



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 05:30 AM EDT

PDB ID : 1HWL
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

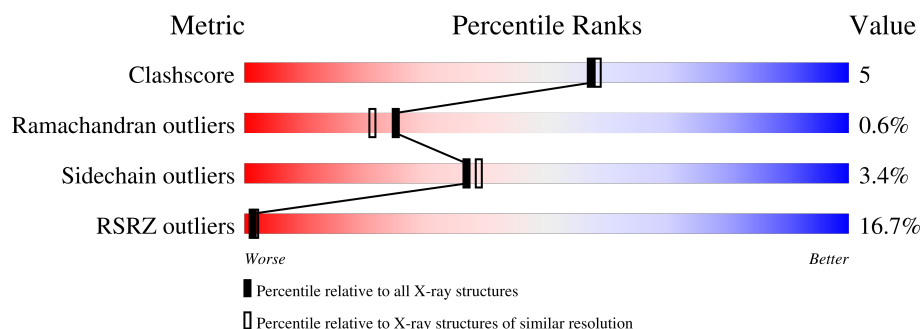
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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	<div> <div>16%</div> <div> <div></div> <div>77%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	467	<div> <div>15%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div></div> <div>15%</div> </div> </div>
1	C	467	<div> <div>15%</div> <div> <div></div> <div>76%</div> <div>9%</div> <div></div> <div>15%</div> </div> </div>
1	D	467	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>8%</div> <div>•</div> <div>18%</div> </div> </div>

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:

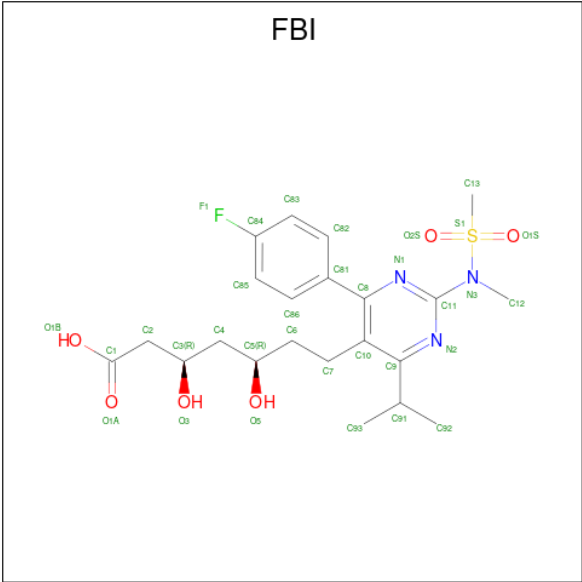
Chain	Residue	Modelled	Actual	Comment	Reference
A	422	GLY	-	insertion	UNP P04035
A	423	ALA	-	insertion	UNP P04035
A	424	MET	-	insertion	UNP P04035
A	425	ALA	-	insertion	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	422	GLY	-	insertion	UNP P04035
B	423	ALA	-	insertion	UNP P04035
B	424	MET	-	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 (three-letter code: 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 (three-letter code: FBI) (formula: $C_{22}H_{30}FN_3O_6S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			33	22	1	3	6	1		
3	B	1	Total	C	F	N	O	S	0	0
			33	22	1	3	6	1		
3	C	1	Total	C	F	N	O	S	0	0
			33	22	1	3	6	1		
3	D	1	Total	C	F	N	O	S	0	0
			33	22	1	3	6	1		

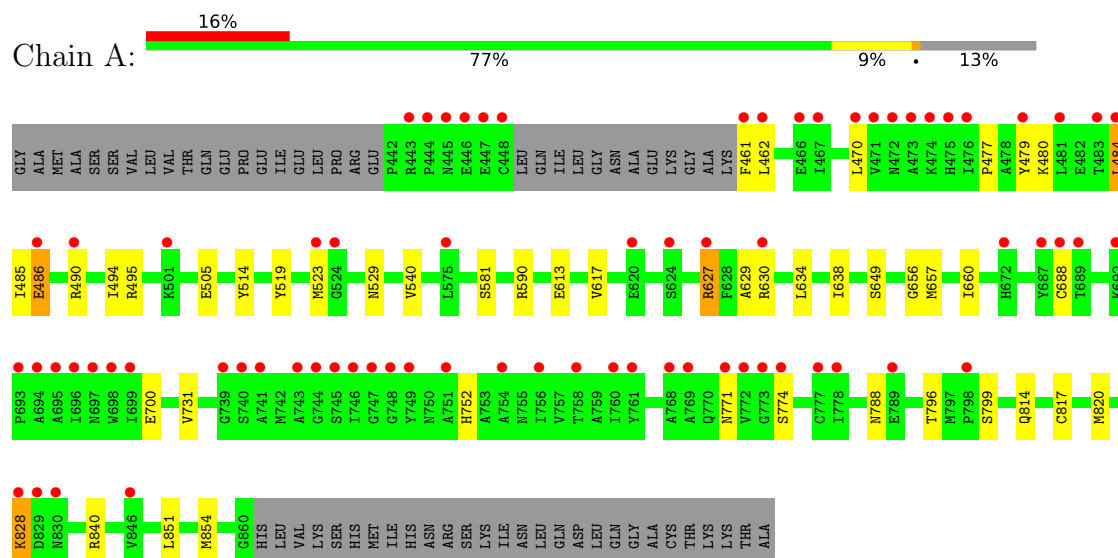
- Molecule 4 is water.

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

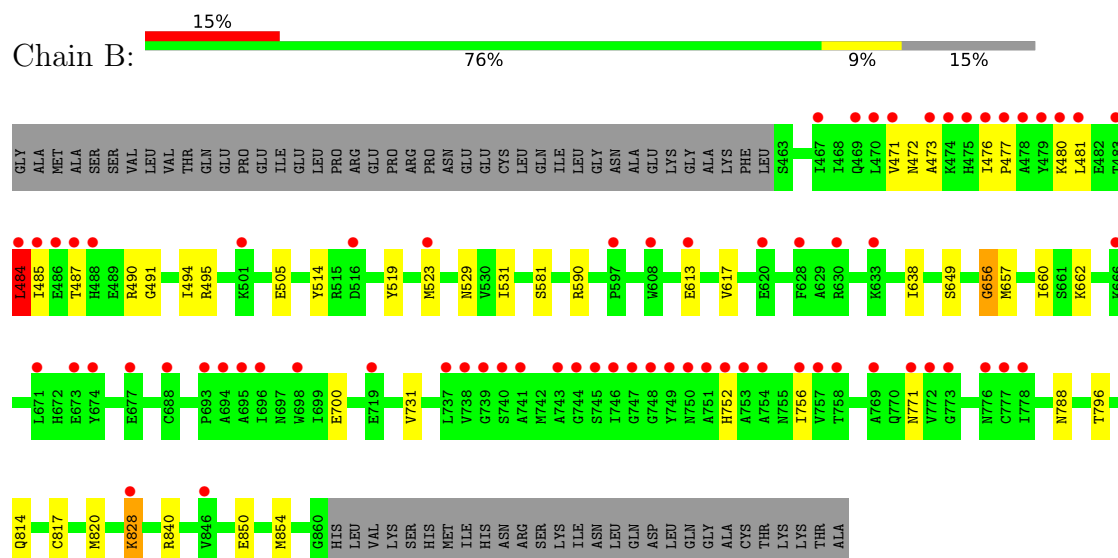
3 Residue-property plots

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.

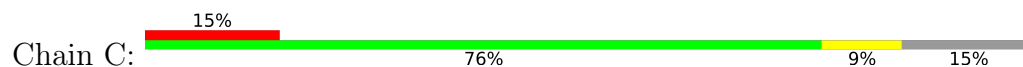
• Molecule 1: HMG-COA REDUCTASE

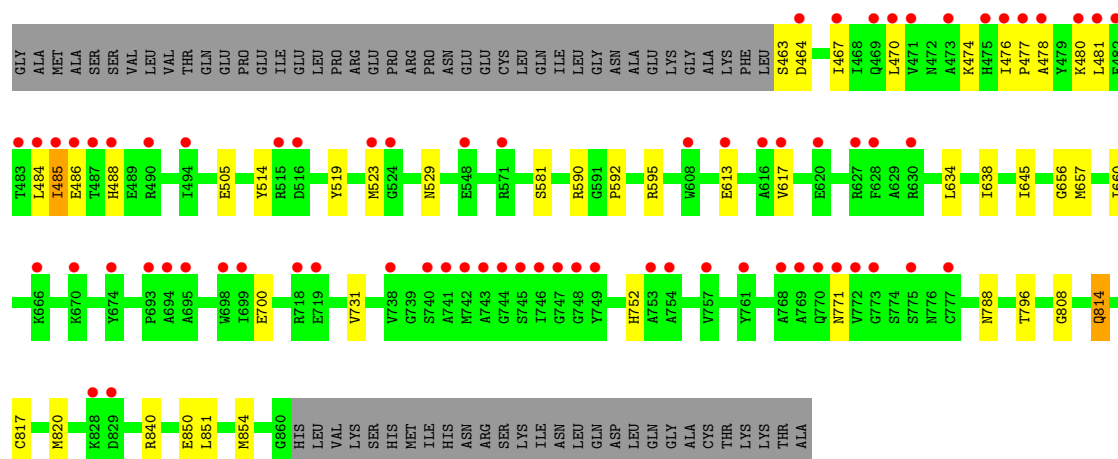


• Molecule 1: HMG-COA REDUCTASE

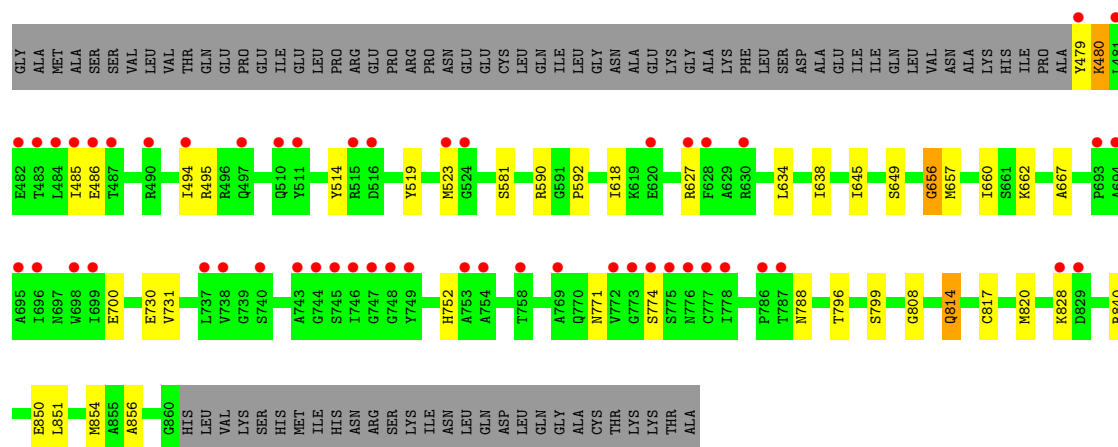
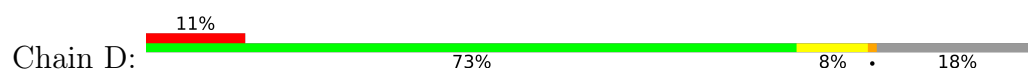


• Molecule 1: HMG-COA REDUCTASE





• 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) 91.7 (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 0.215 , (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)	0.38 , 50.0	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.50	0/3072	0.67	0/4153
1	B	0.50	0/2994	0.67	1/4049 (0.0%)
1	C	0.49	0/2994	0.66	0/4049
1	D	0.54	0/2872	0.68	1/3882 (0.0%)
All	All	0.51	0/11932	0.67	2/16133 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	656	GLY	N-CA-C	5.30	126.34	113.10
1	B	656	GLY	N-CA-C	5.21	126.13	113.10

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	3028	0	3059	29	0
1	B	2952	0	2989	33	0
1	C	2952	0	2989	30	0
1	D	2832	0	2865	29	0
2	A	54	0	24	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	118	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 (118) 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:D:523:MET:HE1	4:D:1055:HOH:O	1.69	0.92
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:A:817:CYS:HA	1:A:820:MET:HE3	1.66	0.77
1:C:817:CYS:HA	1:C:820:MET:HE3	1.66	0.77
1:B:817:CYS:HA	1:B:820:MET:HE3	1.67	0.77
1:D:817:CYS:HA	1:D:820:MET:HE3	1.66	0.76
1:A:523:MET:HE1	4:A:1092:HOH:O	1.87	0.75
3:D:3:FBI:H61	3:D:3:FBI:H91	1.69	0.74
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: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
1:B:523:MET:HE1	4:B:1108:HOH:O	1.95	0.64
2:A:102:ADP:H2	1:B:529:ASN:ND2	1.95	0.63
1:A:485:ILE:HD13	1:A:494:ILE:HD12	1.80	0.63
1:C:523:MET:HE1	4:C:1087:HOH:O	1.99	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:D:519:TYR:O	1:D:523:MET:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:TYR:O	1:B:523:MET:HG2	2.02	0.60
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: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: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: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:D:523:MET:HE3	1:D:523:MET:HA	1.89	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
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: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
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: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:B:471:VAL:C	1:B:473:ALA:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:820:MET:HE2	1:C:820:MET:HB2	1.80	0.46
1:C:478:ALA:O	1:C:481:LEU:HG	2.16	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: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:A:629:ALA:C	1:A:630:ARG:HD2	2.37	0.45
1:B:481:LEU:HD12	1:B:495:ARG:HB2	1.99	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:D:523:MET:HA	1:D:523:MET:CE	2.48	0.43
1:D:820:MET:HE2	1:D:820:MET:HB2	1.81	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
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: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:C:731:VAL:HG12	1:C:854:MET:HE1	2.01	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:523:MET:HA	1:B:523:MET:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:MET:CE	1:A:523:MET:HA	2.51	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%)	22	18
1	B	396/467 (85%)	376 (95%)	17 (4%)	3 (1%)	19	15
1	C	396/467 (85%)	378 (96%)	16 (4%)	2 (0%)	29	26
1	D	380/467 (81%)	364 (96%)	15 (4%)	1 (0%)	41	41
All	All	1575/1868 (84%)	1503 (95%)	63 (4%)	9 (1%)	25	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	472	ASN
1	B	484	LEU
1	A	484	LEU

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Mol	Chain	Res	Type
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%)	311 (96%)	14 (4%)	29	29
1	B	316/375 (84%)	308 (98%)	8 (2%)	47	52
1	C	316/375 (84%)	305 (96%)	11 (4%)	36	38
1	D	303/375 (81%)	293 (97%)	10 (3%)	38	40
All	All	1260/1500 (84%)	1217 (97%)	43 (3%)	37	39

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	505	GLU
1	A	627	ARG
1	A	634	LEU
1	A	657	MET
1	A	688	CYS
1	A	700	GLU
1	A	752	HIS
1	A	788	ASN
1	A	814	GLN
1	A	828	LYS
1	A	851	LEU
1	B	484	LEU

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Mol	Chain	Res	Type
1	B	505	GLU
1	B	657	MET
1	B	700	GLU
1	B	752	HIS
1	B	788	ASN
1	B	814	GLN
1	B	828	LYS
1	C	464	ASP
1	C	470	LEU
1	C	484	LEU
1	C	505	GLU
1	C	634	LEU
1	C	657	MET
1	C	700	GLU
1	C	752	HIS
1	C	788	ASN
1	C	814	GLN
1	C	851	LEU
1	D	480	LYS
1	D	627	ARG
1	D	634	LEU
1	D	657	MET
1	D	700	GLU
1	D	752	HIS
1	D	788	ASN
1	D	814	GLN
1	D	828	LYS
1	D	851	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	D	788	ASN
1	D	830	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 ⓘ

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
2	ADP	C	103	-	24,29,29	1.32	3 (12%)	29,45,45	1.00	2 (6%)
3	FBI	A	2	-	30,34,34	3.68	8 (26%)	37,49,49	2.15	8 (21%)
2	ADP	A	102	-	24,29,29	1.28	2 (8%)	29,45,45	0.74	0
3	FBI	C	4	-	30,34,34	3.68	10 (33%)	37,49,49	2.29	9 (24%)
3	FBI	B	1	-	30,34,34	3.52	9 (30%)	37,49,49	2.16	8 (21%)
3	FBI	D	3	-	30,34,34	3.59	7 (23%)	37,49,49	2.17	9 (24%)
2	ADP	A	101	-	24,29,29	1.27	2 (8%)	29,45,45	0.76	1 (3%)

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	ADP	C	103	-	-	2/12/32/32	0/3/3/3
3	FBI	A	2	-	-	4/29/31/31	0/2/2/2
2	ADP	A	102	-	-	2/12/32/32	0/3/3/3
3	FBI	C	4	-	-	2/29/31/31	0/2/2/2
3	FBI	B	1	-	-	4/29/31/31	0/2/2/2
3	FBI	D	3	-	-	4/29/31/31	0/2/2/2
2	ADP	A	101	-	-	3/12/32/32	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2	FBI	O1S-S1	11.35	1.60	1.43
3	C	4	FBI	O1S-S1	11.19	1.60	1.43
3	D	3	FBI	O2S-S1	10.63	1.59	1.43
3	A	2	FBI	O2S-S1	10.62	1.59	1.43
3	D	3	FBI	O1S-S1	10.56	1.59	1.43
3	B	1	FBI	O1S-S1	10.47	1.59	1.43
3	B	1	FBI	O2S-S1	10.28	1.59	1.43
3	C	4	FBI	O2S-S1	10.27	1.59	1.43
3	C	4	FBI	C81-C8	-9.01	1.38	1.49
3	B	1	FBI	C81-C8	-8.58	1.39	1.49
3	D	3	FBI	C81-C8	-8.49	1.39	1.49
3	A	2	FBI	C81-C8	-8.46	1.39	1.49
3	A	2	FBI	S1-N3	4.81	1.74	1.64
3	D	3	FBI	S1-N3	4.61	1.74	1.64
3	C	4	FBI	C6-C7	-4.54	1.32	1.52
3	D	3	FBI	C9-C91	4.50	1.57	1.51
3	C	4	FBI	S1-N3	4.47	1.74	1.64
3	D	3	FBI	C6-C7	-4.40	1.33	1.52
3	A	2	FBI	C6-C7	-4.24	1.33	1.52
3	B	1	FBI	C6-C7	-4.22	1.33	1.52
3	A	2	FBI	C9-C91	3.95	1.56	1.51
3	C	4	FBI	C9-C91	3.91	1.56	1.51
2	C	103	ADP	C8-N7	-3.83	1.27	1.34
3	B	1	FBI	C9-C91	3.69	1.56	1.51
3	B	1	FBI	S1-N3	3.68	1.72	1.64
2	A	102	ADP	C8-N7	-3.54	1.28	1.34
2	A	101	ADP	C8-N7	-3.54	1.28	1.34
3	D	3	FBI	C10-C9	3.01	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	4	FBI	C7-C10	2.66	1.55	1.52
2	A	101	ADP	O4'-C4'	2.60	1.50	1.45
3	B	1	FBI	C8-C10	2.36	1.45	1.41
3	C	4	FBI	C11-N2	-2.33	1.30	1.34
2	C	103	ADP	O4'-C4'	2.24	1.50	1.45
2	C	103	ADP	C2'-C3'	2.20	1.59	1.53
3	A	2	FBI	C7-C10	2.16	1.55	1.52
3	A	2	FBI	C8-C10	2.16	1.45	1.41
3	B	1	FBI	C83-C84	2.08	1.41	1.37
2	A	102	ADP	O4'-C4'	2.05	1.49	1.45
3	B	1	FBI	C11-N1	-2.04	1.31	1.34
3	C	4	FBI	C83-C84	2.03	1.41	1.37
3	C	4	FBI	C11-N1	-2.02	1.31	1.34

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1	FBI	O2S-S1-O1S	-8.23	106.86	118.59
3	C	4	FBI	O2S-S1-O1S	-8.20	106.90	118.59
3	A	2	FBI	O2S-S1-O1S	-7.44	107.98	118.59
3	D	3	FBI	O2S-S1-O1S	-7.31	108.18	118.59
3	D	3	FBI	O1S-S1-N3	5.24	113.39	107.08
3	C	4	FBI	C7-C6-C5	5.13	124.93	115.05
3	D	3	FBI	C10-C9-N2	-4.46	118.90	122.67
3	A	2	FBI	O2S-S1-N3	4.23	112.18	107.08
3	A	2	FBI	C7-C6-C5	4.10	122.94	115.05
3	A	2	FBI	C10-C9-N2	-4.10	119.20	122.67
3	B	1	FBI	C10-C9-N2	-4.02	119.27	122.67
3	D	3	FBI	C7-C6-C5	3.98	122.70	115.05
3	B	1	FBI	C11-N2-C9	3.93	120.62	116.21
3	B	1	FBI	O2S-S1-N3	3.85	111.72	107.08
3	A	2	FBI	C11-N2-C9	3.82	120.49	116.21
3	B	1	FBI	C7-C6-C5	3.71	122.19	115.05
3	C	4	FBI	O1S-S1-N3	3.57	111.38	107.08
3	B	1	FBI	O1S-S1-N3	3.44	111.22	107.08
3	D	3	FBI	C11-N2-C9	3.42	120.05	116.21
3	C	4	FBI	C10-C9-N2	-3.39	119.81	122.67
3	C	4	FBI	C13-S1-N3	3.39	110.57	106.79
3	C	4	FBI	O2S-S1-N3	3.34	111.10	107.08
3	C	4	FBI	C11-N2-C9	3.33	119.94	116.21
3	D	3	FBI	C13-S1-N3	2.85	109.97	106.79
3	A	2	FBI	C13-S1-N3	2.78	109.89	106.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2	FBI	O1S-S1-N3	2.77	110.42	107.08
3	C	4	FBI	C10-C8-N1	-2.60	118.50	122.78
2	C	103	ADP	C3'-C2'-C1'	2.49	104.73	100.98
3	D	3	FBI	C92-C91-C9	2.46	115.11	110.96
3	C	4	FBI	C82-C81-C8	2.41	124.43	120.61
3	B	1	FBI	C10-C8-N1	-2.39	118.85	122.78
3	D	3	FBI	C10-C8-N1	-2.31	118.97	122.78
2	C	103	ADP	C2'-C3'-C4'	2.31	107.14	102.64
3	D	3	FBI	O2S-S1-N3	2.29	109.83	107.08
3	A	2	FBI	C10-C8-N1	-2.24	119.09	122.78
3	B	1	FBI	C13-S1-N3	2.05	109.07	106.79
2	A	101	ADP	C5-C6-N6	2.01	123.41	120.35

There are no chirality outliers.

All (21) torsion outliers are listed below:

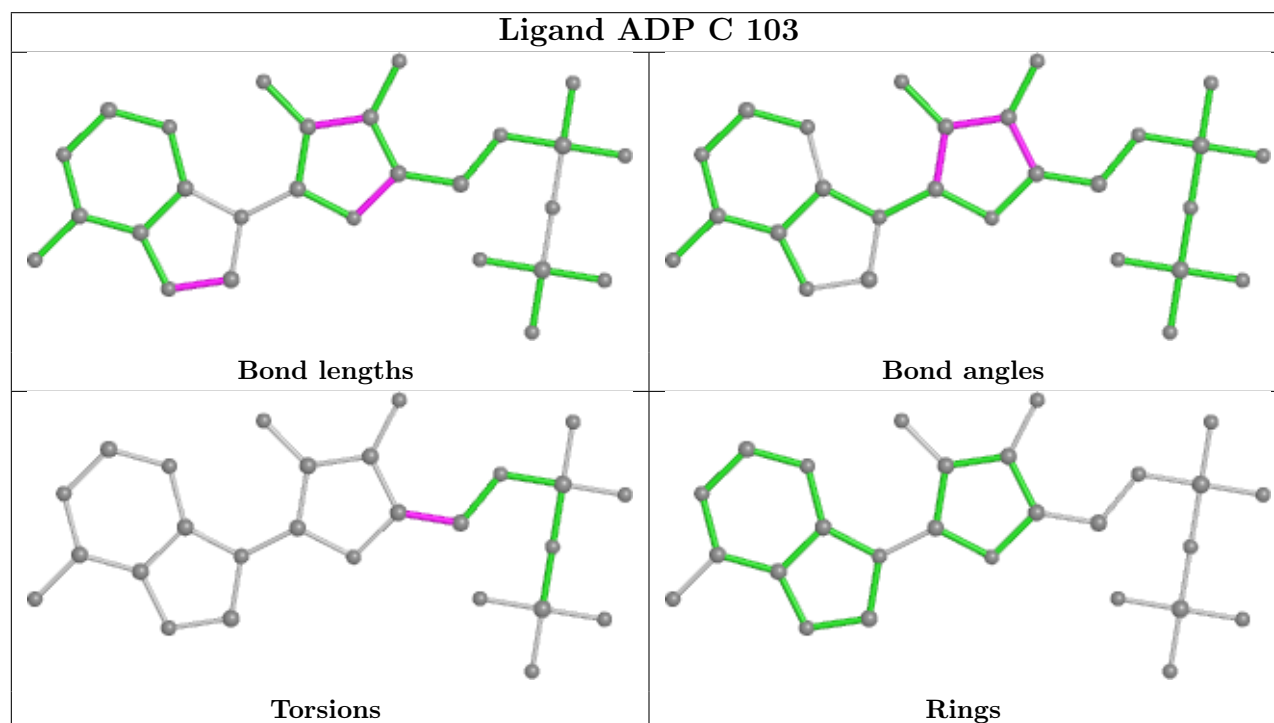
Mol	Chain	Res	Type	Atoms
2	A	101	ADP	O4'-C4'-C5'-O5'
2	A	101	ADP	C3'-C4'-C5'-O5'
3	A	2	FBI	C8-C10-C7-C6
3	A	2	FBI	C9-C10-C7-C6
3	A	2	FBI	C4-C5-C6-C7
3	B	1	FBI	C8-C10-C7-C6
3	B	1	FBI	C9-C10-C7-C6
3	B	1	FBI	C4-C5-C6-C7
3	C	4	FBI	O5-C5-C6-C7
3	D	3	FBI	C8-C10-C7-C6
3	D	3	FBI	C9-C10-C7-C6
3	D	3	FBI	C4-C5-C6-C7
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	102	ADP	O4'-C4'-C5'-O5'
2	A	101	ADP	PA-O3A-PB-O3B

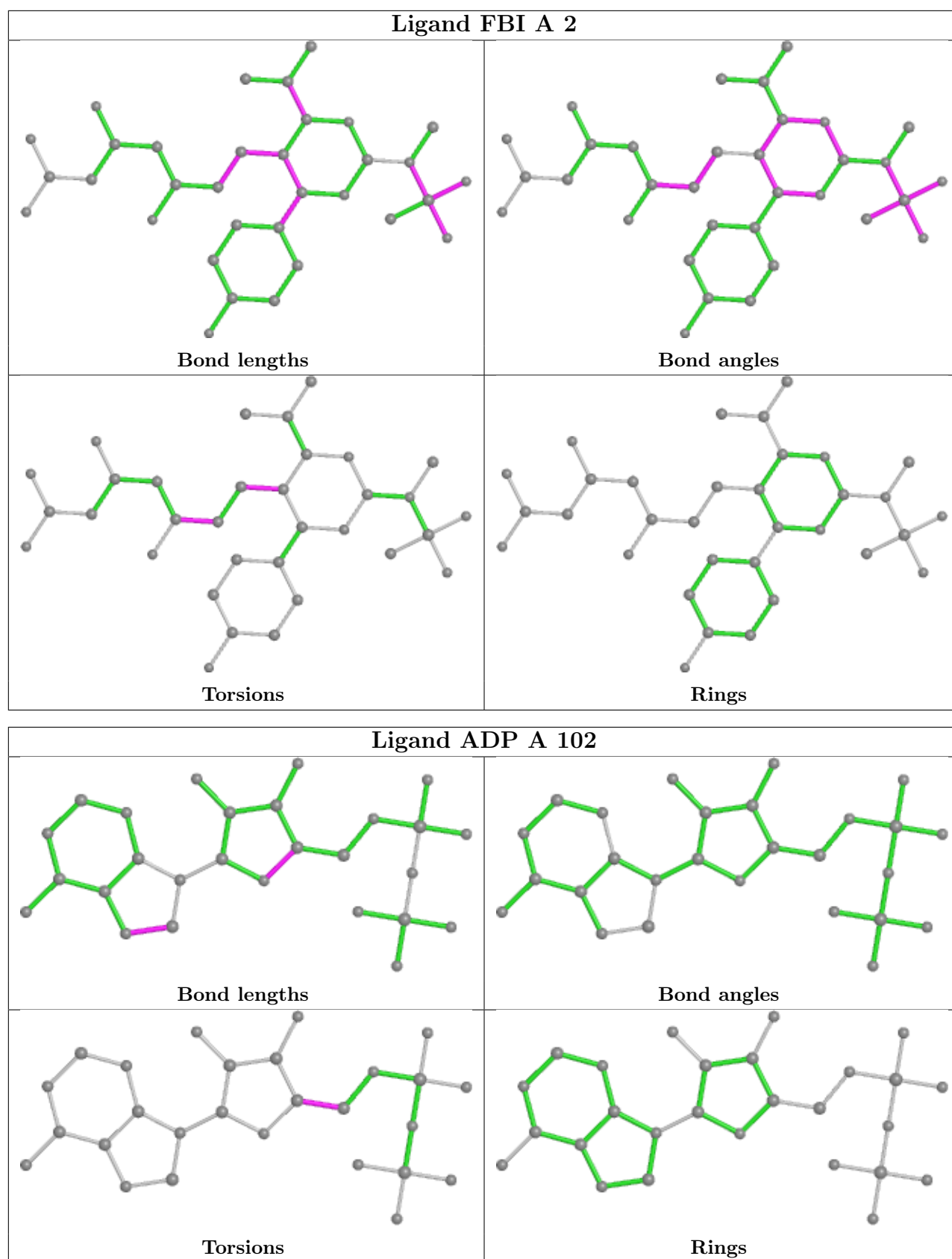
There are no ring outliers.

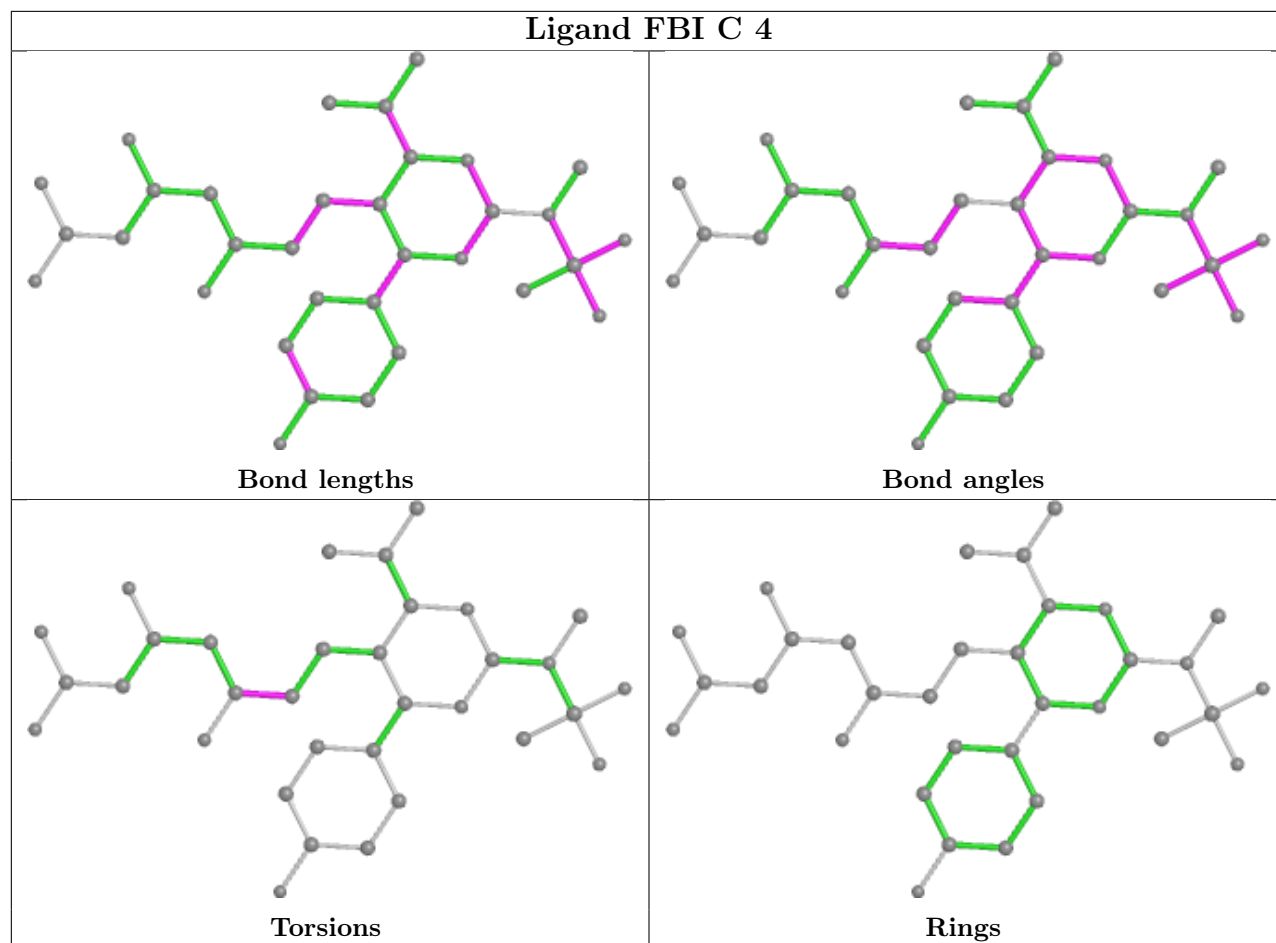
7 monomers are involved in 15 short contacts:

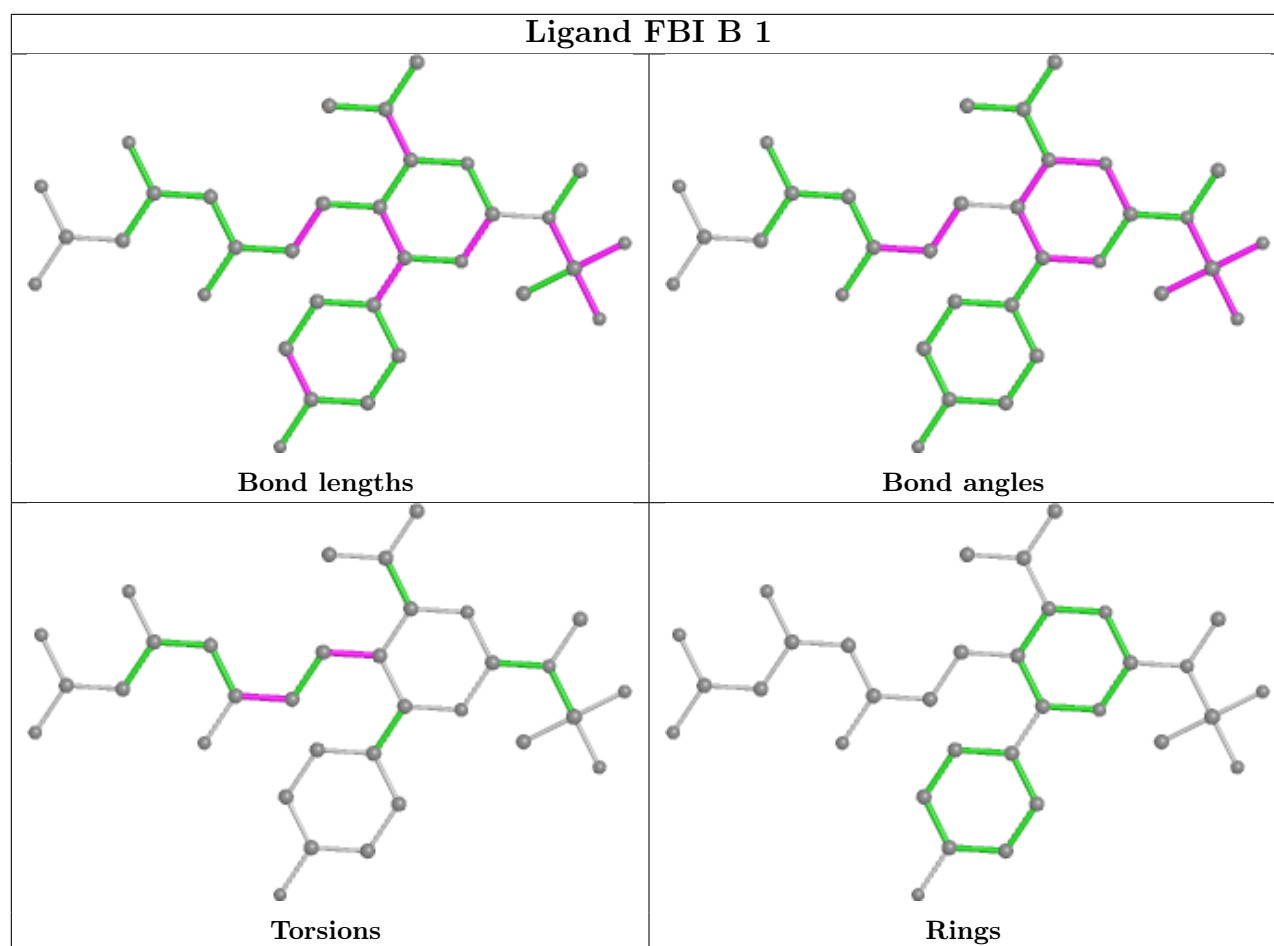
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	103	ADP	2	0
3	A	2	FBI	2	0
2	A	102	ADP	3	0
3	C	4	FBI	2	0
3	B	1	FBI	2	0
3	D	3	FBI	2	0
2	A	101	ADP	2	0

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.

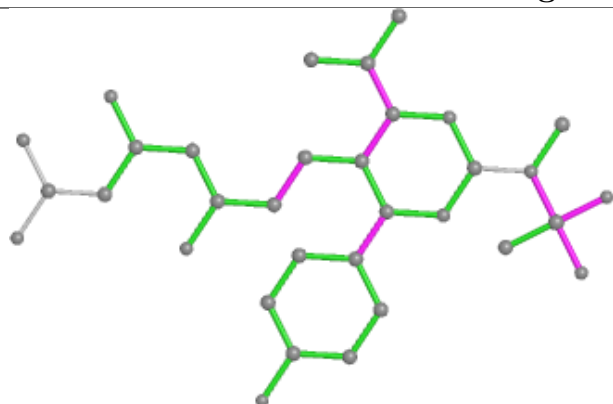




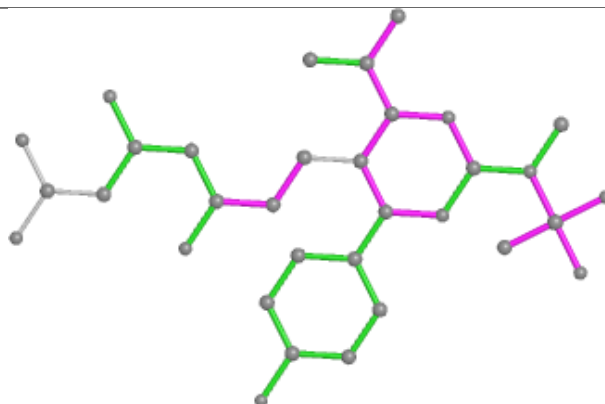




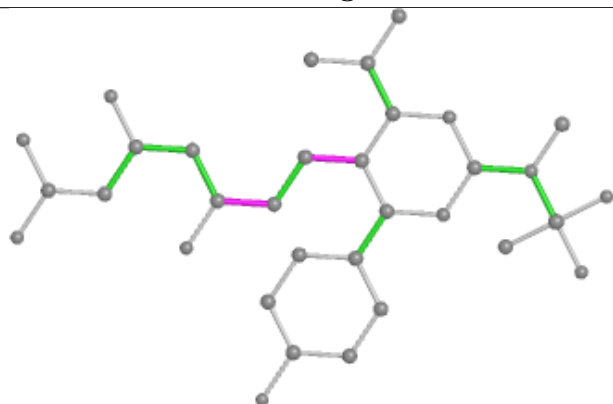
Ligand FBI D 3



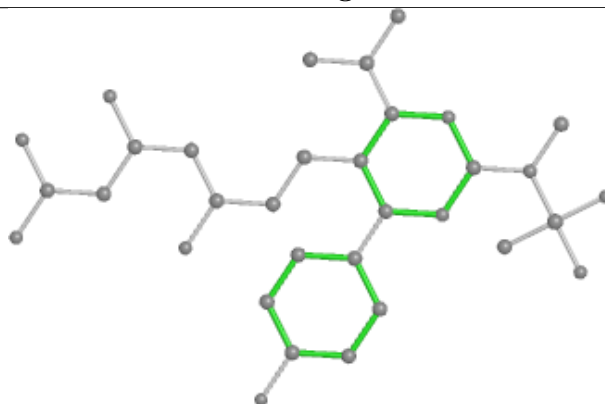
Bond lengths



Bond angles

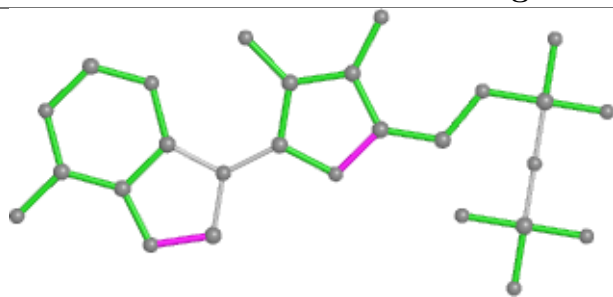


Torsions

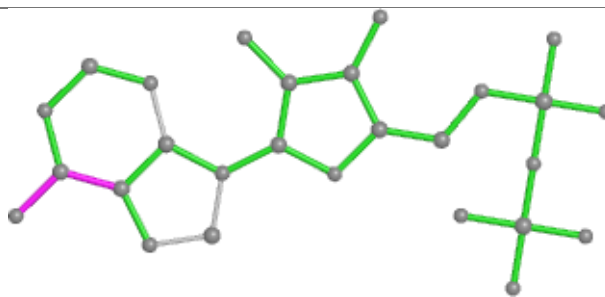


Rings

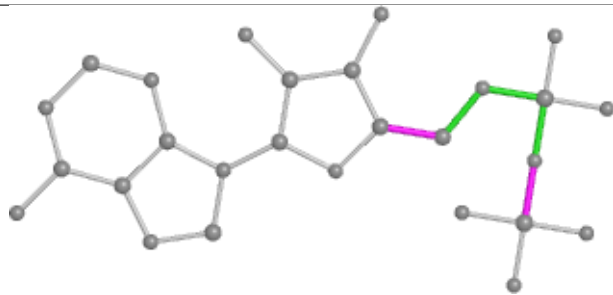
Ligand ADP A 101



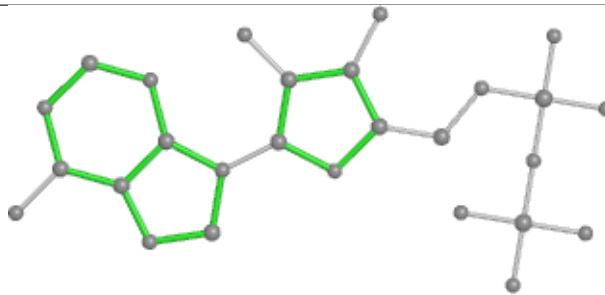
Bond lengths



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%)	0.87	73 (17%) 1 1	35, 52, 90, 97	0
1	B	398/467 (85%)	0.87	70 (17%) 1 1	35, 52, 82, 100	0
1	C	398/467 (85%)	0.84	70 (17%) 1 1	36, 54, 89, 99	0
1	D	382/467 (81%)	0.70	52 (13%) 3 4	35, 50, 75, 100	0
All	All	1585/1868 (84%)	0.82	265 (16%) 1 2	35, 52, 87, 100	0

All (265) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	483	THR	9.6
1	A	484	LEU	8.9
1	D	484	LEU	7.7
1	C	475	HIS	7.5
1	A	473	ALA	7.2
1	A	475	HIS	6.6
1	B	484	LEU	6.4
1	D	479	TYR	6.4
1	C	484	LEU	6.0
1	D	485	ILE	6.0
1	C	483	THR	5.9
1	B	481	LEU	5.9
1	A	476	ILE	5.6
1	A	471	VAL	5.6
1	B	477	PRO	5.6
1	A	483	THR	5.5
1	D	746	ILE	5.5
1	C	485	ILE	5.4
1	B	475	HIS	5.3
1	A	772	VAL	5.2
1	B	476	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	486	GLU	5.2
1	B	478	ALA	5.1
1	B	746	ILE	5.0
1	C	470	LEU	5.0
1	A	746	ILE	4.9
1	A	448	CYS	4.9
1	B	486	GLU	4.8
1	B	485	ILE	4.8
1	B	630	ARG	4.7
1	D	694	ALA	4.7
1	A	446	GLU	4.7
1	B	470	LEU	4.6
1	C	486	GLU	4.6
1	C	471	VAL	4.5
1	A	470	LEU	4.4
1	C	674	TYR	4.4
1	A	694	ALA	4.4
1	B	471	VAL	4.3
1	B	469	GLN	4.3
1	D	627	ARG	4.2
1	D	481	LEU	4.1
1	D	772	VAL	4.1
1	C	627	ARG	4.1
1	D	524	GLY	4.0
1	D	516	ASP	4.0
1	B	693	PRO	3.9
1	A	699	ILE	3.9
1	C	741	ALA	3.9
1	B	694	ALA	3.8
1	A	467	ILE	3.8
1	C	772	VAL	3.8
1	C	694	ALA	3.8
1	B	749	TYR	3.8
1	D	695	ALA	3.8
1	A	777	CYS	3.7
1	D	523	MET	3.7
1	B	479	TYR	3.7
1	A	461	PHE	3.7
1	C	515	ARG	3.7
1	B	754	ALA	3.6
1	D	828	LYS	3.6
1	A	698	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	777	CYS	3.6
1	A	769	ALA	3.6
1	D	743	ALA	3.6
1	C	746	ILE	3.6
1	D	482	GLU	3.6
1	C	628	PHE	3.5
1	C	467	ILE	3.5
1	C	523	MET	3.5
1	C	773	GLY	3.5
1	A	828	LYS	3.5
1	C	476	ILE	3.5
1	D	699	ILE	3.4
1	A	744	GLY	3.4
1	C	769	ALA	3.4
1	A	466	GLU	3.4
1	B	483	THR	3.4
1	B	467	ILE	3.3
1	D	745	SER	3.3
1	C	477	PRO	3.3
1	A	778	ILE	3.3
1	B	698	TRP	3.3
1	B	480	LYS	3.3
1	C	695	ALA	3.3
1	C	718	ARG	3.3
1	B	772	VAL	3.3
1	D	744	GLY	3.3
1	A	474	LYS	3.3
1	A	479	TYR	3.3
1	A	741	ALA	3.3
1	B	741	ALA	3.3
1	C	740	SER	3.2
1	A	630	ARG	3.2
1	B	620	GLU	3.2
1	C	753	ALA	3.2
1	D	696	ILE	3.2
1	B	487	THR	3.2
1	C	473	ALA	3.2
1	C	743	ALA	3.2
1	C	487	THR	3.2
1	D	747	GLY	3.1
1	A	627	ARG	3.1
1	A	773	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	749	TYR	3.1
1	D	693	PRO	3.1
1	A	462	LEU	3.1
1	B	756	ILE	3.1
1	C	757	VAL	3.1
1	B	757	VAL	3.1
1	B	695	ALA	3.1
1	A	689	THR	3.1
1	C	745	SER	3.0
1	B	758	THR	3.0
1	A	748	GLY	3.0
1	C	698	TRP	3.0
1	A	693	PRO	3.0
1	B	743	ALA	3.0
1	A	749	TYR	3.0
1	B	523	MET	3.0
1	B	748	GLY	3.0
1	A	481	LEU	3.0
1	A	447	GLU	3.0
1	C	742	MET	2.9
1	B	474	LYS	2.9
1	C	699	ILE	2.9
1	A	472	ASN	2.9
1	A	754	ALA	2.9
1	A	745	SER	2.9
1	B	778	ILE	2.9
1	D	490	ARG	2.9
1	B	740	SER	2.8
1	C	608	TRP	2.8
1	A	443	ARG	2.8
1	B	473	ALA	2.8
1	C	482	GLU	2.8
1	A	486	GLU	2.8
1	A	829	ASP	2.8
1	D	487	THR	2.8
1	B	516	ASP	2.7
1	C	524	GLY	2.7
1	D	748	GLY	2.7
1	D	630	ARG	2.7
1	D	829	ASP	2.7
1	D	698	TRP	2.7
1	D	511	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	696	ILE	2.7
1	C	829	ASP	2.7
1	B	828	LYS	2.7
1	B	613	GLU	2.7
1	C	693	PRO	2.7
1	C	478	ALA	2.7
1	D	758	THR	2.7
1	A	771	ASN	2.7
1	D	749	TYR	2.6
1	C	738	VAL	2.6
1	C	744	GLY	2.6
1	C	747	GLY	2.6
1	D	777	CYS	2.6
1	D	778	ILE	2.6
1	C	548	GLU	2.6
1	C	754	ALA	2.6
1	A	672	HIS	2.6
1	C	490	ARG	2.6
1	A	798	PRO	2.6
1	A	695	ALA	2.6
1	A	501	LYS	2.6
1	B	737	LEU	2.6
1	B	677	GLU	2.6
1	A	740	SER	2.6
1	A	760	ILE	2.6
1	A	688	CYS	2.6
1	D	786	PRO	2.6
1	C	719	GLU	2.6
1	D	515	ARG	2.5
1	B	753	ALA	2.5
1	D	753	ALA	2.5
1	A	524	GLY	2.5
1	C	469	GLN	2.5
1	A	743	ALA	2.5
1	A	697	ASN	2.5
1	D	775	SER	2.5
1	D	773	GLY	2.5
1	C	771	ASN	2.5
1	A	444	PRO	2.5
1	B	674	TYR	2.5
1	C	464	ASP	2.5
1	D	737	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	770	GLN	2.4
1	A	846	VAL	2.4
1	A	756	ILE	2.4
1	A	830	ASN	2.4
1	C	670	LYS	2.4
1	C	777	CYS	2.4
1	A	758	THR	2.4
1	B	745	SER	2.4
1	B	744	GLY	2.4
1	A	620	GLU	2.4
1	A	523	MET	2.4
1	D	494	ILE	2.4
1	C	666	LYS	2.4
1	C	616	ALA	2.4
1	A	687	TYR	2.4
1	C	761	TYR	2.4
1	B	773	GLY	2.4
1	D	628	PHE	2.3
1	C	480	LYS	2.3
1	C	488	HIS	2.3
1	A	747	GLY	2.3
1	D	740	SER	2.3
1	C	775	SER	2.3
1	B	488	HIS	2.3
1	B	628	PHE	2.3
1	B	769	ALA	2.3
1	B	846	VAL	2.3
1	C	768	ALA	2.3
1	B	719	GLU	2.2
1	B	750	ASN	2.2
1	B	688	CYS	2.2
1	B	751	ALA	2.2
1	B	738	VAL	2.2
1	B	673	GLU	2.2
1	B	696	ILE	2.2
1	C	571	ARG	2.2
1	A	575	LEU	2.2
1	C	481	LEU	2.2
1	C	617	VAL	2.2
1	A	761	TYR	2.2
1	C	748	GLY	2.2
1	B	747	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	624	SER	2.1
1	D	787	THR	2.1
1	B	633	LYS	2.1
1	B	671	LEU	2.1
1	B	776	ASN	2.1
1	A	774	SER	2.1
1	B	666	LYS	2.1
1	A	751	ALA	2.1
1	D	769	ALA	2.1
1	B	608	TRP	2.1
1	B	752	HIS	2.1
1	C	620	GLU	2.1
1	A	692	LYS	2.1
1	C	494	ILE	2.1
1	C	516	ASP	2.1
1	C	613	GLU	2.1
1	A	768	ALA	2.1
1	D	510	GLN	2.1
1	A	739	GLY	2.1
1	B	739	GLY	2.1
1	D	620	GLU	2.0
1	D	774	SER	2.0
1	A	445	ASN	2.0
1	A	490	ARG	2.0
1	D	497	GLN	2.0
1	B	771	ASN	2.0
1	D	776	ASN	2.0
1	B	501	LYS	2.0
1	C	828	LYS	2.0
1	A	789	GLU	2.0
1	B	597	PRO	2.0
1	D	754	ALA	2.0
1	C	630	ARG	2.0
1	D	738	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

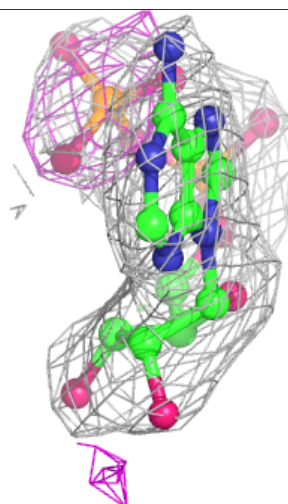
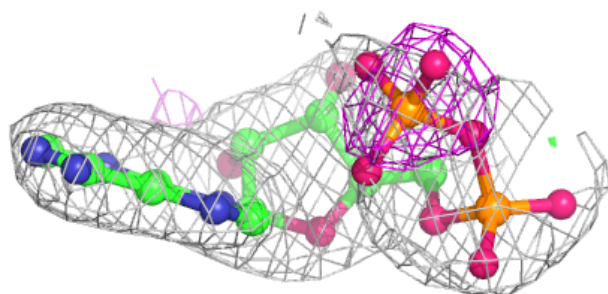
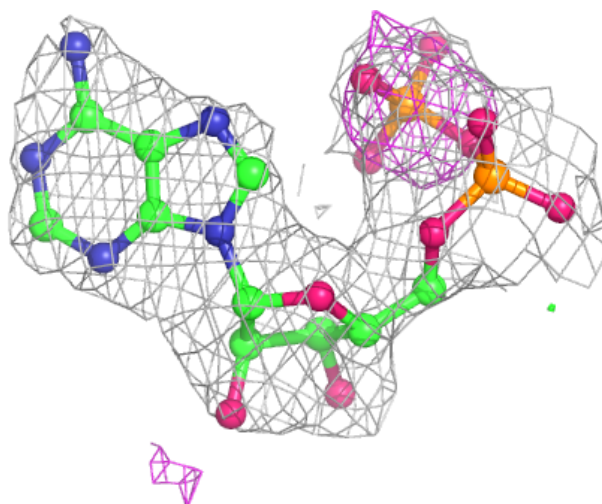
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	A	101	27/27	0.75	0.26	90,93,99,99	0
2	ADP	C	103	27/27	0.78	0.25	83,88,99,99	0
2	ADP	A	102	27/27	0.79	0.26	88,91,99,99	0
3	FBI	D	3	33/33	0.91	0.13	44,51,57,58	0
3	FBI	B	1	33/33	0.93	0.13	46,54,59,59	0
3	FBI	C	4	33/33	0.93	0.14	44,51,57,57	0
3	FBI	A	2	33/33	0.93	0.14	41,48,52,53	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.

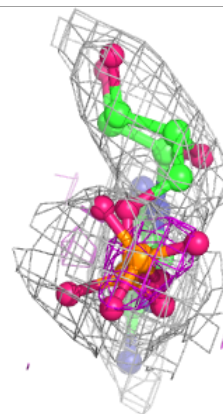
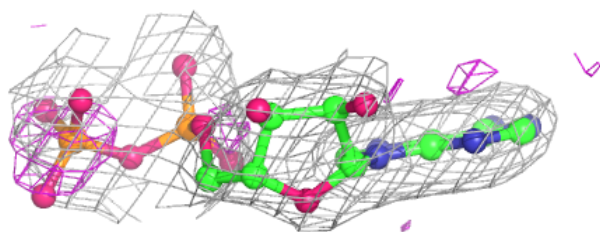
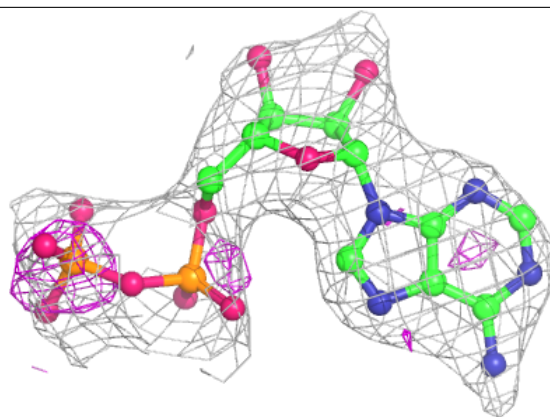
Electron density around ADP A 101:

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

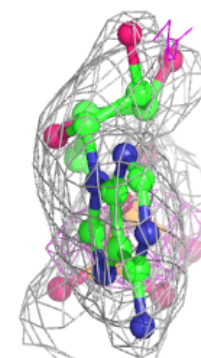
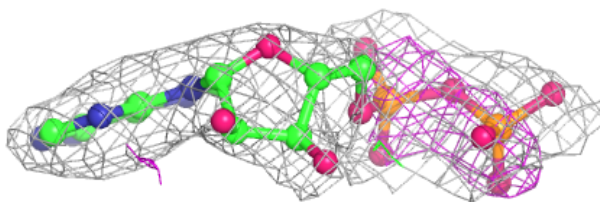
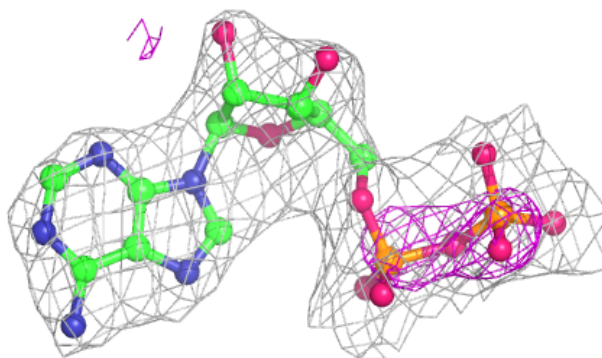


Electron density around ADP C 103:

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

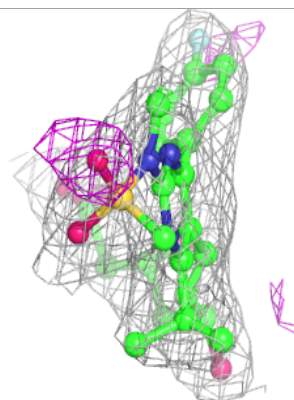
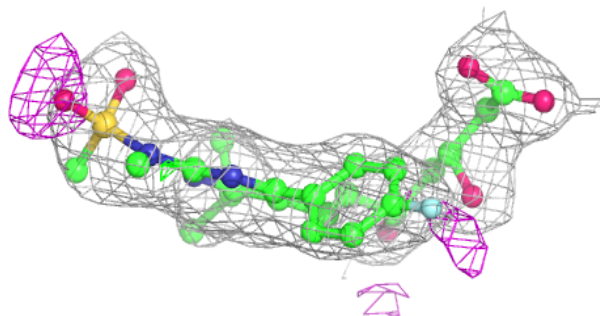
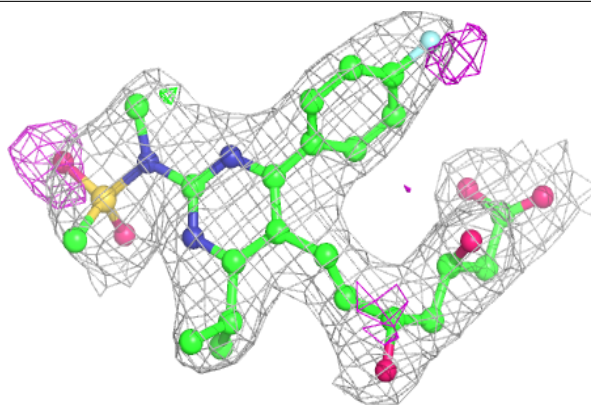
**Electron density around ADP A 102:**

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

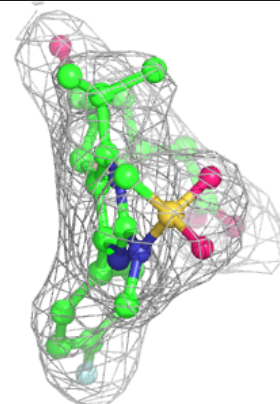
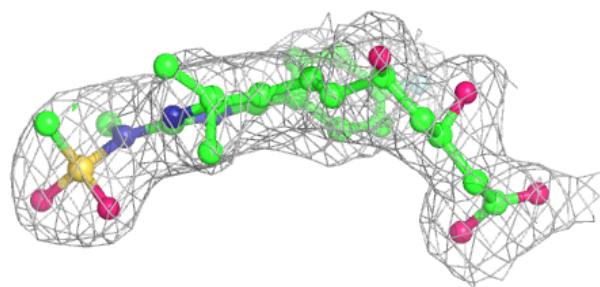
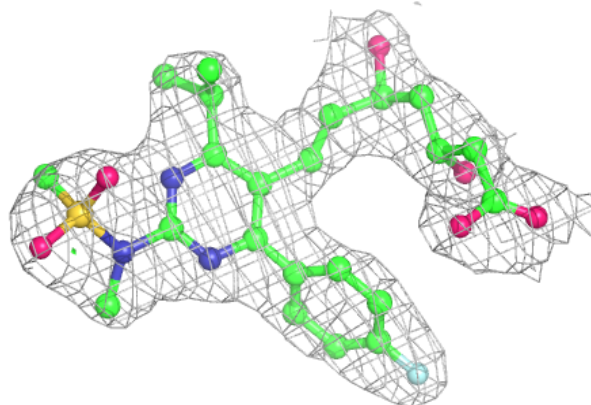


Electron density around FBI D 3:

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

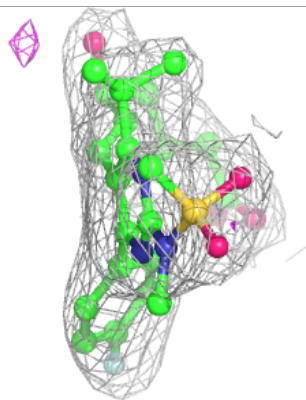
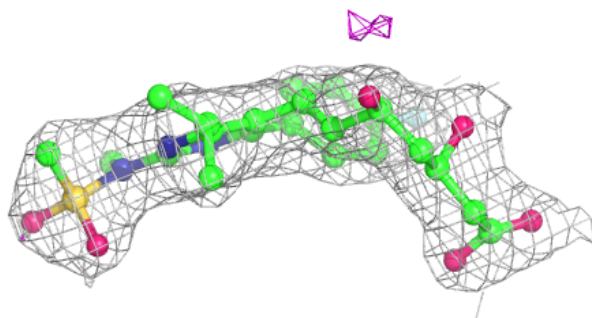
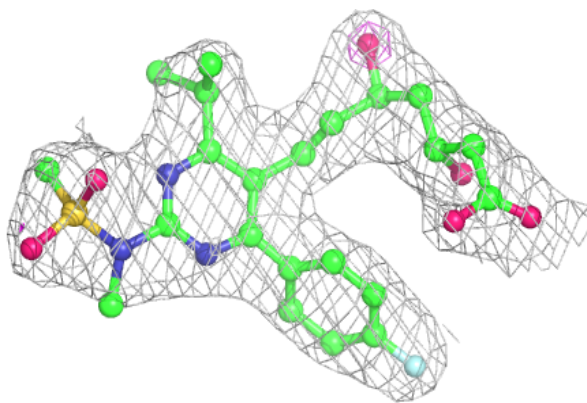
**Electron density around FBI B 1:**

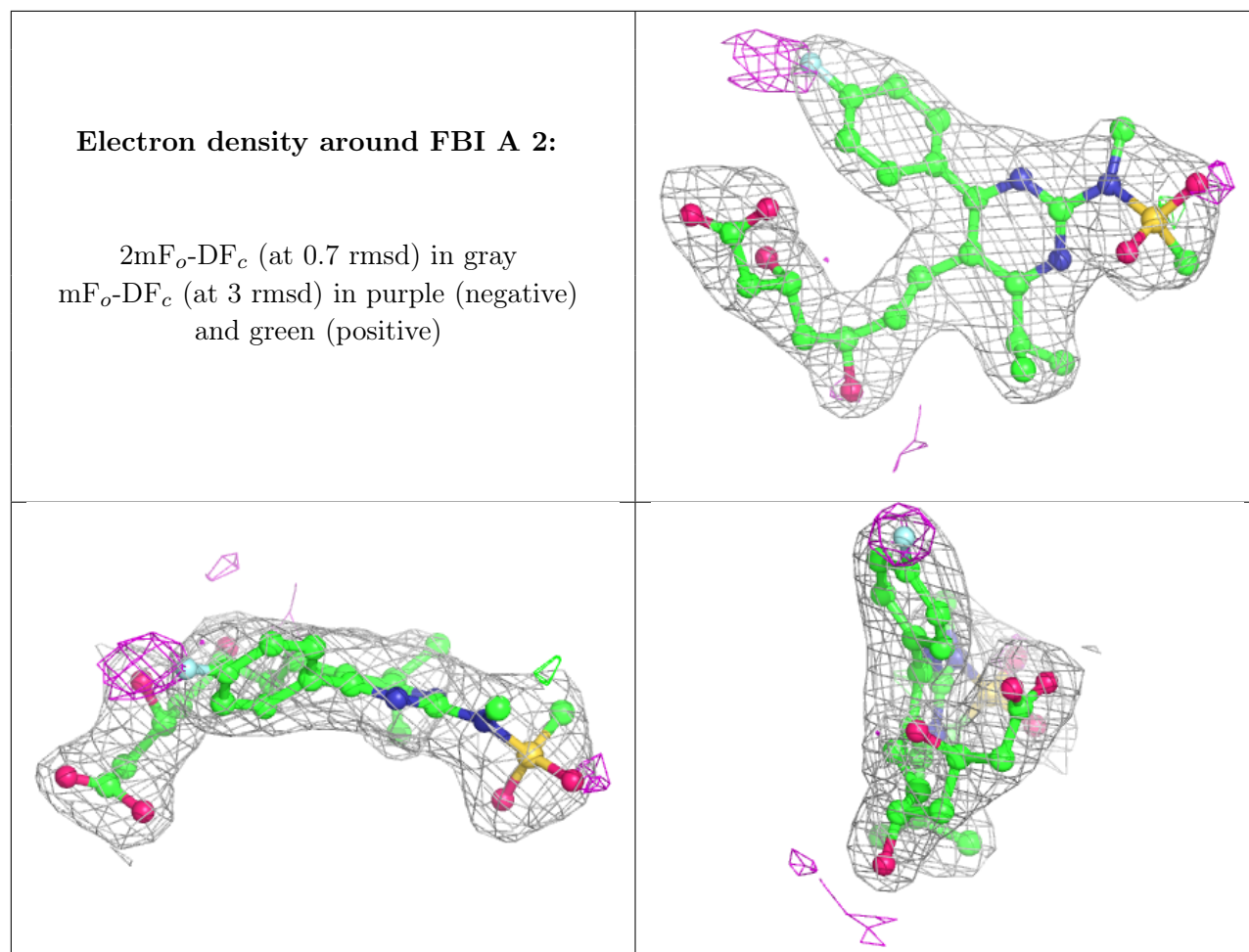
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.