Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 02:11 PM JST

PDB ID	:	8IG0
Title	:	Crystal structure of menin in complex with DS-1594b
Authors	:	Suzuki, M.; Yoneyama, T.; Imai, E.
Deposited on	:	2023-02-20
Resolution	:	2.60 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:

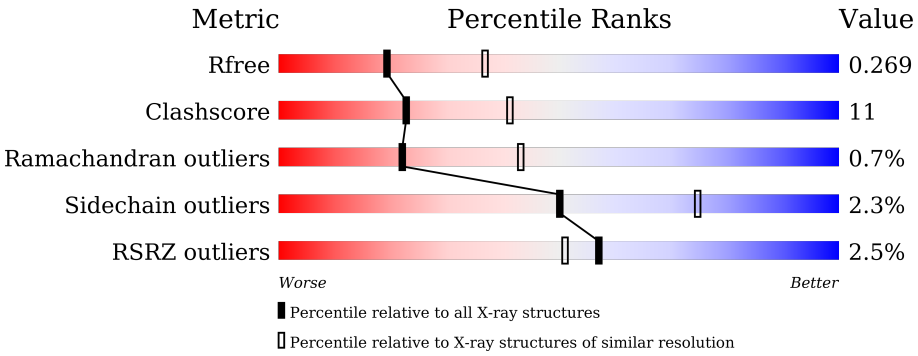
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	550	2% 69% 19% • 12%
1	B	550	3% 65% 23% • 11%
1	C	550	% 66% 21% • 12%
1	D	550	2% 69% 19% • 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15039 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 Menin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3678	2370	621	673	14			
1	B	490	Total	C	N	O	S	0	0	0
			3666	2352	621	679	14			
1	C	483	Total	C	N	O	S	0	0	0
			3687	2369	620	684	14			
1	D	485	Total	C	N	O	S	0	0	0
			3686	2369	623	680	14			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	ALA	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	ALA	deletion	UNP O00255
A	?	-	ALA	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	ALA	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	TRP	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	ALA	deletion	UNP O00255
A	?	-	ARG	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	ARG	deletion	UNP O00255
A	?	-	ARG	deletion	UNP O00255

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ARG	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	ARG	deletion	UNP O00255
A	?	-	ARG	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	SER	deletion	UNP O00255
A	?	-	LYS	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	GLU	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	LYS	deletion	UNP O00255
A	?	-	LYS	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	ALA	deletion	UNP O00255
A	?	-	LEU	deletion	UNP O00255
A	?	-	ASP	deletion	UNP O00255
A	?	-	LYS	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	LEU	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	THR	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	GLN	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	ALA	deletion	UNP O00255
A	?	-	VAL	deletion	UNP O00255
A	?	-	SER	deletion	UNP O00255
A	?	-	GLY	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	ARG	deletion	UNP O00255
A	?	-	LYS	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
A	?	-	PRO	deletion	UNP O00255
B	?	-	ARG	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	ALA	deletion	UNP O00255

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLU	deletion	UNP O00255
B	?	-	ALA	deletion	UNP O00255
B	?	-	ALA	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	ALA	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	TRP	deletion	UNP O00255
B	?	-	GLY	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	ALA	deletion	UNP O00255
B	?	-	ARG	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	GLY	deletion	UNP O00255
B	?	-	ARG	deletion	UNP O00255
B	?	-	ARG	deletion	UNP O00255
B	?	-	ARG	deletion	UNP O00255
B	?	-	GLY	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	ARG	deletion	UNP O00255
B	?	-	ARG	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	SER	deletion	UNP O00255
B	?	-	LYS	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	GLU	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	LYS	deletion	UNP O00255
B	?	-	LYS	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	ALA	deletion	UNP O00255
B	?	-	LEU	deletion	UNP O00255
B	?	-	ASP	deletion	UNP O00255
B	?	-	LYS	deletion	UNP O00255
B	?	-	GLY	deletion	UNP O00255
B	?	-	LEU	deletion	UNP O00255

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	deletion	UNP O00255
B	?	-	THR	deletion	UNP O00255
B	?	-	GLY	deletion	UNP O00255
B	?	-	GLN	deletion	UNP O00255
B	?	-	GLY	deletion	UNP O00255
B	?	-	ALA	deletion	UNP O00255
B	?	-	VAL	deletion	UNP O00255
B	?	-	SER	deletion	UNP O00255
B	?	-	GLY	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	ARG	deletion	UNP O00255
B	?	-	LYS	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
B	?	-	PRO	deletion	UNP O00255
C	?	-	ARG	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	ALA	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	ALA	deletion	UNP O00255
C	?	-	ALA	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	ALA	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	TRP	deletion	UNP O00255
C	?	-	GLY	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	ALA	deletion	UNP O00255
C	?	-	ARG	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	GLY	deletion	UNP O00255
C	?	-	ARG	deletion	UNP O00255
C	?	-	ARG	deletion	UNP O00255
C	?	-	ARG	deletion	UNP O00255
C	?	-	GLY	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	ARG	deletion	UNP O00255
C	?	-	ARG	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	SER	deletion	UNP O00255
C	?	-	LYS	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	GLU	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	LYS	deletion	UNP O00255
C	?	-	LYS	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	ALA	deletion	UNP O00255
C	?	-	LEU	deletion	UNP O00255
C	?	-	ASP	deletion	UNP O00255
C	?	-	LYS	deletion	UNP O00255
C	?	-	GLY	deletion	UNP O00255
C	?	-	LEU	deletion	UNP O00255
C	?	-	GLY	deletion	UNP O00255
C	?	-	THR	deletion	UNP O00255
C	?	-	GLY	deletion	UNP O00255
C	?	-	GLN	deletion	UNP O00255
C	?	-	GLY	deletion	UNP O00255
C	?	-	ALA	deletion	UNP O00255
C	?	-	VAL	deletion	UNP O00255
C	?	-	SER	deletion	UNP O00255
C	?	-	GLY	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	ARG	deletion	UNP O00255
C	?	-	LYS	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
C	?	-	PRO	deletion	UNP O00255
D	?	-	ARG	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255
D	?	-	ALA	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255
D	?	-	ALA	deletion	UNP O00255
D	?	-	ALA	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255
D	?	-	ALA	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	TRP	deletion	UNP O00255
D	?	-	GLY	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255
D	?	-	ALA	deletion	UNP O00255
D	?	-	ARG	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255
D	?	-	GLY	deletion	UNP O00255
D	?	-	ARG	deletion	UNP O00255
D	?	-	ARG	deletion	UNP O00255
D	?	-	ARG	deletion	UNP O00255
D	?	-	GLY	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	ARG	deletion	UNP O00255
D	?	-	ARG	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255
D	?	-	SER	deletion	UNP O00255
D	?	-	LYS	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255
D	?	-	GLU	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	LYS	deletion	UNP O00255
D	?	-	LYS	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	ALA	deletion	UNP O00255
D	?	-	LEU	deletion	UNP O00255
D	?	-	ASP	deletion	UNP O00255
D	?	-	LYS	deletion	UNP O00255
D	?	-	GLY	deletion	UNP O00255
D	?	-	LEU	deletion	UNP O00255
D	?	-	GLY	deletion	UNP O00255
D	?	-	THR	deletion	UNP O00255
D	?	-	GLY	deletion	UNP O00255
D	?	-	GLN	deletion	UNP O00255
D	?	-	GLY	deletion	UNP O00255
D	?	-	ALA	deletion	UNP O00255

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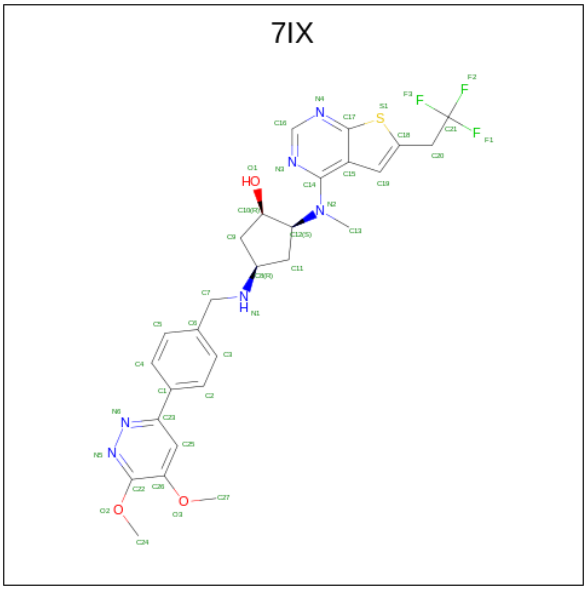
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	VAL	deletion	UNP O00255
D	?	-	SER	deletion	UNP O00255
D	?	-	GLY	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	ARG	deletion	UNP O00255
D	?	-	LYS	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255
D	?	-	PRO	deletion	UNP O00255

- Molecule 2 is (1R,2S,4R)-4-[[4-(5,6-dimethoxypyridazin-3-yl)phenyl]methylamino]-2-[methyl-[6-[2,2,2-tris(fluoranyl)ethyl]thieno[2,3-d]pyrimidin-4-yl]amino]cyclopentan-1-ol (three-letter code: 7IX) (formula: $C_{27}H_{29}F_3N_6O_3S$) (labeled as "Ligand of Interest" by depositor).

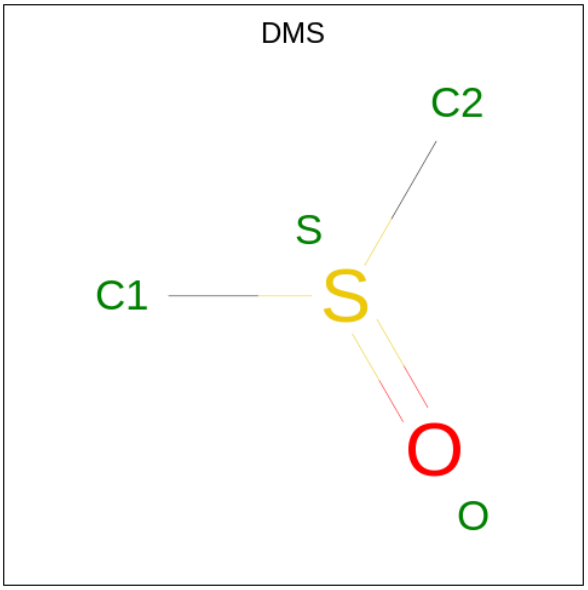


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			40	27	3	6	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			40	27	3	6	3	1		
2	C	1	Total	C	F	N	O	S	0	0
			40	27	3	6	3	1		
2	D	1	Total	C	F	N	O	S	0	0
			40	27	3	6	3	1		

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total X 1 1	0	0
3	B	1	Total X 1 1	0	0
3	C	1	Total X 1 1	0	0
3	D	1	Total X 1 1	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	36	Total O 36 36	0	0
5	B	32	Total O 32 32	0	0

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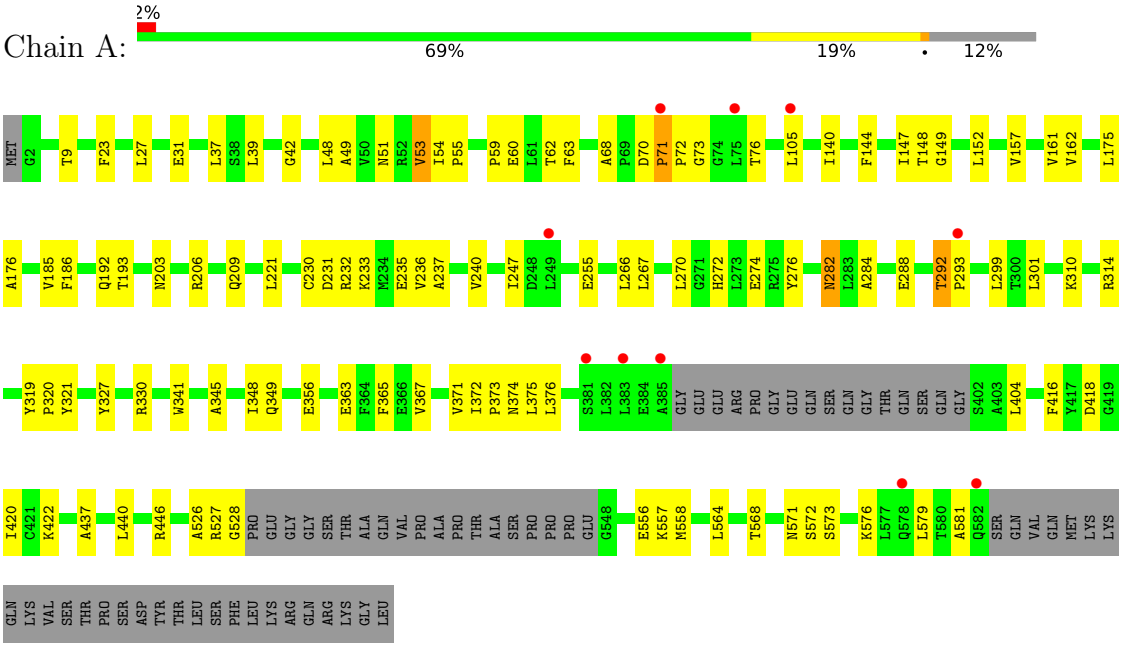
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	36	Total O 36 36	0	0
5	D	38	Total O 38 38	0	0

3 Residue-property plots

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

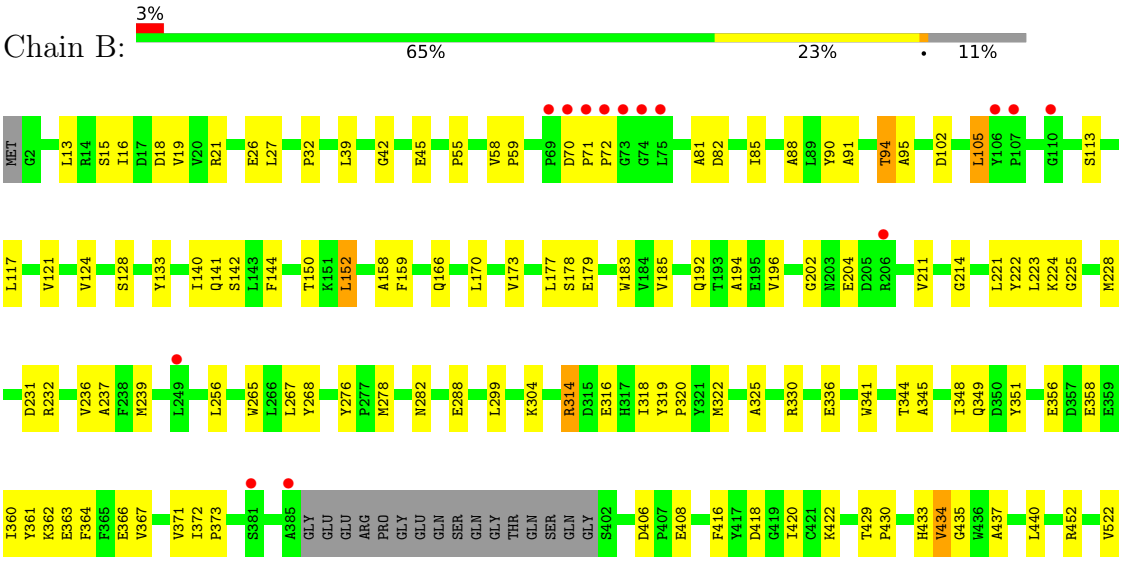
• Molecule 1: Menin

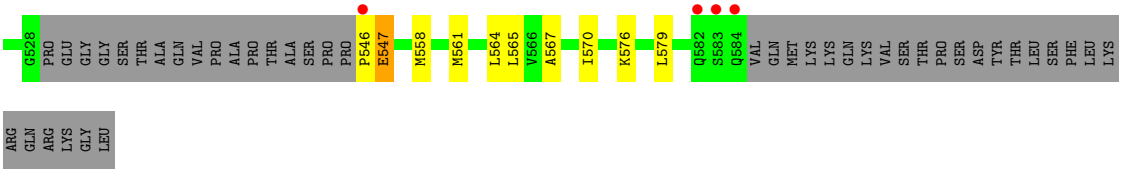
Chain A:



• Molecule 1: Menin

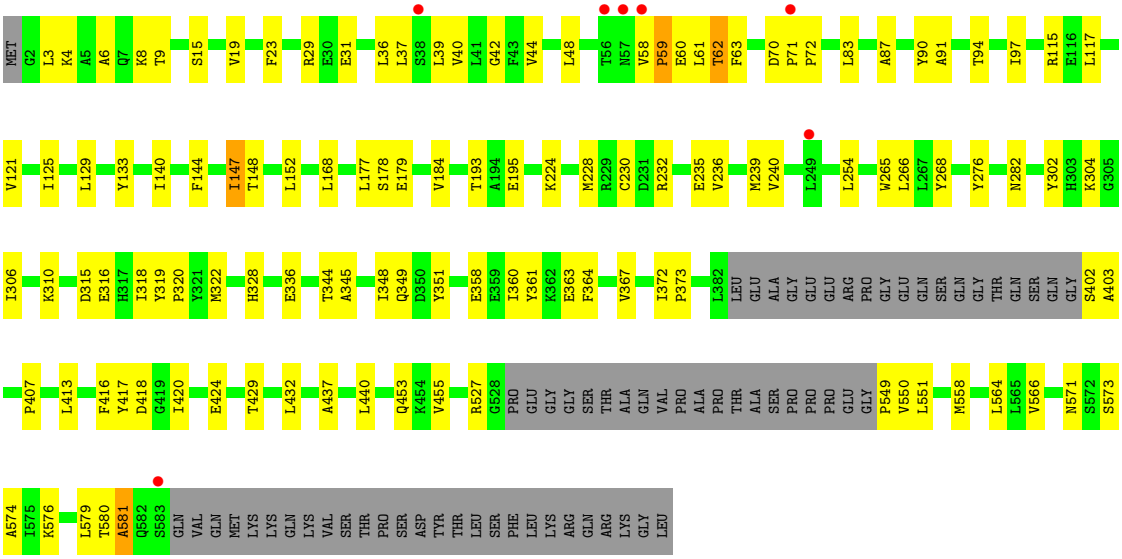
Chain B:





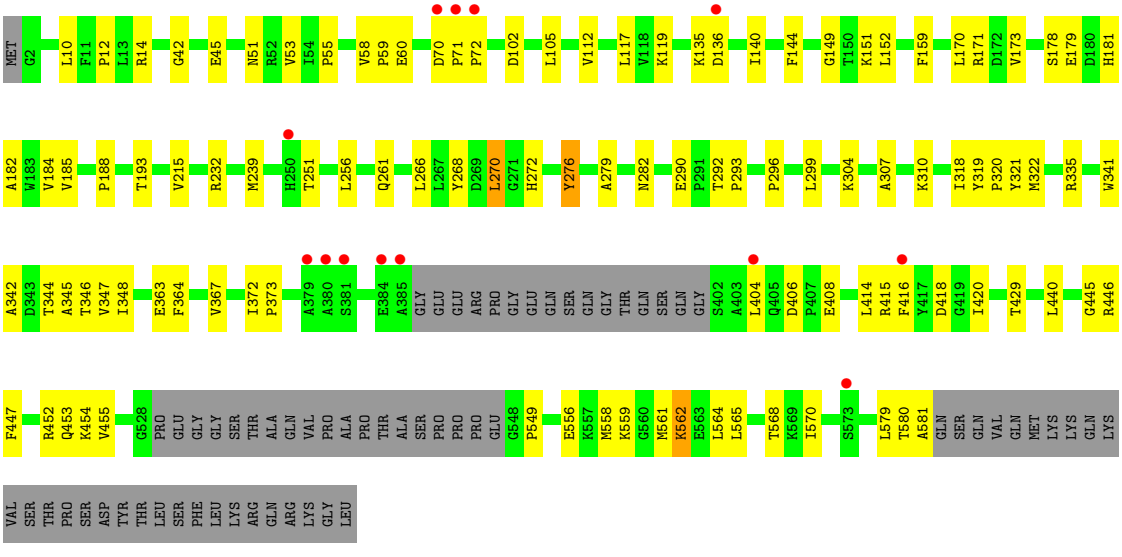
• Molecule 1: Menin

Chain C:



• Molecule 1: Menin

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	141.58Å 70.15Å 144.43Å 90.00° 91.47° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 24.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.00-2.60) 99.8 (24.95-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.212 , 0.266 0.216 , 0.269	Depositor DCC
R_{free} test set	4393 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.006 for l,k,-h 0.015 for h,-k,-l 0.003 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15039	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: UNX, DMS, 7IX

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	0.32	0/3765	0.63	0/5134
1	B	0.31	0/3754	0.65	1/5124 (0.0%)
1	C	0.32	0/3774	0.61	0/5141
1	D	0.33	0/3774	0.64	0/5148
All	All	0.32	0/15067	0.63	1/20547 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	314	ARG	CG-CD-NE	-5.96	99.27	111.80

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	3678	0	3553	76	0
1	B	3666	0	3462	95	0
1	C	3687	0	3558	86	0
1	D	3686	0	3542	78	0
2	A	40	0	0	1	0
2	B	40	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	40	0	0	1	0
2	D	40	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	6	0	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
5	A	36	0	0	2	0
5	B	32	0	0	4	0
5	C	36	0	0	3	0
5	D	38	0	0	3	0
All	All	15039	0	14139	333	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 (333) 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:270:LEU:HB2	1:A:272:HIS:HD2	1.20	1.02
1:C:322:MET:HE3	1:C:360:ILE:HD11	1.43	0.97
1:A:270:LEU:HB2	1:A:272:HIS:CD2	1.98	0.97
1:C:440:LEU:HD23	1:C:579:LEU:HD22	1.60	0.83
1:D:185:VAL:HG12	1:D:193:THR:HG22	1.66	0.78
1:D:363:GLU:O	1:D:367:VAL:HG23	1.83	0.78
1:A:51:ASN:HB2	1:B:202:GLY:HA2	1.66	0.78
1:C:133:TYR:OH	1:D:51:ASN:ND2	2.16	0.78
1:A:51:ASN:ND2	1:B:133:TYR:OH	2.17	0.76
1:C:416:PHE:CZ	1:C:420:ILE:HD11	2.22	0.74
1:B:192:GLN:HA	5:B:803:HOH:O	1.87	0.74
1:C:58:VAL:HG11	1:C:61:LEU:HD12	1.71	0.72
1:C:358:GLU:CB	5:C:814:HOH:O	2.38	0.70
1:B:345:ALA:O	1:B:348:ILE:HG22	1.91	0.69
1:A:270:LEU:CB	1:A:272:HIS:CD2	2.73	0.69
1:B:159:PHE:CZ	1:B:239:MET:HE2	2.28	0.69
1:D:322:MET:HG2	1:D:341:TRP:HZ3	1.58	0.69
1:A:59:PRO:O	1:A:60:GLU:CB	2.42	0.68
1:C:39:LEU:HD23	1:C:144:PHE:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:PHE:CE2	1:B:420:ILE:CD1	2.77	0.68
1:D:580:THR:O	1:D:581:ALA:HB2	1.92	0.67
1:C:322:MET:CE	1:C:360:ILE:HD11	2.23	0.67
1:B:288:GLU:OE1	1:B:330:ARG:NH2	2.23	0.67
1:B:82:ASP:HB3	1:B:85:ILE:HG13	1.77	0.66
1:C:58:VAL:HG13	1:C:59:PRO:HD2	1.78	0.66
1:B:55:PRO:HB2	1:B:58:VAL:CB	2.26	0.65
1:B:416:PHE:CZ	1:B:420:ILE:HD11	2.32	0.65
1:A:440:LEU:HD23	1:A:579:LEU:HD22	1.78	0.65
1:B:345:ALA:HA	1:B:348:ILE:HG22	1.79	0.64
1:D:319:TYR:N	1:D:320:PRO:CD	2.59	0.64
1:B:140:ILE:O	1:B:140:ILE:HG13	1.98	0.64
1:C:36:LEU:O	1:C:40:VAL:HG23	1.98	0.64
1:D:440:LEU:HD23	1:D:579:LEU:HD22	1.78	0.64
1:D:266:LEU:O	1:D:270:LEU:HD12	1.98	0.63
1:B:113:SER:OG	1:B:170:LEU:HD22	1.98	0.63
2:B:700:7IX:C19	2:B:700:7IX:C13	2.77	0.63
1:D:556:GLU:HA	1:D:559:LYS:HG2	1.81	0.62
1:B:159:PHE:HZ	1:B:239:MET:HE2	1.63	0.62
1:B:319:TYR:N	1:B:320:PRO:CD	2.62	0.62
1:C:564:LEU:N	1:C:564:LEU:HD12	2.15	0.62
1:C:319:TYR:N	1:C:320:PRO:CD	2.63	0.62
1:B:322:MET:HG2	1:B:341:TRP:HZ3	1.66	0.61
1:B:564:LEU:HD12	1:B:564:LEU:N	2.16	0.61
1:A:70:ASP:HA	1:A:71:PRO:C	2.22	0.61
1:D:345:ALA:O	1:D:348:ILE:HG22	2.01	0.60
1:C:83:LEU:O	1:C:83:LEU:HD12	2.02	0.60
1:C:31:GLU:OE1	1:C:232:ARG:NH1	2.29	0.60
1:A:176:ALA:HB2	1:A:185:VAL:HG13	1.84	0.60
1:D:268:TYR:OH	1:D:304:LYS:HE3	2.02	0.59
1:C:440:LEU:CD2	1:C:579:LEU:HD22	2.31	0.59
1:A:162:VAL:HG21	1:A:175:LEU:HB2	1.84	0.59
1:B:178:SER:OG	1:B:179:GLU:N	2.36	0.59
1:B:90:TYR:O	1:B:94:THR:OG1	2.21	0.58
1:B:177:LEU:HB2	1:B:228:MET:HB2	1.83	0.58
1:A:416:PHE:CZ	1:A:420:ILE:HD11	2.39	0.58
1:C:6:ALA:O	1:C:9:THR:HG22	2.03	0.58
1:A:556:GLU:OE1	1:A:556:GLU:HA	2.04	0.58
1:B:124:VAL:O	1:B:128:SER:OG	2.20	0.58
1:D:335:ARG:HB3	1:D:335:ARG:NH1	2.19	0.57
1:A:62:THR:HG22	1:A:63:PHE:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD22	1:A:356:GLU:HB3	1.85	0.57
1:B:183:TRP:HB2	1:B:194:ALA:O	2.05	0.57
1:C:178:SER:OG	1:C:179:GLU:N	2.37	0.57
1:A:376:LEU:HB3	1:A:446:ARG:HG2	1.86	0.56
1:A:319:TYR:N	1:A:320:PRO:CD	2.68	0.56
1:C:125:ILE:O	1:C:129:LEU:HD23	2.05	0.56
1:D:440:LEU:CD2	1:D:579:LEU:HD22	2.35	0.56
1:B:70:ASP:HB3	1:B:71:PRO:HA	1.87	0.56
1:D:59:PRO:C	1:D:60:GLU:HG2	2.24	0.56
1:A:186:PHE:O	1:A:192:GLN:HB2	2.05	0.56
1:D:71:PRO:HD2	1:D:72:PRO:HD3	1.88	0.56
1:D:342:ALA:HB1	1:D:415:ARG:HG2	1.88	0.56
1:A:299:LEU:HD13	1:A:327:TYR:CE2	2.41	0.55
1:A:404:LEU:HD22	1:A:446:ARG:O	2.07	0.55
1:B:13:LEU:HB2	1:B:81:ALA:HB3	1.89	0.55
1:D:304:LYS:O	1:D:307:ALA:HB3	2.07	0.55
1:B:319:TYR:N	1:B:320:PRO:HD3	2.21	0.55
1:C:266:LEU:HD12	1:C:266:LEU:O	2.06	0.55
1:B:564:LEU:HD12	1:B:564:LEU:H	1.71	0.55
1:C:91:ALA:HA	1:C:94:THR:HG22	1.89	0.55
1:D:215:VAL:HA	5:D:816:HOH:O	2.07	0.55
1:D:335:ARG:HB3	1:D:335:ARG:HH11	1.72	0.55
1:B:363:GLU:O	1:B:367:VAL:HG23	2.07	0.54
1:D:418:ASP:HA	1:D:558:MET:HG3	1.89	0.54
1:C:236:VAL:O	1:C:240:VAL:HG23	2.07	0.54
1:C:564:LEU:N	1:C:564:LEU:CD1	2.70	0.54
1:C:140:ILE:HG13	1:C:140:ILE:O	2.08	0.54
1:B:214:GLY:HA3	1:B:222:TYR:CD2	2.43	0.54
1:C:42:GLY:HA3	1:C:144:PHE:HB3	1.90	0.53
1:B:117:LEU:O	1:B:121:VAL:HG23	2.09	0.53
1:B:166:GLN:HG3	1:B:232:ARG:NH1	2.24	0.53
1:A:62:THR:CG2	1:A:63:PHE:N	2.72	0.53
1:B:42:GLY:HA3	1:B:144:PHE:HB3	1.90	0.53
1:A:206:ARG:HG2	1:A:209:GLN:OE1	2.09	0.53
1:C:310:LYS:HE3	1:C:315:ASP:OD2	2.09	0.53
1:B:224:LYS:HD3	1:B:351:TYR:CE1	2.44	0.52
1:C:3:LEU:HB2	1:C:8:LYS:HE3	1.91	0.52
1:D:178:SER:OG	1:D:179:GLU:N	2.43	0.52
1:B:16:ILE:HB	5:B:805:HOH:O	2.10	0.52
1:B:418:ASP:HA	1:B:558:MET:HG3	1.91	0.52
1:A:233:LYS:HB3	1:A:272:HIS:ND1	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:437:ALA:HB1	1:C:576:LYS:HG2	1.90	0.52
1:B:429:THR:HG22	1:B:430:PRO:O	2.10	0.51
1:C:59:PRO:HG2	1:C:60:GLU:H	1.75	0.51
1:B:336:GLU:OE1	1:B:336:GLU:N	2.43	0.51
1:A:310:LYS:HE3	1:A:321:TYR:OH	2.11	0.51
1:B:15:SER:O	1:B:19:VAL:HG23	2.10	0.51
1:B:345:ALA:HA	1:B:348:ILE:CG2	2.40	0.51
1:A:148:THR:HG22	1:A:149:GLY:N	2.24	0.51
1:B:561:MET:O	1:B:565:LEU:HG	2.11	0.51
1:C:418:ASP:HA	1:C:558:MET:HG3	1.92	0.51
1:D:71:PRO:N	1:D:72:PRO:CD	2.74	0.51
1:C:71:PRO:O	1:C:72:PRO:C	2.49	0.51
1:D:53:VAL:O	1:D:55:PRO:HD3	2.10	0.51
1:D:261:GLN:NE2	1:D:290:GLU:O	2.41	0.50
1:A:440:LEU:CD2	1:A:579:LEU:HD22	2.40	0.50
1:C:564:LEU:CD1	1:C:564:LEU:H	2.24	0.50
1:D:181:HIS:CG	1:D:182:ALA:H	2.29	0.50
1:A:288:GLU:OE1	1:A:330:ARG:NH2	2.41	0.50
1:B:18:ASP:OD1	1:B:21:ARG:NH1	2.45	0.50
1:B:358:GLU:O	1:B:362:LYS:HG3	2.11	0.50
1:C:70:ASP:C	1:C:72:PRO:HD2	2.32	0.50
1:A:49:ALA:HA	1:A:247:ILE:HG12	1.93	0.50
1:B:236:VAL:O	1:B:239:MET:HG2	2.11	0.50
1:B:406:ASP:OD1	1:B:408:GLU:HB2	2.12	0.50
1:A:42:GLY:HA3	1:A:144:PHE:HB3	1.92	0.50
1:A:418:ASP:HA	1:A:558:MET:HG3	1.93	0.50
1:D:45:GLU:HG3	1:D:256:LEU:CD1	2.41	0.50
1:A:349:GLN:HB2	1:A:422:LYS:HB3	1.92	0.50
1:B:314:ARG:HB2	1:B:316:GLU:HG3	1.92	0.50
1:A:206:ARG:HB2	5:A:802:HOH:O	2.10	0.50
1:A:528:GLY:HA3	1:D:251:THR:HA	1.93	0.50
1:D:173:VAL:O	1:D:232:ARG:NH2	2.45	0.50
1:B:416:PHE:CE2	1:B:420:ILE:HD11	2.47	0.49
1:A:564:LEU:CD1	1:A:564:LEU:N	2.74	0.49
1:C:71:PRO:N	1:C:72:PRO:CD	2.74	0.49
1:A:274:GLU:HA	1:A:274:GLU:OE1	2.12	0.49
1:C:195:GLU:HA	5:C:803:HOH:O	2.11	0.49
1:C:453:GLN:C	1:C:455:VAL:H	2.15	0.49
1:B:221:LEU:HD22	1:B:356:GLU:HB3	1.94	0.49
2:D:700:7IX:C19	2:D:700:7IX:C13	2.91	0.49
1:B:39:LEU:HD23	1:B:144:PHE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:TYR:OH	1:C:304:LYS:HE3	2.12	0.49
2:A:700:7IX:C19	2:A:700:7IX:C13	2.90	0.49
1:C:4:LYS:HE3	1:C:29:ARG:HH22	1.78	0.49
1:C:62:THR:HG22	1:C:63:PHE:H	1.77	0.49
1:C:348:ILE:HG12	1:C:364:PHE:HE2	1.78	0.49
1:B:564:LEU:H	1:B:564:LEU:CD1	2.26	0.48
1:A:282:ASN:C	1:A:282:ASN:HD22	2.15	0.48
1:B:345:ALA:C	1:B:348:ILE:HG22	2.33	0.48
1:D:318:ILE:C	1:D:320:PRO:HD2	2.34	0.48
1:C:140:ILE:O	1:C:152:LEU:HA	2.13	0.48
1:C:402:SER:OG	1:C:403:ALA:N	2.46	0.48
1:A:230:CYS:HB3	1:A:235:GLU:HG3	1.95	0.48
1:C:302:TYR:O	1:C:306:ILE:HG13	2.13	0.48
1:A:237:ALA:HA	1:A:267:LEU:HD13	1.95	0.48
1:B:173:VAL:O	1:B:232:ARG:NH2	2.47	0.48
1:D:140:ILE:O	1:D:152:LEU:HA	2.14	0.48
1:C:455:VAL:HG22	1:C:549:PRO:HB2	1.95	0.48
1:B:71:PRO:O	1:B:72:PRO:C	2.50	0.48
1:B:91:ALA:O	1:B:95:ALA:HB2	2.14	0.48
1:B:223:LEU:O	1:B:225:GLY:N	2.47	0.48
1:B:45:GLU:HA	1:B:256:LEU:HD11	1.96	0.48
1:B:345:ALA:CA	1:B:348:ILE:HG22	2.42	0.48
1:D:45:GLU:HA	1:D:256:LEU:HD11	1.96	0.48
1:C:407:PRO:HB2	1:C:549:PRO:HG2	1.96	0.47
2:C:700:7IX:C13	2:C:700:7IX:C19	2.92	0.47
1:D:416:PHE:CZ	1:D:420:ILE:HD11	2.49	0.47
1:D:580:THR:O	1:D:581:ALA:CB	2.59	0.47
1:D:345:ALA:HA	1:D:348:ILE:HG22	1.97	0.47
1:A:231:ASP:HB2	5:A:822:HOH:O	2.15	0.47
1:B:325:ALA:HB1	1:B:341:TRP:CE2	2.49	0.47
1:D:319:TYR:N	1:D:320:PRO:HD3	2.30	0.47
1:A:365:PHE:CD1	1:A:365:PHE:C	2.88	0.47
1:B:42:GLY:HA3	1:B:144:PHE:CB	2.45	0.47
1:B:361:TYR:CD1	1:B:361:TYR:C	2.88	0.47
1:C:71:PRO:N	1:C:72:PRO:HD2	2.29	0.47
1:D:112:VAL:HG11	1:D:188:PRO:HD3	1.97	0.47
1:D:445:GLY:C	1:D:447:PHE:H	2.17	0.47
1:B:372:ILE:HB	1:B:373:PRO:HD3	1.97	0.47
1:D:453:GLN:C	1:D:455:VAL:H	2.18	0.47
1:A:571:ASN:O	1:A:573:SER:N	2.47	0.47
1:D:404:LEU:HD13	1:D:446:ARG:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:SER:HB2	5:C:811:HOH:O	2.14	0.47
1:A:39:LEU:HD21	1:A:147:ILE:HD12	1.98	0.46
1:A:314:ARG:CZ	1:D:10:LEU:HD21	2.44	0.46
1:B:366:GLU:O	1:B:371:VAL:HG23	2.14	0.46
1:C:15:SER:O	1:C:19:VAL:HG23	2.15	0.46
1:C:97:ILE:HG22	1:C:168:LEU:HD21	1.97	0.46
1:C:416:PHE:CE1	1:C:420:ILE:HD11	2.50	0.46
1:A:71:PRO:HB2	1:A:72:PRO:HD3	1.96	0.46
1:A:236:VAL:O	1:A:240:VAL:HG23	2.15	0.46
1:D:270:LEU:HB3	1:D:272:HIS:CD2	2.50	0.46
1:D:322:MET:HG2	1:D:341:TRP:CZ3	2.43	0.46
1:A:526:ALA:HB1	1:D:251:THR:CG2	2.46	0.46
1:B:561:MET:O	1:B:561:MET:HG3	2.15	0.46
1:C:361:TYR:CD1	1:C:361:TYR:C	2.88	0.46
1:D:455:VAL:HG22	1:D:549:PRO:HG2	1.98	0.46
1:A:527:ARG:O	1:A:528:GLY:C	2.54	0.46
1:B:348:ILE:HG12	1:B:364:PHE:CE2	2.50	0.46
1:A:363:GLU:O	1:A:367:VAL:HG23	2.16	0.46
1:A:437:ALA:HB1	1:A:576:LYS:HG2	1.98	0.46
1:D:320:PRO:HB3	5:D:831:HOH:O	2.15	0.46
1:A:571:ASN:C	1:A:573:SER:H	2.20	0.45
1:C:147:ILE:HD13	1:C:147:ILE:HA	1.68	0.45
1:A:284:ALA:HB2	1:A:301:LEU:HB3	1.98	0.45
1:B:85:ILE:O	1:B:88:ALA:HB3	2.17	0.45
1:B:223:LEU:C	1:B:225:GLY:N	2.69	0.45
1:D:445:GLY:O	1:D:447:PHE:N	2.49	0.45
1:B:159:PHE:HZ	1:B:239:MET:CE	2.27	0.45
1:D:71:PRO:CD	1:D:72:PRO:HD3	2.47	0.45
1:B:433:HIS:O	1:B:435:GLY:N	2.49	0.45
1:C:344:THR:HG22	1:C:364:PHE:CE1	2.52	0.45
1:B:152:LEU:HD23	1:B:152:LEU:HA	1.79	0.45
1:A:157:VAL:O	1:A:161:VAL:HG23	2.17	0.45
1:A:175:LEU:O	1:A:230:CYS:HB2	2.17	0.45
1:A:237:ALA:HA	1:A:267:LEU:CD1	2.46	0.45
1:C:117:LEU:O	1:C:121:VAL:HG23	2.17	0.45
1:C:4:LYS:HE2	1:C:4:LYS:HB2	1.77	0.45
1:B:26:GLU:O	1:B:32:PRO:HB3	2.17	0.45
1:B:452:ARG:CZ	1:B:570:ILE:HD11	2.46	0.45
1:B:91:ALA:O	1:B:95:ALA:CB	2.65	0.45
1:B:567:ALA:HB1	5:B:822:HOH:O	2.16	0.45
1:C:147:ILE:HG22	1:C:148:THR:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:LYS:HB2	1:D:119:LYS:HE3	1.61	0.45
1:C:318:ILE:CG2	1:C:322:MET:HE3	2.48	0.44
1:C:550:VAL:HG12	1:C:551:LEU:N	2.32	0.44
1:A:68:ALA:HB3	1:A:73:GLY:O	2.16	0.44
1:C:416:PHE:CZ	1:C:420:ILE:CD1	2.98	0.44
1:A:371:VAL:O	1:A:375:LEU:HB2	2.17	0.44
1:B:318:ILE:C	1:B:320:PRO:HD2	2.37	0.44
1:C:115:ARG:NH2	1:C:193:THR:O	2.46	0.44
1:C:224:LYS:HE2	1:C:316:GLU:OE2	2.18	0.44
1:D:372:ILE:HB	1:D:373:PRO:HD3	1.99	0.44
1:B:349:GLN:HB2	1:B:422:LYS:HB3	1.98	0.44
1:A:292:THR:HA	1:A:293:PRO:HD3	1.86	0.44
1:D:321:TYR:CE2	1:D:347:VAL:HG21	2.52	0.44
1:B:158:ALA:HA	1:B:196:VAL:HG21	1.99	0.44
1:B:564:LEU:N	1:B:564:LEU:CD1	2.81	0.44
1:D:181:HIS:CG	1:D:182:ALA:N	2.86	0.44
1:D:414:LEU:CD2	1:D:565:LEU:HD13	2.48	0.43
1:B:159:PHE:CZ	1:B:239:MET:CE	3.01	0.43
1:B:268:TYR:OH	1:B:304:LYS:HE3	2.18	0.43
1:C:424:GLU:OE1	1:C:432:LEU:HD12	2.18	0.43
1:C:144:PHE:CZ	1:C:148:THR:HG21	2.54	0.43
1:D:561:MET:O	1:D:561:MET:HG3	2.17	0.43
1:B:440:LEU:HD23	1:B:579:LEU:HD22	2.01	0.43
1:C:83:LEU:CD1	1:C:87:ALA:HB2	2.49	0.43
1:C:254:LEU:HD23	1:C:254:LEU:HA	1.87	0.43
1:A:564:LEU:CD1	1:A:564:LEU:H	2.31	0.43
1:C:90:TYR:CD1	1:C:90:TYR:C	2.92	0.43
1:A:27:LEU:HD13	1:A:270:LEU:HD12	2.01	0.43
1:A:48:LEU:HD13	1:A:255:GLU:HB2	2.01	0.43
1:A:140:ILE:O	1:A:152:LEU:HA	2.18	0.43
1:C:328:HIS:CD2	1:C:336:GLU:HB3	2.54	0.43
1:D:406:ASP:OD2	1:D:408:GLU:HB2	2.18	0.43
1:D:454:LYS:O	1:D:549:PRO:HD2	2.19	0.43
1:A:23:PHE:CE1	1:A:37:LEU:HD22	2.54	0.43
1:A:39:LEU:HD21	1:A:147:ILE:CD1	2.48	0.42
1:C:44:VAL:O	1:C:48:LEU:HB2	2.19	0.42
1:D:136:ASP:HA	5:D:807:HOH:O	2.19	0.42
1:D:414:LEU:HD22	1:D:565:LEU:HD13	2.01	0.42
1:A:185:VAL:HG12	1:A:193:THR:HG22	2.00	0.42
1:B:372:ILE:N	1:B:373:PRO:CD	2.82	0.42
1:C:152:LEU:HA	1:C:152:LEU:HD23	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:PHE:HZ	1:D:239:MET:HE1	1.84	0.42
1:A:557:LYS:HE2	1:A:581:ALA:HB3	2.01	0.42
1:B:360:ILE:HD12	1:B:360:ILE:HA	1.84	0.42
1:B:437:ALA:HB1	1:B:576:LYS:HG2	2.01	0.42
1:C:265:TRP:CE3	1:C:265:TRP:HA	2.54	0.42
1:A:372:ILE:N	1:A:373:PRO:CD	2.83	0.42
1:B:406:ASP:OD1	1:B:406:ASP:C	2.58	0.42
1:C:133:TYR:O	1:C:133:TYR:CD1	2.72	0.42
1:D:102:ASP:OD2	1:D:105:LEU:HG	2.20	0.42
1:C:23:PHE:CE2	1:C:37:LEU:HD22	2.54	0.42
1:C:177:LEU:HB2	1:C:228:MET:HB2	2.00	0.42
1:D:42:GLY:HA3	1:D:144:PHE:HB3	2.01	0.42
1:A:53:VAL:O	1:A:55:PRO:HD3	2.19	0.42
1:A:345:ALA:O	1:A:348:ILE:HG22	2.20	0.42
1:B:102:ASP:HB3	1:B:105:LEU:HD12	2.01	0.42
1:B:231:ASP:O	1:B:232:ARG:C	2.56	0.42
1:C:413:LEU:HD11	1:C:417:TYR:HE1	1.85	0.42
1:D:310:LYS:HE3	1:D:321:TYR:OH	2.20	0.42
1:A:54:ILE:HD13	1:A:63:PHE:CG	2.54	0.41
1:B:27:LEU:HD21	1:B:236:VAL:HG11	2.02	0.41
1:B:141:GLN:HG2	1:B:142:SER:N	2.35	0.41
1:D:453:GLN:NE2	1:D:568:THR:HG23	2.34	0.41
1:A:341:TRP:CZ3	1:A:367:VAL:HG21	2.55	0.41
1:B:223:LEU:C	1:B:225:GLY:H	2.22	0.41
1:B:433:HIS:O	1:B:434:VAL:C	2.59	0.41
1:A:266:LEU:O	1:A:270:LEU:HG	2.20	0.41
1:C:224:LYS:HD3	1:C:351:TYR:CE1	2.55	0.41
1:C:348:ILE:HG12	1:C:364:PHE:CE2	2.55	0.41
1:C:571:ASN:ND2	1:C:574:ALA:HB2	2.36	0.41
1:D:561:MET:O	1:D:565:LEU:HG	2.20	0.41
1:A:299:LEU:HD12	1:A:299:LEU:HA	1.95	0.41
1:C:360:ILE:HD12	1:C:360:ILE:HA	1.91	0.41
1:D:70:ASP:C	1:D:72:PRO:HD2	2.40	0.41
1:D:292:THR:HA	1:D:293:PRO:HD3	1.89	0.41
1:D:564:LEU:HD12	1:D:564:LEU:N	2.35	0.41
1:C:580:THR:O	1:C:581:ALA:HB2	2.21	0.41
1:D:55:PRO:HB3	1:D:58:VAL:HG23	2.03	0.41
1:B:318:ILE:C	1:B:320:PRO:CD	2.88	0.41
1:D:299:LEU:HD12	1:D:299:LEU:HA	1.85	0.41
1:C:39:LEU:HD23	1:C:144:PHE:CA	2.45	0.41
1:D:149:GLY:O	1:D:151:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLU:OE1	1:A:232:ARG:HD2	2.20	0.41
1:A:42:GLY:HA3	1:A:144:PHE:CB	2.51	0.41
1:A:345:ALA:HA	1:A:348:ILE:HG22	2.03	0.41
1:B:237:ALA:HA	1:B:267:LEU:HD13	2.03	0.41
1:B:344:THR:HG22	1:B:364:PHE:CE1	2.55	0.41
1:D:276:TYR:CD1	1:D:279:ALA:HB2	2.55	0.41
1:D:404:LEU:HD23	1:D:404:LEU:HA	1.83	0.41
1:D:452:ARG:CZ	1:D:570:ILE:HD11	2.51	0.41
1:A:564:LEU:N	1:A:564:LEU:HD12	2.35	0.41
1:B:371:VAL:HG21	2:B:700:7IX:O3	2.21	0.41
1:C:230:CYS:HB3	1:C:235:GLU:HG3	2.02	0.40
1:D:346:THR:OG1	1:D:415:ARG:NH1	2.53	0.40
1:D:562:LYS:HE2	1:D:562:LYS:HB3	1.90	0.40
1:B:546:PRO:O	1:B:547:GLU:CB	2.69	0.40
1:C:83:LEU:HD12	1:C:87:ALA:HB2	2.04	0.40
1:D:117:LEU:HD21	1:D:170:LEU:HD21	2.04	0.40
1:A:284:ALA:HB2	1:A:301:LEU:CB	2.52	0.40
1:B:183:TRP:HB3	5:B:810:HOH:O	2.22	0.40
1:C:239:MET:HB3	1:C:239:MET:HE2	1.99	0.40
1:C:345:ALA:HA	1:C:348:ILE:HG22	2.03	0.40
1:C:345:ALA:O	1:C:348:ILE:HG22	2.21	0.40
1:C:363:GLU:O	1:C:367:VAL:HG23	2.21	0.40
1:C:372:ILE:HB	1:C:373:PRO:HD3	2.04	0.40
1:D:59:PRO:O	1:D:60:GLU:HG2	2.21	0.40
1:D:344:THR:HG22	1:D:364:PHE:CZ	2.56	0.40
1:B:265:TRP:HA	1:B:265:TRP:CE3	2.56	0.40
1:D:12:PRO:HG3	1:D:14:ARG:NH1	2.37	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	480/550 (87%)	452 (94%)	25 (5%)	3 (1%)	25	47
1	B	484/550 (88%)	446 (92%)	33 (7%)	5 (1%)	15	32
1	C	477/550 (87%)	441 (92%)	33 (7%)	3 (1%)	25	47
1	D	479/550 (87%)	446 (93%)	31 (6%)	2 (0%)	34	57
All	All	1920/2200 (87%)	1785 (93%)	122 (6%)	13 (1%)	22	43

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	135	LYS
1	B	204	GLU
1	C	59	PRO
1	C	527	ARG
1	A	203	ASN
1	B	59	PRO
1	D	296	PRO
1	A	572	SER
1	B	434	VAL
1	B	547	GLU
1	C	581	ALA
1	B	211	VAL
1	A	71	PRO

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	368/461 (80%)	359 (98%)	9 (2%)	49	74
1	B	359/461 (78%)	349 (97%)	10 (3%)	43	69
1	C	375/461 (81%)	367 (98%)	8 (2%)	53	77
1	D	371/461 (80%)	364 (98%)	7 (2%)	57	79
All	All	1473/1844 (80%)	1439 (98%)	34 (2%)	50	75

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	53	VAL
1	A	76	THR
1	A	105	LEU
1	A	276	TYR
1	A	282	ASN
1	A	292	THR
1	A	374	ASN
1	A	568	THR
1	B	94	THR
1	B	105	LEU
1	B	150	THR
1	B	152	LEU
1	B	185	VAL
1	B	276	TYR
1	B	278	MET
1	B	282	ASN
1	B	299	LEU
1	B	522	VAL
1	C	62	THR
1	C	147	ILE
1	C	184	VAL
1	C	276	TYR
1	C	282	ASN
1	C	349	GLN
1	C	429	THR
1	C	566	VAL
1	D	171	ARG
1	D	184	VAL
1	D	270	LEU
1	D	276	TYR
1	D	282	ASN
1	D	429	THR
1	D	562	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	258	GLN
1	A	282	ASN
1	A	374	ASN
1	B	209	GLN

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	339	GLN
1	B	405	GLN
1	B	453	GLN
1	C	258	GLN
1	C	272	HIS
1	C	282	ASN
1	D	51	ASN
1	D	272	HIS
1	D	282	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are unknown - leaving 8 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	$\#\|Z\| > 2$
4	DMS	A	702	-	3,3,3	0.37	0	3,3,3	0.09	0
2	7IX	A	700	-	41,44,44	1.32	5 (12%)	42,64,64	1.31	7 (16%)
4	DMS	D	702	-	3,3,3	0.38	0	3,3,3	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	7IX	D	700	-	41,44,44	1.23	4 (9%)	42,64,64	1.63	11 (26%)
4	DMS	C	702	-	3,3,3	0.27	0	3,3,3	0.07	0
4	DMS	B	702	-	3,3,3	0.40	0	3,3,3	0.13	0
2	7IX	C	700	-	41,44,44	1.20	4 (9%)	42,64,64	1.42	7 (16%)
2	7IX	B	700	-	41,44,44	1.49	4 (9%)	42,64,64	1.74	12 (28%)

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	7IX	A	700	-	-	3/24/38/38	0/5/5/5
2	7IX	B	700	-	-	3/24/38/38	0/5/5/5
2	7IX	C	700	-	-	5/24/38/38	0/5/5/5
2	7IX	D	700	-	-	5/24/38/38	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700	7IX	C22-N5	6.26	1.37	1.32
2	A	700	7IX	C22-N5	4.74	1.36	1.32
2	C	700	7IX	C22-N5	4.20	1.35	1.32
2	D	700	7IX	C20-C21	4.11	1.54	1.49
2	A	700	7IX	C20-C18	-3.74	1.49	1.50
2	D	700	7IX	C22-N5	3.73	1.35	1.32
2	C	700	7IX	C20-C18	-2.93	1.49	1.50
2	A	700	7IX	C20-C21	2.68	1.52	1.49
2	B	700	7IX	C20-C21	2.63	1.52	1.49
2	A	700	7IX	C1-C23	-2.54	1.44	1.48
2	C	700	7IX	C20-C21	2.47	1.52	1.49
2	A	700	7IX	C14-N3	2.37	1.36	1.33
2	B	700	7IX	C1-C23	-2.34	1.45	1.48
2	B	700	7IX	C14-N3	2.21	1.36	1.33
2	D	700	7IX	C1-C23	-2.15	1.45	1.48
2	C	700	7IX	C14-N3	2.08	1.36	1.33
2	D	700	7IX	C20-C18	-2.02	1.50	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	700	7IX	C24-O2-C22	-4.89	112.36	117.21
2	B	700	7IX	O2-C22-C26	3.76	123.45	116.93
2	C	700	7IX	C6-C7-N1	-3.61	103.74	112.67
2	B	700	7IX	C6-C7-N1	-3.30	104.50	112.67
2	D	700	7IX	C6-C7-N1	-3.27	104.58	112.67
2	B	700	7IX	O1-C10-C12	-3.23	105.46	111.39
2	D	700	7IX	O2-C22-C26	3.15	122.40	116.93
2	D	700	7IX	C1-C23-N6	-3.11	111.14	115.97
2	C	700	7IX	O1-C10-C12	-2.99	105.90	111.39
2	D	700	7IX	C24-O2-C22	-2.92	114.32	117.21
2	D	700	7IX	C7-N1-C8	-2.83	110.10	114.14
2	C	700	7IX	C27-O3-C26	-2.81	113.29	117.53
2	D	700	7IX	C25-C23-N6	2.77	123.75	121.64
2	A	700	7IX	C6-C7-N1	-2.63	106.17	112.67
2	C	700	7IX	F2-C21-F3	2.56	115.84	106.43
2	B	700	7IX	C13-N2-C12	2.55	122.39	118.22
2	B	700	7IX	C2-C1-C23	-2.52	117.30	121.28
2	B	700	7IX	C7-N1-C8	-2.45	110.64	114.14
2	B	700	7IX	C25-C23-N6	2.40	123.47	121.64
2	A	700	7IX	O1-C10-C12	-2.37	107.04	111.39
2	D	700	7IX	C25-C23-C1	2.34	124.97	121.85
2	B	700	7IX	C13-N2-C14	-2.31	114.46	120.40
2	A	700	7IX	F2-C21-F3	2.24	114.68	106.43
2	A	700	7IX	C2-C1-C23	-2.20	117.81	121.28
2	B	700	7IX	C4-C1-C2	2.17	121.92	117.59
2	D	700	7IX	C27-O3-C26	-2.17	114.25	117.53
2	B	700	7IX	C27-O3-C26	-2.17	114.25	117.53
2	C	700	7IX	C13-N2-C12	2.13	121.71	118.22
2	B	700	7IX	F2-C21-F3	2.12	114.23	106.43
2	C	700	7IX	N3-C14-N2	-2.10	114.80	117.06
2	A	700	7IX	C1-C23-N6	-2.08	112.73	115.97
2	A	700	7IX	O2-C22-C26	2.07	120.53	116.93
2	D	700	7IX	N3-C14-N2	-2.07	114.83	117.06
2	A	700	7IX	C22-N5-N6	2.06	121.22	119.32
2	C	700	7IX	C4-C5-C6	-2.05	118.20	121.03
2	D	700	7IX	C7-C6-C3	-2.04	116.68	120.91
2	D	700	7IX	C5-C6-C3	2.00	121.31	118.17

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	7IX	C11-C12-N2-C13

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Mol	Chain	Res	Type	Atoms
2	B	700	7IX	C11-C12-N2-C13
2	C	700	7IX	C18-C20-C21-F1
2	C	700	7IX	C18-C20-C21-F2
2	C	700	7IX	C11-C12-N2-C13
2	D	700	7IX	C18-C20-C21-F3
2	D	700	7IX	C18-C20-C21-F1
2	D	700	7IX	C18-C20-C21-F2
2	B	700	7IX	C10-C12-N2-C13
2	C	700	7IX	C10-C12-N2-C13
2	D	700	7IX	C10-C12-N2-C13
2	D	700	7IX	C11-C12-N2-C13
2	A	700	7IX	C10-C12-N2-C13
2	C	700	7IX	C18-C20-C21-F3
2	A	700	7IX	C15-C14-N2-C13
2	B	700	7IX	N3-C14-N2-C12

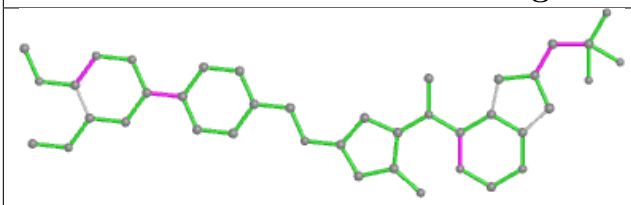
There are no ring outliers.

4 monomers are involved in 5 short contacts:

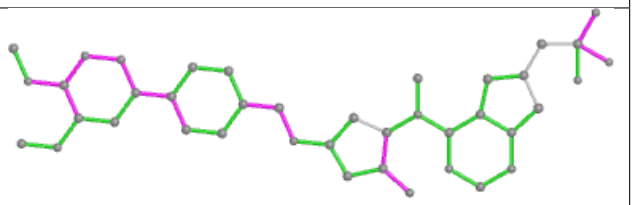
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700	7IX	1	0
2	D	700	7IX	1	0
2	C	700	7IX	1	0
2	B	700	7IX	2	0

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 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.

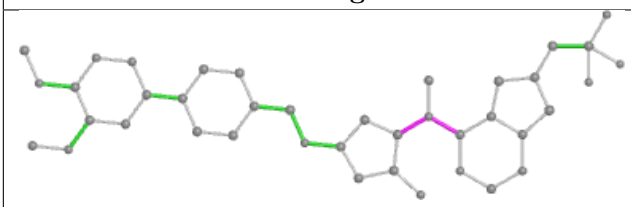
Ligand 7IX A 700



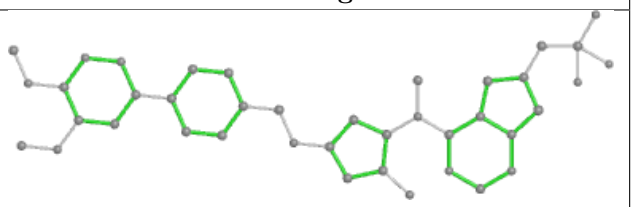
Bond lengths



Bond angles

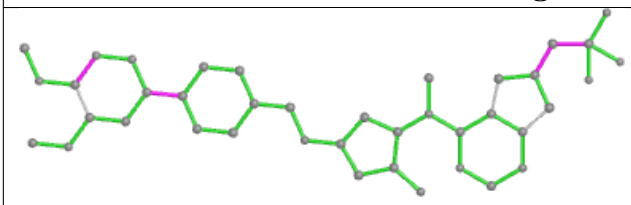


Torsions

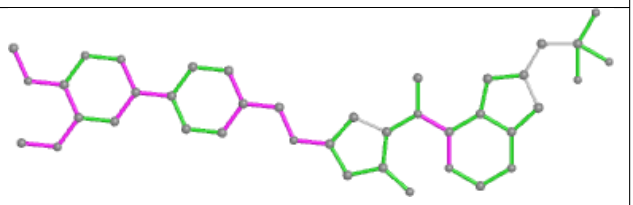


Rings

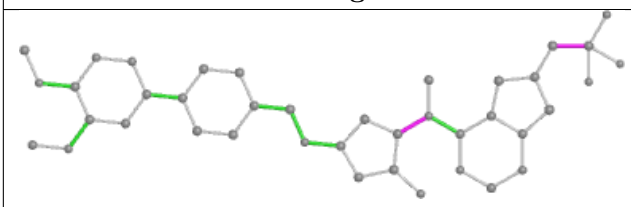
Ligand 7IX D 700



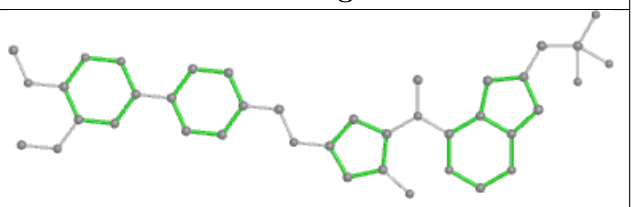
Bond lengths



Bond angles

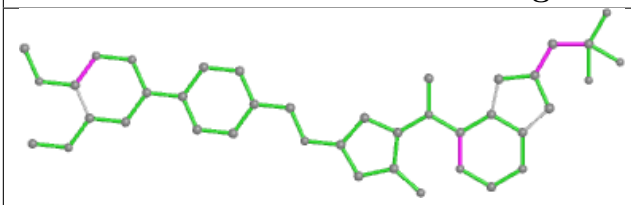


Torsions

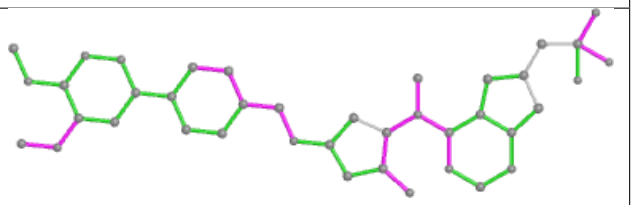


Rings

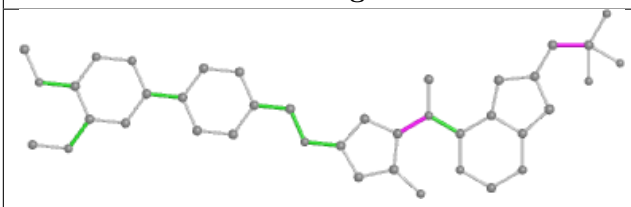
Ligand 7IX C 700



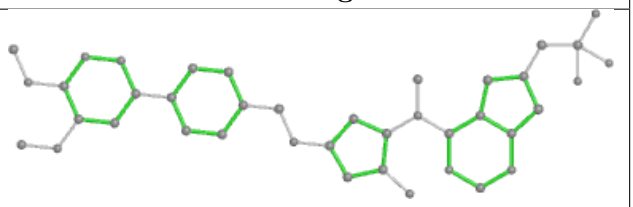
Bond lengths



Bond angles

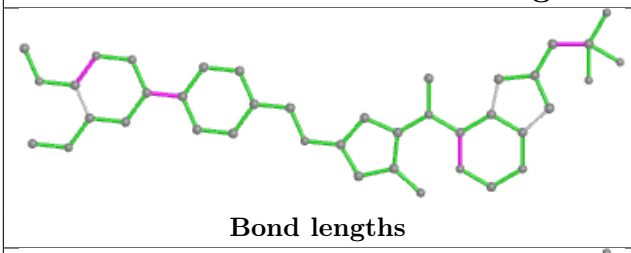


Torsions

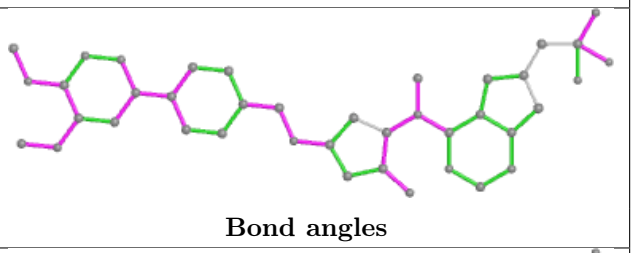


Rings

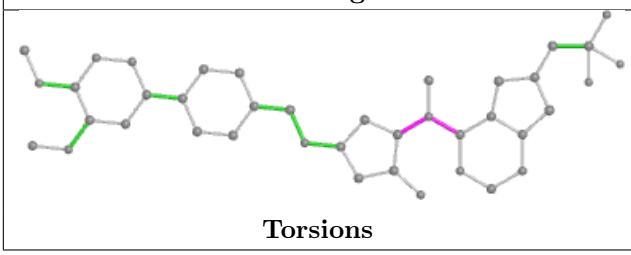
Ligand 7IX B 700



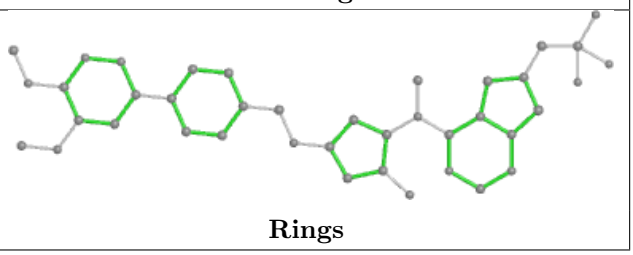
Bond lengths



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	486/550 (88%)	-0.31	10 (2%)	63	58	32, 60, 95, 140	0
1	B	490/550 (89%)	-0.23	18 (3%)	41	34	39, 68, 110, 172	0
1	C	483/550 (87%)	-0.30	7 (1%)	75	71	38, 64, 106, 145	0
1	D	485/550 (88%)	-0.26	13 (2%)	54	48	33, 62, 106, 156	0
All	All	1944/2200 (88%)	-0.28	48 (2%)	57	51	32, 63, 105, 172	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	PRO	8.2
1	D	71	PRO	5.5
1	B	385	ALA	5.3
1	D	385	ALA	4.4
1	B	73	GLY	3.7
1	A	578	GLN	3.5
1	C	71	PRO	3.4
1	C	56	THR	3.3
1	C	58	VAL	3.3
1	B	75	LEU	3.2
1	B	249	LEU	3.2
1	C	38	SER	3.1
1	C	583	SER	3.0
1	B	110	GLY	2.9
1	D	250	HIS	2.8
1	C	249	LEU	2.8
1	B	74	GLY	2.8
1	B	583	SER	2.8
1	A	71	PRO	2.8
1	B	72	PRO	2.8
1	B	106	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	105	LEU	2.6
1	D	72	PRO	2.5
1	D	379	ALA	2.5
1	B	69	PRO	2.5
1	A	385	ALA	2.4
1	B	584	GLN	2.4
1	C	57	ASN	2.4
1	D	136	ASP	2.4
1	A	75	LEU	2.3
1	D	573	SER	2.3
1	B	381	SER	2.2
1	B	546	PRO	2.2
1	D	381	SER	2.2
1	A	582	GLN	2.2
1	B	582	GLN	2.2
1	A	293	PRO	2.1
1	B	107	PRO	2.1
1	B	70	ASP	2.1
1	D	70	ASP	2.1
1	D	384	GLU	2.1
1	A	249	LEU	2.1
1	D	380	ALA	2.1
1	B	206	ARG	2.1
1	A	383	LEU	2.1
1	D	404	LEU	2.1
1	A	381	SER	2.0
1	D	416	PHE	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,

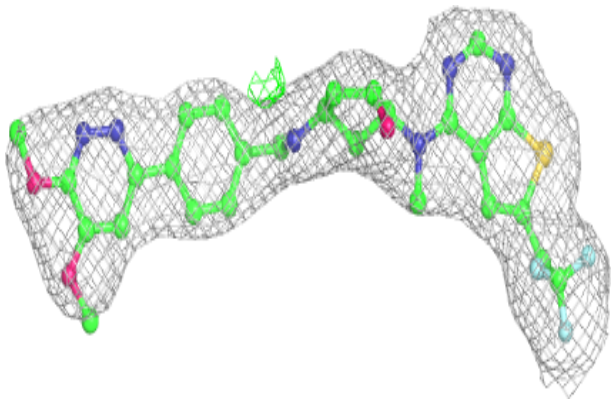
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

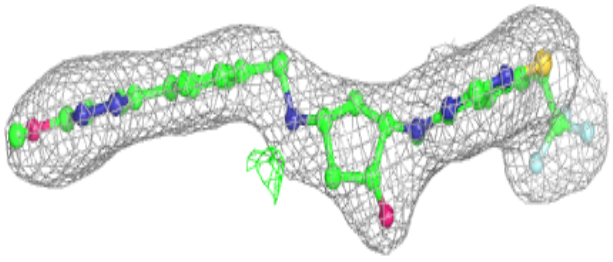
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	D	702	4/4	0.82	0.23	77,85,91,103	0
4	DMS	C	702	4/4	0.89	0.23	98,108,108,115	0
3	UNX	B	701	1/1	0.90	0.33	9,9,9,9	0
4	DMS	B	702	4/4	0.90	0.21	70,92,93,101	0
4	DMS	A	702	4/4	0.91	0.19	74,83,93,103	0
3	UNX	C	701	1/1	0.96	0.43	7,7,7,7	0
3	UNX	D	701	1/1	0.96	0.24	9,9,9,9	0
2	7IX	C	700	40/40	0.97	0.13	36,49,66,70	0
2	7IX	D	700	40/40	0.97	0.10	29,42,52,54	0
3	UNX	A	701	1/1	0.97	0.28	6,6,6,6	0
2	7IX	A	700	40/40	0.97	0.11	33,40,58,64	0
2	7IX	B	700	40/40	0.97	0.11	28,44,53,55	0

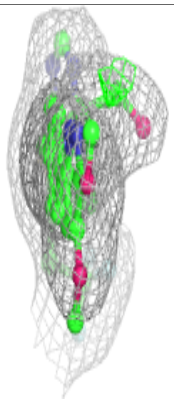
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7IX C 700:

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

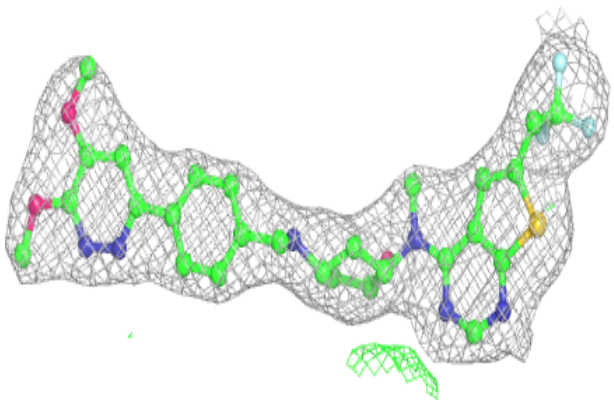


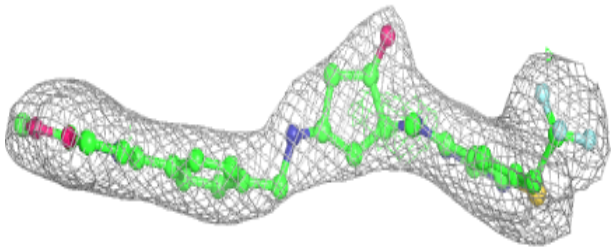


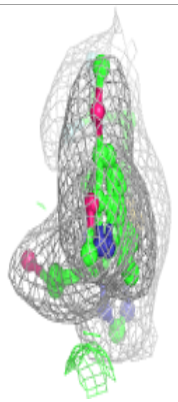


Electron density around 7IX D 700:

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

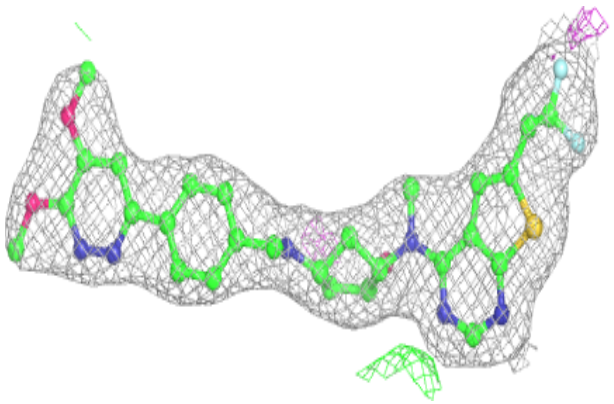


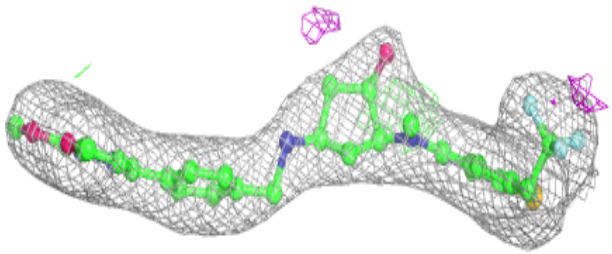


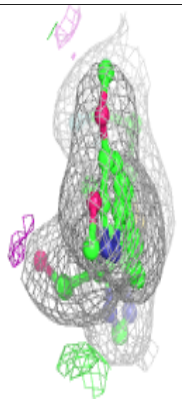


Electron density around 7IX A 700:

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

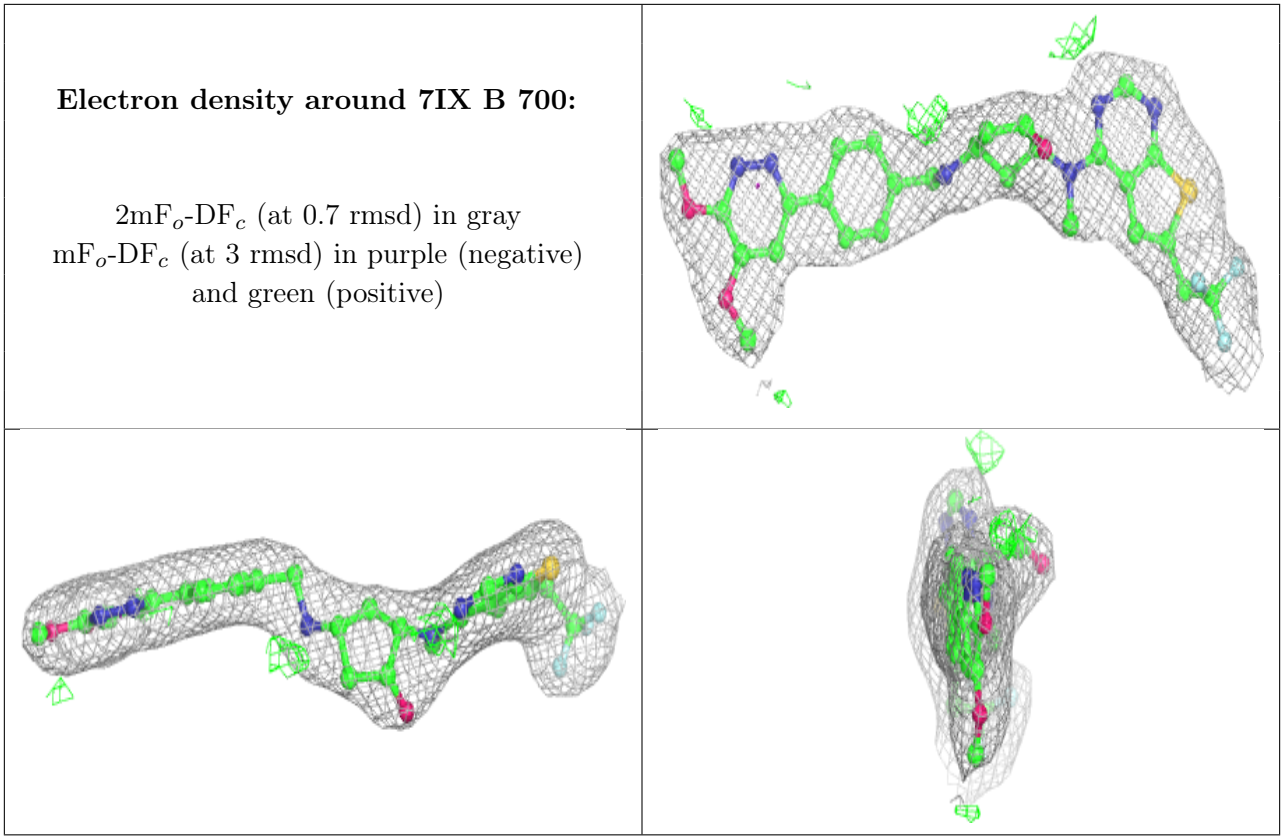






Electron density around 7IX B 700:

$2mF_o$-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.