



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 06:15 pm GMT

PDB ID : 4A36  
Title : Structure of duck RIG-I helicase domain bound to 19-mer dsRNA and ATP transition state analogue  
Authors : Kowalinski, E.; Lunardi, T.; McCarthy, A.A.; Cusack, S.  
Deposited on : 2011-09-30  
Resolution : 3.70 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

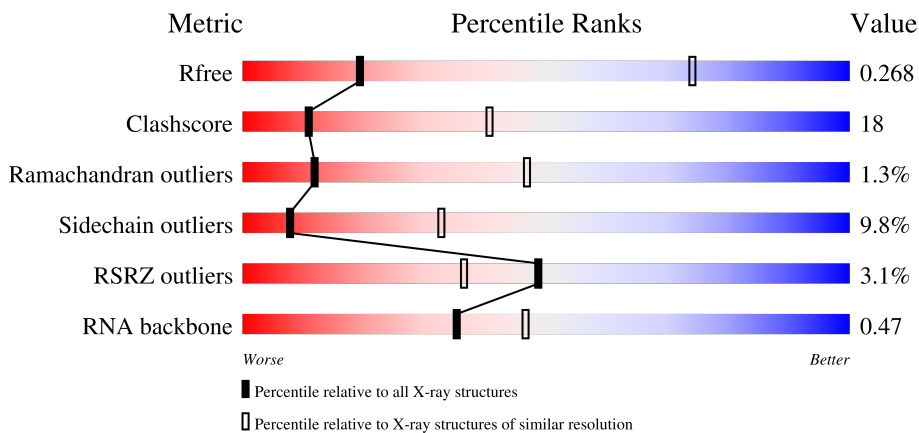
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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))
$R_{free}$	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

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  $\geq 3$ , 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	556	 4% 58% 31% 6%
1	B	556	 2% 57% 32% 5% 6%
2	R	19	 47% 47% 5%
2	T	19	 53% 37% 5% 5%

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Mol	Chain	Length	Quality of chain
3	S	19	
3	U	19	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AF3	B	1796	-	-	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9974 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 RETINOIC ACID INDUCIBLE PROTEIN I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	523	Total 4175	C 2634	N 726	O 789	S 26	0	0	0
1	B	523	Total 4173	C 2635	N 726	O 786	S 26	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLY	-	expression tag	UNP D3TI84
A	240	ALA	-	expression tag	UNP D3TI84
A	241	MET	-	expression tag	UNP D3TI84
B	239	GLY	-	expression tag	UNP D3TI84
B	240	ALA	-	expression tag	UNP D3TI84
B	241	MET	-	expression tag	UNP D3TI84

- Molecule 2 is a RNA chain called 5'-R(\*GP\*CP\*AP\*UP\*GP\*CP\*GP\*AP\*CP\*CP\*UP\*C  
P\*UP\*GP \*UP\*UP\*UP\*GP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	R	19	Total 398	C 179	N 67	O 134	P 18	0	0	0
2	T	18	Total 376	C 169	N 62	O 128	P 17	0	0	0

- Molecule 3 is a RNA chain called 5'-R(\*UP\*CP\*AP\*AP\*AP\*CP\*AP\*GP\*AP\*GP\*GP\*U  
P\*CP\*GP \*CP\*AP\*UP\*GP\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	S	19	Total 404	C 182	N 76	O 128	P 18	0	0	0
3	U	18	Total 384	C 173	N 74	O 120	P 17	0	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

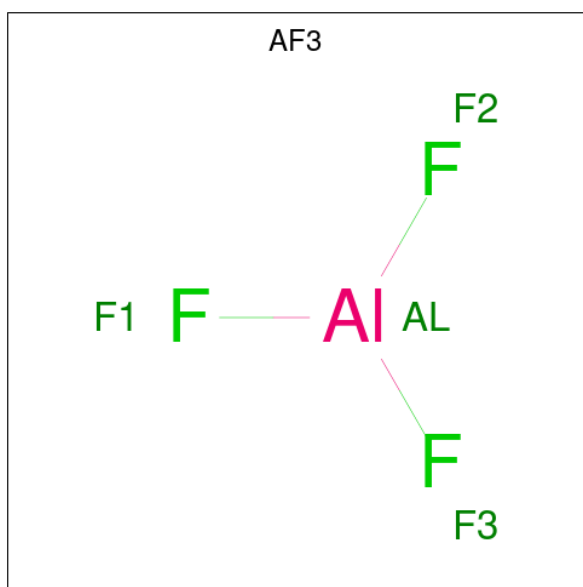


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	27	10	5	10	2	0	0
4	B	1	27	10	5	10	2	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

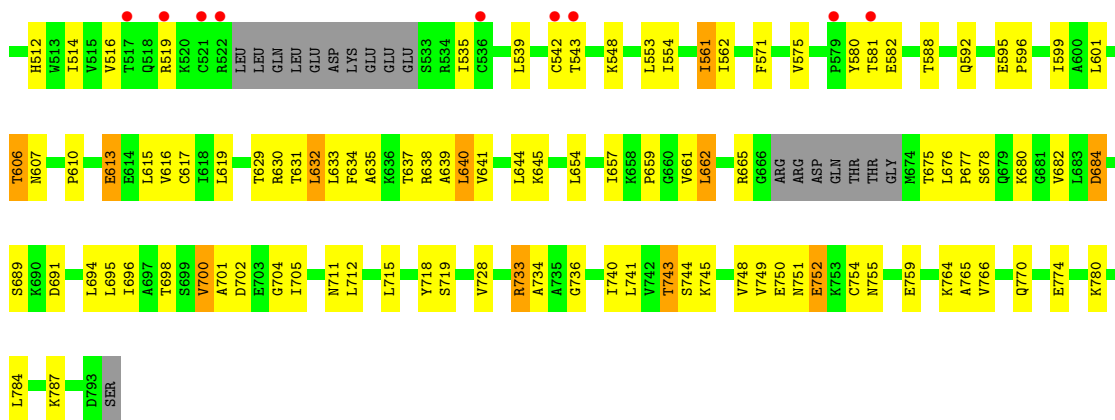
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	1	1	1	0	0
5	B	1	1	1	0	0

- Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula:  $AlF_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
6	A	1	4	1	3	0	0
6	B	1	4	1	3	0	0





● Molecule 2: 5'-R(\*GP\*CP\*AP\*UP\*GP\*CP\*GP\*AP\*CP\*CP\*UP\*CP\*UP\*GP \*UP\*UP\*UP\*GP\*A)-3'



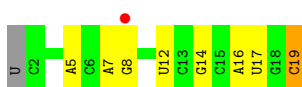
● Molecule 2: 5'-R(\*GP\*CP\*AP\*UP\*GP\*CP\*GP\*AP\*CP\*CP\*UP\*CP\*UP\*GP \*UP\*UP\*UP\*GP\*A)-3'



● Molecule 3: 5'-R(\*UP\*CP\*AP\*AP\*AP\*CP\*AP\*GP\*AP\*GP\*GP\*UP\*CP\*GP \*CP\*AP\*UP\*GP\*C)-3'



● Molecule 3: 5'-R(\*UP\*CP\*AP\*AP\*AP\*CP\*AP\*GP\*AP\*GP\*GP\*UP\*CP\*GP \*CP\*AP\*UP\*GP\*C)-3'





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.27Å 129.27Å 106.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.95 – 3.70 45.95 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.95-3.70) 100.0 (45.95-3.70)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 3.66Å)	Xtrriage
Refinement program	REFMAC 5.6.0116	Depositor
R, $R_{free}$	0.193 , 0.263 0.196 , 0.268	Depositor DCC
$R_{free}$ test set	940 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	98.3	Xtrriage
Anisotropy	0.235	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 66.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.047 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9974	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, ADP, MG

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	0.45	0/4239	0.64	0/5715
1	B	0.45	0/4238	0.64	0/5715
2	R	0.34	0/443	0.73	0/688
2	T	0.30	0/418	0.74	0/649
3	S	0.31	0/452	0.72	0/703
3	U	0.29	0/430	0.73	0/669
All	All	0.43	0/10220	0.66	0/14139

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	719	SER	Peptide
1	B	719	SER	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	4175	0	4231	164	0
1	B	4173	0	4234	165	0
2	R	398	0	205	7	0
2	T	376	0	194	5	0
3	S	404	0	208	11	0
3	U	384	0	198	10	0
4	A	27	0	12	1	0
4	B	27	0	12	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	4	0	0	1	0
6	B	4	0	0	3	0
All	All	9974	0	9294	348	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 18.

All (348) 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:641:VAL:HG13	1:A:696:ILE:HG22	1.35	1.08
1:B:641:VAL:HG13	1:B:696:ILE:HG22	1.40	1.03
1:B:303:VAL:HG12	1:B:304:PRO:HD3	1.47	0.96
1:A:327:ILE:HG22	1:A:349:VAL:HG13	1.52	0.92
1:B:416:VAL:O	1:B:416:VAL:HG13	1.67	0.91
1:B:743:THR:HG22	1:B:745:LYS:H	1.35	0.90
1:A:743:THR:HG22	1:A:745:LYS:H	1.34	0.90
1:B:327:ILE:HG22	1:B:349:VAL:HG13	1.55	0.89
1:A:303:VAL:HG12	1:A:304:PRO:HD3	1.56	0.87
1:A:416:VAL:O	1:A:416:VAL:HG13	1.73	0.87
1:B:269:THR:HG22	1:B:457:LYS:HZ3	1.40	0.86
1:A:335:VAL:HG11	1:A:340:VAL:CG2	2.07	0.84
1:A:350:THR:HG23	1:A:351:PRO:HD2	1.61	0.81
1:B:335:VAL:HG11	1:B:340:VAL:CG2	2.10	0.81
1:B:303:VAL:HG12	1:B:304:PRO:CD	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:THR:HG22	1:A:592:GLN:OE1	1.83	0.79
1:B:335:VAL:HG11	1:B:340:VAL:HG21	1.66	0.78
1:B:269:THR:HG22	1:B:457:LYS:NZ	1.99	0.78
1:B:637:THR:HG23	3:U:16:A:OP1	1.83	0.77
1:A:278:ILE:HD12	1:A:279:LEU:N	1.99	0.77
1:A:335:VAL:HG11	1:A:340:VAL:HG21	1.67	0.77
1:A:390:MET:HE1	1:A:407:ILE:HD12	1.67	0.76
1:A:390:MET:CE	1:A:407:ILE:HD12	2.16	0.75
1:B:694:LEU:HD12	1:B:695:LEU:N	2.01	0.75
1:A:743:THR:HG21	1:A:748:VAL:HB	1.68	0.74
1:A:257:ALA:HB3	1:A:280:ILE:HD12	1.69	0.73
1:B:416:VAL:O	1:B:416:VAL:CG1	2.35	0.73
1:A:733:ARG:NH2	6:A:1796:AF3:F2	2.11	0.73
1:B:743:THR:HG21	1:B:748:VAL:HB	1.70	0.73
1:A:310:LYS:HA	1:A:348:VAL:HG21	1.72	0.72
1:A:641:VAL:HG13	1:A:696:ILE:CG2	2.15	0.72
1:A:297:VAL:HG21	1:A:369:PHE:CE1	2.25	0.72
1:B:641:VAL:HG13	1:B:696:ILE:CG2	2.18	0.72
1:A:303:VAL:HG11	1:A:676:LEU:HD22	1.70	0.72
1:B:278:ILE:C	1:B:278:ILE:HD12	2.11	0.71
1:B:588:THR:HG22	1:B:592:GLN:OE1	1.88	0.71
1:A:702:ASP:HB2	1:A:728:VAL:HG22	1.72	0.71
1:B:462:VAL:HG13	1:B:741:LEU:HD23	1.73	0.71
1:B:350:THR:HG23	1:B:351:PRO:HD2	1.72	0.70
1:B:698:THR:HG21	3:U:17:U:OP1	1.91	0.70
1:B:702:ASP:HB2	1:B:728:VAL:HG22	1.74	0.70
1:A:491:ILE:HG22	1:A:535:ILE:HG23	1.74	0.70
1:B:278:ILE:HD12	1:B:279:LEU:N	2.06	0.69
1:B:631:THR:HB	1:B:694:LEU:HD13	1.74	0.69
1:A:303:VAL:HG12	1:A:304:PRO:CD	2.21	0.69
1:A:278:ILE:HD12	1:A:278:ILE:C	2.13	0.68
1:B:615:LEU:CD2	1:B:619:LEU:HD22	2.22	0.68
1:B:364:THR:HG22	1:B:364:THR:O	1.93	0.68
1:A:631:THR:HB	1:A:694:LEU:HD13	1.74	0.68
1:A:694:LEU:HD12	1:A:695:LEU:N	2.09	0.68
1:A:416:VAL:O	1:A:416:VAL:CG1	2.42	0.67
1:B:297:VAL:HG21	1:B:369:PHE:CE1	2.29	0.67
1:A:273:LYS:HE2	1:A:412:ALA:HB2	1.76	0.67
1:B:581:THR:HG22	1:B:582:GLU:H	1.60	0.67
1:B:255:GLN:HA	1:B:258:ILE:HD12	1.74	0.67
1:B:491:ILE:HG22	1:B:535:ILE:HG23	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:THR:HG22	1:A:582:GLU:H	1.59	0.66
1:A:364:THR:HG22	1:A:364:THR:O	1.95	0.65
1:B:615:LEU:HD21	1:B:619:LEU:HD22	1.77	0.65
1:B:303:VAL:HG11	1:B:676:LEU:HD22	1.78	0.65
1:B:273:LYS:HE2	1:B:412:ALA:HB2	1.78	0.65
1:B:363:LEU:CD1	1:B:368:ILE:HD12	2.27	0.64
1:B:338:GLU:HG2	1:B:362:THR:HG22	1.80	0.64
1:B:429:ILE:HD13	1:B:766:VAL:HG22	1.80	0.64
1:B:390:MET:CE	1:B:407:ILE:HD12	2.28	0.64
1:A:363:LEU:CD1	1:A:368:ILE:HD12	2.28	0.63
1:A:363:LEU:HD11	1:A:368:ILE:HD12	1.80	0.63
1:B:310:LYS:HA	1:B:348:VAL:HG21	1.81	0.63
2:R:13:U:H2'	2:R:14:G:O4'	1.99	0.63
1:A:327:ILE:CG2	1:A:353:ILE:HG21	2.28	0.63
1:A:297:VAL:CG2	1:A:369:PHE:CE1	2.82	0.62
1:B:363:LEU:HD11	1:B:368:ILE:HD12	1.79	0.62
1:B:645:LYS:HD3	1:B:661:VAL:HG23	1.81	0.62
1:A:327:ILE:HG21	1:A:353:ILE:HG21	1.82	0.62
1:A:645:LYS:HD3	1:A:661:VAL:HG23	1.81	0.62
1:B:327:ILE:CG2	1:B:353:ILE:HG21	2.30	0.62
1:A:698:THR:HG21	3:S:17:U:OP1	1.99	0.62
1:B:264:LEU:HD11	1:B:411:THR:HG22	1.82	0.61
1:A:338:GLU:HG2	1:A:362:THR:HG22	1.83	0.61
1:B:374:PHE:CZ	1:B:390:MET:HE2	2.35	0.61
1:B:698:THR:HG23	1:B:700:VAL:CG2	2.31	0.61
1:A:350:THR:HG21	3:S:19:C:OP1	2.01	0.61
1:A:472:PRO:HB2	1:A:601:LEU:HD11	1.83	0.61
1:B:698:THR:HG23	1:B:700:VAL:HG23	1.81	0.61
1:B:733:ARG:NH2	6:B:1796:AF3:F2	2.24	0.61
1:A:275:PHE:CE1	1:A:279:LEU:HD13	2.35	0.60
1:A:390:MET:HG3	1:A:436:LEU:HD23	1.83	0.60
1:A:637:THR:HG23	3:S:16:A:OP1	2.01	0.60
1:B:421:ASN:ND2	1:B:424:GLU:OE1	2.35	0.60
1:B:327:ILE:HG21	1:B:353:ILE:HG21	1.82	0.60
1:A:635:ALA:HB1	1:A:640:LEU:HD13	1.84	0.59
1:B:347:ILE:N	1:B:347:ILE:HD12	2.17	0.59
3:S:10:G:H2'	3:S:11:G:H8	1.67	0.59
1:B:562:ILE:HD12	1:B:562:ILE:H	1.67	0.59
1:B:704:GLY:HA2	6:B:1796:AF3:F3	1.93	0.59
1:A:297:VAL:HG23	1:A:369:PHE:CD1	2.38	0.59
1:A:347:ILE:HD12	1:A:347:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ILE:HD13	1:A:766:VAL:HG22	1.84	0.58
1:A:462:VAL:HG11	1:A:749:VAL:HG13	1.85	0.58
1:A:698:THR:HG23	1:A:700:VAL:HG23	1.85	0.58
1:A:421:ASN:ND2	1:A:424:GLU:OE1	2.36	0.58
1:A:615:LEU:HD21	1:A:619:LEU:HD22	1.87	0.57
1:A:335:VAL:CG1	1:A:340:VAL:CG2	2.81	0.57
1:A:561:ILE:HD12	1:A:561:ILE:H	1.69	0.57
1:B:297:VAL:CG2	1:B:369:PHE:CE1	2.88	0.57
1:A:629:THR:HG23	1:A:711:ASN:HB3	1.87	0.57
3:S:10:G:H2'	3:S:11:G:C8	2.39	0.57
1:A:575:VAL:HG12	1:A:580:TYR:CD1	2.39	0.57
1:B:635:ALA:HB1	1:B:640:LEU:HD13	1.85	0.57
1:B:694:LEU:HD12	1:B:695:LEU:H	1.69	0.57
2:R:5:G:H2'	2:R:6:C:O4'	2.05	0.56
1:B:698:THR:CG2	1:B:700:VAL:HG23	2.36	0.56
1:A:678:SER:O	1:A:682:VAL:HG23	2.06	0.56
1:B:561:ILE:HD12	1:B:561:ILE:H	1.69	0.56
1:B:662:LEU:HD13	1:B:695:LEU:HD21	1.88	0.56
1:A:390:MET:HE1	1:A:407:ILE:CD1	2.34	0.56
1:A:616:VAL:HA	1:A:654:LEU:HD11	1.88	0.55
1:A:615:LEU:CD2	1:A:619:LEU:HD22	2.36	0.55
1:B:468:ARG:NH1	1:B:606:THR:HG22	2.21	0.55
1:B:734:ALA:O	1:B:736:GLY:N	2.39	0.55
1:A:255:GLN:HA	1:A:258:ILE:HD12	1.88	0.55
1:B:273:LYS:HE3	4:B:1794:ADP:O1B	2.07	0.55
1:B:335:VAL:CG1	1:B:340:VAL:CG2	2.84	0.55
2:T:5:G:H2'	2:T:6:C:O4'	2.08	0.54
1:A:273:LYS:HE3	4:A:1794:ADP:O1B	2.08	0.54
1:A:276:VAL:O	1:A:280:ILE:HG12	2.08	0.54
1:A:350:THR:CG2	1:A:351:PRO:HD2	2.34	0.54
1:B:276:VAL:O	1:B:280:ILE:HG12	2.08	0.54
1:B:472:PRO:HB2	1:B:601:LEU:HD11	1.90	0.53
1:B:575:VAL:HG12	1:B:580:TYR:CD1	2.42	0.53
1:A:595:GLU:HG2	1:A:599:ILE:HD11	1.91	0.53
1:B:257:ALA:HB3	1:B:280:ILE:HD12	1.91	0.53
1:B:519:ARG:HH12	3:U:12:U:H5''	1.73	0.53
1:B:297:VAL:HG23	1:B:369:PHE:CD1	2.43	0.53
1:B:425:THR:HG22	1:B:765:ALA:CB	2.39	0.53
1:A:462:VAL:HG13	1:A:741:LEU:HD23	1.89	0.53
1:A:662:LEU:HD13	1:A:695:LEU:HD21	1.89	0.53
1:A:680:LYS:O	1:A:684:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:PHE:CE1	1:B:279:LEU:HD13	2.44	0.53
1:B:571:PHE:O	1:B:575:VAL:HG23	2.09	0.53
2:T:4:U:H2'	2:T:5:G:C8	2.44	0.53
1:A:258:ILE:HG23	1:A:283:HIS:HB3	1.90	0.53
1:B:390:MET:HG3	1:B:436:LEU:HD23	1.91	0.53
1:A:468:ARG:NH1	1:A:606:THR:HG22	2.24	0.52
1:B:347:ILE:HG22	1:B:349:VAL:HG22	1.89	0.52
1:B:390:MET:HE3	1:B:407:ILE:HD12	1.90	0.52
1:B:629:THR:HG23	1:B:711:ASN:HB3	1.91	0.52
1:B:616:VAL:HA	1:B:654:LEU:HD11	1.90	0.52
1:A:575:VAL:HG12	1:A:580:TYR:HD1	1.75	0.52
1:A:698:THR:HG23	1:A:700:VAL:CG2	2.39	0.52
1:A:315:HIS:O	1:A:319:ARG:HD3	2.10	0.52
1:A:330:GLU:HG3	1:A:676:LEU:HD12	1.91	0.52
2:R:4:U:H2'	2:R:5:G:C8	2.45	0.51
2:T:3:A:C2	2:T:4:U:C2	2.98	0.51
1:A:425:THR:HG22	1:A:765:ALA:CB	2.40	0.51
1:A:460:ILE:HG23	1:A:739:CYS:SG	2.51	0.51
1:A:743:THR:HG22	1:A:745:LYS:N	2.15	0.51
1:A:698:THR:CG2	1:A:700:VAL:HG23	2.41	0.51
1:B:462:VAL:HG11	1:B:749:VAL:HG13	1.92	0.51
1:A:275:PHE:CE1	1:A:279:LEU:CD1	2.93	0.51
1:A:562:ILE:HD12	1:A:562:ILE:H	1.75	0.51
1:B:333:SER:OG	3:S:2:C:OP1	2.29	0.51
1:A:634:PHE:CE1	1:A:701:ALA:HB3	2.46	0.50
1:B:258:ILE:HG23	1:B:283:HIS:HB3	1.92	0.50
3:U:5:A:O5'	3:U:5:A:H8	1.94	0.50
1:A:248:SER:O	1:A:251:ILE:HG22	2.11	0.50
1:B:390:MET:HE1	1:B:407:ILE:HD12	1.93	0.50
1:B:575:VAL:HG12	1:B:580:TYR:HD1	1.76	0.50
1:A:327:ILE:CG2	1:A:349:VAL:HG13	2.32	0.50
1:B:595:GLU:HG2	1:B:599:ILE:HD11	1.92	0.50
1:B:468:ARG:HH12	1:B:606:THR:HG22	1.76	0.50
1:B:678:SER:O	1:B:682:VAL:HG23	2.12	0.50
1:A:473:PHE:HA	1:A:476:ILE:HD12	1.92	0.50
1:B:376:GLU:O	1:B:379:ASN:ND2	2.44	0.50
1:B:698:THR:CG2	1:B:700:VAL:CG2	2.89	0.50
1:A:431:SER:HA	1:A:784:LEU:HD23	1.93	0.50
1:B:514:ILE:HG23	1:B:543:THR:HB	1.93	0.49
1:B:315:HIS:O	1:B:319:ARG:HD3	2.13	0.49
1:B:701:ALA:HA	1:B:705:ILE:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:ARG:HH12	1:A:606:THR:HG22	1.77	0.49
1:B:491:ILE:CG2	1:B:535:ILE:HG23	2.42	0.49
1:B:743:THR:HG22	1:B:745:LYS:N	2.16	0.49
1:A:750:GLU:O	1:A:751:ASN:C	2.50	0.49
1:B:330:GLU:HG3	1:B:676:LEU:HD12	1.94	0.49
1:A:328:SER:OG	1:A:329:GLY:N	2.46	0.49
1:B:303:VAL:HG21	1:B:676:LEU:CD1	2.43	0.49
1:B:303:VAL:HG21	1:B:676:LEU:HD11	1.95	0.49
2:R:3:A:C2	2:R:4:U:C2	3.00	0.49
1:A:491:ILE:CG2	1:A:535:ILE:HG23	2.41	0.48
1:B:431:SER:HA	1:B:784:LEU:HD23	1.94	0.48
1:B:469:ILE:O	1:B:469:ILE:HD12	2.12	0.48
1:A:275:PHE:O	1:A:278:ILE:HG13	2.13	0.48
1:A:595:GLU:OE2	1:A:599:ILE:HD11	2.14	0.48
1:B:465:VAL:HG11	1:B:610:PRO:HB2	1.95	0.48
1:B:680:LYS:O	1:B:684:ASP:HB2	2.12	0.48
1:A:469:ILE:HD12	1:A:469:ILE:O	2.14	0.48
1:B:698:THR:CG2	3:U:17:U:OP1	2.59	0.48
1:A:512:HIS:O	1:A:516:VAL:HG23	2.14	0.48
1:A:514:ILE:HG23	1:A:543:THR:HB	1.95	0.48
1:B:506:GLY:O	1:B:554:ILE:HD13	2.13	0.48
1:A:303:VAL:HG21	1:A:676:LEU:CD1	2.44	0.48
1:A:694:LEU:HD12	1:A:695:LEU:H	1.76	0.48
1:A:303:VAL:HG11	1:A:676:LEU:CD2	2.42	0.48
1:B:473:PHE:HA	1:B:476:ILE:HD12	1.94	0.48
1:A:701:ALA:HA	1:A:705:ILE:HD12	1.95	0.47
1:A:707:ILE:O	1:A:707:ILE:HG22	2.15	0.47
1:A:356:ASN:O	1:A:359:GLU:HG2	2.15	0.47
1:A:419:ALA:HB1	1:A:425:THR:N	2.29	0.47
1:A:612:LEU:HD21	1:A:647:CYS:SG	2.55	0.47
1:B:425:THR:CG2	1:B:765:ALA:HB2	2.45	0.47
1:A:676:LEU:N	1:A:677:PRO:HD2	2.30	0.47
1:A:734:ALA:O	1:A:736:GLY:N	2.44	0.47
1:B:303:VAL:CG1	1:B:304:PRO:N	2.78	0.47
1:B:356:ASN:O	1:B:359:GLU:HG2	2.15	0.47
1:B:441:ILE:HB	1:B:770:GLN:NE2	2.30	0.47
1:B:305:VAL:HG22	1:B:705:ILE:HG13	1.97	0.47
1:A:297:VAL:CG2	1:A:369:PHE:CD1	2.98	0.47
1:A:261:LYS:NZ	1:A:774:GLU:OE1	2.49	0.46
1:A:303:VAL:HG21	1:A:676:LEU:HD11	1.97	0.46
1:A:376:GLU:O	1:A:379:ASN:ND2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:GLY:HA2	3:U:19:C:H5''	1.97	0.46
1:B:350:THR:CG2	1:B:351:PRO:HD2	2.43	0.46
1:B:676:LEU:N	1:B:677:PRO:HD2	2.31	0.46
1:B:419:ALA:HB1	1:B:425:THR:N	2.31	0.46
1:B:610:PRO:HA	1:B:613:GLU:HB2	1.98	0.46
1:B:631:THR:HG22	1:B:632:LEU:N	2.31	0.46
2:R:13:U:C2	2:R:14:G:C8	3.04	0.46
1:A:355:VAL:O	1:A:356:ASN:C	2.53	0.46
1:B:254:ALA:HA	1:B:280:ILE:HD11	1.97	0.46
1:B:350:THR:HB	1:B:353:ILE:HD13	1.98	0.46
1:A:778:ALA:O	1:A:782:HIS:ND1	2.49	0.46
1:B:355:VAL:O	1:B:356:ASN:C	2.54	0.46
1:A:390:MET:HE2	1:A:407:ILE:HD12	1.98	0.45
1:A:698:THR:CG2	3:S:17:U:OP1	2.64	0.45
1:B:263:ALA:HB3	1:B:408:LEU:HD12	1.96	0.45
1:A:305:VAL:HG22	1:A:705:ILE:HG13	1.97	0.45
1:A:399:ASN:HD21	1:A:792:ARG:NH2	2.15	0.45
1:B:487:LEU:HD12	1:B:487:LEU:O	2.16	0.45
1:B:328:SER:OG	1:B:329:GLY:N	2.50	0.45
1:A:361:GLY:O	1:A:363:LEU:N	2.50	0.45
1:B:261:LYS:NZ	1:B:774:GLU:OE1	2.48	0.45
1:A:297:VAL:HG21	1:A:369:PHE:CZ	2.50	0.45
1:A:465:VAL:HG11	1:A:610:PRO:HB2	1.99	0.45
1:A:441:ILE:HB	1:A:770:GLN:NE2	2.32	0.45
1:A:571:PHE:O	1:A:575:VAL:HG23	2.17	0.45
1:B:306:TYR:CZ	1:B:328:SER:HB2	2.52	0.45
1:B:327:ILE:CG2	1:B:349:VAL:HG13	2.38	0.45
3:S:7:A:C2	3:S:8:G:C5	3.05	0.45
1:A:749:VAL:HG12	1:A:753:LYS:HE3	1.99	0.45
1:A:615:LEU:C	1:A:615:LEU:HD23	2.37	0.45
1:B:297:VAL:HG21	1:B:369:PHE:CZ	2.52	0.45
1:A:374:PHE:CZ	1:A:390:MET:HE3	2.52	0.45
1:A:425:THR:CG2	1:A:765:ALA:HB2	2.47	0.44
1:A:631:THR:HG22	1:A:632:LEU:N	2.31	0.44
1:B:303:VAL:CG1	1:B:304:PRO:CD	2.91	0.44
1:B:488:MET:HE2	1:B:539:LEU:HD22	1.99	0.44
1:B:615:LEU:HD23	1:B:619:LEU:HD22	1.95	0.44
1:B:596:PRO:HA	1:B:599:ILE:HD12	1.99	0.44
1:A:347:ILE:HG22	1:A:349:VAL:HG22	1.99	0.44
1:B:414:VAL:CG1	1:B:429:ILE:HG12	2.48	0.44
1:A:264:LEU:HD11	1:A:411:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:HD13	1:A:368:ILE:HD12	2.00	0.44
1:B:444:VAL:HG21	1:B:451:LEU:HD22	1.98	0.44
1:B:512:HIS:O	1:B:516:VAL:HG23	2.17	0.44
1:A:487:LEU:HD12	1:A:487:LEU:O	2.18	0.44
1:A:596:PRO:HA	1:A:599:ILE:HD12	2.00	0.44
1:A:762:MET:O	1:A:765:ALA:HB3	2.18	0.44
1:A:476:ILE:HG21	1:A:598:LEU:HD21	1.99	0.44
1:B:361:GLY:O	1:B:363:LEU:N	2.51	0.44
1:A:743:THR:HG22	1:A:744:SER:N	2.33	0.43
1:A:707:ILE:HD12	1:A:707:ILE:N	2.34	0.43
1:B:390:MET:HE1	1:B:407:ILE:CD1	2.48	0.43
1:A:350:THR:HB	1:A:353:ILE:HD13	2.01	0.43
1:A:350:THR:HG21	3:S:19:C:P	2.58	0.43
1:A:521:CYS:SG	1:A:539:LEU:HD12	2.58	0.43
1:A:610:PRO:HA	1:A:613:GLU:HB2	1.99	0.43
1:B:712:LEU:CD1	1:B:740:ILE:HD12	2.48	0.43
1:A:337:VAL:O	1:A:338:GLU:C	2.55	0.43
1:B:363:LEU:HD13	1:B:368:ILE:HD12	1.99	0.43
1:B:634:PHE:CE1	1:B:701:ALA:HB3	2.54	0.43
4:B:1794:ADP:O2B	6:B:1796:AF3:F3	2.27	0.43
1:B:269:THR:H	1:B:457:LYS:HZ1	1.65	0.43
1:A:278:ILE:HG22	1:A:313:PHE:CZ	2.54	0.42
1:A:390:MET:CE	1:A:407:ILE:CD1	2.92	0.42
1:B:490:THR:O	1:B:490:THR:HG22	2.19	0.42
1:A:297:VAL:HG13	1:A:349:VAL:HG23	2.01	0.42
1:A:335:VAL:CG1	1:A:340:VAL:HG23	2.49	0.42
1:B:689:SER:C	1:B:691:ASP:H	2.22	0.42
1:B:702:ASP:HB2	1:B:728:VAL:CG2	2.48	0.42
1:A:715:LEU:HB3	1:A:718:TYR:HB3	2.01	0.42
1:A:275:PHE:CE1	1:A:278:ILE:HD11	2.54	0.42
1:A:429:ILE:HD12	1:A:765:ALA:HB1	2.02	0.42
1:A:488:MET:HE2	1:A:539:LEU:HD22	2.00	0.42
1:A:254:ALA:HA	1:A:280:ILE:HD11	2.00	0.42
1:B:595:GLU:OE2	1:B:599:ILE:HD11	2.20	0.42
1:B:640:LEU:HD22	1:B:644:LEU:CD1	2.50	0.42
1:B:743:THR:HG22	1:B:744:SER:N	2.33	0.42
2:R:16:U:H2'	2:R:17:U:C6	2.55	0.42
1:B:715:LEU:HB3	1:B:718:TYR:HB3	2.02	0.42
2:T:7:G:N2	3:U:14:G:C4	2.88	0.42
1:A:436:LEU:HB2	1:A:438:ILE:HD13	2.01	0.42
1:A:708:VAL:O	1:A:734:ALA:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:16:A:H2'	3:S:17:U:O4'	2.20	0.42
1:A:476:ILE:HD13	1:A:598:LEU:HD23	2.01	0.42
1:A:490:THR:HG22	1:A:490:THR:O	2.20	0.42
1:A:645:LYS:HD3	1:A:661:VAL:CG2	2.49	0.42
1:B:264:LEU:HB2	1:B:438:ILE:HG12	2.02	0.41
1:B:281:CYS:SG	1:B:296:VAL:HG11	2.60	0.41
1:B:404:LEU:HB3	1:B:405:PRO:HD2	2.02	0.41
1:B:297:VAL:CG2	1:B:369:PHE:CD1	3.03	0.41
1:B:422:ILE:HD11	1:B:764:LYS:NZ	2.34	0.41
1:B:750:GLU:O	1:B:751:ASN:C	2.56	0.41
1:A:531:GLU:OE2	1:A:535:ILE:HD11	2.21	0.41
1:A:592:GLN:HA	1:A:595:GLU:HB2	2.01	0.41
1:B:380:THR:OG1	1:B:436:LEU:HD21	2.21	0.41
3:U:16:A:H2'	3:U:17:U:O4'	2.20	0.41
1:A:789:ARG:NH1	1:A:790:VAL:H	2.18	0.41
1:A:404:LEU:HB3	1:A:405:PRO:HD2	2.03	0.41
1:A:765:ALA:O	1:A:769:ILE:HG13	2.21	0.41
1:B:324:VAL:HG22	1:B:346:ILE:HB	2.02	0.41
1:B:357:SER:HA	1:B:360:ASP:HB2	2.02	0.41
1:B:629:THR:HG22	1:B:630:ARG:N	2.34	0.41
1:B:350:THR:HG21	3:U:19:C:OP1	2.21	0.41
1:B:592:GLN:HA	1:B:595:GLU:HB2	2.03	0.41
1:A:357:SER:HA	1:A:360:ASP:HB2	2.03	0.41
1:A:414:VAL:CG1	1:A:429:ILE:HG12	2.50	0.41
1:A:419:ALA:CB	1:A:425:THR:N	2.84	0.41
1:A:664:GLY:C	1:A:665:ARG:HG2	2.42	0.41
1:B:248:SER:O	1:B:251:ILE:HG22	2.21	0.41
1:B:275:PHE:O	1:B:278:ILE:HG13	2.21	0.41
1:B:407:ILE:HG22	1:B:408:LEU:N	2.36	0.41
1:B:419:ALA:CB	1:B:425:THR:N	2.83	0.41
1:B:638:ARG:O	1:B:639:ALA:C	2.58	0.41
2:T:14:G:C2	3:U:7:A:C2	3.08	0.41
1:A:347:ILE:HD12	1:A:347:ILE:H	1.85	0.41
1:A:749:VAL:O	1:A:753:LYS:HG3	2.21	0.41
1:B:335:VAL:CG1	1:B:340:VAL:HG23	2.50	0.41
1:B:615:LEU:HD11	1:B:633:LEU:HD21	2.03	0.41
1:A:698:THR:CG2	1:A:700:VAL:CG2	2.98	0.40
1:A:634:PHE:HE1	1:A:701:ALA:HB3	1.85	0.40
1:B:548:LYS:HG3	1:B:571:PHE:CE1	2.57	0.40
1:B:645:LYS:HD3	1:B:661:VAL:CG2	2.49	0.40
1:A:565:LEU:HD11	1:A:599:ILE:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:VAL:HG13	1:B:349:VAL:HG23	2.03	0.40
1:B:477:ILE:HG21	1:B:553:LEU:HG	2.04	0.40
2:R:7:G:N2	3:S:14:G:C4	2.89	0.40
1:B:581:THR:HG22	1:B:582:GLU:N	2.32	0.40
1:B:752:GLU:O	1:B:755:ASN:HB2	2.21	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	515/556 (93%)	454 (88%)	54 (10%)	7 (1%)	11	45
1	B	515/556 (93%)	452 (88%)	57 (11%)	6 (1%)	13	48
All	All	1030/1112 (93%)	906 (88%)	111 (11%)	13 (1%)	12	47

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	458	PRO
1	B	458	PRO
1	B	461	ASP
1	A	453	ARG
1	A	461	ASP
1	B	453	ARG
1	B	607	ASN
1	A	403	GLN
1	A	607	ASN
1	B	403	GLN
1	B	659	PRO
1	A	416	VAL
1	A	659	PRO

### 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	468/498 (94%)	421 (90%)	47 (10%)	7	32
1	B	468/498 (94%)	423 (90%)	45 (10%)	8	34
All	All	936/996 (94%)	844 (90%)	92 (10%)	8	33

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	SER
1	A	278	ILE
1	A	283	HIS
1	A	302	LYS
1	A	303	VAL
1	A	306	TYR
1	A	315	HIS
1	A	319	ARG
1	A	327	ILE
1	A	333	SER
1	A	342	GLU
1	A	349	VAL
1	A	356	ASN
1	A	362	THR
1	A	363	LEU
1	A	365	SER
1	A	366	LEU
1	A	367	SER
1	A	385	PRO
1	A	414	VAL
1	A	416	VAL
1	A	442	SER
1	A	449	GLN
1	A	453	ARG
1	A	456	ASN
1	A	507	THR
1	A	542	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	561	ILE
1	A	606	THR
1	A	613	GLU
1	A	617	CYS
1	A	632	LEU
1	A	640	LEU
1	A	657	ILE
1	A	662	LEU
1	A	665	ARG
1	A	675	THR
1	A	684	ASP
1	A	700	VAL
1	A	733	ARG
1	A	752	GLU
1	A	754	CYS
1	A	759	GLU
1	A	780	LYS
1	A	787	LYS
1	A	790	VAL
1	A	793	ASP
1	B	248	SER
1	B	278	ILE
1	B	279	LEU
1	B	283	HIS
1	B	302	LYS
1	B	303	VAL
1	B	306	TYR
1	B	315	HIS
1	B	319	ARG
1	B	327	ILE
1	B	333	SER
1	B	349	VAL
1	B	356	ASN
1	B	362	THR
1	B	363	LEU
1	B	365	SER
1	B	366	LEU
1	B	367	SER
1	B	385	PRO
1	B	414	VAL
1	B	416	VAL
1	B	442	SER

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Mol	Chain	Res	Type
1	B	449	GLN
1	B	453	ARG
1	B	507	THR
1	B	542	CYS
1	B	561	ILE
1	B	606	THR
1	B	613	GLU
1	B	617	CYS
1	B	632	LEU
1	B	640	LEU
1	B	657	ILE
1	B	662	LEU
1	B	665	ARG
1	B	675	THR
1	B	684	ASP
1	B	700	VAL
1	B	733	ARG
1	B	743	THR
1	B	752	GLU
1	B	754	CYS
1	B	759	GLU
1	B	780	LYS
1	B	787	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	356	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	R	18/19 (94%)	2 (11%)	0
2	T	17/19 (89%)	3 (17%)	0
3	S	18/19 (94%)	1 (5%)	0
3	U	17/19 (89%)	2 (11%)	0
All	All	70/76 (92%)	8 (11%)	0

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	R	14	G
2	R	15	U
3	S	19	C
2	T	12	C
2	T	13	U
2	T	14	G
3	U	8	G
3	U	19	C

There are no RNA pucker outliers to report.

#### 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 monosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
4	ADP	A	1794	5,6	24,29,29	1.06	3 (12%)	29,45,45	1.54	4 (13%)
6	AF3	A	1796	4	0,3,3	-	-	-	-	-
6	AF3	B	1796	4	0,3,3	-	-	-	-	-
4	ADP	B	1794	5,6	24,29,29	1.03	2 (8%)	29,45,45	1.47	4 (13%)

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
4	ADP	A	1794	5,6	-	0/12/32/32	0/3/3/3
4	ADP	B	1794	5,6	-	1/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1794	ADP	O4'-C1'	2.65	1.44	1.41
4	B	1794	ADP	C5-C4	2.40	1.47	1.40
4	A	1794	ADP	C5-C4	2.26	1.46	1.40
4	B	1794	ADP	C2-N3	2.26	1.35	1.32
4	A	1794	ADP	C2-N3	2.07	1.35	1.32

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1794	ADP	N3-C2-N1	-4.02	122.40	128.68
4	A	1794	ADP	PA-O3A-PB	-3.62	120.40	132.83
4	B	1794	ADP	N3-C2-N1	-3.22	123.64	128.68
4	B	1794	ADP	PA-O3A-PB	-2.95	122.69	132.83
4	B	1794	ADP	C4-C5-N7	-2.59	106.70	109.40
4	A	1794	ADP	O3A-PB-O1B	-2.40	97.89	111.19
4	A	1794	ADP	C4-C5-N7	-2.27	107.04	109.40
4	B	1794	ADP	O3A-PB-O1B	-2.17	99.13	111.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1794	ADP	C5'-O5'-PA-O3A

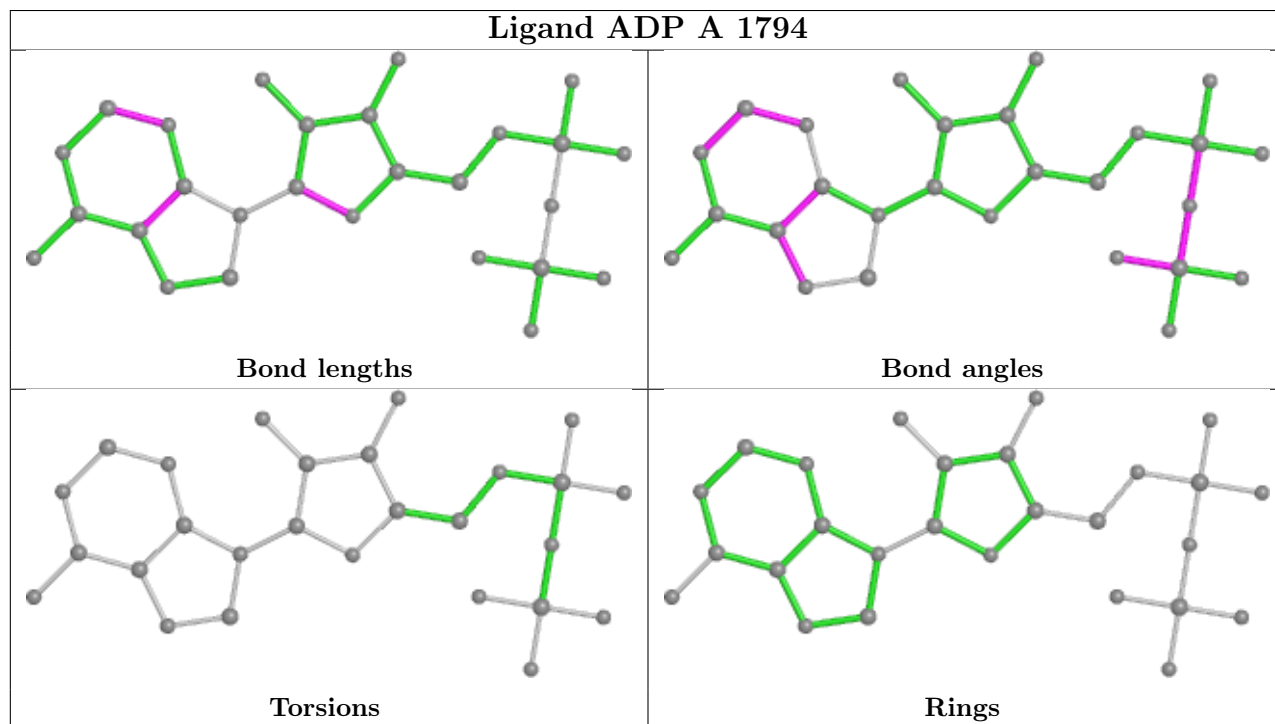
There are no ring outliers.

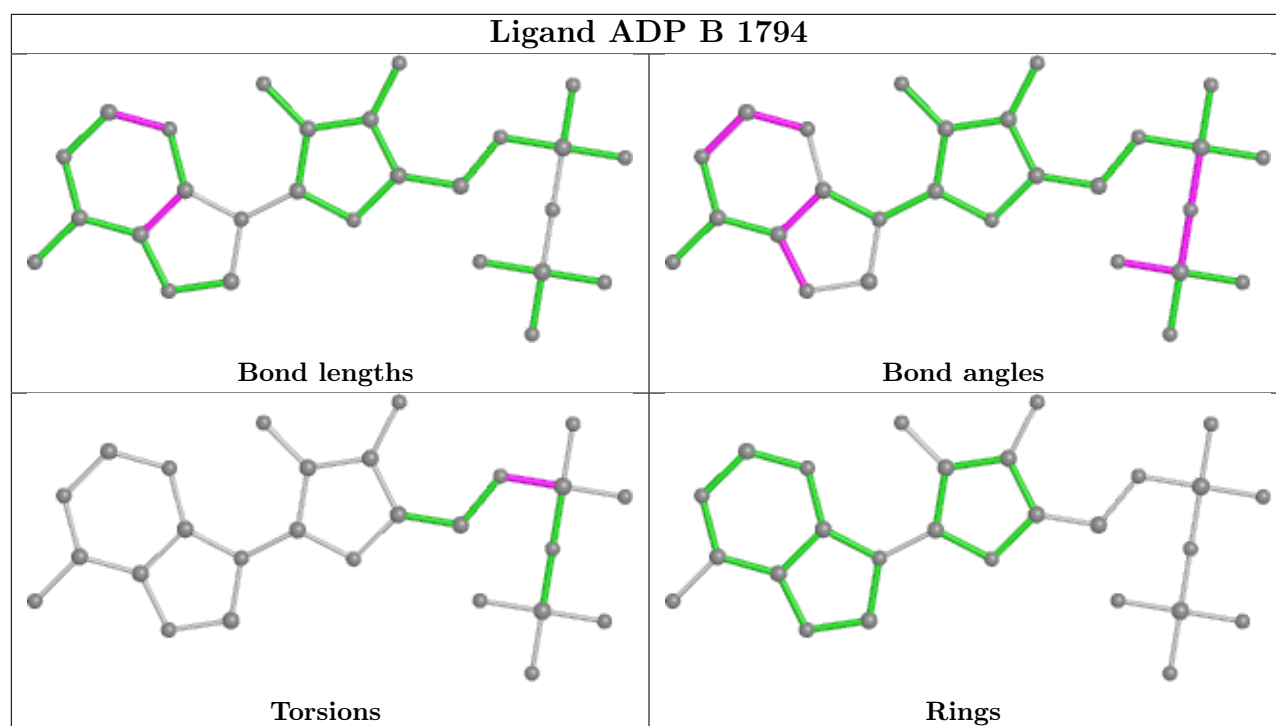
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1794	ADP	1	0
6	A	1796	AF3	1	0
6	B	1796	AF3	3	0
4	B	1794	ADP	2	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





## 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	523/556 (94%)	-0.04	25 (4%) 30 22	57, 104, 211, 264	0
1	B	523/556 (94%)	-0.21	9 (1%) 70 59	56, 96, 164, 207	0
2	R	19/19 (100%)	0.13	0 100 100	73, 114, 141, 155	0
2	T	18/19 (94%)	0.16	0 100 100	85, 113, 204, 208	0
3	S	19/19 (100%)	0.14	0 100 100	74, 105, 152, 165	0
3	U	18/19 (94%)	0.34	1 (5%) 24 17	66, 138, 200, 219	0
All	All	1120/1188 (94%)	-0.10	35 (3%) 49 36	56, 99, 196, 264	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	ILE	5.8
1	A	545	HIS	5.4
1	A	521	CYS	5.0
1	B	581	THR	4.2
1	A	538	ALA	4.1
1	A	488	MET	4.0
1	A	537	ARG	3.8
1	A	512	HIS	3.8
1	B	517	THR	3.7
1	A	542	CYS	3.5
1	A	515	VAL	3.4
1	A	511	GLU	3.4
1	A	534	ARG	3.4
1	B	536	CYS	3.1
1	A	490	THR	2.9
1	B	522	ARG	2.8
1	B	521	CYS	2.7
1	A	485	GLU	2.7
1	A	514	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	517	THR	2.5
1	A	583	LEU	2.5
1	A	582	GLU	2.5
1	A	518	GLN	2.5
1	A	587	LEU	2.5
1	A	470	HIS	2.4
1	B	579	PRO	2.4
1	A	474	ALA	2.3
1	A	600	ALA	2.3
1	A	536	CYS	2.3
1	B	542	CYS	2.3
1	B	543	THR	2.2
1	B	519	ARG	2.1
1	A	575	VAL	2.1
3	U	8	G	2.1
1	A	489	ARG	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](#)

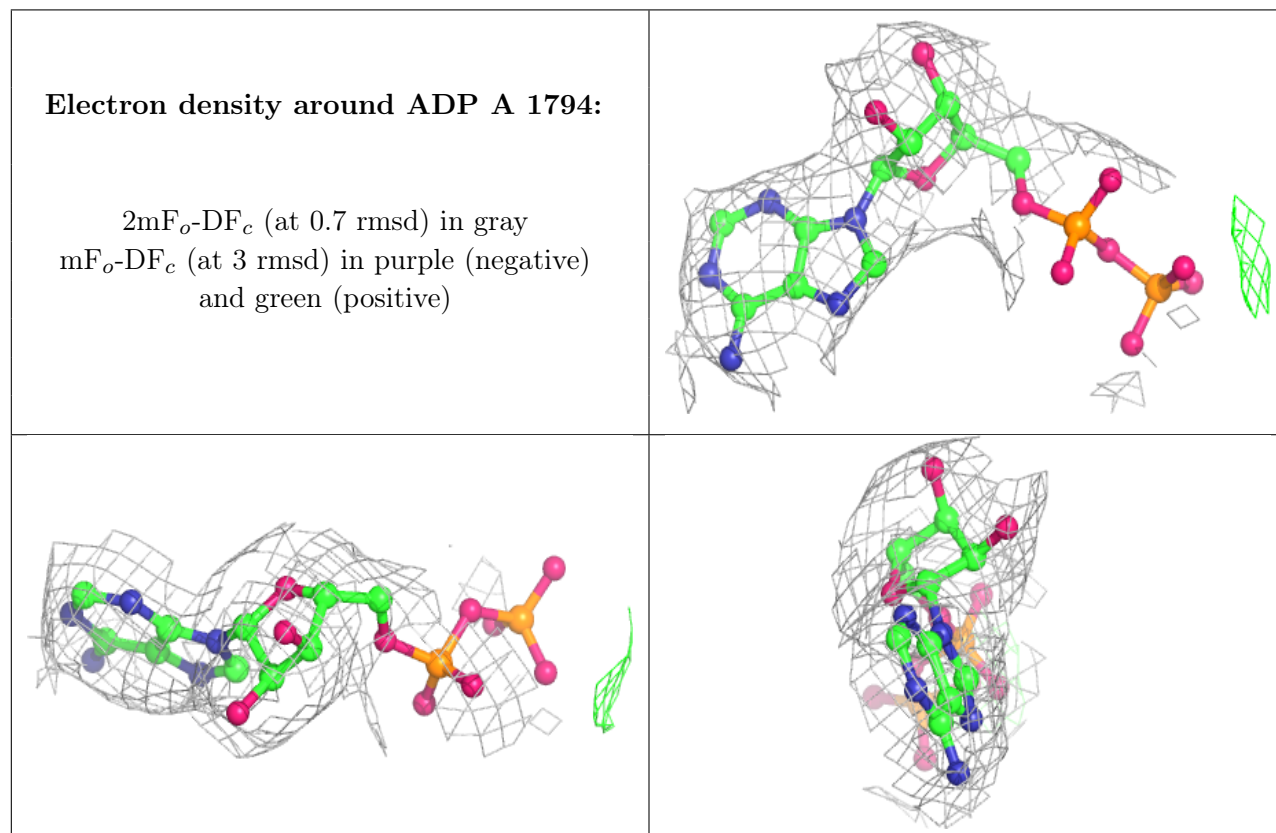
There are no monosaccharides in this entry.

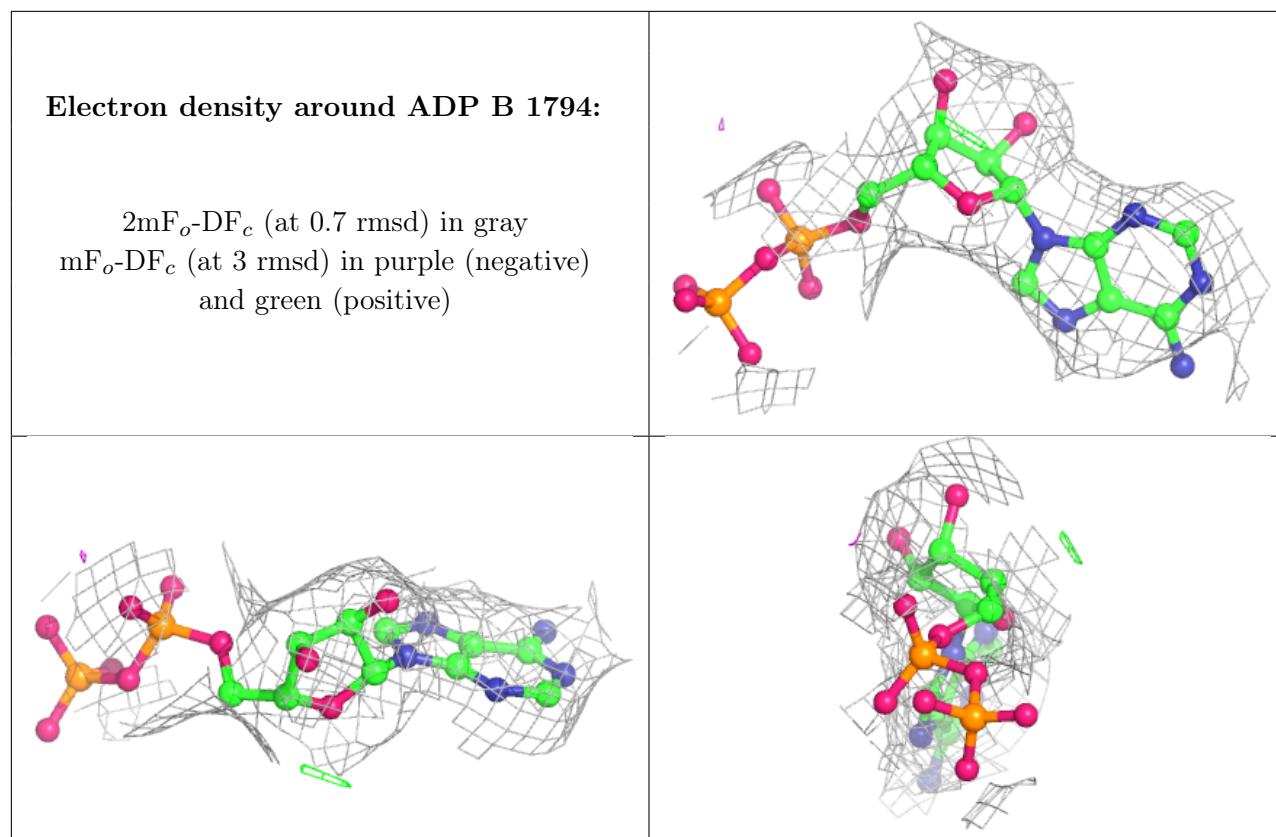
## 6.4 Ligands [i](#)

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, 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
4	ADP	A	1794	27/27	0.92	0.23	60,72,76,80	0
4	ADP	B	1794	27/27	0.94	0.20	60,68,73,76	0
5	MG	A	1795	1/1	0.98	0.34	35,35,35,35	0
5	MG	B	1795	1/1	0.99	0.28	35,35,35,35	0
6	AF3	A	1796	4/4	0.99	0.31	34,35,35,39	0
6	AF3	B	1796	4/4	0.99	0.22	39,40,41,41	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.