



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:15 PM UTC

PDB ID : 3HKY / pdb_00003hky
Title : HCV NS5B polymerase genotype 1b in complex with 1,5 benzodiazepine 6
Authors : Nyanguile, O.; De Bondt, H.L.
Deposited on : 2009-05-26
Resolution : 1.90 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

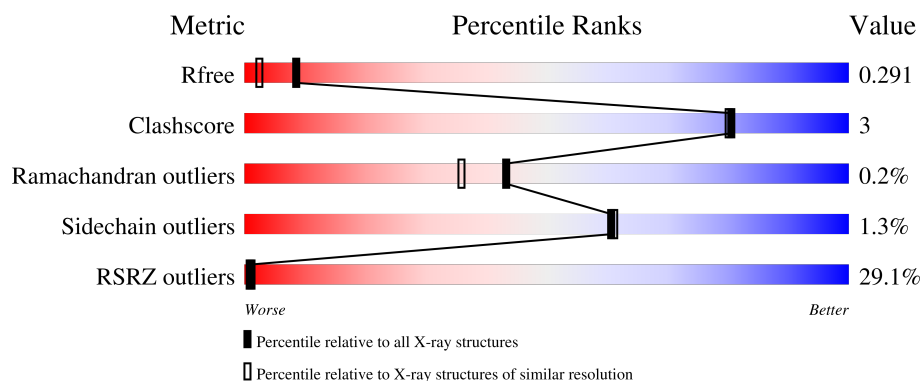
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	581	9% 90% 6% . .
1	B	581	48% 90% 7% .

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
3	SO4	A	581	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9585 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 RNA-directed RNA polymerase.

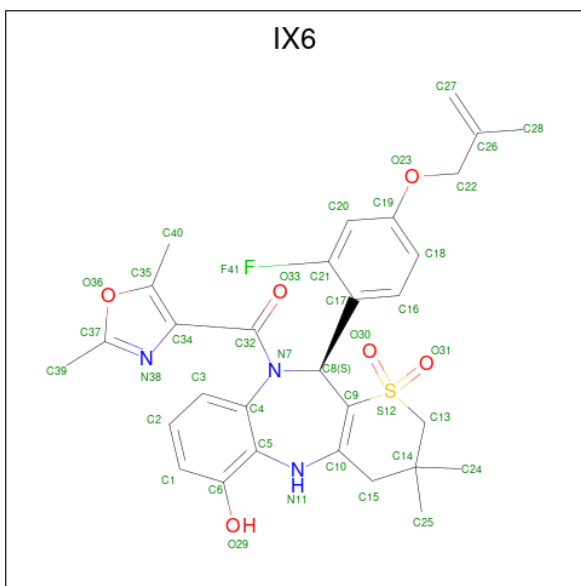
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	564	Total	C	N	O	S	0	5	0
			4426	2783	785	825	33			
1	B	560	Total	C	N	O	S	0	1	0
			4362	2747	771	812	32			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP O92972
A	-1	ALA	-	expression tag	UNP O92972
A	0	SER	-	expression tag	UNP O92972
A	571	LEU	-	expression tag	UNP O92972
A	572	GLU	-	expression tag	UNP O92972
A	573	HIS	-	expression tag	UNP O92972
A	574	HIS	-	expression tag	UNP O92972
A	575	HIS	-	expression tag	UNP O92972
A	576	HIS	-	expression tag	UNP O92972
A	577	HIS	-	expression tag	UNP O92972
A	578	HIS	-	expression tag	UNP O92972
B	-2	MET	-	expression tag	UNP O92972
B	-1	ALA	-	expression tag	UNP O92972
B	0	SER	-	expression tag	UNP O92972
B	571	LEU	-	expression tag	UNP O92972
B	572	GLU	-	expression tag	UNP O92972
B	573	HIS	-	expression tag	UNP O92972
B	574	HIS	-	expression tag	UNP O92972
B	575	HIS	-	expression tag	UNP O92972
B	576	HIS	-	expression tag	UNP O92972
B	577	HIS	-	expression tag	UNP O92972
B	578	HIS	-	expression tag	UNP O92972

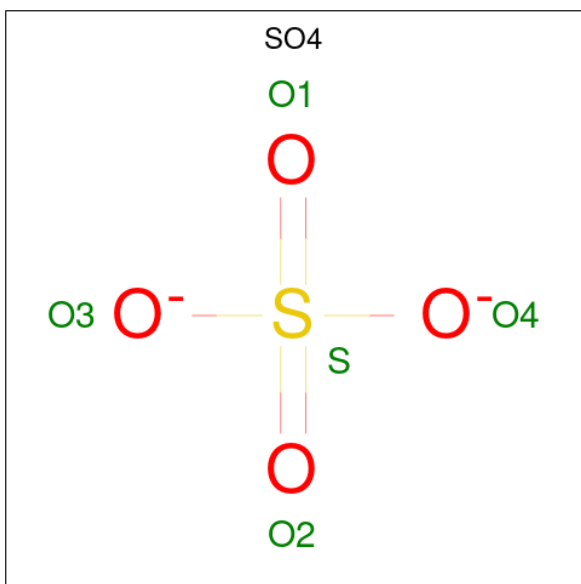
- Molecule 2 is (11S)-10-[(2,5-dimethyl-1,3-oxazol-4-yl)carbonyl]-11-{2-fluoro-4-[(2-methylprop-2-en-1-yl)oxy]phenyl}-3,3-dimethyl-2,3,4,5,10,11-hexahydrothiopyrano[3,2-b][1,5]benzodia

zepin-6-ol 1,1-dioxide (CCD ID: IX6) (formula: $C_{30}H_{32}FN_3O_6S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			41	30	1	3	6	1		
2	B	1	Total	C	F	N	O	S	0	0
			41	30	1	3	6	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

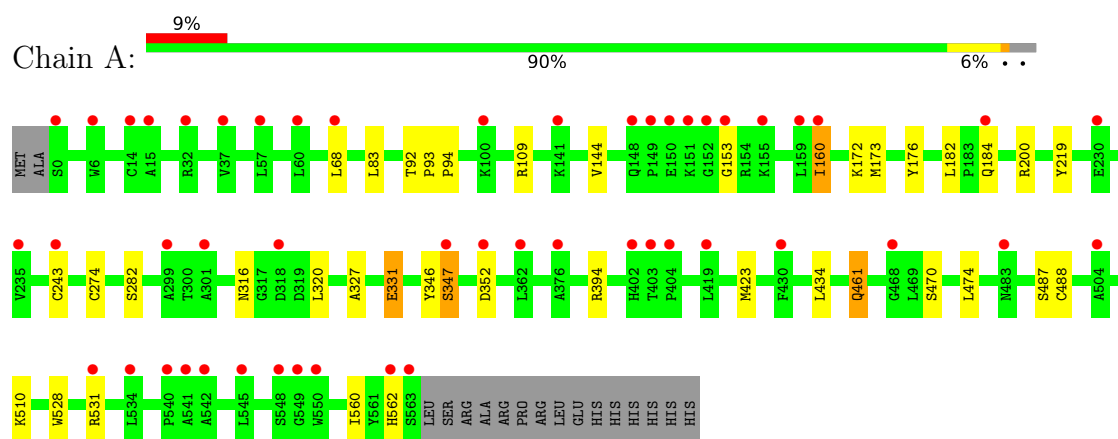
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	402	Total O 403 403	0	1
5	B	270	Total O 270 270	0	0

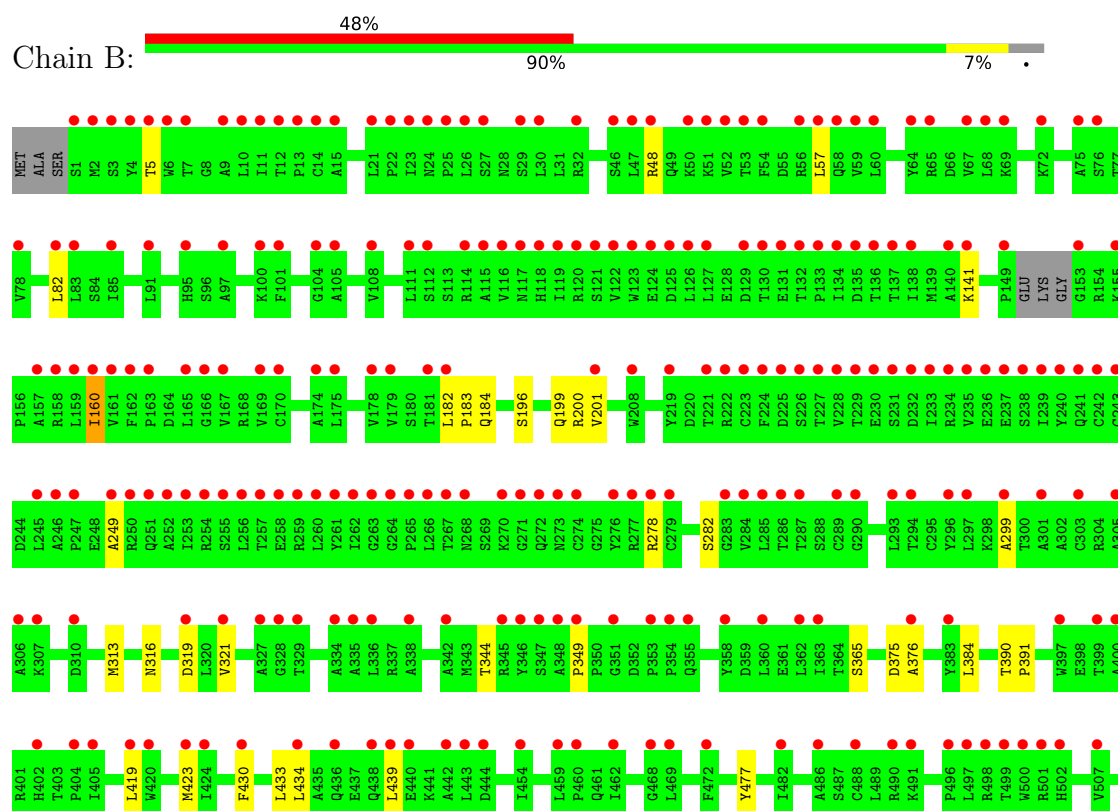
3 Residue-property plots [i](#)

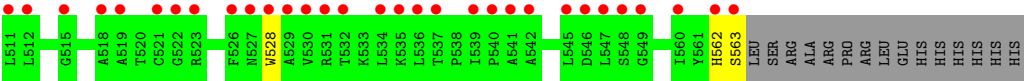
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: RNA-directed RNA polymerase



- Molecule 1: RNA-directed RNA polymerase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.27Å 107.68Å 133.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.90 – 1.90 44.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (44.90-1.90) 99.9 (44.90-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.184 , 0.209 (Not available) , 0.291	Depositor DCC
R_{free} test set	967 reflections (0.80%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9585	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: SO4, CL, IX6

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	0.77	0/4523	0.86	0/6137
1	B	0.65	0/4457	0.78	0/6049
All	All	0.71	0/8980	0.82	0/12186

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	4426	0	4428	22	0
1	B	4362	0	4373	22	0
2	A	41	0	31	0	0
2	B	41	0	31	0	0
3	A	30	0	0	2	0
3	B	10	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	403	0	0	4	0
5	B	270	0	0	4	0
All	All	9585	0	8863	46	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 3.

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)
1:A:488:CYS:HB2	5:A:603:HOH:O	1.76	0.85
1:A:461:GLN:H	1:A:461:GLN:HE21	1.37	0.72
3:A:581:SO4:O1	5:A:616:HOH:O	2.14	0.63
3:A:581:SO4:O4	5:A:671:HOH:O	2.16	0.61
1:A:200:ARG:HH12	1:A:316:ASN:HD21	1.50	0.58
1:B:434:LEU:CD1	1:B:439:LEU:HD11	2.34	0.58
1:B:299:ALA:C	1:B:313:MET:HE1	2.29	0.57
1:A:160:ILE:HD12	1:A:282:SER:OG	2.06	0.56
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.87	0.56
1:B:160:ILE:HD12	1:B:282:SER:OG	2.05	0.56
1:A:182:LEU:HD12	1:A:243:CYS:SG	2.45	0.56
1:B:5:THR:HG23	1:B:278:ARG:HH12	1.71	0.55
1:A:461:GLN:H	1:A:461:GLN:NE2	2.05	0.54
1:B:321:VAL:HG22	1:B:365:SER:HB3	1.89	0.54
1:B:390:THR:HB	1:B:391:PRO:HD3	1.95	0.49
1:B:562:HIS:O	1:B:563:SER:C	2.55	0.49
1:A:200:ARG:HH12	1:A:316:ASN:ND2	2.10	0.49
1:B:419:LEU:HG	1:B:423:MET:CE	2.43	0.48
1:B:201:VAL:HG22	1:B:384:LEU:HG	1.95	0.48
1:A:184:GLN:NE2	5:A:779:HOH:O	2.47	0.48
1:B:184:GLN:NE2	5:B:810:HOH:O	2.47	0.48
1:A:327:ALA:O	1:A:331:GLU:HG3	2.14	0.47
1:A:434:LEU:HD21	1:A:510:LYS:HB2	1.96	0.47
1:B:419:LEU:HD13	1:B:477:TYR:CD1	2.50	0.47
1:A:346:TYR:O	1:A:347:SER:HB3	2.16	0.46
1:B:48:ARG:NH1	5:B:801:HOH:O	2.48	0.46
1:B:375:ASP:OD1	1:B:376:ALA:N	2.46	0.46
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.97	0.45
1:B:196:SER:H	1:B:199:GLN:NE2	2.14	0.45
1:A:327:ALA:O	1:A:331:GLU:CG	2.65	0.45
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.99	0.45
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.97	0.44
1:A:423:MET:HA	1:A:528:TRP:CZ2	2.53	0.44
1:A:470:SER:O	1:A:474:LEU:HG	2.18	0.44
1:A:176:TYR:OH	1:A:562:HIS:HE1	2.01	0.43
1:B:344:THR:HG23	1:B:349:PRO:HB3	2.01	0.43
1:B:200:ARG:HH22	1:B:316:ASN:HD21	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:PHE:O	1:B:434:LEU:HB2	2.19	0.42
1:B:141:LYS:NZ	5:B:585:HOH:O	2.53	0.42
1:A:83:LEU:HB2	1:A:173:MET:HA	2.01	0.42
1:B:182:LEU:N	1:B:183:PRO:CD	2.83	0.42
1:B:423:MET:HA	1:B:528:TRP:CZ2	2.55	0.42
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.94	0.41
1:A:346:TYR:O	1:A:347:SER:CB	2.68	0.41
1:B:375:ASP:HB3	5:B:611:HOH:O	2.20	0.41
1:A:92:THR:O	1:A:109:ARG:HD2	2.22	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	566/581 (97%)	553 (98%)	11 (2%)	2 (0%)	30	22
1	B	556/581 (96%)	548 (99%)	8 (1%)	0	100	100
All	All	1122/1162 (97%)	1101 (98%)	19 (2%)	2 (0%)	43	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	GLY
1	A	347	SER

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	484/495 (98%)	476 (98%)	8 (2%)	53	52
1	B	477/495 (96%)	473 (99%)	4 (1%)	73	75
All	All	961/990 (97%)	949 (99%)	12 (1%)	61	63

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

Mol	Chain	Res	Type
1	A	68	LEU
1	A	160	ILE
1	A	274	CYS
1	A	331	GLU
1	A	352	ASP
1	A	461	GLN
1	A	487	SER
1	A	531	ARG
1	B	57	LEU
1	B	160	ILE
1	B	319	ASP
1	B	433	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	34	HIS
1	A	35	ASN
1	A	49	GLN
1	A	148	GLN
1	A	206	ASN
1	A	316	ASN
1	A	461	GLN
1	A	483	ASN
1	A	514	GLN
1	A	562	HIS
1	B	28	ASN
1	B	35	ASN
1	B	58	GLN
1	B	184	GLN

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Mol	Chain	Res	Type
1	B	199	GLN
1	B	206	ASN
1	B	309	GLN
1	B	316	ASN
1	B	438	GLN
1	B	461	GLN
1	B	483	ASN
1	B	502	HIS
1	B	562	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	IX6	B	579	-	40,45,45	2.90	9 (22%)	56,70,70	2.47	17 (30%)
3	SO4	A	584	-	4,4,4	0.25	0	6,6,6	0.20	0
3	SO4	A	583	-	4,4,4	0.32	0	6,6,6	0.16	0
2	IX6	A	579	-	40,45,45	2.75	7 (17%)	56,70,70	2.52	16 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	580	-	4,4,4	0.19	0	6,6,6	0.13	0
3	SO4	A	586	-	4,4,4	0.28	0	6,6,6	0.13	0
3	SO4	B	582	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	582	-	4,4,4	0.26	0	6,6,6	0.18	0
3	SO4	A	581	-	4,4,4	0.22	0	6,6,6	0.14	0
3	SO4	A	580	-	4,4,4	0.31	0	6,6,6	0.58	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
2	IX6	B	579	-	-	2/17/54/54	0/3/5/5
2	IX6	A	579	-	-	5/17/54/54	0/3/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	579	IX6	O36-C37	-11.41	1.23	1.37
2	A	579	IX6	O36-C37	-11.18	1.23	1.37
2	B	579	IX6	O36-C35	-10.26	1.22	1.38
2	A	579	IX6	O36-C35	-10.11	1.22	1.38
2	B	579	IX6	C32-N7	5.55	1.40	1.35
2	B	579	IX6	C37-N38	5.17	1.36	1.29
2	A	579	IX6	C37-N38	4.36	1.35	1.29
2	A	579	IX6	C32-N7	3.59	1.38	1.35
2	B	579	IX6	C13-S12	2.81	1.80	1.76
2	B	579	IX6	C34-N38	-2.61	1.33	1.38
2	B	579	IX6	C15-C10	2.58	1.53	1.50
2	A	579	IX6	C34-N38	-2.50	1.33	1.38
2	A	579	IX6	C15-C10	2.40	1.53	1.50
2	B	579	IX6	C34-C32	-2.17	1.46	1.49
2	A	579	IX6	C10-N11	2.10	1.39	1.35
2	B	579	IX6	O31-S12	2.09	1.46	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	579	IX6	C4-N7-C32	-6.67	116.33	123.15
2	A	579	IX6	O33-C32-N7	-6.62	112.95	123.01
2	B	579	IX6	O36-C35-C40	6.51	124.40	115.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	579	IX6	O36-C35-C40	6.38	124.23	115.88
2	A	579	IX6	C37-O36-C35	6.36	110.21	104.86
2	B	579	IX6	C14-C15-C10	6.13	120.10	113.40
2	A	579	IX6	C4-N7-C32	-5.92	117.09	123.15
2	A	579	IX6	C14-C15-C10	5.87	119.82	113.40
2	B	579	IX6	C37-O36-C35	5.33	109.34	104.86
2	B	579	IX6	C40-C35-C34	-5.17	126.86	135.15
2	A	579	IX6	C22-O23-C19	4.86	126.33	117.63
2	A	579	IX6	C40-C35-C34	-4.85	127.37	135.15
2	B	579	IX6	O33-C32-N7	-4.82	115.68	123.01
2	B	579	IX6	C22-O23-C19	4.55	125.78	117.63
2	A	579	IX6	C9-C10-N11	-3.78	123.89	126.58
2	B	579	IX6	C9-C10-N11	-3.75	123.91	126.58
2	A	579	IX6	C5-C4-N7	3.34	121.53	119.37
2	A	579	IX6	C35-C34-N38	-3.29	106.67	109.62
2	B	579	IX6	C5-C4-N7	3.26	121.48	119.37
2	A	579	IX6	O36-C37-C39	2.99	123.49	117.49
2	B	579	IX6	C35-C34-N38	-2.97	106.96	109.62
2	B	579	IX6	C20-C21-C17	-2.93	120.68	123.93
2	B	579	IX6	C6-C5-N11	-2.82	114.56	118.99
2	B	579	IX6	O31-S12-O30	-2.80	114.44	117.14
2	B	579	IX6	O36-C37-C39	2.53	122.56	117.49
2	B	579	IX6	C39-C37-N38	-2.41	123.80	128.83
2	A	579	IX6	C20-C21-C17	-2.41	121.25	123.93
2	B	579	IX6	C16-C17-C21	2.39	119.24	116.22
2	A	579	IX6	C6-C5-N11	-2.36	115.28	118.99
2	A	579	IX6	C1-C6-C5	2.29	122.64	118.69
2	A	579	IX6	C39-C37-N38	-2.26	124.12	128.83
2	B	579	IX6	C21-C17-C8	-2.22	117.42	120.71
2	A	579	IX6	O36-C37-N38	-2.08	112.38	114.87

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	579	IX6	O23-C22-C26-C27
2	B	579	IX6	O23-C22-C26-C28
2	A	579	IX6	O33-C32-C34-N38
2	A	579	IX6	O23-C22-C26-C27
2	A	579	IX6	O23-C22-C26-C28
2	A	579	IX6	N7-C32-C34-N38
2	A	579	IX6	O33-C32-N7-C8

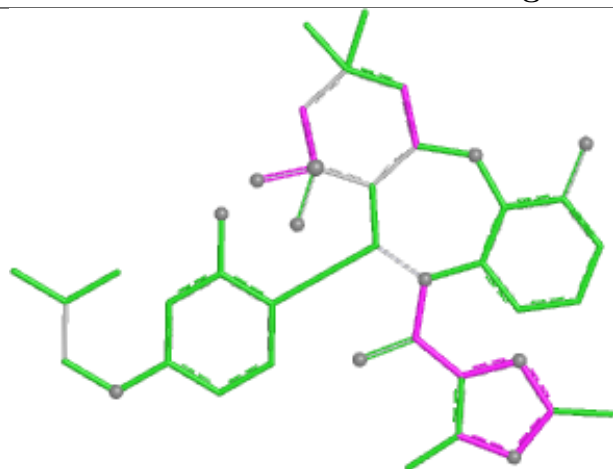
There are no ring outliers.

1 monomer is involved in 2 short contacts:

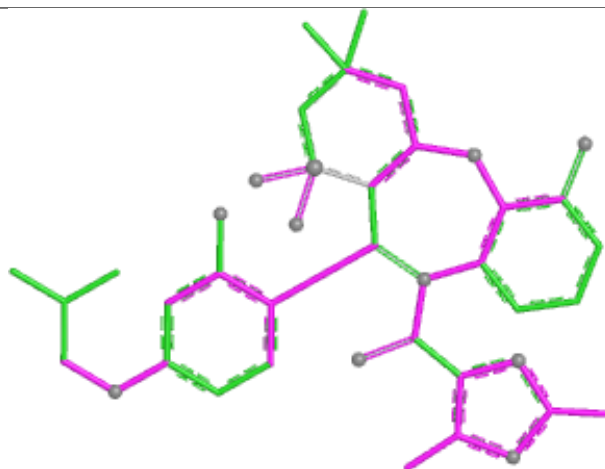
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	581	SO4	2	0

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.

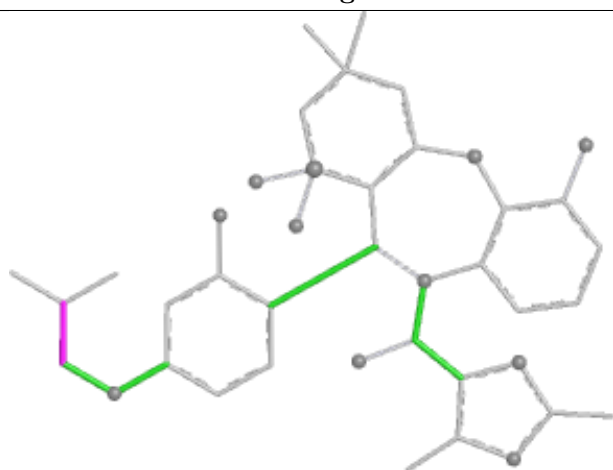
Ligand IX6 B 579



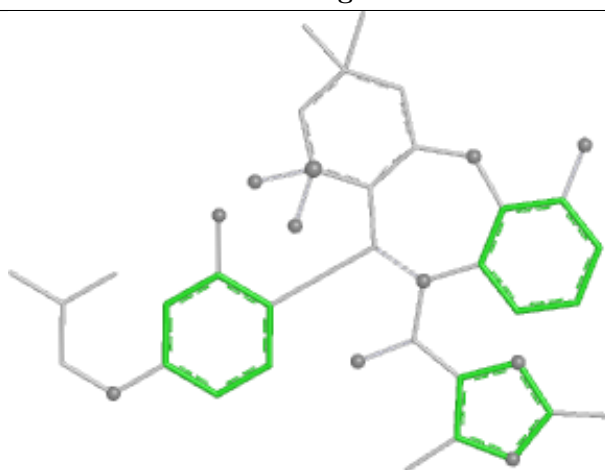
Bond lengths



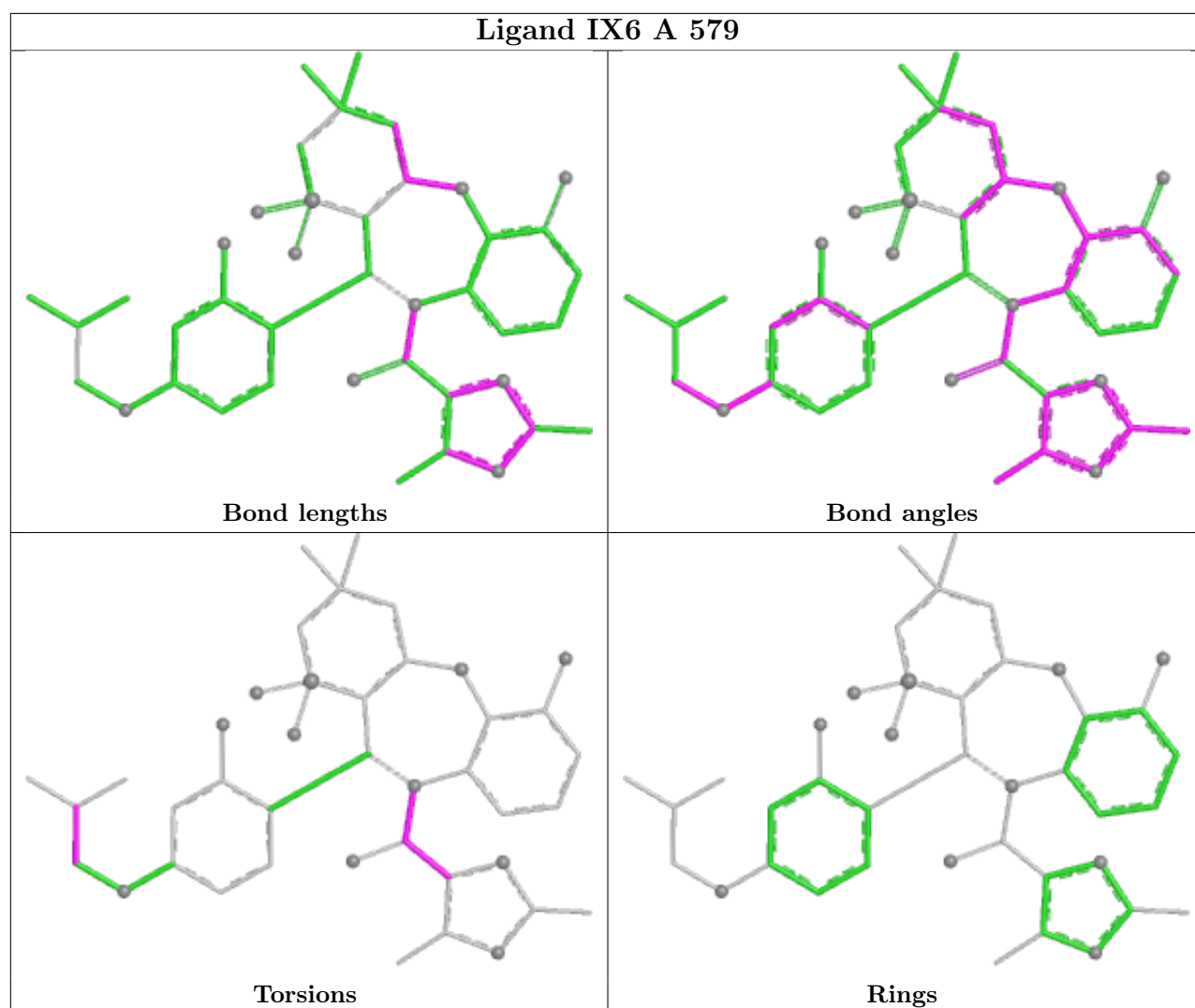
Bond angles



Torsions



Rings



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	564/581 (97%)	1.11	50 (8%)	15 16	21, 45, 62, 99	4 (0%)
1	B	560/581 (96%)	2.11	277 (49%)	0 0	36, 46, 63, 78	0
All	All	1124/1162 (96%)	1.61	327 (29%)	1 1	21, 46, 62, 99	4 (0%)

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	ILE	5.4
1	B	126	LEU	5.4
1	B	6	TRP	5.1
1	B	57	LEU	5.1
1	B	440	GLU	4.8
1	B	134	ILE	4.8
1	B	149	PRO	4.6
1	B	235	VAL	4.6
1	B	541	ALA	4.5
1	B	153	GLY	4.5
1	B	160	ILE	4.4
1	B	4	TYR	4.4
1	B	262	ILE	4.4
1	B	25	PRO	4.3
1	B	52	VAL	4.3
1	B	159	LEU	4.3
1	B	123	TRP	4.3
1	B	542	ALA	4.3
1	B	22	PRO	4.3
1	A	57	LEU	4.2
1	B	228	VAL	4.2
1	B	260	LEU	4.2
1	B	265	PRO	4.2
1	B	1	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	469	LEU	4.1
1	B	59	VAL	4.1
1	B	276	TYR	4.1
1	B	127	LEU	4.0
1	B	26	LEU	3.9
1	B	266	LEU	3.9
1	B	563	SER	3.9
1	B	547	LEU	3.9
1	B	132	THR	3.9
1	B	507	VAL	3.9
1	B	233	ILE	3.8
1	B	5	THR	3.8
1	B	167	VAL	3.8
1	B	231	SER	3.7
1	A	160	ILE	3.7
1	B	67	VAL	3.7
1	B	284	VAL	3.7
1	B	130	THR	3.7
1	A	0	SER	3.7
1	B	255	SER	3.7
1	B	249	ALA	3.6
1	B	253	ILE	3.6
1	B	358	TYR	3.6
1	B	178	VAL	3.6
1	B	264	GLY	3.6
1	B	11	ILE	3.6
1	B	122	VAL	3.6
1	A	563	SER	3.6
1	B	256	LEU	3.6
1	B	274	CYS	3.5
1	A	534	LEU	3.5
1	B	10	LEU	3.5
1	B	245	LEU	3.5
1	B	502	HIS	3.5
1	A	542	ALA	3.5
1	B	257	THR	3.4
1	B	68	LEU	3.4
1	B	545	LEU	3.4
1	A	148	GLN	3.4
1	B	158	ARG	3.4
1	B	208	TRP	3.4
1	B	549	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	400	ALA	3.4
1	B	297	LEU	3.4
1	B	263	GLY	3.3
1	B	500	TRP	3.3
1	B	278	ARG	3.3
1	B	548	SER	3.3
1	B	138	ILE	3.3
1	B	175	LEU	3.3
1	B	229	THR	3.3
1	B	526	PHE	3.3
1	B	133	PRO	3.3
1	B	174	ALA	3.3
1	B	252	ALA	3.3
1	B	285	LEU	3.2
1	A	100	LYS	3.2
1	A	151	LYS	3.2
1	B	119	ILE	3.2
1	B	240	TYR	3.2
1	B	82	LEU	3.2
1	B	534	LEU	3.2
1	B	165	LEU	3.2
1	B	511	LEU	3.2
1	B	121	SER	3.2
1	B	279	CYS	3.2
1	A	15	ALA	3.1
1	B	518	ALA	3.1
1	B	404	PRO	3.1
1	B	515	GLY	3.1
1	A	403	THR	3.1
1	B	247	PRO	3.1
1	B	21	LEU	3.1
1	B	54	PHE	3.1
1	B	273	ASN	3.1
1	B	562	HIS	3.1
1	B	539	ILE	3.1
1	A	152	GLY	3.1
1	B	9	ALA	3.1
1	B	85	ILE	3.0
1	B	60	LEU	3.0
1	B	307	LYS	3.0
1	B	383	TYR	3.0
1	B	430	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	258	GLU	3.0
1	B	14	CYS	3.0
1	B	270	LYS	3.0
1	B	293	LEU	3.0
1	B	46	SER	3.0
1	B	224	PHE	3.0
1	B	125	ASP	3.0
1	B	162	PHE	3.0
1	B	521	CYS	3.0
1	B	454	ILE	3.0
1	B	348	ALA	2.9
1	B	78	VAL	2.9
1	B	238	SER	2.9
1	B	536	LEU	2.9
1	B	267	THR	2.9
1	B	346	TYR	2.9
1	B	223	CYS	2.9
1	B	336	LEU	2.9
1	A	549	GLY	2.9
1	B	161	VAL	2.8
1	B	163	PRO	2.8
1	B	376	ALA	2.8
1	B	129	ASP	2.8
1	B	30	LEU	2.8
1	B	522	GLY	2.8
1	A	402	HIS	2.8
1	B	234	ARG	2.8
1	B	540	PRO	2.8
1	B	135	ASP	2.8
1	B	546	ASP	2.8
1	B	140	ALA	2.8
1	B	490	ARG	2.8
1	B	512	LEU	2.8
1	B	51	LYS	2.8
1	B	100	LYS	2.8
1	B	496	PRO	2.8
1	B	170	CYS	2.8
1	B	289	CYS	2.8
1	B	468	GLY	2.8
1	B	246	ALA	2.7
1	B	442	ALA	2.7
1	B	50	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	545	LEU	2.7
1	B	136	THR	2.7
1	B	111	LEU	2.7
1	B	182	LEU	2.7
1	B	124	GLU	2.7
1	B	230	GLU	2.7
1	B	529	ALA	2.7
1	B	271	GLY	2.7
1	B	351	GLY	2.7
1	B	7	THR	2.7
1	A	184	GLN	2.7
1	A	404	PRO	2.7
1	B	226	SER	2.7
1	B	353	PRO	2.7
1	B	179	VAL	2.7
1	B	105	ALA	2.6
1	B	166	GLY	2.6
1	B	486	ALA	2.6
1	B	225	ASP	2.6
1	B	523	ARG	2.6
1	B	12	THR	2.6
1	B	112	SER	2.6
1	B	460	PRO	2.6
1	B	321	VAL	2.6
1	B	472	PHE	2.6
1	A	149	PRO	2.6
1	A	540	PRO	2.6
1	B	439	LEU	2.6
1	B	497	LEU	2.6
1	B	239	ILE	2.6
1	B	283	GLY	2.6
1	B	69	LYS	2.6
1	A	347	SER	2.6
1	B	24	ASN	2.6
1	B	117	ASN	2.6
1	B	347	SER	2.6
1	B	259	ARG	2.6
1	B	131	GLU	2.6
1	B	116	VAL	2.6
1	B	519	ALA	2.6
1	A	243	CYS	2.5
1	B	56	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	349	PRO	2.5
1	B	434	LEU	2.5
1	B	424	ILE	2.5
1	B	335	ALA	2.5
1	B	3	SER	2.5
1	B	286	THR	2.5
1	B	83	LEU	2.5
1	B	443	LEU	2.5
1	B	459	LEU	2.5
1	A	548	SER	2.5
1	B	32	ARG	2.5
1	B	118	HIS	2.5
1	B	53	THR	2.5
1	B	287	THR	2.5
1	A	155	LYS	2.5
1	B	219	TYR	2.5
1	B	277	ARG	2.5
1	B	272	GLN	2.5
1	B	355	GLN	2.5
1	B	2	MET	2.5
1	B	397	TRP	2.5
1	B	97	ALA	2.5
1	B	399	THR	2.5
1	B	169	VAL	2.5
1	A	141	LYS	2.5
1	A	150	GLU	2.4
1	B	13	PRO	2.4
1	B	251	GLN	2.4
1	B	342	ALA	2.4
1	B	303	CYS	2.4
1	B	488	CYS	2.4
1	A	419	LEU	2.4
1	B	72	LYS	2.4
1	B	527	ASN	2.4
1	B	29	SER	2.4
1	B	242	CYS	2.4
1	B	232	ASP	2.3
1	B	120	ARG	2.3
1	B	250	ARG	2.3
1	B	254	ARG	2.3
1	B	362	LEU	2.3
1	B	237	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	235	VAL	2.3
1	B	114	ARG	2.3
1	B	499	THR	2.3
1	B	532	THR	2.3
1	B	537	THR	2.3
1	B	268	ASN	2.3
1	A	153	GLY	2.3
1	B	328	GLY	2.3
1	B	58	GLN	2.3
1	A	14	CYS	2.3
1	A	159	LEU	2.3
1	B	47	LEU	2.3
1	B	261	TYR	2.3
1	A	376	ALA	2.3
1	A	541	ALA	2.3
1	B	115	ALA	2.3
1	B	301	ALA	2.3
1	B	290	GLY	2.3
1	B	462	ILE	2.3
1	B	498	ARG	2.3
1	B	294	THR	2.3
1	B	360	LEU	2.3
1	B	528	TRP	2.2
1	A	230	GLU	2.2
1	B	64	TYR	2.2
1	B	338	ALA	2.2
1	A	318	ASP	2.2
1	B	405	ILE	2.2
1	B	402	HIS	2.2
1	B	155	LYS	2.2
1	B	48	ARG	2.2
1	B	419	LEU	2.2
1	B	27	SER	2.2
1	A	6	TRP	2.2
1	B	420	TRP	2.2
1	A	562	HIS	2.2
1	B	535	LYS	2.2
1	B	329	THR	2.2
1	B	354	PRO	2.2
1	A	301	ALA	2.2
1	B	75	ALA	2.2
1	B	76	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	91	LEU	2.2
1	B	157	ALA	2.2
1	B	305	ALA	2.2
1	B	334	ALA	2.2
1	B	141	LYS	2.2
1	B	296	TYR	2.1
1	B	363	ILE	2.1
1	B	482	ILE	2.1
1	B	436	GLN	2.1
1	B	438	GLN	2.1
1	B	201	VAL	2.1
1	B	221	THR	2.1
1	A	60	LEU	2.1
1	B	222	ARG	2.1
1	B	501	ARG	2.1
1	B	423	MET	2.1
1	A	504	ALA	2.1
1	B	15	ALA	2.1
1	B	560	ILE	2.1
1	B	310	ASP	2.1
1	A	550	TRP	2.1
1	B	227	THR	2.1
1	B	491	LYS	2.1
1	B	95	HIS	2.1
1	B	306	ALA	2.1
1	A	430	PHE	2.1
1	A	352	ASP	2.1
1	A	32	ARG	2.1
1	B	345	ARG	2.1
1	B	137	THR	2.1
1	B	181	THR	2.1
1	B	236	GLU	2.1
1	A	468	GLY	2.1
1	A	483	ASN	2.1
1	B	108	VAL	2.1
1	B	530	VAL	2.1
1	A	68	LEU	2.1
1	B	299	ALA	2.1
1	B	444	ASP	2.1
1	A	531	ARG	2.1
1	B	101	PHE	2.0
1	B	241	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	37	VAL	2.0
1	A	362	LEU	2.0
1	B	243	CYS	2.0
1	A	299	ALA	2.0
1	B	65	ARG	2.0
1	B	327	ALA	2.0
1	B	319	ASP	2.0
1	B	531	ARG	2.0
1	B	104	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 oligosaccharides 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.

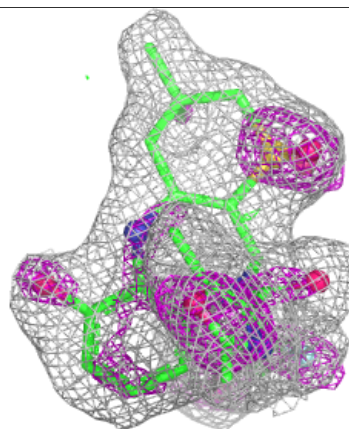
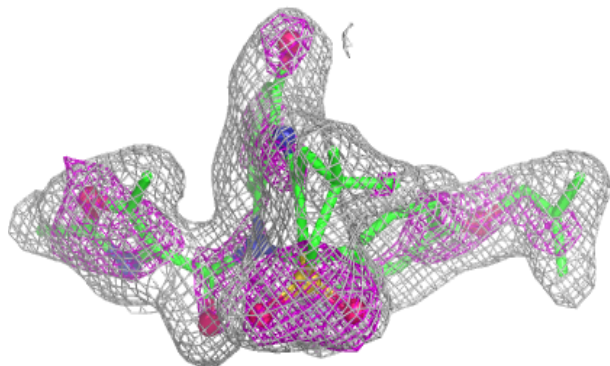
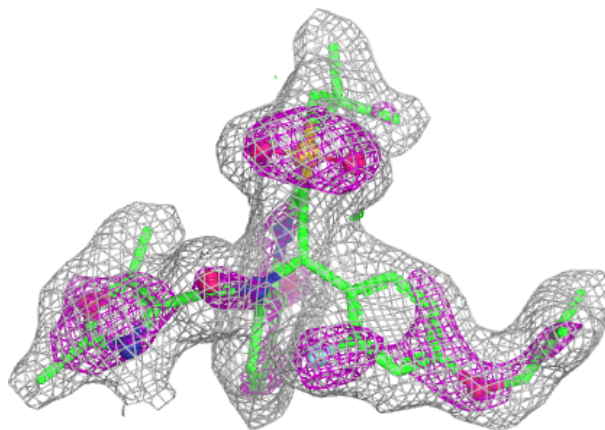
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	A	586	5/5	0.64	0.15	87,87,91,93	0
3	SO4	B	582	5/5	0.66	0.12	100,102,105,105	0
3	SO4	B	580	5/5	0.70	0.17	75,77,83,83	0
3	SO4	A	582	5/5	0.80	0.13	77,80,84,85	0
3	SO4	A	583	5/5	0.85	0.15	52,54,56,60	0
3	SO4	A	584	5/5	0.86	0.14	57,60,64,65	0
3	SO4	A	581	5/5	0.86	0.16	70,72,72,73	0
3	SO4	A	580	5/5	0.90	0.14	44,53,55,58	0
4	CL	A	585	1/1	0.92	0.14	73,73,73,73	0
2	IX6	B	579	41/41	0.93	0.14	32,43,46,48	0
4	CL	B	581	1/1	0.94	0.10	64,64,64,64	0
2	IX6	A	579	41/41	0.96	0.12	25,29,35,39	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.

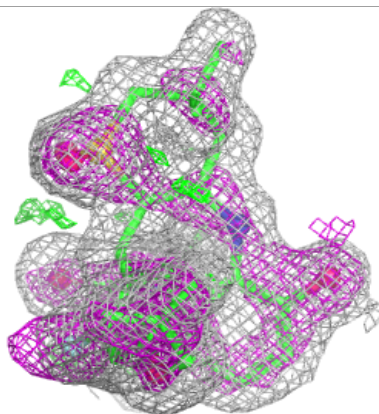
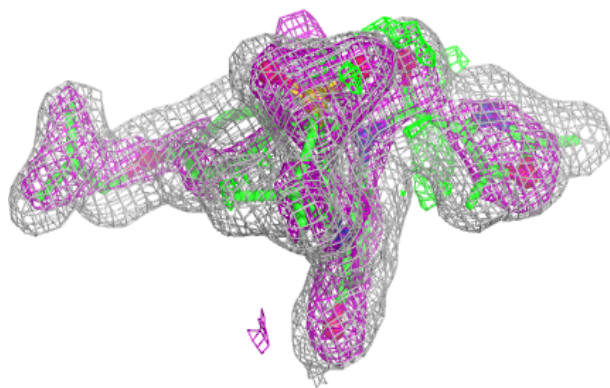
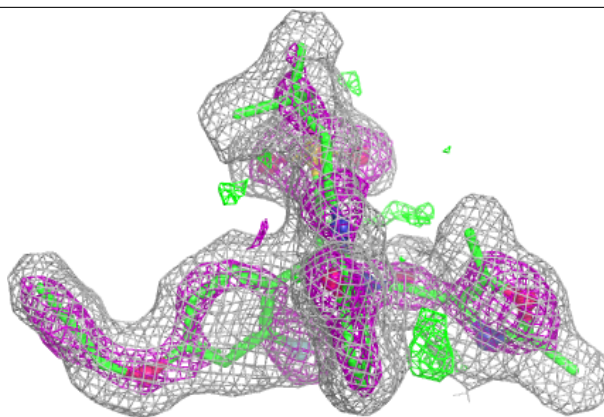
Electron density around IX6 B 579:

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



Electron density around IX6 A 579:

$2mF_o-DF_c$ (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.