Full wwPDB X-ray Structure Validation Report (i)

Aug 26, 2023 – 06:16 PM EDT

PDB ID	:	3EPT
Title	:	Structure of the rebeccamycin biosynthetic enzyme RebC with reduced flavin
Authors	:	Ryan, K.S.; Drennan, C.L.
Deposited on	:	2008-09-30
Resolution	:	2.97 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

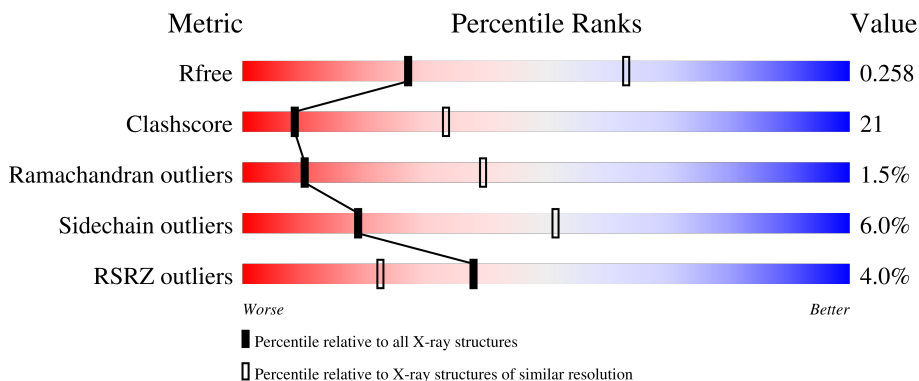|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.97 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	Percentile Ranks	Value
Rfree		0.258
Clashscore		21
Ramachandran outliers		1.5%
Sidechain outliers		6.0%
RSRZ outliers		4.0%

Worse ────────────────── *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	549	5% / 58% / 32% / • / 6%
1	B	549	3% / 57% / 34% / • / 5%

WORLDWIDE
wwPDB
PROTEIN DATA BANK

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8085 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 RebC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	3941	2473	743	715	10	0	0	0
1	B	520	Total	C	N	O	S	0	0	0
			3972	2489	752	721	10			

There are 40 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8KI25
A	-18	GLY	-	expression tag	UNP Q8KI25
A	-17	SER	-	expression tag	UNP Q8KI25
A	-16	SER	-	expression tag	UNP Q8KI25
A	-15	HIS	-	expression tag	UNP Q8KI25
A	-14	HIS	-	expression tag	UNP Q8KI25
A	-13	HIS	-	expression tag	UNP Q8KI25
A	-12	HIS	-	expression tag	UNP Q8KI25
A	-11	HIS	-	expression tag	UNP Q8KI25
A	-10	HIS	-	expression tag	UNP Q8KI25
A	-9	SER	-	expression tag	UNP Q8KI25
A	-8	SER	-	expression tag	UNP Q8KI25
A	-7	GLY	-	expression tag	UNP Q8KI25
A	-6	LEU	-	expression tag	UNP Q8KI25
A	-5	VAL	-	expression tag	UNP Q8KI25
A	-4	PRO	-	expression tag	UNP Q8KI25
A	-3	ARG	-	expression tag	UNP Q8KI25
A	-2	GLY	-	expression tag	UNP Q8KI25
A	-1	SER	-	expression tag	UNP Q8KI25
A	0	HIS	-	expression tag	UNP Q8KI25
B	-19	MET	-	expression tag	UNP Q8KI25
B	-18	GLY	-	expression tag	UNP Q8KI25
B	-17	SER	-	expression tag	UNP Q8KI25
B	-16	SER	-	expression tag	UNP Q8KI25
B	-15	HIS	-	expression tag	UNP Q8KI25

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q8KI25
B	-13	HIS	-	expression tag	UNP Q8KI25
B	-12	HIS	-	expression tag	UNP Q8KI25
B	-11	HIS	-	expression tag	UNP Q8KI25
B	-10	HIS	-	expression tag	UNP Q8KI25
B	-9	SER	-	expression tag	UNP Q8KI25
B	-8	SER	-	expression tag	UNP Q8KI25
B	-7	GLY	-	expression tag	UNP Q8KI25
B	-6	LEU	-	expression tag	UNP Q8KI25
B	-5	VAL	-	expression tag	UNP Q8KI25
B	-4	PRO	-	expression tag	UNP Q8KI25
B	-3	ARG	-	expression tag	UNP Q8KI25
B	-2	GLY	-	expression tag	UNP Q8KI25
B	-1	SER	-	expression tag	UNP Q8KI25
B	0	HIS	-	expression tag	UNP Q8KI25

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is DIHYDROFLAVINE-ADENINE DINUCLEOTIDE (three-letter code: FDA) (formula: $C_{27}H_{35}N_9O_{15}P_2$).
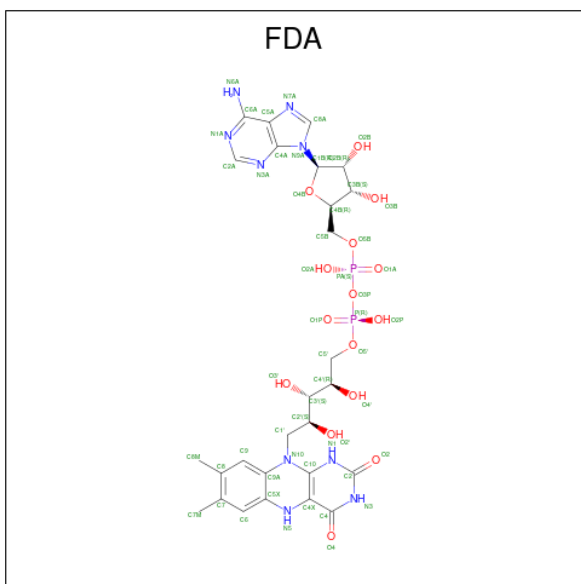
FDA

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

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total 30	O 30	0	0
4	B	35	Total 35	O 35	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: RebC

Chain A:

• Molecule 1: RebC

Chain B:
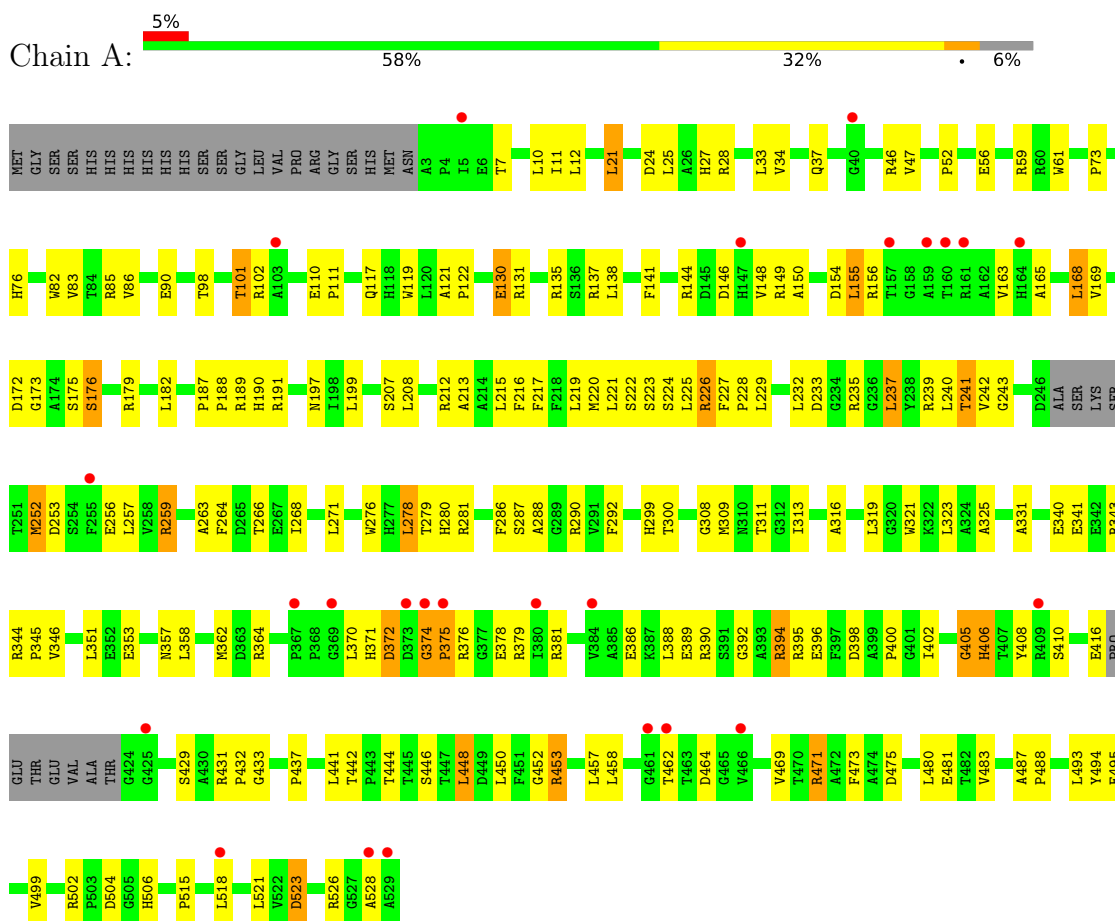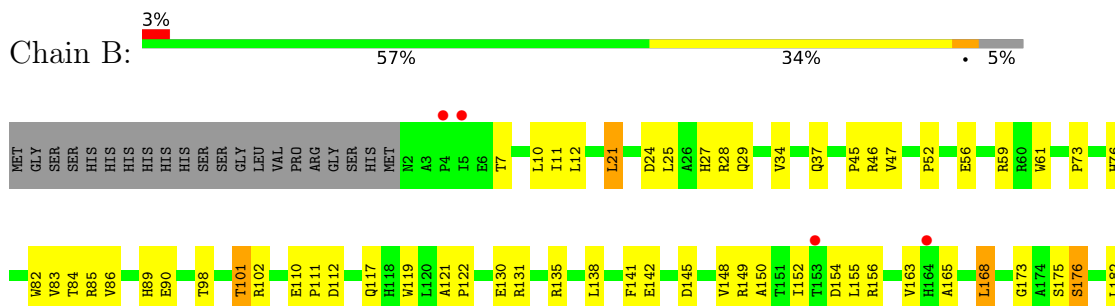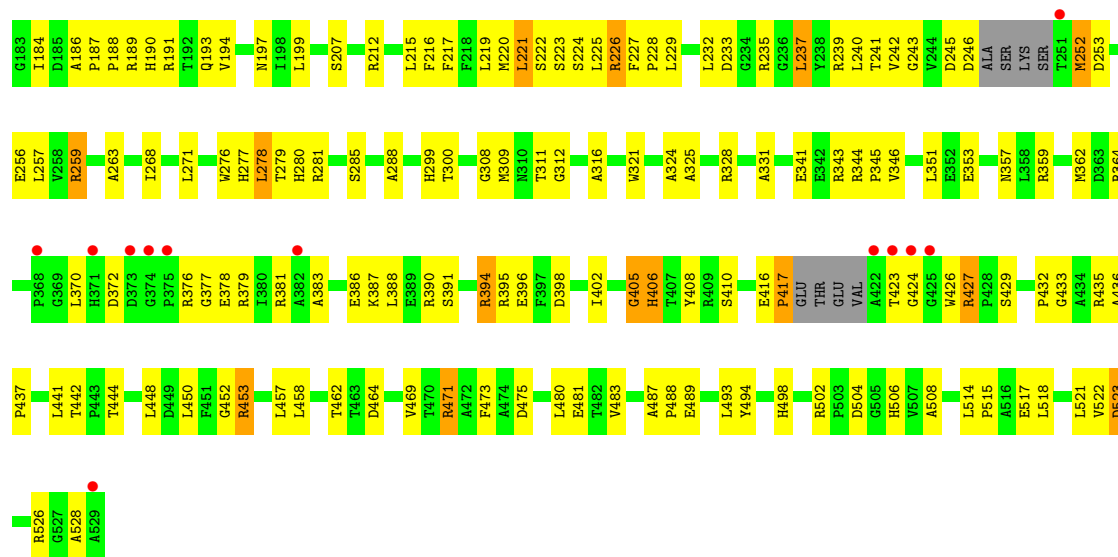
4   Data and refinement statistics   ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.26Å 78.22Å 123.06Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	40.00 – 2.97 37.23 – 2.96	Depositor EDS
% Data completeness (in resolution range)	88.4 (40.00-2.97) 87.6 (37.23-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	3.32 (at 2.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.276 0.208 , 0.258	Depositor DCC
R_{free} test set	1165 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	54.9	Xtriage
Anisotropy	0.434	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 46.0	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	8085	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.38	0/4038	0.64	0/5495
1	B	0.38	0/4070	0.64	0/5540
All	All	0.38	0/8108	0.64	0/11035

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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	3941	0	3861	163	0
1	B	3972	0	3889	165	0
2	A	1	0	0	0	0
3	A	53	0	33	2	0
3	B	53	0	33	2	0
4	A	30	0	0	1	0
4	B	35	0	0	0	0
All	All	8085	0	7816	327	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 21.

All (327) 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:375:PRO:HA	1:A:378:GLU:HB3	1.33	1.07
1:B:188:PRO:HG3	1:B:281:ARG:HH21	1.32	0.92
1:A:188:PRO:HG3	1:A:281:ARG:HH21	1.35	0.91
1:A:82:TRP:HB3	1:A:220:MET:HE2	1.59	0.85
1:B:82:TRP:HB3	1:B:220:MET:HE2	1.60	0.82
1:A:341:GLU:OE2	1:A:410:SER:HB2	1.80	0.81
1:B:416:GLU:HB3	1:B:417:PRO:HD2	1.64	0.80
1:B:252:MET:HG3	1:B:253:ASP:H	1.46	0.79
1:B:341:GLU:OE2	1:B:410:SER:HB2	1.83	0.77
1:B:423:THR:HG22	1:B:424:GLY:H	1.49	0.77
1:B:219:LEU:O	1:B:226:ARG:HA	1.85	0.76
1:A:219:LEU:O	1:A:226:ARG:HA	1.85	0.76
1:A:252:MET:HG3	1:A:253:ASP:H	1.51	0.76
1:B:121:ALA:HB3	1:B:122:PRO:HD3	1.66	0.75
1:A:73:PRO:HB2	1:A:76:HIS:HB2	1.68	0.74
1:A:138:LEU:HD11	1:A:150:ALA:HB1	1.69	0.74
1:A:370:LEU:HD12	1:A:381:ARG:HG2	1.68	0.74
1:B:73:PRO:HB2	1:B:76:HIS:HB2	1.69	0.73
1:A:148:VAL:HG11	1:A:168:LEU:HD12	1.71	0.71
1:B:252:MET:HG3	1:B:253:ASP:N	2.04	0.71
1:B:471:ARG:HD2	1:B:475:ASP:OD1	1.93	0.69
1:B:82:TRP:HB3	1:B:220:MET:CE	2.21	0.68
1:A:154:ASP:O	1:A:156:ARG:N	2.27	0.67
1:B:148:VAL:HG11	1:B:168:LEU:HD12	1.76	0.67
1:A:82:TRP:HB3	1:A:220:MET:CE	2.25	0.67
1:A:188:PRO:HG3	1:A:281:ARG:NH2	2.10	0.67
1:A:462:THR:OG1	1:A:464:ASP:HB2	1.94	0.67
1:A:232:LEU:HD12	1:A:237:LEU:HD22	1.77	0.67
1:B:138:LEU:HD11	1:B:150:ALA:HB1	1.77	0.66
1:A:189:ARG:HD3	1:A:351:LEU:HD13	1.77	0.66
1:B:188:PRO:CG	1:B:281:ARG:HH21	2.08	0.66
1:A:85:ARG:NH1	1:A:263:ALA:HA	2.10	0.65
1:B:370:LEU:HD11	1:B:381:ARG:HG3	1.78	0.65
1:B:299:HIS:CE1	1:B:311:THR:HG22	2.32	0.65
1:A:121:ALA:HB3	1:A:122:PRO:HD3	1.78	0.65
1:B:189:ARG:HD3	1:B:351:LEU:HD13	1.77	0.65
1:B:85:ARG:NH1	1:B:263:ALA:HA	2.12	0.65
1:B:429:SER:O	1:B:437:PRO:HD3	1.96	0.65
1:B:135:ARG:NH1	1:B:156:ARG:HA	2.11	0.65
1:B:232:LEU:HD12	1:B:237:LEU:HD22	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:THR:OG1	1:B:464:ASP:HB2	1.96	0.64
1:A:85:ARG:HH12	1:A:263:ALA:HA	1.62	0.64
1:A:471:ARG:HD2	1:A:475:ASP:OD1	1.97	0.64
1:B:37:GLN:O	1:B:135:ARG:HA	1.98	0.64
1:A:7:THR:O	1:A:165:ALA:HA	1.98	0.64
1:B:135:ARG:HH11	1:B:156:ARG:HA	1.64	0.63
1:A:252:MET:HG3	1:A:253:ASP:N	2.12	0.63
1:B:377:GLY:O	1:B:381:ARG:HB2	1.97	0.63
1:A:429:SER:O	1:A:437:PRO:HD3	1.99	0.62
1:B:357:ASN:OD1	1:B:396:GLU:HG3	1.98	0.62
1:B:59:ARG:HD2	1:B:110:GLU:OE2	1.99	0.62
1:B:199:LEU:HD21	1:B:237:LEU:HD21	1.82	0.62
1:A:325:ALA:HB1	1:A:331:ALA:HB2	1.81	0.62
1:A:515:PRO:HG2	1:A:518:LEU:HD23	1.81	0.62
1:A:37:GLN:O	1:A:135:ARG:HA	1.99	0.62
1:A:416:GLU:HG3	1:A:432:PRO:HD2	1.81	0.62
1:B:457:LEU:HD22	1:B:469:VAL:HG11	1.81	0.61
1:B:309:MET:H	3:B:711:FDA:HN1	1.48	0.61
1:B:353:GLU:HG2	1:B:402:ILE:HG13	1.81	0.61
1:B:47:VAL:H	1:B:117:GLN:NE2	1.99	0.61
1:A:353:GLU:HG2	1:A:402:ILE:HG13	1.83	0.60
1:A:357:ASN:OD1	1:A:396:GLU:HG3	2.01	0.60
1:B:223:SER:O	1:B:226:ARG:HD3	2.00	0.60
1:A:197:ASN:HD22	1:A:239:ARG:HD2	1.66	0.60
1:A:47:VAL:H	1:A:117:GLN:NE2	1.99	0.60
1:A:502:ARG:HG3	1:A:506:HIS:O	2.01	0.60
1:A:191:ARG:HA	1:B:145:ASP:OD1	2.02	0.60
1:B:27:HIS:CE1	1:B:61:TRP:HA	2.37	0.60
1:A:473:PHE:CD1	1:A:480:LEU:HD22	2.37	0.60
1:B:85:ARG:HH12	1:B:263:ALA:HA	1.66	0.60
1:A:199:LEU:HD21	1:A:237:LEU:HD21	1.83	0.59
1:B:489:GLU:OE1	1:B:489:GLU:N	2.25	0.59
1:B:515:PRO:HG2	1:B:518:LEU:HD23	1.83	0.59
1:A:223:SER:O	1:A:226:ARG:HD3	2.02	0.59
1:B:370:LEU:CD1	1:B:381:ARG:HG3	2.33	0.59
1:A:351:LEU:C	1:A:351:LEU:HD23	2.23	0.59
1:A:526:ARG:NH1	1:A:528:ALA:HB2	2.17	0.59
1:A:457:LEU:HD22	1:A:469:VAL:HG11	1.85	0.59
1:B:416:GLU:HG3	1:B:432:PRO:HD2	1.83	0.59
1:B:416:GLU:HB3	1:B:417:PRO:CD	2.33	0.58
1:B:7:THR:O	1:B:165:ALA:HA	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:PRO:HG3	1:B:281:ARG:NH2	2.12	0.58
1:B:473:PHE:CD1	1:B:480:LEU:HD22	2.39	0.58
1:B:325:ALA:HB1	1:B:331:ALA:HB2	1.85	0.58
1:A:52:PRO:O	1:A:56:GLU:HG3	2.03	0.58
1:A:227:PHE:HB3	1:A:228:PRO:HD2	1.85	0.58
1:B:190:HIS:HB2	1:B:280:HIS:CG	2.38	0.58
1:B:227:PHE:HB3	1:B:228:PRO:HD2	1.85	0.58
1:A:253:ASP:HB3	1:A:256:GLU:HB2	1.86	0.57
1:A:309:MET:HB3	3:A:710:FDA:O2	2.04	0.57
1:A:233:ASP:O	1:A:235:ARG:HG3	2.04	0.57
1:B:351:LEU:C	1:B:351:LEU:HD23	2.25	0.57
1:A:199:LEU:CD2	1:A:237:LEU:HD21	2.34	0.57
1:A:480:LEU:HD12	1:A:481:GLU:H	1.70	0.57
1:A:83:VAL:HG12	1:A:90:GLU:HA	1.87	0.57
1:B:480:LEU:HD12	1:B:481:GLU:H	1.69	0.57
1:B:119:TRP:CH2	1:B:233:ASP:HB2	2.40	0.56
1:A:190:HIS:HB2	1:A:280:HIS:CG	2.40	0.56
1:B:12:LEU:HD22	1:B:138:LEU:HD22	1.86	0.56
1:B:502:ARG:HG3	1:B:506:HIS:O	2.04	0.56
1:A:119:TRP:CH2	1:A:233:ASP:HB2	2.40	0.56
1:B:253:ASP:HB3	1:B:256:GLU:HB2	1.86	0.56
1:A:281:ARG:NH1	4:A:723:HOH:O	2.39	0.56
1:B:135:ARG:HH11	1:B:156:ARG:CA	2.20	0.55
1:B:199:LEU:CD2	1:B:237:LEU:HD21	2.36	0.55
1:B:526:ARG:NH1	1:B:528:ALA:HB2	2.21	0.55
1:B:52:PRO:O	1:B:56:GLU:HG3	2.06	0.55
1:B:86:VAL:HG21	1:B:229:LEU:HD13	1.88	0.55
1:B:12:LEU:HD22	1:B:138:LEU:CD2	2.37	0.55
1:A:86:VAL:HG21	1:A:229:LEU:HD13	1.89	0.55
1:B:245:ASP:O	1:B:246:ASP:C	2.45	0.54
1:A:11:ILE:HB	1:A:34:VAL:HG22	1.90	0.54
1:A:364:ARG:HD3	1:A:388:LEU:HD21	1.90	0.54
1:B:189:ARG:O	1:B:190:HIS:CG	2.61	0.54
1:A:59:ARG:HD2	1:A:110:GLU:OE2	2.08	0.53
1:B:217:PHE:O	1:B:228:PRO:HA	2.08	0.53
1:B:489:GLU:H	1:B:489:GLU:CD	2.11	0.53
1:B:83:VAL:HG12	1:B:90:GLU:HA	1.90	0.53
1:B:215:LEU:HG	1:B:216:PHE:CD1	2.44	0.53
1:A:442:THR:C	1:A:444:THR:H	2.12	0.53
1:B:46:ARG:HB2	1:B:117:GLN:HE22	1.74	0.53
1:A:10:LEU:HD22	1:A:163:VAL:CG1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LEU:HD13	1:B:163:VAL:HG11	1.90	0.52
1:A:442:THR:C	1:A:444:THR:N	2.63	0.52
1:B:386:GLU:O	1:B:390:ARG:HG3	2.08	0.52
1:A:28:ARG:CZ	1:A:321:TRP:HB3	2.40	0.52
1:A:208:LEU:HD13	1:A:264:PHE:CD1	2.44	0.52
1:B:11:ILE:HB	1:B:34:VAL:HG22	1.91	0.52
1:B:24:ASP:HB2	1:B:61:TRP:CZ2	2.45	0.52
1:A:325:ALA:CB	1:A:331:ALA:HB2	2.40	0.51
1:A:222:SER:O	1:A:226:ARG:HB3	2.10	0.51
1:A:252:MET:HG2	1:A:257:LEU:HG	1.92	0.51
1:A:259:ARG:HE	1:A:268:ILE:HD12	1.75	0.51
1:A:215:LEU:HG	1:A:216:PHE:CD1	2.45	0.51
1:A:299:HIS:CE1	1:A:311:THR:HG22	2.46	0.51
1:B:222:SER:O	1:B:226:ARG:HB3	2.11	0.51
1:B:353:GLU:HG2	1:B:402:ILE:CG1	2.41	0.51
1:A:12:LEU:HD22	1:A:138:LEU:HD22	1.93	0.51
1:A:502:ARG:HB2	1:A:504:ASP:OD1	2.11	0.51
1:B:325:ALA:CB	1:B:331:ALA:HB2	2.40	0.51
1:B:441:LEU:HD11	1:B:450:LEU:HD11	1.93	0.51
1:A:47:VAL:HG22	1:A:117:GLN:NE2	2.26	0.50
1:B:387:LYS:O	1:B:391:SER:N	2.44	0.50
1:B:46:ARG:H	1:B:117:GLN:NE2	2.08	0.50
1:A:364:ARG:NE	1:A:388:LEU:HD21	2.26	0.50
1:B:442:THR:C	1:B:444:THR:N	2.64	0.50
1:B:453:ARG:HG3	1:B:453:ARG:HH11	1.75	0.50
1:B:502:ARG:HB2	1:B:504:ASP:OD1	2.11	0.50
1:B:142:GLU:HG3	1:B:142:GLU:O	2.12	0.50
1:B:442:THR:C	1:B:444:THR:H	2.14	0.50
1:B:222:SER:O	1:B:226:ARG:HD2	2.11	0.50
1:A:364:ARG:CD	1:A:388:LEU:HD21	2.42	0.50
1:A:12:LEU:HD22	1:A:138:LEU:CD2	2.41	0.49
1:A:226:ARG:NH2	1:A:362:MET:O	2.45	0.49
1:A:287:SER:HB3	1:A:292:PHE:CD2	2.47	0.49
1:B:199:LEU:CD2	1:B:271:LEU:HD12	2.42	0.49
1:A:217:PHE:O	1:A:228:PRO:HA	2.11	0.49
1:B:426:TRP:O	1:B:427:ARG:HG2	2.11	0.49
1:B:182:LEU:HD13	1:B:288:ALA:HB3	1.95	0.49
1:B:437:PRO:HB2	1:B:493:LEU:HD21	1.94	0.49
1:A:199:LEU:CD2	1:A:271:LEU:HD12	2.43	0.49
1:A:344:ARG:HB3	1:A:345:PRO:HD3	1.95	0.49
1:B:84:THR:HG23	1:B:89:HIS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:NH2	1:B:111:PRO:HB2	2.28	0.49
1:A:10:LEU:HD22	1:A:163:VAL:HG11	1.94	0.49
1:A:46:ARG:H	1:A:117:GLN:NE2	2.11	0.49
1:B:480:LEU:HD12	1:B:481:GLU:N	2.28	0.49
1:A:188:PRO:CG	1:A:281:ARG:HH21	2.17	0.48
1:B:523:ASP:O	1:B:528:ALA:HB3	2.13	0.48
1:A:102:ARG:NH2	1:A:111:PRO:HB2	2.28	0.48
1:A:197:ASN:OD1	1:A:276:TRP:NE1	2.44	0.48
1:B:346:VAL:HG13	1:B:406:HIS:CE1	2.48	0.48
1:A:523:ASP:O	1:A:528:ALA:HB3	2.14	0.48
1:B:372:ASP:O	1:B:381:ARG:NH2	2.46	0.48
1:B:394:ARG:NH1	1:B:398:ASP:OD2	2.46	0.48
1:A:46:ARG:HB2	1:A:117:GLN:HE22	1.77	0.48
1:B:173:GLY:O	1:B:176:SER:HB2	2.13	0.48
1:B:416:GLU:O	1:B:417:PRO:C	2.51	0.48
1:A:278:LEU:HD21	1:A:358:LEU:HD22	1.96	0.48
1:A:309:MET:H	3:A:710:FDA:HN1	1.60	0.48
1:B:324:ALA:O	1:B:328:ARG:HG2	2.13	0.48
1:B:344:ARG:HB3	1:B:345:PRO:HD3	1.95	0.48
1:A:27:HIS:CE1	1:A:61:TRP:HA	2.48	0.48
1:A:199:LEU:HD22	1:A:271:LEU:HB2	1.96	0.48
1:A:378:GLU:HA	1:A:381:ARG:NH1	2.29	0.48
1:B:405:GLY:O	1:B:406:HIS:O	2.32	0.48
1:B:11:ILE:HD11	1:B:25:LEU:HD12	1.96	0.47
1:A:441:LEU:HD11	1:A:450:LEU:HD11	1.95	0.47
1:B:98:THR:OG1	1:B:101:THR:HB	2.13	0.47
1:B:199:LEU:HD22	1:B:271:LEU:HB2	1.96	0.47
1:A:56:GLU:O	1:A:59:ARG:HB3	2.14	0.47
1:B:21:LEU:HD22	1:B:25:LEU:HG	1.97	0.47
1:A:137:ARG:CZ	1:A:155:LEU:HD21	2.45	0.47
1:A:154:ASP:C	1:A:156:ARG:H	2.17	0.47
1:A:405:GLY:O	1:A:406:HIS:O	2.33	0.47
1:B:189:ARG:HD3	1:B:351:LEU:CD1	2.44	0.47
1:A:47:VAL:H	1:A:117:GLN:HE21	1.61	0.47
1:A:212:ARG:HE	1:A:212:ARG:HB3	1.53	0.47
1:B:226:ARG:NH2	1:B:362:MET:O	2.47	0.47
1:A:442:THR:O	1:A:444:THR:N	2.47	0.47
1:B:442:THR:O	1:B:444:THR:N	2.47	0.47
1:B:28:ARG:CZ	1:B:321:TRP:HB3	2.45	0.47
1:A:189:ARG:O	1:A:190:HIS:CG	2.68	0.46
1:B:197:ASN:OD1	1:B:276:TRP:NE1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:364:ARG:NE	1:B:388:LEU:HD21	2.31	0.46
1:B:215:LEU:HG	1:B:216:PHE:CE1	2.51	0.46
1:A:319:LEU:CD1	1:A:323:LEU:HG	2.46	0.46
1:A:353:GLU:HG2	1:A:402:ILE:CG1	2.45	0.46
1:A:408:TYR:O	1:A:433:GLY:HA3	2.16	0.46
1:A:119:TRP:C	1:A:122:PRO:HD2	2.37	0.46
1:B:197:ASN:HD22	1:B:239:ARG:HD2	1.80	0.46
1:B:259:ARG:HE	1:B:268:ILE:HD12	1.80	0.46
1:A:319:LEU:HD12	1:A:323:LEU:HG	1.98	0.45
1:B:12:LEU:HD13	1:B:138:LEU:HB2	1.98	0.45
1:A:222:SER:O	1:A:226:ARG:HD2	2.16	0.45
1:B:437:PRO:HG2	1:B:494:TYR:CE1	2.52	0.45
1:A:98:THR:H	1:A:101:THR:HG22	1.82	0.45
1:A:146:ASP:HA	1:A:290:ARG:HE	1.81	0.45
1:A:386:GLU:O	1:A:389:GLU:HB3	2.17	0.45
1:A:346:VAL:HG13	1:A:406:HIS:CE1	2.51	0.45
1:A:395:ARG:HB3	1:A:395:ARG:NH1	2.31	0.45
1:A:437:PRO:HB2	1:A:493:LEU:HD21	1.98	0.45
1:A:12:LEU:HD13	1:A:138:LEU:HB2	1.99	0.45
1:A:135:ARG:HH11	1:A:156:ARG:HA	1.81	0.45
1:A:173:GLY:O	1:A:176:SER:HB2	2.16	0.45
1:A:453:ARG:HG3	1:A:453:ARG:HH11	1.81	0.45
1:B:184:ILE:HD13	1:B:285:SER:HB3	1.98	0.45
1:A:10:LEU:HD13	1:A:163:VAL:HG11	1.98	0.45
1:A:21:LEU:HD22	1:A:25:LEU:HG	1.98	0.45
1:B:47:VAL:H	1:B:117:GLN:HE21	1.65	0.45
1:B:221:LEU:HD23	1:B:221:LEU:O	2.17	0.45
1:B:518:LEU:O	1:B:521:LEU:HB3	2.17	0.45
1:B:28:ARG:NH2	1:B:321:TRP:HB3	2.32	0.44
1:B:379:ARG:C	1:B:381:ARG:H	2.20	0.44
1:A:189:ARG:HD3	1:A:351:LEU:CD1	2.46	0.44
1:A:228:PRO:O	1:A:241:THR:HG22	2.17	0.44
1:B:458:LEU:HD23	1:B:483:VAL:HB	1.99	0.44
1:B:498:HIS:CD2	1:B:514:LEU:HG	2.52	0.44
1:A:154:ASP:C	1:A:156:ARG:N	2.71	0.44
1:A:370:LEU:CD1	1:A:381:ARG:HG2	2.45	0.44
1:B:175:SER:O	1:B:176:SER:C	2.55	0.44
1:A:266:THR:O	1:A:268:ILE:HG13	2.17	0.44
1:A:408:TYR:CE2	1:A:506:HIS:ND1	2.86	0.44
1:A:480:LEU:HD12	1:A:481:GLU:N	2.30	0.44
1:B:28:ARG:NH1	1:B:452:GLY:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ALA:O	1:B:281:ARG:HB2	2.18	0.44
1:B:56:GLU:O	1:B:59:ARG:HB3	2.18	0.44
1:B:408:TYR:O	1:B:433:GLY:HA3	2.18	0.43
1:A:175:SER:O	1:A:176:SER:C	2.56	0.43
1:A:394:ARG:NH1	1:A:398:ASP:OD2	2.51	0.43
1:A:402:ILE:O	1:A:406:HIS:CD2	2.71	0.43
1:A:518:LEU:O	1:A:521:LEU:HB3	2.18	0.43
1:B:27:HIS:NE2	1:B:61:TRP:HA	2.32	0.43
1:B:56:GLU:HA	1:B:110:GLU:HG3	2.00	0.43
1:A:224:SER:HB2	1:A:243:GLY:O	2.18	0.43
1:B:408:TYR:CE2	1:B:506:HIS:ND1	2.87	0.43
1:B:395:ARG:NH1	1:B:395:ARG:HB3	2.33	0.43
1:A:11:ILE:HD11	1:A:25:LEU:HD12	2.01	0.43
1:A:197:ASN:ND2	1:A:239:ARG:HD2	2.32	0.43
1:A:215:LEU:HG	1:A:216:PHE:CE1	2.53	0.43
1:A:494:TYR:HD2	1:A:499:VAL:HG21	1.84	0.43
1:B:187:PRO:HA	1:B:188:PRO:HD3	1.79	0.43
1:A:33:LEU:HD23	1:A:34:VAL:N	2.33	0.43
1:B:212:ARG:HE	1:B:212:ARG:HB3	1.52	0.43
1:A:386:GLU:OE2	1:A:390:ARG:HD2	2.18	0.43
1:A:458:LEU:HD23	1:A:483:VAL:HB	2.00	0.43
1:B:453:ARG:HG3	1:B:453:ARG:NH1	2.34	0.43
1:A:135:ARG:HD2	1:A:156:ARG:HE	1.84	0.43
1:A:405:GLY:O	1:A:406:HIS:C	2.57	0.42
1:B:233:ASP:O	1:B:235:ARG:HG3	2.19	0.42
1:B:309:MET:HB3	3:B:711:FDA:O2	2.20	0.42
1:A:56:GLU:HA	1:A:110:GLU:HG3	2.02	0.42
1:A:182:LEU:HD13	1:A:288:ALA:HB3	2.01	0.42
1:B:45:PRO:HD2	1:B:199:LEU:HD11	2.00	0.42
1:B:487:ALA:HA	1:B:488:PRO:HD2	1.90	0.42
1:A:33:LEU:HD23	1:A:33:LEU:C	2.40	0.42
1:A:208:LEU:HD13	1:A:264:PHE:HB3	2.00	0.42
1:A:371:HIS:O	1:A:372:ASP:C	2.57	0.42
1:A:494:TYR:O	1:A:495:GLU:HB2	2.18	0.42
1:B:152:ILE:N	1:B:152:ILE:HD12	2.34	0.42
1:B:312:GLY:O	1:B:316:ALA:N	2.53	0.42
1:B:226:ARG:HG2	1:B:227:PHE:CE2	2.54	0.42
1:A:390:ARG:C	1:A:392:GLY:H	2.22	0.42
1:B:154:ASP:O	1:B:156:ARG:N	2.52	0.42
1:B:193:GLN:HE22	1:B:362:MET:CE	2.33	0.42
1:B:359:ARG:HG3	1:B:359:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:ARG:C	1:B:383:ALA:H	2.21	0.42
1:B:222:SER:OG	1:B:225:LEU:HB2	2.20	0.41
1:B:252:MET:HG2	1:B:257:LEU:HG	2.02	0.41
1:B:299:HIS:O	1:B:299:HIS:ND1	2.53	0.41
1:A:28:ARG:NH1	1:A:452:GLY:O	2.53	0.41
1:A:343:ARG:O	1:A:344:ARG:C	2.58	0.41
1:A:21:LEU:HD12	1:A:169:VAL:HG11	2.01	0.41
1:A:24:ASP:HB2	1:A:61:TRP:CZ2	2.56	0.41
1:A:141:PHE:HA	1:A:149:ARG:O	2.19	0.41
1:A:374:GLY:O	1:A:376:ARG:N	2.53	0.41
1:A:176:SER:HB3	1:A:179:ARG:NH1	2.35	0.41
1:B:119:TRP:CZ2	1:B:233:ASP:HB2	2.55	0.41
1:B:138:LEU:HD11	1:B:150:ALA:CB	2.47	0.41
1:B:141:PHE:HA	1:B:149:ARG:O	2.21	0.41
1:B:224:SER:HB2	1:B:243:GLY:O	2.21	0.41
1:B:405:GLY:O	1:B:406:HIS:C	2.59	0.41
1:B:278:LEU:HD12	1:B:279:THR:N	2.36	0.41
1:B:502:ARG:HG2	1:B:508:ALA:HB2	2.02	0.41
1:A:437:PRO:HG2	1:A:494:TYR:CE1	2.56	0.41
1:B:52:PRO:HD3	1:B:112:ASP:HB3	2.01	0.41
1:A:130:GLU:O	1:A:130:GLU:OE1	2.38	0.41
1:A:313:ILE:O	1:A:316:ALA:HB3	2.20	0.41
1:A:431:ARG:HG2	1:A:431:ARG:HH11	1.85	0.41
1:A:446:SER:OG	1:A:448:LEU:HB2	2.20	0.41
1:B:119:TRP:C	1:B:122:PRO:HD2	2.41	0.41
1:B:381:ARG:C	1:B:383:ALA:N	2.74	0.41
1:B:522:VAL:O	1:B:526:ARG:HG2	2.21	0.41
1:A:398:ASP:OD1	1:A:400:PRO:HD3	2.20	0.41
1:B:343:ARG:O	1:B:344:ARG:C	2.59	0.41
1:B:194:VAL:HG22	1:B:277:HIS:CD2	2.55	0.40
1:B:379:ARG:C	1:B:381:ARG:N	2.74	0.40
1:A:21:LEU:CD1	1:A:169:VAL:HG11	2.50	0.40
1:A:172:ASP:N	1:A:172:ASP:OD1	2.53	0.40
1:A:187:PRO:HA	1:A:188:PRO:HD3	1.80	0.40
1:A:278:LEU:HD12	1:A:279:THR:N	2.36	0.40
1:A:286:PHE:HB2	1:A:340:GLU:HB2	2.02	0.40
1:A:487:ALA:HA	1:A:488:PRO:HD2	1.89	0.40
1:B:402:ILE:O	1:B:406:HIS:CD2	2.74	0.40
1:A:144:ARG:HG3	1:A:144:ARG:NH1	2.36	0.40
1:B:376:ARG:C	1:B:378:GLU:N	2.74	0.40
1:B:435:ARG:O	1:B:436:ALA:C	2.59	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	510/549 (93%)	461 (90%)	40 (8%)	9 (2%)	8	35
1	B	514/549 (94%)	465 (90%)	43 (8%)	6 (1%)	13	45
All	All	1024/1098 (93%)	926 (90%)	83 (8%)	15 (2%)	10	39

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	LEU
1	A	406	HIS
1	B	155	LEU
1	B	406	HIS
1	A	374	GLY
1	A	405	GLY
1	B	405	GLY
1	A	375	PRO
1	A	176	SER
1	B	176	SER
1	B	453	ARG
1	A	453	ARG
1	A	213	ALA
1	B	308	GLY
1	A	308	GLY

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	397/433 (92%)	374 (94%)	23 (6%)	20	53
1	B	400/433 (92%)	375 (94%)	25 (6%)	18	49
All	All	797/866 (92%)	749 (94%)	48 (6%)	19	51

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	101	THR
1	A	130	GLU
1	A	131	ARG
1	A	168	LEU
1	A	207	SER
1	A	221	LEU
1	A	225	LEU
1	A	226	ARG
1	A	237	LEU
1	A	240	LEU
1	A	241	THR
1	A	242	VAL
1	A	252	MET
1	A	259	ARG
1	A	278	LEU
1	A	300	THR
1	A	372	ASP
1	A	379	ARG
1	A	394	ARG
1	A	448	LEU
1	A	471	ARG
1	A	523	ASP
1	B	21	LEU
1	B	29	GLN
1	B	101	THR
1	B	130	GLU
1	B	131	ARG
1	B	168	LEU
1	B	191	ARG
1	B	207	SER
1	B	221	LEU
1	B	226	ARG
1	B	237	LEU

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Mol	Chain	Res	Type
1	B	240	LEU
1	B	241	THR
1	B	242	VAL
1	B	252	MET
1	B	259	ARG
1	B	278	LEU
1	B	300	THR
1	B	394	ARG
1	B	417	PRO
1	B	427	ARG
1	B	448	LEU
1	B	471	ARG
1	B	517	GLU
1	B	523	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	117	GLN
1	A	193	GLN
1	A	277	HIS
1	A	280	HIS
1	A	355	ASN
1	B	66	GLN
1	B	117	GLN
1	B	193	GLN
1	B	277	HIS
1	B	371	HIS

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
3	FDA	B	711	-	52,58,58	1.62	9 (17%)	60,89,89	1.15	3 (5%)
3	FDA	A	710	-	52,58,58	1.70	11 (21%)	60,89,89	1.12	4 (6%)

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	FDA	B	711	-	-	4/30/50/50	0/6/6/6
3	FDA	A	710	-	-	3/30/50/50	0/6/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	710	FDA	C5X-C9A	5.02	1.46	1.40
3	B	711	FDA	C5X-C9A	4.09	1.45	1.40
3	A	710	FDA	C4A-N3A	4.08	1.41	1.35
3	B	711	FDA	C9A-N10	3.96	1.48	1.41
3	A	710	FDA	C9A-N10	3.71	1.47	1.41
3	B	711	FDA	C4X-N5	3.66	1.43	1.35
3	B	711	FDA	C4A-N3A	3.57	1.40	1.35
3	B	711	FDA	C1'-C2'	3.50	1.57	1.52
3	A	710	FDA	C1'-C2'	3.33	1.57	1.52
3	A	710	FDA	C4X-N5	3.19	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	710	FDA	C2B-C1B	-3.15	1.49	1.53
3	B	711	FDA	C7M-C7	3.14	1.57	1.51
3	A	710	FDA	C2A-N3A	2.79	1.36	1.32
3	A	710	FDA	C5'-C4'	-2.73	1.47	1.51
3	A	710	FDA	C7M-C7	2.71	1.56	1.51
3	B	711	FDA	C2A-N3A	2.63	1.36	1.32
3	B	711	FDA	C5'-C4'	-2.57	1.48	1.51
3	A	710	FDA	C2-N3	2.52	1.41	1.37
3	B	711	FDA	C9-C8	2.23	1.42	1.39
3	A	710	FDA	C9-C8	2.10	1.42	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	711	FDA	O2-C2-N3	-3.12	115.93	121.82
3	A	710	FDA	O2-C2-N3	-2.72	116.69	121.82
3	A	710	FDA	O4B-C1B-C2B	-2.64	103.07	106.93
3	A	710	FDA	C9A-C5X-N5	2.37	122.72	119.56
3	B	711	FDA	C9A-C9-C8	2.29	123.91	119.30
3	B	711	FDA	O4B-C1B-C2B	-2.10	103.86	106.93
3	A	710	FDA	N3-C2-N1	2.09	119.17	115.80

There are no chirality outliers.
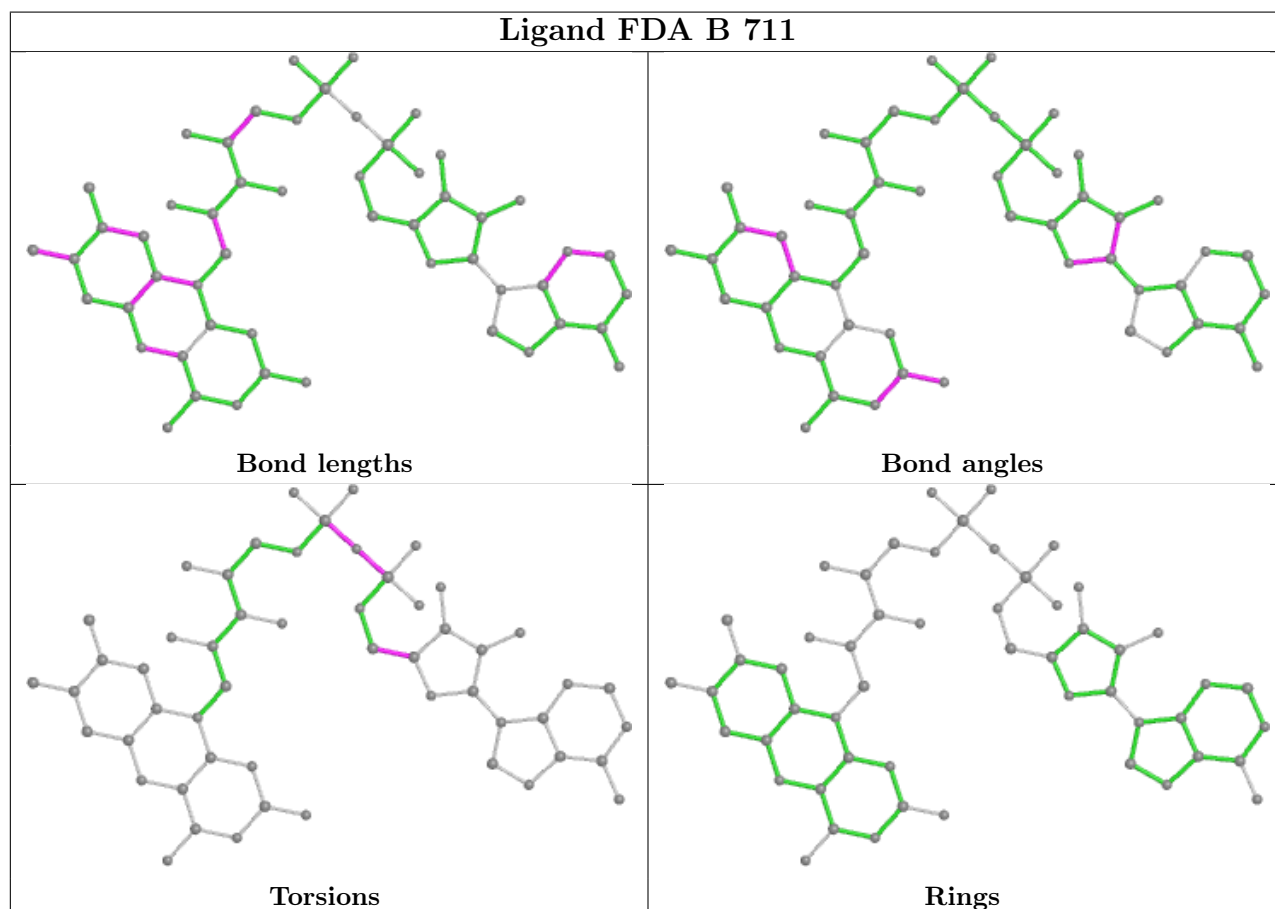
All (7) torsion outliers are listed below:

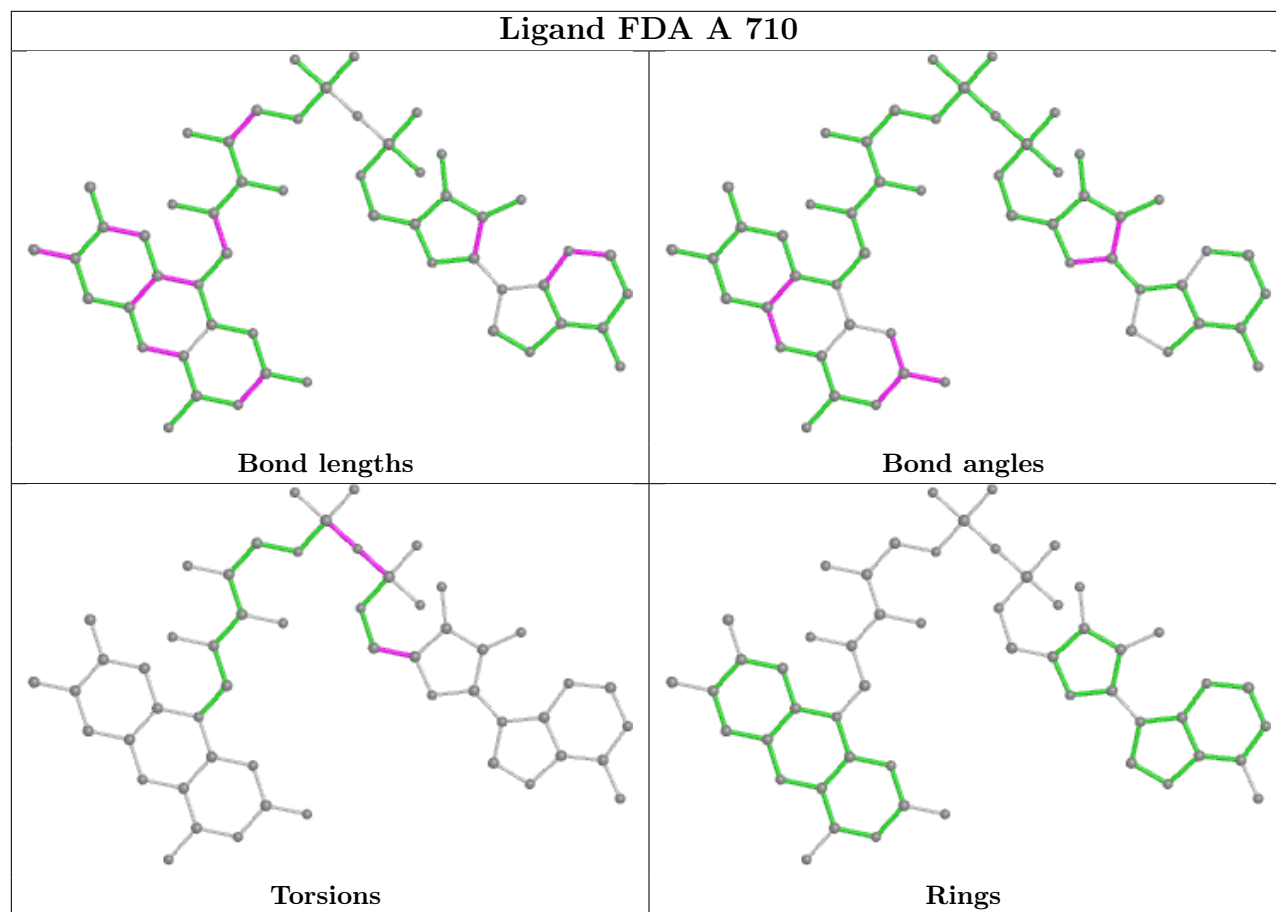| Mol	Chain	Res	Type	Atoms
3	A	710	FDA	PA-O3P-P-O5'
3	B	711	FDA	PA-O3P-P-O5'
3	A	710	FDA	P-O3P-PA-O1A
3	B	711	FDA	P-O3P-PA-O1A
3	A	710	FDA	O4B-C4B-C5B-O5B
3	B	711	FDA	O4B-C4B-C5B-O5B
3	B	711	FDA	P-O3P-PA-O2A

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	711	FDA	2	0
3	A	710	FDA	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand FDA B 711

Bond lengths

Bond angles

Torsions

Rings

Ligand FDA A 710

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Fit of model and data ⓘ

6.1　Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	516/549 (93%)	0.09	25 (4%)	30	18	22, 47, 72, 97	0
1	B	520/549 (94%)	0.12	16 (3%)	49	30	24, 42, 69, 92	0
All	All	1036/1098 (94%)	0.11	41 (3%)	38	23	22, 44, 70, 97	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	374	GLY	5.6
1	B	423	THR	4.7
1	B	422	ALA	4.4
1	B	425	GLY	4.3
1	B	4	PRO	3.9
1	B	424	GLY	3.8
1	B	251	THR	3.7
1	B	375	PRO	3.7
1	B	382	ALA	3.6
1	A	529	ALA	3.5
1	B	374	GLY	3.4
1	A	159	ALA	3.4
1	A	367	PRO	3.3
1	B	529	ALA	3.3
1	B	373	ASP	3.1
1	A	375	PRO	2.9
1	B	5	ILE	2.8
1	A	255	PHE	2.8
1	A	373	ASP	2.6
1	B	153	THR	2.6
1	A	5	ILE	2.6
1	A	160	THR	2.6
1	A	161	ARG	2.5
1	A	425	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	147	HIS	2.4
1	B	368	PRO	2.4
1	A	409	ARG	2.4
1	A	157	THR	2.3
1	B	164	HIS	2.3
1	A	40	GLY	2.3
1	A	528	ALA	2.2
1	A	466	VAL	2.2
1	B	371	HIS	2.2
1	A	164	HIS	2.2
1	A	462	THR	2.2
1	A	103	ALA	2.2
1	A	461	GLY	2.1
1	A	384	VAL	2.0
1	A	380	ILE	2.0
1	A	518	LEU	2.0
1	A	369	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)
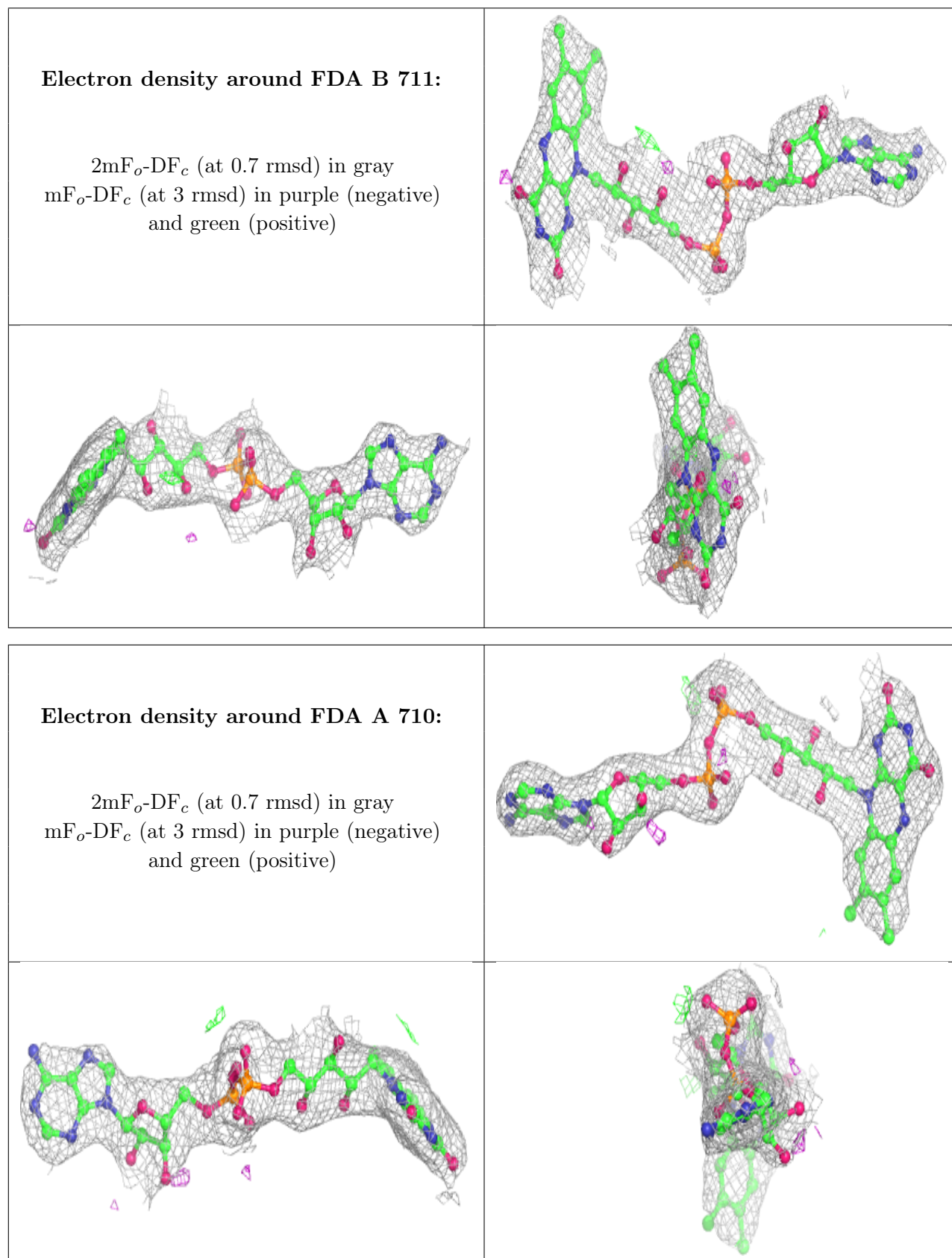
There are no monosaccharides in this entry.

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	NA	A	530	1/1	0.93	0.29	23,23,23,23	0
3	FDA	B	711	53/53	0.94	0.18	30,39,42,44	0
3	FDA	A	710	53/53	0.95	0.17	28,38,42,43	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 B 711:

$2mF_o$-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 710:

$2mF_o$-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 ⓘ

There are no such residues in this entry.