Full wwPDB X-ray Structure Validation Report ⓘ

Jun 11, 2024 – 09:22 PM EDT

PDB ID	:	2WTU
Title	:	Crystal structure of Escherichia coli MutS in complex with a 16 basepair oligo containing an A.A mismatch.
Authors	:	Natrajan, G.; Lebbink, J.H.; Reumer, A.; Fish, A.; Winterwerp, H.H.; Sixma, T.K.
Deposited on	:	2009-09-22
Resolution	:	3.40 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 ⓘ 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:

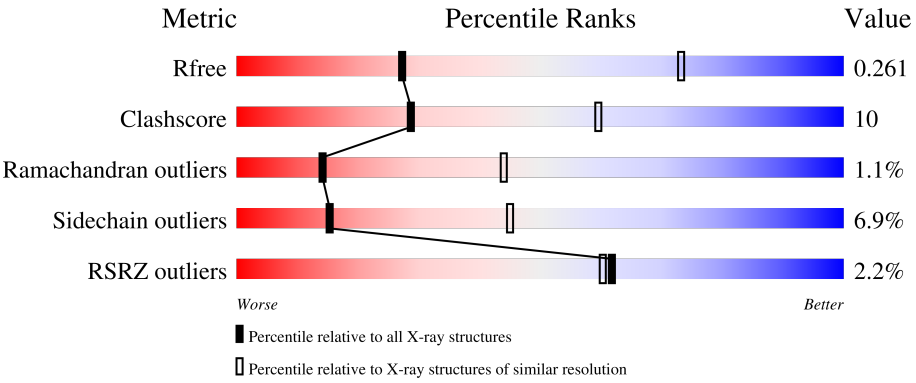
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 3.40 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))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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	800	% 74% 23%
1	B	800	3% 66% 24% 8%
2	E	16	6% 69% 31%
3	F	16	38% 56% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 12753 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 DNA MISMATCH REPAIR PROTEIN MUTS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	791	Total	C	N	O	S	0	0	0
			6225	3915	1106	1175	29			
1	B	738	Total	C	N	O	S	0	0	0
			5803	3646	1031	1100	26			

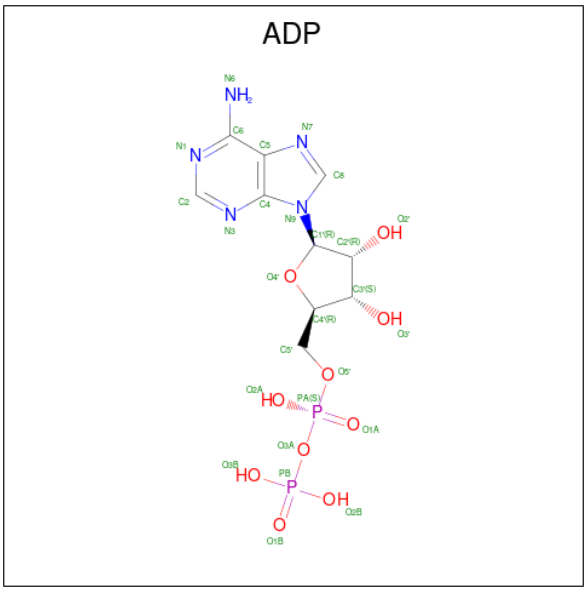
- Molecule 2 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	16	Total	C	N	O	P	0	0	0
			324	154	65	90	15			

- Molecule 3 is a DNA chain called DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	16	Total	C	N	O	P	0	0	0
			330	156	60	98	16			

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



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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

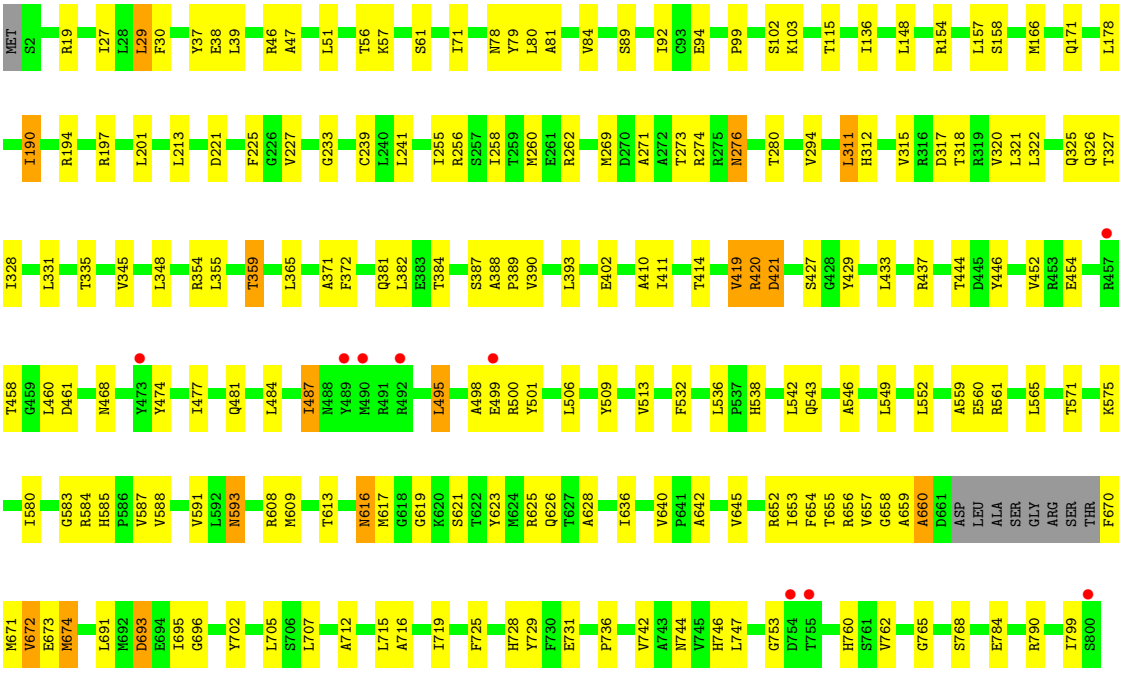
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	16	Total	O	0	0
			16	16		
6	E	1	Total	O	0	0
			1	1		
6	F	1	Total	O	0	0
			1	1		

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.

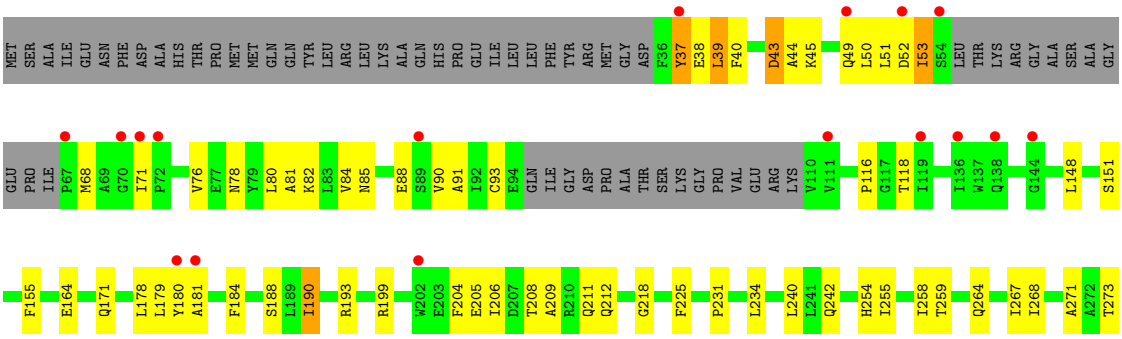
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

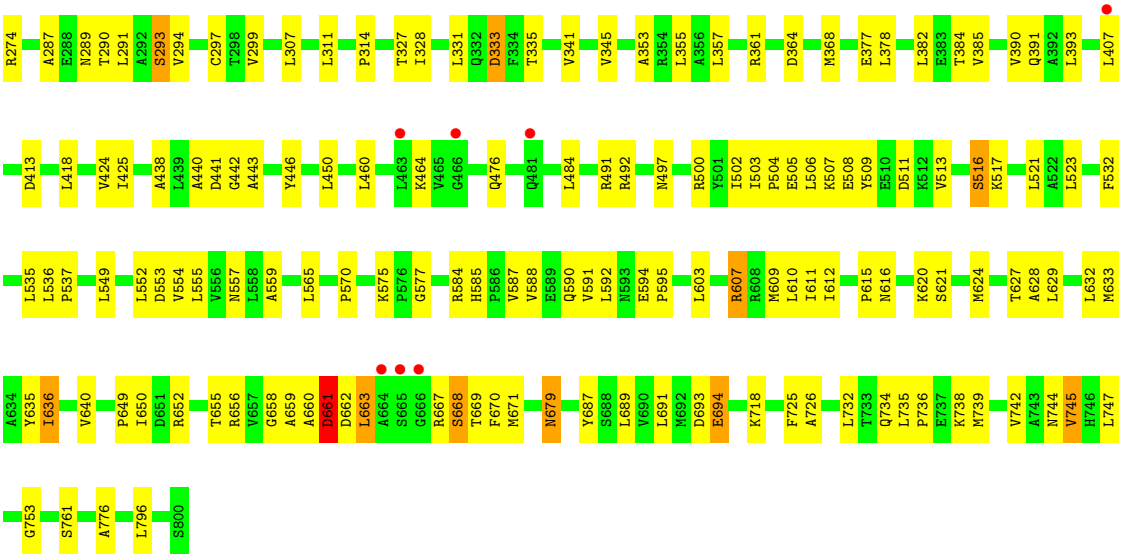
Chain A:



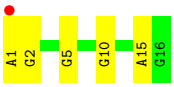
• Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

Chain B:

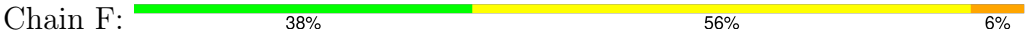


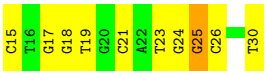


• Molecule 2: DNA



• Molecule 3: DNA





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	91.11Å 137.89Å 161.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.40 46.34 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.40) 99.8 (46.34-3.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.73 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.203 , 0.263 0.204 , 0.261	Depositor DCC
R_{free} test set	1446 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	74.0	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 45.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12753	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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

5.1 Standard geometry

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

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	0.38	0/6331	0.59	0/8569
1	B	0.40	0/5897	0.59	0/7981
2	E	0.71	0/364	1.50	8/559 (1.4%)
3	F	0.81	0/369	1.68	8/568 (1.4%)
All	All	0.42	0/12961	0.70	16/17677 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	21	DC	O4'-C1'-N1	7.77	113.44	108.00
2	E	1	DA	O4'-C1'-N9	7.61	113.33	108.00
3	F	25	DG	O4'-C1'-N9	7.37	113.16	108.00
2	E	5	DG	O4'-C1'-N9	7.33	113.13	108.00
2	E	10	DG	O4'-C4'-C3'	-7.27	101.59	104.50
3	F	18	DG	O4'-C4'-C3'	-7.01	101.70	104.50
3	F	15	DC	O4'-C1'-N1	6.82	112.77	108.00
2	E	10	DG	C1'-O4'-C4'	-6.57	103.53	110.10
3	F	17	DG	O4'-C1'-N9	6.35	112.44	108.00
3	F	26	DC	O4'-C1'-C2'	-6.34	100.83	105.90
2	E	15	DA	O4'-C1'-N9	6.05	112.23	108.00
3	F	26	DC	C1'-O4'-C4'	-5.96	104.14	110.10
2	E	1	DA	O4'-C1'-C2'	-5.43	101.56	105.90
2	E	1	DA	P-O3'-C3'	5.31	126.08	119.70
2	E	5	DG	O4'-C1'-C2'	-5.24	101.71	105.90
3	F	25	DG	P-O3'-C3'	5.23	125.98	119.70

There are no chirality outliers.

There are no planarity outliers.

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	6225	0	6266	124	0
1	B	5803	0	5840	120	0
2	E	324	0	179	1	0
3	F	330	0	181	4	0
4	A	27	0	12	1	0
5	A	2	0	0	2	0
5	B	1	0	0	1	0
6	A	23	0	0	1	0
6	B	16	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	12753	0	12478	244	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 10.

All (244) 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:655:THR:HG22	1:B:691:LEU:HD12	1.51	0.90
1:B:517:LYS:HE2	5:B:1801:CL:CL	2.16	0.82
1:A:345:VAL:HG11	1:A:549:LEU:HD13	1.60	0.81
1:A:154:ARG:NH1	5:A:1803:CL:CL	2.54	0.77
1:B:311:LEU:HD23	1:B:636:ILE:HD12	1.67	0.76
1:B:38:GLU:O	1:B:39:LEU:HB2	1.84	0.74
1:A:460:LEU:HD22	1:A:481:GLN:HB3	1.70	0.72
1:B:355:LEU:HD22	1:B:368:MET:HE3	1.70	0.71
1:B:297:CYS:HB2	1:B:557:ASN:HD21	1.55	0.71
1:B:594:GLU:HG3	1:B:595:PRO:HD2	1.74	0.70
1:B:311:LEU:HD23	1:B:636:ILE:CD1	2.22	0.69
1:B:385:VAL:HG11	1:B:390:VAL:HG11	1.75	0.69
1:A:705:LEU:HD13	1:A:729:TYR:CD1	2.28	0.68
1:B:40:PHE:HA	1:B:43:ASP:OD1	1.93	0.68
1:B:355:LEU:HD22	1:B:368:MET:CE	2.24	0.68
1:B:633:MET:O	1:B:636:ILE:HG22	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:GLN:O	1:A:384:THR:HG22	1.96	0.66
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.78	0.66
1:A:393:LEU:HD13	1:A:552:LEU:CD1	2.27	0.65
1:A:609:MET:HE3	1:A:716:ALA:HB2	1.79	0.65
1:B:667:ARG:HB2	1:B:671:MET:HG2	1.79	0.65
1:B:585:HIS:CD2	1:B:588:VAL:HG23	2.32	0.64
1:A:328:ILE:HG23	1:A:559:ALA:HA	1.78	0.64
1:B:662:ASP:HB3	1:B:663:LEU:HA	1.80	0.63
1:A:157:LEU:HD23	1:A:157:LEU:C	2.18	0.62
1:B:80:LEU:HD21	1:B:90:VAL:HG11	1.81	0.62
1:A:707:LEU:HD11	1:B:776:ALA:HB2	1.82	0.61
1:B:327:THR:HG23	1:B:390:VAL:HG22	1.83	0.60
1:B:294:VAL:HG21	1:B:587:VAL:HA	1.84	0.59
1:A:262:ARG:NH1	6:A:2007:HOH:O	2.35	0.59
1:A:157:LEU:HD23	1:A:158:SER:N	2.17	0.59
1:B:82:LYS:HA	1:B:85:ASN:HB2	1.84	0.59
1:A:580:ILE:HG21	1:A:583:GLY:HA3	1.84	0.59
1:A:657:VAL:HA	1:A:693:ASP:HB2	1.85	0.59
1:A:39:LEU:HD13	1:A:47:ALA:CB	2.33	0.59
1:A:178:LEU:HD11	1:A:190:ILE:HD11	1.85	0.58
1:A:372:PHE:CZ	1:A:542:LEU:HD21	2.37	0.58
1:B:660:ALA:HA	1:B:661:ASP:CB	2.33	0.58
1:A:213:LEU:HD23	1:A:241:LEU:HD22	1.85	0.58
1:A:628:ALA:HB2	1:A:691:LEU:HD11	1.85	0.58
1:A:348:LEU:HD23	1:A:546:ALA:HB2	1.86	0.57
1:A:640:VAL:HG11	1:A:645:VAL:HG21	1.87	0.57
1:A:393:LEU:HD13	1:A:552:LEU:HD13	1.87	0.57
1:B:628:ALA:HB2	1:B:691:LEU:HD11	1.86	0.56
1:B:570:PRO:HD3	1:B:640:VAL:HG22	1.87	0.56
1:A:388:ALA:HB3	1:A:389:PRO:HD3	1.88	0.56
1:B:287:ALA:O	1:B:290:THR:HG22	2.06	0.56
1:A:487:ILE:HD12	1:A:487:ILE:H	1.71	0.56
1:B:609:MET:HB3	1:B:742:VAL:HG22	1.87	0.55
1:A:655:THR:HG23	1:A:657:VAL:HG23	1.87	0.55
1:B:49:GLN:HB3	1:B:50:LEU:HD12	1.88	0.55
1:A:89:SER:HB3	1:A:115:THR:HG22	1.88	0.55
1:B:290:THR:HG23	1:B:293:SER:H	1.72	0.55
1:A:674:MET:CE	1:A:707:LEU:HD13	2.38	0.54
1:B:40:PHE:O	1:B:44:ALA:N	2.40	0.54
1:A:625:ARG:NH2	1:A:657:VAL:HG11	2.23	0.54
1:B:450:LEU:O	1:B:450:LEU:HD23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:NH1	1:A:543:GLN:OE1	2.41	0.54
1:A:331:LEU:O	1:A:335:THR:HG23	2.08	0.54
1:A:136:ILE:HD11	1:A:166:MET:SD	2.48	0.54
1:A:276:ASN:HD21	1:A:625:ARG:HH21	1.56	0.54
1:A:355:LEU:HD12	1:A:532:PHE:HD1	1.73	0.53
1:A:37:TYR:OH	1:A:94:GLU:OE2	2.21	0.53
1:B:353:ALA:O	1:B:357:LEU:HD13	2.08	0.53
1:A:695:ILE:C	1:A:695:ILE:HD12	2.29	0.53
1:B:181:ALA:HB2	1:B:204:PHE:CE2	2.42	0.53
1:A:674:MET:HA	1:A:674:MET:HE2	1.91	0.52
1:A:746:HIS:ND1	1:A:765:GLY:O	2.30	0.52
1:B:382:LEU:HD11	1:B:552:LEU:HD21	1.91	0.52
1:A:660:ALA:HB1	1:A:672:VAL:HG21	1.92	0.52
1:B:212:GLN:HG2	1:B:242:GLN:NE2	2.25	0.52
1:B:345:VAL:HG21	1:B:549:LEU:HD22	1.91	0.52
1:B:407:LEU:HD21	1:B:535:LEU:HD21	1.92	0.52
1:A:593:ASN:OD1	1:A:593:ASN:N	2.42	0.52
1:B:151:SER:O	1:B:353:ALA:HB2	2.10	0.52
1:A:561:ARG:NH1	1:A:565:LEU:HD11	2.25	0.51
1:A:715:LEU:HD23	1:A:719:ILE:HD12	1.92	0.51
1:A:509:TYR:O	1:A:513:VAL:HG12	2.10	0.51
1:B:267:ILE:HB	1:B:314:PRO:HG2	1.92	0.51
1:A:227:VAL:HG12	1:A:260:MET:HB2	1.91	0.51
1:B:184:PHE:CE2	1:B:190:ILE:HD12	2.45	0.51
1:B:440:ALA:HB2	1:B:516:SER:HB3	1.91	0.51
1:B:291:LEU:HD22	1:B:629:LEU:HD22	1.94	0.50
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.93	0.50
1:A:608:ARG:NH1	1:A:716:ALA:O	2.44	0.50
1:B:446:TYR:CG	1:B:509:TYR:HE1	2.29	0.50
1:A:372:PHE:HZ	1:A:542:LEU:HD21	1.76	0.50
1:A:495:LEU:N	1:A:495:LEU:HD12	2.27	0.50
2:E:2:DG:N2	3:F:30:DT:O2	2.45	0.50
1:A:365:LEU:HD12	1:A:411:ILE:HD11	1.93	0.50
1:A:29:LEU:HD12	1:A:30:PHE:N	2.26	0.50
1:A:269:MET:O	1:A:274:ARG:NH1	2.45	0.49
1:A:585:HIS:ND1	1:A:588:VAL:HG23	2.27	0.49
1:B:273:THR:HA	1:B:655:THR:OG1	2.11	0.49
1:B:38:GLU:O	1:B:39:LEU:CB	2.57	0.49
1:B:84:VAL:HG13	1:B:116:PRO:HA	1.93	0.49
1:B:393:LEU:HD13	1:B:552:LEU:HD12	1.92	0.49
1:B:464:LYS:NZ	3:F:19:DT:OP1	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:620:LYS:HG3	1:B:747:LEU:HD12	1.94	0.49
1:A:294:VAL:HG21	1:A:587:VAL:HA	1.94	0.49
1:B:205:GLU:O	1:B:209:ALA:HB2	2.12	0.49
1:A:619:GLY:C	1:A:747:LEU:HD22	2.32	0.49
1:B:736:PRO:HG2	1:B:744:ASN:ND2	2.28	0.49
1:B:615:PRO:HD2	1:B:747:LEU:O	2.13	0.48
1:A:657:VAL:HG13	1:A:693:ASP:OD2	2.12	0.48
1:A:273:THR:HG21	1:A:653:ILE:O	2.13	0.48
1:A:419:VAL:O	1:A:421:ASP:N	2.47	0.48
1:A:695:ILE:HD12	1:A:696:GLY:N	2.28	0.48
1:B:662:ASP:HB3	1:B:663:LEU:CA	2.43	0.48
1:A:157:LEU:HD21	1:A:233:GLY:HA3	1.96	0.47
1:B:655:THR:CG2	1:B:691:LEU:HD12	2.35	0.47
1:B:663:LEU:H	1:B:663:LEU:HD13	1.79	0.47
1:B:299:VAL:HG22	1:B:553:ASP:OD1	2.14	0.47
1:B:476:GLN:HE21	1:B:500:ARG:HE	1.60	0.47
1:A:736:PRO:HG2	1:A:744:ASN:ND2	2.29	0.47
1:A:327:THR:HG23	1:A:390:VAL:CG2	2.45	0.47
1:A:623:TYR:HD1	1:A:626:GLN:HE21	1.62	0.47
1:B:327:THR:HG23	1:B:390:VAL:CG2	2.45	0.47
1:B:443:ALA:HB1	1:B:513:VAL:HG23	1.96	0.47
1:A:201:LEU:C	1:A:201:LEU:HD13	2.35	0.47
1:A:280:THR:OG1	1:A:312:HIS:HE1	1.97	0.47
1:A:419:VAL:O	1:A:420:ARG:C	2.53	0.47
1:A:736:PRO:HG2	1:A:744:ASN:HD22	1.80	0.47
1:B:588:VAL:HG13	1:B:592:LEU:HG	1.96	0.47
1:A:136:ILE:HG22	1:A:178:LEU:CD2	2.45	0.46
1:A:609:MET:CE	1:A:716:ALA:HB2	2.44	0.46
1:B:502:ILE:HG21	1:B:507:LYS:HE2	1.95	0.46
1:B:393:LEU:HD13	1:B:552:LEU:CD1	2.45	0.46
1:A:136:ILE:CG2	1:A:178:LEU:HD21	2.45	0.46
1:A:410:ALA:HA	1:A:429:TYR:CD1	2.50	0.46
1:A:157:LEU:HD22	1:A:260:MET:HG3	1.97	0.46
1:A:454:GLU:O	1:A:458:THR:HG23	2.16	0.46
1:A:642:ALA:HB3	1:A:645:VAL:HG23	1.97	0.46
1:B:148:LEU:HB3	1:B:240:LEU:HD21	1.97	0.46
1:B:80:LEU:CD2	1:B:90:VAL:HG11	2.45	0.46
1:B:660:ALA:HA	1:B:661:ASP:HB3	1.97	0.46
1:A:609:MET:HE1	1:A:712:ALA:O	2.16	0.46
1:A:705:LEU:HD21	1:A:731:GLU:HB2	1.98	0.46
1:A:621:SER:HB3	1:A:625:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:735:LEU:N	1:B:736:PRO:CD	2.79	0.45
1:B:88:GLU:O	1:B:90:VAL:HG23	2.16	0.45
1:B:254:HIS:CE1	1:B:357:LEU:HD11	2.51	0.45
1:B:148:LEU:HD11	1:B:255:ILE:HD13	1.96	0.45
1:B:171:GLN:HG2	1:B:271:ALA:HA	1.97	0.45
1:B:693:ASP:HA	1:B:726:ALA:HB3	1.98	0.45
1:A:387:SER:OG	1:A:390:VAL:HG23	2.16	0.45
1:A:433:LEU:HD21	1:A:437:ARG:NH2	2.32	0.45
1:A:495:LEU:HD11	1:A:500:ARG:HD2	1.99	0.45
1:A:359:THR:O	1:A:359:THR:HG23	2.16	0.45
1:B:382:LEU:O	1:B:391:GLN:NE2	2.49	0.45
1:B:438:ALA:O	1:B:442:GLY:N	2.48	0.45
1:A:178:LEU:CD1	1:A:190:ILE:HD11	2.46	0.44
1:A:674:MET:HE3	1:A:707:LEU:HD13	1.97	0.44
1:B:53:ILE:HD13	1:B:71:ILE:HG22	1.99	0.44
1:B:734:GLN:O	1:B:738:LYS:HG2	2.17	0.44
1:A:99:PRO:HA	1:A:102:SER:HB2	1.99	0.44
1:A:585:HIS:CE1	1:A:588:VAL:HG23	2.53	0.44
1:A:588:VAL:HA	1:A:591:VAL:HG12	1.99	0.44
1:B:659:ALA:O	1:B:660:ALA:HB3	2.18	0.44
1:A:157:LEU:C	1:A:157:LEU:CD2	2.84	0.44
1:A:616:ASN:O	1:A:617:MET:HB2	2.18	0.44
1:B:82:LYS:HA	1:B:85:ASN:CB	2.48	0.44
1:B:627:THR:HG22	1:B:689:LEU:HD21	1.99	0.44
1:B:424:VAL:HG13	1:B:425:ILE:HG12	2.00	0.44
1:B:635:TYR:OH	1:B:649:PRO:HA	2.18	0.44
1:A:171:GLN:HG2	1:A:271:ALA:HA	2.00	0.44
1:B:460:LEU:HD21	1:B:484:LEU:HB2	1.99	0.44
1:A:728:HIS:ND1	5:A:1802:CL:CL	2.88	0.44
1:B:503:ILE:HB	1:B:504:PRO:HD2	2.00	0.44
1:B:611:ILE:HD13	1:B:725:PHE:HB3	2.00	0.44
1:A:148:LEU:HD21	1:A:255:ILE:HD11	2.00	0.43
1:A:652:ARG:HD3	1:A:654:PHE:CZ	2.53	0.43
1:A:799:ILE:HG22	1:A:799:ILE:O	2.18	0.43
1:B:90:VAL:HG12	1:B:91:ALA:N	2.33	0.43
1:B:164:GLU:HG2	1:B:679:ASN:OD1	2.17	0.43
1:B:735:LEU:HD22	1:B:739:MET:SD	2.58	0.43
1:A:658:GLY:O	1:A:659:ALA:HB3	2.19	0.43
1:B:612:ILE:HG12	1:B:745:VAL:HG23	2.00	0.43
1:A:538:HIS:O	1:A:542:LEU:HB2	2.19	0.43
1:B:341:VAL:HG11	1:B:378:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD21	1:A:92:ILE:HD11	2.00	0.43
1:A:335:THR:HB	1:A:560:GLU:HB2	1.99	0.43
1:B:179:LEU:HD22	1:B:199:ARG:HD3	2.01	0.43
1:A:609:MET:HB3	1:A:742:VAL:HG22	2.00	0.43
1:A:705:LEU:HD13	1:A:729:TYR:CG	2.53	0.43
1:B:327:THR:HG22	1:B:331:LEU:HD12	1.99	0.43
1:B:377:GLU:OE1	1:B:377:GLU:HA	2.19	0.43
1:A:78:ASN:O	1:A:81:ALA:HB3	2.18	0.43
1:A:315:VAL:HG12	1:A:317:ASP:H	1.84	0.43
1:B:355:LEU:HD12	1:B:532:PHE:CD1	2.54	0.43
1:A:674:MET:HE1	1:A:707:LEU:CD1	2.49	0.42
1:B:268:ILE:HB	1:B:652:ARG:HG2	2.00	0.42
1:B:450:LEU:HD23	1:B:450:LEU:C	2.39	0.42
1:B:621:SER:HA	1:B:624:MET:HE3	2.00	0.42
3:F:24:DG:H2"	3:F:25:DG:H8	1.84	0.42
1:A:355:LEU:HD12	1:A:532:PHE:CD1	2.53	0.42
1:B:668:SER:HB3	1:B:669:THR:O	2.19	0.42
1:A:345:VAL:HG13	1:A:371:ALA:HB1	1.99	0.42
1:B:333:ASP:OD1	1:B:333:ASP:N	2.52	0.42
1:A:317:ASP:OD2	1:A:320:VAL:HG23	2.19	0.42
1:B:505:GLU:O	1:B:508:GLU:HB3	2.19	0.42
1:A:136:ILE:CD1	1:A:166:MET:SD	3.07	0.42
1:A:311:LEU:HD12	1:A:636:ILE:HD13	2.01	0.42
1:B:45:LYS:O	1:B:49:GLN:HB2	2.20	0.42
1:B:231:PRO:HA	1:B:234:LEU:HD12	2.02	0.42
1:B:71:ILE:CD1	1:B:76:VAL:HG23	2.50	0.42
1:A:474:TYR:HB2	1:A:500:ARG:HB3	2.02	0.42
1:B:594:GLU:HG3	1:B:595:PRO:CD	2.48	0.42
1:B:225:PHE:HB3	1:B:258:ILE:O	2.19	0.42
1:B:536:LEU:N	1:B:537:PRO:CD	2.82	0.42
1:A:446:TYR:CE2	1:A:509:TYR:CD2	3.08	0.42
1:B:446:TYR:CB	1:B:509:TYR:HE1	2.32	0.42
1:A:623:TYR:CE1	1:A:762:VAL:HG21	2.54	0.41
1:B:361:ARG:O	1:B:364:ASP:HB2	2.20	0.41
1:A:89:SER:OG	1:A:197:ARG:NH2	2.53	0.41
1:A:410:ALA:HB2	1:A:429:TYR:CE1	2.56	0.41
1:B:71:ILE:HD11	1:B:76:VAL:HG23	2.02	0.41
1:B:693:ASP:O	1:B:694:GLU:C	2.59	0.41
1:A:51:LEU:HD22	1:A:79:TYR:HD1	1.86	0.41
1:A:318:THR:HG22	1:A:322:LEU:HD12	2.02	0.41
1:B:650:ILE:HA	1:B:687:TYR:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ILE:HD12	1:A:501:TYR:CE2	2.56	0.41
1:A:674:MET:CE	1:A:707:LEU:CD1	2.98	0.41
1:A:354:ARG:HB3	1:A:359:THR:HG22	2.03	0.41
1:A:56:THR:OG1	1:A:57:LYS:N	2.53	0.41
1:A:382:LEU:HD11	1:A:552:LEU:HD21	2.03	0.41
1:B:40:PHE:O	1:B:44:ALA:CB	2.68	0.41
1:B:503:ILE:HG13	1:B:506:LEU:HB2	2.02	0.41
1:A:225:PHE:HB3	1:A:258:ILE:O	2.21	0.41
1:A:495:LEU:HD13	1:A:498:ALA:HB3	2.03	0.41
1:B:118:THR:OG1	1:B:118:THR:O	2.36	0.41
1:B:307:LEU:HD13	1:B:554:VAL:HG13	2.03	0.41
1:B:565:LEU:HD22	1:B:590:GLN:NE2	2.36	0.41
1:B:577:GLY:HA2	1:B:603:LEU:O	2.21	0.41
1:B:656:ARG:NH2	1:B:658:GLY:O	2.54	0.41
1:A:27:ILE:HG21	1:A:89:SER:HB2	2.02	0.41
1:A:321:LEU:O	1:A:325:GLN:HG3	2.21	0.41
1:A:652:ARG:HD3	1:A:654:PHE:CE2	2.56	0.41
1:B:607:ARG:CZ	1:B:610:LEU:HD21	2.51	0.41
1:B:289:ASN:OD1	1:B:591:VAL:HG21	2.20	0.40
1:A:71:ILE:HG22	3:F:23:DT:H4'	2.02	0.40
1:A:760:HIS:HB3	4:A:1801:ADP:C6	2.56	0.40
1:A:702:TYR:CD1	1:B:796:LEU:HD13	2.56	0.40
1:B:81:ALA:O	1:B:85:ASN:HB2	2.22	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	787/800 (98%)	743 (94%)	38 (5%)	6 (1%)	19 51
1	B	732/800 (92%)	652 (89%)	69 (9%)	11 (2%)	10 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1519/1600 (95%)	1395 (92%)	107 (7%)	17 (1%)	14 44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	ARG
1	B	39	LEU
1	B	413	ASP
1	A	660	ALA
1	A	671	MET
1	B	52	ASP
1	B	694	GLU
1	B	753	GLY
1	A	753	GLY
1	A	784	GLU
1	B	264	GLN
1	B	37	TYR
1	B	616	ASN
1	B	670	PHE
1	A	61	SER
1	B	218	GLY
1	B	661	ASP

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	657/664 (99%)	613 (93%)	44 (7%)	16 46
1	B	613/664 (92%)	569 (93%)	44 (7%)	14 43
All	All	1270/1328 (96%)	1182 (93%)	88 (7%)	15 45

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG

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Mol	Chain	Res	Type
1	A	29	LEU
1	A	38	GLU
1	A	46	ARG
1	A	84	VAL
1	A	103	LYS
1	A	190	ILE
1	A	194	ARG
1	A	221	ASP
1	A	239	CYS
1	A	276	ASN
1	A	311	LEU
1	A	326	GLN
1	A	359	THR
1	A	402	GLU
1	A	414	THR
1	A	419	VAL
1	A	421	ASP
1	A	427	SER
1	A	444	THR
1	A	452	VAL
1	A	461	ASP
1	A	468	ASN
1	A	484	LEU
1	A	487	ILE
1	A	495	LEU
1	A	499	GLU
1	A	506	LEU
1	A	536	LEU
1	A	571	THR
1	A	575	LYS
1	A	584	ARG
1	A	593	ASN
1	A	613	THR
1	A	616	ASN
1	A	656	ARG
1	A	670	PHE
1	A	672	VAL
1	A	673	GLU
1	A	674	MET
1	A	693	ASP
1	A	725	PHE
1	A	768	SER

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Mol	Chain	Res	Type
1	A	790	ARG
1	B	37	TYR
1	B	43	ASP
1	B	51	LEU
1	B	53	ILE
1	B	68	MET
1	B	78	ASN
1	B	93	CYS
1	B	155	PHE
1	B	178	LEU
1	B	180	TYR
1	B	188	SER
1	B	190	ILE
1	B	193	ARG
1	B	206	ILE
1	B	208	THR
1	B	211	GLN
1	B	259	THR
1	B	274	ARG
1	B	293	SER
1	B	333	ASP
1	B	335	THR
1	B	384	THR
1	B	418	LEU
1	B	441	ASP
1	B	491	ARG
1	B	492	ARG
1	B	497	ASN
1	B	511	ASP
1	B	516	SER
1	B	521	LEU
1	B	523	LEU
1	B	575	LYS
1	B	584	ARG
1	B	607	ARG
1	B	632	LEU
1	B	636	ILE
1	B	661	ASP
1	B	663	LEU
1	B	668	SER
1	B	679	ASN
1	B	718	LYS

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Mol	Chain	Res	Type
1	B	732	LEU
1	B	745	VAL
1	B	761	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	312	HIS
1	A	493	GLN
1	A	566	ASN
1	A	590	GLN
1	A	616	ASN
1	A	643	GLN
1	A	734	GLN
1	A	744	ASN
1	B	242	GLN
1	B	332	GLN
1	B	339	GLN
1	B	344	GLN
1	B	476	GLN
1	B	538	HIS
1	B	557	ASN
1	B	566	ASN
1	B	585	HIS
1	B	590	GLN
1	B	593	ASN
1	B	714	ASN
1	B	717	ASN
1	B	734	GLN
1	B	744	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ADP	A	1801	-	24,29,29	0.90	1 (4%)	29,45,45	1.19	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	1801	-	-	2/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	ADP	C2-N3	2.21	1.35	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1801	ADP	N3-C2-N1	-4.11	123.10	128.67
4	A	1801	ADP	C4-C5-N7	-2.10	107.12	109.34

There are no chirality outliers.

All (2) torsion outliers are listed below:

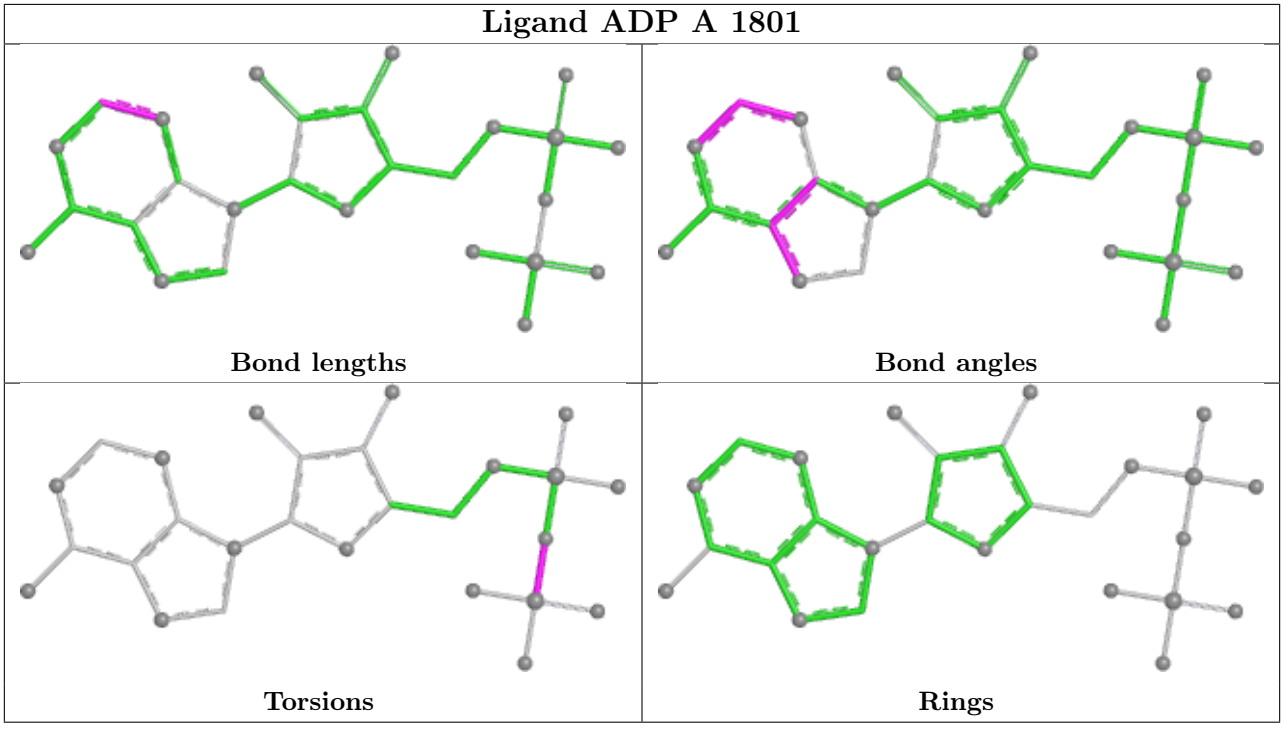
Mol	Chain	Res	Type	Atoms
4	A	1801	ADP	PA-O3A-PB-O2B
4	A	1801	ADP	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1801	ADP	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.



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

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	791/800 (98%)	0.15	9 (1%) 80 79	39, 56, 72, 88	0
1	B	738/800 (92%)	0.32	24 (3%) 46 45	32, 64, 90, 121	0
2	E	16/16 (100%)	0.49	1 (6%) 20 21	51, 64, 115, 126	0
3	F	16/16 (100%)	0.31	0 100 100	51, 73, 92, 107	0
All	All	1561/1632 (95%)	0.23	34 (2%) 62 60	32, 60, 84, 126	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	TYR	5.6
1	B	71	ILE	4.0
1	B	180	TYR	3.8
1	A	754	ASP	3.8
1	B	72	PRO	3.2
1	A	755	THR	3.1
1	B	181	ALA	3.0
1	B	665	SER	2.9
1	B	407	LEU	2.9
1	B	144	GLY	2.8
1	B	136	ILE	2.7
1	A	489	TYR	2.7
2	E	1	DA	2.6
1	A	490	MET	2.5
1	B	466	GLY	2.5
1	B	666	GLY	2.4
1	A	473	TYR	2.4
1	A	492	ARG	2.4
1	B	664	ALA	2.3
1	B	67	PRO	2.3
1	B	70	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	54	SER	2.3
1	B	89	SER	2.3
1	B	202	TRP	2.2
1	B	111	VAL	2.2
1	B	138	GLN	2.2
1	A	800	SER	2.1
1	B	52	ASP	2.1
1	A	457	ARG	2.1
1	B	463	LEU	2.1
1	A	499	GLU	2.0
1	B	49	GLN	2.0
1	B	481	GLN	2.0
1	B	119	ILE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

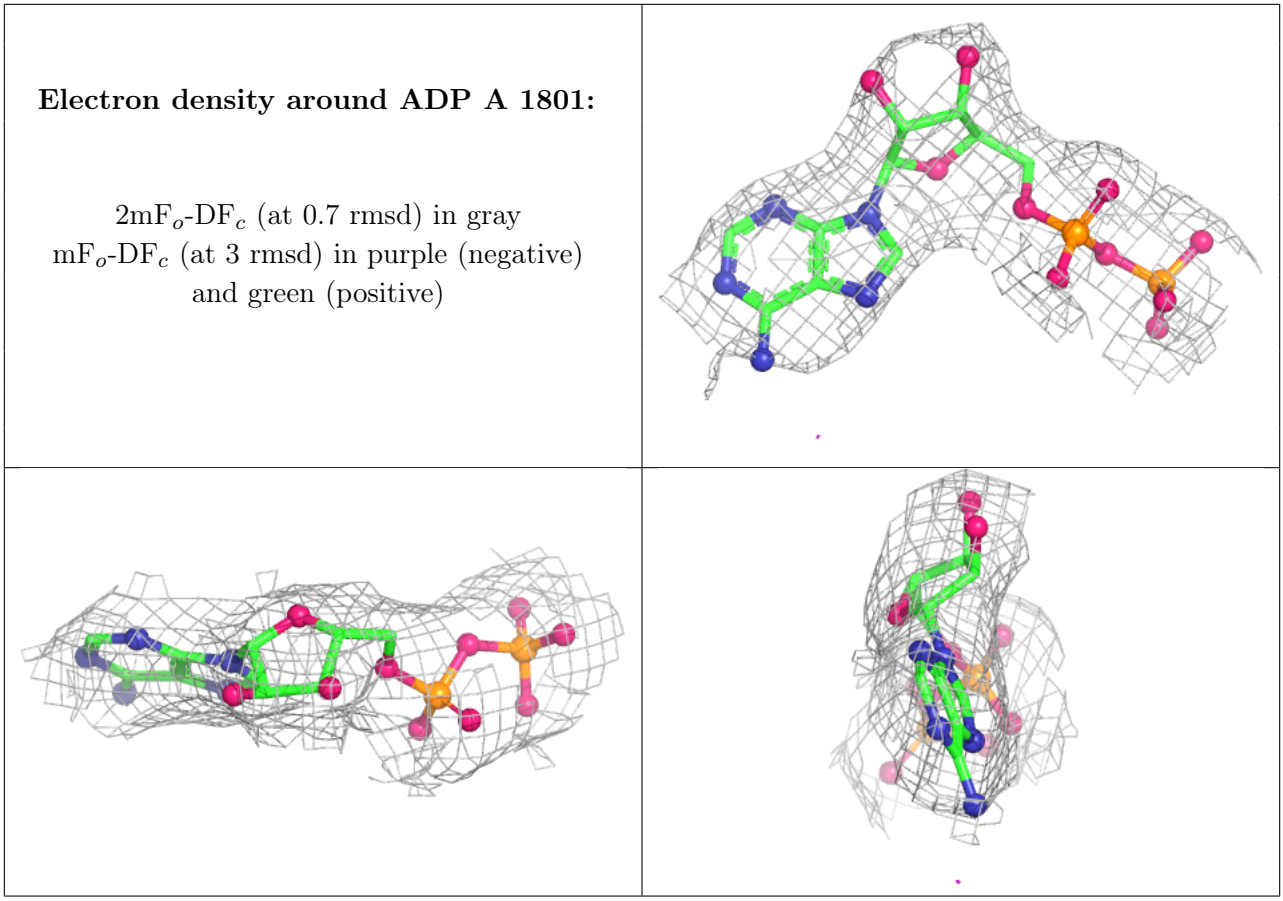
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	CL	A	1802	1/1	0.57	0.33	30,30,30,30	0
5	CL	A	1803	1/1	0.82	0.18	30,30,30,30	0
5	CL	B	1801	1/1	0.92	0.30	30,30,30,30	0
4	ADP	A	1801	27/27	0.95	0.18	62,65,66,66	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 1801:

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



6.5 Other polymers

There are no such residues in this entry.