:O	1:A:104:LEU:HA	2.16	0.46
2:D:116:THR:HA	2:D:148:PHE:O	2.15	0.46
1:C:120:PRO:HG2	1:C:130:ALA:HB1	1.98	0.46
1:A:27(A):SER:HA	1:A:68:GLY:O	2.16	0.46
1:C:25:SER:OG	1:C:69:THR:HA	2.15	0.46
2:D:36:TRP:HA	2:D:91:TYR:O	2.16	0.46
1:A:47:LEU:O	1:A:58:VAL:HG21	2.16	0.46
1:A:25:SER:HB2	1:A:27:GLN:O	2.15	0.46
2:B:115:LYS:O	2:B:117:THR:N	2.48	0.46
1:C:61:ARG:HD2	1:C:77:ARG:O	2.15	0.46
2:B:23:LYS:HE2	2:B:77:THR:HG23	1.97	0.45
1:A:19:ALA:HB3	1:A:75:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:VAL:HA	1:C:95:PRO:HA	1.80	0.45
2:D:47:TYR:O	2:D:60:ASN:HB2	2.16	0.45
1:A:149:LYS:HB2	1:A:193:THR:HB	1.98	0.45
1:C:36:TYR:HE2	2:D:103:TRP:HE1	1.65	0.45
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.99	0.45
1:A:160:LEU:HD23	1:A:178:THR:HB	1.98	0.45
1:C:149:LYS:HB2	1:C:193:THR:HB	1.99	0.45
1:A:143:ASP:O	1:A:198:HIS:HD2	2.01	0.44
1:A:181:LEU:HD22	1:A:185:GLU:HG2	1.97	0.44
2:D:24:SER:OG	2:D:34:MET:SD	2.69	0.44
2:D:93:ALA:HB1	2:D:100(B):MET:HB3	1.99	0.44
1:A:2:VAL:HG21	1:A:93:HIS:CD2	2.52	0.44
1:A:146:VAL:HA	1:A:195:GLU:O	2.18	0.44
2:D:121:VAL:HG22	2:D:144:VAL:HG13	2.00	0.44
1:A:149:LYS:HA	1:A:154:GLU:HA	1.99	0.44
2:B:70:THR:OG1	2:B:79:TYR:HB2	2.18	0.44
1:C:104:LEU:HD23	1:C:104:LEU:HA	1.87	0.43
2:D:172:HIS:HB2	2:D:190:SER:OG	2.18	0.43
1:A:83:LEU:HD11	1:A:106:ILE:HD11	2.00	0.43
2:B:11:LEU:HA	2:B:110:THR:O	2.17	0.43
1:A:120:PRO:HD2	1:A:186:TYR:OH	2.19	0.43
2:B:93:ALA:HA	2:B:102:TYR:O	2.19	0.43
1:A:145:ASN:HB3	1:A:197:THR:HB	2.00	0.43
2:B:13:LYS:HG2	2:B:14:PRO:HD2	2.00	0.43
2:D:14:PRO:HD2	2:D:113:SER:HB3	2.01	0.43
2:D:122:TYR:HA	2:D:123:PRO:HD2	1.86	0.43
1:A:6:GLN:HG3	1:A:88:CYS:SG	2.59	0.43
1:C:118:PHE:HE2	1:C:135:PHE:CD2	2.36	0.43
1:A:193:THR:HG23	1:A:208:SER:OG	2.19	0.43
1:A:201:SER:HB3	1:A:203:SER:O	2.19	0.43
2:B:52:SER:HB3	2:B:56:VAL:H	1.84	0.43
1:A:61:ARG:HB3	1:A:77:ARG:NH1	2.33	0.42
2:B:148:PHE:O	2:B:212:HIS:HE1	2.03	0.42
1:A:86:TYR:HE2	1:A:104:LEU:HD11	1.84	0.42
2:B:12:VAL:HG23	2:B:111:VAL:HG22	2.02	0.42
2:B:70:THR:HB	2:B:79:TYR:HD2	1.84	0.42
2:B:179:GLN:N	2:B:184:LEU:O	2.52	0.42
2:B:125:ALA:O	2:B:127:VAL:N	2.53	0.42
2:B:112:SER:HB3	2:B:148:PHE:CZ	2.54	0.41
2:B:2:VAL:HG21	2:B:27:TYR:CD1	2.55	0.41
2:B:4:LEU:HD12	2:B:104:GLY:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:151:PRO:O	2:D:212:HIS:HD2	2.04	0.41
1:C:46:LEU:HD22	2:D:101:ASP:HA	2.02	0.41
1:A:47:LEU:HD11	1:A:86:TYR:HE1	1.85	0.41
1:A:54:ARG:HG2	1:A:58:VAL:HB	2.01	0.41
2:D:127:VAL:O	2:D:129:GLY:N	2.53	0.41
1:C:95:PRO:HD3	2:D:61:GLN:OE1	2.20	0.41
1:C:149:LYS:HA	1:C:153:SER:O	2.21	0.41
1:C:197:THR:HG23	1:C:204:PRO:HG3	2.03	0.41
1:A:21:ILE:O	1:A:72:THR:HA	2.20	0.41
2:D:34:MET:HE3	2:D:78:ALA:HB2	2.02	0.41
2:D:51:ILE:HA	2:D:56:VAL:O	2.21	0.41
1:A:111:ALA:HB3	1:A:139:PHE:HA	2.02	0.40
2:D:38:ARG:O	2:D:45:LEU:HA	2.21	0.40
1:A:113:PRO:HG3	1:A:144:ILE:HD11	2.03	0.40
1:C:118:PHE:HE1	2:D:126:PRO:HA	1.86	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	214/219 (98%)	187 (87%)	21 (10%)	6 (3%)	5 7
1	C	214/219 (98%)	196 (92%)	14 (6%)	4 (2%)	8 13
2	B	215/218 (99%)	176 (82%)	29 (14%)	10 (5%)	2 2
2	D	215/218 (99%)	187 (87%)	17 (8%)	11 (5%)	2 2
All	All	858/874 (98%)	746 (87%)	81 (9%)	31 (4%)	3 4

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	VAL
1	A	171	SER
1	A	200	THR
2	B	62	LYS
2	B	116	THR
2	B	183	ASP
1	C	51	VAL
1	C	200	THR
2	D	29	PHE
2	D	98	ASN
2	D	127	VAL
2	D	128	CYS
2	B	44	SER
2	B	53	TYR
2	B	98	ASN
2	B	163	SER
2	D	25	SER
2	D	41	HIS
2	D	76	SER
2	D	134	THR
2	D	196	SER
1	A	138	ASN
1	C	169	LYS
1	A	60	ASP
2	B	130	ASP
2	D	97	GLY
1	A	109	ALA
1	C	199	LYS
2	B	126	PRO
2	D	169	GLY
2	B	26	GLY

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	193/196 (98%)	170 (88%)	23 (12%)	5 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	193/196 (98%)	169 (88%)	24 (12%)	4 9
2	B	184/187 (98%)	156 (85%)	28 (15%)	3 5
2	D	184/187 (98%)	160 (87%)	24 (13%)	4 7
All	All	754/766 (98%)	655 (87%)	99 (13%)	4 7

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	8	PRO
1	A	12	PRO
1	A	22	SER
1	A	25	SER
1	A	27(A)	SER
1	A	43	SER
1	A	45	LYS
1	A	48	ILE
1	A	69	THR
1	A	76	SER
1	A	77	ARG
1	A	91	THR
1	A	94	VAL
1	A	96	PRO
1	A	104	LEU
1	A	132	VAL
1	A	156	GLN
1	A	182	THR
1	A	183	LYS
1	A	199	LYS
1	A	200	THR
1	A	202	THR
2	B	29	PHE
2	B	32	PHE
2	B	44	SER
2	B	62	LYS
2	B	70	THR
2	B	74	SER
2	B	77	THR
2	B	84	SER
2	B	105	HIS
2	B	108	SER

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Mol	Chain	Res	Type
2	B	115	LYS
2	B	119	PRO
2	B	127	VAL
2	B	133	THR
2	B	134	THR
2	B	138	VAL
2	B	140	LEU
2	B	149	PRO
2	B	151	PRO
2	B	165	SER
2	B	166	LEU
2	B	179	GLN
2	B	183	ASP
2	B	203	GLN
2	B	209	ASN
2	B	218	LYS
2	B	219	VAL
2	B	220	ASP
1	C	1	ASP
1	C	8	PRO
1	C	18	GLN
1	C	43	SER
1	C	51	VAL
1	C	54	ARG
1	C	56	SER
1	C	91	THR
1	C	95	PRO
1	C	122	SER
1	C	127	SER
1	C	163	TRP
1	C	164	THR
1	C	170	ASP
1	C	175	MET
1	C	181	LEU
1	C	182	THR
1	C	184	ASP
1	C	197	THR
1	C	200	THR
1	C	202	THR
1	C	203	SER
1	C	204	PRO
1	C	211	ARG

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Mol	Chain	Res	Type
2	D	2	VAL
2	D	7	SER
2	D	10	GLU
2	D	13	LYS
2	D	14	PRO
2	D	18	VAL
2	D	24	SER
2	D	32	PHE
2	D	34	MET
2	D	72	ASP
2	D	75	SER
2	D	119	PRO
2	D	133	THR
2	D	137	SER
2	D	140	LEU
2	D	149	PRO
2	D	151	PRO
2	D	152	VAL
2	D	166	LEU
2	D	179	GLN
2	D	188	SER
2	D	194	THR
2	D	208	CYS
2	D	209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	53	ASN
2	B	35	ASN
2	B	203	GLN
2	B	209	ASN
1	C	18	GLN
2	D	35	ASN

5.3.3 RNA

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)

2 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	$\#\|Z\| > 2$
3	DGX	B	228	-	42,42,62	0.91	2 (4%)	63,68,98	1.41	10 (15%)
3	DGX	D	228	-	42,42,62	0.63	0	63,68,98	1.26	4 (6%)

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	DGX	B	228	-	-	2/8/101/141	0/6/6/8
3	DGX	D	228	-	-	2/8/101/141	0/6/6/8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	228	DGX	C14-C8	3.27	1.58	1.54
3	B	228	DGX	O14-C14	2.37	1.47	1.44

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	228	DGX	C19-C10-C1	-4.66	100.75	108.26
3	D	228	DGX	C19-C10-C1	-4.33	101.29	108.26
3	D	228	DGX	C9-C11-C12	-3.71	109.41	114.30
3	B	228	DGX	C11-C9-C10	-3.28	110.35	113.73
3	B	228	DGX	C10-C9-C8	3.27	116.81	112.00
3	D	228	DGX	C1-C10-C5	2.63	111.66	107.77
3	B	228	DGX	C7-C8-C14	2.58	113.94	111.39
3	D	228	DGX	C11-C9-C10	-2.40	111.25	113.73
3	B	228	DGX	C1X-O3-C3	2.32	119.83	115.20
3	B	228	DGX	C4-C3-C2	-2.32	108.54	111.54
3	B	228	DGX	C15-C14-C8	2.31	119.29	116.05
3	B	228	DGX	C11-C9-C8	-2.27	105.78	110.50
3	B	228	DGX	C11-C12-C13	2.19	115.81	112.54
3	B	228	DGX	C1-C10-C5	2.17	110.97	107.77

There are no chirality outliers.

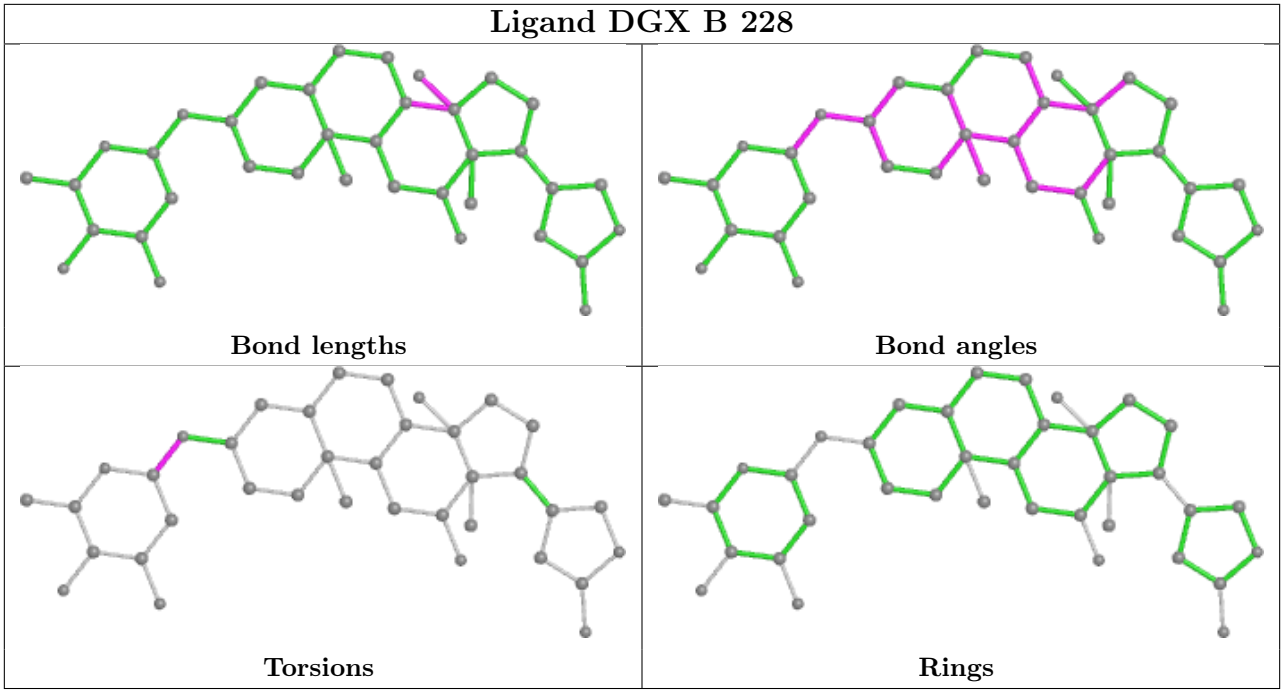
All (4) torsion outliers are listed below:

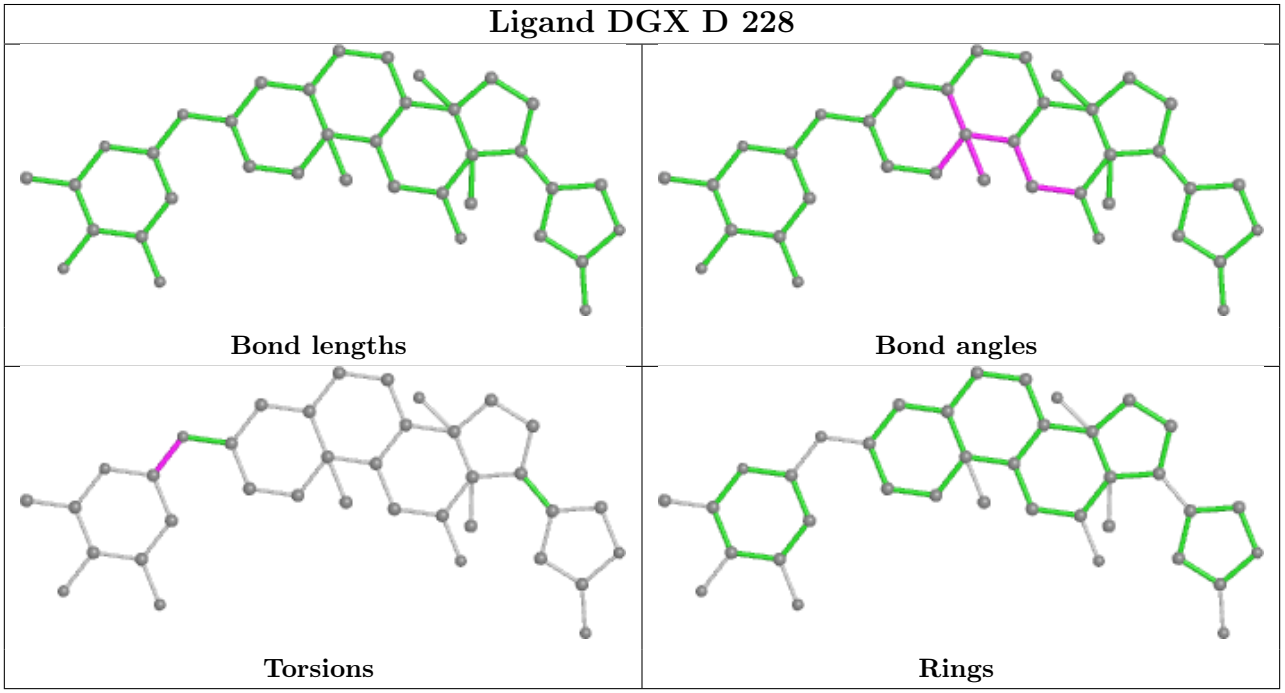
Mol	Chain	Res	Type	Atoms
3	B	228	DGX	C2X-C1X-O3-C3
3	D	228	DGX	C2X-C1X-O3-C3
3	B	228	DGX	O5X-C1X-O3-C3
3	D	228	DGX	O5X-C1X-O3-C3

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 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.





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, 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	216/219 (98%)	-0.59	0 100 100	2, 17, 30, 38	0
1	C	216/219 (98%)	-0.61	0 100 100	2, 17, 35, 64	0
2	B	217/218 (99%)	-0.24	7 (3%) 47 51	3, 24, 51, 60	0
2	D	217/218 (99%)	-0.34	5 (2%) 60 63	3, 21, 47, 62	0
All	All	866/874 (99%)	-0.45	12 (1%) 75 77	2, 20, 42, 64	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	27	TYR	6.6
2	D	27	TYR	6.4
2	B	29	PHE	5.2
2	B	134	THR	4.6
2	B	129	GLY	4.5
2	D	29	PHE	4.4
2	D	2	VAL	3.7
2	B	26	GLY	3.0
2	D	28	ILE	2.8
2	D	53	TYR	2.5
2	B	133	THR	2.5
2	B	73	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands (i)

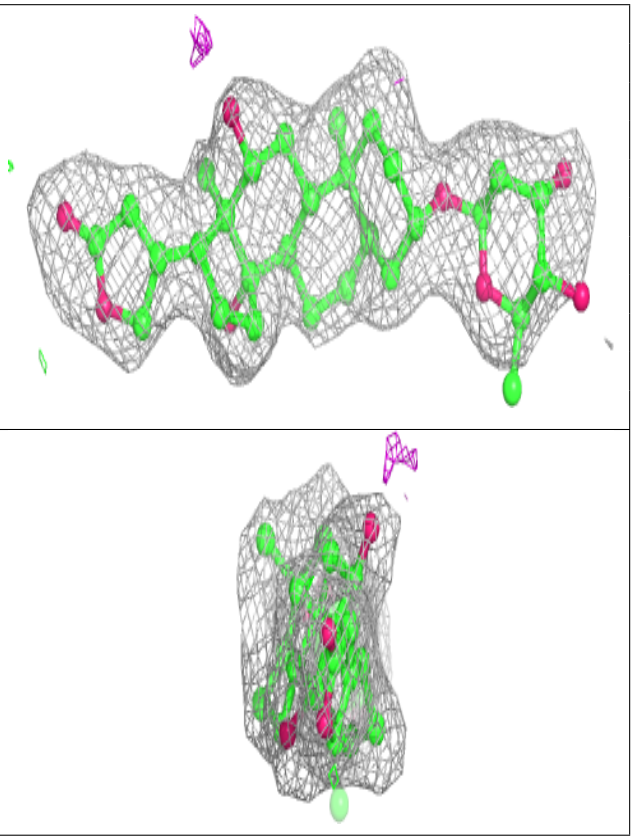
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

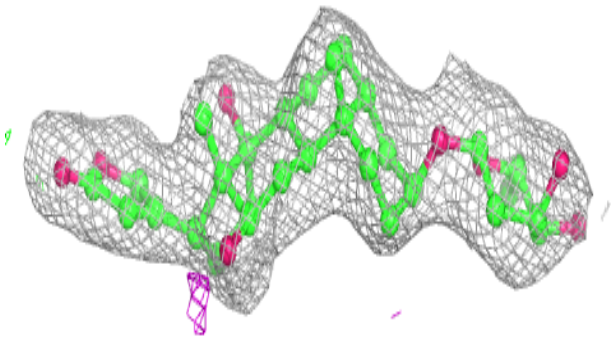
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DGX	D	228	37/55	0.89	0.14	27,38,54,55	0
3	DGX	B	228	37/55	0.91	0.14	8,20,48,51	0

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 DGX D 228:

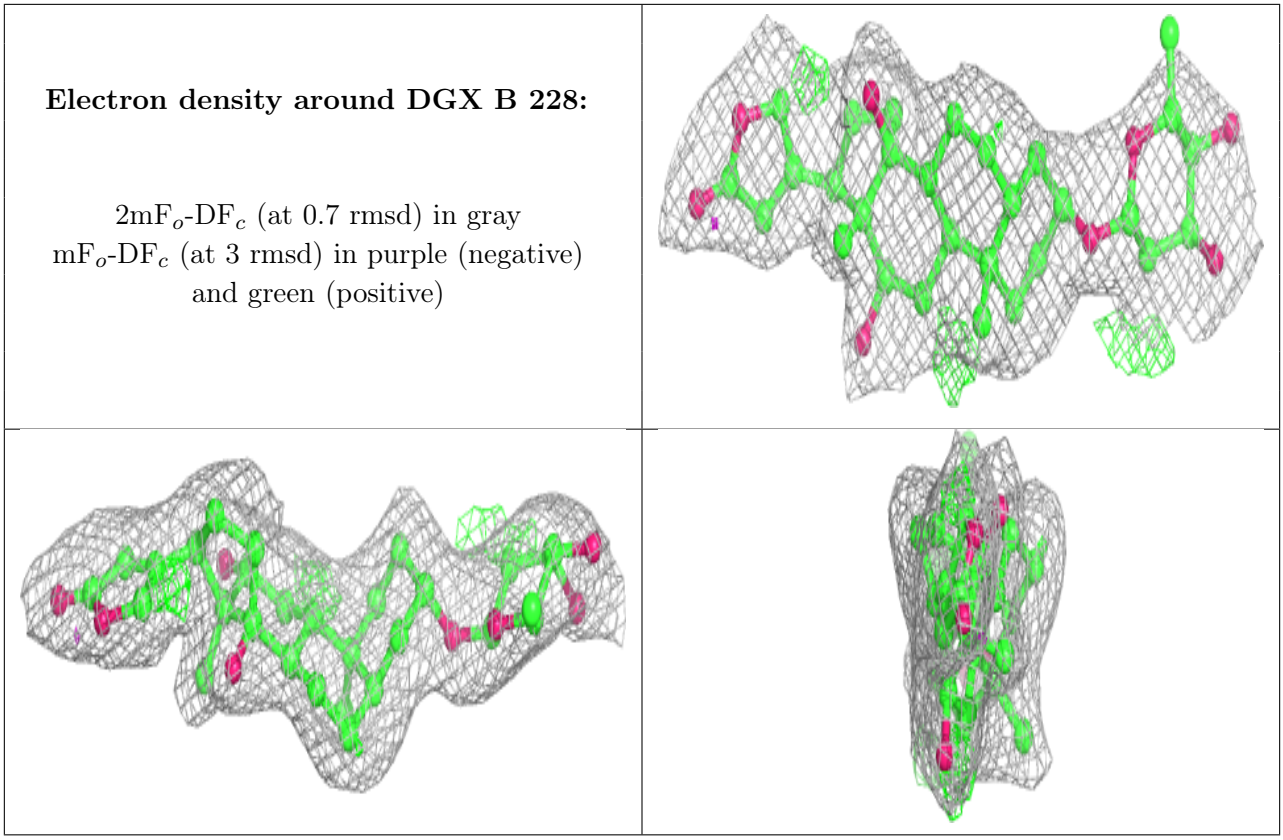
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around DGX B 228:

$2mF_o$-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.