



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:13 AM UTC

PDB ID : 4IOL / pdb_00004iol
Title : N10-formyltetrahydrofolate synthetase from *Moorella thermoacetica* with ADP/ZD9 and XPO
Authors : Stec, B.
Deposited on : 2013-01-08
Resolution : 2.56 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

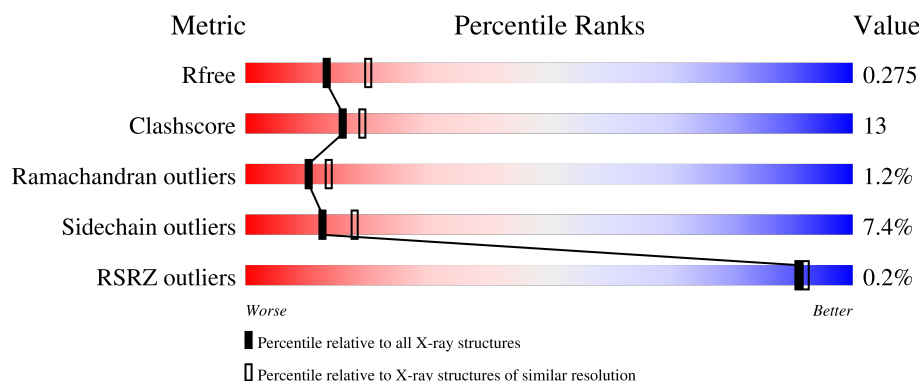
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	559	 77% 21% .
1	B	559	 60% 38% .

2 Entry composition [i](#)

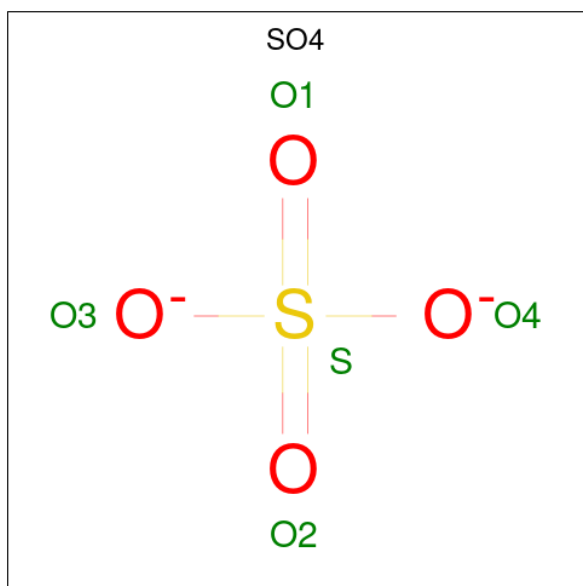
There are 6 unique types of molecules in this entry. The entry contains 8654 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	557	Total	C	N	O	S	0	0	0
			4195	2661	721	792	21			
1	B	557	Total	C	N	O	S	0	0	0
			4195	2661	721	792	21			

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



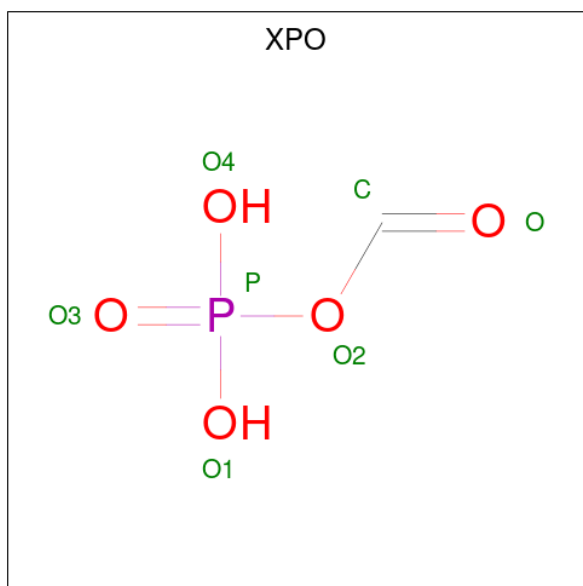
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- # ADP

Chemical structure of ZD9, a pyrimidine derivative. The structure features a pyrimidine ring with a carbonyl group at C1 (O7), an NH group at N2, and an NH group at N4. A side chain is attached at C5, consisting of a methylene group (C12) linked to an NH group (N13), which is further linked to a propyne group (C14-C15-C16). The atoms are color-coded: carbons are green, nitrogens are blue, and oxygen is red.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			18	14	3	1		

- Molecule 5 is formyl phosphate (CCD ID: XPO) (formula: $\text{CH}_3\text{O}_5\text{P}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	1
			7	1	5	1		

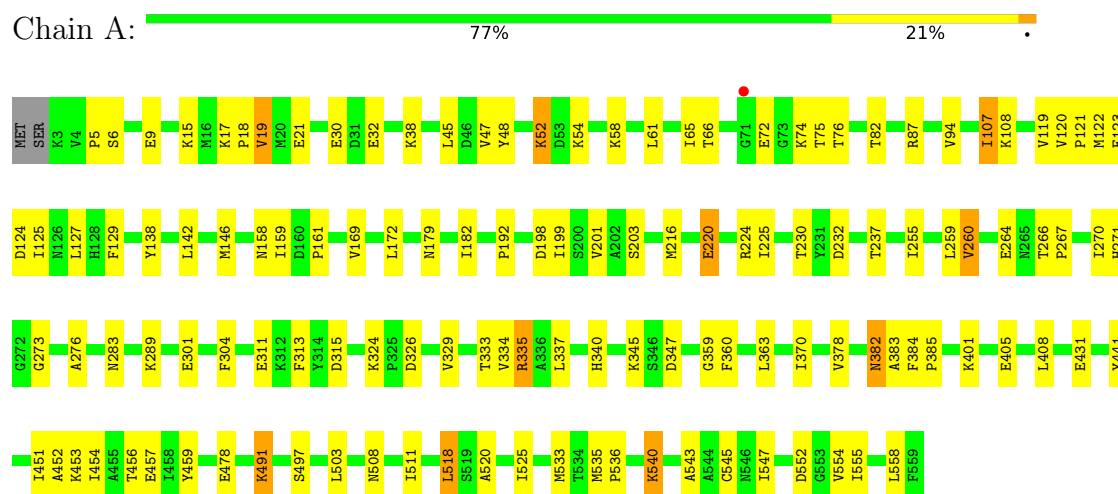
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	118	Total	O	0	0
			118	118		
6	B	47	Total	O	0	0
			47	47		

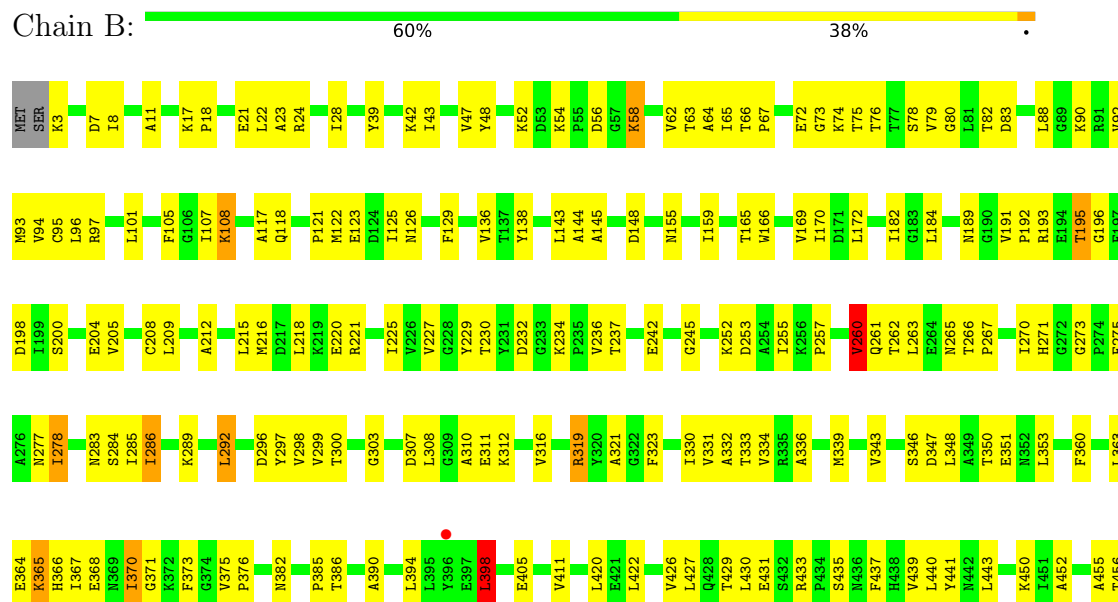
3 Residue-property plots

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



• Molecule 1: Formate--tetrahydrofolate ligase



E457	I458	Y459		D462	G463	V464		E469		G481	Y482	G483		V487		A490	K491	T492		S495	F496	S497	D498	D499	M500	T501	K502		R507	N508		I511		A522		I525	V526	P527	I528		I532	M533	T534		K540	R541	P542		C545		F559
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	160.37Å 160.37Å 258.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	122.30 – 2.56 122.30 – 2.56	Depositor EDS
% Data completeness (in resolution range)	88.2 (122.30-2.56) 88.2 (122.30-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.57Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.190 , 0.279 0.190 , 0.275	Depositor DCC
R_{free} test set	1822 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8654	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: ZD9, SO4, ADP, XPO

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	0.84	0/4266	1.04	4/5778 (0.1%)
1	B	0.75	0/4266	1.06	8/5778 (0.1%)
All	All	0.80	0/8532	1.05	12/11556 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	458	ILE	N-CA-C	6.54	117.53	111.45
1	B	191	VAL	CA-C-N	-6.03	113.55	119.76
1	B	191	VAL	C-N-CA	-6.03	113.55	119.76
1	B	204	GLU	N-CA-C	-5.77	105.12	111.82
1	B	457	GLU	N-CA-C	5.60	117.07	111.07
1	A	451	ILE	N-CA-C	5.53	115.73	110.42
1	A	54	LYS	CA-C-N	-5.53	114.89	120.31
1	A	54	LYS	C-N-CA	-5.53	114.89	120.31
1	B	296	ASP	N-CA-C	-5.44	106.81	113.50
1	B	398	LEU	N-CA-C	5.25	117.75	111.71
1	A	47	VAL	CB-CA-C	-5.19	105.32	111.97
1	B	39	TYR	N-CA-C	5.07	119.19	112.30

There are no chirality outliers.

There are no planarity outliers.

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	4195	0	4278	82	0
1	B	4195	0	4278	149	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
3	A	27	0	12	5	0
3	B	27	0	12	2	0
4	A	18	0	15	5	0
5	A	7	0	3	1	0
6	A	118	0	0	7	0
6	B	47	0	0	6	0
All	All	8654	0	8598	225	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 13.

All (225) 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:308:LEU:O	1:B:312:LYS:HG3	1.51	1.10
1:B:8:ILE:HA	1:B:122:MET:HE1	1.38	1.05
1:B:376:PRO:HD3	1:B:435:SER:HB2	1.44	0.98
1:A:405:GLU:HG2	6:A:791:HOH:O	1.66	0.96
1:B:422:LEU:O	1:B:426:VAL:HG23	1.73	0.88
1:A:383:ALA:HB2	1:A:408:LEU:HD11	1.57	0.86
1:B:126:ASN:HD22	1:B:559:PHE:HE1	1.22	0.86
1:A:491:LYS:HE3	1:A:497:SER:O	1.77	0.83
1:B:360:PHE:CE1	1:B:364:GLU:HB2	2.15	0.81
1:B:376:PRO:HD3	1:B:435:SER:CB	2.12	0.80
1:B:125:ILE:HD13	1:B:129:PHE:CE1	2.17	0.79
1:B:42:LYS:HD3	1:B:253:ASP:O	1.83	0.79
1:B:343:VAL:HG13	1:B:347:ASP:HB2	1.69	0.72
1:B:195:THR:OG1	1:B:196:GLY:N	2.22	0.72
1:B:126:ASN:ND2	1:B:559:PHE:HE1	1.87	0.72
1:B:455:ALA:HA	1:B:459:TYR:HD2	1.54	0.71
1:B:353:LEU:HD21	1:B:390:ALA:HB1	1.71	0.71
1:B:308:LEU:O	1:B:312:LYS:CG	2.35	0.70
1:B:339:MET:HG3	1:B:348:LEU:HD21	1.75	0.69
1:B:138:TYR:HB2	6:B:739:HOH:O	1.93	0.68
1:B:78:SER:O	1:B:299:VAL:HG11	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:MET:HG2	1:B:267:PRO:HB2	1.74	0.67
1:B:455:ALA:HA	1:B:459:TYR:CD2	2.29	0.67
1:B:429:THR:HG23	1:B:433:ARG:HD3	1.76	0.66
1:B:129:PHE:HD2	6:B:740:HOH:O	1.79	0.66
1:B:23:ALA:HA	1:B:28:ILE:HD12	1.78	0.66
1:A:385:PRO:HD3	4:A:603[B]:ZD9:H39	1.77	0.66
1:B:262:THR:HG22	1:B:263:LEU:N	2.11	0.65
1:B:330:ILE:HD11	1:B:370:ILE:HD13	1.78	0.65
1:A:383:ALA:HB2	1:A:408:LEU:CD1	2.28	0.64
1:B:8:ILE:CD1	1:B:122:MET:HE3	2.28	0.64
1:B:360:PHE:HE1	1:B:364:GLU:HB2	1.62	0.64
1:B:427:LEU:O	1:B:431:GLU:HG2	1.98	0.64
1:B:495:SER:OG	1:B:502:LYS:O	2.16	0.63
1:B:373:PHE:CE2	1:B:440:LEU:HB2	2.33	0.62
1:A:199:ILE:N	1:A:535:MET:HE2	2.15	0.62
1:B:136:VAL:HG13	1:B:205:VAL:HG12	1.81	0.62
1:A:337:LEU:O	1:A:359:GLY:HA3	2.00	0.61
1:B:364:GLU:O	1:B:368:GLU:HG3	2.00	0.61
1:B:271:HIS:ND1	1:B:284:SER:OG	2.29	0.61
1:B:330:ILE:CD1	1:B:370:ILE:HD13	2.31	0.61
1:A:87:ARG:HH21	1:A:264:GLU:CD	2.09	0.60
1:A:6:SER:OG	1:A:9:GLU:HG3	2.01	0.60
1:A:543:ALA:O	1:A:547:ILE:HG13	2.01	0.60
1:B:8:ILE:HD12	1:B:122:MET:CE	2.32	0.59
1:A:216:MET:HG2	6:A:806:HOH:O	2.02	0.59
1:B:11:ALA:HB2	1:B:118:GLN:OE1	2.03	0.59
1:B:286:ILE:HD12	6:B:728:HOH:O	2.01	0.59
1:A:179:ASN:ND2	1:B:189:ASN:HD22	2.01	0.59
1:B:182:ILE:O	1:B:192:PRO:HA	2.03	0.59
1:B:67:PRO:HD3	6:B:743:HOH:O	2.04	0.58
1:A:61:LEU:HD13	1:A:313:PHE:CD2	2.39	0.58
1:B:278:ILE:HG23	1:B:532:ILE:HG21	1.86	0.58
1:B:440:LEU:HG	1:B:440:LEU:O	2.03	0.58
1:B:58:LYS:HD3	1:B:430:LEU:HD22	1.84	0.58
1:B:169:VAL:HB	1:B:200:SER:HA	1.85	0.57
1:B:376:PRO:CD	1:B:435:SER:CB	2.81	0.57
1:A:120:VAL:HB	1:A:121:PRO:HA	1.87	0.57
1:B:8:ILE:HD13	1:B:122:MET:HE3	1.87	0.57
1:B:376:PRO:CD	1:B:435:SER:HB2	2.29	0.56
1:B:260:VAL:HG21	1:B:270:ILE:HD12	1.86	0.56
1:B:289:LYS:HB3	1:B:323:PHE:HZ	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLY:HA2	2:B:601:SO4:O2	2.06	0.56
1:B:363:LEU:O	1:B:367:ILE:HG13	2.05	0.56
1:A:74:LYS:H	3:A:602[A]:ADP:PB	2.29	0.56
1:B:121:PRO:O	1:B:125:ILE:HG12	2.06	0.56
1:B:292:LEU:HD23	1:B:298:VAL:HG21	1.88	0.55
1:B:88:LEU:HD21	1:B:420:LEU:CD2	2.36	0.55
1:A:452:ALA:O	1:A:456:THR:HG23	2.06	0.55
1:A:19:VAL:HG22	1:A:38:LYS:O	2.07	0.55
1:B:79:VAL:HG11	1:B:117:ALA:O	2.06	0.55
1:A:172:LEU:HG	1:B:138:TYR:CZ	2.42	0.55
1:B:278:ILE:CG2	1:B:532:ILE:HG21	2.37	0.55
1:A:198:ASP:C	1:A:535:MET:HE2	2.32	0.54
1:A:220:GLU:OE1	1:A:224:ARG:NH2	2.41	0.54
1:A:453:LYS:HE2	6:A:710:HOH:O	2.07	0.54
1:B:62:VAL:HG21	1:B:78:SER:HA	1.90	0.53
1:A:311:GLU:OE1	1:A:315:ASP:OD1	2.27	0.53
1:B:65:ILE:HA	1:B:366:HIS:CD2	2.44	0.53
1:B:125:ILE:HD12	1:B:270:ILE:HD13	1.91	0.53
1:B:166:TRP:HB2	1:B:227:VAL:HA	1.91	0.53
1:B:394:LEU:O	1:B:398:LEU:HD12	2.09	0.52
1:A:179:ASN:HD22	1:B:189:ASN:HD22	1.58	0.52
1:B:143:LEU:HD23	1:B:166:TRP:CE2	2.44	0.52
1:A:545:CYS:HA	1:B:242:GLU:O	2.09	0.52
1:B:80:GLY:HA3	1:B:411:VAL:HG11	1.92	0.52
1:B:215:LEU:HA	1:B:255:ILE:CD1	2.39	0.52
1:B:95:CYS:O	1:B:96:LEU:HD23	2.10	0.52
1:B:83:ASP:OD1	1:B:262:THR:HG21	2.10	0.52
1:B:8:ILE:HD12	1:B:122:MET:HE3	1.92	0.52
1:B:277:ASN:OD1	1:B:278:ILE:N	2.39	0.52
1:A:142:LEU:O	1:A:146:MET:HG3	2.10	0.51
1:B:143:LEU:HD23	1:B:166:TRP:NE1	2.26	0.51
1:B:343:VAL:HG13	1:B:347:ASP:CB	2.39	0.51
1:B:225:ILE:O	1:B:237:THR:HA	2.11	0.51
1:B:67:PRO:HA	1:B:72:GLU:CD	2.36	0.51
1:B:63:THR:O	1:B:331:VAL:HG23	2.12	0.50
1:B:75:THR:O	1:B:76:THR:C	2.54	0.50
1:A:75:THR:HA	1:A:301:GLU:OE2	2.11	0.50
1:B:221:ARG:NH1	1:B:522:ALA:O	2.43	0.50
1:B:229:TYR:CD1	1:B:229:TYR:N	2.78	0.50
1:B:497:SER:HA	1:B:511:ILE:HD11	1.92	0.50
1:B:441:TYR:CD1	1:B:450:LYS:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:PRO:HD3	4:A:603[B]:ZD9:C39	2.42	0.49
1:B:88:LEU:HD21	1:B:420:LEU:HD23	1.95	0.49
1:B:17:LYS:O	1:B:18:PRO:C	2.53	0.49
1:B:307:ASP:N	1:B:307:ASP:OD1	2.45	0.49
1:A:75:THR:N	5:A:604[C]:XPO:O2	2.46	0.49
1:A:385:PRO:HG3	4:A:603[B]:ZD9:H39	1.95	0.48
1:B:92:VAL:HA	1:B:297:TYR:O	2.14	0.48
1:B:94:VAL:HA	1:B:299:VAL:O	2.13	0.48
1:B:285:ILE:HD13	1:B:321:ALA:HB2	1.95	0.48
1:A:335:ARG:HG3	6:A:808:HOH:O	2.12	0.48
1:A:276:ALA:HB3	1:A:304:PHE:CD2	2.49	0.48
1:A:82:THR:HG22	1:A:266:THR:HG21	1.96	0.48
1:A:125:ILE:HA	1:A:129:PHE:CD1	2.48	0.48
1:A:385:PRO:CD	4:A:603[B]:ZD9:H39	2.43	0.48
1:B:22:LEU:HD11	1:B:261:GLN:NE2	2.29	0.48
1:A:453:LYS:O	1:A:457:GLU:HB2	2.14	0.48
1:B:8:ILE:CD1	1:B:122:MET:CE	2.91	0.48
1:B:48:TYR:HE1	6:B:729:HOH:O	1.97	0.48
1:A:169:VAL:HG11	1:A:203:SER:HB2	1.95	0.47
1:B:262:THR:HG22	1:B:263:LEU:H	1.77	0.47
1:A:547:ILE:O	1:B:245:GLY:HA3	2.14	0.47
1:B:74:LYS:O	1:B:78:SER:HB2	2.14	0.47
1:B:283:ASN:HD21	1:B:300:THR:HG1	1.60	0.47
1:A:61:LEU:HD13	1:A:313:PHE:CE2	2.49	0.47
1:A:17:LYS:O	1:A:18:PRO:C	2.55	0.47
1:A:552:ASP:HB2	1:A:554:VAL:HG23	1.96	0.47
1:B:79:VAL:CG1	1:B:117:ALA:O	2.62	0.47
1:B:101:LEU:CD2	1:B:105:PHE:HE1	2.28	0.47
1:B:481:GLY:C	1:B:483:GLY:H	2.23	0.47
1:A:30:GLU:C	1:A:32:GLU:H	2.23	0.46
1:A:82:THR:OG1	1:A:94:VAL:HB	2.16	0.46
1:A:182:ILE:O	1:A:192:PRO:HA	2.14	0.46
1:B:107:ILE:O	1:B:108:LYS:HB2	2.15	0.46
1:A:382:ASN:ND2	6:A:813:HOH:O	2.48	0.46
1:B:208:CYS:O	1:B:209:LEU:C	2.59	0.46
1:A:533:MET:HE3	1:A:536:PRO:HG3	1.97	0.46
1:B:169:VAL:HA	1:B:198:ASP:O	2.16	0.46
1:B:370:ILE:O	1:B:371:GLY:C	2.58	0.46
1:A:72:GLU:HB2	3:A:602[A]:ADP:O2B	2.16	0.46
1:B:159:ILE:HA	1:B:230:THR:HA	1.97	0.46
1:B:333:THR:HB	1:B:336:ALA:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:PRO:HA	1:B:72:GLU:OE2	2.15	0.46
1:A:441:TYR:CE2	1:A:454:ILE:HD11	2.52	0.45
1:B:198:ASP:OD1	1:B:534:THR:OG1	2.34	0.45
1:A:48:TYR:CD1	1:A:289:LYS:HG3	2.51	0.45
1:A:382:ASN:OD1	3:A:602[A]:ADP:N7	2.50	0.45
1:A:459:TYR:HD2	1:A:511:ILE:HD11	1.82	0.45
1:B:56:ASP:HB3	1:B:292:LEU:HD13	1.97	0.45
1:B:262:THR:CG2	1:B:263:LEU:N	2.80	0.45
1:B:310:ALA:O	1:B:311:GLU:C	2.60	0.45
1:A:45:LEU:HD23	6:A:805:HOH:O	2.15	0.45
1:B:82:THR:HG21	1:B:94:VAL:HB	1.98	0.45
1:B:216:MET:HE2	1:B:216:MET:HA	1.97	0.45
1:B:490:ALA:HB3	1:B:528:ILE:HA	1.99	0.45
1:B:382:ASN:HD21	3:B:602:ADP:HN61	1.65	0.45
1:A:459:TYR:CD2	1:A:511:ILE:HD11	2.52	0.45
1:B:462:ASP:OD2	1:B:508:ASN:HA	2.16	0.45
1:B:376:PRO:CD	1:B:435:SER:HB3	2.46	0.44
1:B:441:TYR:CE1	1:B:450:LYS:HD3	2.52	0.44
1:A:119:VAL:HG11	1:A:270:ILE:HD11	1.99	0.44
1:A:124:ASP:O	1:A:129:PHE:HA	2.16	0.44
1:A:271:HIS:O	1:A:283:ASN:HB2	2.17	0.44
1:B:144:ALA:O	1:B:145:ALA:C	2.61	0.44
1:B:437:PHE:CD1	1:B:437:PHE:C	2.96	0.44
1:B:21:GLU:O	1:B:24:ARG:HB2	2.18	0.44
1:A:201:VAL:HB	1:A:273:GLY:O	2.17	0.44
1:A:138:TYR:CZ	1:B:172:LEU:HG	2.52	0.44
1:B:339:MET:CG	1:B:348:LEU:HD21	2.47	0.44
1:B:17:LYS:HG3	1:B:265:ASN:CG	2.43	0.44
1:B:507:ARG:O	1:B:508:ASN:HB2	2.17	0.44
1:A:124:ASP:HB3	6:A:758:HOH:O	2.17	0.43
1:B:499:ASP:HB3	1:B:502:LYS:HG3	2.00	0.43
1:A:385:PRO:CG	4:A:603[B]:ZD9:H39	2.49	0.43
1:B:292:LEU:HD23	1:B:298:VAL:CG2	2.48	0.43
1:A:518:LEU:HD21	1:A:520:ALA:HB2	1.99	0.43
1:B:107:ILE:HG13	1:B:108:LYS:H	1.84	0.43
1:A:87:ARG:NH2	1:A:264:GLU:OE2	2.49	0.43
1:A:138:TYR:CZ	1:B:101:LEU:HD13	2.53	0.43
1:B:125:ILE:HD13	1:B:129:PHE:CD1	2.54	0.43
1:A:333:THR:HG22	1:A:382:ASN:HB3	2.01	0.43
1:A:334:VAL:O	1:A:335:ARG:C	2.62	0.43
1:A:555:ILE:HG21	1:A:558:LEU:HD23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:602[A]:ADP:O1A	3:A:602[A]:ADP:H8	2.01	0.43
1:B:375:VAL:HA	1:B:376:PRO:HD3	1.90	0.43
1:A:329:VAL:HA	1:A:378:VAL:O	2.19	0.43
1:A:540:LYS:H	1:A:540:LYS:HG3	1.56	0.43
1:A:382:ASN:HD22	1:A:382:ASN:HA	1.68	0.42
1:B:73:GLY:HA2	3:B:602:ADP:O5'	2.18	0.42
1:A:360:PHE:O	1:A:363:LEU:N	2.53	0.42
1:B:79:VAL:O	1:B:82:THR:HB	2.18	0.42
1:B:90:LYS:HB3	1:B:297:TYR:CD2	2.53	0.42
1:A:123:GLU:O	1:A:127:LEU:HG	2.19	0.42
1:B:8:ILE:CA	1:B:122:MET:HE1	2.29	0.42
1:B:365:LYS:HG3	1:B:496:PHE:CE1	2.55	0.42
1:B:260:VAL:HB	1:B:261:GLN:H	1.68	0.42
1:A:74:LYS:HB3	3:A:602[A]:ADP:O1B	2.19	0.42
1:A:255:ILE:O	1:A:255:ILE:HG13	2.20	0.42
1:B:464:VAL:HA	1:B:511:ILE:O	2.20	0.42
1:B:319:ARG:HE	1:B:443:LEU:HD21	1.85	0.41
1:A:266:THR:CG2	1:A:267:PRO:HD2	2.50	0.41
1:B:155:ASN:N	6:B:706:HOH:O	2.52	0.41
1:B:236:VAL:HG12	1:B:237:THR:N	2.34	0.41
1:B:257:PRO:HA	1:B:271:HIS:CD2	2.56	0.41
1:A:52:LYS:HB3	1:A:52:LYS:HE2	1.73	0.41
1:B:64:ALA:HA	1:B:331:VAL:H	1.86	0.41
1:B:125:ILE:CD1	1:B:129:PHE:CE1	2.97	0.41
1:B:525:ILE:HG22	1:B:527:PRO:HD3	2.02	0.41
1:B:212:ALA:HB2	1:B:218:LEU:HD13	2.03	0.41
1:A:124:ASP:O	1:A:129:PHE:CA	2.69	0.41
1:A:259:LEU:O	1:A:260:VAL:HG13	2.20	0.41
1:B:184:LEU:CD2	1:B:192:PRO:HB3	2.51	0.41
1:B:452:ALA:O	1:B:456:THR:HG22	2.21	0.41
1:A:66:THR:HB	1:A:340:HIS:CE1	2.56	0.40
1:A:159:ILE:O	1:A:161:PRO:HD3	2.21	0.40
1:B:43:ILE:CG2	1:B:47:VAL:HG21	2.50	0.40
1:B:331:VAL:HG12	1:B:332:ALA:H	1.86	0.40
1:A:158:ASN:O	1:A:230:THR:HA	2.21	0.40
1:A:58:LYS:HA	1:A:326:ASP:OD2	2.21	0.40
1:A:225:ILE:O	1:A:237:THR:HA	2.21	0.40
1:B:148:ASP:CG	1:B:193:ARG:HH21	2.28	0.40
1:B:542:PRO:HD2	1:B:545:CYS:SG	2.61	0.40
1:A:61:LEU:HD13	1:A:313:PHE:CG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	555/559 (99%)	503 (91%)	46 (8%)	6 (1%)	11	15
1	B	555/559 (99%)	475 (86%)	73 (13%)	7 (1%)	9	12
All	All	1110/1118 (99%)	978 (88%)	119 (11%)	13 (1%)	10	14

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	260	VAL
1	B	108	LYS
1	B	252	LYS
1	A	107	ILE
1	A	335	ARG
1	A	122	MET
1	B	7	ASP
1	A	5	PRO
1	B	492	THR
1	B	273	GLY
1	B	385	PRO
1	B	260	VAL
1	A	65	ILE

5.3.2 Protein sidechains

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	439/441 (100%)	415 (94%)	24 (6%)	19	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	439/441 (100%)	398 (91%)	41 (9%)	8 11
All	All	878/882 (100%)	813 (93%)	65 (7%)	13 18

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LYS
1	A	19	VAL
1	A	21	GLU
1	A	52	LYS
1	A	76	THR
1	A	107	ILE
1	A	108	LYS
1	A	220	GLU
1	A	232	ASP
1	A	324	LYS
1	A	345	LYS
1	A	347	ASP
1	A	370	ILE
1	A	382	ASN
1	A	384	PHE
1	A	401	LYS
1	A	431	GLU
1	A	478	GLU
1	A	491	LYS
1	A	503	LEU
1	A	508	ASN
1	A	518	LEU
1	A	525	ILE
1	A	540	LYS
1	B	3	LYS
1	B	52	LYS
1	B	54	LYS
1	B	58	LYS
1	B	66	THR
1	B	97	ARG
1	B	123	GLU
1	B	165	THR
1	B	170	ILE
1	B	195	THR
1	B	220	GLU
1	B	232	ASP

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Mol	Chain	Res	Type
1	B	234	LYS
1	B	260	VAL
1	B	266	THR
1	B	275	PHE
1	B	278	ILE
1	B	286	ILE
1	B	292	LEU
1	B	316	VAL
1	B	319	ARG
1	B	334	VAL
1	B	346	SER
1	B	350	THR
1	B	351	GLU
1	B	365	LYS
1	B	370	ILE
1	B	386	THR
1	B	398	LEU
1	B	405	GLU
1	B	439	VAL
1	B	464	VAL
1	B	469	GLU
1	B	487	VAL
1	B	498	ASP
1	B	500	MET
1	B	507	ARG
1	B	526	VAL
1	B	533	MET
1	B	540	LYS
1	B	541	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	ASN
1	A	179	ASN
1	A	283	ASN
1	A	382	ASN
1	A	438	HIS
1	A	484	ASN
1	B	12	GLN
1	B	29	GLN
1	B	126	ASN

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Mol	Chain	Res	Type
1	B	149	ASN
1	B	153	GLN
1	B	158	ASN
1	B	179	ASN
1	B	265	ASN
1	B	382	ASN
1	B	438	HIS
1	B	465	ASN

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](#)

8 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
4	ZD9	A	603[B]	-	17,19,19	1.60	3 (17%)	23,26,26	1.98	6 (26%)
2	SO4	B	601	-	4,4,4	0.49	0	6,6,6	0.23	0
3	ADP	A	602[A]	-	28,29,29	1.44	4 (14%)	43,45,45	1.90	10 (23%)
5	XPO	A	604[C]	-	5,6,6	3.58	3 (60%)	6,8,8	0.79	0
3	ADP	B	602	-	28,29,29	1.56	5 (17%)	43,45,45	1.84	10 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	603	-	4,4,4	0.48	0	6,6,6	0.22	0
2	SO4	A	605	-	4,4,4	0.53	0	6,6,6	0.37	0
2	SO4	A	601	-	4,4,4	0.60	0	6,6,6	0.55	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	ZD9	A	603[B]	-	-	0/3/5/5	0/2/2/2
3	ADP	B	602	-	-	4/16/32/32	0/3/3/3
3	ADP	A	602[A]	-	-	5/16/32/32	0/3/3/3
5	XPO	A	604[C]	-	-	0/0/4/4	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	604[C]	XPO	P-O2	6.43	1.71	1.59
4	A	603[B]	ZD9	C12-N13	-5.20	1.37	1.45
3	A	602[A]	ADP	C5-C4	4.62	1.47	1.39
3	B	602	ADP	C5-C4	4.53	1.47	1.39
3	B	602	ADP	PA-O3A	4.02	1.63	1.59
5	A	604[C]	XPO	P-O3	3.87	1.62	1.50
3	A	602[A]	ADP	C5-C6	2.98	1.49	1.41
3	A	602[A]	ADP	PA-O3A	2.94	1.62	1.59
3	B	602	ADP	C5-N7	-2.45	1.34	1.39
3	B	602	ADP	C8-N7	2.44	1.36	1.31
3	B	602	ADP	C5-C6	2.34	1.47	1.41
3	A	602[A]	ADP	C8-N7	2.25	1.36	1.31
5	A	604[C]	XPO	P-O4	2.09	1.62	1.54
4	A	603[B]	ZD9	C3-N4	2.06	1.36	1.31
4	A	603[B]	ZD9	C1-N2	-2.01	1.34	1.37

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602[A]	ADP	C5-C4-N3	-5.87	118.63	126.72
4	A	603[B]	ZD9	C1-N2-C3	-5.87	120.68	123.87
3	B	602	ADP	C5-C4-N3	-5.53	119.10	126.72
3	B	602	ADP	N3-C4-N9	4.68	135.13	127.17
3	A	602[A]	ADP	N3-C4-N9	4.59	134.98	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602[A]	ADP	C4-C5-N7	-3.97	106.04	110.58
3	A	602[A]	ADP	C2-N3-C4	3.91	121.38	111.83
3	B	602	ADP	N3-C2-N1	-3.82	122.80	128.58
3	B	602	ADP	C2-N3-C4	3.78	121.06	111.83
3	A	602[A]	ADP	N3-C2-N1	-3.54	123.22	128.58
4	A	603[B]	ZD9	C6-C1-N2	3.54	118.67	114.93
4	A	603[B]	ZD9	C5-N4-C3	3.15	121.30	118.16
3	A	602[A]	ADP	C5-N7-C8	3.00	108.17	103.45
4	A	603[B]	ZD9	C6-C5-N4	-2.98	119.41	122.41
3	A	602[A]	ADP	C4-N9-C8	2.85	108.73	105.74
3	B	602	ADP	C4-N9-C8	2.75	108.62	105.74
4	A	603[B]	ZD9	C9-C12-N13	2.73	118.65	113.15
3	B	602	ADP	C4-C5-N7	-2.68	107.52	110.58
4	A	603[B]	ZD9	C11-C10-C9	2.58	120.27	117.99
3	A	602[A]	ADP	C6-C5-N7	2.42	136.75	132.09
3	B	602	ADP	C5-N7-C8	2.41	107.23	103.45
3	B	602	ADP	C2'-C3'-C4'	2.37	107.19	102.61
3	A	602[A]	ADP	N9-C8-N7	-2.30	110.67	113.94
3	B	602	ADP	N9-C8-N7	-2.17	110.86	113.94
3	B	602	ADP	C3'-C2'-C1'	2.07	105.39	101.46
3	A	602[A]	ADP	C2-N1-C6	2.07	122.13	118.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602[A]	ADP	C5'-O5'-PA-O3A
3	B	602	ADP	PA-O3A-PB-O2B
3	A	602[A]	ADP	O4'-C4'-C5'-O5'
3	B	602	ADP	C3'-C4'-C5'-O5'
3	B	602	ADP	O4'-C4'-C5'-O5'
3	A	602[A]	ADP	C3'-C4'-C5'-O5'
3	A	602[A]	ADP	C4'-C5'-O5'-PA
3	A	602[A]	ADP	C5'-O5'-PA-O1A
3	B	602	ADP	C4'-C5'-O5'-PA

There are no ring outliers.

5 monomers are involved in 14 short contacts:

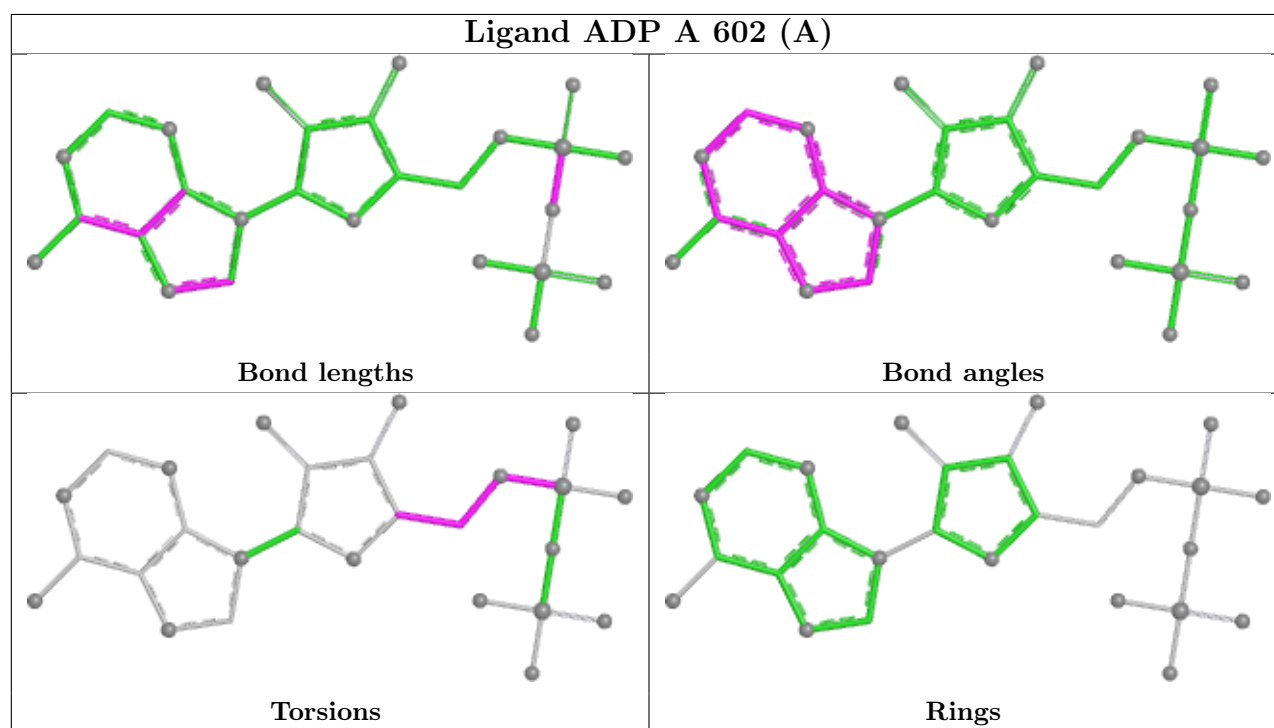
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603[B]	ZD9	5	0

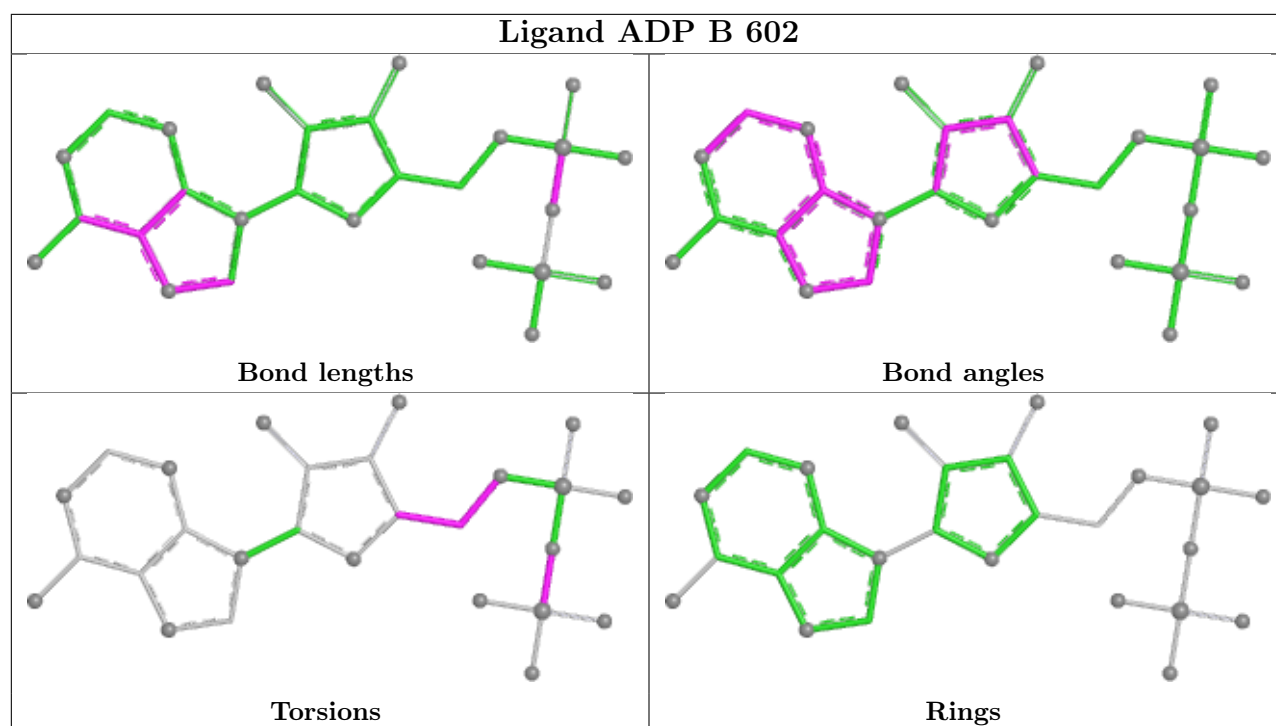
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	SO4	1	0
3	A	602[A]	ADP	5	0
5	A	604[C]	XPO	1	0
3	B	602	ADP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	557/559 (99%)	-0.60	1 (0%) 91 92	33, 49, 79, 129	0
1	B	557/559 (99%)	-0.02	1 (0%) 91 92	31, 72, 107, 149	0
All	All	1114/1118 (99%)	-0.31	2 (0%) 91 92	31, 60, 102, 149	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	396	TYR	2.3
1	A	71	GLY	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

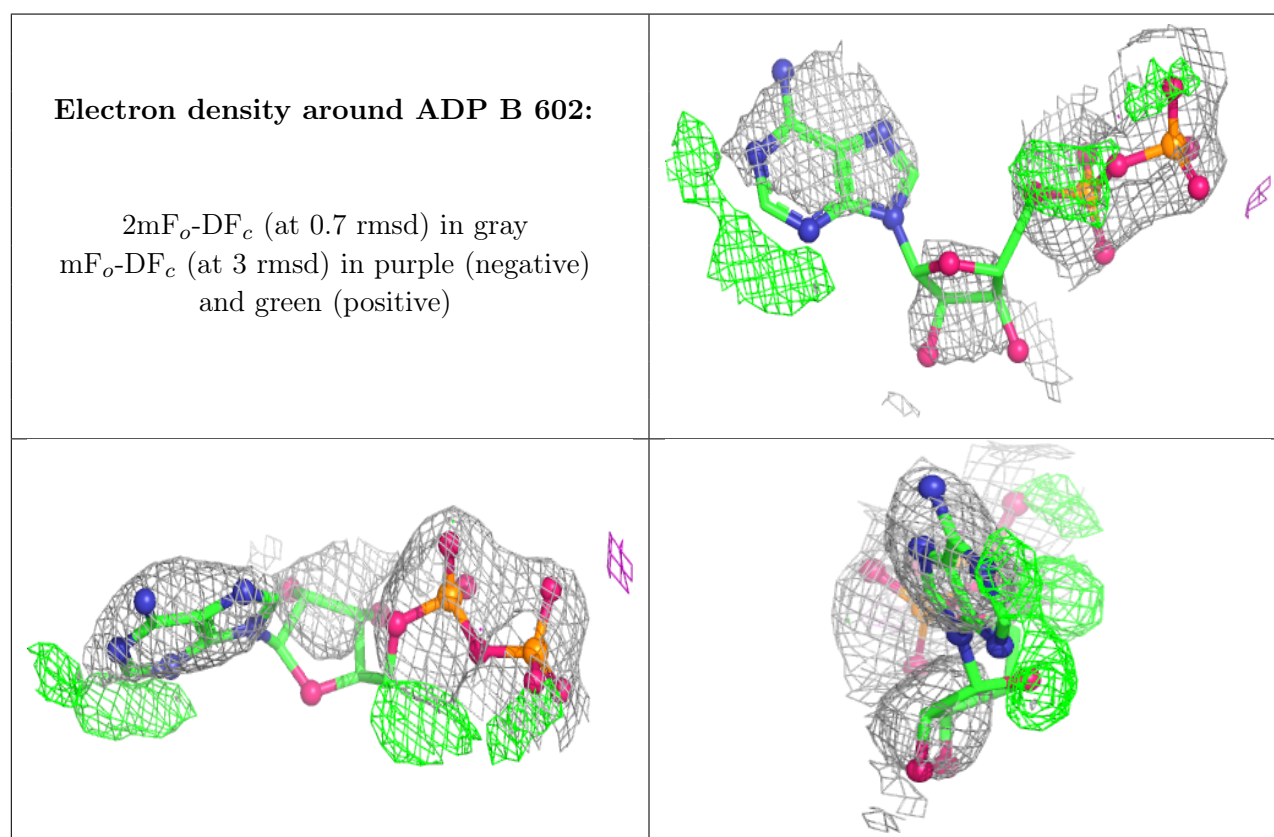
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ADP	B	602	27/27	0.82	0.15	59,71,80,81	27
2	SO4	A	605	5/5	0.83	0.09	88,94,109,113	0
4	ZD9	A	603[B]	18/18	0.85	0.21	53,56,67,69	18

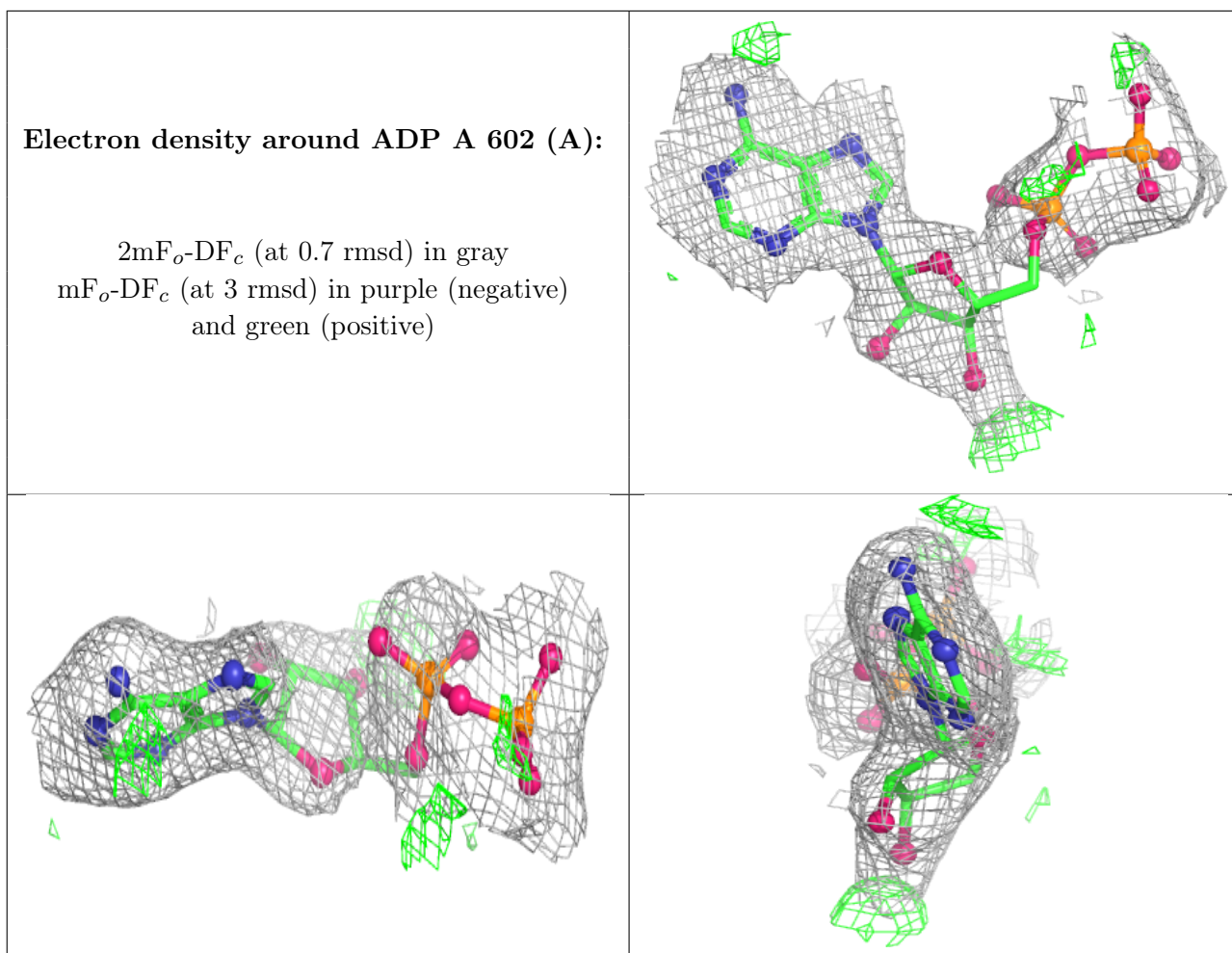
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	601	5/5	0.91	0.10	76,87,93,95	0
2	SO4	B	603	5/5	0.93	0.08	92,98,103,104	0
3	ADP	A	602[A]	27/27	0.93	0.09	48,64,76,81	27
2	SO4	A	601	5/5	0.95	0.08	50,64,70,70	0
5	XPO	A	604[C]	7/7	0.96	0.11	57,60,66,68	7

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





6.5 Other polymers [i](#)

There are no such residues in this entry.