



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:25 PM UTC

PDB ID : 4CY8 / pdb_00004cy8
Title : 2-hydroxybiphenyl 3-monooxygenase (HbpA) in complex with FAD
Authors : Jensen, C.N.; Farrugia, J.E.; Frank, A.; Man, H.; Hart, S.; Turkenburg, J.P.; Grogan, G.
Deposited on : 2014-04-10
Resolution : 2.03 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

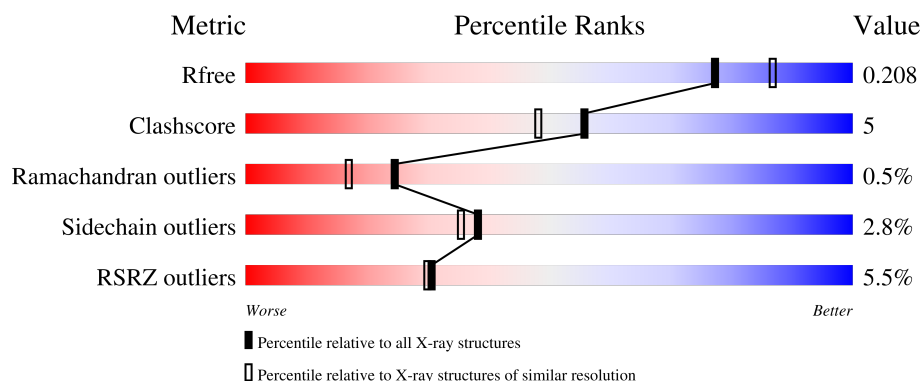
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	586	
1	B	586	
1	C	586	
1	D	586	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17641 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.

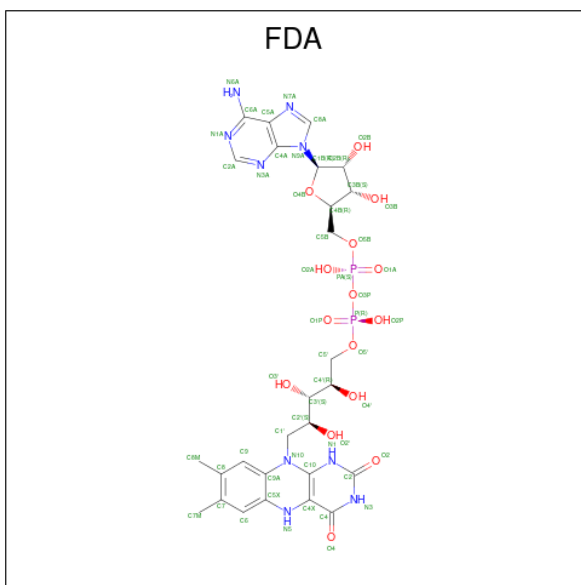
- Molecule 1 is a protein called 2-HYDROXYBIPHENYL 3-MONOOXYGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	539	Total	C	N	O	S	0	0	0
			3999	2533	700	748	18			
1	B	535	Total	C	N	O	S	0	0	0
			3939	2491	696	734	18			
1	C	530	Total	C	N	O	S	0	0	0
			3916	2472	693	734	17			
1	D	537	Total	C	N	O	S	0	0	0
			3968	2514	694	742	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	347	GLN	THR	engineered mutation	UNP O06647
B	347	GLN	THR	engineered mutation	UNP O06647
C	347	GLN	THR	engineered mutation	UNP O06647
D	347	GLN	THR	engineered mutation	UNP O06647

- Molecule 2 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (CCD ID: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

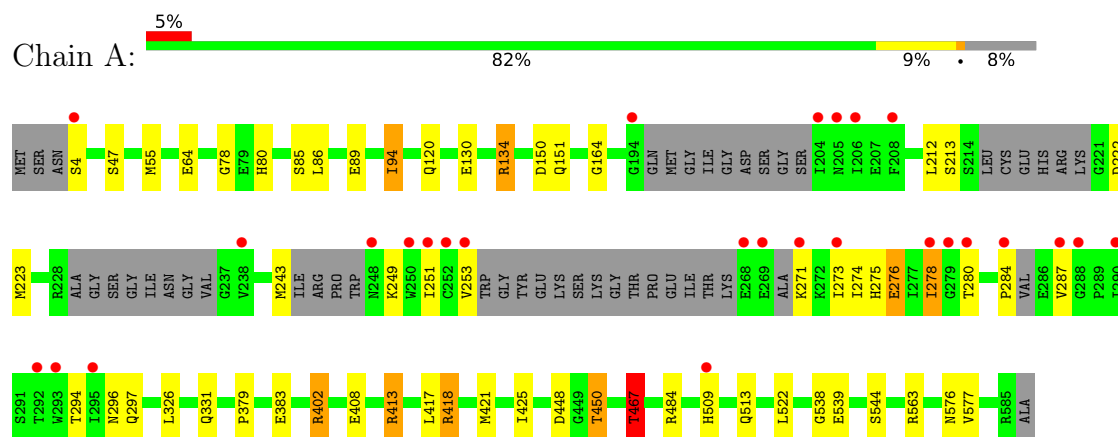
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	417	Total O 417 417	0	0
3	B	417	Total O 417 417	0	0
3	C	404	Total O 404 404	0	0
3	D	369	Total O 369 369	0	0

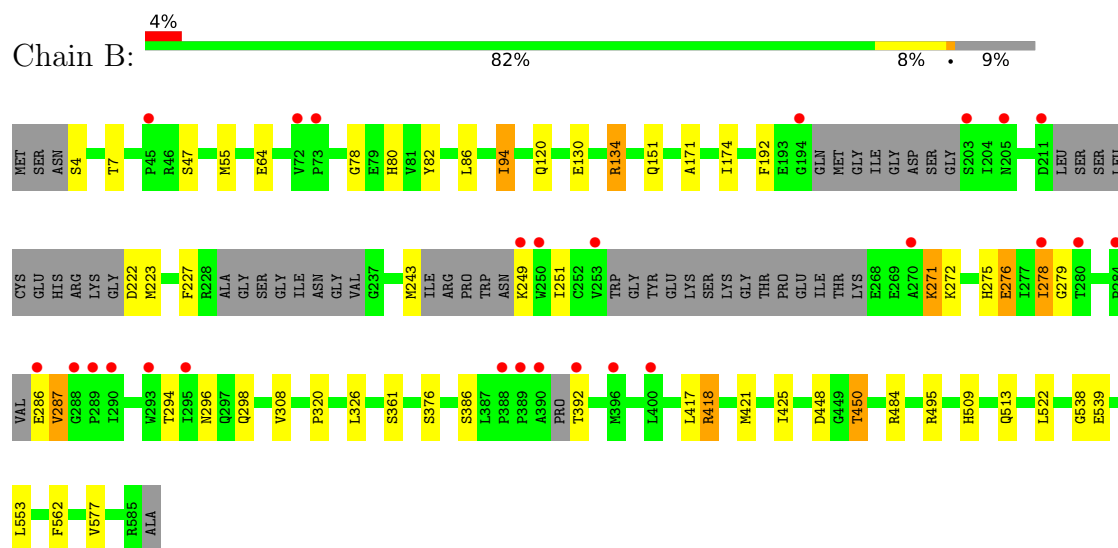
3 Residue-property plots [i](#)

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.

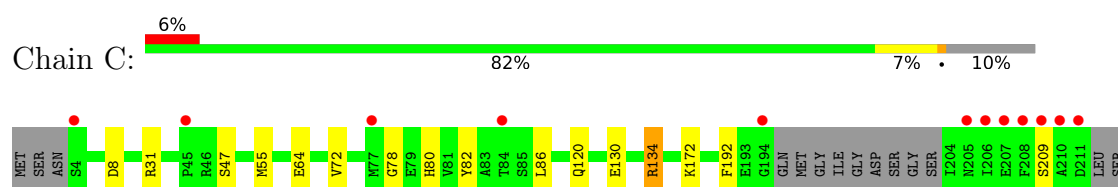
• Molecule 1: 2-HYDROXYBIPHENYL 3-MONOOXYGENASE

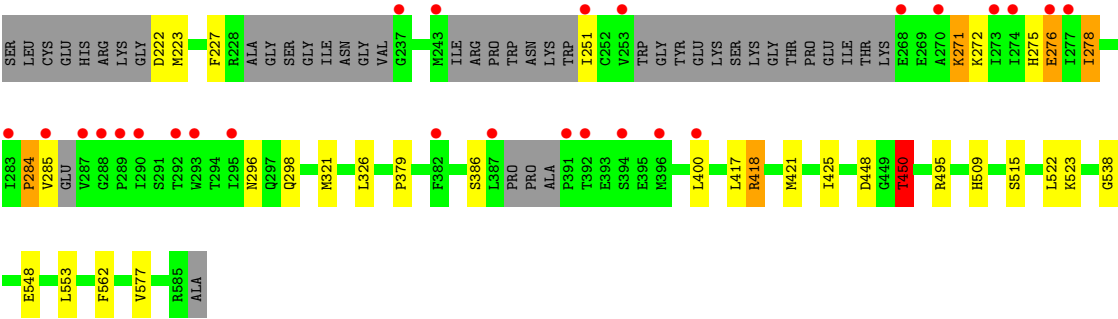


• Molecule 1: 2-HYDROXYBIPHENYL 3-MONOOXYGENASE

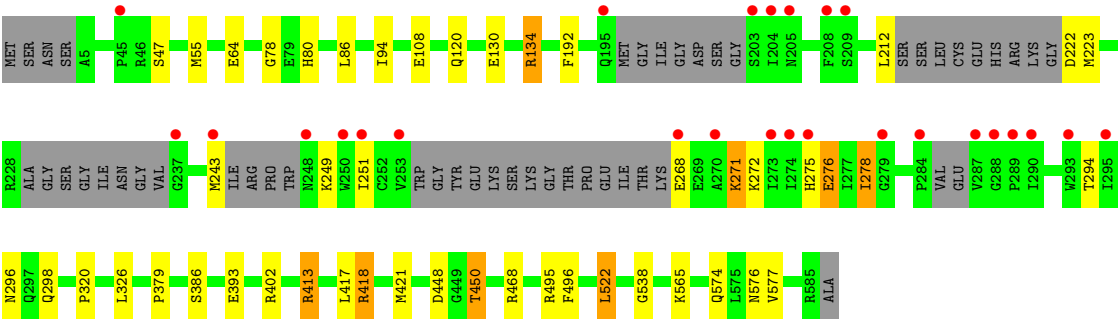
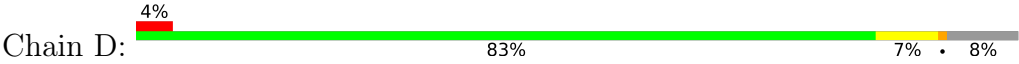


• Molecule 1: 2-HYDROXYBIPHENYL 3-MONOOXYGENASE





● Molecule 1: 2-HYDROXYBIPHENYL 3-MONOOXYGENASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.00Å 96.18Å 102.16Å 114.09° 95.80° 109.31°	Depositor
Resolution (Å)	59.53 – 2.03 59.53 – 2.03	Depositor EDS
% Data completeness (in resolution range)	90.0 (59.53-2.03) 90.0 (59.53-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.169 , 0.202 (Not available) , 0.208	Depositor DCC
R_{free} test set	7349 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17641	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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: FDA

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	1.11	2/4080 (0.0%)	1.06	10/5541 (0.2%)
1	B	1.10	2/4017 (0.0%)	1.02	5/5454 (0.1%)
1	C	1.11	4/3990 (0.1%)	1.02	6/5415 (0.1%)
1	D	1.12	1/4048 (0.0%)	1.00	4/5500 (0.1%)
All	All	1.11	9/16135 (0.1%)	1.03	25/21910 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	9

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	418	ARG	CD-NE	-7.86	1.35	1.46
1	A	418	ARG	CD-NE	-7.28	1.36	1.46
1	C	418	ARG	CD-NE	-5.85	1.38	1.46
1	B	418	ARG	CD-NE	-5.35	1.38	1.46
1	B	361	SER	N-CA	5.31	1.51	1.46
1	C	515	SER	CA-C	5.08	1.59	1.52
1	A	331	GLN	CA-C	5.03	1.59	1.52
1	C	72	VAL	CA-C	5.02	1.57	1.53
1	C	548	GLU	N-CA	-5.00	1.40	1.46

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ILE	N-CA-CB	-8.96	102.06	111.64
1	A	418	ARG	NE-CZ-NH2	-8.41	111.63	119.20
1	A	467	THR	N-CA-CB	-8.09	98.19	110.73
1	C	418	ARG	NE-CZ-NH2	-7.39	112.55	119.20
1	B	94	ILE	N-CA-CB	-7.16	103.98	111.64
1	B	78	GLY	N-CA-C	7.02	122.78	113.37
1	D	418	ARG	NE-CZ-NH2	-7.00	112.90	119.20
1	A	94	ILE	CB-CA-C	6.75	115.94	109.33
1	B	418	ARG	NE-CZ-NH2	-6.75	113.13	119.20
1	A	78	GLY	N-CA-C	6.34	121.87	113.37
1	D	78	GLY	N-CA-C	6.04	121.47	114.16
1	A	379	PRO	N-CA-C	6.04	118.07	110.70
1	B	94	ILE	CB-CA-C	5.72	114.94	109.33
1	C	78	GLY	N-CA-C	5.65	120.94	113.37
1	C	272	LYS	N-CA-C	-5.59	106.35	112.72
1	A	418	ARG	NE-CZ-NH1	5.56	127.06	121.50
1	C	450	THR	CB-CA-C	5.44	116.70	108.86
1	B	272	LYS	N-CA-C	-5.34	106.54	112.57
1	C	400	LEU	N-CA-C	5.25	117.00	111.28
1	D	379	PRO	N-CA-C	5.20	117.04	110.70
1	C	379	PRO	N-CA-C	5.15	116.98	110.70
1	A	150	ASP	CA-C-N	5.14	127.69	120.28
1	A	150	ASP	C-N-CA	5.14	127.69	120.28
1	A	467	THR	OG1-CB-CG2	5.13	119.57	109.30
1	D	272	LYS	N-CA-C	-5.06	106.95	112.72

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	LYS	Peptide
1	A	278	ILE	Peptide
1	B	271	LYS	Peptide
1	B	278	ILE	Peptide
1	C	271	LYS	Peptide
1	C	278	ILE	Peptide
1	C	284	PRO	Peptide
1	D	271	LYS	Peptide
1	D	278	ILE	Peptide

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	3999	0	3847	46	4
1	B	3939	0	3758	39	0
1	C	3916	0	3748	36	0
1	D	3968	0	3805	30	0
2	A	53	0	33	2	0
2	B	53	0	33	3	0
2	C	53	0	33	3	0
2	D	53	0	33	3	0
3	A	417	0	0	20	0
3	B	417	0	0	18	1
3	C	404	0	0	13	3
3	D	369	0	0	8	0
All	All	17641	0	15290	147	4

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 (147) 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:B:308:VAL:HG22	3:B:2169:HOH:O	1.49	1.10
1:B:174:ILE:HB	3:B:2169:HOH:O	1.51	1.10
1:A:296:ASN:HB2	3:A:2209:HOH:O	1.53	1.07
1:C:425:ILE:HG22	3:C:2257:HOH:O	1.56	1.01
1:D:576:ASN:HB3	3:D:2364:HOH:O	1.67	0.93
1:B:539:GLU:HG2	3:B:2189:HOH:O	1.72	0.89
1:A:284:PRO:N	3:A:2206:HOH:O	2.06	0.87
1:A:4:SER:CB	3:A:2002:HOH:O	2.23	0.87
1:D:320:PRO:O	3:D:2179:HOH:O	1.93	0.84
1:A:539:GLU:HG2	3:A:2196:HOH:O	1.78	0.82
1:A:425:ILE:HG22	3:A:2303:HOH:O	1.79	0.81
1:A:467:THR:HG21	1:A:544:SER:O	1.79	0.81
1:B:425:ILE:HG22	3:B:2272:HOH:O	1.81	0.81
1:A:164:GLY:O	3:A:2174:HOH:O	1.98	0.81
1:A:275:HIS:O	1:A:276:GLU:CB	2.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:LEU:H	2:A:1586:FDA:HN1	1.31	0.79
1:C:275:HIS:O	1:C:276:GLU:CB	2.33	0.77
1:B:278:ILE:CB	3:B:2194:HOH:O	2.34	0.76
1:C:8:ASP:OD2	3:C:2005:HOH:O	2.03	0.75
1:A:576:ASN:HB3	3:A:2411:HOH:O	1.85	0.75
1:C:82:TYR:HD1	1:C:227:PHE:HE1	1.31	0.74
1:D:275:HIS:O	1:D:276:GLU:CB	2.36	0.73
1:D:108:GLU:CD	3:D:2087:HOH:O	2.32	0.71
1:B:275:HIS:O	1:B:276:GLU:CB	2.39	0.70
1:D:418:ARG:HD2	3:D:2243:HOH:O	1.90	0.70
1:A:576:ASN:OD1	3:A:2369:HOH:O	2.12	0.67
1:D:268:GLU:N	3:D:2159:HOH:O	2.27	0.67
1:A:418:ARG:HD2	3:A:2297:HOH:O	1.94	0.67
1:D:418:ARG:CD	3:D:2243:HOH:O	2.43	0.67
1:B:279:GLY:HA2	3:B:2194:HOH:O	1.94	0.66
1:C:425:ILE:HB	3:C:2256:HOH:O	1.95	0.66
1:B:418:ARG:CD	3:B:2267:HOH:O	2.42	0.66
1:B:418:ARG:HD2	3:B:2267:HOH:O	1.96	0.66
1:B:326:LEU:H	2:B:1586:FDA:HN1	1.43	0.65
1:C:321:MET:HE2	3:C:2199:HOH:O	1.97	0.65
1:C:209:SER:O	1:C:285:VAL:CB	2.45	0.64
1:C:326:LEU:H	2:C:1586:FDA:HN1	1.44	0.64
1:A:85:SER:OG	3:A:2080:HOH:O	2.15	0.64
1:C:82:TYR:HD1	1:C:227:PHE:CE1	2.15	0.63
1:A:418:ARG:CD	3:A:2297:HOH:O	2.48	0.61
3:A:2382:HOH:O	1:C:418:ARG:HD2	2.01	0.61
1:B:275:HIS:CB	3:B:2195:HOH:O	2.49	0.61
1:A:467:THR:CG2	1:A:563:ARG:HH11	2.14	0.60
1:A:274:ILE:O	1:A:278:ILE:HG22	2.02	0.60
1:A:243:MET:HG2	1:A:249:LYS:O	2.03	0.59
1:B:275:HIS:HA	3:B:2194:HOH:O	2.02	0.59
1:B:320:PRO:O	3:B:2214:HOH:O	2.16	0.58
1:B:243:MET:HG2	1:B:249:LYS:O	2.03	0.58
1:C:523:LYS:CB	3:C:2331:HOH:O	2.51	0.58
1:D:243:MET:HG2	1:D:249:LYS:O	2.03	0.58
1:A:212:LEU:HD22	1:A:278:ILE:HD11	1.85	0.58
1:C:31:ARG:HD2	3:C:2016:HOH:O	2.04	0.58
1:B:495:ARG:NE	3:B:2341:HOH:O	2.21	0.57
1:C:222:ASP:CB	3:C:2077:HOH:O	2.53	0.56
3:A:2382:HOH:O	1:C:418:ARG:CD	2.53	0.56
1:B:130:GLU:OE2	1:B:134:ARG:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:OE2	1:A:134:ARG:HD2	2.05	0.56
1:C:130:GLU:OE2	1:C:134:ARG:HD2	2.05	0.55
1:D:130:GLU:OE2	1:D:134:ARG:HD2	2.06	0.55
1:B:418:ARG:HD3	3:B:2267:HOH:O	2.05	0.55
1:A:418:ARG:HD3	1:C:538:GLY:HA3	1.88	0.55
1:C:284:PRO:HA	3:C:2181:HOH:O	2.07	0.54
1:D:326:LEU:H	2:D:1586:FDA:HN1	1.55	0.54
1:B:55:MET:HE3	1:B:64:GLU:HG3	1.90	0.54
1:B:80:HIS:CD2	1:B:223:MET:HB3	2.43	0.54
1:C:80:HIS:CD2	1:C:223:MET:HB3	2.43	0.54
1:B:392:THR:CB	3:B:2259:HOH:O	2.56	0.53
1:D:393:GLU:CB	3:D:2226:HOH:O	2.57	0.53
1:A:538:GLY:HA3	1:C:418:ARG:HD3	1.91	0.53
1:A:222:ASP:CB	3:A:2078:HOH:O	2.57	0.52
1:B:538:GLY:HA3	1:D:418:ARG:HD3	1.92	0.52
1:A:425:ILE:CG2	3:A:2303:HOH:O	2.48	0.52
1:C:425:ILE:CG2	3:C:2257:HOH:O	2.33	0.52
1:D:402:ARG:NE	1:D:413:ARG:NH2	2.58	0.51
1:C:55:MET:HE3	1:C:64:GLU:HG3	1.91	0.51
1:D:402:ARG:CD	1:D:413:ARG:HH21	2.23	0.51
1:D:55:MET:HE3	1:D:64:GLU:HG3	1.92	0.51
1:A:55:MET:HE3	1:A:64:GLU:HG3	1.92	0.50
1:A:467:THR:HG22	1:A:563:ARG:HH11	1.76	0.50
1:A:278:ILE:HG23	1:A:280:THR:H	1.76	0.50
1:C:417:LEU:HG	1:C:421:MET:HE2	1.94	0.50
1:C:509:HIS:ND1	3:C:2339:HOH:O	2.35	0.50
1:B:4:SER:C	3:B:2002:HOH:O	2.55	0.49
1:B:222:ASP:CB	3:B:2080:HOH:O	2.60	0.49
1:B:286:GLU:O	1:B:287:VAL:CB	2.60	0.49
1:A:417:LEU:HG	1:A:421:MET:HE2	1.94	0.49
1:D:86:LEU:HB3	1:D:278:ILE:O	2.13	0.49
1:B:484:ARG:NH1	3:B:2336:HOH:O	2.28	0.48
1:D:192:PHE:HB3	1:D:298:GLN:HG2	1.94	0.48
1:B:47:SER:HA	2:B:1586:FDA:C4X	2.42	0.48
1:C:86:LEU:HB3	1:C:278:ILE:O	2.12	0.48
1:A:326:LEU:C	1:A:326:LEU:HD23	2.38	0.48
1:D:326:LEU:C	1:D:326:LEU:HD23	2.39	0.48
1:B:86:LEU:HB3	1:B:278:ILE:O	2.13	0.48
1:B:47:SER:HA	2:B:1586:FDA:N5	2.29	0.47
1:A:86:LEU:HB3	1:A:278:ILE:O	2.13	0.47
1:C:192:PHE:HB3	1:C:298:GLN:HG2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:ASP:OD1	1:C:450:THR:HG22	2.14	0.47
1:D:402:ARG:HG2	3:D:2231:HOH:O	2.13	0.47
1:A:80:HIS:CD2	1:A:223:MET:HB3	2.49	0.47
1:C:495:ARG:NE	3:C:2325:HOH:O	2.19	0.47
1:D:80:HIS:CD2	1:D:223:MET:HB3	2.49	0.47
1:C:82:TYR:CD1	1:C:227:PHE:CE1	3.01	0.47
1:B:47:SER:OG	1:B:120:GLN:HB2	2.14	0.47
1:C:172:LYS:HE2	3:C:2134:HOH:O	2.14	0.46
1:D:402:ARG:HD2	1:D:413:ARG:NH2	2.31	0.46
1:D:448:ASP:OD1	1:D:450:THR:HG22	2.16	0.46
1:B:192:PHE:HB3	1:B:298:GLN:HG2	1.98	0.46
1:A:448:ASP:OD1	1:A:450:THR:HG22	2.16	0.45
1:D:402:ARG:CD	1:D:413:ARG:NH2	2.80	0.45
1:B:448:ASP:OD1	1:B:450:THR:HG22	2.17	0.45
1:A:47:SER:OG	1:A:120:GLN:HB2	2.17	0.45
1:C:425:ILE:HD12	3:C:2256:HOH:O	2.17	0.45
1:C:284:PRO:O	1:C:285:VAL:CB	2.65	0.44
1:D:47:SER:HA	2:D:1586:FDA:C4X	2.47	0.44
1:B:417:LEU:HG	1:B:421:MET:HE2	2.00	0.44
1:B:418:ARG:HD3	1:D:538:GLY:HA3	1.99	0.44
1:C:47:SER:HA	2:C:1586:FDA:N5	2.32	0.44
1:A:275:HIS:HA	1:A:278:ILE:HG22	1.99	0.44
1:D:47:SER:HA	2:D:1586:FDA:N5	2.32	0.44
1:D:47:SER:OG	1:D:120:GLN:HB2	2.18	0.44
1:B:326:LEU:C	1:B:326:LEU:HD23	2.43	0.44
1:A:278:ILE:HD13	1:A:278:ILE:HG21	1.82	0.44
1:A:484:ARG:HD2	3:A:2181:HOH:O	2.17	0.44
1:A:509:HIS:NE2	1:A:513:GLN:OE1	2.51	0.43
1:A:297:GLN:HG2	3:A:2210:HOH:O	2.17	0.43
1:C:47:SER:OG	1:C:120:GLN:HB2	2.19	0.43
1:A:89:GLU:CB	3:A:2278:HOH:O	2.67	0.43
1:B:82:TYR:HD2	1:B:227:PHE:CE1	2.37	0.43
1:D:417:LEU:HG	1:D:421:MET:HE2	2.01	0.42
1:D:496:PHE:HB2	1:D:522:LEU:HD12	2.01	0.42
1:A:402:ARG:HD3	1:A:402:ARG:HA	1.79	0.42
1:B:7:THR:O	1:B:171:ALA:HA	2.19	0.42
1:C:47:SER:HA	2:C:1586:FDA:C4X	2.50	0.42
1:D:450:THR:HG23	1:D:468:ARG:HE	1.84	0.42
1:A:273:ILE:O	1:A:275:HIS:O	2.38	0.41
1:A:467:THR:HG22	1:A:563:ARG:NH1	2.34	0.41
1:C:553:LEU:HB3	1:C:562:PHE:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:VAL:HG23	3:A:2202:HOH:O	2.18	0.41
1:A:151:GLN:HG3	3:A:2160:HOH:O	2.20	0.41
1:A:47:SER:HA	2:A:1586:FDA:N5	2.35	0.41
1:B:376:SER:HB3	3:B:2256:HOH:O	2.21	0.41
1:A:467:THR:HG23	1:A:563:ARG:HH11	1.82	0.41
1:A:413:ARG:H	1:A:413:ARG:HG2	1.75	0.40
1:C:326:LEU:C	1:C:326:LEU:HD23	2.46	0.40
1:B:509:HIS:NE2	1:B:513:GLN:OE1	2.54	0.40
1:B:553:LEU:HB3	1:B:562:PHE:HB3	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ARG:NH2	3:C:2248:HOH:O[1_455]	0.87	1.33
1:A:383:GLU:OE2	3:B:2330:HOH:O[1_565]	1.54	0.66
1:A:402:ARG:CZ	3:C:2248:HOH:O[1_455]	1.62	0.58
1:A:402:ARG:NE	3:C:2248:HOH:O[1_455]	2.07	0.13

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	523/586 (89%)	507 (97%)	13 (2%)	3 (1%)	21	12
1	B	519/586 (89%)	505 (97%)	11 (2%)	3 (1%)	21	12
1	C	514/586 (88%)	500 (97%)	12 (2%)	2 (0%)	30	22
1	D	523/586 (89%)	508 (97%)	13 (2%)	2 (0%)	30	22
All	All	2079/2344 (89%)	2020 (97%)	49 (2%)	10 (0%)	24	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	VAL
1	B	287	VAL
1	A	276	GLU
1	B	276	GLU
1	C	276	GLU
1	D	276	GLU
1	B	271	LYS
1	C	271	LYS
1	D	271	LYS
1	A	213	SER

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	395/467 (85%)	384 (97%)	11 (3%)	38	35
1	B	380/467 (81%)	370 (97%)	10 (3%)	40	38
1	C	382/467 (82%)	375 (98%)	7 (2%)	51	52
1	D	388/467 (83%)	373 (96%)	15 (4%)	28	22
All	All	1545/1868 (83%)	1502 (97%)	43 (3%)	38	35

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

Mol	Chain	Res	Type
1	A	94	ILE
1	A	134	ARG
1	A	251	ILE
1	A	294	THR
1	A	402	ARG
1	A	408	GLU
1	A	413	ARG
1	A	450	THR
1	A	467	THR
1	A	522	LEU
1	A	577	VAL
1	B	94	ILE

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Mol	Chain	Res	Type
1	B	134	ARG
1	B	151	GLN
1	B	251	ILE
1	B	294	THR
1	B	296	ASN
1	B	386	SER
1	B	450	THR
1	B	522	LEU
1	B	577	VAL
1	C	134	ARG
1	C	251	ILE
1	C	296	ASN
1	C	386	SER
1	C	450	THR
1	C	522	LEU
1	C	577	VAL
1	D	94	ILE
1	D	134	ARG
1	D	212	LEU
1	D	222	ASP
1	D	251	ILE
1	D	294	THR
1	D	296	ASN
1	D	386	SER
1	D	413	ARG
1	D	450	THR
1	D	495	ARG
1	D	522	LEU
1	D	565	LYS
1	D	574	GLN
1	D	577	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	296	ASN
1	A	297	GLN
1	A	366	GLN
1	B	366	GLN
1	B	516	GLN
1	C	297	GLN
1	D	366	GLN

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](#)

4 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	FDA	B	1586	-	57,58,58	2.02	13 (22%)	78,89,89	1.93	21 (26%)
2	FDA	D	1586	-	57,58,58	2.05	15 (26%)	78,89,89	1.89	22 (28%)
2	FDA	A	1586	-	57,58,58	1.80	13 (22%)	78,89,89	1.76	19 (24%)
2	FDA	C	1586	-	57,58,58	2.04	12 (21%)	78,89,89	1.72	22 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FDA	B	1586	-	-	1/34/50/50	0/6/6/6
2	FDA	D	1586	-	-	1/34/50/50	0/6/6/6
2	FDA	A	1586	-	-	0/34/50/50	0/6/6/6
2	FDA	C	1586	-	-	0/34/50/50	0/6/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1586	FDA	C5X-C9A	8.79	1.50	1.40
2	A	1586	FDA	C5X-C9A	8.30	1.49	1.40
2	D	1586	FDA	C5X-C9A	7.90	1.49	1.40
2	B	1586	FDA	C5X-C9A	7.74	1.49	1.40
2	B	1586	FDA	PA-O3P	6.71	1.66	1.59
2	D	1586	FDA	P-O3P	5.21	1.65	1.59
2	D	1586	FDA	C5A-C4A	4.15	1.46	1.39
2	B	1586	FDA	P-O3P	4.07	1.63	1.59
2	C	1586	FDA	C8-C7	4.00	1.50	1.40
2	A	1586	FDA	C5X-N5	-3.92	1.33	1.39
2	C	1586	FDA	P-O3P	3.91	1.63	1.59
2	B	1586	FDA	C5X-N5	-3.88	1.33	1.39
2	D	1586	FDA	C1'-C2'	3.83	1.58	1.52
2	C	1586	FDA	C5X-N5	-3.82	1.33	1.39
2	C	1586	FDA	C4X-C4	3.80	1.53	1.41
2	C	1586	FDA	C5A-C4A	3.70	1.45	1.39
2	D	1586	FDA	C8-C7	3.64	1.49	1.40
2	D	1586	FDA	C5X-N5	-3.48	1.34	1.39
2	A	1586	FDA	C5A-C4A	3.42	1.45	1.39
2	B	1586	FDA	O2-C2	3.40	1.30	1.23
2	D	1586	FDA	C5'-C4'	3.36	1.56	1.51
2	B	1586	FDA	C8-C7	3.34	1.49	1.40
2	C	1586	FDA	C8A-N7A	3.10	1.37	1.31
2	C	1586	FDA	PA-O3P	3.01	1.62	1.59
2	B	1586	FDA	C5A-N7A	-2.99	1.33	1.39
2	C	1586	FDA	O4-C4	2.95	1.29	1.23
2	D	1586	FDA	O4-C4	2.85	1.29	1.23
2	A	1586	FDA	C8-C7	2.81	1.47	1.40
2	D	1586	FDA	C4X-C4	2.80	1.50	1.41
2	D	1586	FDA	O2-C2	2.76	1.29	1.23
2	A	1586	FDA	C5A-N7A	-2.70	1.34	1.39
2	B	1586	FDA	C4X-C4	2.69	1.49	1.41
2	A	1586	FDA	C4A-N9A	-2.60	1.32	1.37
2	A	1586	FDA	C6-C7	-2.58	1.36	1.39
2	A	1586	FDA	P-O3P	2.55	1.62	1.59
2	A	1586	FDA	PA-O3P	2.44	1.62	1.59
2	B	1586	FDA	C5A-C4A	2.37	1.43	1.39
2	A	1586	FDA	C1'-C2'	2.36	1.55	1.52
2	B	1586	FDA	C10-N10	2.32	1.42	1.38
2	B	1586	FDA	C8A-N7A	2.31	1.36	1.31
2	C	1586	FDA	C1'-C2'	2.29	1.55	1.52
2	A	1586	FDA	C4X-C4	2.26	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1586	FDA	C10-N10	2.22	1.42	1.38
2	D	1586	FDA	C2-N3	2.18	1.41	1.37
2	D	1586	FDA	C2-N1	-2.18	1.33	1.37
2	B	1586	FDA	C1'-C2'	2.17	1.55	1.52
2	D	1586	FDA	C4A-N9A	-2.15	1.33	1.37
2	D	1586	FDA	C5A-N7A	-2.12	1.35	1.39
2	A	1586	FDA	C5A-C6A	2.10	1.46	1.41
2	C	1586	FDA	C10-N1	-2.10	1.33	1.37
2	B	1586	FDA	O4-C4	2.09	1.27	1.23
2	D	1586	FDA	C4A-N3A	2.06	1.38	1.34
2	C	1586	FDA	C4A-N9A	-2.00	1.33	1.37

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1586	FDA	C4A-N9A-C8A	4.90	110.88	105.74
2	C	1586	FDA	C5A-C4A-N3A	-4.89	119.98	126.72
2	A	1586	FDA	N3A-C4A-N9A	4.78	135.30	127.17
2	D	1586	FDA	N3A-C4A-N9A	4.73	135.22	127.17
2	B	1586	FDA	C5A-C4A-N3A	-4.70	120.24	126.72
2	D	1586	FDA	N3A-C2A-N1A	-4.69	121.49	128.58
2	C	1586	FDA	N3-C2-N1	4.56	122.90	115.74
2	A	1586	FDA	C5A-C4A-N3A	-4.54	120.47	126.72
2	B	1586	FDA	N3A-C4A-N9A	4.43	134.71	127.17
2	D	1586	FDA	C4A-N9A-C8A	4.41	110.37	105.74
2	B	1586	FDA	N3A-C2A-N1A	-4.29	122.08	128.58
2	B	1586	FDA	O3P-PA-O1A	-4.14	98.25	110.70
2	D	1586	FDA	O2-C2-N1	-4.02	114.72	121.86
2	B	1586	FDA	C4A-N9A-C8A	3.98	109.92	105.74
2	B	1586	FDA	O4-C4-C4X	-3.89	117.89	127.26
2	B	1586	FDA	C4'-C3'-C2'	-3.88	107.11	113.57
2	B	1586	FDA	C5A-C6A-N6A	-3.87	113.71	123.29
2	B	1586	FDA	N9A-C8A-N7A	-3.74	108.62	113.94
2	D	1586	FDA	C2A-N3A-C4A	3.67	120.79	111.83
2	A	1586	FDA	N9A-C8A-N7A	-3.64	108.78	113.94
2	C	1586	FDA	C4A-C5A-N7A	-3.61	106.46	110.58
2	B	1586	FDA	N6A-C6A-N1A	3.59	126.37	118.38
2	D	1586	FDA	C5A-C4A-N3A	-3.58	121.78	126.72
2	A	1586	FDA	O3P-PA-O1A	-3.53	100.08	110.70
2	A	1586	FDA	N3-C2-N1	3.53	121.28	115.74
2	B	1586	FDA	C2A-N3A-C4A	3.50	120.37	111.83
2	D	1586	FDA	O3P-PA-O1A	-3.48	100.23	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1586	FDA	N3A-C4A-N9A	3.35	132.87	127.17
2	D	1586	FDA	O4-C4-C4X	-3.30	119.31	127.26
2	D	1586	FDA	C5A-C6A-N6A	-3.24	115.26	123.29
2	C	1586	FDA	C2B-C1B-N9A	3.20	121.25	113.30
2	A	1586	FDA	O4-C4-C4X	-3.19	119.57	127.26
2	C	1586	FDA	C4A-N9A-C8A	3.17	109.06	105.74
2	C	1586	FDA	C2A-N3A-C4A	3.15	119.53	111.83
2	D	1586	FDA	N3-C2-N1	3.15	120.69	115.74
2	D	1586	FDA	O3B-C3B-C4B	-3.12	102.11	111.08
2	B	1586	FDA	C4A-N9A-C1B	-3.04	119.52	126.63
2	C	1586	FDA	C5'-C4'-C3'	-2.98	106.60	112.22
2	C	1586	FDA	N9A-C8A-N7A	-2.95	109.75	113.94
2	B	1586	FDA	C4-N3-C2	-2.94	122.32	126.37
2	D	1586	FDA	C4-N3-C2	-2.90	122.38	126.37
2	C	1586	FDA	C4-N3-C2	-2.88	122.41	126.37
2	A	1586	FDA	C2A-N3A-C4A	2.87	118.83	111.83
2	A	1586	FDA	C5A-N7A-C8A	2.84	107.92	103.45
2	A	1586	FDA	N3A-C2A-N1A	-2.84	124.28	128.58
2	A	1586	FDA	C4-N3-C2	-2.81	122.50	126.37
2	B	1586	FDA	O5B-PA-O1A	2.80	120.03	108.94
2	B	1586	FDA	N3-C2-N1	2.77	120.09	115.74
2	D	1586	FDA	C4A-N9A-C1B	-2.75	120.20	126.63
2	D	1586	FDA	C2B-C1B-N9A	2.72	120.07	113.30
2	C	1586	FDA	O2-C2-N3	-2.69	117.08	121.86
2	B	1586	FDA	C5A-N7A-C8A	2.65	107.61	103.45
2	D	1586	FDA	N6A-C6A-N1A	2.65	124.28	118.38
2	C	1586	FDA	C5A-N7A-C8A	2.63	107.59	103.45
2	D	1586	FDA	C5A-C4A-N9A	-2.58	103.00	105.81
2	B	1586	FDA	O2P-P-O3P	-2.57	100.34	107.27
2	B	1586	FDA	C4-C4X-N5	2.53	122.85	116.37
2	D	1586	FDA	C6A-C5A-C4A	-2.48	113.79	117.18
2	C	1586	FDA	C4-C4X-N5	2.44	122.61	116.37
2	C	1586	FDA	O4'-C4'-C3'	2.42	114.91	109.25
2	A	1586	FDA	C4-C4X-N5	2.40	122.51	116.37
2	A	1586	FDA	N6A-C6A-N1A	2.40	123.72	118.38
2	D	1586	FDA	C4'-C3'-C2'	-2.37	109.62	113.57
2	C	1586	FDA	N3A-C2A-N1A	-2.36	125.02	128.58
2	A	1586	FDA	C2B-C1B-N9A	2.35	119.15	113.30
2	B	1586	FDA	C2B-C1B-N9A	2.32	119.08	113.30
2	A	1586	FDA	O2A-PA-O5B	2.30	118.01	107.57
2	D	1586	FDA	C4-C4X-N5	2.30	122.25	116.37
2	A	1586	FDA	O4B-C1B-C2B	-2.30	101.70	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1586	FDA	C4'-C3'-C2'	-2.29	109.76	113.57
2	A	1586	FDA	C4X-C4-N3	2.28	118.38	112.13
2	B	1586	FDA	C4X-C4-N3	2.26	118.34	112.13
2	D	1586	FDA	O4B-C1B-N9A	-2.26	103.75	108.09
2	C	1586	FDA	C6-C5X-C9A	2.20	122.20	119.80
2	C	1586	FDA	C6A-C5A-N7A	2.20	136.32	132.09
2	B	1586	FDA	O2-C2-N1	-2.17	118.01	121.86
2	C	1586	FDA	O3P-PA-O1A	-2.13	104.28	110.70
2	A	1586	FDA	C4A-C5A-N7A	-2.13	108.14	110.58
2	C	1586	FDA	O4B-C1B-N9A	-2.11	104.03	108.09
2	D	1586	FDA	O4-C4-N3	2.07	124.00	120.11
2	C	1586	FDA	O3B-C3B-C4B	-2.06	105.18	111.08
2	C	1586	FDA	C4A-N9A-C1B	-2.05	121.83	126.63
2	D	1586	FDA	O3P-P-O1P	2.04	116.84	110.70
2	A	1586	FDA	C4'-C3'-C2'	-2.02	110.21	113.57

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1586	FDA	P-O3P-PA-O1A
2	D	1586	FDA	O4B-C4B-C5B-O5B

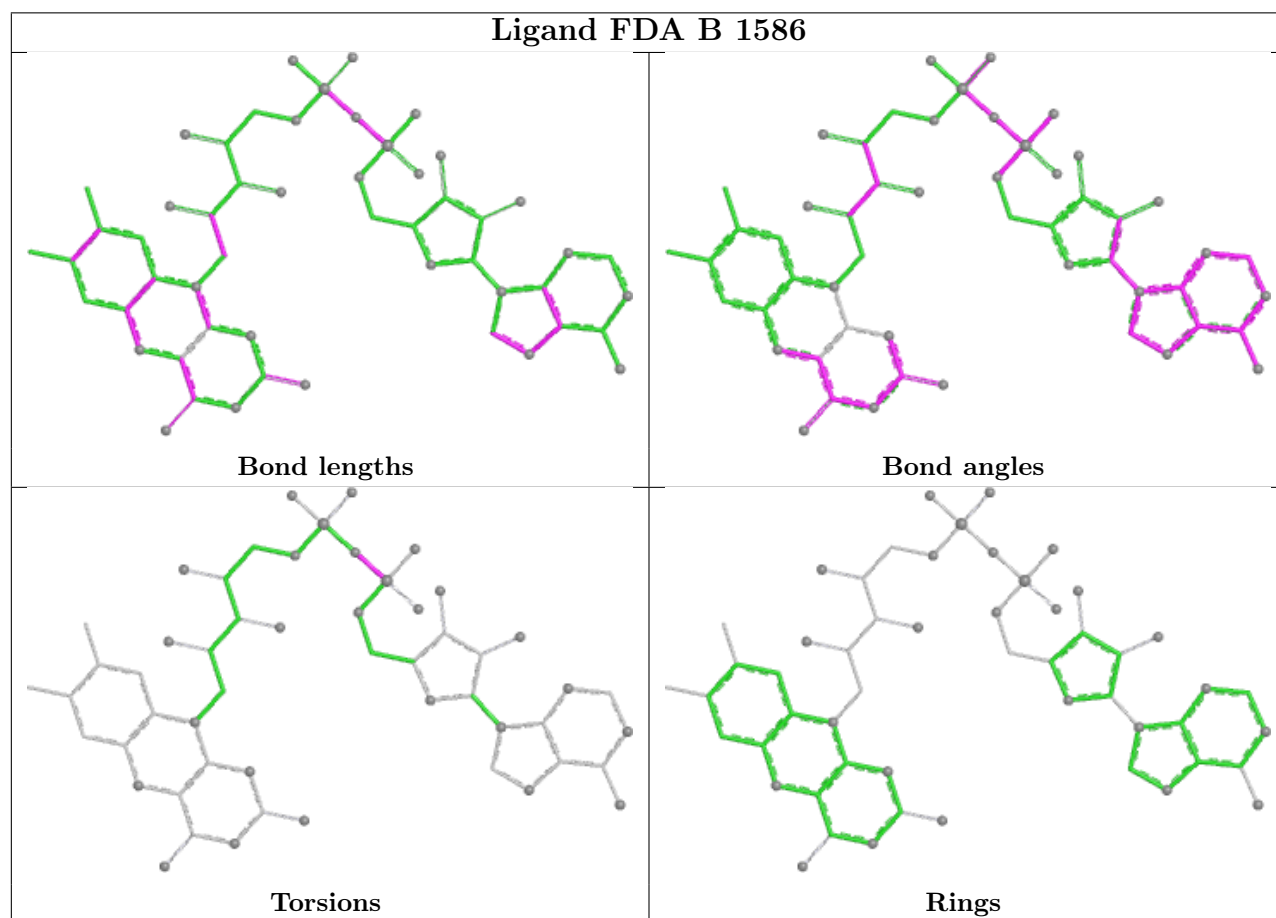
There are no ring outliers.

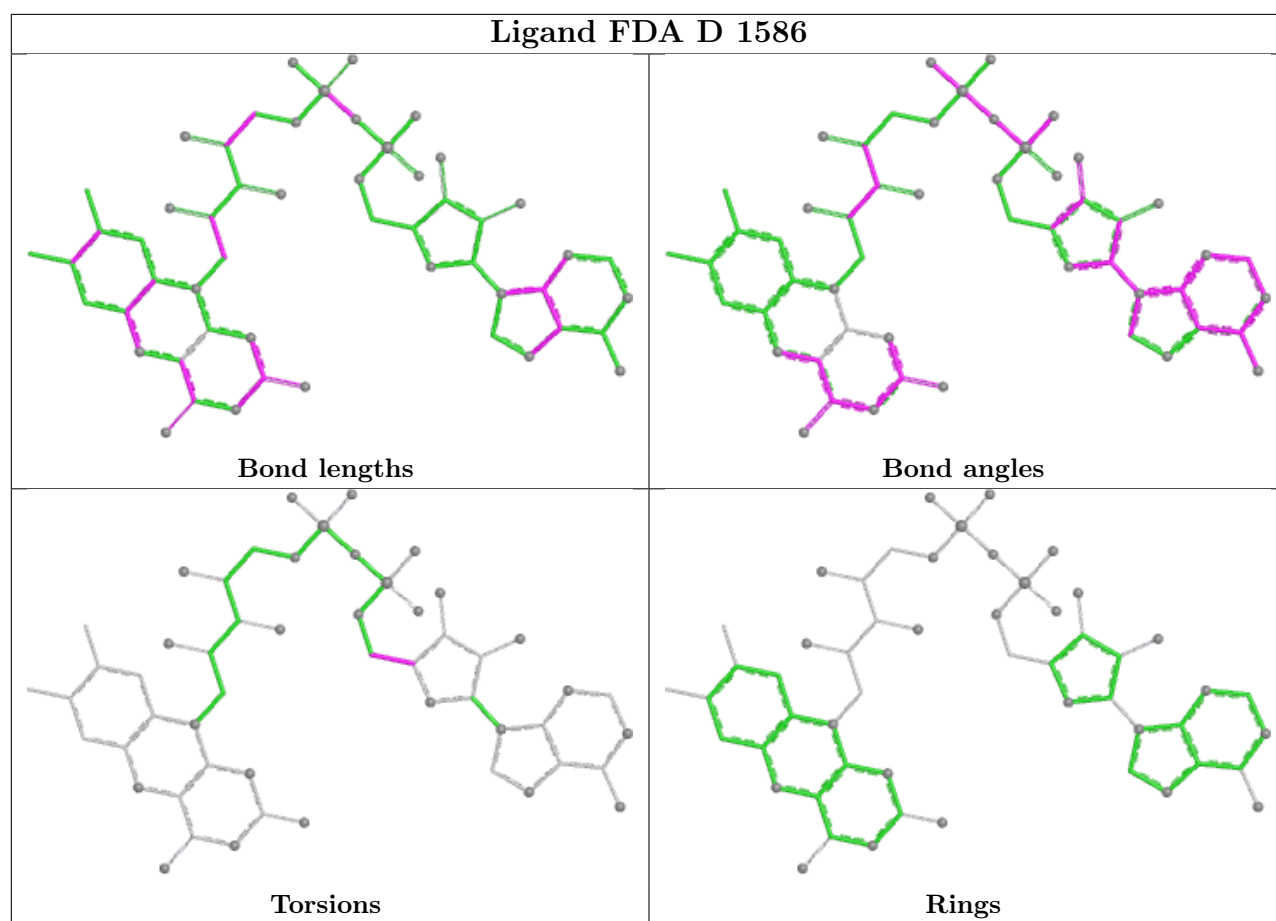
4 monomers are involved in 11 short contacts:

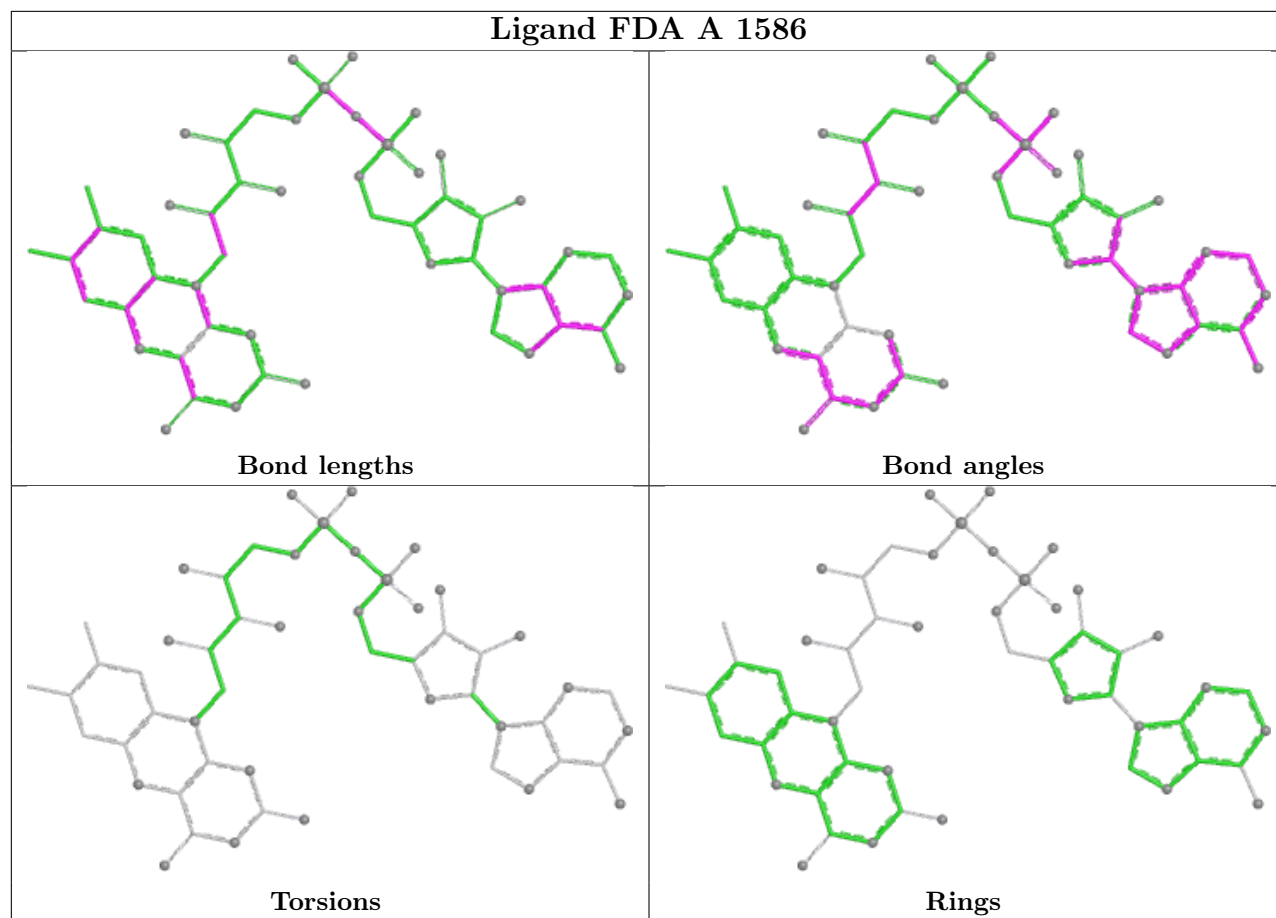
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1586	FDA	3	0
2	D	1586	FDA	3	0
2	A	1586	FDA	2	0
2	C	1586	FDA	3	0

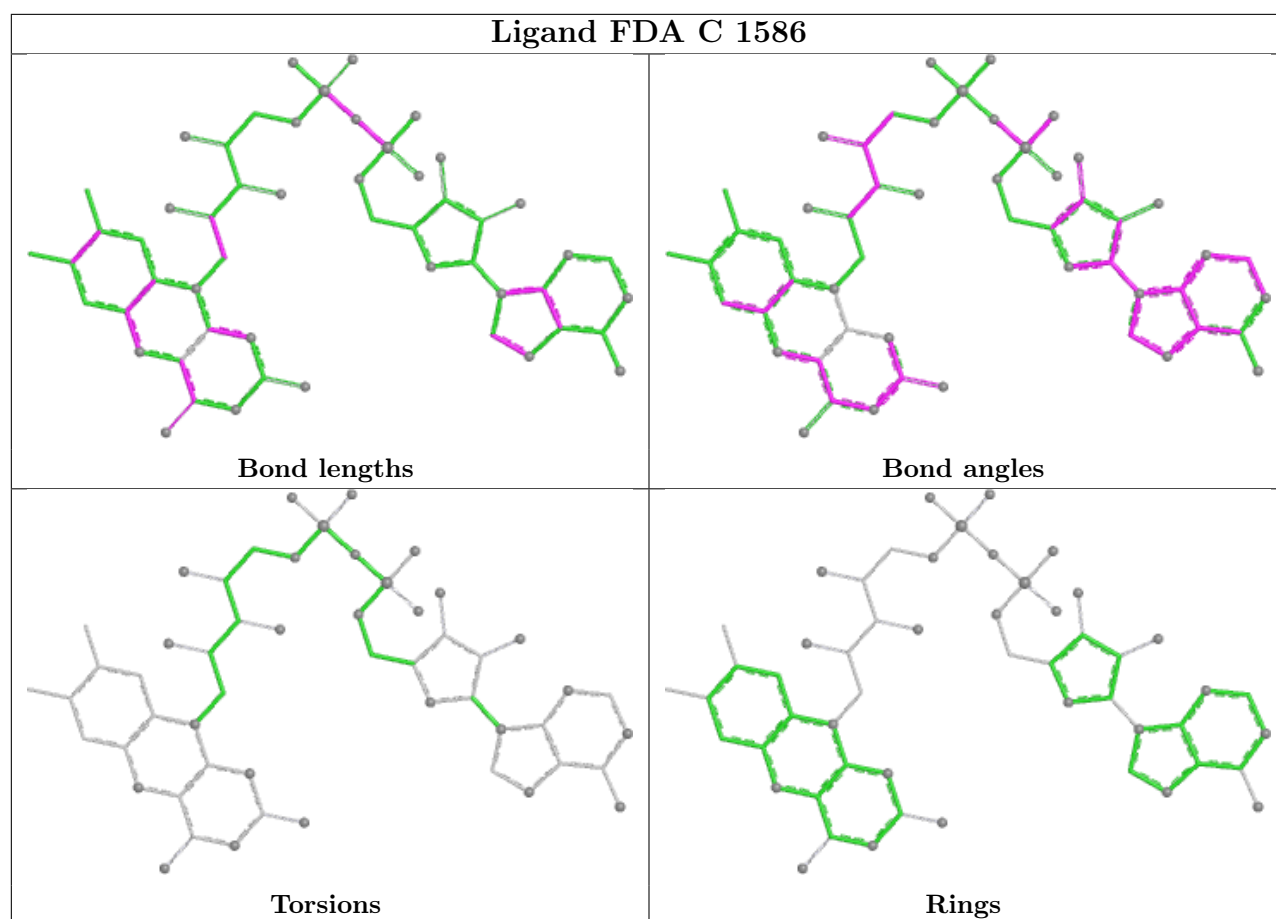
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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	539/586 (91%)	0.04	27 (5%) 34 33	19, 32, 66, 93	0
1	B	535/586 (91%)	0.04	26 (4%) 35 34	19, 31, 73, 113	0
1	C	530/586 (90%)	0.04	38 (7%) 21 20	18, 30, 75, 93	0
1	D	537/586 (91%)	0.06	26 (4%) 35 35	19, 33, 71, 99	0
All	All	2141/2344 (91%)	0.05	117 (5%) 30 30	18, 31, 71, 113	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	390	ALA	5.4
1	A	253	VAL	5.2
1	C	387	LEU	4.5
1	B	253	VAL	4.5
1	B	284	PRO	4.3
1	C	396	MET	4.3
1	C	287	VAL	4.2
1	C	391	PRO	4.2
1	B	72	VAL	4.0
1	A	194	GLY	3.8
1	D	204	ILE	3.7
1	D	273	ILE	3.7
1	D	248	ASN	3.7
1	A	290	ILE	3.7
1	A	284	PRO	3.6
1	A	295	ILE	3.6
1	D	287	VAL	3.6
1	A	271	LYS	3.5
1	C	290	ILE	3.5
1	C	251	ILE	3.4
1	A	287	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	293	TRP	3.4
1	B	211	ASP	3.4
1	B	295	ILE	3.4
1	A	204	ILE	3.3
1	C	295	ILE	3.3
1	C	205	ASN	3.3
1	C	270	ALA	3.3
1	A	269	GLU	3.3
1	C	243	MET	3.2
1	D	251	ILE	3.1
1	D	208	PHE	3.1
1	B	389	PRO	3.1
1	C	285	VAL	3.1
1	D	250	TRP	3.1
1	D	293	TRP	3.1
1	C	194	GLY	3.1
1	A	248	ASN	3.1
1	D	284	PRO	3.1
1	D	289	PRO	3.1
1	B	203	SER	3.1
1	D	290	ILE	3.1
1	C	288	GLY	3.0
1	D	288	GLY	3.0
1	B	286	GLU	3.0
1	C	253	VAL	3.0
1	D	205	ASN	2.9
1	B	293	TRP	2.9
1	D	274	ILE	2.9
1	D	275	HIS	2.9
1	B	205	ASN	2.9
1	B	249	LYS	2.9
1	C	276	GLU	2.9
1	A	278	ILE	2.8
1	A	4	SER	2.8
1	C	211	ASP	2.8
1	C	283	ILE	2.8
1	C	394	SER	2.8
1	D	243	MET	2.8
1	A	252	CYS	2.8
1	C	208	PHE	2.7
1	A	293	TRP	2.7
1	D	195	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	273	ILE	2.7
1	A	268	GLU	2.6
1	B	400	LEU	2.6
1	C	206	ILE	2.6
1	C	210	ALA	2.6
1	B	73	PRO	2.6
1	B	250	TRP	2.6
1	C	400	LEU	2.6
1	A	206	ILE	2.5
1	D	253	VAL	2.5
1	C	209	SER	2.5
1	C	273	ILE	2.5
1	C	392	THR	2.4
1	B	396	MET	2.4
1	A	238	VAL	2.4
1	D	203	SER	2.4
1	A	280	THR	2.4
1	C	289	PRO	2.4
1	D	45	PRO	2.4
1	B	270	ALA	2.4
1	C	292	THR	2.4
1	C	382	PHE	2.4
1	B	278	ILE	2.4
1	C	4	SER	2.4
1	C	84	THR	2.4
1	D	270	ALA	2.3
1	D	209	SER	2.3
1	A	292	THR	2.3
1	A	509	HIS	2.3
1	B	290	ILE	2.3
1	A	205	ASN	2.3
1	D	237	GLY	2.3
1	A	250	TRP	2.3
1	C	268	GLU	2.2
1	B	194	GLY	2.2
1	C	237	GLY	2.2
1	D	279	GLY	2.2
1	B	280	THR	2.2
1	C	277	ILE	2.2
1	D	295	ILE	2.2
1	A	288	GLY	2.2
1	C	77	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	289	PRO	2.1
1	D	268	GLU	2.1
1	B	392	THR	2.1
1	A	251	ILE	2.1
1	A	279	GLY	2.1
1	C	45	PRO	2.1
1	A	208	PHE	2.1
1	B	45	PRO	2.0
1	B	388	PRO	2.0
1	C	274	ILE	2.0
1	C	207	GLU	2.0
1	B	288	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

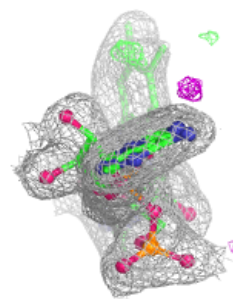
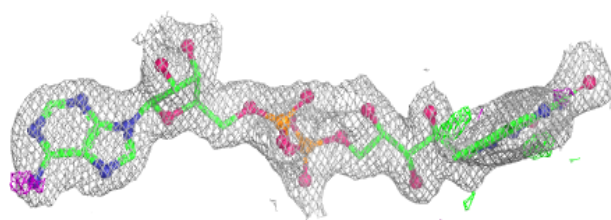
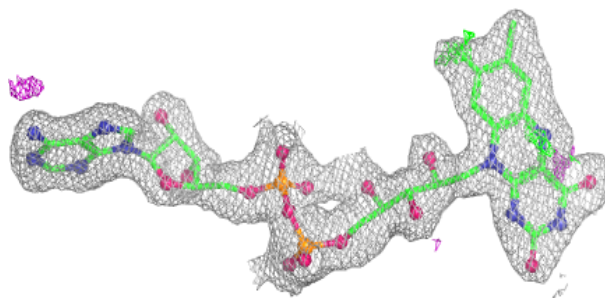
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FDA	C	1586	53/53	0.96	0.07	23,30,42,48	0
2	FDA	B	1586	53/53	0.97	0.07	23,30,42,51	0
2	FDA	D	1586	53/53	0.97	0.07	25,33,40,45	0
2	FDA	A	1586	53/53	0.98	0.05	21,29,34,40	0

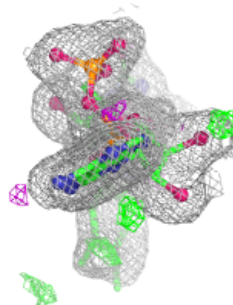
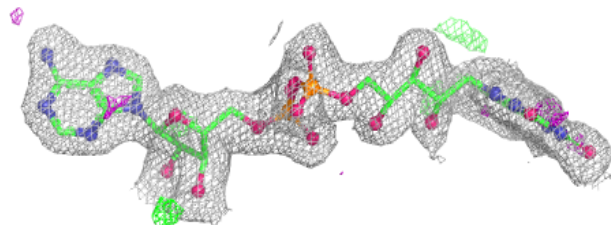
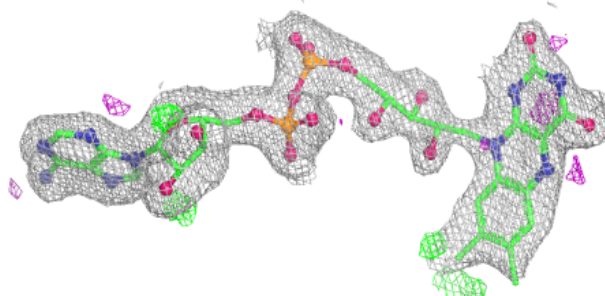
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FDA C 1586:

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

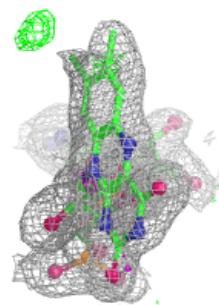
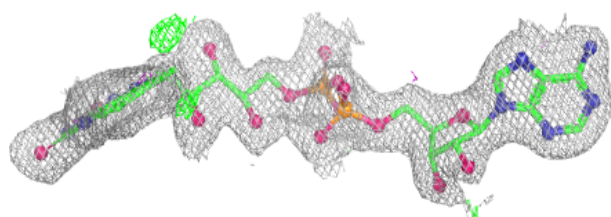
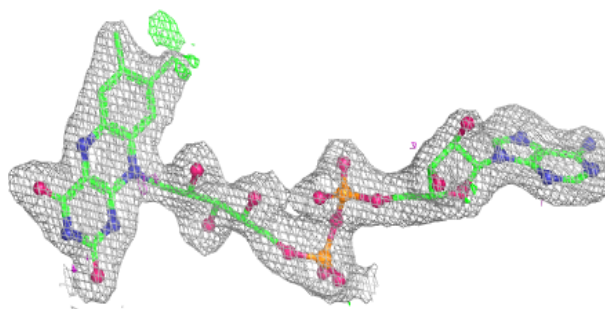
**Electron density around FDA B 1586:**

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

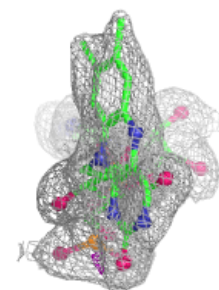
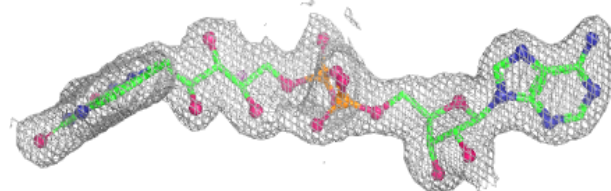
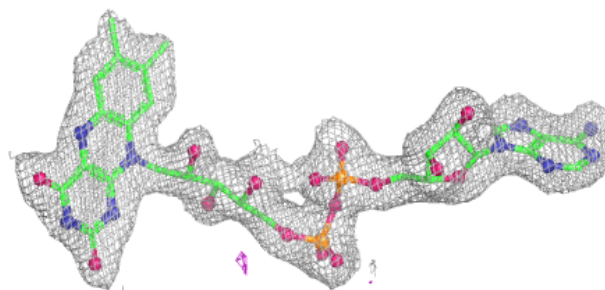


Electron density around FDA D 1586:

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

**Electron density around FDA A 1586:**

$2mF_o-DF_c$ (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.