



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:23 AM UTC

PDB ID : 3EPT / pdb\_00003ept  
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](mailto: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>.

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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

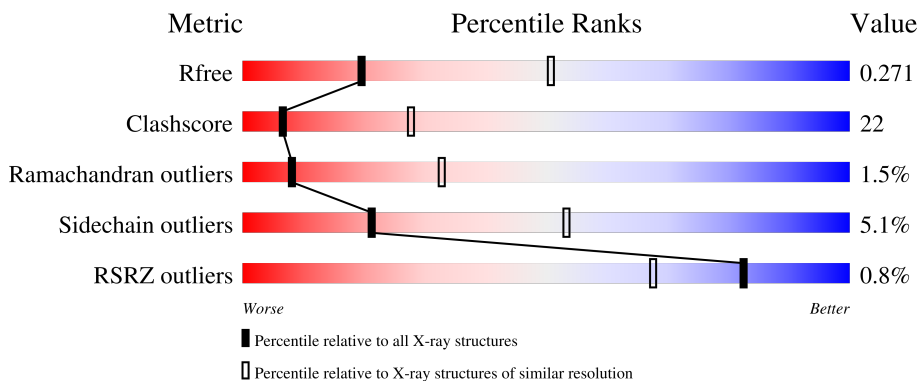
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.97 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (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  $\geq 3$ , 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	549	
1	B	549	

## 2 Entry composition [i](#)

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	3972	2489	752	721	10	0	0	0

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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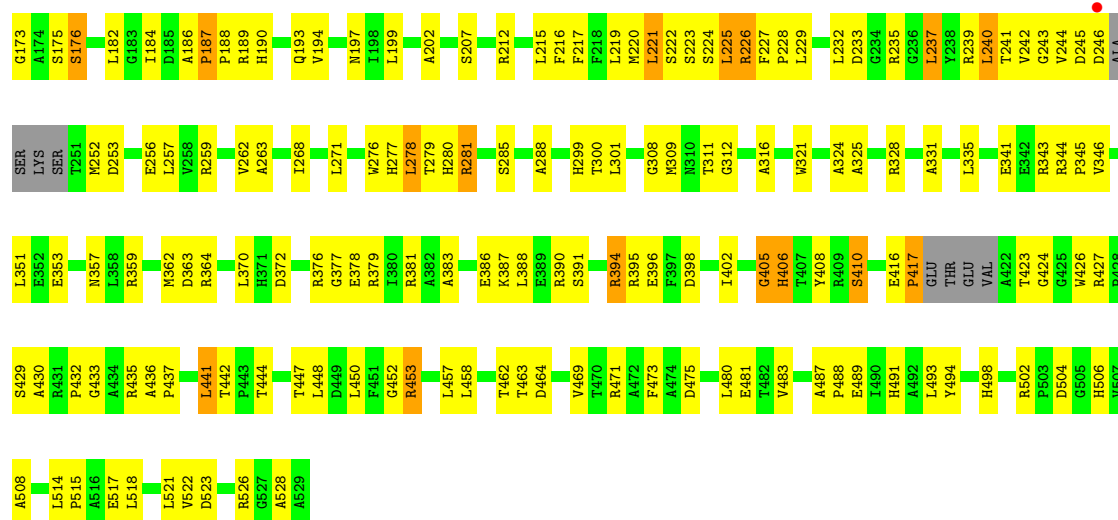


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is water.

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





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.26Å 78.22Å 123.06Å 90.00° 98.66° 90.00°	Depositor
Resolution (Å)	40.00 – 2.97 40.00 – 2.97	Depositor EDS
% Data completeness (in resolution range)	88.4 (40.00-2.97) 88.4 (40.00-2.97)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.95Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.276 0.221 , 0.271	Depositor DCC
$R_{free}$ test set	1165 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtrriage
Anisotropy	0.434	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	8085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FDA, NA

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	0.47	0/4038	0.97	14/5495 (0.3%)
1	B	0.49	0/4070	0.98	16/5540 (0.3%)
All	All	0.48	0/8108	0.97	30/11035 (0.3%)

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	GLY	N-CA-C	-8.57	103.57	114.37
1	A	410	SER	N-CA-C	7.05	118.81	108.86
1	B	410	SER	N-CA-C	6.74	118.37	108.86
1	A	202	ALA	CA-C-N	6.36	127.78	119.84
1	A	202	ALA	C-N-CA	6.36	127.78	119.84
1	A	463	THR	N-CA-C	-6.27	104.94	112.59
1	B	463	THR	N-CA-C	-6.01	105.13	112.88
1	B	202	ALA	CA-C-N	5.98	127.31	119.84
1	B	202	ALA	C-N-CA	5.98	127.31	119.84
1	B	156	ARG	N-CA-C	-5.95	106.66	112.97
1	A	262	VAL	N-CA-C	5.84	116.56	107.28
1	B	441	LEU	N-CA-C	-5.78	105.33	112.90
1	B	262	VAL	N-CA-C	5.73	116.39	107.28
1	A	335	LEU	N-CA-C	5.56	117.80	111.02
1	A	441	LEU	N-CA-C	-5.47	105.73	112.90
1	A	3	ALA	CA-C-N	5.41	125.72	119.93
1	A	3	ALA	C-N-CA	5.41	125.72	119.93
1	B	430	ALA	N-CA-C	-5.31	105.11	113.02
1	A	430	ALA	N-CA-C	-5.20	105.67	113.89
1	B	491	HIS	N-CA-C	-5.15	105.66	111.28
1	B	42	ILE	N-CA-C	5.12	115.96	108.58
1	B	447	THR	N-CA-C	-5.11	105.84	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	PRO	CA-C-N	5.07	124.98	119.76
1	B	187	PRO	C-N-CA	5.07	124.98	119.76
1	B	335	LEU	N-CA-C	5.07	117.20	111.02
1	A	379	ARG	N-CA-C	-5.07	106.93	113.01
1	A	281	ARG	N-CA-C	5.05	117.63	108.69
1	A	491	HIS	N-CA-C	-5.05	105.77	111.28
1	B	281	ARG	N-CA-C	5.05	117.63	108.69
1	A	229	LEU	N-CA-C	-5.03	99.22	108.02

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	3941	0	3861	170	0
1	B	3972	0	3889	173	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	342	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 22.

All (342) 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:82:TRP:HB3	1:B:220:MET:HE2	1.45	0.96
1:A:82:TRP:HB3	1:A:220:MET:HE2	1.50	0.92
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.67
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
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:351:LEU:C	1:A:351:LEU:HD23	2.23	0.64
1:A:7:THR:O	1:A:165:ALA:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ARG:HH11	1:B:156:ARG:HA	1.64	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:B:351:LEU:C	1:B:351:LEU:HD23	2.25	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:A:252:MET:HG3	1:A:253:ASP:N	2.12	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:245:ASP:O	1:B:246:ASP:C	2.45	0.59
1:B:370:LEU:CD1	1:B:381:ARG:HG3	2.33	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
1:B:188:PRO:HG3	1:B:281:ARG:NH2	2.12	0.58
1:B:489:GLU:H	1:B:489:GLU:CD	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:442:THR:C	1:A:444:THR:H	2.12	0.57
1:A:233:ASP:O	1:A:235:ARG:HG3	2.04	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:A:442:THR:C	1:A:444:THR:N	2.63	0.55
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:442:THR:C	1:B:444:THR:H	2.14	0.55
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: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:B:416:GLU:O	1:B:417:PRO:C	2.51	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
1:B:10:LEU:HD13	1:B:163:VAL:HG11	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:442:THR:C	1:B:444:THR:N	2.64	0.52
1:A:154:ASP:C	1:A:156:ARG:H	2.17	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:A:119:TRP:C	1:A:122:PRO:HD2	2.37	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: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:193:GLN:NE2	1:A:362:MET:HE2	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:H	1:A:117:GLN:NE2	2.11	0.49
1:A:154:ASP:C	1:A:156:ARG:N	2.71	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:175:SER:O	1:B:176:SER:C	2.55	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: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:175:SER:O	1:A:176:SER:C	2.56	0.48
1:A:199:LEU:HD22	1:A:271:LEU:HB2	1.96	0.48
1:B:379:ARG:C	1:B:381:ARG:H	2.20	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:A:405:GLY:O	1:A:406:HIS:C	2.57	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: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:B:193:GLN:NE2	1:B:362:MET:HE2	2.29	0.47
1:A:33:LEU:C	1:A:33:LEU:HD23	2.40	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:A:371:HIS:O	1:A:372:ASP:C	2.57	0.47
1:B:226:ARG:NH2	1:B:362:MET:O	2.47	0.47
1:A:390:ARG:C	1:A:392:GLY:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:364:ARG:NE	1:B:388:LEU:HD21	2.31	0.46
1:B:381:ARG:C	1:B:383:ALA:H	2.21	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:B:405:GLY:O	1:B:406:HIS:C	2.59	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:B:119:TRP:C	1:B:122:PRO:HD2	2.41	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:B:379:ARG:C	1:B:381:ARG:N	2.74	0.45
1:A:437:PRO:HB2	1:A:493:LEU:HD21	1.98	0.45
1:B:343:ARG:O	1:B:344:ARG:C	2.59	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:B:435:ARG:O	1:B:436:ALA:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:370:LEU:CD1	1:A:381:ARG:HG2	2.45	0.44
1:B:376:ARG:C	1:B:378:GLU:N	2.74	0.44
1:A:266:THR:O	1:A:268:ILE:HG13	2.17	0.44
1:A:343:ARG:O	1:A:344:ARG:C	2.58	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
1:B:186:ALA:O	1:B:281:ARG:HB2	2.18	0.44
1:B:376:ARG:C	1:B:378:GLU:H	2.25	0.44
1:A:388:LEU:O	1:A:389:GLU:C	2.61	0.44
1:B:56:GLU:O	1:B:59:ARG:HB3	2.18	0.44
1:B:28:ARG:C	1:B:29:GLN:HG2	2.43	0.43
1:B:408:TYR:O	1:B:433:GLY:HA3	2.18	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:363:ASP:O	1:A:364:ARG:C	2.61	0.42
1:B:98:THR:O	1:B:99:ALA:C	2.61	0.42
1:B:233:ASP:O	1:B:235:ARG:HG3	2.19	0.42
1:B:381:ARG:C	1:B:383:ALA:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:208:LEU:HD13	1:A:264:PHE:HB3	2.00	0.42
1:A:390:ARG:C	1:A:392:GLY:N	2.77	0.42
1:B:363:ASP:O	1:B:364:ARG:C	2.63	0.42
1:A:494:TYR:O	1:A:495:GLU:HB2	2.18	0.42
1:B:50:ILE:HG12	1:B:309:MET:HE1	2.01	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:115:CYS:O	1:A:116:PRO:C	2.63	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
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:B:33:LEU:HD23	1:B:33:LEU:C	2.46	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:359:ARG:O	1:A:360:ARG:C	2.64	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: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:381:ARG:C	1:A:383:ALA:N	2.79	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: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:A:399:ALA:O	1:A:400:PRO:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:VAL:HG22	1:B:277:HIS:CD2	2.55	0.40
1:A:21:LEU:CD1	1:A:169:VAL:HG11	2.50	0.40
1:B:240:LEU:C	1:B:240:LEU:HD22	2.47	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

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/549 (93%)	461 (90%)	40 (8%)	9 (2%)	6	28
1	B	514/549 (94%)	465 (90%)	43 (8%)	6 (1%)	10	38
All	All	1024/1098 (93%)	926 (90%)	83 (8%)	15 (2%)	8	33

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

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Mol	Chain	Res	Type
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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	397/433 (92%)	378 (95%)	19 (5%)	23	55
1	B	400/433 (92%)	378 (94%)	22 (6%)	19	51
All	All	797/866 (92%)	756 (95%)	41 (5%)	21	53

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	101	THR
1	A	123	LEU
1	A	130	GLU
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	244	VAL
1	A	252	MET
1	A	278	LEU
1	A	300	THR

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Mol	Chain	Res	Type
1	A	394	ARG
1	A	448	LEU
1	B	21	LEU
1	B	101	THR
1	B	123	LEU
1	B	130	GLU
1	B	131	ARG
1	B	168	LEU
1	B	207	SER
1	B	221	LEU
1	B	225	LEU
1	B	226	ARG
1	B	237	LEU
1	B	240	LEU
1	B	241	THR
1	B	242	VAL
1	B	244	VAL
1	B	278	LEU
1	B	300	THR
1	B	301	LEU
1	B	394	ARG
1	B	417	PRO
1	B	448	LEU
1	B	517	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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	A	477	HIS
1	A	498	HIS
1	A	513	HIS
1	B	27	HIS
1	B	66	GLN
1	B	117	GLN
1	B	193	GLN
1	B	277	HIS

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Mol	Chain	Res	Type
1	B	371	HIS
1	B	477	HIS
1	B	498	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	-	57,58,58	1.56	9 (15%)	78,89,89	1.10	4 (5%)
3	FDA	A	710	-	57,58,58	1.57	9 (15%)	78,89,89	1.07	3 (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
3	FDA	B	711	-	-	3/34/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FDA	A	710	-	-	2/34/50/50	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	710	FDA	C5X-C9A	5.20	1.46	1.40
3	B	711	FDA	C5X-C9A	4.25	1.45	1.40
3	B	711	FDA	C9A-N10	4.01	1.48	1.41
3	B	711	FDA	C4X-N5	3.93	1.43	1.35
3	A	710	FDA	C9A-N10	3.76	1.47	1.41
3	A	710	FDA	C4A-N3A	3.67	1.41	1.34
3	B	711	FDA	C1'-C2'	3.55	1.57	1.52
3	A	710	FDA	C4X-N5	3.43	1.42	1.35
3	A	710	FDA	C1'-C2'	3.38	1.57	1.52
3	B	711	FDA	C7M-C7	3.36	1.57	1.51
3	B	711	FDA	C4A-N3A	3.30	1.40	1.34
3	A	710	FDA	C7M-C7	2.90	1.56	1.51
3	A	710	FDA	C5'-C4'	-2.85	1.47	1.51
3	B	711	FDA	C5'-C4'	-2.68	1.48	1.51
3	A	710	FDA	C2-N3	2.65	1.41	1.37
3	B	711	FDA	C9-C8	2.37	1.42	1.39
3	A	710	FDA	C9-C8	2.23	1.42	1.39
3	B	711	FDA	C2-N3	2.03	1.40	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	711	FDA	O2-C2-N3	-3.34	115.93	121.86
3	A	710	FDA	O2-C2-N3	-2.91	116.69	121.86
3	A	710	FDA	C9A-C5X-N5	2.75	122.72	119.37
3	B	711	FDA	C4'-C3'-C2'	-2.36	109.64	113.57
3	B	711	FDA	C9A-C9-C8	2.33	123.91	119.22
3	B	711	FDA	C9A-C5X-N5	2.29	122.16	119.37
3	A	710	FDA	N3-C2-N1	2.18	119.17	115.74

There are no chirality outliers.

All (5) 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'

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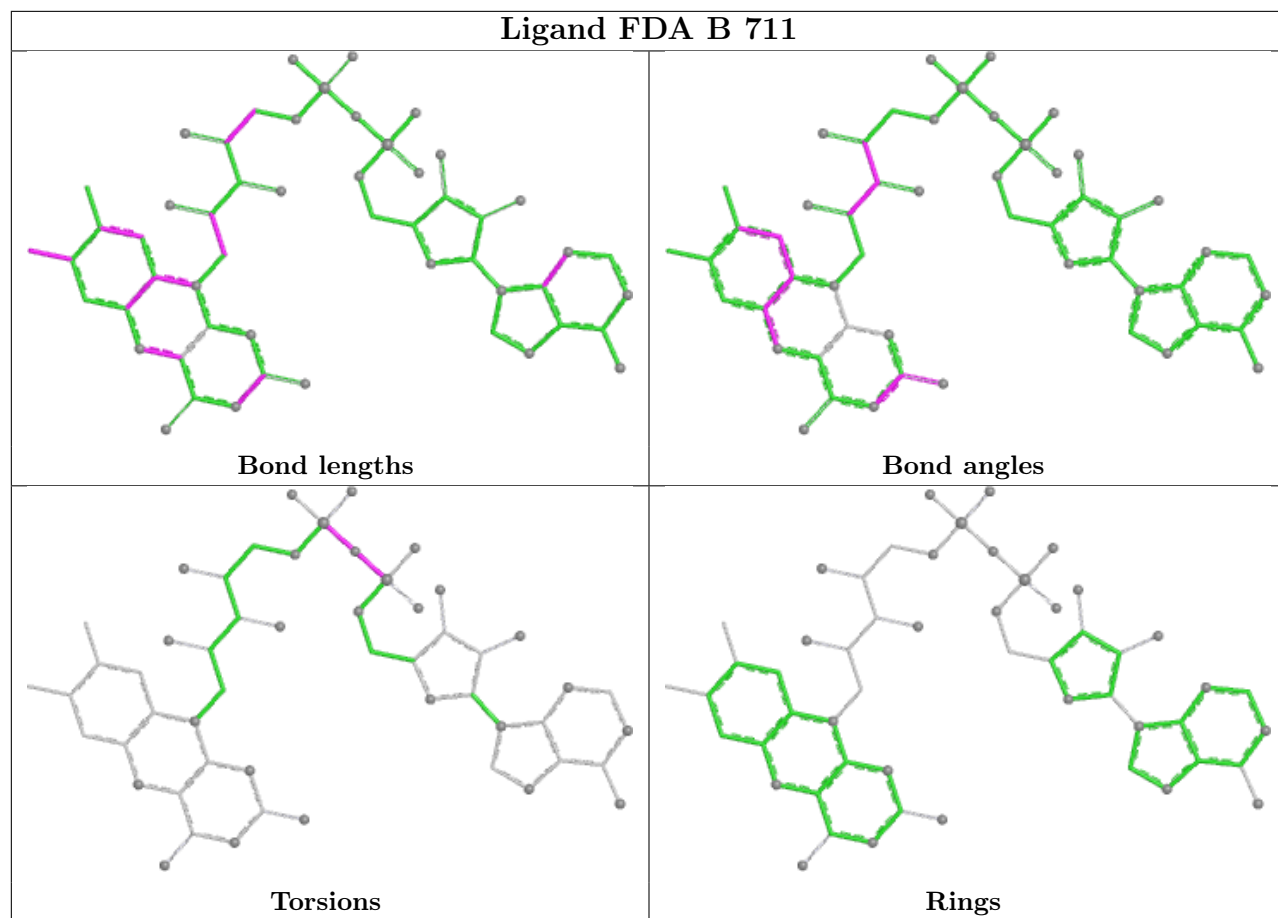
Mol	Chain	Res	Type	Atoms
3	A	710	FDA	P-O3P-PA-O1A
3	B	711	FDA	P-O3P-PA-O1A
3	B	711	FDA	P-O3P-PA-O2A

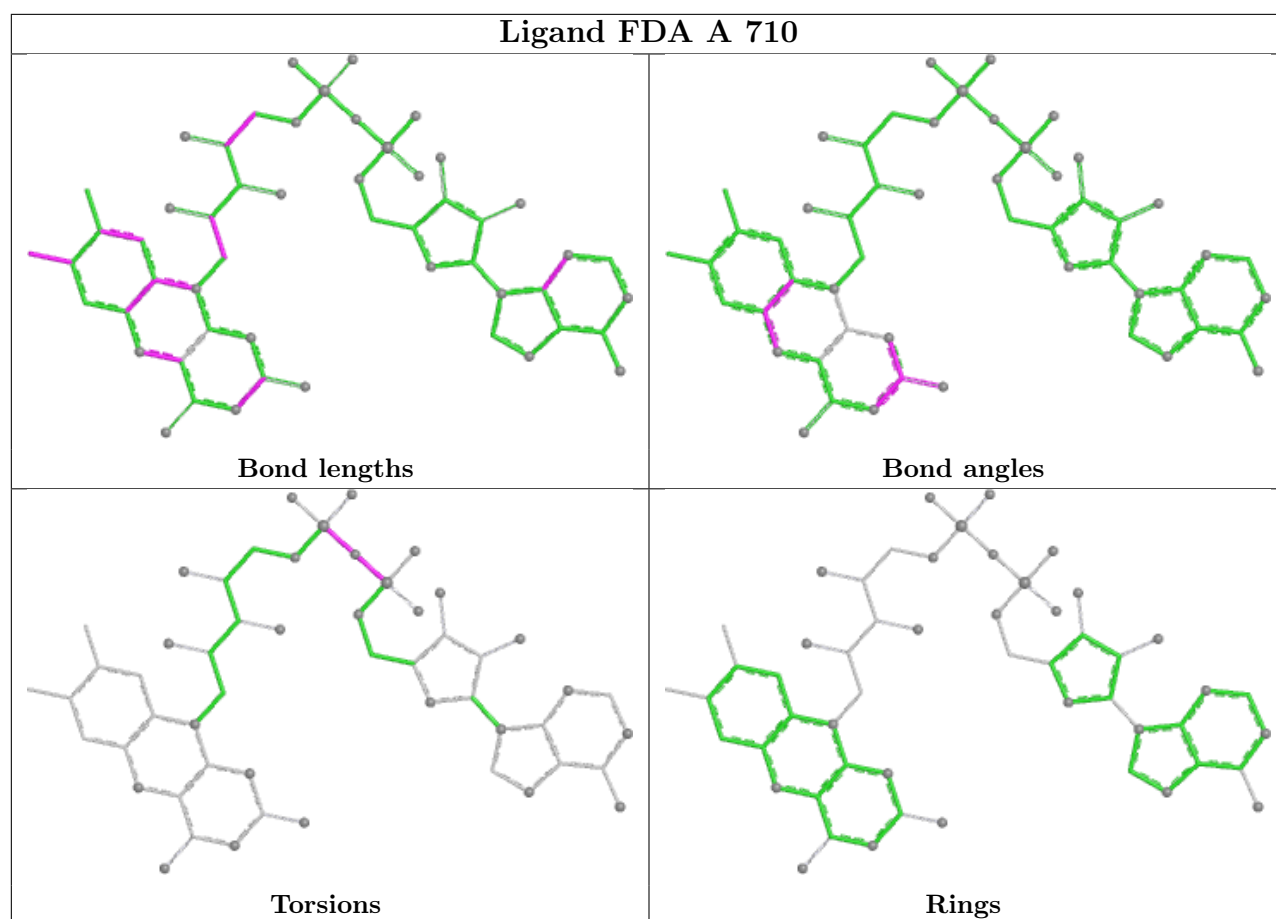
There are no ring outliers.

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 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	516/549 (93%)	-0.04	6 (1%) 76 59	22, 47, 72, 97	0
1	B	520/549 (94%)	-0.12	2 (0%) 88 79	24, 42, 69, 92	0
All	All	1036/1098 (94%)	-0.08	8 (0%) 82 67	22, 44, 70, 97	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	PHE	3.2
1	A	246	ASP	2.8
1	B	2	ASN	2.3
1	A	377	GLY	2.3
1	B	246	ASP	2.3
1	A	466	VAL	2.1
1	A	251	THR	2.1
1	A	380	ILE	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.

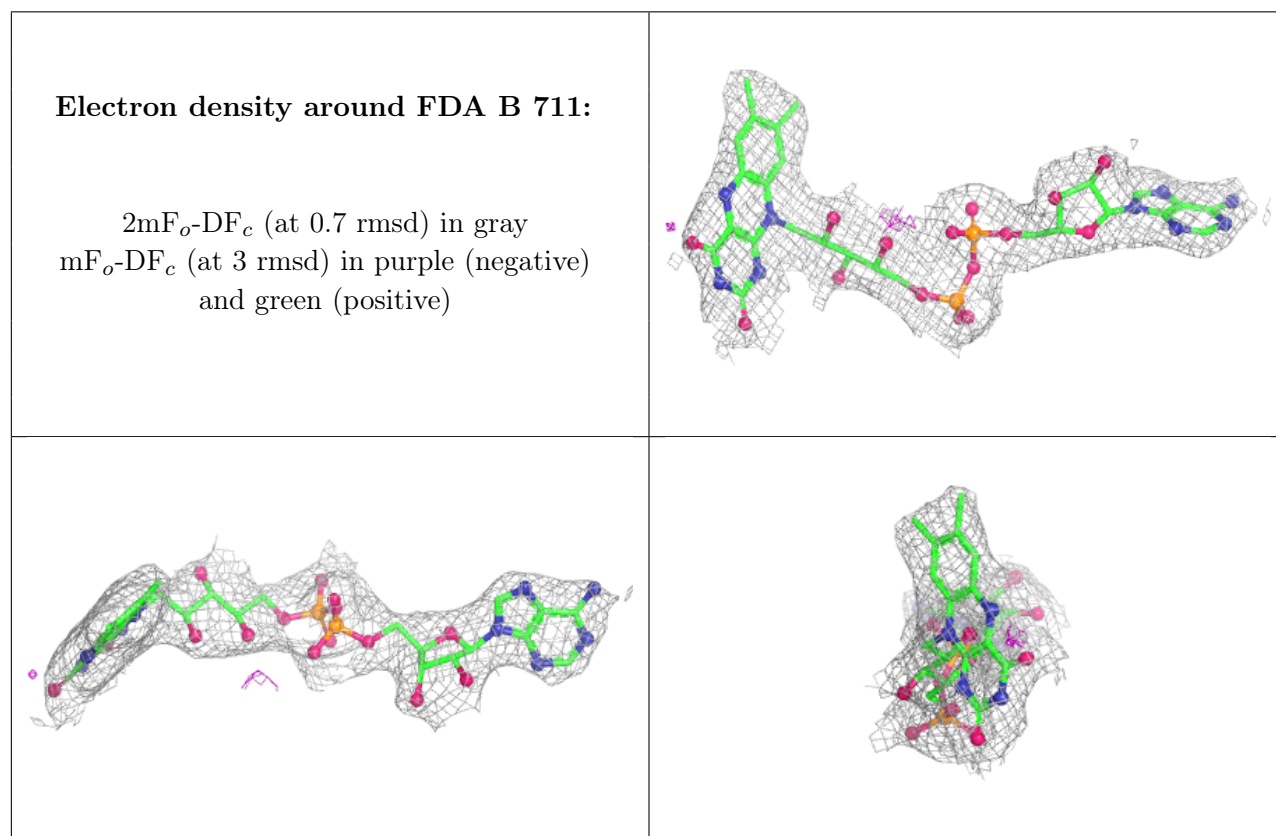
### 6.4 Ligands [i](#)

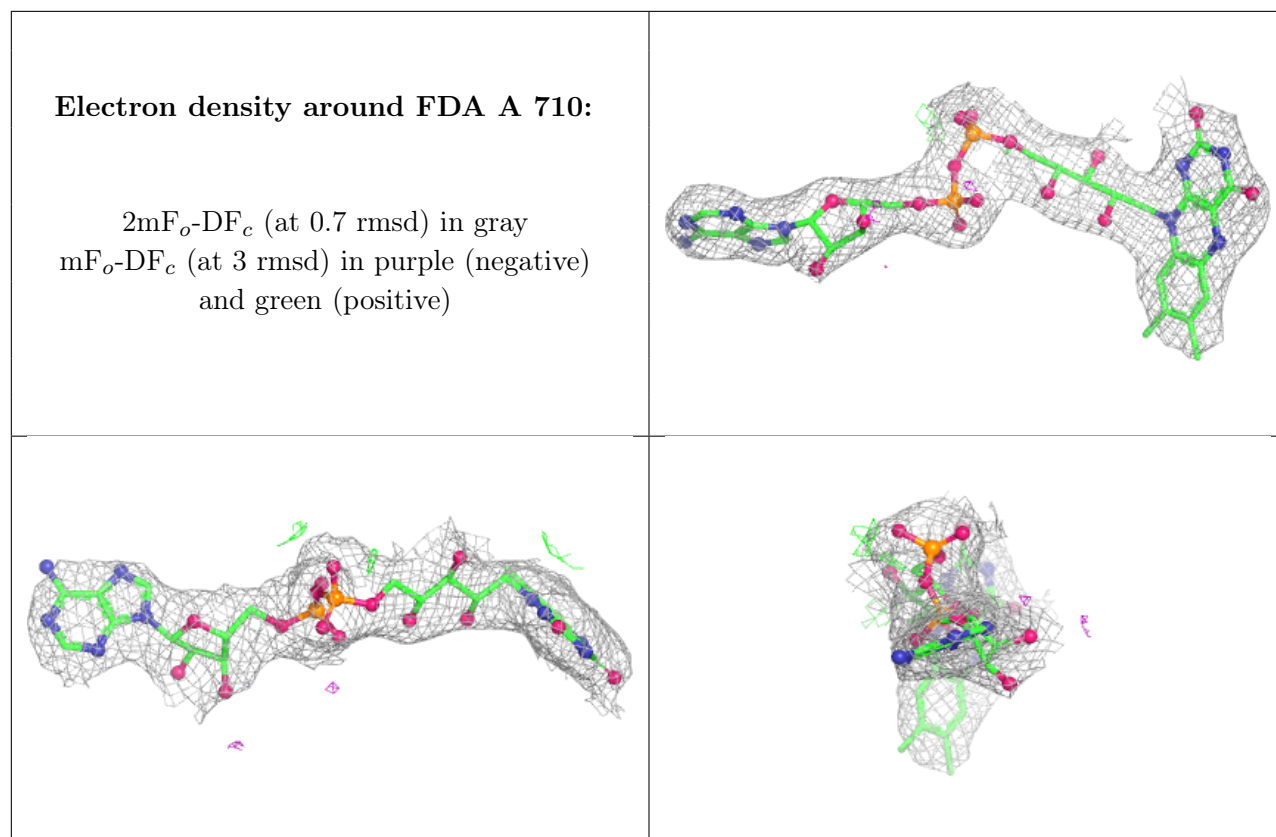
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	FDA	B	711	53/53	0.94	0.08	30,39,42,44	0
3	FDA	A	710	53/53	0.95	0.08	28,38,42,43	0
2	NA	A	530	1/1	0.95	0.13	23,23,23,23	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.





## 6.5 Other polymers [i](#)

There are no such residues in this entry.