Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 02:20 PM BST

PDB ID	:	4JJZ
Title	:	Crystal Structure of N10-Formyltetrahydrofolate Synthetase with ADP and Formylphosphate
Authors	:	Celeste, L.R.; Lovelace, L.L.; Lebioda, L.
Deposited on	:	2013-03-08
Resolution	:	2.50 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 following versions of software and data (see references ⓘ) were used in the production of this report:

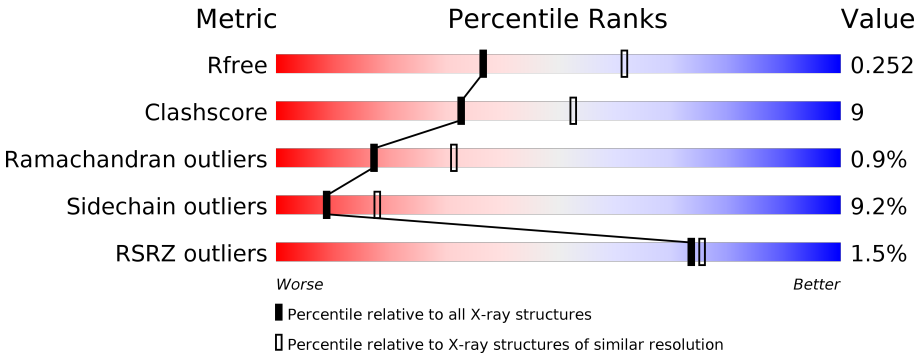
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	559	2% 84% 12%
1	B	559	2% 80% 14%

2 Entry composition

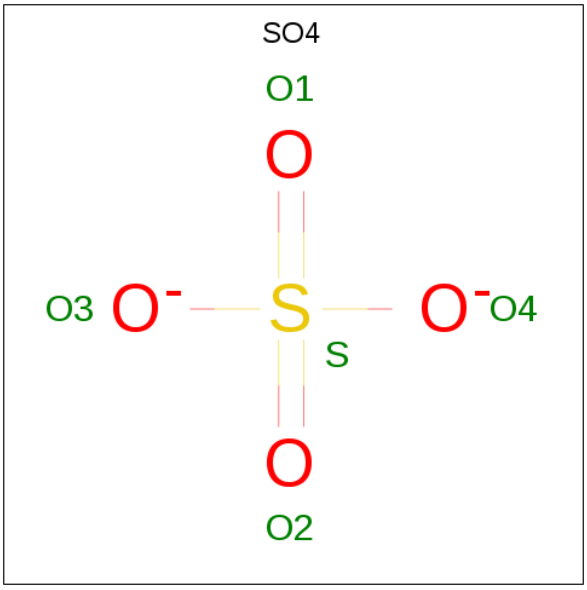
There are 8 unique types of molecules in this entry. The entry contains 8458 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Formate--tetrahydrofolate ligase.

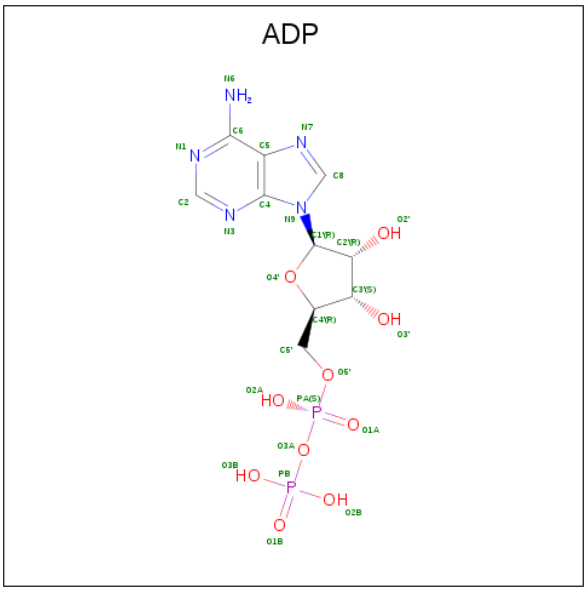
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4073	2591	693	768	21			
1	B	552	Total	C	N	O	S	0	0	0
			4108	2604	706	777	21			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



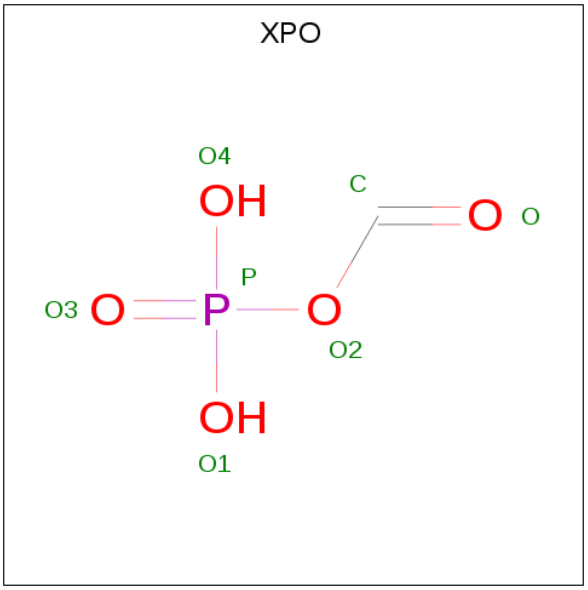
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



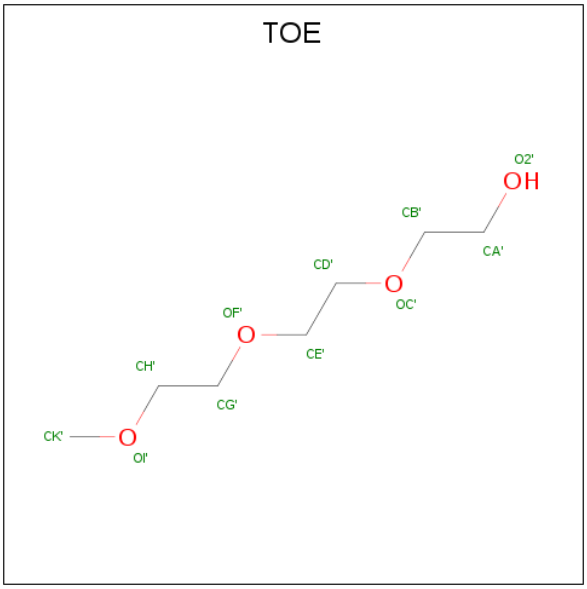
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is formyl phosphate (three-letter code: XPO) (formula: CH_3O_5P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			7	1	5	1		
4	B	1	Total	C	O	P	0	1
			14	2	10	2		

- Molecule 5 is 2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHOXYL (three-letter code: TOE) (formula: $C_7H_{16}O_4$).

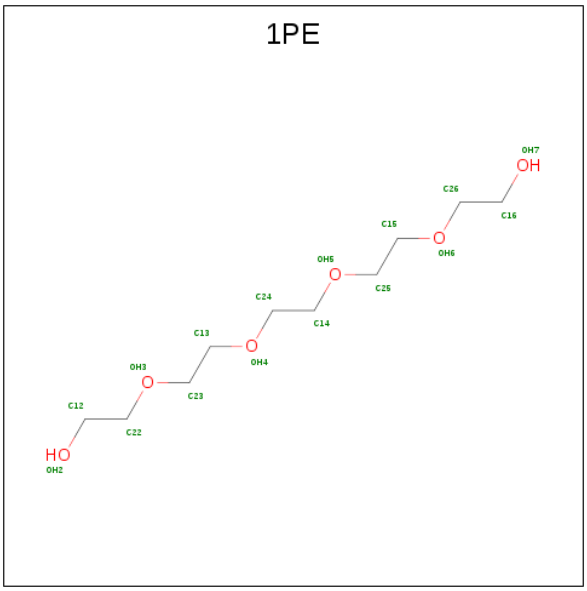


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 11 7 4	0	0
5	B	1	Total C O 11 7 4	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 7 4 3	0	0

- Molecule 8 is water.

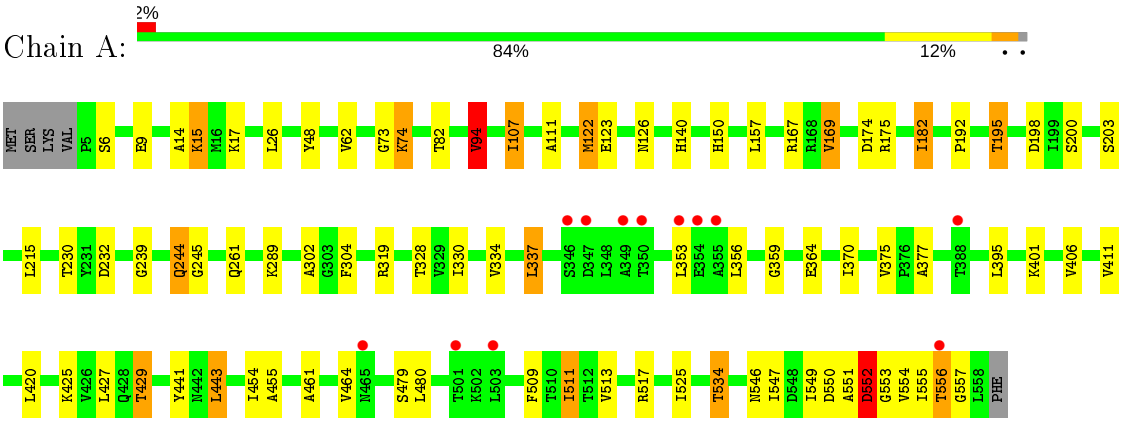
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	86	Total O 86 86	0	0
8	B	75	Total O 75 75	0	0

3 Residue-property plots (i)

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

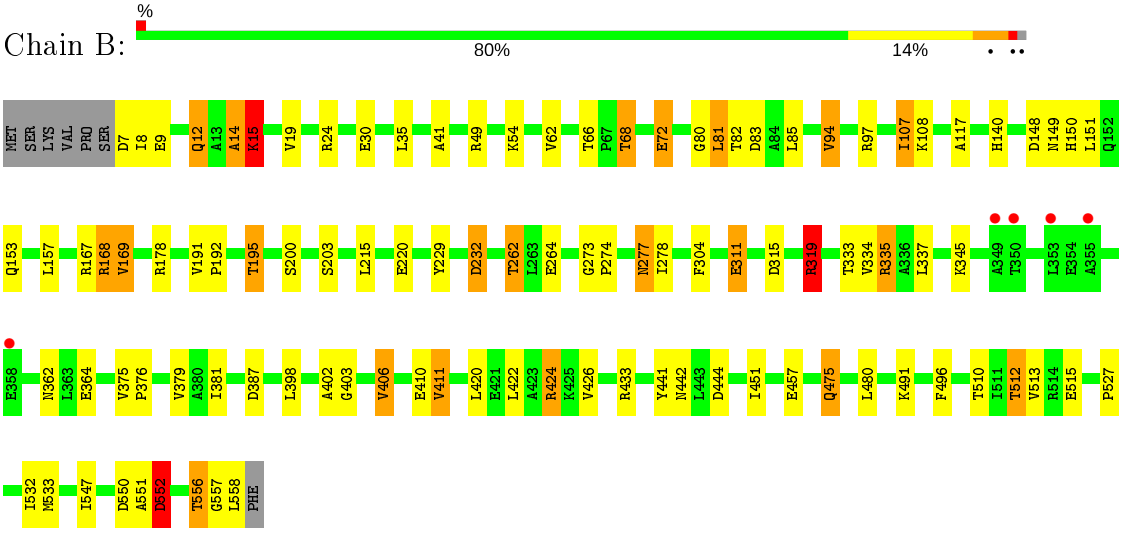
- Molecule 1: Formate--tetrahydrofolate ligase

Chain A:



- Molecule 1: Formate--tetrahydrofolate ligase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	91.17Å 212.98Å 53.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 2.50 47.77 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.6 (47.81-2.50) 91.6 (47.77-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.51Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.251 0.188 , 0.252	Depositor DCC
R_{free} test set	1694 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.987	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8458	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.5568e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, XPO, ADP, 1PE, SO4, TOE

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	0.61	0/4143	0.79	1/5631 (0.0%)
1	B	0.62	0/4177	0.84	4/5669 (0.1%)
All	All	0.62	0/8320	0.81	5/11300 (0.0%)

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 (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	168	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	B	168	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	94	VAL	CB-CA-C	-5.83	100.31	111.40
1	B	15	LYS	N-CA-C	5.65	126.25	111.00
1	B	319	ARG	NE-CZ-NH2	-5.55	117.52	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	14	ALA	Peptide

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	4073	0	4077	76	0
1	B	4108	0	4138	71	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	7	0	2	0	0
4	B	14	0	5	1	0
5	A	11	0	16	0	0
5	B	11	0	16	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	B	7	0	9	3	0
8	A	86	0	0	7	0
8	B	75	0	0	7	0
All	All	8458	0	8287	145	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 9.

All (145) 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:547:ILE:CG1	1:A:556:THR:CG2	1.76	1.57
1:A:547:ILE:HG12	1:A:556:THR:CG2	1.32	1.56
1:A:547:ILE:CA	1:A:556:THR:HG21	1.47	1.43
1:A:547:ILE:CB	1:A:556:THR:HG21	1.72	1.18
1:A:547:ILE:HA	1:A:556:THR:CG2	1.70	1.18
1:A:547:ILE:CG1	1:A:556:THR:HG23	1.62	1.11
1:A:547:ILE:HG13	1:A:556:THR:CG2	1.70	1.08
1:A:547:ILE:HA	1:A:556:THR:HG21	1.26	1.06
1:B:83:ASP:OD2	1:B:262:THR:HG21	1.60	1.02
1:A:547:ILE:CB	1:A:556:THR:CG2	2.34	1.00
1:A:547:ILE:HG13	1:A:556:THR:HG23	1.28	0.99
1:A:547:ILE:HG12	1:A:556:THR:HG22	1.00	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ILE:CA	1:A:556:THR:CG2	2.27	0.96
1:A:547:ILE:HG12	1:A:556:THR:HG23	1.32	0.86
1:A:547:ILE:HA	1:A:556:THR:CB	2.08	0.84
1:A:547:ILE:CG1	1:A:556:THR:HG21	1.70	0.81
1:A:547:ILE:N	1:A:556:THR:HG21	1.95	0.79
1:B:232:ASP:HB2	8:B:761:HOH:O	1.83	0.76
1:B:12:GLN:HE21	1:B:12:GLN:N	1.83	0.76
1:A:107:ILE:HG22	8:A:763:HOH:O	1.87	0.75
1:B:335:ARG:HH22	1:B:387:ASP:CB	2.00	0.75
1:A:319:ARG:NH2	1:A:441:TYR:O	2.20	0.74
1:B:232:ASP:CB	8:B:761:HOH:O	2.36	0.74
1:A:244:GLN:HE21	1:A:244:GLN:H	1.37	0.73
1:B:140:HIS:HD2	1:B:203:SER:OG	1.71	0.73
1:A:140:HIS:HD2	1:A:203:SER:OG	1.73	0.72
1:A:547:ILE:CG1	1:A:556:THR:HG22	1.79	0.71
1:A:546:ASN:C	1:A:556:THR:OG1	2.29	0.70
1:B:148:ASP:OD2	1:B:168:ARG:NH2	2.23	0.68
1:B:319:ARG:NH2	1:B:441:TYR:O	2.27	0.65
1:A:198:ASP:CG	1:A:534:THR:HG23	2.18	0.64
1:A:150:HIS:HE1	1:A:157:LEU:H	1.47	0.63
1:A:546:ASN:O	1:A:556:THR:OG1	2.15	0.63
1:A:82:THR:HG21	1:A:94:VAL:HG22	1.83	0.61
1:B:12:GLN:NE2	1:B:12:GLN:N	2.49	0.61
1:B:557:GLY:O	1:B:558:LEU:O	2.19	0.60
1:A:546:ASN:HB2	1:A:556:THR:OG1	2.01	0.60
1:A:174:ASP:OD2	1:B:168:ARG:NH1	2.35	0.59
1:B:402:ALA:N	1:B:403:GLY:HA2	2.17	0.59
1:A:239:GLY:HA2	1:A:244:GLN:HE22	1.68	0.59
1:A:175:ARG:HH12	1:B:149:ASN:HD22	1.49	0.58
1:A:455:ALA:HB1	1:A:511:ILE:HD11	1.84	0.58
1:A:425:LYS:O	1:A:429:THR:HG22	2.04	0.58
1:B:195:THR:HG21	8:B:706:HOH:O	2.03	0.57
1:A:547:ILE:HA	1:A:556:THR:HB	1.85	0.57
1:A:454:ILE:HD13	1:A:454:ILE:N	2.21	0.56
1:B:140:HIS:HD2	1:B:203:SER:HG	1.53	0.55
1:B:169:VAL:HG13	1:B:200:SER:HA	1.89	0.55
1:B:140:HIS:HE1	1:B:167:ARG:O	1.90	0.55
1:B:169:VAL:HG13	1:B:200:SER:OG	2.06	0.55
1:B:491:LYS:HE3	1:B:496:PHE:O	2.07	0.55
1:B:66:THR:H	1:B:362:ASN:HD21	1.56	0.54
1:A:546:ASN:O	1:A:556:THR:CB	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ALA:CB	1:A:511:ILE:HD11	2.37	0.54
1:A:546:ASN:C	1:A:556:THR:HG1	2.10	0.54
1:A:556:THR:O	1:A:556:THR:HG23	2.07	0.54
1:A:547:ILE:HG13	1:A:556:THR:HG21	1.55	0.54
1:B:178:ARG:HD3	1:B:533:MET:CE	2.38	0.53
1:A:461:ALA:HB2	1:A:509:PHE:CE1	2.43	0.53
1:A:48:TYR:CZ	1:A:289:LYS:HE3	2.43	0.53
1:A:198:ASP:CG	1:A:534:THR:CG2	2.77	0.53
1:B:195:THR:HG23	8:B:730:HOH:O	2.09	0.53
1:A:557:GLY:HA3	8:A:770:HOH:O	2.09	0.52
1:B:192:PRO:HG2	7:B:605:1PE:OH6	2.09	0.52
1:B:376:PRO:HB3	1:B:433:ARG:HE	1.75	0.52
1:B:424:ARG:HB2	1:B:424:ARG:HH11	1.75	0.51
1:B:68:THR:HB	1:B:72:GLU:OE1	2.11	0.51
1:B:150:HIS:HE1	1:B:157:LEU:H	1.58	0.50
1:A:74:LYS:HE3	1:A:302:ALA:O	2.10	0.50
1:B:14:ALA:O	1:B:15:LYS:CB	2.60	0.50
1:A:443:LEU:CD1	8:A:760:HOH:O	2.60	0.50
1:A:169:VAL:HG13	1:A:200:SER:OG	2.12	0.50
1:B:311:GLU:HG2	8:B:743:HOH:O	2.11	0.50
1:B:451:ILE:HD12	1:B:527:PRO:HG2	1.93	0.50
1:B:192:PRO:HD2	7:B:605:1PE:C25	2.42	0.49
1:B:80:GLY:HA3	1:B:411:VAL:HG11	1.94	0.49
1:A:17:LYS:H	1:A:261:GLN:HE22	1.59	0.49
1:A:547:ILE:CB	1:A:556:THR:HG22	2.28	0.49
1:B:149:ASN:HD21	1:B:153:GLN:HE21	1.60	0.48
1:A:546:ASN:CB	1:A:556:THR:OG1	2.62	0.48
1:A:195:THR:HG21	8:A:715:HOH:O	2.13	0.48
1:B:191:VAL:O	1:B:191:VAL:HG13	2.13	0.48
1:B:178:ARG:HD3	1:B:533:MET:HE3	1.96	0.48
1:A:443:LEU:HD12	8:A:760:HOH:O	2.12	0.48
1:A:330:ILE:HD11	1:A:370:ILE:HG13	1.97	0.47
1:A:140:HIS:HD2	1:A:203:SER:HG	1.62	0.47
1:A:239:GLY:HA2	1:A:244:GLN:NE2	2.30	0.47
1:A:48:TYR:CE2	1:A:289:LYS:HE3	2.50	0.47
1:B:192:PRO:HD2	7:B:605:1PE:H252	1.97	0.46
1:B:80:GLY:HA3	1:B:411:VAL:CG1	2.45	0.46
1:B:107:ILE:H	1:B:107:ILE:HD12	1.81	0.46
1:B:82:THR:HG21	1:B:94:VAL:HG22	1.98	0.46
1:A:107:ILE:CB	8:A:763:HOH:O	2.64	0.46
1:B:512:THR:HG23	8:B:739:HOH:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:VAL:HB	1:B:406:VAL:HG13	1.98	0.45
1:A:546:ASN:O	1:A:556:THR:HB	2.16	0.45
1:A:140:HIS:HE1	1:A:167:ARG:O	1.99	0.45
1:A:198:ASP:OD1	1:A:534:THR:CG2	2.64	0.45
1:B:402:ALA:H	1:B:403:GLY:HA2	1.82	0.45
1:B:475:GLN:HA	1:B:475:GLN:OE1	2.16	0.45
1:A:549:ILE:HB	1:A:554:VAL:HG22	1.99	0.45
1:B:278:ILE:HD11	1:B:532:ILE:HG12	1.98	0.45
1:B:335:ARG:H	1:B:335:ARG:CD	2.29	0.45
1:B:169:VAL:CG1	1:B:200:SER:HA	2.46	0.44
1:B:169:VAL:CG1	1:B:200:SER:OG	2.65	0.44
1:A:14:ALA:O	1:A:15:LYS:CB	2.66	0.44
1:B:422:LEU:O	1:B:426:VAL:HG23	2.17	0.44
1:B:515:GLU:HG3	5:B:604:TOE:H14	2.00	0.44
1:B:547:ILE:CG1	1:B:556:THR:HB	2.48	0.43
1:A:550:ASP:C	1:A:552:ASP:H	2.21	0.43
1:B:151:LEU:HD13	1:B:191:VAL:HG11	2.00	0.43
1:A:517:ARG:HH22	1:A:534:THR:HG21	1.84	0.43
1:A:328:THR:O	1:A:377:ALA:HA	2.18	0.43
1:B:232:ASP:HB3	8:B:761:HOH:O	2.12	0.43
1:B:273:GLY:N	1:B:274:PRO:CD	2.81	0.43
1:B:81:LEU:HD22	1:B:85:LEU:HD11	2.01	0.43
1:A:140:HIS:CD2	1:A:203:SER:OG	2.62	0.42
1:A:550:ASP:O	1:A:552:ASP:N	2.52	0.42
1:B:140:HIS:CE1	1:B:167:ARG:O	2.71	0.42
1:A:111:ALA:H	1:A:126:ASN:HD21	1.67	0.42
1:A:244:GLN:HG2	1:A:245:GLY:N	2.33	0.42
1:B:97:ARG:HH22	4:B:603[A]:XPO:P	2.43	0.42
1:B:315:ASP:O	1:B:319:ARG:HD2	2.19	0.42
1:A:230:THR:OG1	1:A:232:ASP:OD2	2.26	0.42
1:B:169:VAL:HG13	1:B:200:SER:CA	2.49	0.42
1:B:262:THR:HG23	1:B:264:GLU:H	1.85	0.41
1:B:191:VAL:O	1:B:191:VAL:CG1	2.67	0.41
1:B:277:ASN:HD22	1:B:278:ILE:N	2.18	0.41
1:B:333:THR:HB	1:B:335:ARG:HE	1.85	0.41
1:B:547:ILE:HG12	1:B:556:THR:HB	2.02	0.41
1:A:182:ILE:O	1:A:192:PRO:HA	2.20	0.41
1:A:511:ILE:H	1:A:511:ILE:HG12	1.81	0.41
1:B:229:TYR:CD1	1:B:229:TYR:N	2.88	0.41
1:B:550:ASP:C	1:B:552:ASP:H	2.24	0.41
1:A:334:VAL:HG13	1:A:356:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:ARG:HH22	1:B:30:GLU:HB2	1.86	0.41
1:A:337:LEU:O	1:A:359:GLY:HA3	2.21	0.41
1:A:553:GLY:HA3	8:A:762:HOH:O	2.21	0.41
1:A:122:MET:HE3	1:A:123:GLU:HA	2.02	0.41
1:B:82:THR:OG1	1:B:94:VAL:HG22	2.21	0.41
1:B:334:VAL:HB	1:B:335:ARG:CZ	2.51	0.41
1:B:35:LEU:HD23	1:B:41:ALA:HB2	2.03	0.41
1:A:150:HIS:CE1	1:A:157:LEU:H	2.35	0.40
1:B:442:ASN:OD1	1:B:444:ASP:N	2.48	0.40
1:B:117:ALA:HB2	1:B:411:VAL:HG13	2.03	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	552/559 (99%)	517 (94%)	30 (5%)	5 (1%)	17	31
1	B	550/559 (98%)	516 (94%)	29 (5%)	5 (1%)	17	31
All	All	1102/1118 (99%)	1033 (94%)	59 (5%)	10 (1%)	17	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	551	ALA
1	B	15	LYS
1	B	551	ALA
1	A	304	PHE
1	A	552	ASP
1	B	552	ASP
1	B	556	THR
1	A	15	LYS

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Mol	Chain	Res	Type
1	B	304	PHE
1	A	73	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	412/441 (93%)	377 (92%)	35 (8%)	10 21
1	B	422/441 (96%)	380 (90%)	42 (10%)	7 15
All	All	834/882 (95%)	757 (91%)	77 (9%)	9 18

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	9	GLU
1	A	26	LEU
1	A	62	VAL
1	A	74	LYS
1	A	94	VAL
1	A	107	ILE
1	A	122	MET
1	A	169	VAL
1	A	182	ILE
1	A	195	THR
1	A	215	LEU
1	A	244	GLN
1	A	337	LEU
1	A	353	LEU
1	A	364	GLU
1	A	375	VAL
1	A	395	LEU
1	A	401	LYS
1	A	406	VAL
1	A	411	VAL

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Mol	Chain	Res	Type
1	A	420	LEU
1	A	427	LEU
1	A	429	THR
1	A	443	LEU
1	A	464	VAL
1	A	479	SER
1	A	480	LEU
1	A	511	ILE
1	A	513	VAL
1	A	525	ILE
1	A	534	THR
1	A	552	ASP
1	A	555	ILE
1	A	556	THR
1	B	7	ASP
1	B	8	ILE
1	B	9	GLU
1	B	12	GLN
1	B	19	VAL
1	B	49	ARG
1	B	54	LYS
1	B	62	VAL
1	B	68	THR
1	B	72	GLU
1	B	81	LEU
1	B	94	VAL
1	B	107	ILE
1	B	108	LYS
1	B	169	VAL
1	B	195	THR
1	B	215	LEU
1	B	220	GLU
1	B	232	ASP
1	B	262	THR
1	B	277	ASN
1	B	311	GLU
1	B	319	ARG
1	B	335	ARG
1	B	337	LEU
1	B	345	LYS
1	B	364	GLU
1	B	375	VAL

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Mol	Chain	Res	Type
1	B	381	ILE
1	B	398	LEU
1	B	406	VAL
1	B	410	GLU
1	B	411	VAL
1	B	420	LEU
1	B	424	ARG
1	B	457	GLU
1	B	475	GLN
1	B	480	LEU
1	B	510	THR
1	B	512	THR
1	B	513	VAL
1	B	552	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	140	HIS
1	A	149	ASN
1	A	150	HIS
1	A	153	GLN
1	A	244	GLN
1	A	261	GLN
1	A	265	ASN
1	A	283	ASN
1	A	484	ASN
1	B	12	GLN
1	B	140	HIS
1	B	149	ASN
1	B	150	HIS
1	B	265	ASN
1	B	277	ASN
1	B	283	ASN
1	B	362	ASN
1	B	382	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
7	1PE	B	605	-	6,6,15	1.59	1 (16%)	5,5,14	2.09	2 (40%)
4	XPO	A	603	6	5,6,6	1.35	1 (20%)	6,8,8	1.75	2 (33%)
2	SO4	A	601	-	4,4,4	0.50	0	6,6,6	0.46	0
2	SO4	B	601	-	4,4,4	0.53	0	6,6,6	0.84	0
4	XPO	B	603[B]	6	5,6,6	0.86	0	6,8,8	1.25	1 (16%)
4	XPO	B	603[A]	6	5,6,6	0.86	0	6,8,8	1.65	2 (33%)
5	TOE	A	604	-	10,10,10	0.75	0	9,9,9	0.78	0
5	TOE	B	604	-	10,10,10	0.76	0	9,9,9	0.80	0
3	ADP	B	602	6	24,29,29	1.03	2 (8%)	29,45,45	1.51	5 (17%)
3	ADP	A	602	6	24,29,29	1.14	3 (12%)	29,45,45	1.57	5 (17%)

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
7	1PE	B	605	-	-	2/4/4/13	-
4	XPO	A	603	6	-	0/0/4/4	-
4	XPO	B	603[B]	6	-	0/0/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	XPO	B	603[A]	6	-	0/0/4/4	-
5	TOE	A	604	-	-	4/8/8/8	-
5	TOE	B	604	-	-	5/8/8/8	-
3	ADP	B	602	6	-	0/12/32/32	0/3/3/3
3	ADP	A	602	6	-	0/12/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	ADP	C5-C4	2.77	1.48	1.40
3	A	602	ADP	C2-N3	2.70	1.36	1.32
3	B	602	ADP	C5-C4	2.21	1.46	1.40
4	A	603	XPO	P-O2	2.13	1.62	1.59
3	A	602	ADP	O4'-C1'	2.12	1.44	1.41
3	B	602	ADP	O4'-C1'	2.09	1.44	1.41
7	B	605	1PE	OH6-C26	2.06	1.51	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	ADP	N3-C2-N1	-4.29	121.97	128.68
3	B	602	ADP	N3-C2-N1	-3.94	122.52	128.68
3	A	602	ADP	PA-O3A-PB	-3.89	119.49	132.83
3	B	602	ADP	PA-O3A-PB	-3.53	120.71	132.83
4	A	603	XPO	O4-P-O2	-3.08	95.61	105.24
7	B	605	1PE	C26-OH6-C15	3.03	126.41	113.29
4	A	603	XPO	O4-P-O1	2.77	118.23	107.64
3	B	602	ADP	O3B-PB-O2B	2.73	118.06	107.64
3	A	602	ADP	C2-N1-C6	2.59	123.19	118.75
3	B	602	ADP	C4-C5-N7	-2.49	106.81	109.40
3	B	602	ADP	C1'-N9-C4	-2.48	122.28	126.64
7	B	605	1PE	OH7-C16-C26	2.41	125.78	111.81
4	B	603[A]	XPO	O4-P-O2	-2.24	98.24	105.24
3	A	602	ADP	O3B-PB-O2B	2.19	116.00	107.64
3	A	602	ADP	C1'-N9-C4	-2.19	122.80	126.64
4	B	603[A]	XPO	O4-P-O3	2.15	119.10	110.68
4	B	603[B]	XPO	O4-P-O1	2.12	115.75	107.64

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	604	TOE	OC'-CD'-CE'-OF'
5	A	604	TOE	OF'-CG'-CH'-OI'
7	B	605	1PE	OH6-C15-C25-OH5
5	B	604	TOE	O2'-CA'-CB'-OC'
5	B	604	TOE	OF'-CG'-CH'-OI'
5	B	604	TOE	CE'-CD'-OC'-CB'
5	A	604	TOE	CH'-CG'-OF'-CE'
5	A	604	TOE	CE'-CD'-OC'-CB'
5	A	604	TOE	O2'-CA'-CB'-OC'
5	B	604	TOE	CH'-CG'-OF'-CE'
7	B	605	1PE	OH7-C16-C26-OH6

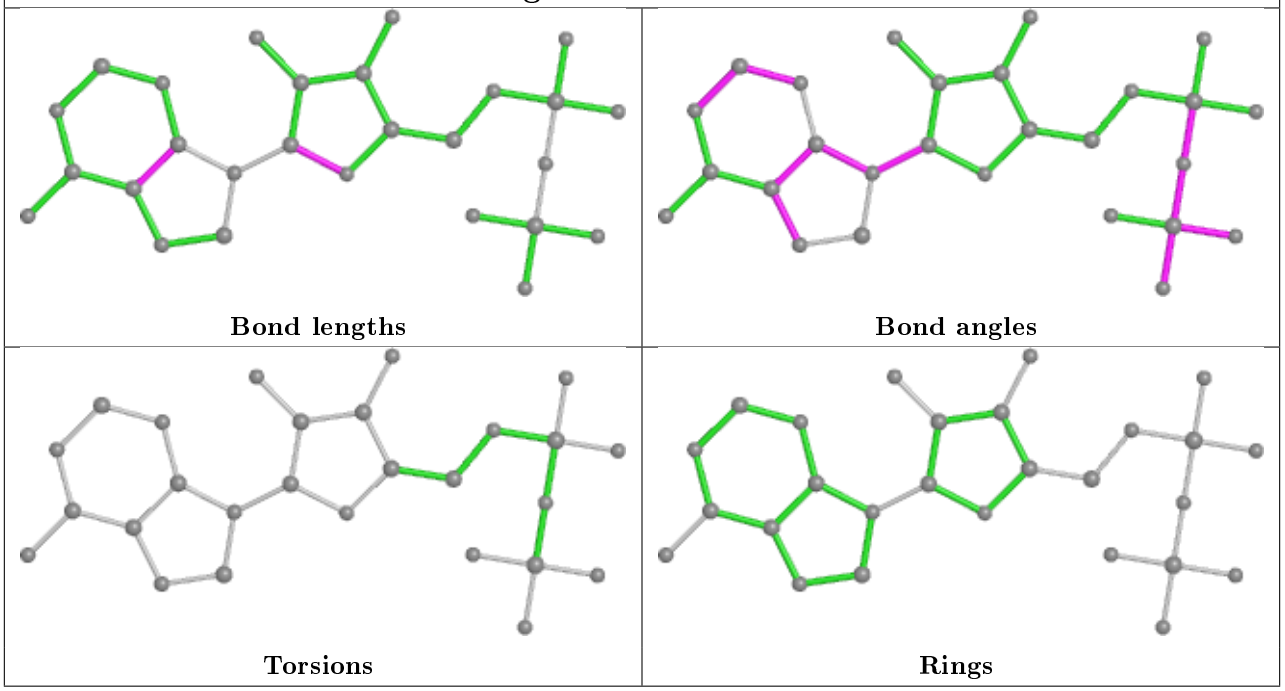
There are no ring outliers.

3 monomers are involved in 5 short contacts:

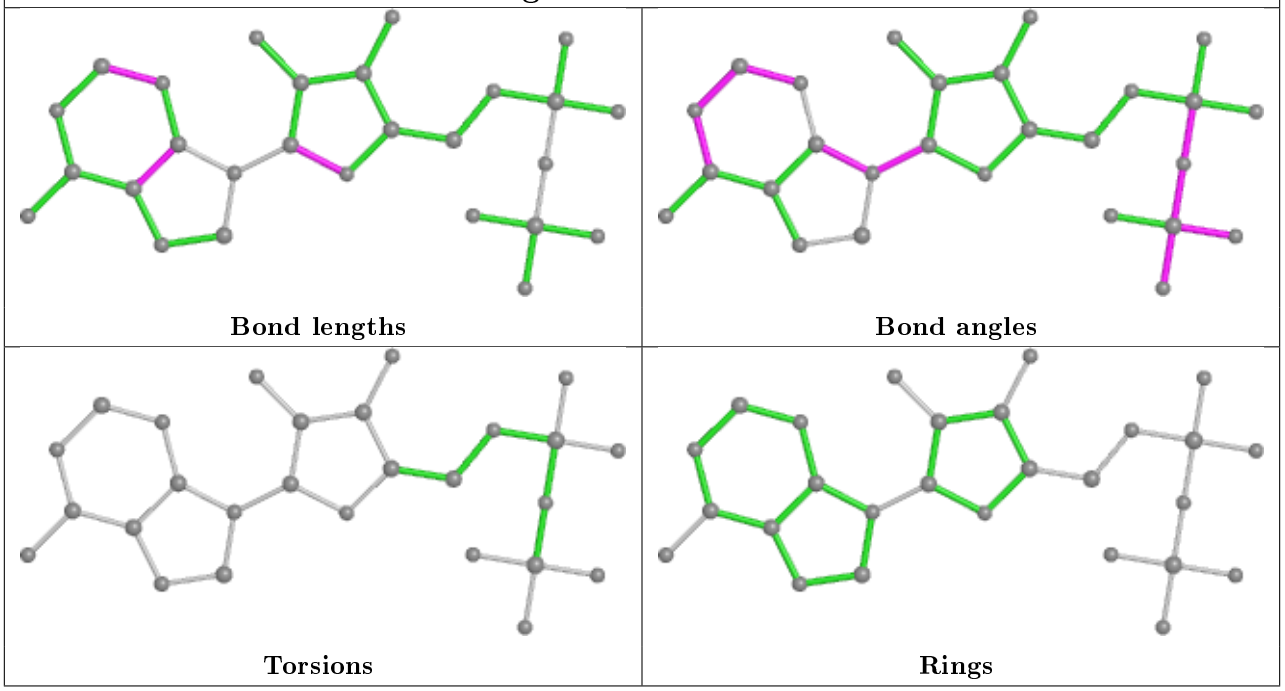
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	605	1PE	3	0
4	B	603[A]	XPO	1	0
5	B	604	TOE	1	0

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

Ligand ADP B 602



Ligand ADP A 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	554/559 (99%)	-0.07	12 (2%) 62 65	16, 41, 70, 92	0
1	B	552/559 (98%)	-0.19	5 (0%) 84 86	17, 37, 63, 84	0
All	All	1106/1118 (98%)	-0.13	17 (1%) 73 75	16, 39, 66, 92	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	346	SER	4.2
1	A	355	ALA	3.9
1	A	556	THR	3.8
1	A	353	LEU	3.5
1	A	354	GLU	3.4
1	A	347	ASP	3.4
1	A	501	THR	2.8
1	A	465	ASN	2.6
1	B	349	ALA	2.6
1	A	350	THR	2.5
1	A	349	ALA	2.5
1	B	355	ALA	2.4
1	A	388	THR	2.2
1	B	353	LEU	2.2
1	B	358	GLU	2.1
1	B	350	THR	2.1
1	A	503	LEU	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

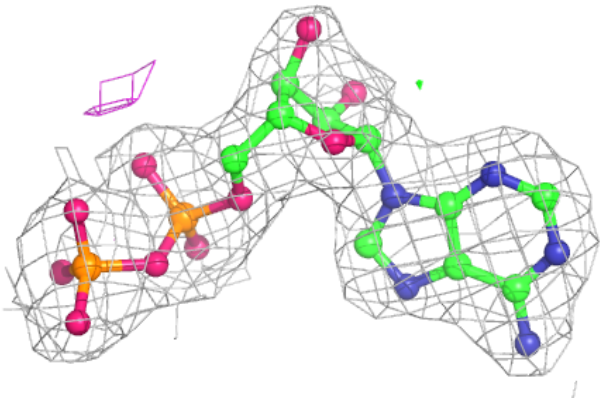
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

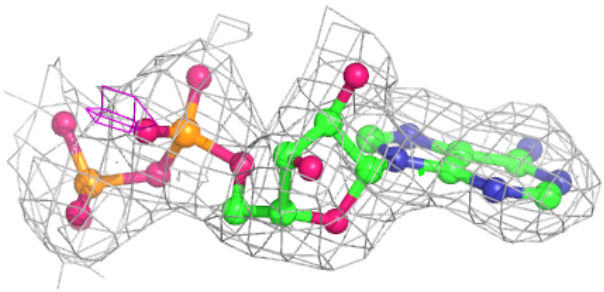
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MG	A	605	1/1	0.84	0.09	29,29,29,29	0
7	1PE	B	605	7/16	0.87	0.33	18,20,24,25	0
5	TOE	A	604	11/11	0.89	0.17	29,33,40,41	0
5	TOE	B	604	11/11	0.95	0.14	28,30,42,42	0
6	MG	B	606	1/1	0.97	0.07	24,24,24,24	0
2	SO4	B	601	5/5	0.97	0.10	37,39,42,45	0
4	XPO	B	603[B]	7/7	0.97	0.15	21,24,29,29	7
4	XPO	B	603[A]	7/7	0.97	0.15	18,20,22,22	7
4	XPO	A	603	7/7	0.97	0.10	37,41,45,46	0
2	SO4	A	601	5/5	0.97	0.09	40,40,43,47	0
3	ADP	B	602	27/27	0.98	0.10	24,35,38,40	0
3	ADP	A	602	27/27	0.98	0.10	26,29,33,34	0

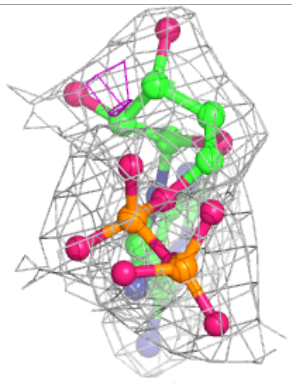
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 602:

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

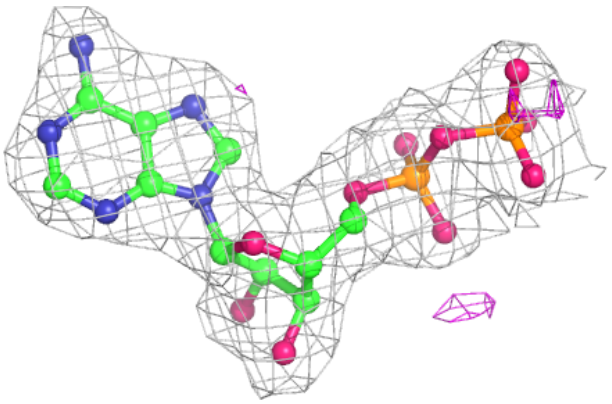


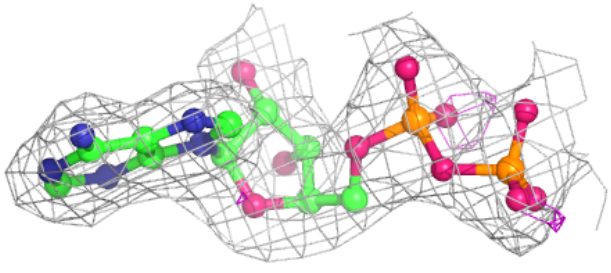


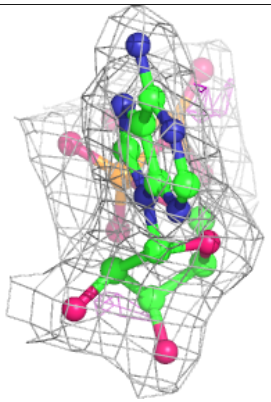


Electron density around ADP A 602:

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







6.5 Other polymers (i)

There are no such residues in this entry.