



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:31 PM UTC

PDB ID : 4NH0 / pdb_00004nh0
Title : Cytoplasmic domain of the Thermomonospora curvata Type VII Secretion ATPase EccC
Authors : Rosenberg, O.S.; Cox, J.S.; Stroud, R.M.; Strauli, N.; Dovala, D.
Deposited on : 2013-11-03
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

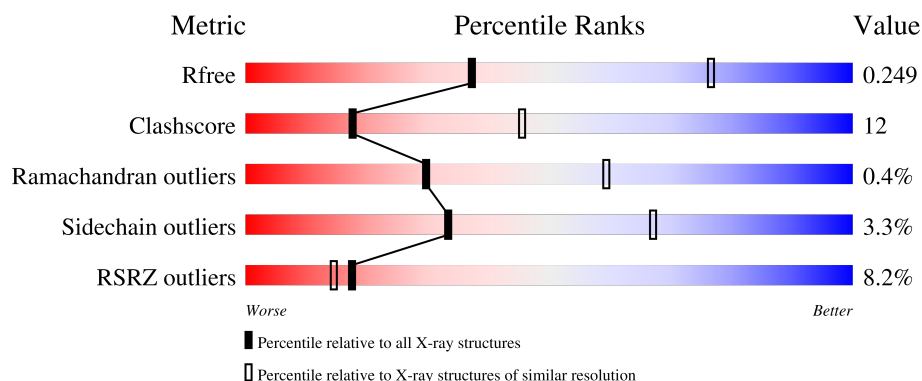
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	1147	4% 58% 16% • 25%
1	B	1147	8% 55% 18% • 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13435 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 Cell divisionFtsK/SpoIIIE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	861	Total	C	N	O	S	0	0	0
			6663	4212	1181	1249	21			
1	B	859	Total	C	N	O	S	0	0	0
			6626	4186	1175	1244	21			

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	MET	-	expression tag	UNP D1A4G7
A	170	HIS	-	expression tag	UNP D1A4G7
A	171	HIS	-	expression tag	UNP D1A4G7
A	172	HIS	-	expression tag	UNP D1A4G7
A	173	HIS	-	expression tag	UNP D1A4G7
A	174	HIS	-	expression tag	UNP D1A4G7
A	175	HIS	-	expression tag	UNP D1A4G7
A	176	HIS	-	expression tag	UNP D1A4G7
A	177	HIS	-	expression tag	UNP D1A4G7
A	178	GLY	-	expression tag	UNP D1A4G7
A	179	GLY	-	expression tag	UNP D1A4G7
A	180	SER	-	expression tag	UNP D1A4G7
A	181	GLU	-	expression tag	UNP D1A4G7
A	182	PHE	-	expression tag	UNP D1A4G7
A	183	SER	-	expression tag	UNP D1A4G7
A	184	ILE	-	expression tag	UNP D1A4G7
A	185	ASP	-	expression tag	UNP D1A4G7
A	186	GLY	-	expression tag	UNP D1A4G7
A	187	GLY	-	expression tag	UNP D1A4G7
A	188	SER	-	expression tag	UNP D1A4G7
A	189	LEU	-	expression tag	UNP D1A4G7
A	190	GLU	-	expression tag	UNP D1A4G7
A	191	VAL	-	expression tag	UNP D1A4G7
A	192	LEU	-	expression tag	UNP D1A4G7
A	193	PHE	-	expression tag	UNP D1A4G7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	194	GLN	-	expression tag	UNP D1A4G7
A	195	GLY	-	expression tag	UNP D1A4G7
A	196	PRO	-	expression tag	UNP D1A4G7
A	197	SER	-	expression tag	UNP D1A4G7
A	198	SER	-	expression tag	UNP D1A4G7
A	199	PRO	-	expression tag	UNP D1A4G7
B	169	MET	-	expression tag	UNP D1A4G7
B	170	HIS	-	expression tag	UNP D1A4G7
B	171	HIS	-	expression tag	UNP D1A4G7
B	172	HIS	-	expression tag	UNP D1A4G7
B	173	HIS	-	expression tag	UNP D1A4G7
B	174	HIS	-	expression tag	UNP D1A4G7
B	175	HIS	-	expression tag	UNP D1A4G7
B	176	HIS	-	expression tag	UNP D1A4G7
B	177	HIS	-	expression tag	UNP D1A4G7
B	178	GLY	-	expression tag	UNP D1A4G7
B	179	GLY	-	expression tag	UNP D1A4G7
B	180	SER	-	expression tag	UNP D1A4G7
B	181	GLU	-	expression tag	UNP D1A4G7
B	182	PHE	-	expression tag	UNP D1A4G7
B	183	SER	-	expression tag	UNP D1A4G7
B	184	ILE	-	expression tag	UNP D1A4G7
B	185	ASP	-	expression tag	UNP D1A4G7
B	186	GLY	-	expression tag	UNP D1A4G7
B	187	GLY	-	expression tag	UNP D1A4G7
B	188	SER	-	expression tag	UNP D1A4G7
B	189	LEU	-	expression tag	UNP D1A4G7
B	190	GLU	-	expression tag	UNP D1A4G7
B	191	VAL	-	expression tag	UNP D1A4G7
B	192	LEU	-	expression tag	UNP D1A4G7
B	193	PHE	-	expression tag	UNP D1A4G7
B	194	GLN	-	expression tag	UNP D1A4G7
B	195	GLY	-	expression tag	UNP D1A4G7
B	196	PRO	-	expression tag	UNP D1A4G7
B	197	SER	-	expression tag	UNP D1A4G7
B	198	SER	-	expression tag	UNP D1A4G7
B	199	PRO	-	expression tag	UNP D1A4G7

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

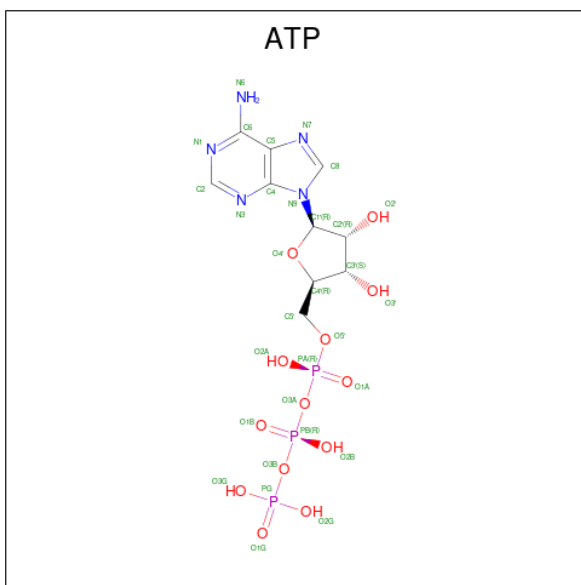


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 5 is water.

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

Chain B: 8% 55% 18% 25%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	251.82Å 116.32Å 174.11Å 90.00° 102.70° 90.00°	Depositor
Resolution (Å)	48.93 – 2.90 48.93 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.93-2.90) 86.2 (48.93-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.52 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.226 , 0.246 0.232 , 0.249	Depositor DCC
R_{free} test set	1523 reflections (1.41%)	wwPDB-VP
Wilson B-factor (Å ²)	67.3	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13435	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ATP, 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	0.34	0/6813	0.75	3/9264 (0.0%)
1	B	0.39	0/6774	0.82	17/9215 (0.2%)
All	All	0.37	0/13587	0.79	20/18479 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1020	ARG	N-CA-C	9.96	123.50	108.46
1	A	999	ASP	CA-C-N	6.28	126.02	119.05
1	A	999	ASP	C-N-CA	6.28	126.02	119.05
1	A	563	GLY	N-CA-C	-6.02	98.91	113.18
1	B	809	PHE	N-CA-C	5.87	120.46	113.12
1	B	768	VAL	CA-C-N	5.74	123.85	119.66
1	B	768	VAL	C-N-CA	5.74	123.85	119.66
1	B	579	ALA	CA-C-N	-5.71	112.70	119.84
1	B	579	ALA	C-N-CA	-5.71	112.70	119.84
1	B	638	ASP	N-CA-C	-5.70	105.06	111.28
1	B	692	SER	CB-CA-C	-5.69	109.50	117.23
1	B	543	ARG	N-CA-C	-5.63	105.22	111.36
1	B	579	ALA	N-CA-C	-5.41	102.77	109.64
1	B	999	ASP	CA-C-N	5.23	124.89	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	999	ASP	C-N-CA	5.23	124.89	119.56
1	B	640	HIS	N-CA-C	5.14	116.97	111.36
1	B	679	ALA	CB-CA-C	-5.10	110.29	117.23
1	B	580	PRO	CA-N-CD	-5.08	104.89	112.00
1	B	601	LYS	CA-C-N	5.00	124.78	119.28
1	B	601	LYS	C-N-CA	5.00	124.78	119.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	807	ARG	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	6663	0	6636	128	0
1	B	6626	0	6588	204	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	62	0	24	1	0
4	B	62	0	24	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	13435	0	13272	332	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 12.

All (332) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:HD21	1:B:633:LYS:CB	1.81	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:CD2	1:B:633:LYS:HB2	1.87	1.05
1:B:629:LEU:HD21	1:B:633:LYS:HB2	1.08	1.03
1:B:1122:LYS:NZ	4:B:1404:ATP:O2B	1.97	0.97
1:B:764:PRO:O	1:B:813:ARG:NH2	2.02	0.93
1:B:631:GLU:N	1:B:631:GLU:OE2	2.02	0.92
1:B:628:ARG:NH2	1:B:650:PHE:CG	2.38	0.91
1:B:636:GLY:O	1:B:640:HIS:HD2	1.52	0.91
1:A:1006:ASP:OD2	1:A:1009:LYS:N	2.04	0.89
1:A:442:GLN:O	1:A:464:LYS:NZ	2.07	0.87
1:B:905:GLU:OE2	1:B:963:ARG:NH1	2.08	0.86
1:B:644:ARG:HH11	1:B:644:ARG:HG3	1.38	0.85
1:A:442:GLN:HG3	1:A:445:ARG:HH12	1.42	0.82
1:A:543:ARG:NH1	1:A:806:ASP:OD2	2.13	0.81
1:B:471:MET:O	1:B:642:SER:OG	1.97	0.81
1:B:807:ARG:HG2	1:B:812:ARG:H	1.45	0.81
1:A:1148:ASP:OD2	1:A:1152:SER:N	2.13	0.80
1:B:628:ARG:HH21	1:B:650:PHE:CB	1.95	0.79
1:A:832:GLY:O	1:A:835:THR:OG1	1.99	0.79
1:A:1006:ASP:HB3	1:A:1009:LYS:HG3	1.65	0.79
1:B:561:HIS:CD2	1:B:562:SER:H	2.01	0.78
1:B:636:GLY:O	1:B:640:HIS:CD2	2.35	0.78
1:A:1006:ASP:CB	1:A:1009:LYS:HG3	2.14	0.78
1:B:644:ARG:HG3	1:B:644:ARG:NH1	1.98	0.78
1:B:807:ARG:NE	1:B:811:GLN:H	1.82	0.78
1:B:813:ARG:HG2	1:B:813:ARG:HH11	1.49	0.77
1:B:572:GLU:OE2	1:B:575:ARG:HG2	1.85	0.77
1:A:542:ASP:OD2	1:A:601:LYS:NZ	2.17	0.76
1:B:743:LEU:HD13	1:B:744:PHE:H	1.50	0.75
1:B:629:LEU:HD22	1:B:630:GLU:H	1.52	0.74
1:B:630:GLU:HG2	1:B:633:LYS:HG2	1.69	0.74
1:B:629:LEU:CD2	1:B:630:GLU:H	2.01	0.73
1:B:807:ARG:HE	1:B:811:GLN:H	1.35	0.73
1:A:555:ARG:NH2	1:A:585:PRO:O	2.21	0.73
1:B:629:LEU:HD23	1:B:633:LYS:HG3	1.71	0.73
1:B:807:ARG:HD2	1:B:807:ARG:C	2.14	0.73
1:B:575:ARG:HG2	1:B:575:ARG:HH11	1.52	0.72
1:B:837:LYS:NZ	4:B:1405:ATP:O2B	2.20	0.72
1:B:891:ARG:NH1	1:B:1096:GLU:OE2	2.24	0.71
1:B:629:LEU:CD2	1:B:633:LYS:CG	2.68	0.71
1:B:637:LEU:O	1:B:641:LEU:HG	1.90	0.71
1:B:743:LEU:HD13	1:B:744:PHE:N	2.05	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:629:LEU:HD11	1:B:634:LEU:HD21	1.71	0.71
1:B:691:VAL:HG23	1:B:692:SER:H	1.55	0.69
1:B:1033:LEU:O	1:B:1035:ARG:N	2.26	0.69
1:B:629:LEU:CD2	1:B:633:LYS:CB	2.58	0.68
1:B:807:ARG:HD2	1:B:808:PRO:N	2.08	0.68
1:B:464:LYS:NZ	1:B:468:GLN:O	2.27	0.68
1:A:1001:TYR:HD1	1:A:1002:GLU:H	1.39	0.68
1:B:807:ARG:HE	1:B:810:ASP:N	1.93	0.67
1:A:904:ARG:NE	1:A:931:ASP:OD2	2.23	0.67
1:B:692:SER:OG	1:B:693:GLY:N	2.26	0.66
1:A:1006:ASP:CG	1:A:1009:LYS:HG3	2.21	0.66
1:B:1200:ARG:HH21	1:B:1236:ARG:HG2	1.60	0.66
1:B:487:GLU:OE2	1:B:692:SER:N	2.29	0.66
1:B:432:ASP:HB3	1:B:435:VAL:HG22	1.78	0.65
1:B:655:SER:OG	1:B:661:VAL:O	2.14	0.65
1:B:804:LEU:HD11	1:B:813:ARG:HB3	1.78	0.65
1:A:432:ASP:HB3	1:A:435:VAL:HG22	1.78	0.64
1:A:975:SER:OG	1:A:980:GLU:OE1	2.16	0.64
1:B:975:SER:OG	1:B:980:GLU:OE1	2.15	0.64
1:B:629:LEU:CD2	1:B:633:LYS:HG3	2.28	0.64
1:A:573:LYS:O	1:A:577:GLU:N	2.30	0.63
1:B:766:LEU:H	1:B:813:ARG:HH22	1.47	0.63
1:A:658:VAL:HG23	1:A:659:LEU:HG	1.81	0.62
1:A:681:GLU:N	1:A:681:GLU:OE1	2.33	0.62
1:A:442:GLN:HG3	1:A:445:ARG:NH1	2.12	0.62
1:B:743:LEU:HA	1:B:746:VAL:HB	1.80	0.62
1:B:1177:ARG:HG2	1:B:1177:ARG:HH11	1.65	0.62
1:B:813:ARG:HG2	1:B:813:ARG:NH1	2.12	0.62
1:B:805:VAL:HA	1:B:1029:PHE:HA	1.82	0.62
1:B:888:ASP:HB3	1:B:1070:MET:HE1	1.82	0.62
1:A:543:ARG:NH2	1:A:763:LEU:O	2.33	0.61
1:B:654:GLU:CD	1:B:654:GLU:H	2.07	0.61
1:A:645:ILE:HG12	1:A:676:LEU:HD23	1.83	0.61
1:A:1189:PRO:HD2	1:A:1192:LEU:HD11	1.83	0.61
1:B:542:ASP:HA	1:B:545:TYR:HB3	1.82	0.61
1:A:920:ARG:NH1	1:A:935:ASP:OD2	2.34	0.60
1:B:628:ARG:NH2	1:B:650:PHE:CD2	2.68	0.60
1:B:1036:ILE:HG12	1:B:1052:THR:HG22	1.82	0.60
1:B:1020:ARG:CG	1:B:1030:LEU:HA	2.32	0.60
1:B:810:ASP:HB3	1:B:812:ARG:NH1	2.17	0.60
1:B:644:ARG:HH11	1:B:644:ARG:CG	2.12	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:ARG:NH1	1:A:765:PRO:HA	2.18	0.59
1:A:1006:ASP:OD2	1:A:1008:LYS:N	2.34	0.59
1:B:628:ARG:NH2	1:B:650:PHE:CB	2.62	0.59
1:B:1148:ASP:OD2	1:B:1152:SER:N	2.34	0.59
1:A:568:LEU:HD13	1:A:619:GLY:HA3	1.84	0.59
1:B:1006:ASP:OD2	1:B:1009:LYS:HG3	2.02	0.59
1:B:772:LEU:HD23	1:B:850:LEU:HD12	1.83	0.59
1:B:923:ARG:NH1	1:B:933:PHE:O	2.35	0.59
1:B:807:ARG:NE	1:B:811:GLN:N	2.49	0.59
1:B:764:PRO:O	1:B:766:LEU:N	2.36	0.59
1:B:575:ARG:HH11	1:B:575:ARG:CG	2.16	0.58
1:A:508:VAL:HG23	1:A:587:LEU:HD11	1.83	0.58
1:A:525:ARG:NH1	1:A:755:GLY:O	2.37	0.58
1:B:629:LEU:HD22	1:B:630:GLU:N	2.18	0.58
1:B:996:ARG:HD3	1:B:1013:VAL:HG22	1.85	0.58
1:B:1037:ASP:OD1	1:B:1038:GLY:N	2.36	0.58
1:A:476:LEU:HB2	1:A:641:LEU:HD13	1.86	0.58
1:B:422:LEU:HD23	1:B:449:PRO:HB2	1.85	0.58
1:B:807:ARG:HE	1:B:809:PHE:C	2.12	0.58
1:B:541:VAL:HG11	1:B:601:LYS:HG3	1.86	0.57
1:A:1001:TYR:CD1	1:A:1002:GLU:N	2.69	0.57
1:B:804:LEU:O	1:B:1030:LEU:N	2.37	0.57
1:B:643:TYR:C	1:B:644:ARG:HD3	2.29	0.57
1:A:837:LYS:O	1:A:840:MET:N	2.38	0.57
1:A:838:SER:OG	4:A:1405:ATP:O1B	2.23	0.57
1:B:572:GLU:O	1:B:575:ARG:HB3	2.05	0.57
1:A:559:LEU:HD21	1:A:584:MET:HE1	1.87	0.57
1:B:613:ARG:NH1	1:B:614:LEU:HD21	2.20	0.57
1:B:859:PHE:HB2	1:B:878:VAL:HG12	1.86	0.56
1:B:810:ASP:HB3	1:B:812:ARG:HH12	1.70	0.56
1:B:1117:ASP:O	1:B:1122:LYS:HE2	2.05	0.56
1:B:1120:CYS:SG	1:B:1122:LYS:HE3	2.45	0.56
1:B:630:GLU:OE2	1:B:633:LYS:NZ	2.33	0.56
1:B:475:GLY:HA3	1:B:643:TYR:CZ	2.41	0.56
1:B:561:HIS:HD2	1:B:562:SER:H	1.53	0.56
1:B:1020:ARG:HD3	1:B:1030:LEU:HA	1.88	0.56
1:B:804:LEU:HD21	1:B:813:ARG:HD3	1.88	0.56
1:B:864:PHE:H	1:B:941:ASP:HB3	1.71	0.55
1:A:771:THR:OG1	1:A:773:ASP:OD1	2.24	0.55
1:A:1035:ARG:HH12	1:A:1044:THR:HG23	1.71	0.55
1:A:462:ASP:OD2	1:A:464:LYS:HE2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:GLN:HA	1:B:445:ARG:NH1	2.22	0.55
1:B:1117:ASP:O	1:B:1122:LYS:CE	2.54	0.55
1:B:1294:GLY:O	1:B:1310:THR:OG1	2.24	0.54
1:B:757:GLU:HG2	1:B:758:PRO:HD2	1.90	0.54
1:A:573:LYS:O	1:A:577:GLU:HB2	2.07	0.54
1:B:822:GLY:O	1:B:824:ALA:N	2.38	0.54
1:B:483:SER:HB2	1:B:647:LEU:HB3	1.88	0.54
1:B:494:LEU:HG	1:B:498:MET:HE2	1.88	0.54
1:B:1054:LYS:NZ	1:B:1058:GLU:OE2	2.38	0.54
1:B:628:ARG:HH21	1:B:650:PHE:HB3	1.71	0.54
1:A:1134:ILE:HG12	1:A:1159:THR:HG21	1.90	0.54
1:A:638:ASP:CG	1:A:644:ARG:HH22	2.16	0.53
1:B:432:ASP:OD1	1:B:434:ALA:N	2.41	0.53
1:B:631:GLU:HA	1:B:657:VAL:HG21	1.89	0.53
1:A:1126:LEU:HD21	1:A:1245:ALA:HB2	1.90	0.53
1:A:807:ARG:HD3	1:A:1027:TYR:CE2	2.43	0.53
1:A:1144:LEU:HD23	1:A:1209:PHE:HB2	1.90	0.53
1:A:1277:LYS:H	1:A:1277:LYS:HD2	1.73	0.53
1:B:631:GLU:OE1	1:B:653:MET:SD	2.67	0.53
1:B:561:HIS:O	1:B:562:SER:OG	2.26	0.53
1:B:593:GLU:OE2	1:B:627:GLN:CG	2.57	0.53
1:B:693:GLY:O	1:B:743:LEU:HD12	2.09	0.52
1:A:1126:LEU:HD12	1:A:1211:VAL:HG13	1.91	0.52
1:B:690:TYR:HD1	1:B:692:SER:HB3	1.73	0.52
1:B:561:HIS:CD2	1:B:562:SER:N	2.75	0.52
1:B:595:SER:OG	1:B:633:LYS:NZ	2.42	0.52
1:B:629:LEU:HD23	1:B:633:LYS:CG	2.36	0.52
1:B:920:ARG:NH1	1:B:935:ASP:OD2	2.43	0.52
1:B:629:LEU:HD11	1:B:634:LEU:CD2	2.40	0.52
1:A:1023:THR:HG22	1:A:1025:ASP:H	1.74	0.51
1:A:1037:ASP:OD1	1:A:1038:GLY:N	2.43	0.51
1:B:1001:TYR:CD2	1:B:1002:GLU:HG3	2.44	0.51
1:B:1071:LEU:HD12	1:B:1072:PRO:HD2	1.91	0.51
1:B:1248:MET:HE2	1:B:1276:ASN:H	1.76	0.51
1:B:572:GLU:OE2	1:B:572:GLU:HA	2.09	0.51
1:B:593:GLU:OE2	1:B:627:GLN:HG3	2.10	0.51
1:A:1183:MET:HE2	1:A:1240:LEU:HB2	1.93	0.51
1:A:1035:ARG:HA	1:A:1052:THR:HG21	1.93	0.51
1:B:1048:GLY:O	1:B:1051:THR:OG1	2.26	0.51
1:A:494:LEU:HG	1:A:498:MET:HE2	1.92	0.51
1:A:572:GLU:O	1:A:575:ARG:HB3	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1183:MET:HB3	1:B:1238:ILE:HD12	1.93	0.51
1:A:1143:ARG:HE	1:A:1163:ILE:HD11	1.76	0.50
1:B:419:LEU:HD22	1:B:491:THR:HG23	1.93	0.50
1:A:759:HIS:NE2	1:A:811:GLN:OE1	2.42	0.50
1:B:1177:ARG:HG2	1:B:1177:ARG:NH1	2.27	0.50
1:B:693:GLY:C	1:B:743:LEU:HD12	2.37	0.50
1:A:558:HIS:ND1	1:A:562:SER:OG	2.44	0.50
1:A:591:LEU:HD21	1:A:597:LEU:HD13	1.93	0.50
1:A:999:ASP:OD1	1:A:1001:TYR:N	2.44	0.50
1:B:572:GLU:HA	1:B:575:ARG:HB3	1.93	0.50
1:B:828:GLY:HA3	1:B:989:LEU:HD13	1.94	0.50
1:B:1180:LYS:HD2	1:B:1227:PRO:HB2	1.93	0.50
1:B:1242:LEU:HD23	1:B:1244:ILE:HD11	1.94	0.50
1:A:796:GLY:HA2	1:A:852:HIS:CD2	2.47	0.49
1:B:807:ARG:HD3	1:B:810:ASP:H	1.76	0.49
1:A:1193:THR:HG23	1:A:1196:GLN:H	1.77	0.49
1:B:832:GLY:O	1:B:837:LYS:NZ	2.46	0.49
1:B:782:SER:OG	1:B:783:ALA:N	2.44	0.49
1:B:872:LEU:HB3	1:B:875:LEU:HD12	1.95	0.49
1:B:565:TYR:CD2	1:B:571:TYR:HA	2.47	0.48
1:B:592:ASP:HA	1:B:625:ALA:HB3	1.95	0.48
1:B:654:GLU:O	1:B:658:VAL:HG13	2.13	0.48
1:B:691:VAL:O	1:B:743:LEU:HD11	2.13	0.48
1:A:866:GLY:H	1:A:884:ARG:HH22	1.60	0.48
1:A:1148:ASP:CG	1:A:1152:SER:H	2.17	0.48
1:B:1035:ARG:HA	1:B:1052:THR:HG21	1.96	0.48
1:A:522:GLU:HG3	1:A:530:ILE:HD12	1.96	0.48
1:A:828:GLY:HA3	1:A:989:LEU:HD13	1.94	0.48
1:B:1020:ARG:HG3	1:B:1029:PHE:O	2.12	0.48
1:A:552:MET:HG3	1:A:610:MET:HE3	1.95	0.48
1:A:1191:ASP:OD1	1:A:1191:ASP:N	2.42	0.48
1:B:641:LEU:N	1:B:641:LEU:HD23	2.27	0.48
1:B:568:LEU:HD13	1:B:584:MET:HE3	1.96	0.48
1:B:807:ARG:HE	1:B:811:GLN:N	2.07	0.48
1:B:1148:ASP:OD2	1:B:1153:LEU:N	2.44	0.48
1:B:1035:ARG:NH2	1:B:1044:THR:O	2.47	0.48
1:A:657:VAL:HG23	1:A:658:VAL:HG13	1.95	0.48
1:A:794:TRP:HA	1:A:797:ARG:HG3	1.96	0.48
1:B:690:TYR:CD1	1:B:692:SER:HB3	2.49	0.47
1:B:769:PRO:HA	1:B:1030:LEU:HD23	1.95	0.47
1:A:419:LEU:HD21	1:A:495:ALA:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:ASP:HA	1:A:1308:ILE:HA	1.96	0.47
1:A:1151:ARG:HB3	1:A:1154:LEU:HD21	1.95	0.47
1:B:416:ASN:HB3	1:B:690:TYR:CE2	2.49	0.47
1:B:629:LEU:CD2	1:B:630:GLU:N	2.73	0.47
1:B:545:TYR:CE1	1:B:607:LEU:HB2	2.49	0.47
1:B:854:PRO:HG2	1:B:1060:TRP:CD1	2.48	0.47
1:A:1218:VAL:O	1:A:1223:ASN:ND2	2.42	0.47
1:B:807:ARG:HD2	1:B:808:PRO:CA	2.44	0.47
1:B:631:GLU:OE1	1:B:653:MET:CG	2.62	0.47
1:B:1248:MET:HG3	1:B:1275:GLY:HA2	1.97	0.47
1:B:575:ARG:CG	1:B:575:ARG:NH1	2.73	0.47
1:A:558:HIS:O	1:A:562:SER:OG	2.33	0.47
1:A:593:GLU:N	1:A:625:ALA:O	2.47	0.47
1:A:810:ASP:HB3	1:A:812:ARG:NH1	2.30	0.47
1:A:442:GLN:HA	1:A:445:ARG:NH1	2.30	0.46
1:A:1178:ASP:OD1	1:A:1178:ASP:N	2.38	0.46
1:B:675:TYR:CE1	1:B:685:ARG:HD3	2.50	0.46
1:B:807:ARG:NE	1:B:810:ASP:N	2.63	0.46
1:A:1242:LEU:HD12	1:A:1244:ILE:HD11	1.96	0.46
1:B:1187:LEU:HA	1:B:1188:PRO:HD3	1.81	0.46
1:A:1014:PRO:HG2	1:A:1020:ARG:NH1	2.31	0.46
1:B:629:LEU:HD23	1:B:630:GLU:H	1.80	0.46
1:B:995:LEU:HA	1:B:1021:GLY:HA3	1.98	0.46
1:A:1277:LYS:HD2	1:A:1277:LYS:N	2.31	0.46
1:B:953:LEU:HA	1:B:956:SER:HB3	1.96	0.46
1:A:837:LYS:HB2	1:A:837:LYS:HE2	1.25	0.46
1:A:1302:ARG:C	1:A:1304:GLY:H	2.22	0.46
1:B:580:PRO:C	1:B:581:LEU:HD12	2.40	0.46
1:B:632:GLY:O	1:B:633:LYS:C	2.57	0.46
1:B:675:TYR:HE1	1:B:685:ARG:HD3	1.81	0.46
1:B:1039:ASP:OD1	1:B:1040:THR:N	2.49	0.46
1:A:416:ASN:ND2	1:A:687:LYS:NZ	2.63	0.45
1:A:1248:MET:HE3	1:A:1279:GLU:HG3	1.96	0.45
1:B:696:ASP:OD1	1:B:697:GLU:N	2.49	0.45
1:A:1183:MET:HB3	1:A:1238:ILE:HD12	1.98	0.45
1:B:462:ASP:OD1	1:B:464:LYS:HE3	2.17	0.45
1:B:1122:LYS:NZ	4:B:1404:ATP:O1G	2.49	0.45
1:B:552:MET:HE2	1:B:610:MET:HE3	1.97	0.45
1:B:628:ARG:CG	1:B:629:LEU:N	2.79	0.45
1:B:1020:ARG:CD	1:B:1030:LEU:HA	2.47	0.45
1:B:476:LEU:HB2	1:B:641:LEU:HD13	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:ASP:CG	1:A:644:ARG:NH2	2.75	0.45
1:A:837:LYS:O	1:A:839:THR:N	2.49	0.45
1:B:1200:ARG:HA	1:B:1202:TRP:CZ3	2.52	0.45
1:A:1001:TYR:O	1:A:1002:GLU:HB2	2.17	0.45
1:B:503:GLU:HB2	1:B:756:PRO:HG2	1.98	0.45
1:B:1020:ARG:HD3	1:B:1030:LEU:CA	2.47	0.45
1:A:518:PHE:HB3	1:A:521:MET:HG3	1.99	0.44
1:B:1148:ASP:CG	1:B:1152:SER:H	2.25	0.44
1:A:693:GLY:O	1:A:743:LEU:N	2.46	0.44
1:B:667:LEU:HA	1:B:668:PRO:HD3	1.86	0.44
1:B:1166:ALA:HB2	1:B:1175:LEU:HD12	1.98	0.44
1:A:1111:HIS:ND1	1:A:1242:LEU:HB2	2.33	0.44
1:A:1006:ASP:CG	1:A:1009:LYS:CG	2.89	0.44
1:B:1188:PRO:HB3	1:B:1192:LEU:HD12	2.00	0.44
1:A:1202:TRP:CE2	1:A:1203:TRP:HD1	2.35	0.44
1:A:1199:SER:HG	1:A:1201:SER:HG	1.65	0.44
1:B:994:GLU:OE2	1:B:997:LEU:HD21	2.18	0.44
1:B:799:HIS:NE2	1:B:819:ASP:OD1	2.51	0.44
1:A:992:LYS:HD2	1:A:1004:GLU:HG2	1.99	0.43
1:B:883:THR:OG1	1:B:884:ARG:N	2.52	0.43
1:B:442:GLN:O	1:B:464:LYS:HE2	2.18	0.43
1:B:691:VAL:HG23	1:B:692:SER:N	2.30	0.43
1:B:542:ASP:HA	1:B:545:TYR:CB	2.47	0.43
1:B:654:GLU:O	1:B:657:VAL:HG12	2.18	0.43
1:A:443:ARG:HA	1:A:464:LYS:NZ	2.33	0.43
1:A:652:ALA:O	1:A:656:ARG:HG3	2.18	0.43
1:B:446:LEU:HD23	1:B:463:ILE:HG13	2.01	0.43
1:B:796:GLY:HA2	1:B:852:HIS:CD2	2.53	0.43
1:A:1230:GLU:H	1:A:1230:GLU:HG2	1.57	0.43
1:B:432:ASP:HB3	1:B:435:VAL:CG2	2.47	0.43
1:B:593:GLU:OE2	1:B:627:GLN:HG2	2.19	0.43
1:B:462:ASP:O	1:B:471:MET:HB2	2.19	0.43
1:B:864:PHE:HB2	1:B:942:ASN:HB3	2.01	0.43
1:B:1189:PRO:HD2	1:B:1192:LEU:HD11	2.00	0.43
1:A:837:LYS:O	1:A:838:SER:C	2.61	0.43
1:A:839:THR:O	1:A:843:THR:HG23	2.18	0.43
1:A:1110:PRO:HG2	1:A:1111:HIS:CD2	2.54	0.43
1:B:741:GLU:HB2	1:B:742:SER:HB3	2.01	0.43
1:B:834:GLN:HB3	4:B:1405:ATP:H5'1	2.01	0.43
1:B:476:LEU:HB2	1:B:641:LEU:CD1	2.49	0.42
1:A:422:LEU:HD23	1:A:449:PRO:HB2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:ASP:OD2	1:A:1153:LEU:N	2.52	0.42
1:A:543:ARG:HH12	1:A:765:PRO:HA	1.84	0.42
1:A:1035:ARG:NH2	1:A:1037:ASP:OD2	2.49	0.42
1:B:1298:PHE:HB2	1:B:1308:ILE:HD13	2.02	0.42
1:B:453:ASP:OD1	1:B:457:ARG:N	2.52	0.42
1:B:654:GLU:CD	1:B:654:GLU:N	2.77	0.42
1:B:1095:ASP:HA	1:B:1308:ILE:HA	2.01	0.42
1:A:906:GLN:O	1:A:910:GLU:HG3	2.19	0.42
1:A:1054:LYS:HZ3	1:A:1058:GLU:CD	2.26	0.42
1:A:1143:ARG:NE	1:A:1163:ILE:HD11	2.34	0.42
1:B:1302:ARG:C	1:B:1304:GLY:H	2.28	0.42
1:A:884:ARG:H	1:A:884:ARG:HG2	1.61	0.42
1:A:1223:ASN:HA	1:A:1224:PRO:HD3	1.85	0.42
1:A:471:MET:HA	1:A:678:PHE:CD1	2.55	0.42
1:A:832:GLY:C	1:A:835:THR:OG1	2.63	0.42
1:A:1014:PRO:HB3	1:A:1017:ARG:HG3	2.01	0.42
1:A:1048:GLY:O	1:A:1052:THR:HG23	2.20	0.41
1:B:555:ARG:NH2	1:B:585:PRO:O	2.51	0.41
1:B:798:LEU:HD11	1:B:920:ARG:NH1	2.35	0.41
1:B:863:ASP:OD2	1:B:867:GLY:HA2	2.19	0.41
1:A:1179:ILE:O	1:A:1183:MET:HG2	2.20	0.41
1:A:1189:PRO:HA	1:A:1190:PRO:HD3	1.87	0.41
1:A:613:ARG:HE	1:A:614:LEU:CD1	2.33	0.41
1:B:743:LEU:O	1:B:747:VAL:N	2.43	0.41
1:A:1036:ILE:HG13	1:A:1052:THR:HG22	2.02	0.41
1:B:429:TYR:HE1	1:B:695:VAL:HG21	1.85	0.41
1:A:949:ASP:OD1	1:A:949:ASP:N	2.54	0.41
1:A:1187:LEU:HA	1:A:1188:PRO:HD3	1.81	0.41
1:A:484:GLY:N	2:A:1401:SO4:O4	2.54	0.41
1:A:533:ASN:HD21	1:A:536:GLU:CD	2.29	0.41
1:A:818:LEU:HG	1:A:991:THR:HG21	2.03	0.41
1:A:954:GLU:O	1:A:958:THR:OG1	2.27	0.41
1:A:437:TRP:CZ2	1:A:751:LEU:HD12	2.56	0.41
1:A:571:TYR:CE1	1:A:581:LEU:HD13	2.56	0.41
1:B:629:LEU:HD22	1:B:630:GLU:O	2.21	0.41
1:B:1020:ARG:HG2	1:B:1030:LEU:HD12	2.03	0.41
1:A:551:GLU:OE1	1:A:555:ARG:NH1	2.53	0.40
1:A:679:ALA:HB3	1:A:681:GLU:OE1	2.21	0.40
1:A:1146:PHE:HD2	1:A:1153:LEU:HD23	1.85	0.40
1:A:864:PHE:H	1:A:941:ASP:HB3	1.86	0.40
1:B:950:TYR:HB3	1:B:953:LEU:HD13	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1065:ALA:HA	1:B:1066:PRO:HD3	1.97	0.40
1:A:864:PHE:HB2	1:A:942:ASN:H	1.86	0.40
1:B:906:GLN:O	1:B:910:GLU:HG3	2.20	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	857/1147 (75%)	799 (93%)	56 (6%)	2 (0%)	43	72
1	B	855/1147 (74%)	793 (93%)	58 (7%)	4 (0%)	24	54
All	All	1712/2294 (75%)	1592 (93%)	114 (7%)	6 (0%)	30	59

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	808	PRO
1	A	577	GLU
1	B	823	GLY
1	B	1034	PRO
1	A	580	PRO
1	B	693	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	709/953 (74%)	690 (97%)	19 (3%)	39	73
1	B	703/953 (74%)	676 (96%)	27 (4%)	29	64
All	All	1412/1906 (74%)	1366 (97%)	46 (3%)	33	67

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	572	GLU
1	A	573	LYS
1	A	577	GLU
1	A	630	GLU
1	A	695	VAL
1	A	766	LEU
1	A	768	VAL
1	A	785	HIS
1	A	807	ARG
1	A	818	LEU
1	A	837	LYS
1	A	838	SER
1	A	1023	THR
1	A	1036	ILE
1	A	1043	GLU
1	A	1074	VAL
1	A	1134	ILE
1	A	1151	ARG
1	A	1230	GLU
1	B	534	LEU
1	B	560	ARG
1	B	575	ARG
1	B	576	MET
1	B	577	GLU
1	B	590	VAL
1	B	601	LYS
1	B	606	GLU
1	B	629	LEU
1	B	630	GLU
1	B	631	GLU
1	B	638	ASP
1	B	641	LEU
1	B	644	ARG
1	B	654	GLU
1	B	658	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	742	SER
1	B	743	LEU
1	B	771	THR
1	B	775	LEU
1	B	802	VAL
1	B	807	ARG
1	B	906	GLN
1	B	1013	VAL
1	B	1025	ASP
1	B	1058	GLU
1	B	1154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	ASN
1	B	561	HIS
1	B	640	HIS
1	B	877	HIS
1	B	959	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	ATP	A	1405	3	32,33,33	1.38	4 (12%)	48,52,52	1.75	9 (18%)
4	ATP	A	1404	3	32,33,33	1.36	4 (12%)	48,52,52	1.76	9 (18%)
2	SO4	B	1401	-	4,4,4	0.23	0	6,6,6	0.09	0
4	ATP	B	1405	3	32,33,33	1.39	4 (12%)	48,52,52	1.76	9 (18%)
4	ATP	B	1404	3	32,33,33	1.36	4 (12%)	48,52,52	1.74	9 (18%)
2	SO4	A	1401	-	4,4,4	0.23	0	6,6,6	0.08	0

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	ATP	A	1404	3	-	1/22/38/38	0/3/3/3
4	ATP	B	1404	3	-	0/22/38/38	0/3/3/3
4	ATP	A	1405	3	-	0/22/38/38	0/3/3/3
4	ATP	B	1405	3	-	0/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1405	ATP	C5-C4	4.73	1.47	1.39
4	A	1405	ATP	C5-C4	4.70	1.47	1.39
4	B	1404	ATP	C5-C4	4.66	1.47	1.39
4	A	1404	ATP	C5-C4	4.64	1.47	1.39
4	A	1405	ATP	C5-C6	2.74	1.48	1.41
4	B	1405	ATP	C5-C6	2.72	1.48	1.41
4	B	1404	ATP	C5-C6	2.69	1.48	1.41
4	A	1404	ATP	C5-C6	2.68	1.48	1.41
4	A	1405	ATP	C8-N7	2.34	1.36	1.31
4	B	1405	ATP	C8-N7	2.34	1.36	1.31
4	B	1404	ATP	C5-N7	-2.33	1.34	1.39
4	A	1404	ATP	C5-N7	-2.32	1.34	1.39
4	A	1404	ATP	C8-N7	2.30	1.36	1.31
4	B	1405	ATP	C5-N7	-2.25	1.35	1.39
4	B	1404	ATP	C8-N7	2.25	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1405	ATP	C5-N7	-2.24	1.35	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1404	ATP	C5-C4-N3	-5.95	118.52	126.72
4	B	1405	ATP	C5-C4-N3	-5.92	118.56	126.72
4	B	1404	ATP	C5-C4-N3	-5.89	118.61	126.72
4	A	1405	ATP	C5-C4-N3	-5.87	118.63	126.72
4	B	1404	ATP	N3-C4-N9	4.67	135.11	127.17
4	B	1405	ATP	N3-C4-N9	4.67	135.11	127.17
4	A	1404	ATP	N3-C4-N9	4.64	135.06	127.17
4	A	1405	ATP	N3-C4-N9	4.63	135.04	127.17
4	A	1404	ATP	C2-N3-C4	3.72	120.92	111.83
4	B	1405	ATP	C2-N3-C4	3.71	120.88	111.83
4	A	1405	ATP	C2-N3-C4	3.69	120.84	111.83
4	B	1404	ATP	C2-N3-C4	3.67	120.80	111.83
4	A	1404	ATP	C4-C5-N7	-3.53	106.55	110.58
4	B	1405	ATP	C4-C5-N7	-3.46	106.62	110.58
4	B	1404	ATP	C4-C5-N7	-3.45	106.63	110.58
4	A	1405	ATP	C4-C5-N7	-3.45	106.64	110.58
4	B	1405	ATP	N3-C2-N1	-3.22	123.70	128.58
4	A	1405	ATP	N3-C2-N1	-3.21	123.73	128.58
4	A	1404	ATP	N3-C2-N1	-3.16	123.80	128.58
4	B	1404	ATP	N3-C2-N1	-3.15	123.81	128.58
4	A	1404	ATP	C5-N7-C8	2.57	107.50	103.45
4	B	1405	ATP	C4-N9-C8	2.56	108.42	105.74
4	B	1404	ATP	C4-N9-C8	2.55	108.42	105.74
4	A	1405	ATP	C4-N9-C8	2.55	108.41	105.74
4	B	1405	ATP	C5-N7-C8	2.52	107.40	103.45
4	B	1404	ATP	C5-N7-C8	2.51	107.39	103.45
4	A	1404	ATP	C4-N9-C8	2.50	108.36	105.74
4	A	1405	ATP	C5-N7-C8	2.49	107.36	103.45
4	A	1404	ATP	C3'-C2'-C1'	2.39	105.98	101.46
4	A	1405	ATP	C3'-C2'-C1'	2.35	105.91	101.46
4	B	1405	ATP	C3'-C2'-C1'	2.30	105.81	101.46
4	B	1404	ATP	C3'-C2'-C1'	2.28	105.78	101.46
4	A	1404	ATP	C6-C5-N7	2.06	136.05	132.09
4	A	1405	ATP	C6-C5-N7	2.03	136.00	132.09
4	B	1405	ATP	C6-C5-N7	2.02	135.99	132.09
4	B	1404	ATP	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

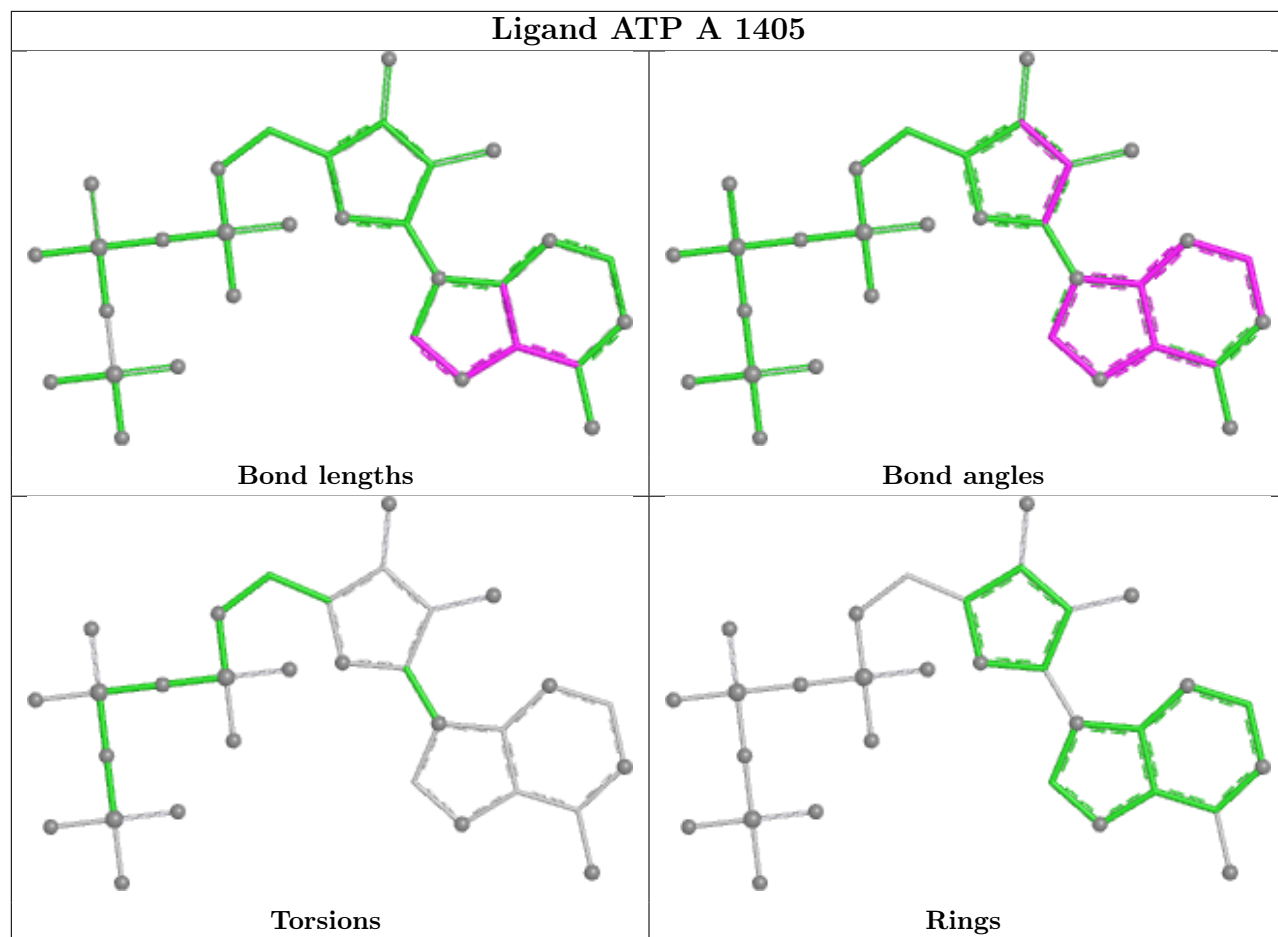
Mol	Chain	Res	Type	Atoms
4	A	1404	ATP	PG-O3B-PB-O2B

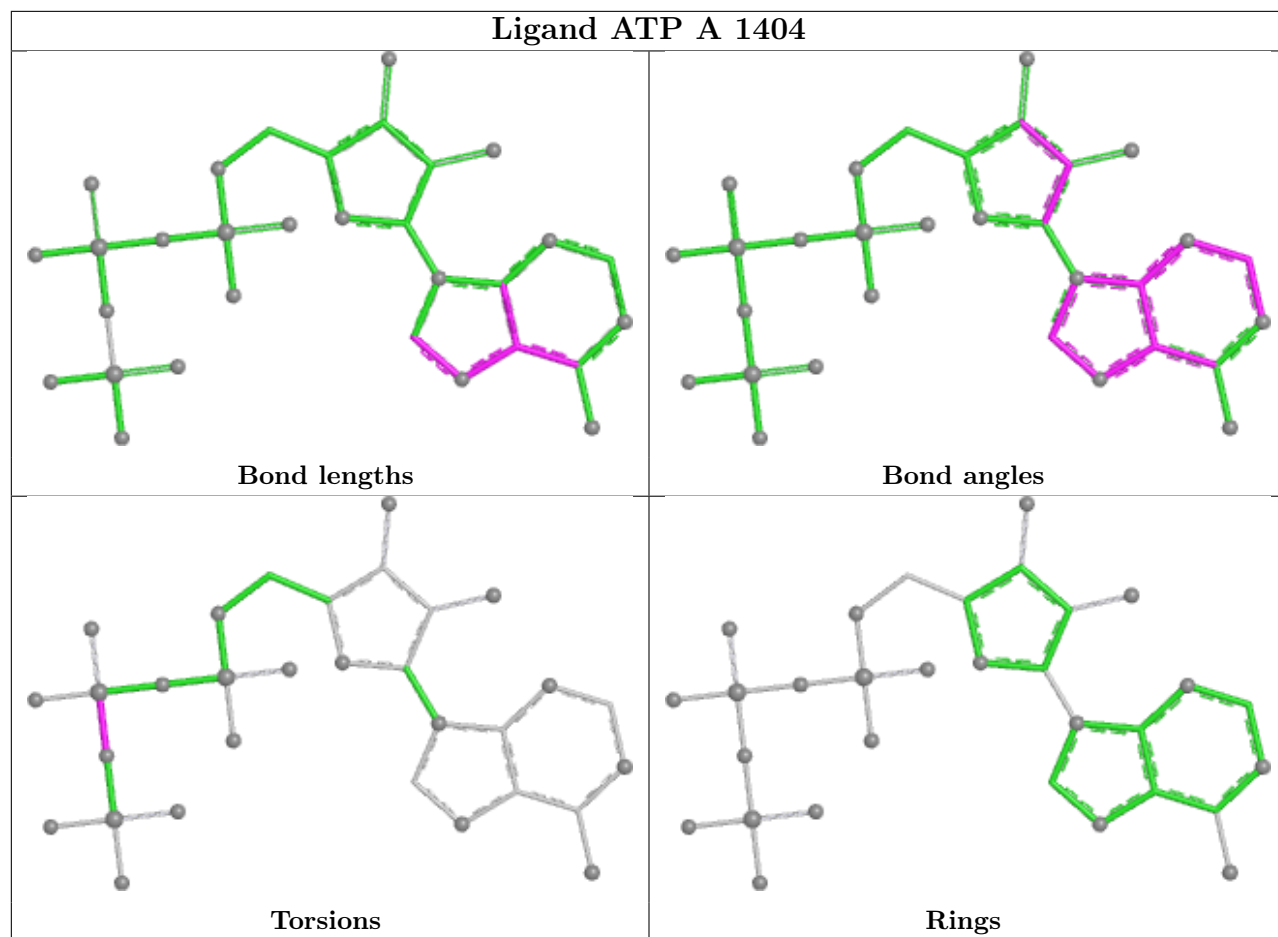
There are no ring outliers.

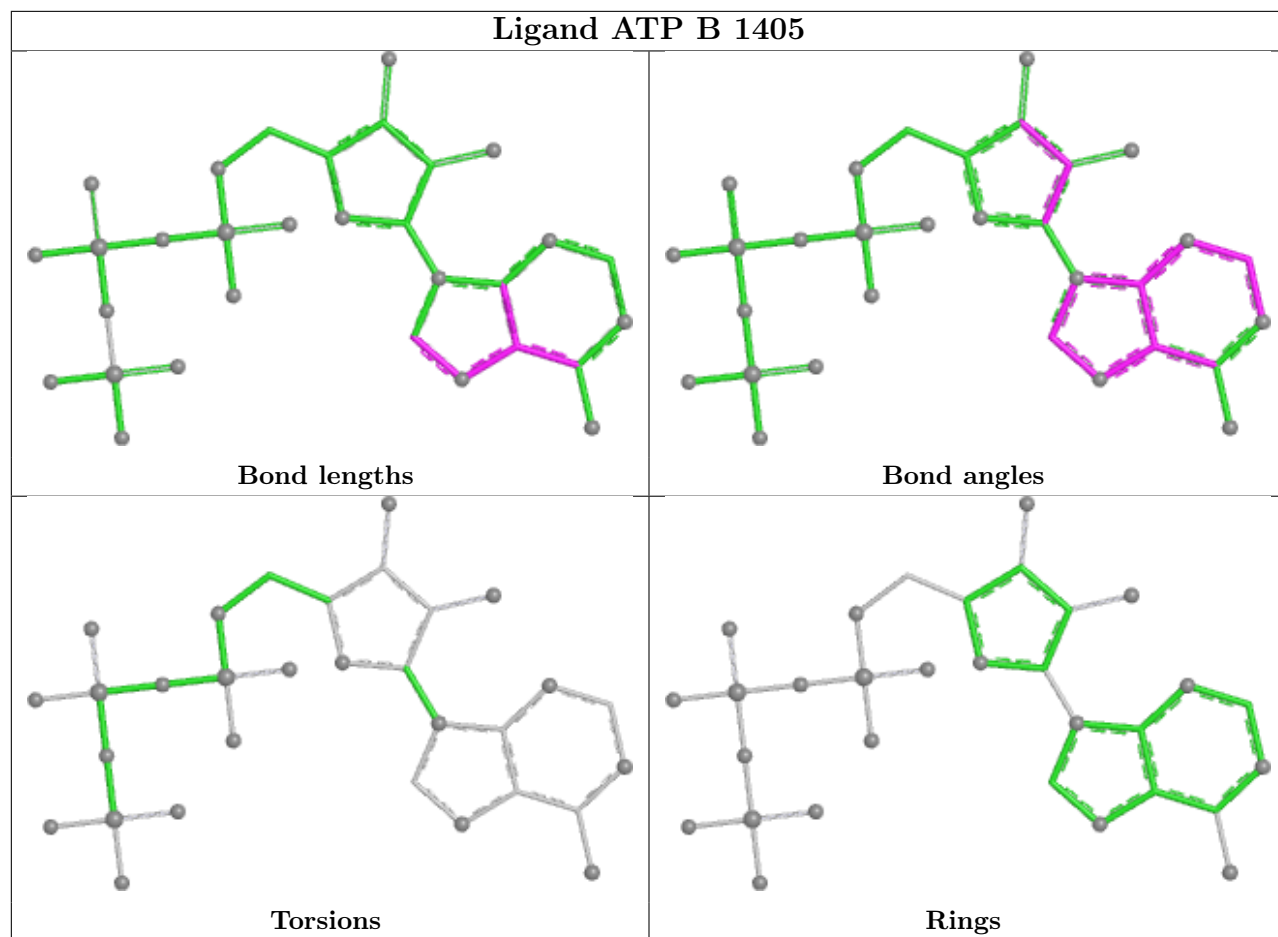
4 monomers are involved in 6 short contacts:

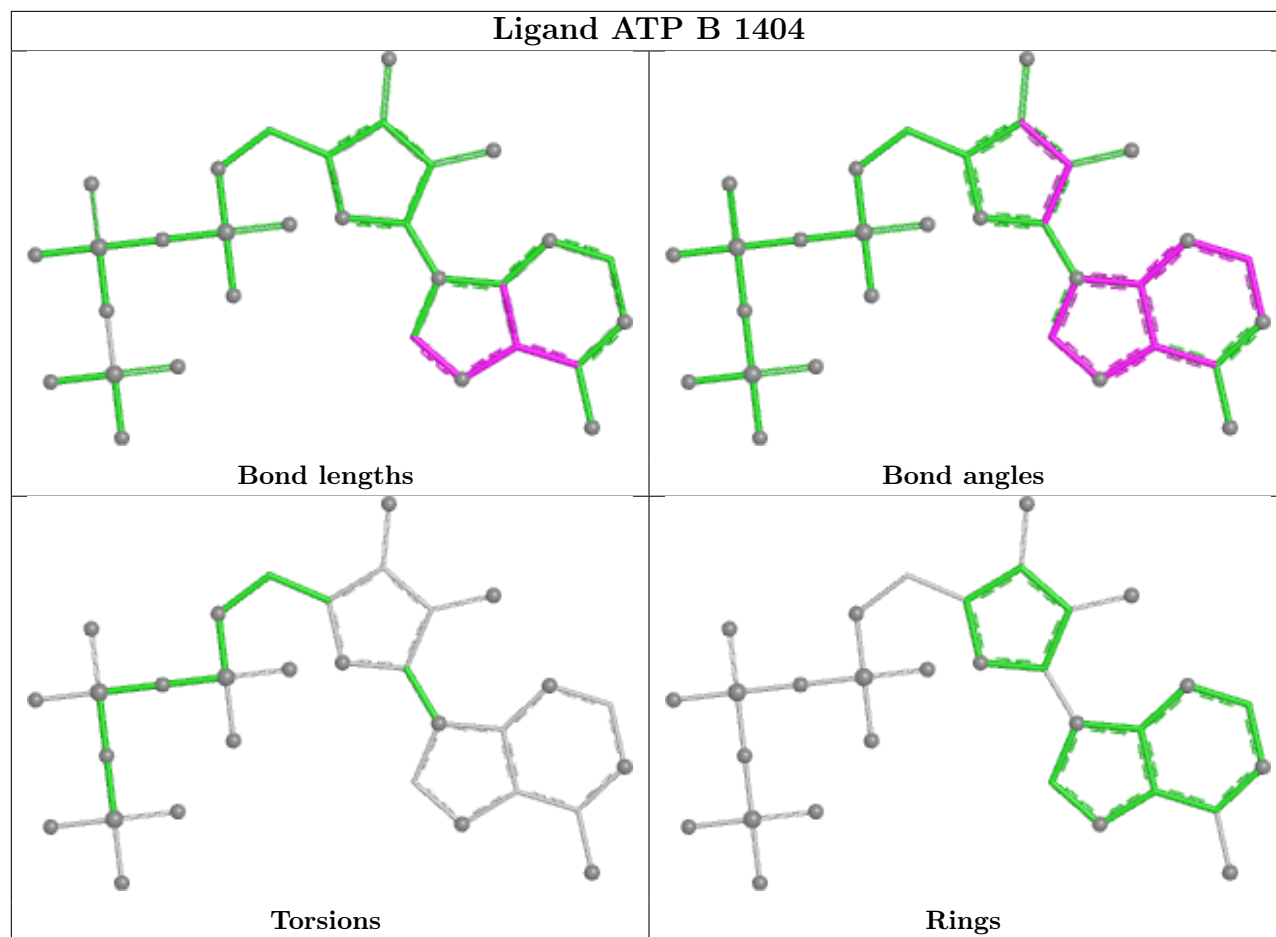
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1405	ATP	1	0
4	B	1405	ATP	2	0
4	B	1404	ATP	2	0
2	A	1401	SO4	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	861/1147 (75%)	0.46	44 (5%)	33	26	44, 80, 113, 151	0
1	B	859/1147 (74%)	0.76	97 (11%)	10	9	35, 84, 128, 161	0
All	All	1720/2294 (74%)	0.61	141 (8%)	17	14	35, 82, 125, 161	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	697	GLU	6.4
1	B	1014	PRO	6.1
1	B	1020	ARG	5.3
1	A	414	SER	5.0
1	B	766	LEU	5.0
1	B	816	TYR	4.9
1	A	1001	TYR	4.5
1	B	1030	LEU	4.5
1	B	652	ALA	4.4
1	A	695	VAL	4.4
1	B	1027	TYR	4.3
1	A	1007	ARG	4.3
1	B	1021	GLY	4.2
1	B	794	TRP	4.2
1	B	1001	TYR	4.2
1	B	579	ALA	4.0
1	B	636	GLY	4.0
1	B	1029	PHE	4.0
1	B	1012	ASN	3.9
1	B	435	VAL	3.9
1	B	637	LEU	3.8
1	B	546	ASP	3.7
1	B	650	PHE	3.7
1	B	542	ASP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	697	GLU	3.4
1	A	680	THR	3.4
1	B	646	GLY	3.3
1	B	793	GLU	3.3
1	A	690	TYR	3.2
1	A	681	GLU	3.2
1	B	772	LEU	3.2
1	B	808	PRO	3.2
1	B	814	ASP	3.2
1	B	634	LEU	3.2
1	A	415	ALA	3.2
1	B	633	LYS	3.1
1	B	741	GLU	3.1
1	A	740	SER	3.1
1	B	765	PRO	3.0
1	B	580	PRO	3.0
1	B	778	PRO	3.0
1	A	1027	TYR	3.0
1	B	807	ARG	3.0
1	A	653	MET	2.9
1	A	1023	THR	2.9
1	B	609	VAL	2.9
1	B	639	THR	2.9
1	B	678	PHE	2.9
1	A	1000	PRO	2.9
1	B	414	SER	2.9
1	B	1024	ARG	2.9
1	B	1177	ARG	2.9
1	A	599	SER	2.9
1	A	884	ARG	2.8
1	B	662	PRO	2.8
1	B	1002	GLU	2.8
1	B	638	ASP	2.8
1	B	806	ASP	2.8
1	B	545	TYR	2.8
1	B	631	GLU	2.7
1	B	1315	SER	2.7
1	B	1018	PRO	2.7
1	A	1177	ARG	2.7
1	B	429	TYR	2.7
1	A	698	GLU	2.7
1	A	1002	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	562	SER	2.7
1	A	694	PRO	2.6
1	A	885	LEU	2.6
1	B	809	PHE	2.6
1	B	557	GLU	2.6
1	B	805	VAL	2.6
1	A	565	TYR	2.6
1	A	1287	LYS	2.6
1	B	1022	LEU	2.6
1	B	532	THR	2.6
1	B	613	ARG	2.5
1	A	784	ALA	2.5
1	B	1010	ALA	2.5
1	B	680	THR	2.5
1	B	1017	ARG	2.5
1	A	1230	GLU	2.5
1	B	565	TYR	2.5
1	B	616	ARG	2.4
1	B	415	ALA	2.4
1	A	1178	ASP	2.4
1	B	669	PRO	2.4
1	B	1025	ASP	2.4
1	B	813	ARG	2.4
1	B	1026	GLY	2.4
1	B	529	ALA	2.4
1	B	473	PRO	2.4
1	A	1191	ASP	2.4
1	B	784	ALA	2.3
1	B	1028	HIS	2.3
1	A	575	ARG	2.3
1	B	561	HIS	2.3
1	A	678	PHE	2.3
1	B	604	PHE	2.3
1	B	581	LEU	2.3
1	B	632	GLY	2.3
1	B	538	LEU	2.2
1	B	764	PRO	2.2
1	B	417	MET	2.2
1	B	783	ALA	2.2
1	B	743	LEU	2.2
1	A	1179	ILE	2.2
1	A	571	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	912	GLY	2.2
1	A	481	THR	2.2
1	B	1023	THR	2.2
1	B	576	MET	2.2
1	B	912	GLY	2.2
1	A	573	LYS	2.2
1	A	630	GLU	2.2
1	A	613	ARG	2.2
1	B	1008	LYS	2.2
1	A	596	GLU	2.2
1	B	438	ARG	2.1
1	A	444	ASN	2.1
1	B	694	PRO	2.1
1	B	770	PRO	2.1
1	B	767	ASP	2.1
1	A	983	THR	2.1
1	B	1287	LYS	2.1
1	A	1221	SER	2.1
1	A	469	GLY	2.1
1	A	1017	ARG	2.1
1	B	454	ALA	2.1
1	B	691	VAL	2.1
1	B	1013	VAL	2.1
1	B	596	GLU	2.1
1	A	435	VAL	2.1
1	B	515	GLY	2.1
1	B	522	GLU	2.1
1	B	868	THR	2.0
1	B	434	ALA	2.0
1	B	817	TRP	2.0
1	B	544	MET	2.0
1	B	584	MET	2.0
1	A	816	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

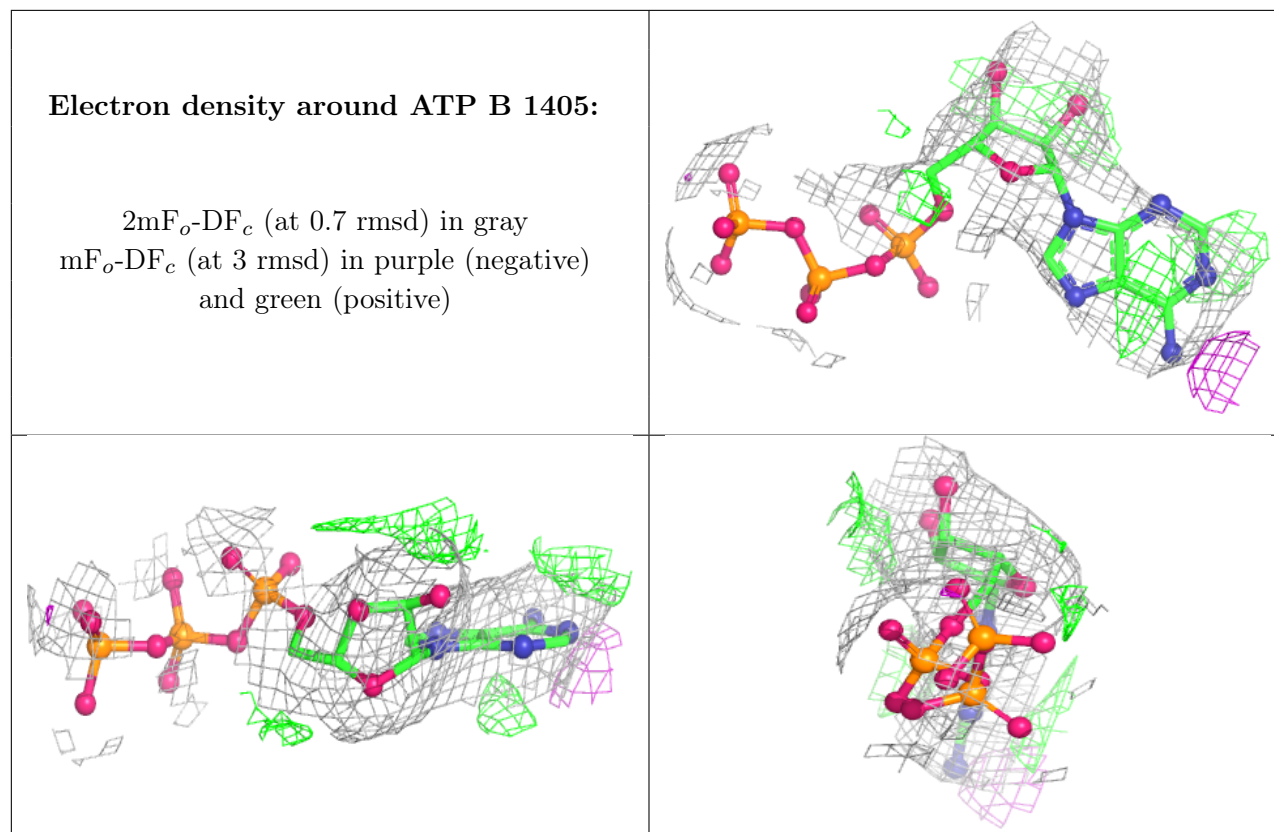
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

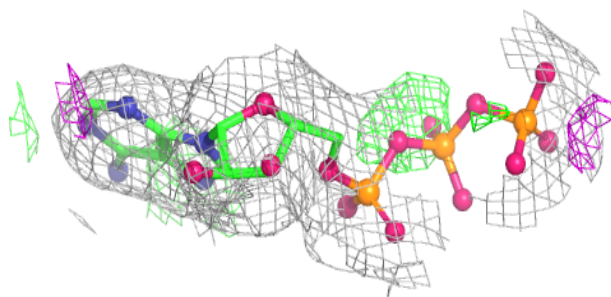
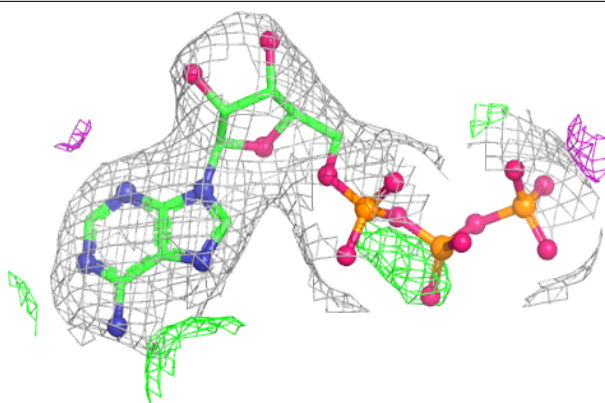
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	1401	5/5	0.90	0.08	97,105,124,150	0
2	SO4	A	1401	5/5	0.91	0.09	72,86,91,93	0
4	ATP	B	1405	31/31	0.93	0.11	69,117,135,141	0
4	ATP	A	1404	31/31	0.95	0.08	61,73,96,101	0
4	ATP	A	1405	31/31	0.96	0.09	65,92,108,113	0
4	ATP	B	1404	31/31	0.97	0.07	34,63,78,97	0
3	MG	A	1402	1/1	0.98	0.04	82,82,82,82	0
3	MG	A	1403	1/1	0.98	0.05	77,77,77,77	0
3	MG	B	1402	1/1	0.99	0.03	59,59,59,59	0
3	MG	B	1403	1/1	0.99	0.03	86,86,86,86	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.

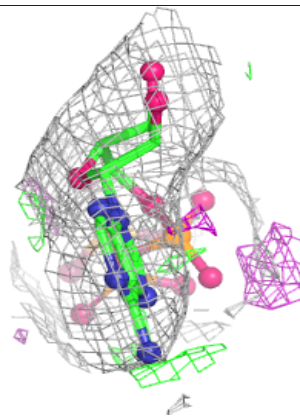
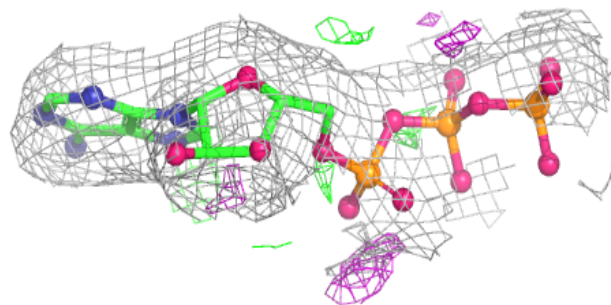
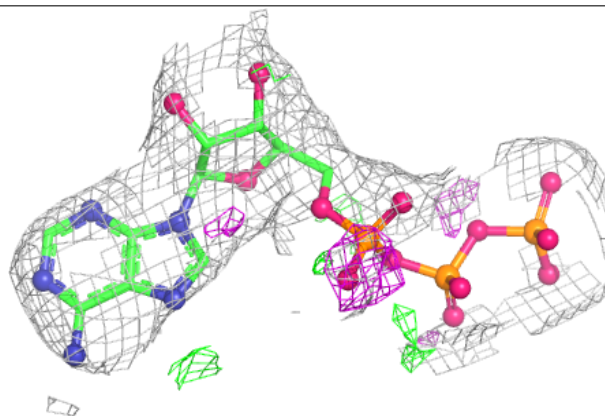


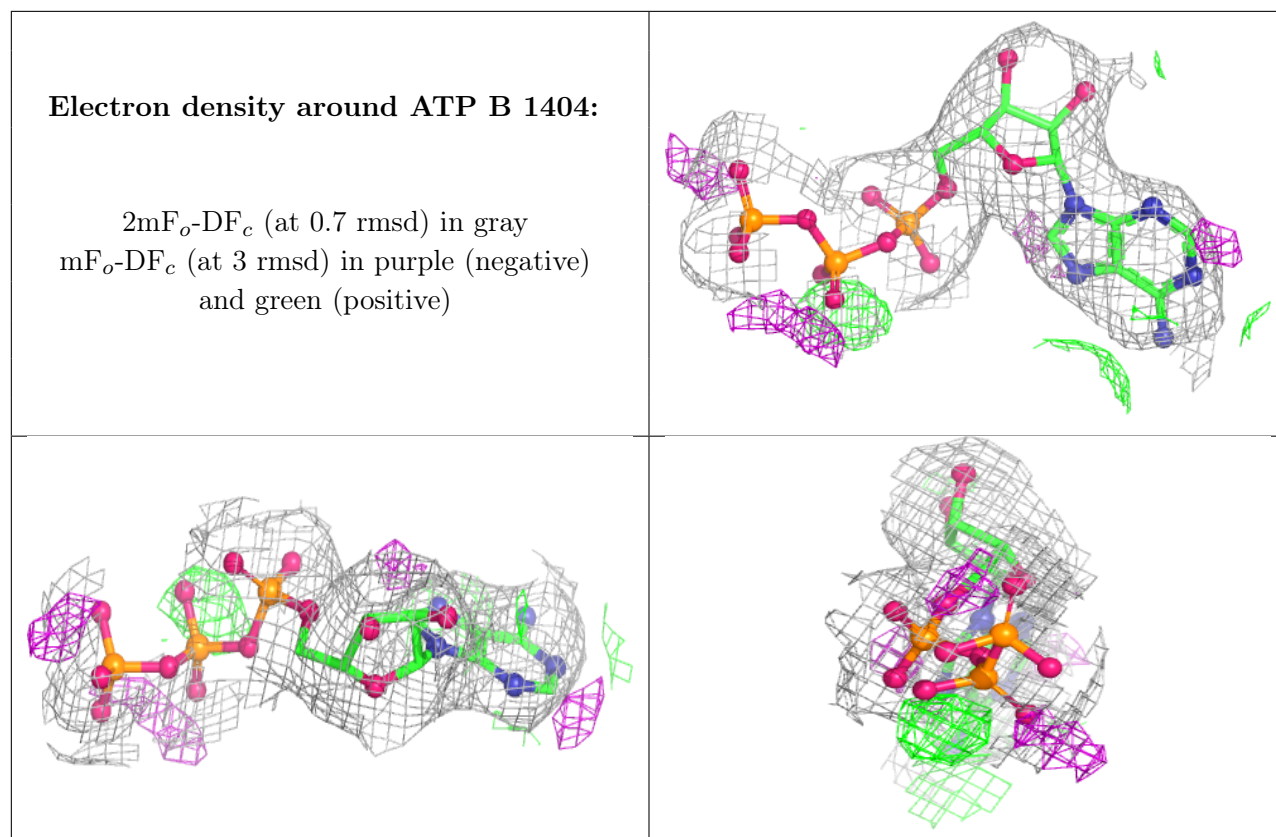
Electron density around ATP A 1404:

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

**Electron density around ATP A 1405:**

$2mF_o-DF_c$ (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.