Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 03:39 am BST

PDB ID	:	1W5S
Title	:	Structure of the Aeropyrum Pernix ORC2 protein (ADP form)
Authors	:	Singleton, M.R.; Morales, R.; Grainge, I.; Cook, N.; Isupov, M.N.; Wigley, D.B.
Deposited on	:	2004-08-09
Resolution	:	2.40 Å(reported)

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

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

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

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

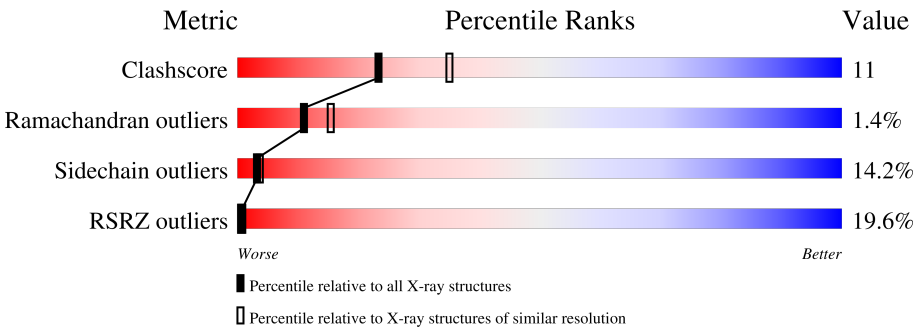
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	412	23% 64% 24% 6% • 5%
1	B	412	15% 71% 20% • • •

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
2	SO4	A	501	-	-	X	-
2	SO4	B	501	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6390 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.

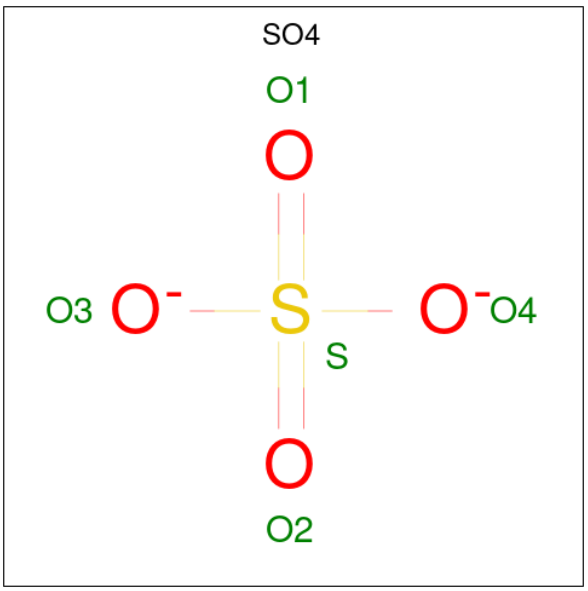
- Molecule 1 is a protein called ORIGIN RECOGNITION COMPLEX SUBUNIT 2 ORC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	3080	1959	543	568	10	0	0	0
1	B	396	3122	1984	550	578	10	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

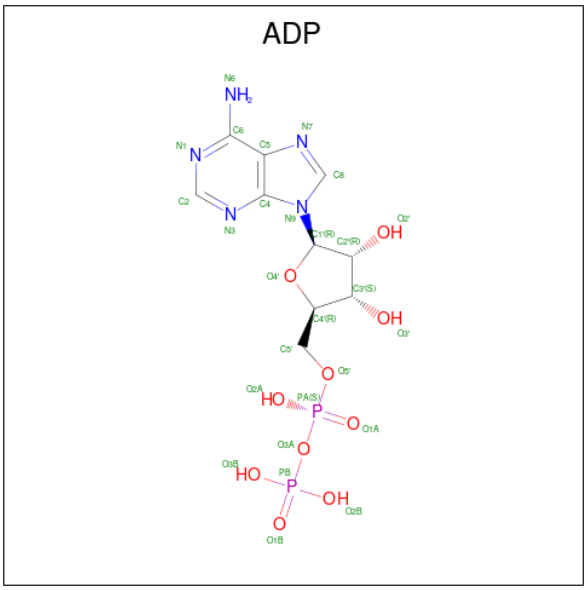
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q9YFU8
A	2	LYS	-	expression tag	UNP Q9YFU8
A	3	VAL	-	expression tag	UNP Q9YFU8
B	1	MET	-	expression tag	UNP Q9YFU8
B	2	LYS	-	expression tag	UNP Q9YFU8
B	3	VAL	-	expression tag	UNP Q9YFU8

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



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

- 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
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
3	B	1	27	10	5	10	2	0	0

- Molecule 4 is water.

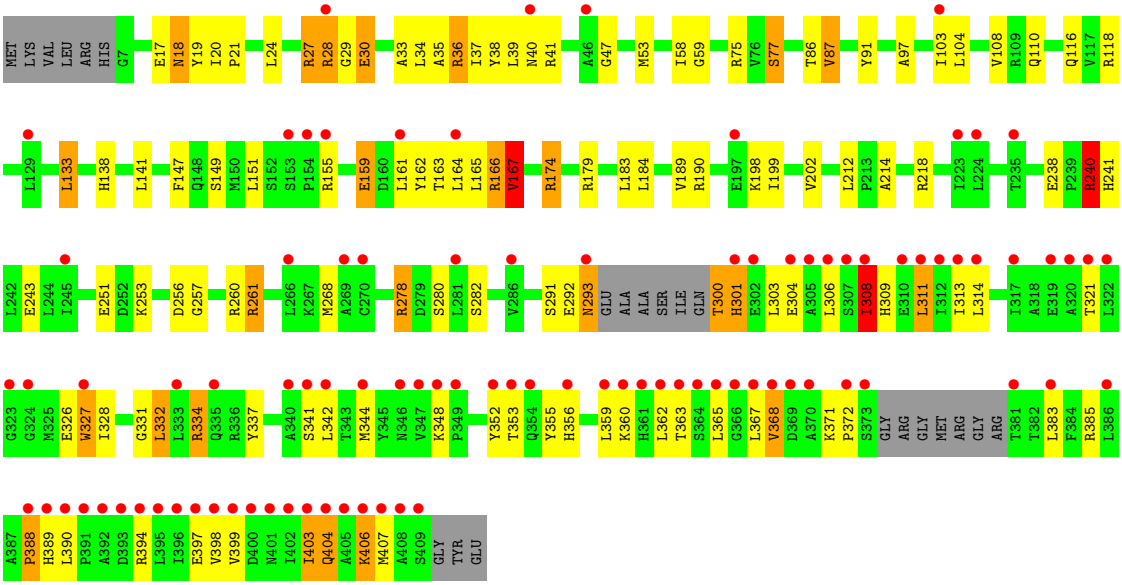
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	62	62	62	0	0
			Total	O		
4	B	52	52	52	0	0

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.

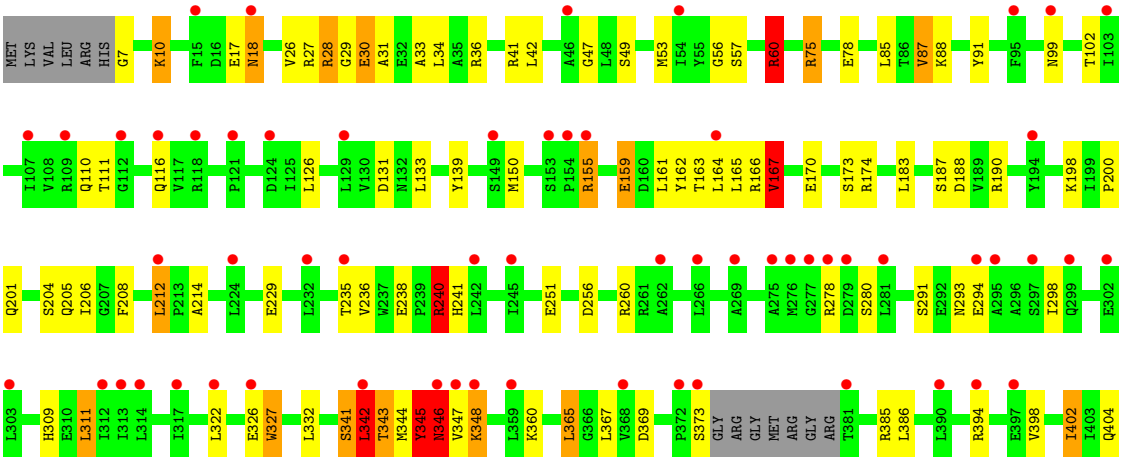
• Molecule 1: ORIGIN RECOGNITION COMPLEX SUBUNIT 2 ORC2

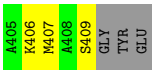
Chain A:



• Molecule 1: ORIGIN RECOGNITION COMPLEX SUBUNIT 2 ORC2

Chain B:




A405
K406
M407
A408
S409
GLY
TYR
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	67.50Å 101.91Å 255.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	129.10 – 2.40 19.78 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (129.10-2.40) 98.4 (19.78-2.40)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.56 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.212 , 0.286 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	33.7	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 59.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6390	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ADP

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	0.96	2/3130 (0.1%)	0.94	10/4232 (0.2%)
1	B	0.96	2/3173 (0.1%)	1.00	10/4292 (0.2%)
All	All	0.96	4/6303 (0.1%)	0.97	20/8524 (0.2%)

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	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	38	TYR	CD1-CE1	5.76	1.48	1.39
1	B	17	GLU	CB-CG	5.25	1.62	1.52
1	B	256	ASP	CB-CG	-5.23	1.40	1.51
1	A	17	GLU	CG-CD	5.04	1.59	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	B	60	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	167	VAL	CB-CA-C	-6.74	98.59	111.40
1	B	47	GLY	N-CA-C	-6.57	96.68	113.10
1	A	260	ARG	NE-CZ-NH1	6.47	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	260	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	B	27	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	167	VAL	CB-CA-C	-5.99	100.02	111.40
1	B	212	LEU	CB-CG-CD1	5.95	121.12	111.00
1	A	41	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	A	133	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	240	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	60	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	256	ASP	CB-CA-C	-5.56	99.29	110.40
1	A	240	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	B	240	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	218	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	75	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	261	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	B	256	ASP	CB-CA-C	-5.02	100.37	110.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ARG	Peptide
1	B	346	ASN	Peptide
1	B	7	GLY	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	3080	0	3157	85	0
1	B	3122	0	3198	75	0
2	A	10	0	0	2	0
2	B	10	0	0	5	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	62	0	0	11	0
4	B	52	0	0	11	0
All	All	6390	0	6379	143	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 11.

All (143) 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:33:ALA:CB	1:B:33:ALA:HB1	1.96	0.96
1:A:238:GLU:H	1:A:241:HIS:HD2	1.15	0.94
1:A:33:ALA:CB	1:B:33:ALA:CB	2.49	0.88
1:A:33:ALA:HB1	1:B:33:ALA:CB	2.02	0.88
1:B:30:GLU:C	4:B:2005:HOH:O	2.13	0.85
1:B:30:GLU:O	1:B:34:LEU:HD13	1.76	0.85
1:A:33:ALA:HB1	1:B:33:ALA:HB1	1.63	0.80
1:A:352:TYR:HB3	4:A:2026:HOH:O	1.80	0.80
1:A:389:HIS:HA	1:B:204:SER:OG	1.84	0.78
1:A:238:GLU:H	1:A:241:HIS:CD2	2.01	0.77
1:B:60:ARG:HD3	1:B:214:ALA:HB2	1.70	0.74
1:B:28:ARG:HG2	1:B:29:GLY:N	2.03	0.73
1:B:30:GLU:HG2	4:B:2004:HOH:O	1.87	0.73
1:A:321:THR:HG23	1:B:201:GLN:OE1	1.90	0.72
1:A:33:ALA:HB2	1:B:33:ALA:CB	2.18	0.72
1:A:91:TYR:H	1:A:110:GLN:HE22	1.39	0.71
1:B:60:ARG:HD2	2:B:500:SO4:O2	1.90	0.70
1:B:238:GLU:H	1:B:241:HIS:HD2	1.40	0.70
1:A:34:LEU:O	1:A:37:ILE:N	2.26	0.68
1:B:78:GLU:HB3	4:B:2017:HOH:O	1.93	0.68
1:A:33:ALA:CB	1:B:33:ALA:HB2	2.24	0.68
1:A:174:ARG:NH1	4:A:2036:HOH:O	2.06	0.66
1:A:240:ARG:NH2	2:A:501:SO4:O2	2.28	0.66
1:A:389:HIS:CA	1:B:204:SER:OG	2.42	0.66
1:A:399:VAL:O	1:A:403:ILE:HB	1.96	0.65
1:A:314:LEU:HD13	1:A:362:LEU:HD22	1.79	0.65
1:B:33:ALA:HB3	4:B:2005:HOH:O	1.98	0.64
1:A:199:ILE:HD12	1:A:202:VAL:HG21	1.81	0.63
1:B:42:LEU:HD13	1:B:85:LEU:HD13	1.81	0.62
1:A:40:ASN:ND2	4:A:2006:HOH:O	2.31	0.62
1:A:33:ALA:HB2	1:B:33:ALA:HB1	1.79	0.61
1:B:28:ARG:NH2	4:B:2004:HOH:O	2.31	0.61
1:A:355:TYR:CZ	1:A:359:LEU:HD11	2.35	0.60
1:A:388:PRO:C	1:B:204:SER:OG	2.39	0.60
1:A:30:GLU:O	1:A:34:LEU:HD13	2.01	0.59
1:A:29:GLY:HA3	1:B:36:ARG:HG2	1.85	0.59
1:B:309:HIS:CD2	4:B:2045:HOH:O	2.57	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:LYS:NZ	1:B:229:GLU:O	2.28	0.58
1:B:26:VAL:O	1:B:28:ARG:NH2	2.36	0.58
1:B:126:LEU:HD21	1:B:167:VAL:HG13	1.85	0.58
1:B:342:LEU:O	1:B:346:ASN:OD1	2.20	0.58
1:A:28:ARG:HG2	1:A:29:GLY:N	2.18	0.58
1:A:174:ARG:CD	4:A:2036:HOH:O	2.52	0.57
1:B:309:HIS:HD2	4:B:2045:HOH:O	1.86	0.57
1:A:33:ALA:HB2	1:B:33:ALA:HB2	1.86	0.57
1:A:389:HIS:HB3	1:B:204:SER:HB2	1.87	0.57
1:A:164:LEU:O	1:A:167:VAL:HG22	2.04	0.57
1:A:241:HIS:HE1	2:A:501:SO4:O4	1.86	0.56
1:B:409:SER:OG	4:B:2051:HOH:O	1.93	0.56
1:A:389:HIS:N	1:B:204:SER:OG	2.38	0.56
1:B:34:LEU:CD2	1:B:208:PHE:CZ	2.88	0.56
1:A:363:THR:HA	1:A:368:VAL:O	2.06	0.55
1:A:356:HIS:O	1:A:360:LYS:HG3	2.07	0.55
1:A:97:ALA:HB1	1:A:103:ILE:HG13	1.89	0.55
1:A:159:GLU:O	1:A:163:THR:HG23	2.07	0.55
1:B:31:ALA:N	4:B:2005:HOH:O	2.36	0.55
1:B:398:VAL:O	1:B:402:ILE:HG23	2.07	0.55
1:B:159:GLU:O	1:B:163:THR:HG23	2.07	0.55
1:B:75:ARG:NH1	4:B:2016:HOH:O	2.40	0.54
1:B:91:TYR:H	1:B:110:GLN:HE22	1.56	0.54
1:A:199:ILE:HD12	1:A:202:VAL:CG2	2.38	0.53
1:A:59:GLY:HA2	1:A:301:HIS:HB3	1.90	0.53
1:B:53:MET:HE2	1:B:206:ILE:HD13	1.91	0.53
1:A:313:ILE:HG13	1:A:337:TYR:CD1	2.44	0.52
1:A:243:GLU:OE2	4:A:2051:HOH:O	2.18	0.52
1:B:18:ASN:HD22	1:B:18:ASN:H	1.57	0.52
1:A:33:ALA:HB1	1:B:33:ALA:HB2	1.88	0.52
1:A:326:GLU:O	1:A:327:TRP:HB2	2.10	0.52
1:B:99:ASN:HD22	1:B:155:ARG:NH1	2.08	0.52
1:A:306:LEU:HB2	1:A:311:LEU:HD22	1.92	0.51
1:A:29:GLY:N	4:A:2005:HOH:O	2.44	0.51
1:B:402:ILE:CD1	1:B:406:LYS:HD2	2.41	0.50
1:A:104:LEU:O	1:A:108:VAL:HG13	2.11	0.50
1:B:341:SER:O	1:B:345:TYR:O	2.29	0.50
1:A:20:ILE:HG22	1:A:21:PRO:HD2	1.93	0.50
1:A:34:LEU:O	1:A:35:ALA:C	2.49	0.50
1:B:33:ALA:O	1:B:36:ARG:HB3	2.12	0.50
1:B:34:LEU:HD21	1:B:208:PHE:CZ	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:VAL:HG11	1:A:389:HIS:CB	2.42	0.49
1:A:337:TYR:O	1:A:341:SER:OG	2.21	0.49
1:A:138:HIS:O	1:A:179:ARG:HD3	2.13	0.49
1:A:53:MET:HE2	1:A:184:LEU:HD12	1.93	0.49
1:A:388:PRO:HB3	1:B:200:PRO:HB2	1.93	0.49
1:A:58:ILE:CG2	1:A:390:LEU:HD21	2.42	0.49
1:A:404:GLN:HE21	1:A:407:MET:HB3	1.78	0.48
1:A:18:ASN:HD22	1:A:19:TYR:N	2.11	0.48
1:A:334:ARG:HD3	4:A:2059:HOH:O	2.13	0.48
1:B:56:GLY:O	1:B:188:ASP:HA	2.13	0.48
1:A:308:ILE:HD12	1:A:309:HIS:CD2	2.49	0.48
1:B:34:LEU:HD23	1:B:208:PHE:CZ	2.49	0.48
1:B:53:MET:CE	1:B:206:ILE:HD13	2.44	0.47
1:B:240:ARG:NH2	2:B:501:SO4:S	2.87	0.47
1:A:331:GLY:O	1:A:334:ARG:HB3	2.13	0.47
1:B:190:ARG:NH1	1:B:365:LEU:O	2.47	0.47
1:A:189:VAL:HG11	1:A:389:HIS:HB3	1.96	0.47
1:A:300:THR:HB	1:A:304:GLU:OE2	2.15	0.47
1:B:99:ASN:OD1	1:B:102:THR:OG1	2.26	0.47
1:B:343:THR:OG1	1:B:344:MET:N	2.48	0.47
1:A:162:TYR:CD2	1:A:166:ARG:HD2	2.49	0.47
1:B:164:LEU:O	1:B:167:VAL:HG22	2.15	0.47
1:A:77:SER:HA	1:A:87:VAL:HG13	1.98	0.46
1:B:241:HIS:HE1	2:B:501:SO4:O1	1.97	0.46
1:A:174:ARG:HD2	4:A:2036:HOH:O	2.15	0.46
1:B:87:VAL:HB	1:B:139:TYR:HB2	1.97	0.46
1:B:346:ASN:OD1	1:B:346:ASN:N	2.48	0.46
1:B:240:ARG:NH2	2:B:501:SO4:O3	2.48	0.46
1:A:371:LYS:HB3	1:A:383:LEU:HB2	1.98	0.46
1:B:163:THR:HG22	1:B:170:GLU:OE2	2.16	0.46
1:A:214:ALA:HB1	1:A:257:GLY:HA3	1.98	0.45
1:A:306:LEU:O	1:A:406:LYS:NZ	2.49	0.45
1:B:204:SER:HB3	4:B:2031:HOH:O	2.15	0.45
1:B:294:GLU:H	1:B:294:GLU:CD	2.18	0.45
1:A:162:TYR:HD2	1:A:166:ARG:HD2	1.81	0.45
1:A:261:ARG:HH21	1:A:293:ASN:HB3	1.81	0.45
1:A:268:MET:HE1	1:A:292:GLU:HG3	1.99	0.45
1:B:57:SER:HB2	1:B:60:ARG:HG3	1.99	0.45
1:A:328:ILE:HD11	1:A:332:LEU:HD13	1.98	0.44
1:B:278:ARG:HG3	1:B:280:SER:O	2.16	0.44
1:A:24:LEU:HD13	1:A:27:ARG:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ASP:OD2	1:B:385:ARG:NE	2.50	0.44
1:A:33:ALA:O	1:A:36:ARG:HB3	2.17	0.44
1:A:29:GLY:CA	4:A:2005:HOH:O	2.65	0.44
1:A:311:LEU:HD12	1:A:399:VAL:HG13	2.00	0.44
1:A:190:ARG:NH1	1:A:365:LEU:O	2.49	0.43
1:A:303:LEU:HD23	1:A:306:LEU:HD12	2.00	0.43
1:B:342:LEU:O	1:B:343:THR:C	2.58	0.43
1:B:386:LEU:HD12	1:B:386:LEU:HA	1.84	0.42
1:A:342:LEU:HD13	1:A:348:LYS:HA	2.01	0.42
1:B:311:LEU:HD21	1:B:402:ILE:HD11	2.01	0.42
1:A:33:ALA:O	1:A:36:ARG:N	2.53	0.42
1:A:292:GLU:O	1:A:293:ASN:C	2.58	0.41
1:B:309:HIS:HE1	1:B:348:LYS:O	2.02	0.41
1:A:334:ARG:CD	4:A:2059:HOH:O	2.69	0.41
1:B:402:ILE:HD12	1:B:406:LYS:HD2	2.03	0.41
1:B:208:PHE:CD1	1:B:208:PHE:C	2.94	0.41
1:A:147:PHE:CE2	1:A:151:LEU:HD11	2.56	0.41
1:A:278:ARG:HG3	1:A:280:SER:O	2.21	0.41
1:B:326:GLU:O	1:B:327:TRP:HB2	2.20	0.41
1:A:365:LEU:HB3	1:A:367:LEU:HD13	2.02	0.41
1:B:88:LYS:NZ	1:B:111:THR:O	2.46	0.41
1:B:240:ARG:NH2	2:B:501:SO4:O1	2.54	0.41
1:A:30:GLU:HG2	4:A:2005:HOH:O	2.21	0.40
1:A:278:ARG:HH21	1:A:282:SER:HB3	1.87	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	384/412 (93%)	356 (93%)	21 (6%)	7 (2%)	8 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	392/412 (95%)	372 (95%)	16 (4%)	4 (1%)	15	23
All	All	776/824 (94%)	728 (94%)	37 (5%)	11 (1%)	11	15

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	342	LEU
1	B	343	THR
1	A	47	GLY
1	A	301	HIS
1	A	327	TRP
1	A	372	PRO
1	B	49	SER
1	B	345	TYR
1	A	86	THR
1	A	388	PRO
1	A	308	ILE

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	328/344 (95%)	284 (87%)	44 (13%)	4	4
1	B	332/344 (96%)	282 (85%)	50 (15%)	3	3
All	All	660/688 (96%)	566 (86%)	94 (14%)	3	4

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	28	ARG
1	A	30	GLU
1	A	36	ARG
1	A	39	LEU

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Mol	Chain	Res	Type
1	A	75	ARG
1	A	77	SER
1	A	87	VAL
1	A	116	GLN
1	A	118	ARG
1	A	133	LEU
1	A	141	LEU
1	A	149	SER
1	A	155	ARG
1	A	159	GLU
1	A	161	LEU
1	A	165	LEU
1	A	166	ARG
1	A	167	VAL
1	A	174	ARG
1	A	183	LEU
1	A	198	LYS
1	A	212	LEU
1	A	240	ARG
1	A	251	GLU
1	A	253	LYS
1	A	278	ARG
1	A	291	SER
1	A	293	ASN
1	A	300	THR
1	A	308	ILE
1	A	311	LEU
1	A	332	LEU
1	A	334	ARG
1	A	344	MET
1	A	353	THR
1	A	368	VAL
1	A	385	ARG
1	A	394	ARG
1	A	397	GLU
1	A	398	VAL
1	A	403	ILE
1	A	404	GLN
1	A	406	LYS
1	B	10	LYS
1	B	18	ASN
1	B	28	ARG

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Mol	Chain	Res	Type
1	B	30	GLU
1	B	41	ARG
1	B	60	ARG
1	B	87	VAL
1	B	116	GLN
1	B	131	ASP
1	B	133	LEU
1	B	150	MET
1	B	155	ARG
1	B	159	GLU
1	B	161	LEU
1	B	162	TYR
1	B	165	LEU
1	B	166	ARG
1	B	167	VAL
1	B	173	SER
1	B	174	ARG
1	B	183	LEU
1	B	187	SER
1	B	198	LYS
1	B	205	GLN
1	B	212	LEU
1	B	235	THR
1	B	236	VAL
1	B	240	ARG
1	B	251	GLU
1	B	291	SER
1	B	293	ASN
1	B	298	ILE
1	B	311	LEU
1	B	322	LEU
1	B	327	TRP
1	B	332	LEU
1	B	341	SER
1	B	342	LEU
1	B	345	TYR
1	B	346	ASN
1	B	347	VAL
1	B	348	LYS
1	B	360	LYS
1	B	365	LEU
1	B	367	LEU

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Mol	Chain	Res	Type
1	B	373	SER
1	B	394	ARG
1	B	402	ILE
1	B	404	GLN
1	B	407	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	110	GLN
1	A	116	GLN
1	A	241	HIS
1	A	293	ASN
1	A	404	GLN
1	B	18	ASN
1	B	110	GLN
1	B	241	HIS
1	B	293	ASN
1	B	329	ASN
1	B	389	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	SO4	A	501	-	4,4,4	0.18	0	6,6,6	0.64	0
2	SO4	B	500	-	4,4,4	0.34	0	6,6,6	0.44	0
2	SO4	A	500	-	4,4,4	0.16	0	6,6,6	0.86	0
3	ADP	A	700	-	24,29,29	1.28	5 (20%)	29,45,45	1.21	4 (13%)
3	ADP	B	700	-	24,29,29	1.03	2 (8%)	29,45,45	1.47	5 (17%)
2	SO4	B	501	-	4,4,4	0.29	0	6,6,6	0.36	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
3	ADP	A	700	-	-	2/12/32/32	0/3/3/3
3	ADP	B	700	-	-	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	700	ADP	O4'-C1'	2.67	1.44	1.41
3	A	700	ADP	C2-N3	2.66	1.36	1.32
3	B	700	ADP	C2-N3	2.53	1.36	1.32
3	B	700	ADP	O4'-C1'	2.40	1.44	1.41
3	A	700	ADP	C4-N3	-2.30	1.32	1.35
3	A	700	ADP	C5-C4	2.16	1.46	1.40
3	A	700	ADP	C2-N1	2.15	1.37	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	700	ADP	N3-C2-N1	-3.50	123.20	128.68
3	B	700	ADP	N3-C2-N1	-3.47	123.26	128.68
3	B	700	ADP	N6-C6-N1	3.13	125.07	118.57
3	B	700	ADP	C5-C6-N6	-3.11	115.62	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	700	ADP	N6-C6-N1	2.50	123.75	118.57
3	B	700	ADP	O4'-C4'-C5'	-2.37	101.58	109.37
3	A	700	ADP	PA-O3A-PB	-2.13	125.50	132.83
3	A	700	ADP	O2A-PA-O1A	2.13	122.78	112.24
3	B	700	ADP	O4'-C1'-C2'	-2.11	103.84	106.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	ADP	PA-O3A-PB-O2B
3	A	700	ADP	PA-O3A-PB-O3B

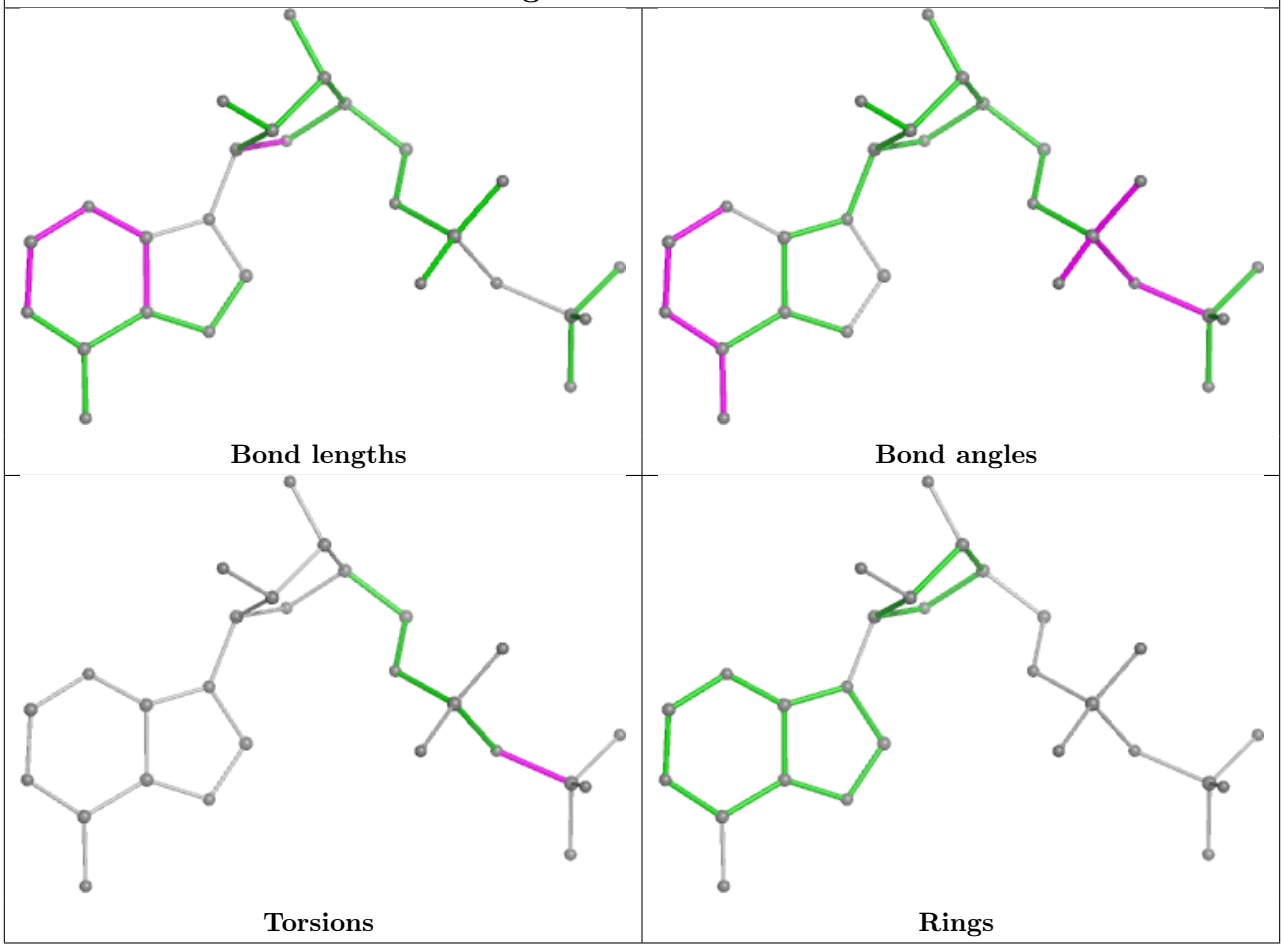
There are no ring outliers.

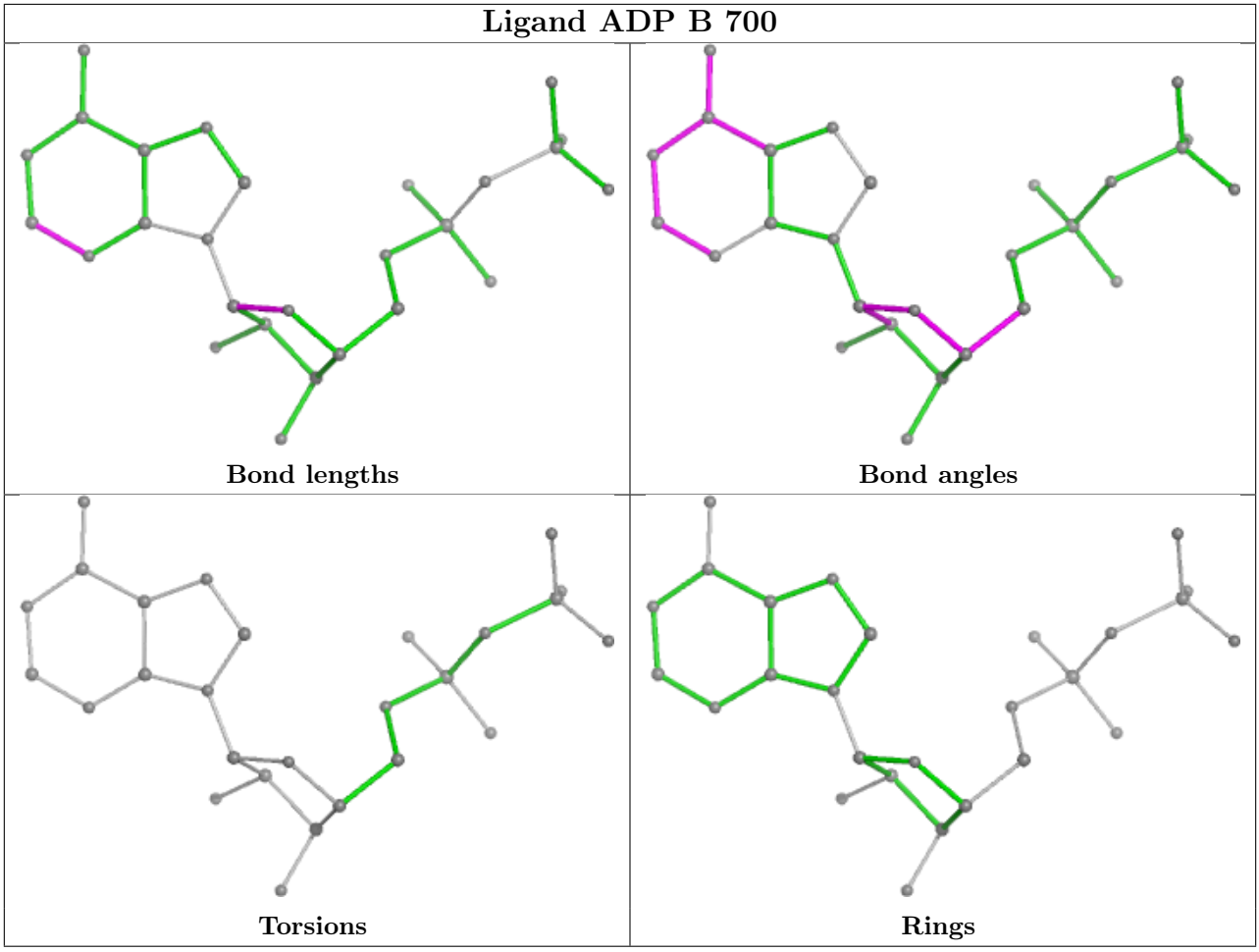
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	2	0
2	B	500	SO4	1	0
2	B	501	SO4	4	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 A 700





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	390/412 (94%)	1.16	94 (24%)	0	0	30, 38, 48, 56	0
1	B	396/412 (96%)	0.84	60 (15%)	2	1	29, 38, 49, 54	0
All	All	786/824 (95%)	1.00	154 (19%)	1	0	29, 38, 48, 56	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	SER	9.2
1	A	347	VAL	6.8
1	A	359	LEU	6.5
1	B	346	ASN	6.0
1	B	373	SER	6.0
1	B	372	PRO	5.9
1	A	394	ARG	5.9
1	A	405	ALA	5.8
1	A	372	PRO	5.8
1	A	305	ALA	5.7
1	A	301	HIS	5.7
1	A	397	GLU	5.6
1	A	362	LEU	5.5
1	A	396	ILE	5.4
1	A	368	VAL	5.4
1	B	277	GLY	5.4
1	A	314	LEU	5.4
1	A	346	ASN	5.1
1	A	365	LEU	5.0
1	A	342	LEU	5.0
1	A	404	GLN	5.0
1	B	279	ASP	4.9
1	A	366	GLY	4.9
1	A	312	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	317	ILE	4.6
1	A	320	ALA	4.6
1	A	197	GLU	4.5
1	A	373	SER	4.5
1	A	361	HIS	4.5
1	A	313	ILE	4.4
1	A	390	LEU	4.3
1	A	344	MET	4.3
1	A	408	ALA	4.2
1	A	46	ALA	4.2
1	A	352	TYR	4.1
1	B	153	SER	4.0
1	B	314	LEU	4.0
1	B	394	ARG	4.0
1	A	392	ALA	3.9
1	A	341	SER	3.9
1	A	363	THR	3.8
1	A	266	LEU	3.8
1	B	266	LEU	3.8
1	A	360	LYS	3.8
1	A	322	LEU	3.8
1	A	348	LYS	3.7
1	A	349	PRO	3.7
1	B	297	SER	3.7
1	A	399	VAL	3.7
1	B	342	LEU	3.6
1	B	245	ILE	3.5
1	A	354	GLN	3.5
1	A	302	GLU	3.4
1	A	235	THR	3.4
1	A	401	ASN	3.4
1	A	402	ILE	3.4
1	A	400	ASP	3.3
1	B	194	TYR	3.3
1	B	322	LEU	3.3
1	A	321	THR	3.3
1	B	294	GLU	3.3
1	A	306	LEU	3.2
1	A	398	VAL	3.2
1	A	224	LEU	3.2
1	A	381	THR	3.2
1	B	275	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	406	LYS	3.2
1	B	18	ASN	3.2
1	A	353	THR	3.2
1	B	155	ARG	3.2
1	A	340	ALA	3.1
1	A	28	ARG	3.1
1	A	407	MET	3.1
1	B	299	GLN	3.1
1	A	335	GLN	3.0
1	B	121	PRO	3.0
1	A	324	GLY	3.0
1	A	164	LEU	3.0
1	A	307	SER	3.0
1	B	381	THR	3.0
1	B	109	ARG	2.9
1	B	313	ILE	2.9
1	A	333	LEU	2.9
1	B	302	GLU	2.9
1	A	323	GLY	2.8
1	A	311	LEU	2.8
1	B	124	ASP	2.8
1	A	364	SER	2.8
1	B	129	LEU	2.8
1	A	40	ASN	2.8
1	B	326	GLU	2.8
1	B	164	LEU	2.7
1	B	397	GLU	2.7
1	B	112	GLY	2.7
1	B	278	ARG	2.7
1	B	312	ILE	2.7
1	A	319	GLU	2.6
1	B	262	ALA	2.6
1	B	359	LEU	2.6
1	A	153	SER	2.6
1	B	235	THR	2.6
1	A	308	ILE	2.6
1	A	388	PRO	2.6
1	B	54	ILE	2.6
1	B	269	ALA	2.5
1	A	154	PRO	2.5
1	A	269	ALA	2.5
1	B	46	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	155	ARG	2.5
1	B	295	ALA	2.5
1	B	95	PHE	2.4
1	A	356	HIS	2.4
1	B	281	LEU	2.4
1	A	304	GLU	2.4
1	A	327	TRP	2.4
1	A	367	LEU	2.4
1	A	395	LEU	2.4
1	A	393	ASP	2.3
1	A	223	ILE	2.3
1	A	370	ALA	2.3
1	A	383	LEU	2.3
1	B	154	PRO	2.3
1	A	245	ILE	2.3
1	A	386	LEU	2.3
1	B	99	ASN	2.3
1	A	281	LEU	2.3
1	B	224	LEU	2.3
1	A	161	LEU	2.3
1	B	276	MET	2.2
1	A	293	ASN	2.2
1	B	107	ILE	2.2
1	B	212	LEU	2.2
1	A	103	ILE	2.2
1	B	232	LEU	2.2
1	A	310	GLU	2.2
1	B	347	VAL	2.2
1	B	317	ILE	2.2
1	B	303	LEU	2.1
1	B	118	ARG	2.1
1	B	348	LYS	2.1
1	A	389	HIS	2.1
1	A	403	ILE	2.1
1	B	15	PHE	2.1
1	A	129	LEU	2.1
1	A	270	CYS	2.1
1	B	242	LEU	2.1
1	B	149	SER	2.1
1	B	390	LEU	2.1
1	A	391	PRO	2.0
1	A	286	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	116	GLN	2.0
1	B	368	VAL	2.0
1	B	103	ILE	2.0
1	A	369	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

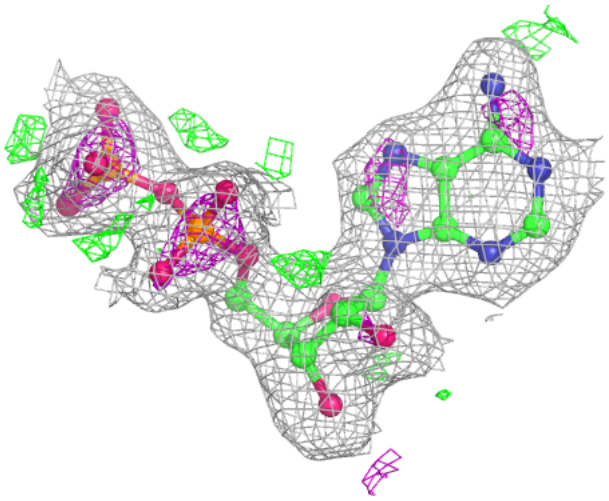
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

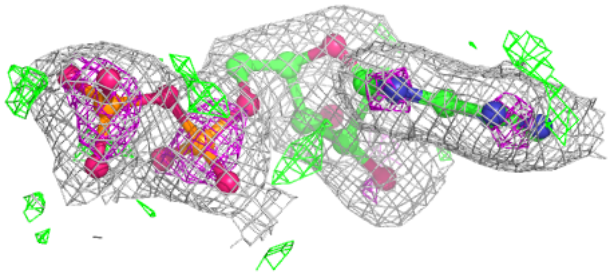
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ADP	A	700	27/27	0.96	0.12	18,21,24,27	0
3	ADP	B	700	27/27	0.97	0.10	22,25,30,33	0
2	SO4	A	501	5/5	0.98	0.23	46,49,51,53	0
2	SO4	B	501	5/5	0.98	0.24	46,46,48,49	0
2	SO4	B	500	5/5	0.99	0.12	30,32,34,35	0
2	SO4	A	500	5/5	0.99	0.12	31,34,36,40	0

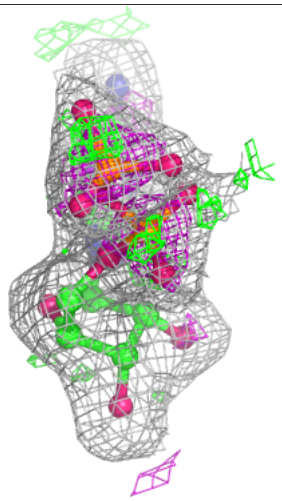
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 700:

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

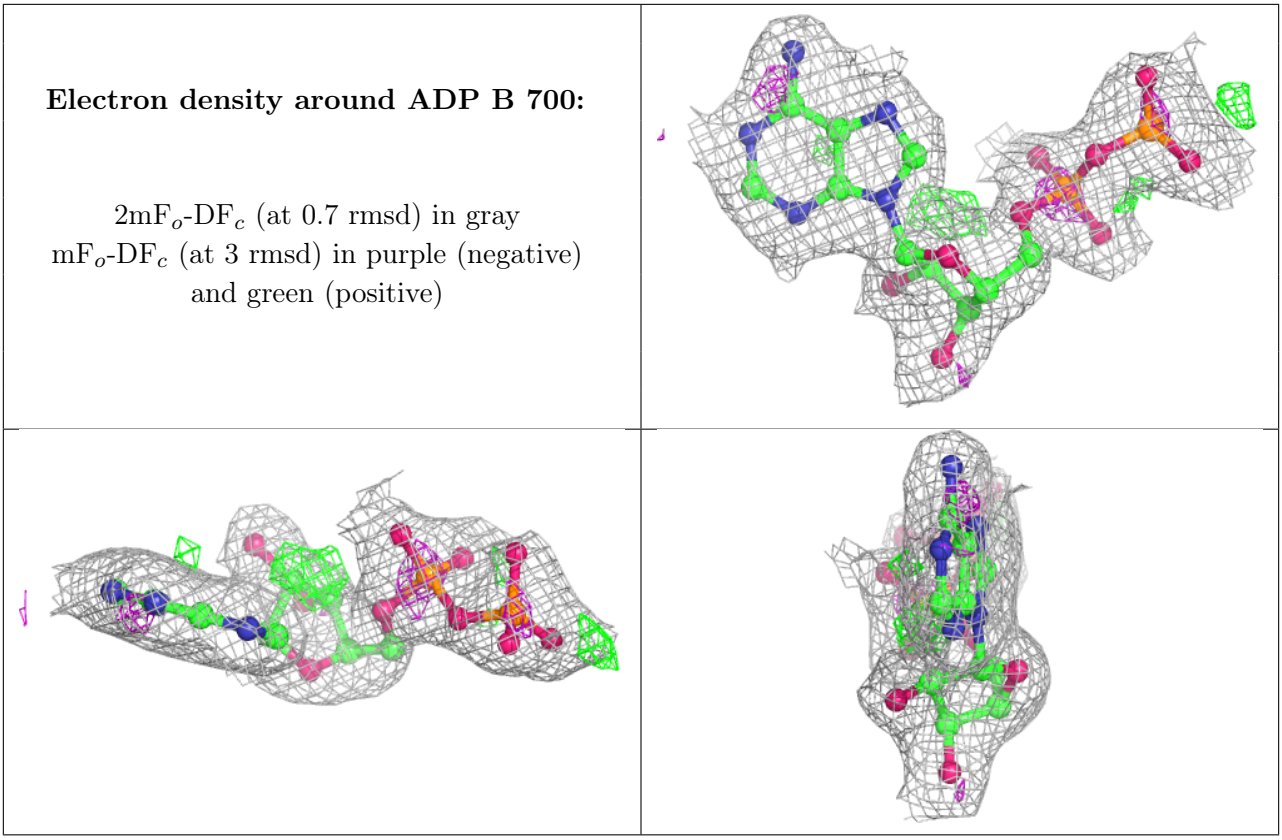






Electron density around ADP B 700:

$2mF_o$-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.