Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 11:37 PM EDT

PDB ID	:	2D3Z
Title	:	X-ray crystal structure of hepatitis C virus RNA-dependent RNA polymerase in complex with non-nucleoside analogue inhibitor
Authors	:	Biswal, B.K.; Wang, M.; Cherney, M.M.; Chan, L.; Yannopoulos, C.G.; Bilimoria, D.; Bedard, J.; James, M.N.G.
Deposited on	:	2005-10-04
Resolution	:	1.80 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:

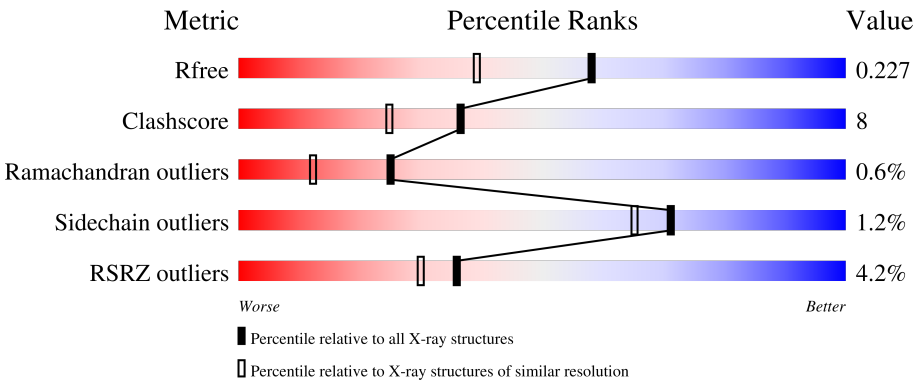
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	570	5% 82% 15% • •
1	B	570	3% 84% 13% • •

2 Entry composition (i)

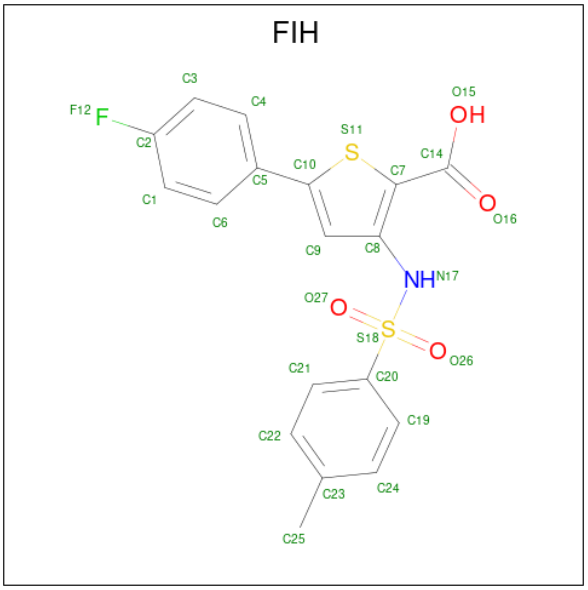
There are 3 unique types of molecules in this entry. The entry contains 10043 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	560	4356	2748	767	810	31	0	0	0
1	B	559	4344	2740	766	807	31	0	0	0

- Molecule 2 is 5-(4-FLUOROPHENYL)-3-{[(4-METHYLPHENYL)SULFONYL]AMINO}THIOPHENE-2-CARBOXYLIC ACID (three-letter code: FIH) (formula: $C_{18}H_{14}FNO_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
2	A	1	26	18	1	1	4	2	0	0
2	B	1	26	18	1	1	4	2	0	0

- Molecule 3 is water.

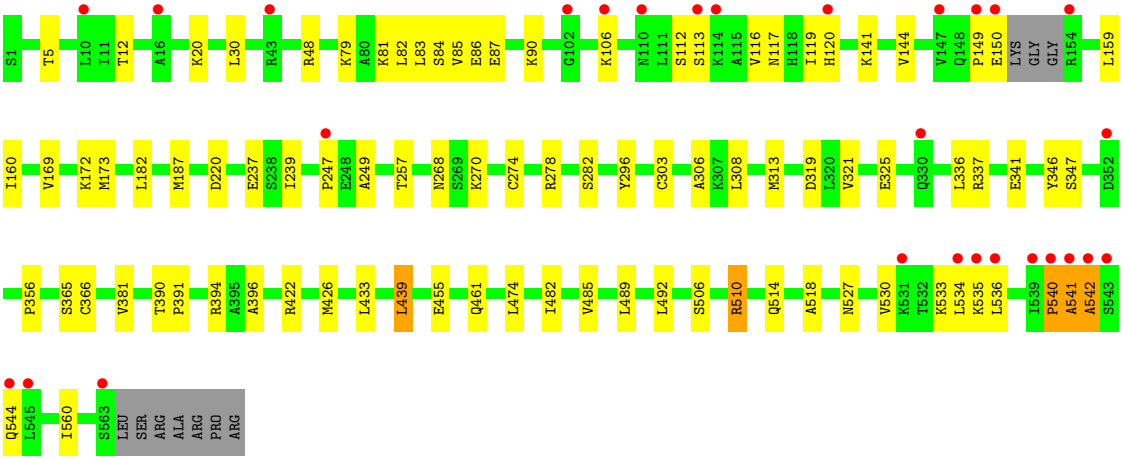
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	617	617	617	0	0
			Total	O		
3	B	674	674	674	0	0

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.

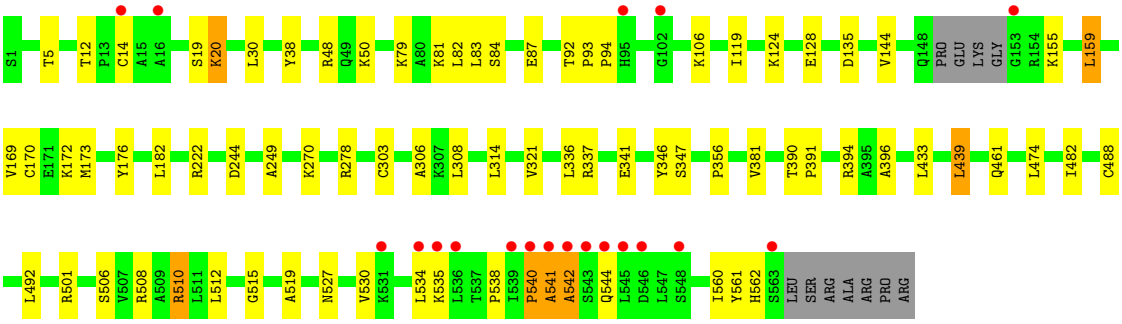
- Molecule 1: polyprotein

Chain A:



- Molecule 1: polyprotein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.75Å 106.13Å 127.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.11 – 1.80 33.11 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (33.11-1.80) 89.7 (33.11-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 1.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.199 , 0.232 0.192 , 0.227	Depositor DCC
R_{free} test set	4795 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10043	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.08 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.8047e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: FIH

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	0.29	0/4451	0.56	0/6041
1	B	0.29	0/4438	0.57	0/6022
All	All	0.29	0/8889	0.57	0/12063

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4356	0	4370	74	0
1	B	4344	0	4360	65	0
2	A	26	0	13	1	0
2	B	26	0	13	1	0
3	A	617	0	0	9	0
3	B	674	0	0	9	0
All	All	10043	0	8756	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 8.

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)
1:A:321:VAL:HG21	1:A:365:SER:HB3	1.38	1.02
1:B:170:CYS:HA	1:B:173:MET:HE3	1.41	1.00
1:B:5:THR:HG23	1:B:278:ARG:HH12	1.29	0.95
1:A:5:THR:HG23	1:A:278:ARG:HH12	1.37	0.89
1:A:321:VAL:CG2	1:A:365:SER:HB3	2.02	0.88
1:A:12:THR:HG21	1:A:270:LYS:HD3	1.57	0.86
1:A:79:LYS:HE2	1:A:81:LYS:HE2	1.59	0.84
1:B:81:LYS:HA	1:B:81:LYS:HE2	1.59	0.82
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.66	0.78
1:A:541:ALA:HB1	1:A:544:GLN:HE21	1.46	0.78
1:B:12:THR:HG21	1:B:270:LYS:HD3	1.64	0.78
1:A:535:LYS:HG3	1:A:536:LEU:H	1.48	0.77
1:B:381:VAL:HG11	1:B:474:LEU:CD2	2.16	0.76
1:A:337:ARG:O	1:A:341:GLU:HG3	1.88	0.74
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.20	0.72
1:A:381:VAL:HG11	1:A:474:LEU:HD22	1.72	0.70
1:B:381:VAL:HG11	1:B:474:LEU:HD22	1.74	0.70
1:A:510:ARG:HH11	1:A:510:ARG:HG2	1.57	0.68
1:A:321:VAL:HG21	1:A:365:SER:CB	2.21	0.66
1:B:527:ASN:HD21	1:B:534:LEU:H	1.42	0.65
1:A:239:ILE:HG12	3:A:2523:HOH:O	1.96	0.65
1:A:83:LEU:HB2	1:A:173:MET:HA	1.78	0.64
1:A:81:LYS:HD3	3:A:2041:HOH:O	1.98	0.64
1:B:541:ALA:O	1:B:544:GLN:HG2	1.98	0.64
1:B:5:THR:HG21	1:B:278:ARG:HH22	1.63	0.64
1:A:149:PRO:O	1:A:150:GLU:HG3	1.99	0.61
1:B:336:LEU:HD12	1:B:356:PRO:HD3	1.82	0.61
1:B:508:ARG:NH1	1:B:512:LEU:HD11	2.15	0.61
1:A:541:ALA:O	1:A:544:GLN:HG2	2.01	0.61
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.83	0.61
1:B:222:ARG:HD3	3:B:3633:HOH:O	2.02	0.60
1:A:422:ARG:HA	1:A:426:MET:HE2	1.84	0.60
1:B:5:THR:HG22	3:B:3296:HOH:O	2.02	0.59
1:B:506:SER:O	1:B:510:ARG:HD3	2.02	0.59
1:B:510:ARG:HG2	1:B:510:ARG:HH11	1.66	0.59
1:A:455:GLU:HB3	3:A:2107:HOH:O	2.03	0.58
1:B:337:ARG:O	1:B:341:GLU:HG3	2.02	0.58
1:B:381:VAL:HG11	1:B:474:LEU:HD21	1.85	0.58
1:A:510:ARG:HG2	1:A:510:ARG:NH1	2.19	0.58
1:B:461:GLN:HG3	3:B:3190:HOH:O	2.02	0.58
1:A:527:ASN:HD21	1:A:534:LEU:H	1.51	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:ARG:O	1:A:426:MET:HE2	2.06	0.56
1:A:535:LYS:HG3	1:A:536:LEU:N	2.17	0.56
1:A:5:THR:HG21	1:A:278:ARG:HH22	1.70	0.56
1:B:50:LYS:HB3	1:B:50:LYS:NZ	2.21	0.55
1:A:461:GLN:HB3	1:A:542:ALA:HA	1.88	0.55
1:B:106:LYS:HB2	3:B:3552:HOH:O	2.07	0.55
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.90	0.54
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.88	0.54
1:A:506:SER:O	1:A:510:ARG:HD3	2.08	0.54
1:A:84:SER:OG	1:A:87:GLU:HG3	2.08	0.53
1:B:5:THR:HG23	1:B:278:ARG:NH1	2.10	0.53
1:B:19:SER:H	1:B:20:LYS:NZ	2.07	0.53
1:A:514:GLN:HB2	1:A:518:ALA:HB3	1.90	0.53
1:B:182:LEU:C	1:B:182:LEU:HD23	2.29	0.53
1:A:182:LEU:HD23	1:A:182:LEU:C	2.29	0.53
1:A:325:GLU:HG3	3:A:2225:HOH:O	2.09	0.52
1:B:510:ARG:HG2	3:B:3257:HOH:O	2.09	0.52
1:B:48:ARG:HG2	1:B:159:LEU:HD13	1.90	0.52
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.40	0.52
1:A:381:VAL:HG11	1:A:474:LEU:HD21	1.93	0.51
1:A:83:LEU:HD13	3:A:2050:HOH:O	2.09	0.51
1:B:461:GLN:HE21	1:B:541:ALA:C	2.12	0.51
1:B:433:LEU:HB3	1:B:439:LEU:HD12	1.92	0.51
1:A:510:ARG:O	1:A:514:GLN:HG2	2.11	0.51
1:B:501:ARG:HD2	3:B:3303:HOH:O	2.10	0.51
1:B:510:ARG:HG2	1:B:510:ARG:NH1	2.26	0.50
1:A:346:TYR:O	1:A:347:SER:HB3	2.11	0.50
1:B:508:ARG:HE	1:B:530:VAL:HG11	1.77	0.50
1:B:461:GLN:HE21	1:B:542:ALA:N	2.10	0.49
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.93	0.49
1:A:527:ASN:O	1:A:530:VAL:HG22	2.12	0.49
1:B:482:ILE:HG23	2:B:3001:FIH:H4	1.94	0.49
1:A:535:LYS:CG	1:A:536:LEU:H	2.23	0.49
1:A:81:LYS:HG2	3:A:2470:HOH:O	2.12	0.48
1:A:306:ALA:HB3	1:A:308:LEU:HD13	1.95	0.48
1:A:485:VAL:O	1:A:489:LEU:HG	2.13	0.48
1:A:187:MET:HE1	1:A:296:TYR:HB2	1.96	0.48
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.95	0.48
1:A:433:LEU:HB3	1:A:439:LEU:HD12	1.96	0.47
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.96	0.47
1:A:390:THR:HB	1:A:391:PRO:HD3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:TYR:OH	1:B:155:LYS:HG2	2.14	0.47
1:A:482:ILE:HG23	2:A:2001:FIH:H4	1.96	0.47
1:B:124:LYS:O	1:B:128:GLU:HG3	2.15	0.47
1:A:5:THR:HG23	1:A:278:ARG:NH1	2.18	0.47
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.95	0.47
1:B:83:LEU:HB2	1:B:173:MET:HA	1.97	0.47
1:A:113:SER:O	1:A:117:ASN:ND2	2.48	0.47
1:B:81:LYS:HE3	3:B:3162:HOH:O	2.15	0.46
1:A:541:ALA:HB1	1:A:544:GLN:NE2	2.22	0.46
1:B:84:SER:OG	1:B:87:GLU:HG3	2.15	0.46
1:A:220:ASP:HB2	3:A:2468:HOH:O	2.15	0.46
1:A:141:LYS:HE2	1:A:160:ILE:HB	1.98	0.46
1:A:422:ARG:HA	1:A:426:MET:CE	2.46	0.45
1:A:86:GLU:O	1:A:90:LYS:HG3	2.16	0.45
1:B:346:TYR:O	1:B:347:SER:HB3	2.16	0.45
1:A:187:MET:HE3	1:A:296:TYR:CD2	2.51	0.45
1:B:510:ARG:NH1	3:B:3257:HOH:O	2.50	0.45
1:B:135:ASP:HB2	3:B:3479:HOH:O	2.17	0.45
1:A:149:PRO:HG2	1:A:150:GLU:H	1.82	0.45
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.99	0.44
1:A:172:LYS:HE3	1:A:560:ILE:HD13	2.00	0.44
1:B:5:THR:CG2	1:B:278:ARG:HH22	2.29	0.44
1:B:19:SER:H	1:B:20:LYS:HZ3	1.65	0.43
1:B:508:ARG:HH22	1:B:534:LEU:HD21	1.82	0.43
1:A:313:MET:HE2	3:A:2273:HOH:O	2.17	0.43
1:A:381:VAL:O	1:A:381:VAL:HG13	2.19	0.43
1:B:461:GLN:HE21	1:B:542:ALA:HA	1.83	0.43
1:B:488:CYS:O	1:B:492:LEU:HD13	2.18	0.43
1:A:313:MET:HB2	1:A:313:MET:HE3	1.86	0.43
1:A:422:ARG:CA	1:A:426:MET:HE2	2.47	0.43
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.89	0.43
1:A:237:GLU:HG3	1:A:257:THR:OG1	2.19	0.42
1:A:533:LYS:N	1:A:533:LYS:HD2	2.34	0.42
1:B:492:LEU:HD12	1:B:492:LEU:N	2.34	0.42
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.58	0.42
1:A:319:ASP:CG	1:A:366:CYS:H	2.22	0.42
1:B:79:LYS:HA	1:B:244:ASP:HB3	2.02	0.42
1:A:540:PRO:O	1:A:542:ALA:N	2.53	0.42
1:B:390:THR:HB	1:B:391:PRO:HD3	2.01	0.42
1:B:540:PRO:O	1:B:542:ALA:N	2.52	0.42
1:B:336:LEU:HD23	1:B:336:LEU:HA	1.89	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:LEU:HD12	1:A:492:LEU:N	2.35	0.42
1:A:85:VAL:HG21	1:A:120:HIS:CE1	2.55	0.41
1:B:176:TYR:OH	1:B:562:HIS:HE1	2.02	0.41
1:B:535:LYS:O	1:B:535:LYS:HG3	2.20	0.41
1:A:321:VAL:CG2	1:A:365:SER:CB	2.86	0.41
1:B:82:LEU:HD21	1:B:249:ALA:HB2	2.02	0.41
1:A:160:ILE:HA	1:A:282:SER:OG	2.20	0.41
1:A:82:LEU:HD13	1:A:249:ALA:HB2	2.03	0.41
1:A:247:PRO:HD2	3:A:2373:HOH:O	2.21	0.41
1:B:30:LEU:HD23	1:B:396:ALA:HA	2.02	0.41
1:A:30:LEU:HD23	1:A:396:ALA:HA	2.03	0.41
1:B:381:VAL:HG13	1:B:381:VAL:O	2.21	0.41
1:A:112:SER:O	1:A:116:VAL:HG23	2.20	0.40
1:B:306:ALA:HB3	1:B:308:LEU:HD13	2.02	0.40
1:B:527:ASN:ND2	1:B:534:LEU:H	2.16	0.40
1:B:92:THR:HA	1:B:93:PRO:HD3	1.97	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	556/570 (98%)	543 (98%)	10 (2%)	3 (0%)	29 15
1	B	555/570 (97%)	541 (98%)	10 (2%)	4 (1%)	22 10
All	All	1111/1140 (98%)	1084 (98%)	20 (2%)	7 (1%)	25 12

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	PRO
1	B	540	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	541	ALA
1	B	541	ALA
1	A	542	ALA
1	B	542	ALA
1	B	538	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	478/485 (99%)	473 (99%)	5 (1%)	76	71
1	B	476/485 (98%)	470 (99%)	6 (1%)	69	62
All	All	954/970 (98%)	943 (99%)	11 (1%)	71	65

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	106	LYS
1	A	303	CYS
1	A	439	LEU
1	A	510	ARG
1	B	14	CYS
1	B	20	LYS
1	B	159	LEU
1	B	303	CYS
1	B	439	LEU
1	B	510	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	117	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	148	GLN
1	A	273	ASN
1	A	309	GLN
1	A	374	HIS
1	A	527	ASN
1	A	544	GLN
1	B	49	GLN
1	B	120	HIS
1	B	184	GLN
1	B	273	ASN
1	B	330	GLN
1	B	374	HIS
1	B	436	GLN
1	B	446	GLN
1	B	461	GLN
1	B	483	ASN
1	B	514	GLN
1	B	527	ASN
1	B	544	GLN
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 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	$\#\|Z\| > 2$
2	FIH	B	3001	-	24,28,28	2.60	14 (58%)	27,41,41	1.94	3 (11%)
2	FIH	A	2001	-	24,28,28	2.54	14 (58%)	27,41,41	1.96	3 (11%)

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	FIH	B	3001	-	-	1/9/19/19	0/3/3/3
2	FIH	A	2001	-	-	1/9/19/19	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	FIH	C9-C8	6.32	1.45	1.39
2	A	2001	FIH	C9-C8	5.75	1.44	1.39
2	A	2001	FIH	S18-N17	4.48	1.70	1.63
2	B	3001	FIH	S18-N17	4.45	1.70	1.63
2	A	2001	FIH	C1-C2	3.09	1.43	1.37
2	A	2001	FIH	C6-C1	3.03	1.43	1.36
2	B	3001	FIH	C6-C1	3.01	1.43	1.36
2	B	3001	FIH	C1-C2	3.01	1.43	1.37
2	B	3001	FIH	C19-C20	2.96	1.43	1.38
2	A	2001	FIH	C20-S18	2.94	1.81	1.76
2	A	2001	FIH	C19-C20	2.90	1.43	1.38
2	B	3001	FIH	C21-C20	2.85	1.43	1.38
2	B	3001	FIH	C20-S18	2.79	1.80	1.76
2	A	2001	FIH	C21-C20	2.74	1.43	1.38
2	B	3001	FIH	C3-C2	2.73	1.42	1.37
2	B	3001	FIH	C4-C3	2.68	1.42	1.36
2	B	3001	FIH	C8-N17	2.66	1.47	1.42
2	A	2001	FIH	C3-C2	2.62	1.42	1.37
2	A	2001	FIH	C8-N17	2.62	1.47	1.42
2	B	3001	FIH	O26-S18	2.56	1.46	1.43
2	A	2001	FIH	O27-S18	2.55	1.46	1.43
2	A	2001	FIH	C4-C3	2.51	1.42	1.36
2	B	3001	FIH	C22-C21	2.46	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	FIH	C22-C21	2.40	1.42	1.38
2	B	3001	FIH	O27-S18	2.40	1.46	1.43
2	A	2001	FIH	C24-C19	2.38	1.42	1.38
2	A	2001	FIH	O26-S18	2.34	1.46	1.43
2	B	3001	FIH	C24-C19	2.27	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2001	FIH	O27-S18-O26	-6.22	111.96	119.52
2	B	3001	FIH	O27-S18-O26	-6.22	111.97	119.52
2	A	2001	FIH	C20-S18-N17	6.18	114.55	106.88
2	B	3001	FIH	C20-S18-N17	5.91	114.20	106.88
2	B	3001	FIH	C3-C2-C1	-3.10	118.73	122.80
2	A	2001	FIH	C3-C2-C1	-3.03	118.83	122.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	3001	FIH	C8-N17-S18-O26
2	A	2001	FIH	C8-N17-S18-O26

There are no ring outliers.

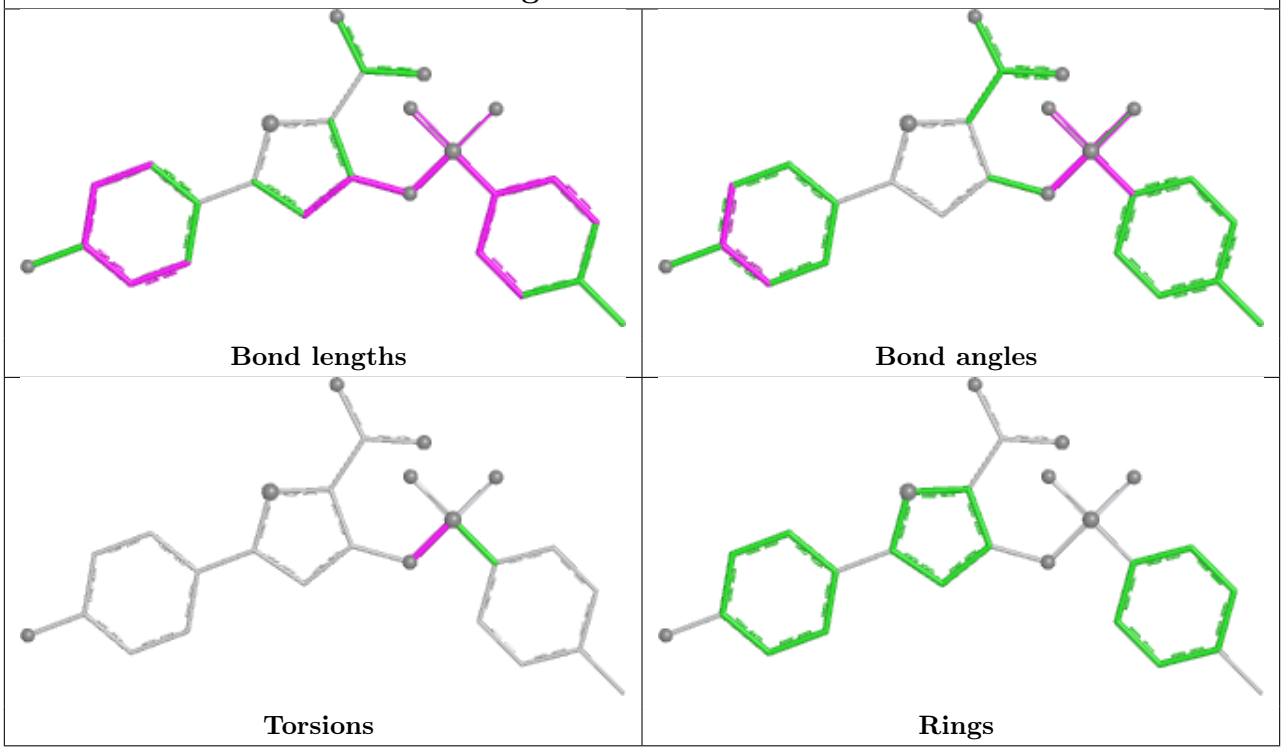
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3001	FIH	1	0
2	A	2001	FIH	1	0

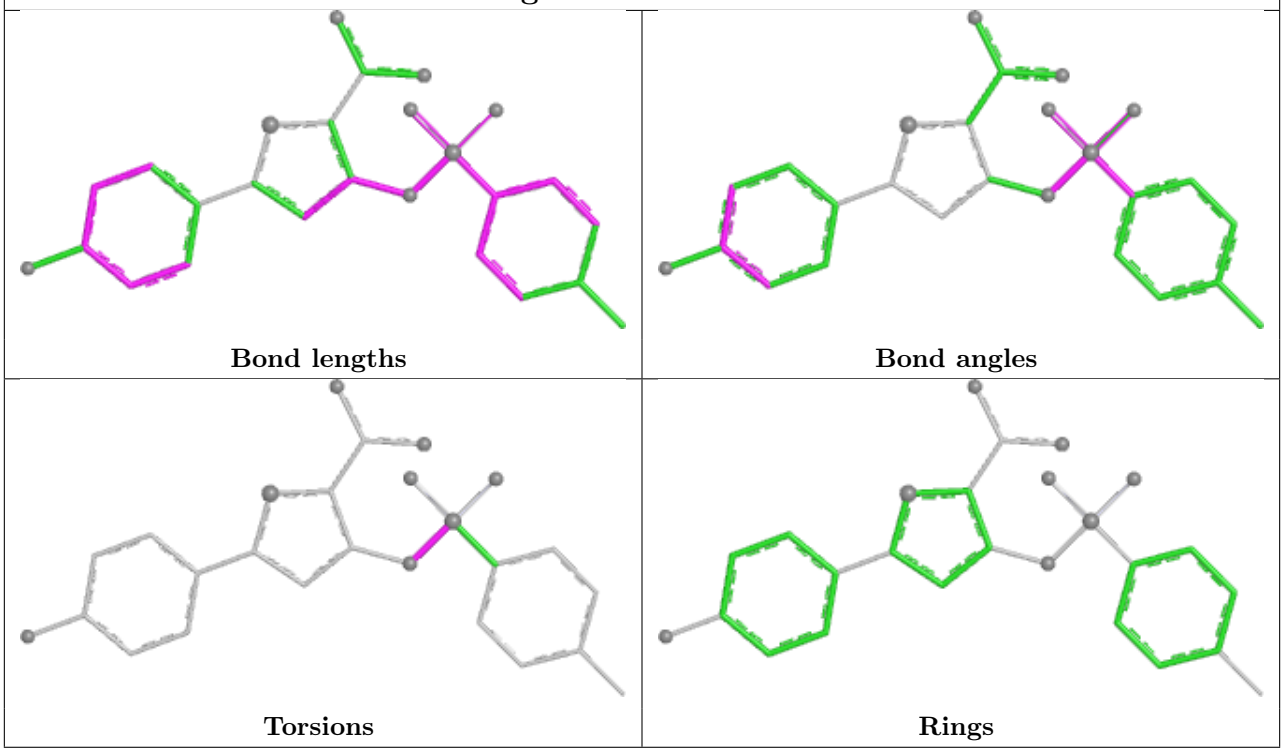
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 FIH B 3001



Ligand FIH A 2001



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	560/570 (98%)	0.12	28 (5%)	28	23	10, 18, 40, 66	0
1	B	559/570 (98%)	-0.03	19 (3%)	45	39	9, 17, 33, 66	0
All	All	1119/1140 (98%)	0.05	47 (4%)	36	30	9, 18, 38, 66	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	542	ALA	15.2
1	A	541	ALA	10.6
1	B	541	ALA	9.5
1	B	542	ALA	9.4
1	B	545	LEU	7.4
1	A	543	SER	6.4
1	A	563	SER	6.0
1	B	563	SER	6.0
1	B	543	SER	5.9
1	B	544	GLN	5.8
1	A	536	LEU	5.3
1	B	536	LEU	5.3
1	A	535	LYS	5.2
1	B	539	ILE	5.0
1	B	534	LEU	5.0
1	A	540	PRO	4.9
1	B	548	SER	4.5
1	A	150	GLU	4.1
1	B	531	LYS	4.1
1	A	539	ILE	4.1
1	B	535	LYS	4.0
1	A	149	PRO	3.9
1	B	540	PRO	3.7
1	A	545	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	95	HIS	3.1
1	A	330	GLN	2.9
1	B	546	ASP	2.8
1	A	110	ASN	2.7
1	B	153	GLY	2.7
1	A	544	GLN	2.7
1	A	531	LYS	2.6
1	A	352	ASP	2.6
1	B	14	CYS	2.6
1	A	16	ALA	2.5
1	B	16	ALA	2.5
1	A	43	ARG	2.5
1	A	247	PRO	2.3
1	B	102	GLY	2.3
1	A	106	LYS	2.3
1	A	102	GLY	2.3
1	A	534	LEU	2.2
1	A	120	HIS	2.1
1	A	154	ARG	2.1
1	A	147	VAL	2.1
1	A	114	LYS	2.1
1	A	113	SER	2.1
1	A	10	LEU	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, 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.

Continued on next page...

Continued from previous page...

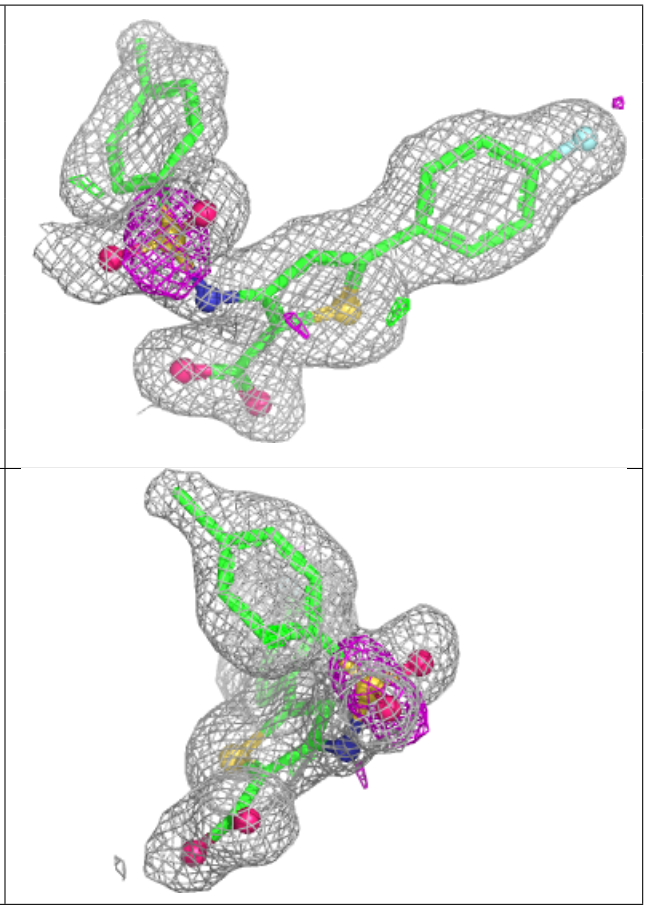
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

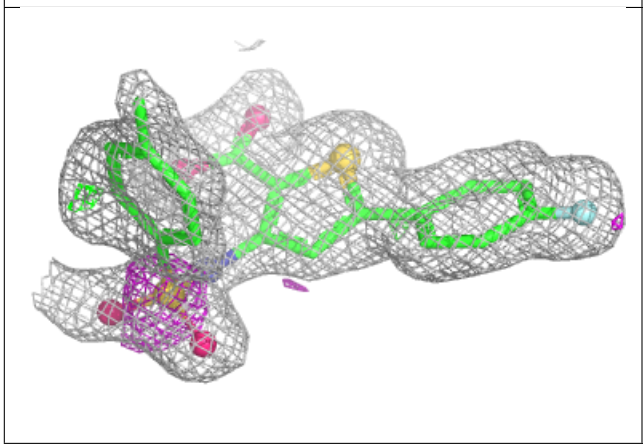
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FIH	A	2001	26/26	0.89	0.13	18,23,29,32	0
2	FIH	B	3001	26/26	0.92	0.14	17,25,29,30	0

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 FIH A 2001:

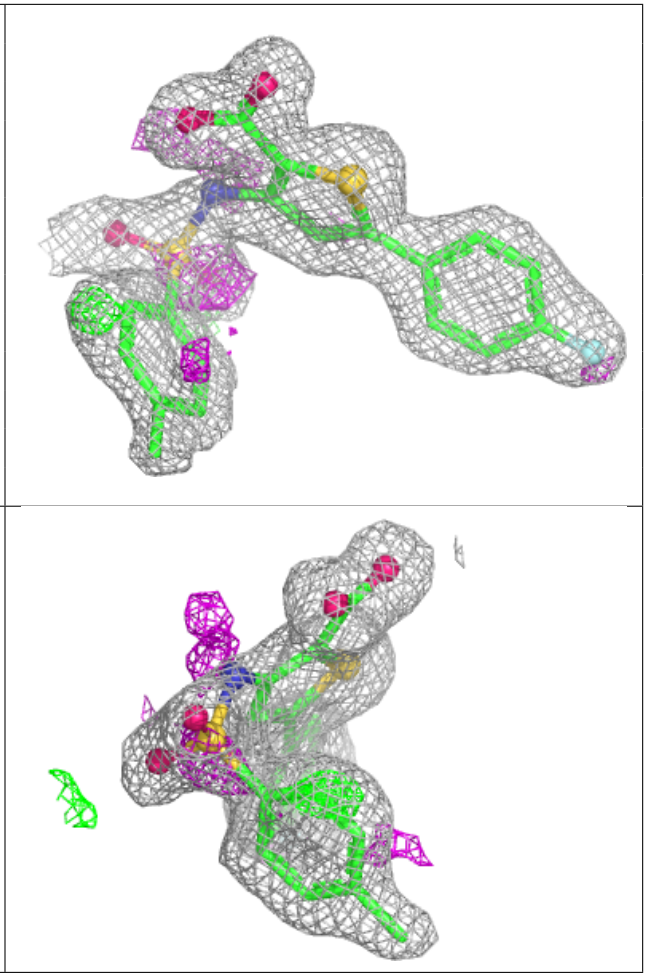
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)





Electron density around FIH B 3001:

$2mF_o$-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.