



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:14 PM UTC

PDB ID : 1HWL / pdb_00001hwl
Title : COMPLEX OF THE CATALYTIC PORTION OF HUMAN HMG-COA REDUCTASE WITH ROSUVASTATIN (FORMALLY KNOWN AS ZD4522)
Authors : Istvan, E.S.; Deisenhofer, J.
Deposited on : 2001-01-09
Resolution : 2.10 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

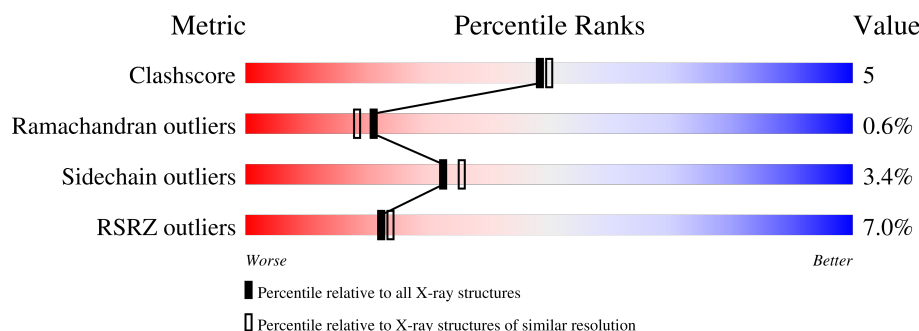
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	467	5% 75% 12% • 13%
1	B	467	6% 73% 11% • 15%
1	C	467	7% 74% 10% • 15%
1	D	467	6% 70% 11% • 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12159 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.

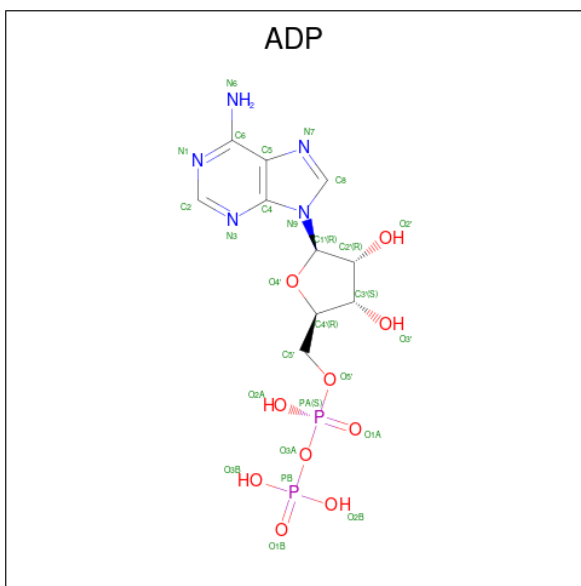
- Molecule 1 is a protein called HMG-COA REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	407	Total	C	N	O	S	0	0	0
			3028	1886	531	581	30			
1	B	398	Total	C	N	O	S	0	0	0
			2952	1838	518	567	29			
1	C	398	Total	C	N	O	S	0	0	0
			2952	1838	518	567	29			
1	D	382	Total	C	N	O	S	0	0	0
			2832	1762	497	544	29			

There are 20 discrepancies between the modelled and reference sequences:

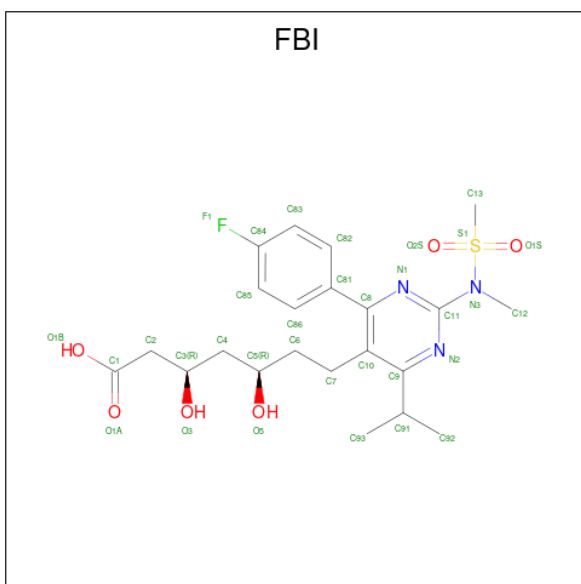
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	insertion	UNP P04035
A	423	ALA	-	insertion	UNP P04035
A	424	MET	-	insertion	UNP P04035
A	425	ALA	-	insertion	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	422	GLY	-	insertion	UNP P04035
B	423	ALA	-	insertion	UNP P04035
B	424	MET	-	insertion	UNP P04035
B	425	ALA	-	insertion	UNP P04035
B	485	ILE	MET	engineered mutation	UNP P04035
C	422	GLY	-	insertion	UNP P04035
C	423	ALA	-	insertion	UNP P04035
C	424	MET	-	insertion	UNP P04035
C	425	ALA	-	insertion	UNP P04035
C	485	ILE	MET	engineered mutation	UNP P04035
D	422	GLY	-	insertion	UNP P04035
D	423	ALA	-	insertion	UNP P04035
D	424	MET	-	insertion	UNP P04035
D	425	ALA	-	insertion	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is 7-[4-(4-FLUORO-PHENYL)-6-ISOPROPYL-2-(METHANESULFONYL-METHYL-AMINO)-PYRIMIDIN-5-YL]-3,5-DIHYDROXY-HEPTANOIC ACID (CCD ID: FBI) (formula: $C_{22}H_{30}FN_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	
			33	22	1	3	6	1	
3	B	1	Total	C	F	N	O	S	
			33	22	1	3	6	1	
3	C	1	Total	C	F	N	O	S	
			33	22	1	3	6	1	
3	D	1	Total	C	F	N	O	S	
			33	22	1	3	6	1	

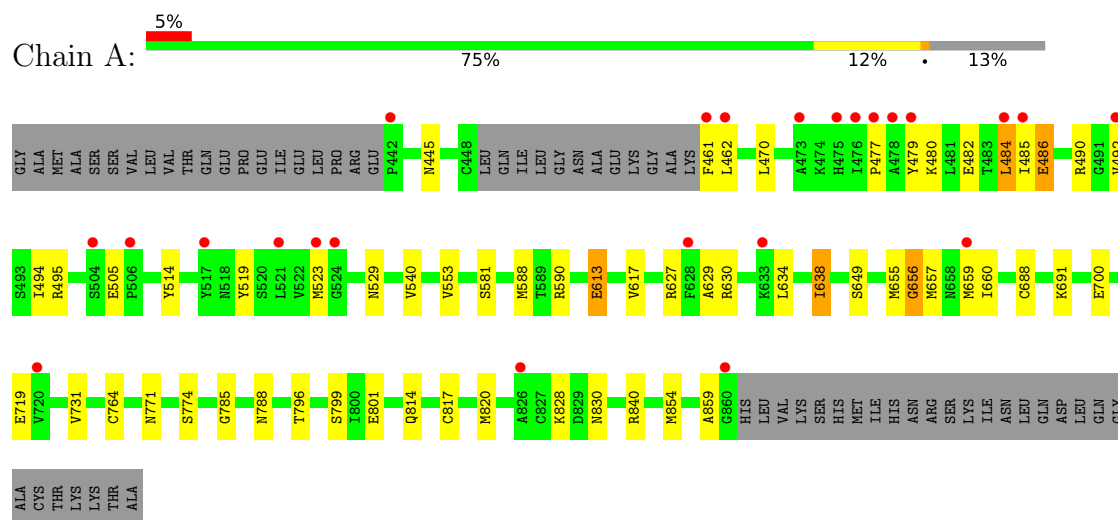
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O		
			49	49	0	0
4	B	41	Total	O		
			41	41	0	0
4	C	44	Total	O		
			44	44	0	0
4	D	48	Total	O		
			48	48	0	0

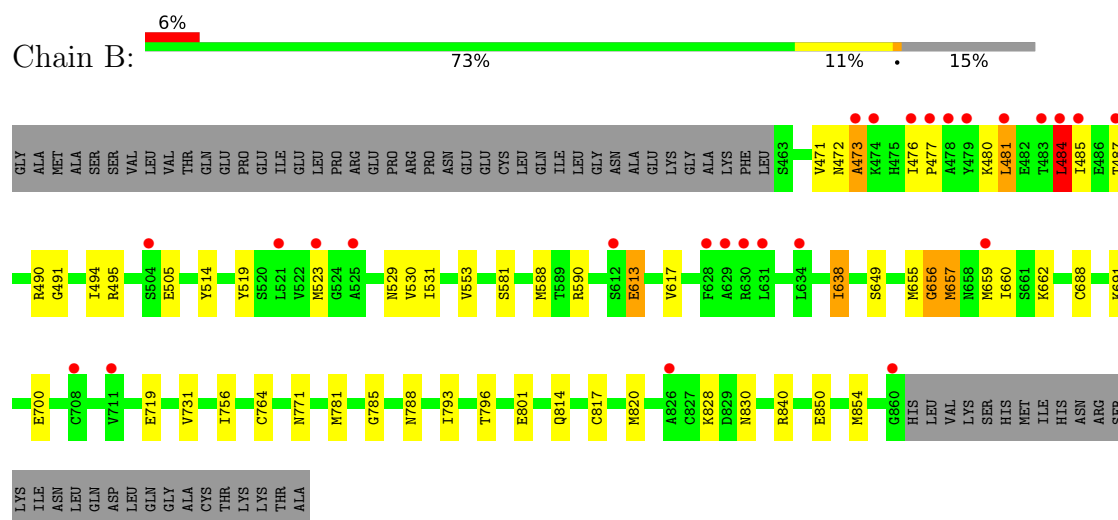
3 Residue-property plots [i](#)

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.

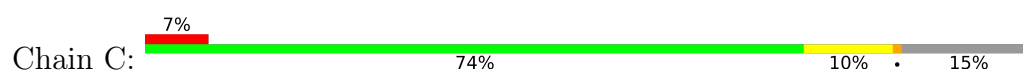
• Molecule 1: HMG-COA REDUCTASE

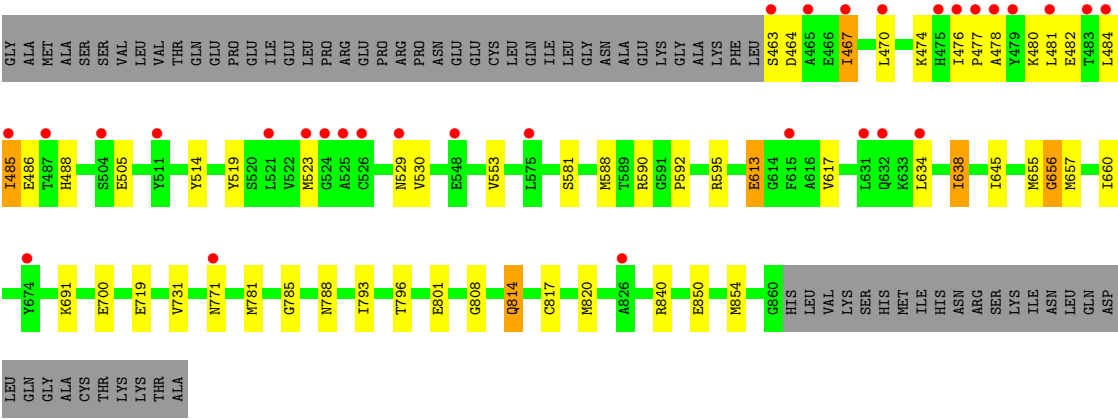


• Molecule 1: HMG-COA REDUCTASE

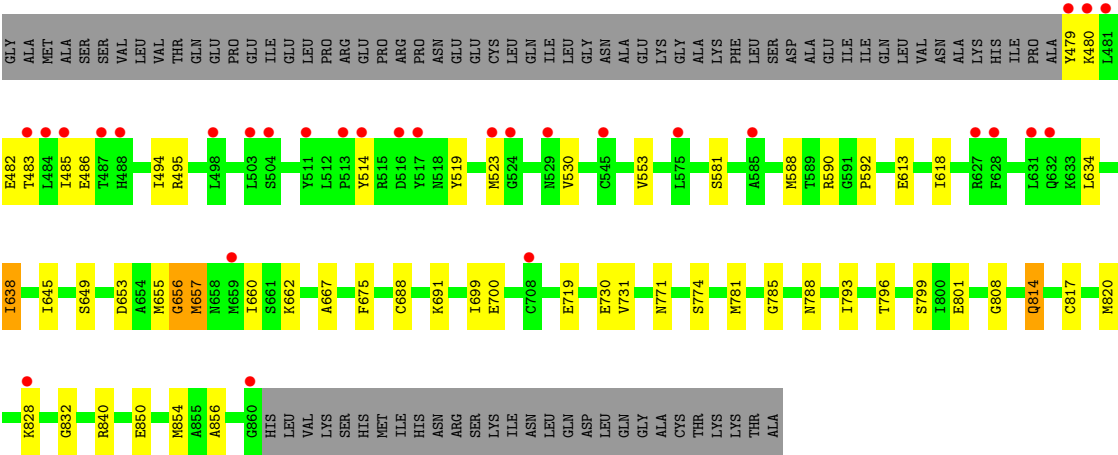


• Molecule 1: HMG-COA REDUCTASE





● Molecule 1: HMG-COA REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.43Å 172.51Å 79.99Å 90.00° 117.36° 90.00°	Depositor
Resolution (Å)	43.29 – 2.10 43.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.6 (43.29-2.10) 91.9 (43.29-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 2.10Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.219 , 0.239 0.216 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12159	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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: ADP, FBI

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	0.62	1/3072 (0.0%)	1.01	12/4153 (0.3%)
1	B	0.62	1/2994 (0.0%)	1.02	13/4049 (0.3%)
1	C	0.60	0/2994	0.99	9/4049 (0.2%)
1	D	0.66	0/2872	1.01	12/3882 (0.3%)
All	All	0.63	2/11932 (0.0%)	1.01	46/16133 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	659	MET	SD-CE	5.94	1.94	1.79
1	A	659	MET	SD-CE	5.35	1.93	1.79

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	553	VAL	N-CA-C	10.50	118.36	107.76
1	A	553	VAL	N-CA-C	10.41	118.27	107.76
1	C	553	VAL	N-CA-C	10.24	118.11	107.76
1	B	553	VAL	N-CA-C	9.90	117.76	107.76
1	D	656	GLY	N-CA-C	7.99	126.34	115.32
1	B	656	GLY	N-CA-C	7.83	126.13	115.32
1	A	655	MET	N-CA-C	-7.59	103.00	111.28
1	B	785	GLY	CA-C-N	7.32	126.85	119.24
1	B	785	GLY	C-N-CA	7.32	126.85	119.24
1	A	656	GLY	N-CA-C	7.17	125.21	115.32
1	B	655	MET	N-CA-C	-7.05	103.60	111.28
1	C	656	GLY	N-CA-C	6.99	125.12	115.27
1	D	655	MET	N-CA-C	-6.61	104.07	111.28
1	D	719	GLU	N-CA-C	6.43	119.60	111.69
1	B	473	ALA	N-CA-C	-6.38	103.94	112.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	GLU	N-CA-C	6.19	119.30	111.69
1	D	785	GLY	CA-C-N	6.17	125.39	118.97
1	D	785	GLY	C-N-CA	6.17	125.39	118.97
1	C	655	MET	N-CA-C	-6.15	104.58	111.28
1	A	859	ALA	N-CA-C	6.11	117.61	111.07
1	A	785	GLY	CA-C-N	6.08	125.29	118.97
1	A	785	GLY	C-N-CA	6.08	125.29	118.97
1	B	719	GLU	N-CA-C	6.03	119.11	111.69
1	C	785	GLY	CA-C-N	6.03	125.24	118.97
1	C	785	GLY	C-N-CA	6.03	125.24	118.97
1	C	719	GLU	N-CA-C	5.88	118.92	111.69
1	D	691	LYS	N-CA-C	5.86	120.01	112.86
1	A	691	LYS	N-CA-C	5.76	119.89	112.86
1	B	481	LEU	N-CA-C	5.74	117.34	111.14
1	C	691	LYS	N-CA-C	5.66	119.76	112.86
1	D	530	VAL	N-CA-C	5.61	116.31	109.30
1	B	691	LYS	N-CA-C	5.60	119.69	112.86
1	A	445	ASN	N-CA-C	5.56	118.06	111.33
1	D	483	THR	N-CA-C	-5.49	106.58	113.28
1	D	675	PHE	CA-C-N	5.45	125.28	119.28
1	D	675	PHE	C-N-CA	5.45	125.28	119.28
1	B	530	VAL	N-CA-C	5.38	116.03	109.30
1	C	530	VAL	N-CA-C	5.31	115.94	109.30
1	D	699	ILE	N-CA-C	5.29	116.77	111.00
1	A	830	ASN	CA-C-N	5.28	125.58	119.93
1	A	830	ASN	C-N-CA	5.28	125.58	119.93
1	B	764	CYS	N-CA-C	5.24	118.69	112.72
1	C	467	ILE	N-CA-C	-5.22	105.44	110.72
1	A	764	CYS	N-CA-C	5.11	118.55	112.72
1	B	830	ASN	CA-C-N	5.10	126.21	119.84
1	B	830	ASN	C-N-CA	5.10	126.21	119.84

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	3028	0	3059	33	0
1	B	2952	0	2989	37	0
1	C	2952	0	2989	33	0
1	D	2832	0	2865	32	0
2	A	54	0	24	5	0
2	C	27	0	12	2	0
3	A	33	0	29	2	0
3	B	33	0	29	2	0
3	C	33	0	29	2	0
3	D	33	0	29	2	0
4	A	49	0	0	1	0
4	B	41	0	0	1	0
4	C	44	0	0	1	0
4	D	48	0	0	1	0
All	All	12159	0	12054	132	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 5.

All (132) 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:828:LYS:HD2	1:A:828:LYS:H	1.40	0.85
1:B:828:LYS:HD2	1:B:828:LYS:H	1.41	0.85
1:C:485:ILE:HG22	1:C:486:GLU:H	1.44	0.82
1:D:523:MET:HE1	4:D:1055:HOH:O	1.87	0.75
1:A:817:CYS:HA	1:A:820:MET:HE3	1.69	0.75
3:D:3:FBI:H61	3:D:3:FBI:H91	1.69	0.74
1:D:523:MET:HE3	1:D:523:MET:HA	1.68	0.74
1:C:817:CYS:HA	1:C:820:MET:HE3	1.69	0.74
1:D:817:CYS:HA	1:D:820:MET:HE3	1.69	0.73
1:B:817:CYS:HA	1:B:820:MET:HE3	1.69	0.73
1:A:523:MET:HE3	1:A:523:MET:HA	1.73	0.71
1:C:523:MET:HA	1:C:523:MET:HE3	1.72	0.71
3:B:1:FBI:H61	3:B:1:FBI:H91	1.74	0.70
1:A:629:ALA:O	1:A:630:ARG:HD2	1.92	0.69
2:A:102:ADP:H2	1:B:529:ASN:HD22	1.39	0.68
1:B:523:MET:HA	1:B:523:MET:HE3	1.76	0.68
1:B:828:LYS:H	1:B:828:LYS:CD	2.06	0.68
1:C:485:ILE:HG22	1:C:486:GLU:N	2.07	0.68
1:A:828:LYS:H	1:A:828:LYS:CD	2.07	0.68
2:A:102:ADP:H2	1:B:529:ASN:ND2	1.95	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ILE:HD13	1:A:494:ILE:HD12	1.80	0.63
1:D:588:MET:HE1	1:D:801:GLU:HG2	1.81	0.62
1:D:480:LYS:H	1:D:480:LYS:HD3	1.65	0.62
3:A:2:FBI:H61	3:A:2:FBI:H91	1.81	0.62
1:C:519:TYR:O	1:C:523:MET:HG2	2.00	0.62
1:A:523:MET:HE1	4:A:1092:HOH:O	2.01	0.60
1:D:519:TYR:O	1:D:523:MET:HG2	2.02	0.60
1:B:519:TYR:O	1:B:523:MET:HG2	2.02	0.60
1:A:588:MET:HE1	1:A:801:GLU:HG2	1.84	0.59
1:A:519:TYR:O	1:A:523:MET:HG2	2.03	0.59
1:D:485:ILE:HG22	1:D:486:GLU:N	2.18	0.58
1:B:487:THR:HG23	1:B:490:ARG:HB3	1.85	0.58
1:C:529:ASN:HD22	2:C:103:ADP:H2	1.52	0.58
3:A:2:FBI:H72	3:A:2:FBI:C86	2.34	0.57
1:B:781:MET:HE2	1:B:793:ILE:HD12	1.85	0.57
1:D:781:MET:HE2	1:D:793:ILE:HD12	1.87	0.56
1:C:485:ILE:CG2	1:C:486:GLU:H	2.17	0.56
1:D:656:GLY:O	1:D:660:ILE:HG12	2.06	0.56
1:C:588:MET:HE1	1:C:801:GLU:HG2	1.88	0.55
1:D:581:SER:OG	1:D:840:ARG:HD2	2.07	0.55
1:C:529:ASN:ND2	2:C:103:ADP:H2	2.05	0.54
1:C:781:MET:HE2	1:C:793:ILE:HD12	1.90	0.54
1:A:529:ASN:ND2	2:A:101:ADP:H2	2.05	0.54
1:C:581:SER:OG	1:C:840:ARG:HD2	2.08	0.54
1:C:656:GLY:O	1:C:660:ILE:HG12	2.07	0.54
1:A:581:SER:OG	1:A:840:ARG:HD2	2.08	0.54
1:A:771:ASN:OD1	1:B:771:ASN:ND2	2.41	0.54
1:B:476:ILE:HD13	1:B:484:LEU:HD23	1.90	0.53
3:D:3:FBI:H72	3:D:3:FBI:C86	2.38	0.53
1:B:588:MET:HE1	1:B:801:GLU:HG2	1.90	0.53
2:A:102:ADP:C2	1:B:529:ASN:ND2	2.77	0.53
1:C:771:ASN:OD1	1:D:771:ASN:ND2	2.42	0.52
1:A:771:ASN:ND2	1:B:771:ASN:OD1	2.43	0.52
1:B:471:VAL:C	1:B:473:ALA:H	2.17	0.52
1:B:581:SER:OG	1:B:840:ARG:HD2	2.09	0.52
1:C:477:PRO:HD2	1:C:480:LYS:HD2	1.92	0.52
1:A:485:ILE:CD1	1:A:494:ILE:HD12	2.40	0.51
1:B:485:ILE:HG22	1:B:487:THR:H	1.74	0.51
1:A:479:TYR:HA	1:A:495:ARG:NH1	2.26	0.51
1:B:656:GLY:O	1:B:660:ILE:HG12	2.10	0.51
1:B:487:THR:HG23	1:B:490:ARG:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:ALA:C	1:A:630:ARG:HD2	2.37	0.50
1:C:771:ASN:ND2	1:D:771:ASN:OD1	2.44	0.49
1:B:796:THR:HG21	1:C:638:ILE:O	2.13	0.49
1:B:613:GLU:O	1:B:617:VAL:HG23	2.13	0.49
1:C:485:ILE:CG2	1:C:486:GLU:N	2.76	0.48
1:B:731:VAL:HG12	1:B:854:MET:HE1	1.96	0.48
1:D:479:TYR:HA	1:D:495:ARG:NH1	2.28	0.48
1:B:485:ILE:CD1	1:B:494:ILE:HD12	2.44	0.47
1:D:731:VAL:HG12	1:D:854:MET:CE	2.44	0.47
3:C:4:FBI:H123	1:D:856:ALA:HB1	1.96	0.47
1:A:731:VAL:HG12	1:A:854:MET:HE1	1.96	0.47
1:C:731:VAL:HG12	1:C:854:MET:CE	2.44	0.47
1:A:529:ASN:HD22	2:A:101:ADP:H2	1.61	0.47
1:A:613:GLU:O	1:A:617:VAL:HG23	2.15	0.47
3:B:1:FBI:H72	3:B:1:FBI:C86	2.45	0.47
1:B:523:MET:HE1	4:B:1108:HOH:O	2.14	0.47
1:C:463:SER:O	1:C:467:ILE:HG12	2.15	0.47
1:C:613:GLU:O	1:C:617:VAL:HG23	2.15	0.47
1:A:627:ARG:HG2	1:A:627:ARG:HH11	1.79	0.46
1:C:478:ALA:O	1:C:481:LEU:HG	2.16	0.46
1:C:523:MET:HE1	4:C:1087:HOH:O	2.15	0.46
1:D:731:VAL:HG12	1:D:854:MET:HE1	1.97	0.46
1:A:477:PRO:HD2	1:A:480:LYS:HD2	1.97	0.46
1:B:731:VAL:HG12	1:B:854:MET:CE	2.46	0.46
1:A:638:ILE:O	1:D:796:THR:HG21	2.15	0.45
1:C:482:GLU:HG2	1:C:523:MET:HE2	1.97	0.45
1:D:774:SER:HA	1:D:799:SER:O	2.17	0.45
1:A:731:VAL:HG12	1:A:854:MET:CE	2.46	0.45
1:B:657:MET:HA	1:B:657:MET:HE2	1.99	0.45
1:B:481:LEU:HD12	1:B:495:ARG:HB2	1.99	0.45
1:C:731:VAL:HG12	1:C:854:MET:HE1	1.98	0.45
1:D:590:ARG:HA	1:D:590:ARG:HD3	1.84	0.45
1:D:485:ILE:HG22	1:D:486:GLU:H	1.83	0.44
1:D:649:SER:HB3	1:D:660:ILE:HD12	1.98	0.44
1:A:656:GLY:O	1:A:660:ILE:HG12	2.17	0.44
1:A:490:ARG:HD3	1:A:490:ARG:HA	1.73	0.44
1:D:485:ILE:CD1	1:D:494:ILE:HD12	2.48	0.43
1:B:590:ARG:HD3	1:B:590:ARG:HA	1.84	0.43
1:C:592:PRO:HD2	1:C:645:ILE:O	2.17	0.43
1:C:481:LEU:O	1:C:485:ILE:HD12	2.19	0.43
1:D:485:ILE:CG2	1:D:486:GLU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:657:MET:HE2	1:D:657:MET:HA	2.00	0.43
1:D:662:LYS:HE2	1:D:662:LYS:HB3	1.83	0.42
1:B:638:ILE:O	1:C:796:THR:HG21	2.19	0.42
1:C:488:HIS:CD2	1:C:523:MET:HG3	2.54	0.42
1:A:649:SER:HB3	1:A:660:ILE:HD12	2.02	0.42
1:B:484:LEU:HD12	1:B:484:LEU:HA	1.89	0.42
1:D:592:PRO:HD2	1:D:645:ILE:O	2.20	0.42
1:D:653:ASP:CG	1:D:832:GLY:H	2.28	0.42
1:B:477:PRO:HD2	1:B:480:LYS:HD2	2.01	0.42
1:C:595:ARG:HH22	1:D:730:GLU:HG2	1.84	0.42
1:A:482:GLU:HG3	1:A:523:MET:HE2	2.02	0.42
1:A:613:GLU:H	1:A:613:GLU:CD	2.28	0.42
1:B:485:ILE:HD12	1:B:491:GLY:HA2	2.01	0.42
1:C:808:GLY:O	1:C:814:GLN:HG3	2.20	0.42
1:A:796:THR:HG21	1:D:638:ILE:O	2.20	0.42
1:D:850:GLU:O	1:D:854:MET:HG2	2.19	0.42
1:A:461:PHE:HB3	1:A:462:LEU:HD12	2.03	0.41
1:B:756:ILE:N	1:B:756:ILE:HD12	2.35	0.41
1:C:850:GLU:O	1:C:854:MET:HG2	2.21	0.41
1:A:540:VAL:CG2	1:B:531:ILE:HD13	2.51	0.41
1:B:662:LYS:HB3	1:B:662:LYS:HE2	1.84	0.41
1:D:618:ILE:HG23	1:D:667:ALA:HB1	2.03	0.41
1:B:649:SER:HB3	1:B:660:ILE:HD12	2.03	0.40
1:B:850:GLU:O	1:B:854:MET:HG2	2.22	0.40
3:C:4:FBI:H3	3:C:4:FBI:H62	1.89	0.40
1:A:590:ARG:HD3	1:A:590:ARG:HA	1.80	0.40
1:A:774:SER:HA	1:A:799:SER:O	2.21	0.40
1:C:474:LYS:HB2	1:C:476:ILE:HG13	2.04	0.40
1:C:590:ARG:HA	1:C:590:ARG:HD3	1.82	0.40
1:D:808:GLY:O	1:D:814:GLN:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	403/467 (86%)	385 (96%)	15 (4%)	3 (1%)	18	15
1	B	396/467 (85%)	376 (95%)	17 (4%)	3 (1%)	16	12
1	C	396/467 (85%)	378 (96%)	16 (4%)	2 (0%)	24	22
1	D	380/467 (81%)	364 (96%)	15 (4%)	1 (0%)	36	36
All	All	1575/1868 (84%)	1503 (95%)	63 (4%)	9 (1%)	21	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	472	ASN
1	B	484	LEU
1	A	484	LEU
1	A	486	GLU
1	D	514	TYR
1	A	514	TYR
1	B	514	TYR
1	C	514	TYR
1	C	485	ILE

5.3.2 Protein sidechains ⓘ

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	325/375 (87%)	312 (96%)	13 (4%)	28	29
1	B	316/375 (84%)	307 (97%)	9 (3%)	38	43
1	C	316/375 (84%)	305 (96%)	11 (4%)	32	35
1	D	303/375 (81%)	293 (97%)	10 (3%)	33	37
All	All	1260/1500 (84%)	1217 (97%)	43 (3%)	32	35

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	470	LEU
1	A	484	LEU
1	A	486	GLU
1	A	492	VAL
1	A	505	GLU
1	A	613	GLU
1	A	634	LEU
1	A	638	ILE
1	A	657	MET
1	A	688	CYS
1	A	700	GLU
1	A	788	ASN
1	A	814	GLN
1	B	484	LEU
1	B	505	GLU
1	B	613	GLU
1	B	638	ILE
1	B	657	MET
1	B	688	CYS
1	B	700	GLU
1	B	788	ASN
1	B	814	GLN
1	C	464	ASP
1	C	470	LEU
1	C	484	LEU
1	C	505	GLU
1	C	613	GLU
1	C	634	LEU
1	C	638	ILE
1	C	657	MET
1	C	700	GLU
1	C	788	ASN
1	C	814	GLN
1	D	482	GLU
1	D	613	GLU
1	D	634	LEU
1	D	638	ILE
1	D	657	MET
1	D	688	CYS
1	D	700	GLU
1	D	788	ASN
1	D	814	GLN
1	D	828	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	469	GLN
1	A	736	ASN
1	A	788	ASN
1	B	529	ASN
1	B	672	HIS
1	B	788	ASN
1	C	488	HIS
1	C	672	HIS
1	C	788	ASN
1	D	488	HIS
1	D	497	GLN
1	D	736	ASN
1	D	788	ASN

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](#)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FBI	D	3	-	33,34,34	3.66	9 (27%)	43,49,49	2.31	12 (27%)
2	ADP	A	102	-	28,29,29	1.59	4 (14%)	43,45,45	0.72	0
3	FBI	C	4	-	33,34,34	3.72	10 (30%)	43,49,49	2.43	13 (30%)
2	ADP	C	103	-	28,29,29	1.38	5 (17%)	43,45,45	0.88	2 (4%)
2	ADP	A	101	-	28,29,29	1.44	4 (14%)	43,45,45	0.72	1 (2%)
3	FBI	A	2	-	33,34,34	3.72	9 (27%)	43,49,49	2.29	12 (27%)
3	FBI	B	1	-	33,34,34	3.58	11 (33%)	43,49,49	2.29	11 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FBI	D	3	-	-	5/31/31/31	0/2/2/2
2	ADP	A	102	-	-	2/16/32/32	0/3/3/3
3	FBI	C	4	-	-	3/31/31/31	0/2/2/2
2	ADP	C	103	-	-	2/16/32/32	0/3/3/3
2	ADP	A	101	-	-	3/16/32/32	0/3/3/3
3	FBI	A	2	-	-	7/31/31/31	0/2/2/2
3	FBI	B	1	-	-	7/31/31/31	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	FBI	O1S-S1	11.56	1.60	1.43
3	C	4	FBI	O1S-S1	11.39	1.60	1.43
3	D	3	FBI	O2S-S1	10.82	1.59	1.43
3	A	2	FBI	O2S-S1	10.81	1.59	1.43
3	D	3	FBI	O1S-S1	10.75	1.59	1.43
3	B	1	FBI	O1S-S1	10.66	1.59	1.43
3	B	1	FBI	O2S-S1	10.46	1.59	1.43
3	C	4	FBI	O2S-S1	10.44	1.59	1.43
3	C	4	FBI	C81-C8	-9.34	1.38	1.49
3	B	1	FBI	C81-C8	-8.89	1.39	1.49
3	D	3	FBI	C81-C8	-8.80	1.39	1.49
3	A	2	FBI	C81-C8	-8.77	1.39	1.49
3	A	2	FBI	S1-N3	6.26	1.74	1.64
3	D	3	FBI	S1-N3	6.01	1.74	1.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	FBI	S1-N3	5.83	1.74	1.64
2	A	102	ADP	PA-O3A	5.48	1.65	1.59
3	B	1	FBI	S1-N3	4.84	1.72	1.64
3	C	4	FBI	C6-C7	-4.82	1.32	1.52
3	D	3	FBI	C6-C7	-4.67	1.33	1.52
3	D	3	FBI	C9-C91	4.52	1.57	1.51
3	A	2	FBI	C6-C7	-4.50	1.33	1.52
3	B	1	FBI	C6-C7	-4.48	1.33	1.52
3	C	4	FBI	O1A-C1	4.28	1.36	1.22
3	B	1	FBI	O1A-C1	4.18	1.35	1.22
3	D	3	FBI	O1A-C1	4.15	1.35	1.22
2	A	101	ADP	PA-O3A	4.05	1.63	1.59
3	A	2	FBI	C9-C91	3.97	1.56	1.51
3	C	4	FBI	C9-C91	3.93	1.56	1.51
3	B	1	FBI	C9-C91	3.71	1.56	1.51
3	A	2	FBI	O1B-C1	-3.28	1.20	1.30
3	A	2	FBI	O1A-C1	3.12	1.32	1.22
3	D	3	FBI	C10-C9	3.10	1.45	1.41
2	C	103	ADP	C8-N9	-3.03	1.32	1.37
2	A	101	ADP	C8-N9	-2.98	1.32	1.37
2	C	103	ADP	PA-O3A	2.86	1.62	1.59
3	B	1	FBI	O1B-C1	-2.73	1.21	1.30
2	A	102	ADP	C1'-N9	2.68	1.53	1.46
2	A	102	ADP	C8-N9	-2.63	1.33	1.37
2	A	101	ADP	O4'-C4'	2.61	1.50	1.45
2	C	103	ADP	C1'-N9	2.56	1.53	1.46
3	C	4	FBI	O1B-C1	-2.52	1.22	1.30
3	D	3	FBI	O1B-C1	-2.46	1.22	1.30
3	B	1	FBI	C8-C10	2.42	1.45	1.41
2	A	101	ADP	C1'-N9	2.37	1.52	1.46
2	C	103	ADP	O4'-C4'	2.26	1.50	1.45
2	C	103	ADP	C2'-C3'	2.21	1.59	1.53
3	A	2	FBI	C8-C10	2.21	1.45	1.41
3	C	4	FBI	C11-N2	-2.19	1.30	1.34
2	A	102	ADP	O4'-C4'	2.06	1.49	1.45
3	B	1	FBI	C83-C84	2.05	1.41	1.37
3	B	1	FBI	C10-C9	2.02	1.44	1.41
3	C	4	FBI	C83-C84	2.00	1.41	1.37

All (51) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	FBI	O2S-S1-O1S	-7.76	106.86	118.46
3	C	4	FBI	O2S-S1-O1S	-7.73	106.90	118.46
3	A	2	FBI	O2S-S1-O1S	-7.01	107.98	118.46
3	D	3	FBI	O2S-S1-O1S	-6.88	108.18	118.46
3	C	4	FBI	C7-C6-C5	6.06	124.93	114.95
3	D	3	FBI	O1S-S1-N3	5.46	113.39	107.14
3	A	2	FBI	C7-C6-C5	4.86	122.94	114.95
3	B	1	FBI	C12-N3-C11	4.85	125.14	116.39
3	D	3	FBI	C7-C6-C5	4.71	122.70	114.95
3	C	4	FBI	C8-N1-C11	4.53	120.67	116.27
3	A	2	FBI	O2S-S1-N3	4.40	112.18	107.14
3	B	1	FBI	C7-C6-C5	4.40	122.19	114.95
3	D	3	FBI	C10-C9-N2	-4.32	118.90	122.55
3	A	2	FBI	C8-N1-C11	4.23	120.38	116.27
3	D	3	FBI	C12-N3-C11	4.19	123.94	116.39
3	A	2	FBI	C12-N3-C11	4.17	123.91	116.39
3	D	3	FBI	C8-N1-C11	4.02	120.18	116.27
3	B	1	FBI	C11-N2-C9	4.00	120.62	116.20
3	B	1	FBI	O2S-S1-N3	4.00	111.72	107.14
3	C	4	FBI	C12-N3-C11	3.97	123.55	116.39
3	A	2	FBI	C10-C9-N2	-3.96	119.20	122.55
3	A	2	FBI	C11-N2-C9	3.89	120.49	116.20
3	B	1	FBI	C10-C9-N2	-3.89	119.27	122.55
3	C	4	FBI	O1S-S1-N3	3.70	111.38	107.14
3	B	1	FBI	C8-N1-C11	3.63	119.80	116.27
3	B	1	FBI	O1S-S1-N3	3.57	111.22	107.14
3	D	3	FBI	C11-N2-C9	3.49	120.05	116.20
3	C	4	FBI	O1A-C1-C2	-3.48	112.15	122.84
3	C	4	FBI	O2S-S1-N3	3.46	111.10	107.14
3	D	3	FBI	O1A-C1-C2	-3.40	112.42	122.84
3	C	4	FBI	C11-N2-C9	3.39	119.94	116.20
3	A	2	FBI	O1B-C1-C2	3.28	124.19	114.00
3	D	3	FBI	O1B-C1-C2	3.27	124.16	114.00
3	C	4	FBI	C10-C9-N2	-3.25	119.81	122.55
3	C	4	FBI	O1B-C1-C2	3.21	123.97	114.00
3	A	2	FBI	O1A-C1-C2	-3.11	113.28	122.84
3	C	4	FBI	C13-S1-N3	3.07	110.57	106.82
3	B	1	FBI	O1B-C1-C2	2.98	123.27	114.00
3	B	1	FBI	O1A-C1-C2	-2.97	113.72	122.84
3	A	2	FBI	O1S-S1-N3	2.86	110.42	107.14
3	C	4	FBI	C10-C8-N1	-2.71	118.50	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3	FBI	C13-S1-N3	2.58	109.97	106.82
3	A	2	FBI	C13-S1-N3	2.51	109.89	106.82
3	B	1	FBI	C10-C8-N1	-2.49	118.85	122.75
3	D	3	FBI	C10-C8-N1	-2.41	118.97	122.75
3	D	3	FBI	O2S-S1-N3	2.35	109.83	107.14
3	C	4	FBI	C82-C81-C8	2.35	124.43	120.62
2	C	103	ADP	C2'-C3'-C4'	2.34	107.14	102.61
3	A	2	FBI	C10-C8-N1	-2.33	119.09	122.75
2	A	101	ADP	C4-N9-C8	2.15	108.00	105.74
2	C	103	ADP	C4-N9-C8	2.08	107.93	105.74

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	101	ADP	O4'-C4'-C5'-O5'
2	A	101	ADP	C3'-C4'-C5'-O5'
3	A	2	FBI	C8-C10-C7-C6
3	A	2	FBI	C9-C10-C7-C6
3	A	2	FBI	C4-C5-C6-C7
3	B	1	FBI	C8-C10-C7-C6
3	B	1	FBI	C9-C10-C7-C6
3	B	1	FBI	C4-C5-C6-C7
3	C	4	FBI	O5-C5-C6-C7
3	D	3	FBI	C8-C10-C7-C6
3	D	3	FBI	C9-C10-C7-C6
3	D	3	FBI	C4-C5-C6-C7
3	A	2	FBI	O5-C5-C6-C7
3	B	1	FBI	O5-C5-C6-C7
3	D	3	FBI	O5-C5-C6-C7
3	C	4	FBI	C4-C5-C6-C7
2	C	103	ADP	O4'-C4'-C5'-O5'
2	C	103	ADP	C3'-C4'-C5'-O5'
2	A	102	ADP	C3'-C4'-C5'-O5'
2	A	101	ADP	PA-O3A-PB-O3B
2	A	102	ADP	O4'-C4'-C5'-O5'
3	C	4	FBI	C12-N3-S1-O1S
3	A	2	FBI	C12-N3-S1-O2S
3	B	1	FBI	C12-N3-S1-O1S
3	D	3	FBI	C12-N3-S1-O2S
3	A	2	FBI	N2-C11-N3-C12
3	A	2	FBI	N1-C11-N3-C12

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Mol	Chain	Res	Type	Atoms
3	B	1	FBI	N2-C11-N3-C12
3	B	1	FBI	N1-C11-N3-C12

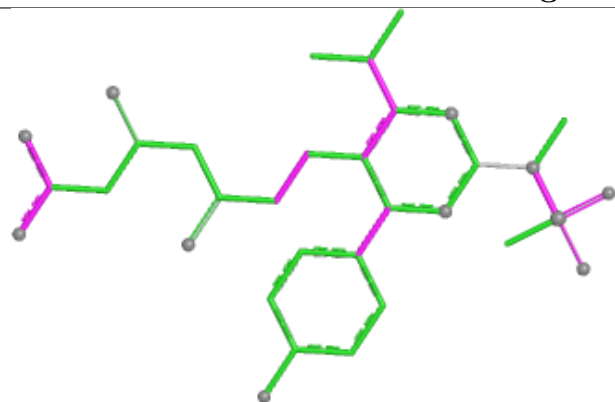
There are no ring outliers.

7 monomers are involved in 15 short contacts:

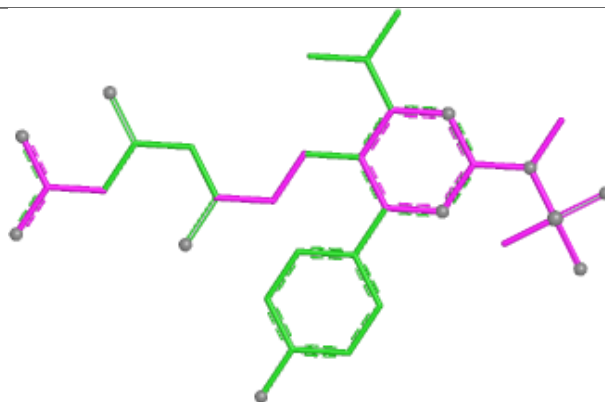
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	3	FBI	2	0
2	A	102	ADP	3	0
3	C	4	FBI	2	0
2	C	103	ADP	2	0
2	A	101	ADP	2	0
3	A	2	FBI	2	0
3	B	1	FBI	2	0

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.

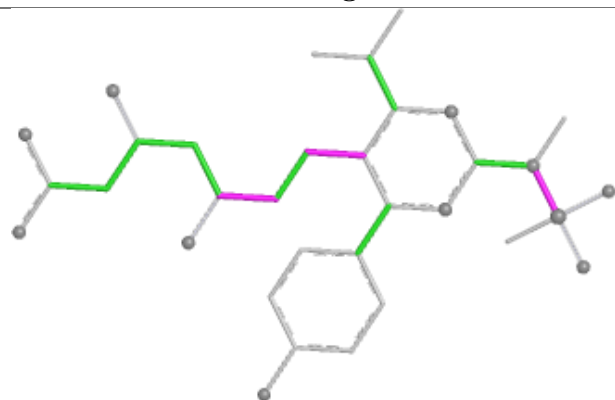
Ligand FBI D 3



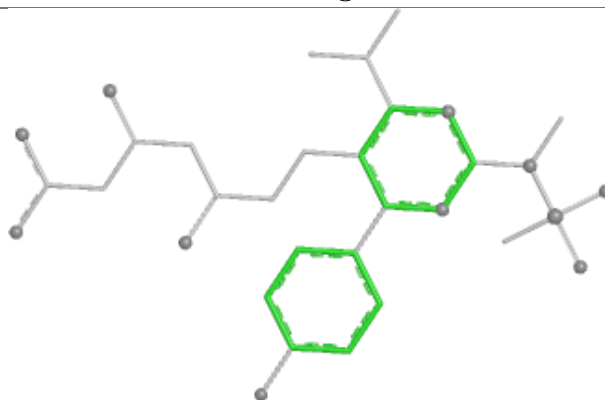
Bond lengths



Bond angles

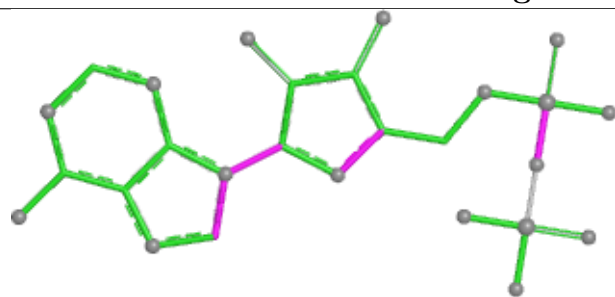


Torsions

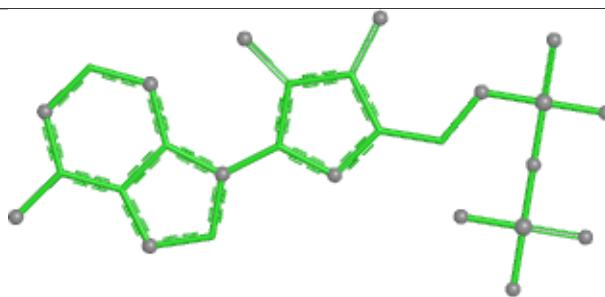


Rings

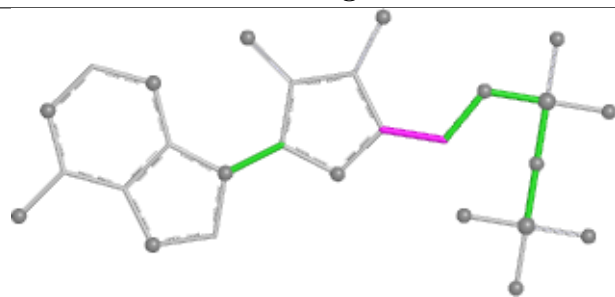
Ligand ADP A 102



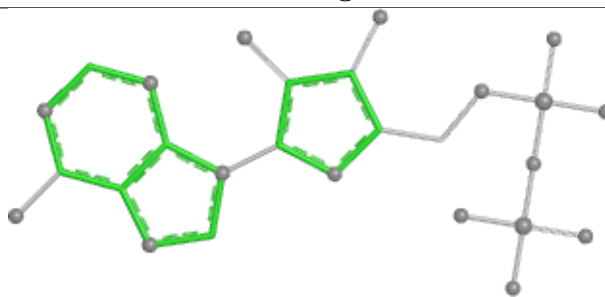
Bond lengths



Bond angles

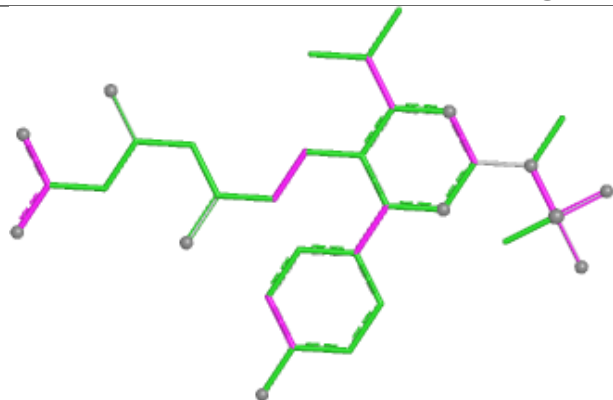


Torsions

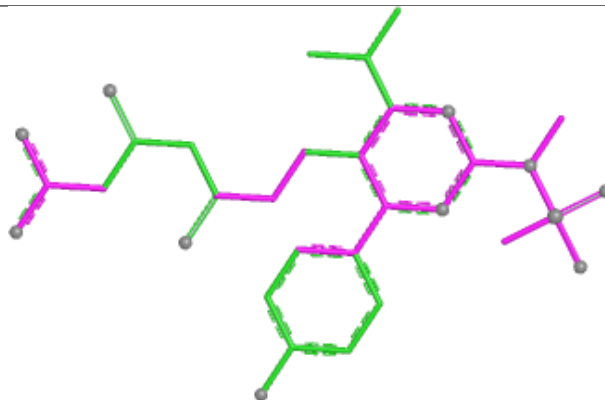


Rings

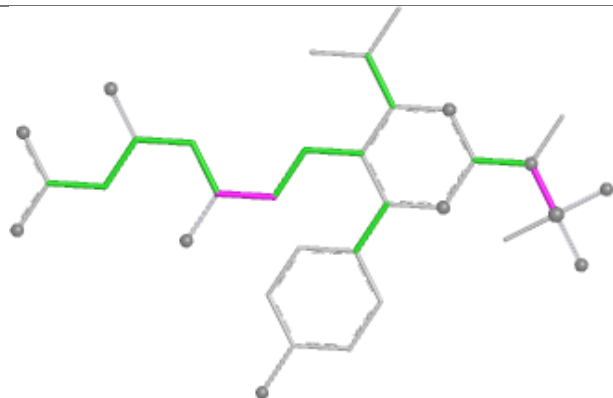
Ligand FBI C 4



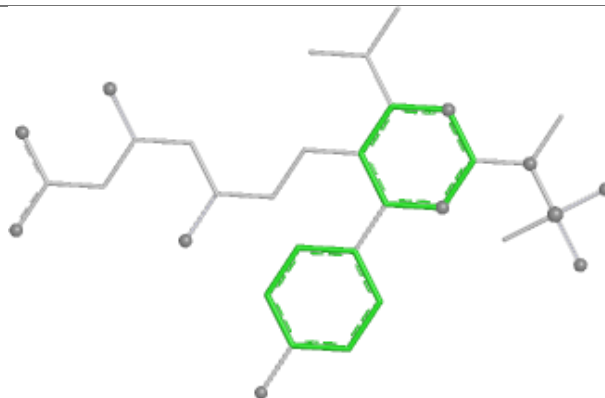
Bond lengths



Bond angles

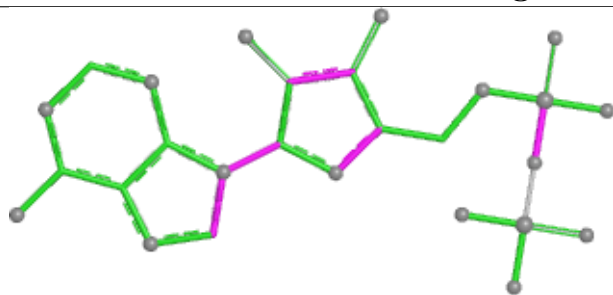


Torsions

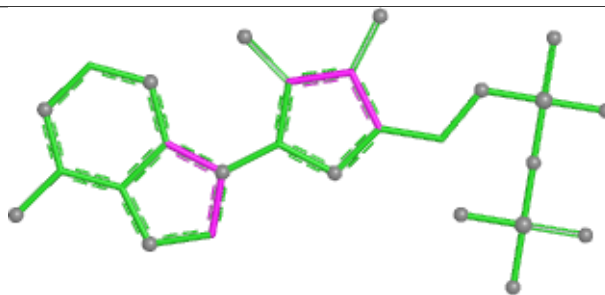


Rings

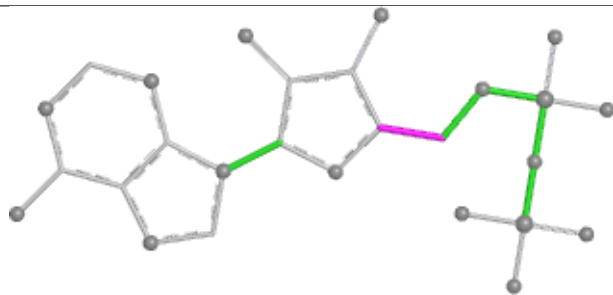
Ligand ADP C 103



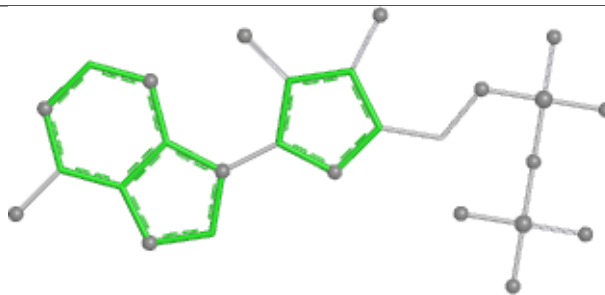
Bond lengths



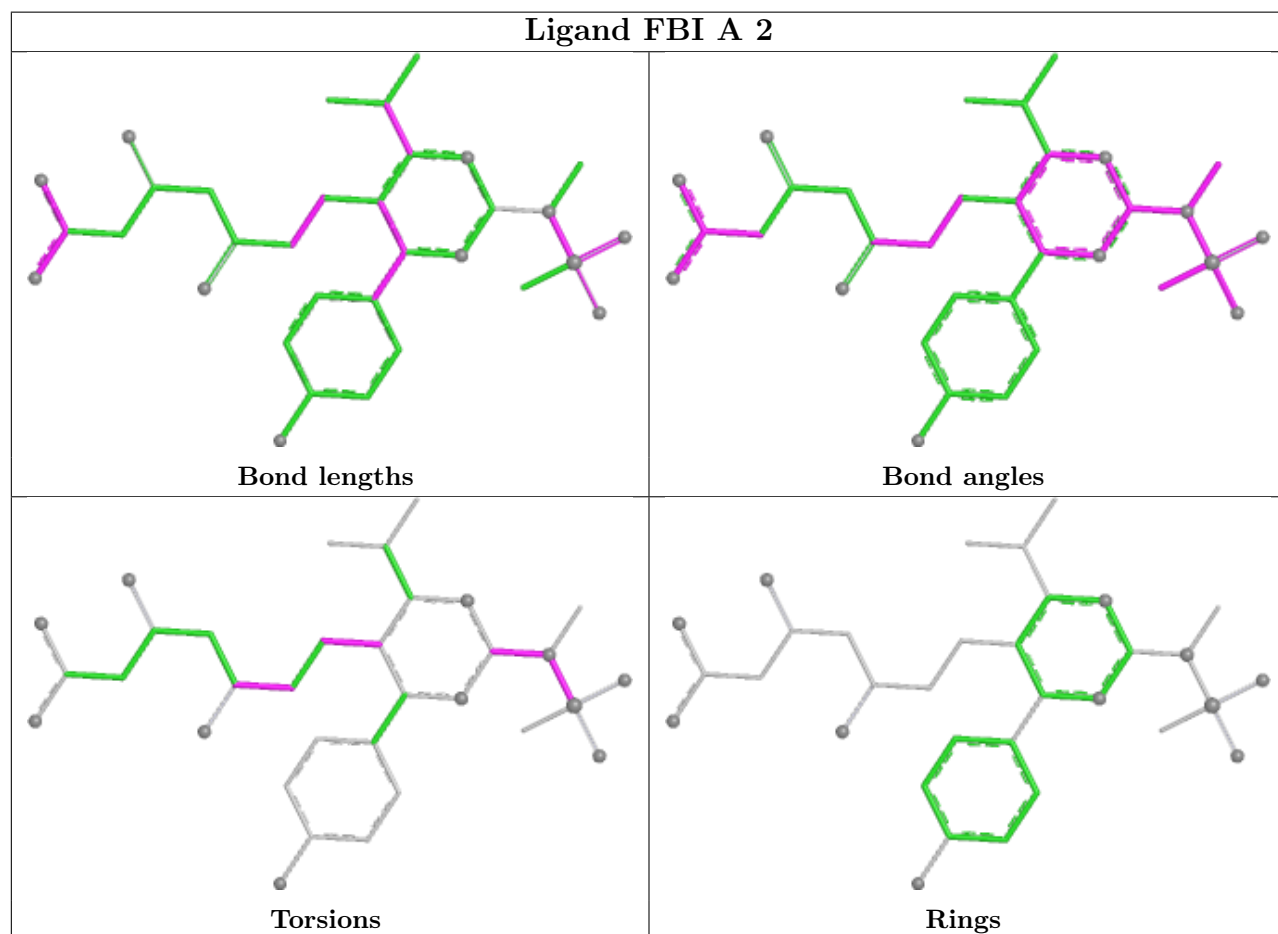
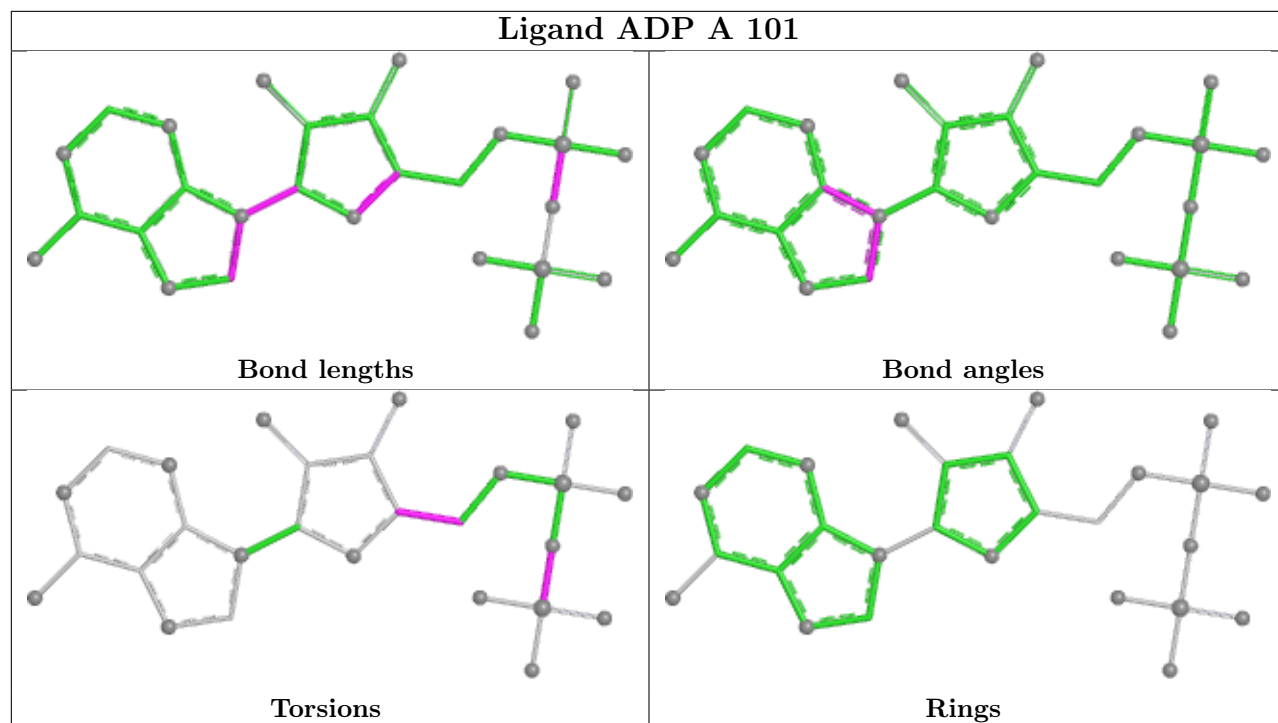
Bond angles

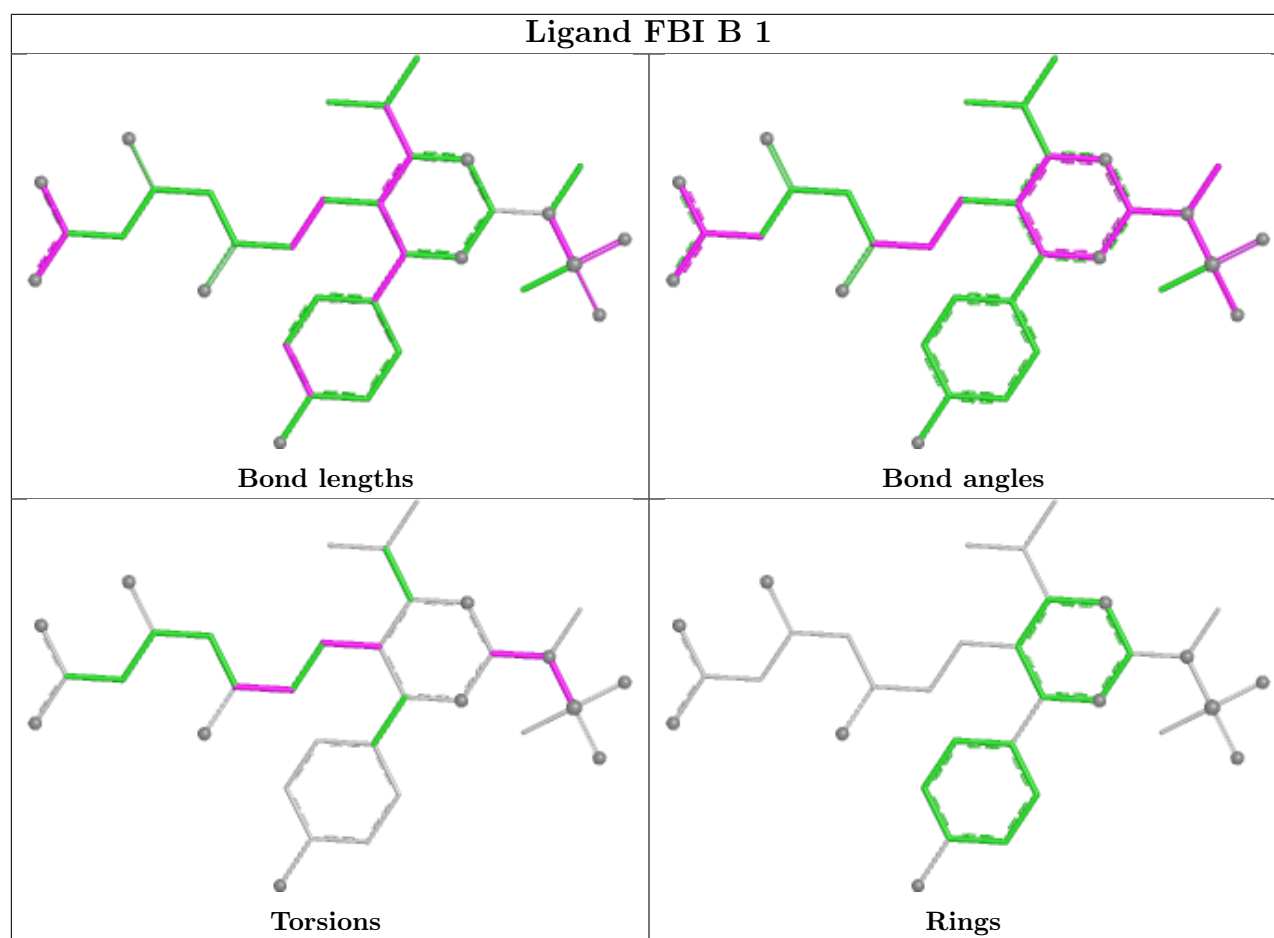


Torsions



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	407/467 (87%)	0.68	24 (5%)	28	30	35, 52, 90, 97	0
1	B	398/467 (85%)	0.66	26 (6%)	25	26	35, 52, 82, 100	0
1	C	398/467 (85%)	0.72	31 (7%)	19	20	36, 54, 89, 99	0
1	D	382/467 (81%)	0.56	30 (7%)	18	20	35, 50, 75, 100	0
All	All	1585/1868 (84%)	0.66	111 (7%)	22	24	35, 52, 87, 100	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	LEU	5.8
1	A	461	PHE	5.7
1	D	483	THR	5.0
1	A	476	ILE	5.0
1	B	478	ALA	4.9
1	C	476	ILE	4.8
1	C	484	LEU	4.5
1	A	442	PRO	4.4
1	B	476	ILE	4.2
1	D	484	LEU	4.0
1	D	479	TYR	3.9
1	C	523	MET	3.9
1	C	463	SER	3.8
1	A	524	GLY	3.8
1	A	478	ALA	3.7
1	D	485	ILE	3.6
1	C	487	THR	3.5
1	D	487	THR	3.4
1	C	475	HIS	3.2
1	B	630	ARG	3.2
1	C	504	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	477	PRO	3.2
1	A	860	GLY	3.2
1	B	629	ALA	3.1
1	B	479	TYR	3.1
1	D	480	LYS	3.0
1	B	481	LEU	3.0
1	D	523	MET	3.0
1	C	634	LEU	2.9
1	C	526	CYS	2.9
1	D	632	GLN	2.9
1	C	478	ALA	2.9
1	B	521	LEU	2.8
1	D	529	ASN	2.8
1	D	481	LEU	2.8
1	D	514	TYR	2.8
1	C	477	PRO	2.8
1	B	484	LEU	2.8
1	C	481	LEU	2.8
1	A	523	MET	2.7
1	C	674	TYR	2.7
1	B	477	PRO	2.7
1	C	485	ILE	2.7
1	B	631	LEU	2.7
1	D	585	ALA	2.6
1	C	479	TYR	2.6
1	B	473	ALA	2.6
1	D	503	LEU	2.6
1	A	492	VAL	2.6
1	A	473	ALA	2.6
1	B	523	MET	2.5
1	B	659	MET	2.5
1	C	524	GLY	2.5
1	A	462	LEU	2.5
1	D	860	GLY	2.5
1	A	479	TYR	2.5
1	B	483	THR	2.5
1	C	465	ALA	2.5
1	C	575	LEU	2.5
1	D	516	ASP	2.5
1	C	525	ALA	2.4
1	D	828	LYS	2.4
1	A	521	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	488	HIS	2.4
1	D	708	CYS	2.4
1	C	632	GLN	2.4
1	D	628	PHE	2.4
1	A	633	LYS	2.4
1	B	708	CYS	2.4
1	C	631	LEU	2.3
1	A	506	PRO	2.3
1	C	771	ASN	2.3
1	D	524	GLY	2.3
1	C	529	ASN	2.3
1	B	634	LEU	2.3
1	B	485	ILE	2.2
1	C	826	ALA	2.2
1	C	470	LEU	2.2
1	D	627	ARG	2.2
1	A	485	ILE	2.2
1	C	483	THR	2.2
1	A	720	VAL	2.2
1	B	826	ALA	2.2
1	B	504	SER	2.2
1	B	612	SER	2.2
1	D	545	CYS	2.1
1	A	517	TYR	2.1
1	B	711	VAL	2.1
1	B	860	GLY	2.1
1	A	826	ALA	2.1
1	A	504	SER	2.1
1	C	521	LEU	2.1
1	D	498	LEU	2.1
1	A	628	PHE	2.1
1	B	525	ALA	2.1
1	D	575	LEU	2.1
1	C	548	GLU	2.1
1	B	474	LYS	2.1
1	C	467	ILE	2.1
1	B	628	PHE	2.1
1	D	504	SER	2.1
1	A	659	MET	2.0
1	A	475	HIS	2.0
1	C	615	PHE	2.0
1	D	659	MET	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	631	LEU	2.0
1	B	487	THR	2.0
1	D	513	PRO	2.0
1	C	511	TYR	2.0
1	D	511	TYR	2.0
1	D	517	TYR	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](#)

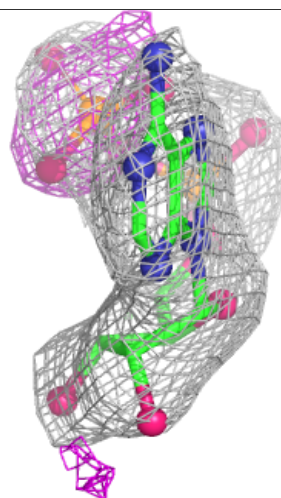
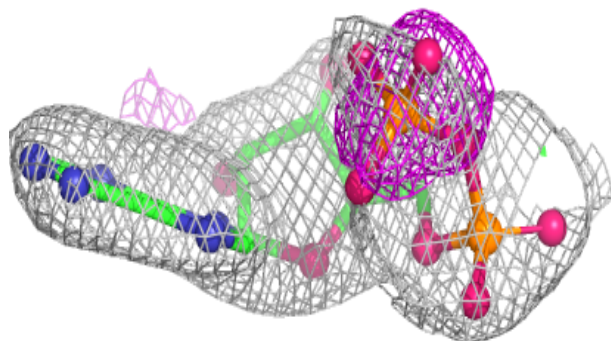
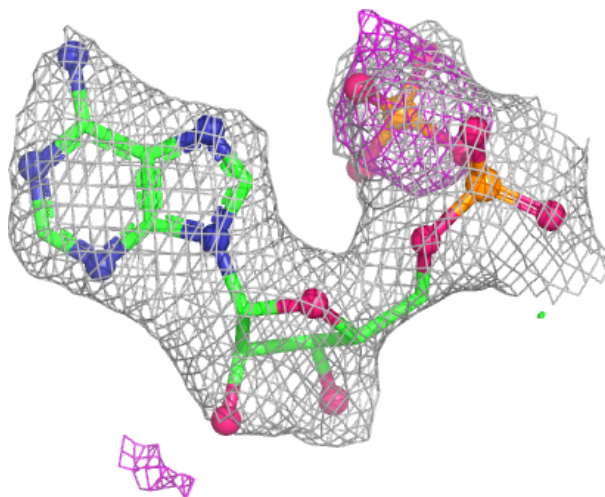
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	101	27/27	0.79	0.13	90,93,99,99	0
2	ADP	A	102	27/27	0.80	0.12	88,91,99,99	0
2	ADP	C	103	27/27	0.83	0.12	83,88,99,99	0
3	FBI	D	3	33/33	0.92	0.10	44,51,57,58	0
3	FBI	A	2	33/33	0.93	0.10	41,48,52,53	0
3	FBI	C	4	33/33	0.94	0.10	44,51,57,57	0
3	FBI	B	1	33/33	0.94	0.10	46,54,59,59	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.

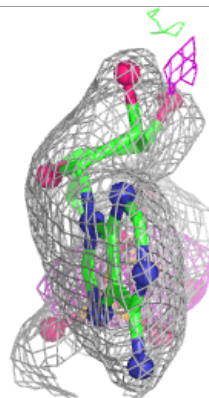
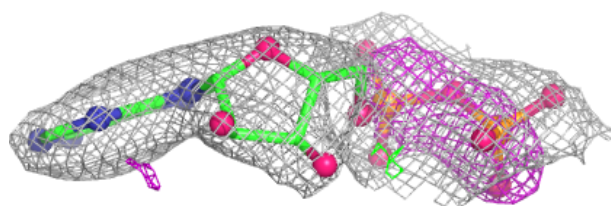
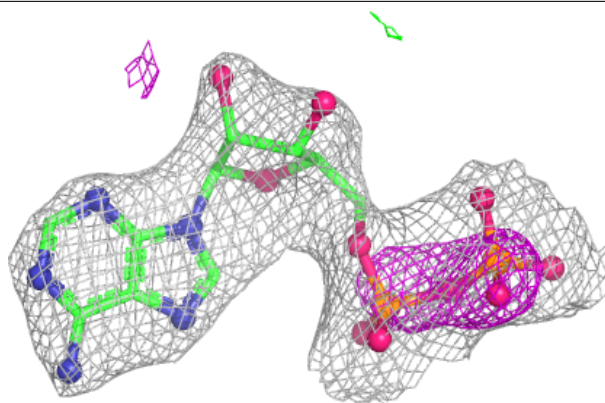
Electron density around ADP A 101:

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

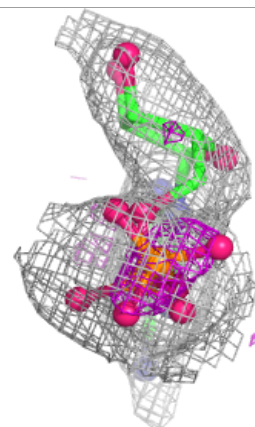
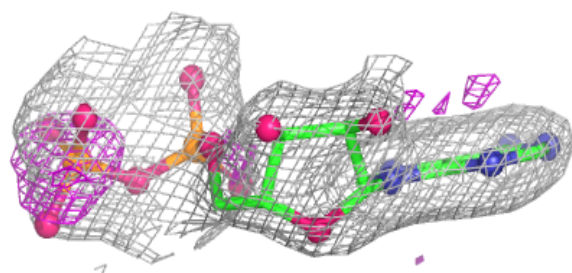
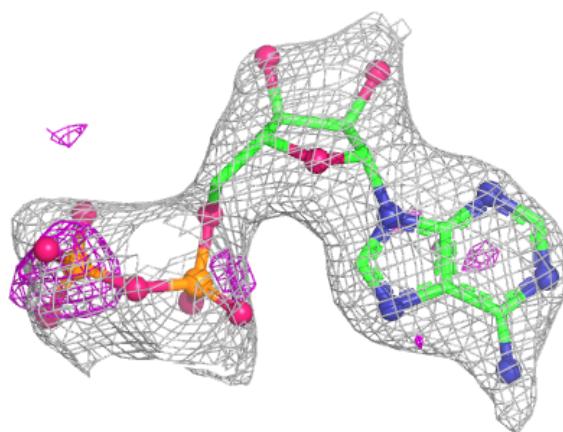


Electron density around ADP A 102:

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

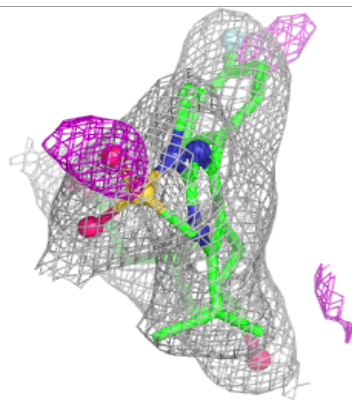
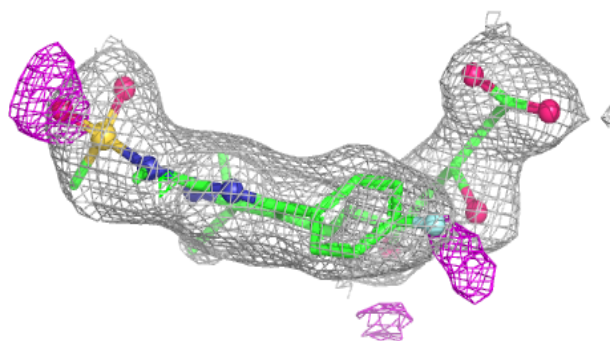
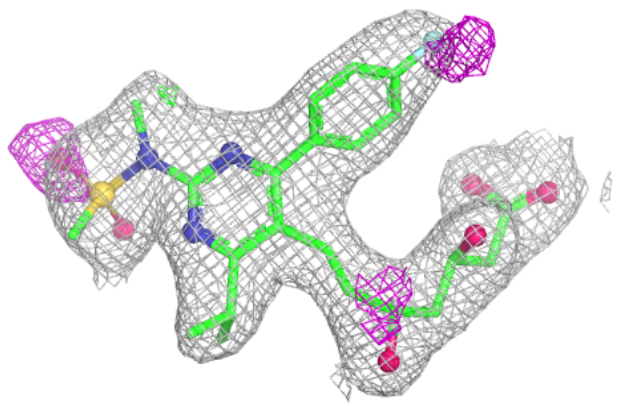
**Electron density around ADP C 103:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



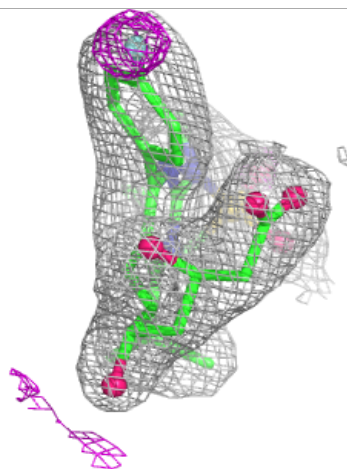
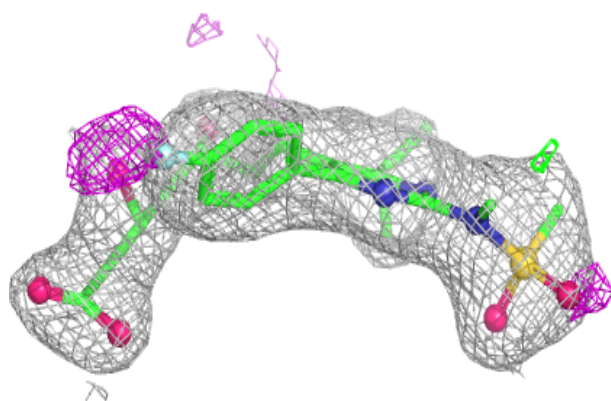
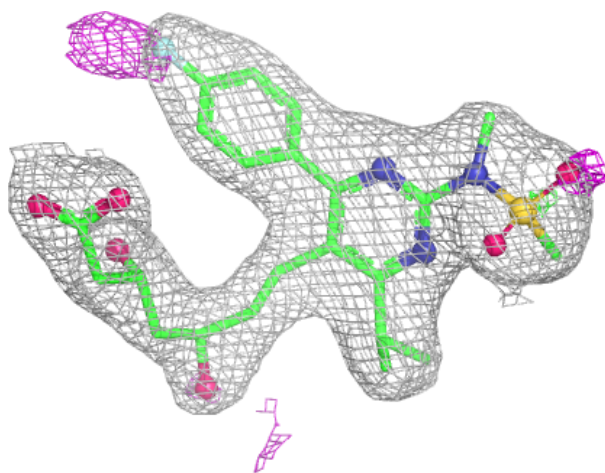
Electron density around FBI D 3:

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



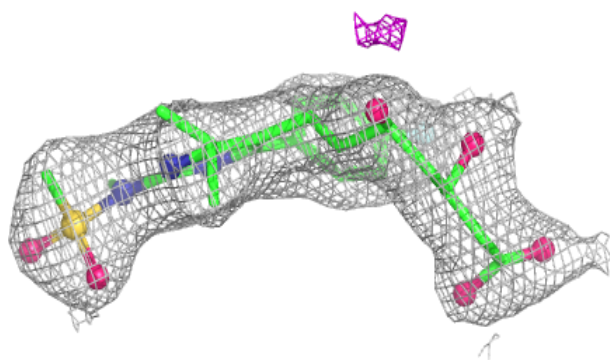
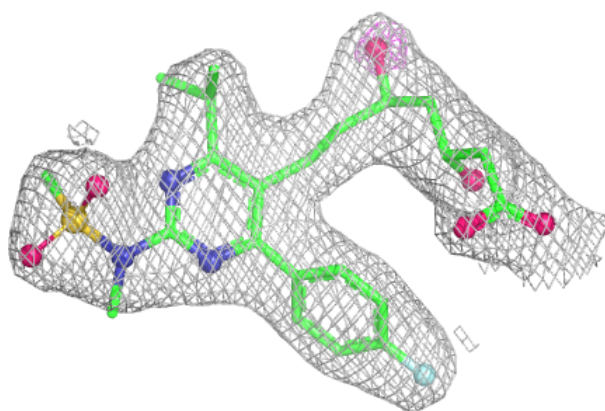
Electron density around FBI A 2:

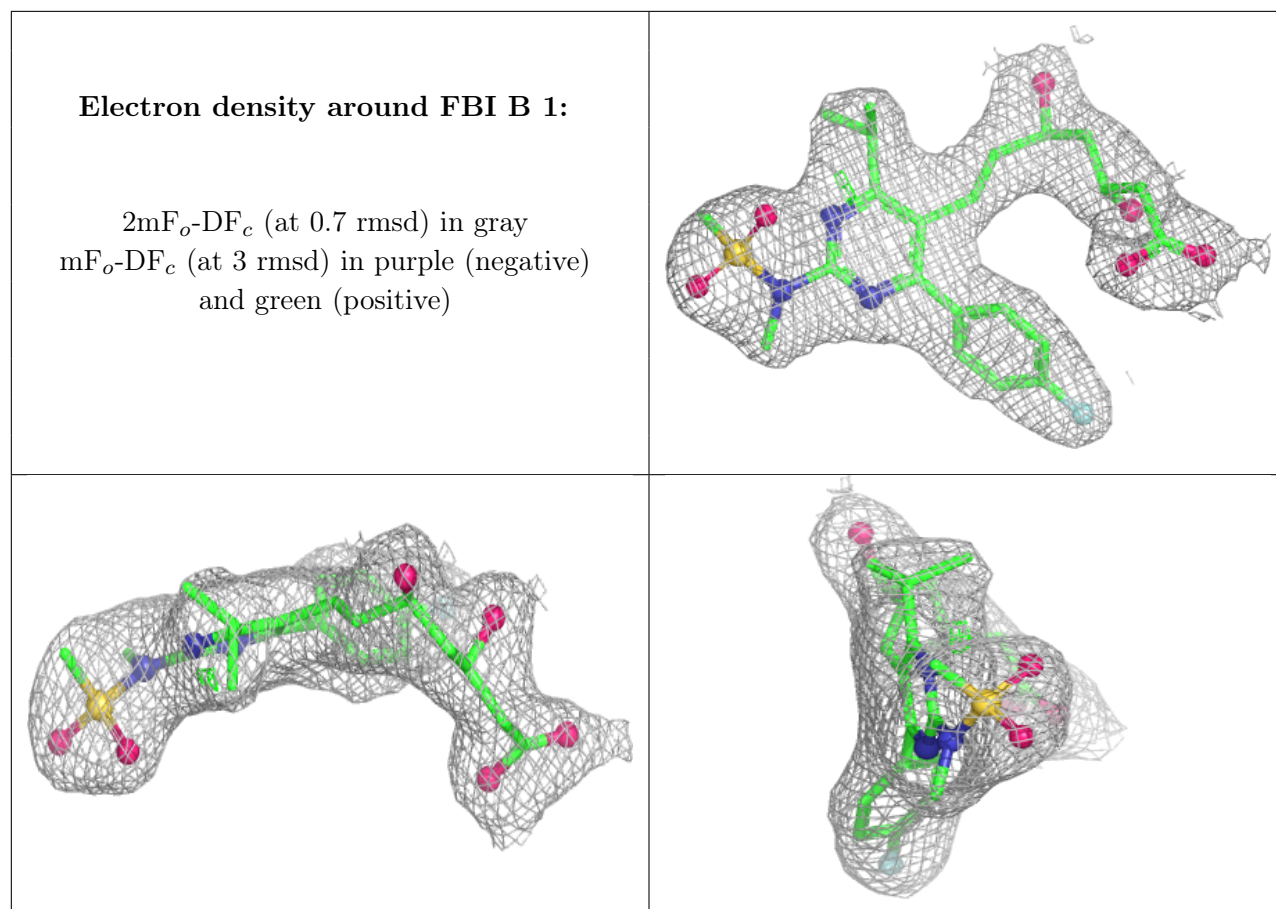
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around FBI C 4:

$2mF_o-DF_c$ (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.