Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:32 pm BST

PDB ID	:	1E3M
Title	:	The crystal structure of E. coli MutS binding to DNA with a G:T mismatch
Authors	:	Lamers, M.H.; Perrakis, A.; Enzlin, J.H.; Winterwerp, H.H.K.; De Wind, N.; Sixma, T.K.
Deposited on	:	2000-06-19
Resolution	:	2.20 Å(reported)

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

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

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

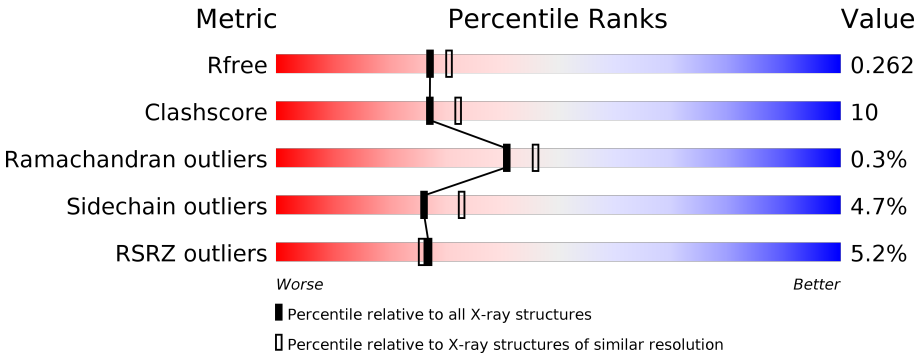
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	800	5% 76% 20%
1	B	800	4% 70% 22% 6%
2	E	30	10% 53% 7% 40%
3	F	30	3% 30% 27% 43%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13392 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	788	Total	C	N	O	S	Se	0	0	0
			6207	3905	1103	1170	6	23			
1	B	754	Total	C	N	O	S	Se	0	0	0
			5964	3756	1060	1120	6	22			

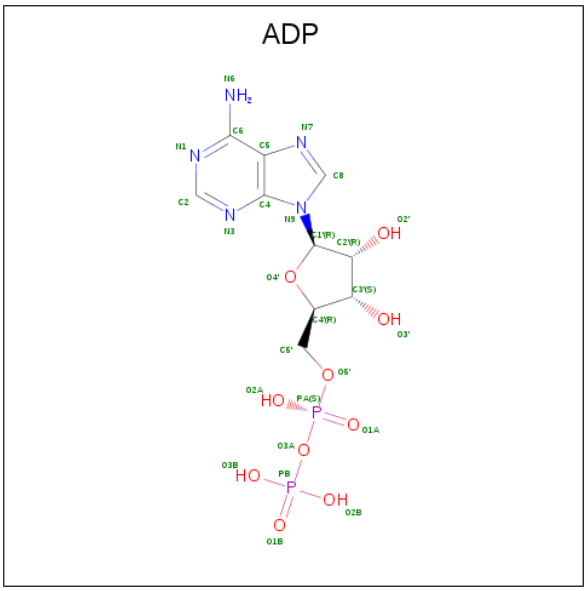
- Molecule 2 is a DNA chain called 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP*CP*AP*CP*CP*AP* GP*TP*GP*TP*CP*AP*GP*CP*GP*TP*CP*CP*TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	P	0	0	0
			367	174	72	104	17			

- Molecule 3 is a DNA chain called 5'-D(*AP*TP*AP*GP*GP*AP*CP*GP*CP*TP*GP*AP*CP*AP*CP* TP*GP*GP*TP*GP*CP*TP*TP*GP*GP*CP*AP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	17	Total	C	N	O	P	0	0	0
			347	166	62	103	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 MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is water.

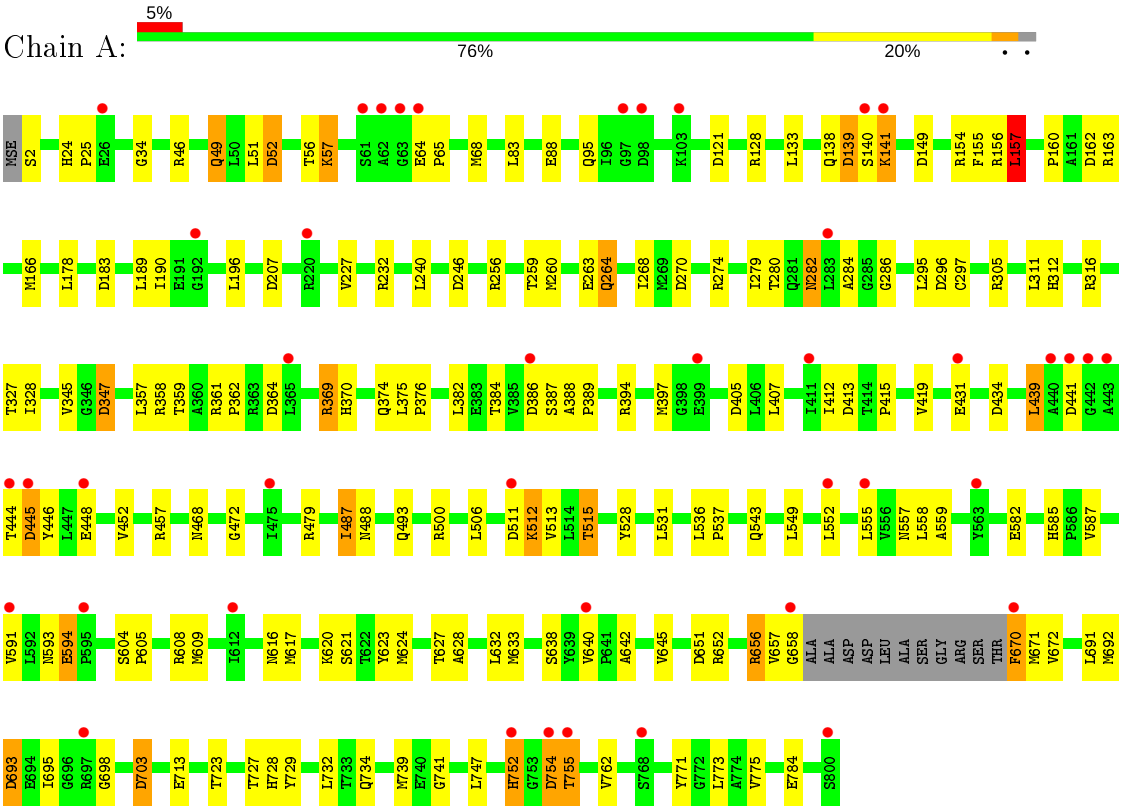
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	228	Total	O	0	0
			228	228		
6	B	223	Total	O	0	0
			223	223		
6	E	11	Total	O	0	0
			11	11		
6	F	16	Total	O	0	0
			16	16		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

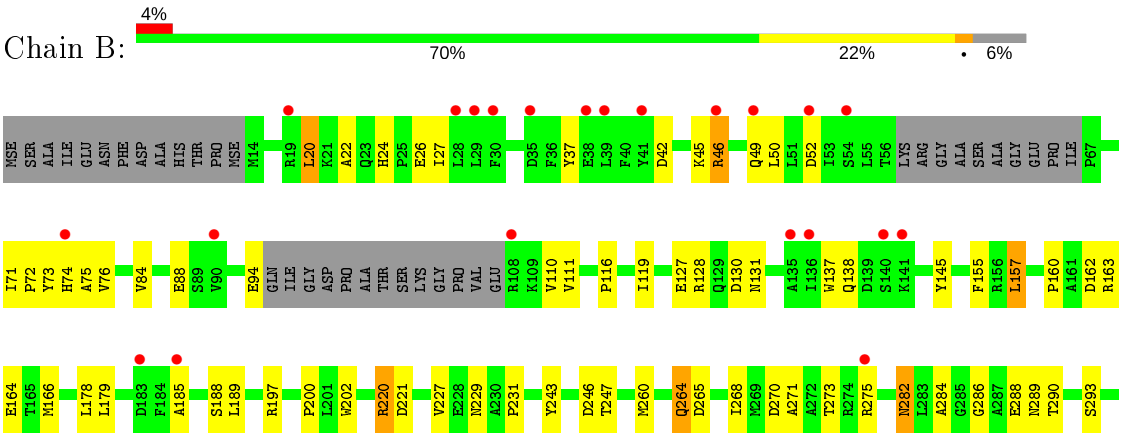
- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

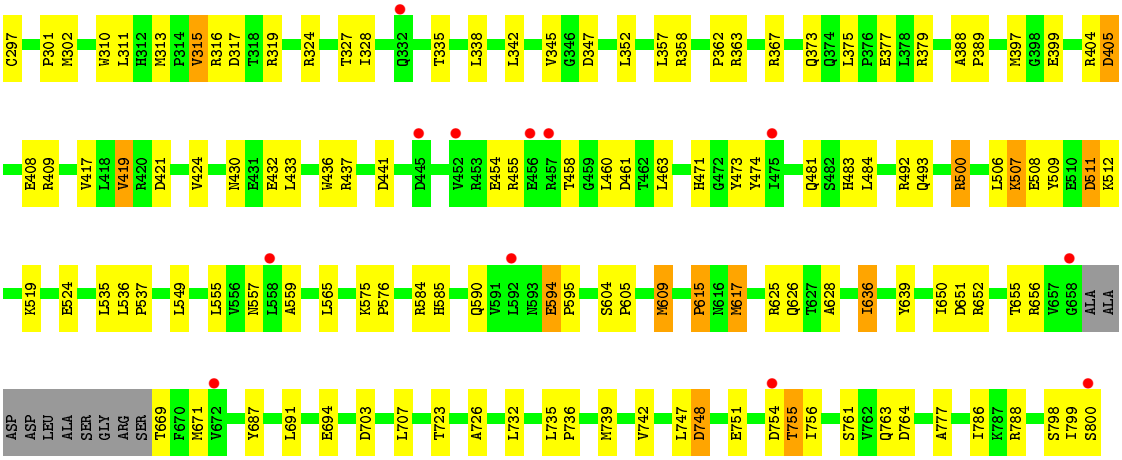
Chain A:



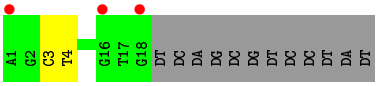
- Molecule 1: DNA MISMATCH REPAIR PROTEIN MUTS

Chain B:

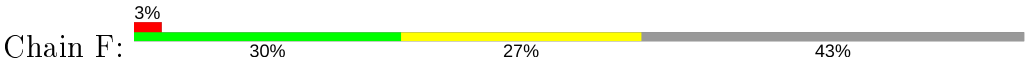


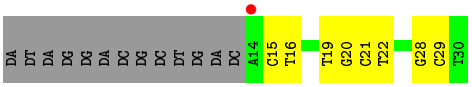


• Molecule 2: 5'-D(*AP*GP*CP*TP*GP*CP*CP*AP*GP*GP*CP*AP*CP*CP*AP* GP*TP* GP*TP*CP*AP*GP*CP*GP*TP*CP*CP*TP*AP*T)-3'



• Molecule 3: 5'-D(*AP*TP*AP*GP*GP*AP*CP*GP*CP*TP*GP*AP*CP*AP*CP* TP*GP* GP*TP*GP*CP*TP*TP*GP*GP*CP*AP*GP*CP*T)-3'





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	89.96Å 92.37Å 261.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.20) 98.7 (19.98-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.228 , 0.266 0.224 , 0.262	Depositor DCC
R_{free} test set	2199 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 35.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13392	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: MG, 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	0.51	0/6290	0.73	22/8475 (0.3%)
1	B	0.50	1/6041 (0.0%)	0.72	18/8136 (0.2%)
2	E	0.82	0/412	1.14	0/634
3	F	0.83	0/388	1.38	3/598 (0.5%)
All	All	0.53	1/13131 (0.0%)	0.77	43/17843 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	609	MSE	SE-CE	-6.72	1.55	1.95

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	693	ASP	CB-CG-OD2	7.06	124.66	118.30
1	B	748	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	162	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	246	ASP	CB-CG-OD2	6.19	123.88	118.30
1	A	207	ASP	CB-CG-OD2	5.97	123.67	118.30
1	B	421	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	52	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	347	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	130	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	270	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	296	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	265	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	413	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	139	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	121	ASP	CB-CG-OD2	5.62	123.36	118.30
3	F	22	DT	N3-C4-O4	5.61	123.27	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	162	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	445	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	511	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	246	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	42	ASP	CB-CG-OD2	5.47	123.22	118.30
3	F	22	DT	C5-C4-O4	-5.47	121.07	124.90
1	A	441	ASP	CB-CG-OD2	5.44	123.20	118.30
3	F	22	DT	O4'-C1'-N1	-5.39	104.22	108.00
1	A	754	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	434	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	347	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	149	ASP	CB-CG-OD2	5.34	123.11	118.30
1	B	511	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	270	ASP	CB-CG-OD2	5.33	123.10	118.30
1	B	703	ASP	CB-CG-OD2	5.32	123.08	118.30
1	A	703	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	764	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	183	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	52	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	441	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	651	ASP	CB-CG-OD2	5.22	122.99	118.30
1	B	754	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	461	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	405	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	157	LEU	CA-CB-CG	5.07	126.96	115.30
1	B	405	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	386	ASP	CB-CG-OD2	5.03	122.82	118.30

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	6207	0	6251	120	0
1	B	5964	0	6018	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	367	0	202	4	0
3	F	347	0	194	4	0
4	A	27	0	12	0	0
5	A	2	0	0	0	0
6	A	228	0	0	9	0
6	B	223	0	0	11	0
6	E	11	0	0	0	0
6	F	16	0	0	0	0
All	All	13392	0	12677	258	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 (258) 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:133:LEU:HG	1:A:240:LEU:HD11	1.40	1.02
1:A:727:THR:HG21	1:A:732:LEU:HD12	1.44	0.98
1:A:141:LYS:H	1:A:141:LYS:HD2	1.31	0.93
1:A:34:GLY:H	1:A:95:GLN:HE22	1.15	0.92
1:B:84:VAL:HG13	1:B:116:PRO:HA	1.52	0.92
1:A:727:THR:HG22	1:A:729:TYR:H	1.35	0.89
1:A:282:ASN:HD22	1:A:284:ALA:H	1.26	0.84
1:B:24:HIS:CD2	1:B:110:VAL:HG21	2.13	0.84
1:B:37:TYR:CE2	1:B:76:VAL:HG21	2.14	0.83
1:B:37:TYR:HE2	1:B:76:VAL:HG21	1.44	0.82
1:B:160:PRO:HG2	1:B:166:MSE:SE	2.29	0.82
1:A:305:ARG:NH2	1:A:347:ASP:OD2	2.13	0.81
1:A:46:ARG:NH2	1:A:88:GLU:OE1	2.15	0.79
1:A:397:MSE:HE1	1:A:552:LEU:HD22	1.67	0.77
1:B:311:LEU:HD23	1:B:636:ILE:HD12	1.66	0.77
1:B:735:LEU:HD22	1:B:739:MSE:HE2	1.67	0.76
1:B:327:THR:HG21	1:B:555:LEU:HD13	1.67	0.75
1:A:141:LYS:HD3	1:A:232:ARG:HH12	1.52	0.75
1:B:264:GLN:H	1:B:264:GLN:HE21	1.32	0.75
1:B:656:ARG:O	1:B:656:ARG:HG3	1.87	0.74
1:B:669:THR:HG22	1:B:671:MSE:H	1.52	0.74
1:A:439:LEU:HD22	1:A:439:LEU:H	1.50	0.74
1:A:34:GLY:H	1:A:95:GLN:NE2	1.84	0.74
1:B:290:THR:HG23	1:B:293:SER:H	1.50	0.73
1:B:282:ASN:HD22	1:B:284:ALA:H	1.37	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:799:ILE:HG22	1:B:799:ILE:O	1.90	0.71
1:B:20:LEU:HD21	1:B:110:VAL:HG23	1.72	0.70
1:B:157:LEU:HD23	1:B:157:LEU:O	1.91	0.70
1:B:94:GLU:HA	1:B:94:GLU:OE1	1.90	0.69
1:B:290:THR:HG22	1:B:293:SER:HB3	1.73	0.69
1:A:752:HIS:ND1	1:A:752:HIS:N	2.40	0.69
1:B:282:ASN:HD21	1:B:286:GLY:H	1.39	0.69
1:B:575:LYS:HB3	1:B:576:PRO:HD2	1.75	0.68
1:A:754:ASP:O	1:A:755:THR:HB	1.94	0.68
1:A:616:ASN:O	1:A:617:MSE:HB2	1.95	0.67
1:B:288:GLU:HG2	1:B:289:ASN:ND2	2.10	0.66
1:B:128:ARG:NH2	6:B:2028:HOH:O	2.29	0.66
1:A:64:GLU:O	6:A:2029:HOH:O	2.14	0.65
1:B:751:GLU:OE2	6:B:2205:HOH:O	2.14	0.65
1:B:290:THR:CG2	1:B:293:SER:H	2.10	0.65
1:B:430:ASN:HD22	1:B:433:LEU:H	1.44	0.64
1:B:163:ARG:HH12	1:B:188:SER:HB2	1.63	0.64
1:B:282:ASN:HD22	1:B:284:ALA:N	1.95	0.63
1:A:327:THR:HG21	1:A:555:LEU:HD13	1.80	0.63
1:B:639:TYR:OH	6:B:2180:HOH:O	2.13	0.63
1:A:282:ASN:HD22	1:A:284:ALA:N	1.93	0.62
1:B:471:HIS:CE1	1:B:493:GLN:HB2	2.34	0.62
1:A:593:ASN:O	1:A:594:GLU:HB3	1.98	0.62
1:B:474:TYR:CE1	1:B:500:ARG:HD2	2.33	0.62
1:B:316:ARG:HD3	1:B:650:ILE:O	2.00	0.62
1:B:26:GLU:HG3	1:B:27:ILE:HG13	1.80	0.62
1:B:799:ILE:CG2	1:B:799:ILE:O	2.48	0.62
1:B:163:ARG:HG3	1:B:189:LEU:HD21	1.82	0.62
1:A:128:ARG:NE	6:A:2048:HOH:O	2.16	0.61
1:B:282:ASN:ND2	1:B:286:GLY:H	1.99	0.60
1:B:362:PRO:HG3	1:B:419:VAL:HG13	1.83	0.60
1:B:268:ILE:HB	1:B:652:ARG:HG2	1.82	0.60
1:A:632:LEU:C	1:A:632:LEU:HD23	2.22	0.60
1:A:394:ARG:HA	1:A:397:MSE:HE3	1.84	0.59
1:B:483:HIS:CE1	1:B:484:LEU:HG	2.37	0.59
1:B:328:ILE:HG23	1:B:559:ALA:HA	1.82	0.59
1:A:133:LEU:CG	1:A:240:LEU:HD11	2.25	0.59
1:A:621:SER:OG	1:A:693:ASP:OD2	2.20	0.59
1:B:297:CYS:H	1:B:557:ASN:HD21	1.51	0.59
1:B:363:ARG:O	1:B:367:ARG:HG3	2.04	0.58
1:B:46:ARG:NH1	1:B:88:GLU:OE2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:GLY:HA3	1:A:703:ASP:HB3	1.86	0.58
1:A:295:LEU:HD11	1:A:633:MSE:HE3	1.85	0.58
1:B:345:VAL:HG11	1:B:549:LEU:HD13	1.86	0.58
1:B:735:LEU:HD22	1:B:739:MSE:CE	2.35	0.57
1:A:536:LEU:N	1:A:537:PRO:HD2	2.20	0.57
1:A:604:SER:HB2	1:A:605:PRO:CD	2.34	0.57
1:B:628:ALA:HB2	1:B:691:LEU:HD11	1.86	0.56
1:A:274:ARG:HG3	1:A:279:ILE:HD12	1.87	0.56
1:A:727:THR:HG23	6:A:2201:HOH:O	2.05	0.56
1:B:437:ARG:NH2	1:B:524:GLU:OE2	2.33	0.56
1:B:375:LEU:O	1:B:379:ARG:HG3	2.06	0.56
3:F:28:DG:H2"	3:F:29:DC:H5"	1.88	0.56
1:B:739:MSE:HE3	1:B:742:VAL:HG21	1.88	0.56
1:B:282:ASN:ND2	1:B:284:ALA:H	2.02	0.55
1:B:313:MSE:HE2	6:B:2088:HOH:O	2.06	0.55
1:A:412:ILE:HD11	1:A:415:PRO:HA	1.88	0.55
1:B:655:THR:O	1:B:655:THR:OG1	2.15	0.55
1:B:157:LEU:C	1:B:157:LEU:HD23	2.26	0.54
1:B:454:GLU:O	1:B:458:THR:HG23	2.07	0.54
1:A:24:HIS:N	1:A:25:PRO:HD3	2.23	0.53
1:A:609:MSE:HE2	1:A:723:THR:HG21	1.90	0.53
1:A:190:ILE:HG23	1:A:196:LEU:HD11	1.90	0.53
1:A:282:ASN:ND2	1:A:284:ALA:H	2.02	0.53
1:B:310:TRP:CB	1:B:636:ILE:HD11	2.38	0.53
1:B:73:TYR:O	1:B:76:VAL:HG23	2.09	0.53
1:B:227:VAL:HG12	1:B:260:MSE:HB2	1.90	0.53
1:B:22:ALA:HB3	6:B:2003:HOH:O	2.08	0.53
1:A:157:LEU:C	1:A:157:LEU:HD23	2.30	0.52
1:A:141:LYS:NZ	6:A:2053:HOH:O	2.19	0.52
1:A:282:ASN:HD21	1:A:286:GLY:H	1.57	0.52
1:A:388:ALA:HB3	1:A:389:PRO:HD3	1.89	0.52
1:B:310:TRP:HB3	1:B:636:ILE:HD11	1.91	0.52
2:E:3:DC:H2"	2:E:4:DT:C5'	2.39	0.52
1:A:632:LEU:O	1:A:632:LEU:HD23	2.10	0.52
1:A:227:VAL:HG12	1:A:260:MSE:HB2	1.92	0.52
1:B:609:MSE:HE2	1:B:723:THR:HG21	1.92	0.52
1:A:670:PHE:N	1:A:670:PHE:CD2	2.79	0.51
1:A:692:MSE:HE3	1:A:695:ILE:HD13	1.93	0.51
1:B:271:ALA:HB1	1:B:275:ARG:HH21	1.75	0.51
1:B:273:THR:HG23	1:B:655:THR:HG23	1.93	0.51
1:B:474:TYR:HA	1:B:506:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:VAL:HG23	1:A:591:VAL:O	2.10	0.51
1:A:670:PHE:N	1:A:670:PHE:HD2	2.09	0.51
1:B:430:ASN:HD21	1:B:432:GLU:HB2	1.76	0.50
1:B:575:LYS:CB	1:B:576:PRO:HD2	2.41	0.50
3:F:15:DC:H2"	3:F:16:DT:H5'	1.93	0.50
1:B:72:PRO:HG2	1:B:75:ALA:HB3	1.93	0.50
1:A:46:ARG:NE	6:A:2021:HOH:O	2.22	0.50
1:A:582:GLU:O	1:A:642:ALA:HA	2.12	0.50
1:A:394:ARG:O	1:A:397:MSE:HG2	2.10	0.50
1:A:263:GLU:HB3	1:A:268:ILE:HD11	1.93	0.50
1:B:324:ARG:O	1:B:328:ILE:HG13	2.11	0.50
1:A:628:ALA:HB2	1:A:691:LEU:HD11	1.92	0.50
1:B:24:HIS:HD2	1:B:110:VAL:HG21	1.74	0.50
2:E:3:DC:H2"	2:E:4:DT:H5"	1.93	0.50
1:A:160:PRO:HG2	1:A:166:MSE:SE	2.62	0.50
1:B:145:TYR:CG	1:B:166:MSE:HE1	2.47	0.50
1:A:439:LEU:HB3	1:A:512:LYS:HZ1	1.76	0.49
1:A:56:THR:OG1	1:A:57:LYS:N	2.45	0.49
1:A:620:LYS:HG2	1:A:747:LEU:HD13	1.94	0.49
1:A:297:CYS:H	1:A:557:ASN:ND2	2.09	0.49
1:A:357:LEU:O	1:A:358:ARG:HB2	2.10	0.49
1:A:359:THR:O	1:A:359:THR:HG22	2.12	0.49
1:A:640:VAL:HG11	1:A:645:VAL:HG21	1.94	0.49
1:B:46:ARG:O	1:B:50:LEU:HG	2.11	0.49
1:B:509:TYR:CD2	1:B:512:LYS:HD2	2.48	0.49
1:A:623:TYR:CE1	1:A:762:VAL:HG21	2.48	0.49
1:A:370:HIS:O	1:A:374:GLN:HG2	2.12	0.49
1:A:468:ASN:O	1:A:472:GLY:N	2.36	0.49
1:B:317:ASP:OD1	1:B:319:ARG:HB2	2.11	0.48
1:B:220:ARG:HG3	1:B:221:ASP:N	2.28	0.48
1:B:594:GLU:HG3	1:B:595:PRO:HD2	1.94	0.48
1:B:138:GLN:HE22	1:B:185:ALA:HB3	1.77	0.48
1:A:156:ARG:HD3	1:A:259:THR:HB	1.96	0.48
1:A:604:SER:HB2	1:A:605:PRO:HD2	1.96	0.48
1:A:608:ARG:HH11	1:A:608:ARG:HG3	1.78	0.48
1:B:405:ASP:OD2	1:B:409:ARG:NH1	2.47	0.48
1:A:656:ARG:NH1	1:A:658:GLY:HA2	2.28	0.48
1:A:670:PHE:CG	1:A:671:MSE:N	2.82	0.48
1:A:256:ARG:HH21	1:A:543:GLN:NE2	2.12	0.48
1:B:652:ARG:NH1	6:B:2182:HOH:O	2.43	0.47
1:A:154:ARG:NH2	6:A:2059:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:PRO:HD2	1:B:417:VAL:O	2.14	0.47
1:A:68:MSE:HE1	3:F:21:DC:H1'	1.96	0.47
1:B:229:ASN:C	1:B:231:PRO:HD3	2.34	0.47
1:A:282:ASN:ND2	1:A:286:GLY:H	2.13	0.47
1:B:271:ALA:CB	1:B:275:ARG:HH21	2.27	0.47
1:B:282:ASN:C	1:B:282:ASN:HD22	2.17	0.47
1:B:138:GLN:NE2	1:B:185:ALA:HB3	2.29	0.47
1:B:625:ARG:NE	6:B:2177:HOH:O	2.44	0.47
1:A:446:TYR:CD1	1:A:446:TYR:C	2.89	0.47
1:A:713:GLU:HG3	1:A:739:MSE:SE	2.65	0.47
1:A:512:LYS:HA	1:A:515:THR:OG1	2.14	0.46
1:A:141:LYS:N	1:A:141:LYS:HD2	2.15	0.46
1:A:46:ARG:NH2	6:A:2022:HOH:O	2.46	0.46
1:A:133:LEU:HG	1:A:240:LEU:CD1	2.29	0.46
1:B:474:TYR:CA	1:B:506:LEU:HD21	2.44	0.46
1:B:282:ASN:ND2	1:B:284:ALA:N	2.61	0.46
1:B:474:TYR:CD1	1:B:500:ARG:HD2	2.50	0.46
1:B:388:ALA:HB3	1:B:389:PRO:HD3	1.98	0.46
1:A:624:MSE:O	1:A:627:THR:HB	2.16	0.46
1:A:493:GLN:NE2	1:A:500:ARG:HH11	2.14	0.45
1:A:608:ARG:NH1	1:A:741:GLY:HA3	2.30	0.45
1:A:46:ARG:NH2	1:A:88:GLU:CD	2.70	0.45
1:B:373:GLN:O	6:B:2113:HOH:O	2.21	0.45
1:A:369:ARG:HG3	1:A:407:LEU:HB3	1.97	0.45
1:B:243:TYR:O	1:B:247:THR:HG23	2.17	0.45
1:B:460:LEU:HD22	1:B:481:GLN:HB3	1.98	0.45
1:B:71:ILE:O	1:B:71:ILE:HG13	2.16	0.45
1:A:141:LYS:HB2	1:A:232:ARG:NH2	2.31	0.45
1:A:656:ARG:HH12	1:A:658:GLY:HA2	1.81	0.45
1:A:651:ASP:OD1	1:A:652:ARG:N	2.50	0.45
1:A:369:ARG:HG3	1:A:407:LEU:CB	2.46	0.45
1:B:748:ASP:OD1	1:B:748:ASP:C	2.54	0.44
1:A:448:GLU:O	1:A:452:VAL:HG23	2.18	0.44
1:A:141:LYS:H	1:A:141:LYS:CD	2.05	0.44
1:B:111:VAL:HG22	1:B:111:VAL:O	2.16	0.44
1:B:388:ALA:N	1:B:389:PRO:CD	2.80	0.44
1:A:280:THR:OG1	1:A:312:HIS:HE1	2.01	0.44
1:A:49:GLN:HE21	1:A:49:GLN:HB3	1.65	0.44
1:A:670:PHE:CE2	1:A:672:VAL:HG23	2.52	0.44
1:B:404:ARG:O	1:B:408:GLU:HG3	2.18	0.44
1:A:2:SER:N	6:A:2001:HOH:O	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HD21	1:A:83:LEU:HG	1.98	0.44
1:B:507:LYS:HD2	1:B:507:LYS:HA	1.66	0.44
1:A:773:LEU:CD2	1:B:707:LEU:HG	2.47	0.44
1:A:419:VAL:HG21	1:A:528:TYR:CE2	2.53	0.44
1:B:315:VAL:HG23	6:B:2073:HOH:O	2.18	0.44
1:B:200:PRO:HB2	1:B:202:TRP:CD1	2.52	0.43
1:B:377:GLU:OE1	1:B:377:GLU:HA	2.18	0.43
1:B:536:LEU:N	1:B:537:PRO:CD	2.80	0.43
1:B:777:ALA:HA	1:B:786:ILE:HD11	2.00	0.43
1:A:657:VAL:O	1:A:657:VAL:HG12	2.19	0.43
1:B:310:TRP:HB3	1:B:636:ILE:CG1	2.49	0.43
1:A:457:ARG:NH2	6:A:2148:HOH:O	2.50	0.43
1:B:179:LEU:HD23	1:B:197:ARG:HB2	2.00	0.43
1:A:139:ASP:HB2	1:A:232:ARG:HH11	1.83	0.43
1:A:274:ARG:HE	1:A:312:HIS:HD2	1.64	0.43
1:A:487:ILE:HD13	1:A:487:ILE:HA	1.81	0.43
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.93	0.43
1:B:615:PRO:HB2	1:B:617:MSE:HG2	1.99	0.43
1:A:328:ILE:HG23	1:A:559:ALA:HA	2.01	0.43
1:A:375:LEU:HB2	1:A:376:PRO:HD3	2.01	0.43
1:B:436:TRP:CH2	1:B:519:LYS:HD2	2.54	0.43
1:A:139:ASP:HB2	1:A:232:ARG:NH1	2.34	0.42
1:B:375:LEU:HD22	1:B:397:MSE:HG2	2.00	0.42
1:B:650:ILE:HA	1:B:687:TYR:O	2.19	0.42
1:A:163:ARG:HG2	1:A:189:LEU:HD21	2.01	0.42
1:B:436:TRP:CZ2	1:B:519:LYS:HD2	2.54	0.42
1:A:138:GLN:CG	1:A:139:ASP:N	2.81	0.42
1:A:728:HIS:ND1	1:A:728:HIS:N	2.67	0.42
1:B:164:GLU:H	1:B:164:GLU:CD	2.23	0.42
1:B:747:LEU:HD23	1:B:761:SER:O	2.20	0.42
1:A:345:VAL:HG11	1:A:549:LEU:HD13	2.02	0.42
1:A:439:LEU:HB3	1:A:512:LYS:NZ	2.35	0.42
1:A:585:HIS:CE1	1:A:587:VAL:HB	2.55	0.42
1:B:508:GLU:O	1:B:511:ASP:HB2	2.20	0.42
1:B:20:LEU:CD2	1:B:110:VAL:HG23	2.45	0.42
1:B:131:ASN:ND2	6:B:2035:HOH:O	2.50	0.42
1:A:558:LEU:HD13	1:A:638:SER:HB2	2.02	0.42
1:B:473:TYR:O	1:B:507:LYS:NZ	2.52	0.42
1:A:361:ARG:O	1:A:364:ASP:HB2	2.20	0.41
2:E:3:DC:H2"	2:E:4:DT:H5'	2.03	0.41
1:A:493:GLN:HE22	1:A:500:ARG:HH11	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ARG:NE	6:B:2145:HOH:O	2.50	0.41
1:A:382:LEU:HD11	1:A:552:LEU:HD21	2.01	0.41
1:A:617:MSE:SE	1:B:671:MSE:HG3	2.71	0.41
1:B:585:HIS:HA	1:B:626:GLN:HB2	2.02	0.41
1:A:362:PRO:HG3	1:A:419:VAL:HG22	2.03	0.41
1:B:290:THR:HG22	1:B:293:SER:CB	2.45	0.41
1:B:310:TRP:HB2	1:B:636:ILE:HD11	2.03	0.41
1:B:669:THR:CG2	1:B:671:MSE:HB2	2.50	0.41
1:B:798:SER:C	1:B:800:SER:H	2.24	0.41
2:E:3:DC:C2'	2:E:4:DT:H5"	2.50	0.41
1:A:604:SER:CB	1:A:605:PRO:CD	2.98	0.41
1:B:127:GLU:HG3	1:B:301:PRO:HB3	2.02	0.41
3:F:19:DT:H2'	3:F:20:DG:C8	2.56	0.41
1:A:282:ASN:C	1:A:282:ASN:HD22	2.24	0.41
1:A:64:GLU:HA	1:A:65:PRO:HD2	1.81	0.41
1:B:84:VAL:HG11	1:B:119:ILE:HD13	2.01	0.41
1:B:565:LEU:HD22	1:B:590:GLN:NE2	2.36	0.41
1:B:735:LEU:HB2	1:B:736:PRO:HD3	2.03	0.41
1:B:755:THR:HB	1:B:756:ILE:H	1.58	0.41
1:B:604:SER:HB2	1:B:605:PRO:HD2	2.03	0.40
1:A:359:THR:CG2	1:A:359:THR:O	2.69	0.40
1:A:771:TYR:O	1:A:775:VAL:HG23	2.21	0.40
1:A:264:GLN:O	1:A:316:ARG:HD3	2.22	0.40
1:B:455:ARG:HD2	1:B:463:LEU:O	2.22	0.40
1:B:655:THR:HG22	1:B:691:LEU:HD12	2.02	0.40
1:B:37:TYR:CD2	1:B:76:VAL:HG21	2.54	0.40
1:B:694:GLU:N	1:B:726:ALA:O	2.46	0.40
1:B:72:PRO:HB2	1:B:74:HIS:ND1	2.37	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	784/800 (98%)	753 (96%)	29 (4%)	2 (0%)	41	46
1	B	746/800 (93%)	718 (96%)	25 (3%)	3 (0%)	34	37
All	All	1530/1600 (96%)	1471 (96%)	54 (4%)	5 (0%)	41	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	594	GLU
1	A	755	THR
1	B	46	ARG
1	B	45	LYS
1	B	617	MSE

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	656/640 (102%)	625 (95%)	31 (5%)	26	33
1	B	631/640 (99%)	601 (95%)	30 (5%)	25	32
All	All	1287/1280 (100%)	1226 (95%)	61 (5%)	26	33

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	52	ASP
1	A	57	LYS
1	A	140	SER
1	A	141	LYS
1	A	155	PHE
1	A	157	LEU
1	A	178	LEU
1	A	264	GLN
1	A	282	ASN
1	A	311	LEU

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Mol	Chain	Res	Type
1	A	369	ARG
1	A	384	THR
1	A	387	SER
1	A	431	GLU
1	A	439	LEU
1	A	444	THR
1	A	445	ASP
1	A	479	ARG
1	A	487	ILE
1	A	488	ASN
1	A	506	LEU
1	A	512	LYS
1	A	513	VAL
1	A	515	THR
1	A	531	LEU
1	A	656	ARG
1	A	670	PHE
1	A	734	GLN
1	A	752	HIS
1	A	784	GLU
1	B	20	LEU
1	B	49	GLN
1	B	137	TRP
1	B	155	PHE
1	B	157	LEU
1	B	178	LEU
1	B	220	ARG
1	B	264	GLN
1	B	282	ASN
1	B	302	MSE
1	B	315	VAL
1	B	335	THR
1	B	338	LEU
1	B	352	LEU
1	B	357	LEU
1	B	399	GLU
1	B	419	VAL
1	B	424	VAL
1	B	492	ARG
1	B	500	ARG
1	B	507	LYS
1	B	535	LEU

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Mol	Chain	Res	Type
1	B	584	ARG
1	B	594	GLU
1	B	615	PRO
1	B	636	ILE
1	B	732	LEU
1	B	755	THR
1	B	763	GLN
1	B	788	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	95	GLN
1	A	171	GLN
1	A	248	GLN
1	A	282	ASN
1	A	312	HIS
1	A	488	ASN
1	A	493	GLN
1	A	543	GLN
1	A	557	ASN
1	A	602	ASN
1	A	606	GLN
1	A	616	ASN
1	A	683	ASN
1	A	734	GLN
1	B	24	HIS
1	B	131	ASN
1	B	138	GLN
1	B	264	GLN
1	B	282	ASN
1	B	430	ASN
1	B	543	GLN
1	B	557	ASN
1	B	717	ASN
1	B	791	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 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	5	24,29,29	1.17	2 (8%)	29,45,45	1.45	3 (10%)

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	5	-	0/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1801	ADP	C2-N3	3.75	1.38	1.32
4	A	1801	ADP	C2-N1	2.38	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1801	ADP	N3-C2-N1	-5.73	119.73	128.68
4	A	1801	ADP	C3'-C2'-C1'	2.89	105.33	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1801	ADP	O2B-PB-O3A	2.31	112.39	104.64

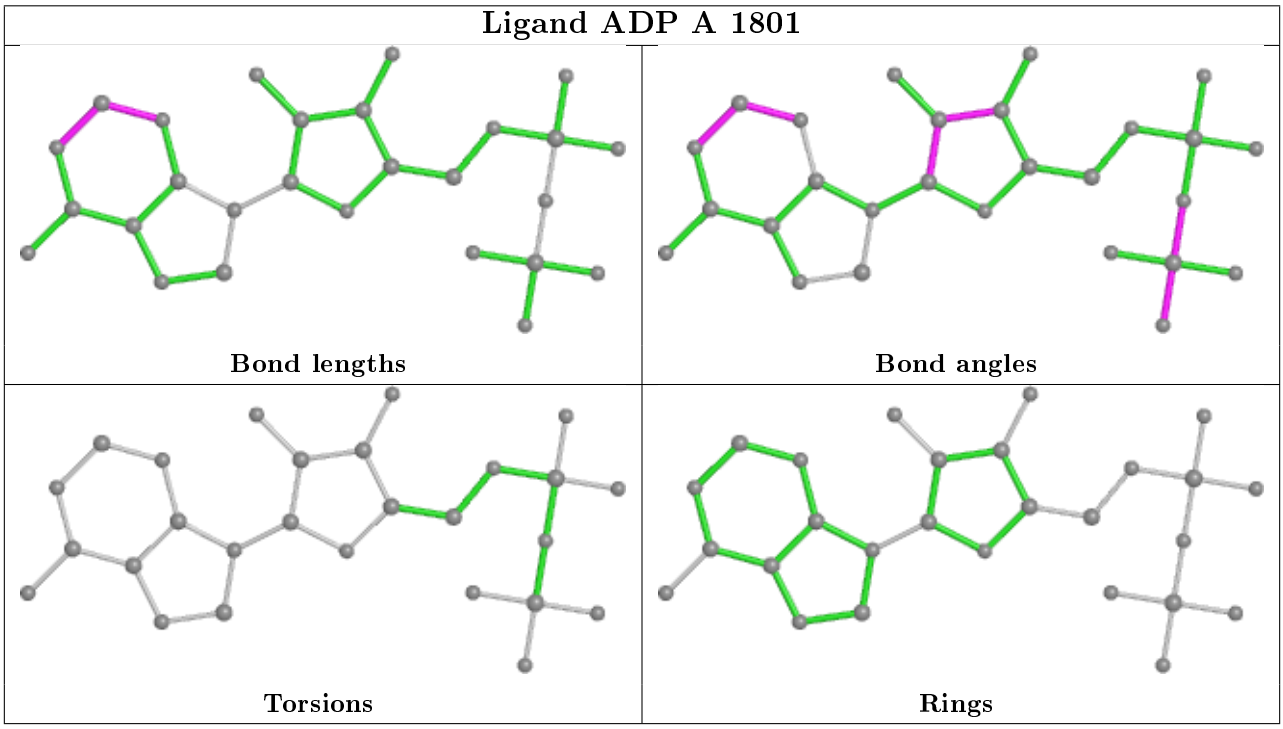
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	765/800 (95%)	0.18	42 (5%) 25 24	30, 44, 61, 82	0
1	B	732/800 (91%)	0.20	34 (4%) 32 31	26, 44, 66, 83	0
2	E	18/30 (60%)	0.20	3 (16%) 1 1	39, 50, 95, 101	0
3	F	17/30 (56%)	-0.22	1 (5%) 22 21	38, 50, 83, 92	0
All	All	1532/1660 (92%)	0.19	80 (5%) 27 26	26, 44, 65, 101	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	THR	6.9
2	E	18	DG	5.3
1	B	29	LEU	5.1
1	B	800	SER	4.4
1	B	28	LEU	4.2
1	A	658	GLY	4.1
1	B	41	TYR	4.0
1	B	475	ILE	3.9
1	A	140	SER	3.8
1	A	800	SER	3.7
1	B	30	PHE	3.6
1	A	62	ALA	3.5
1	B	52	ASP	3.5
1	A	475	ILE	3.4
1	A	441	ASP	3.3
1	A	192	GLY	3.2
1	A	768	SER	3.2
2	E	1	DA	3.2
1	B	658	GLY	3.2
1	B	183	ASP	3.1
1	B	140	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	19	ARG	3.1
1	A	752	HIS	3.0
1	B	141	LYS	3.0
1	A	754	ASP	2.9
1	B	135	ALA	2.9
1	B	35	ASP	2.9
1	A	141	LYS	2.9
1	B	39	LEU	2.8
1	A	443	ALA	2.8
1	B	74	HIS	2.7
1	B	672	VAL	2.7
1	B	452	VAL	2.7
1	A	445	ASP	2.7
1	A	511	ASP	2.7
1	B	90	VAL	2.7
2	E	16	DG	2.6
1	A	98	ASP	2.6
1	B	592	LEU	2.6
1	A	103	LYS	2.6
1	B	108	ARG	2.6
1	A	63	GLY	2.6
1	A	755	THR	2.6
1	A	220	ARG	2.6
1	A	563	TYR	2.6
3	F	14	DA	2.6
1	B	46	ARG	2.6
1	A	365	LEU	2.5
1	A	61	SER	2.5
1	B	54	SER	2.5
1	A	386	ASP	2.5
1	A	555	LEU	2.5
1	A	448	GLU	2.4
1	A	64	GLU	2.4
1	A	697	ARG	2.3
1	A	670	PHE	2.3
1	A	552	LEU	2.3
1	A	640	VAL	2.3
1	A	431	GLU	2.3
1	A	26	GLU	2.3
1	B	136	ILE	2.3
1	A	595	PRO	2.3
1	A	612	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	558	LEU	2.2
1	B	275	ARG	2.2
1	A	442	GLY	2.2
1	B	49	GLN	2.2
1	B	456	GLU	2.2
1	A	97	GLY	2.2
1	A	591	VAL	2.2
1	B	445	ASP	2.2
1	B	457	ARG	2.2
1	A	399	GLU	2.2
1	A	411	ILE	2.2
1	A	283	LEU	2.2
1	B	38	GLU	2.1
1	B	754	ASP	2.1
1	B	332	GLN	2.1
1	A	440	ALA	2.1
1	B	185	ALA	2.1

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 carbohydrates 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.

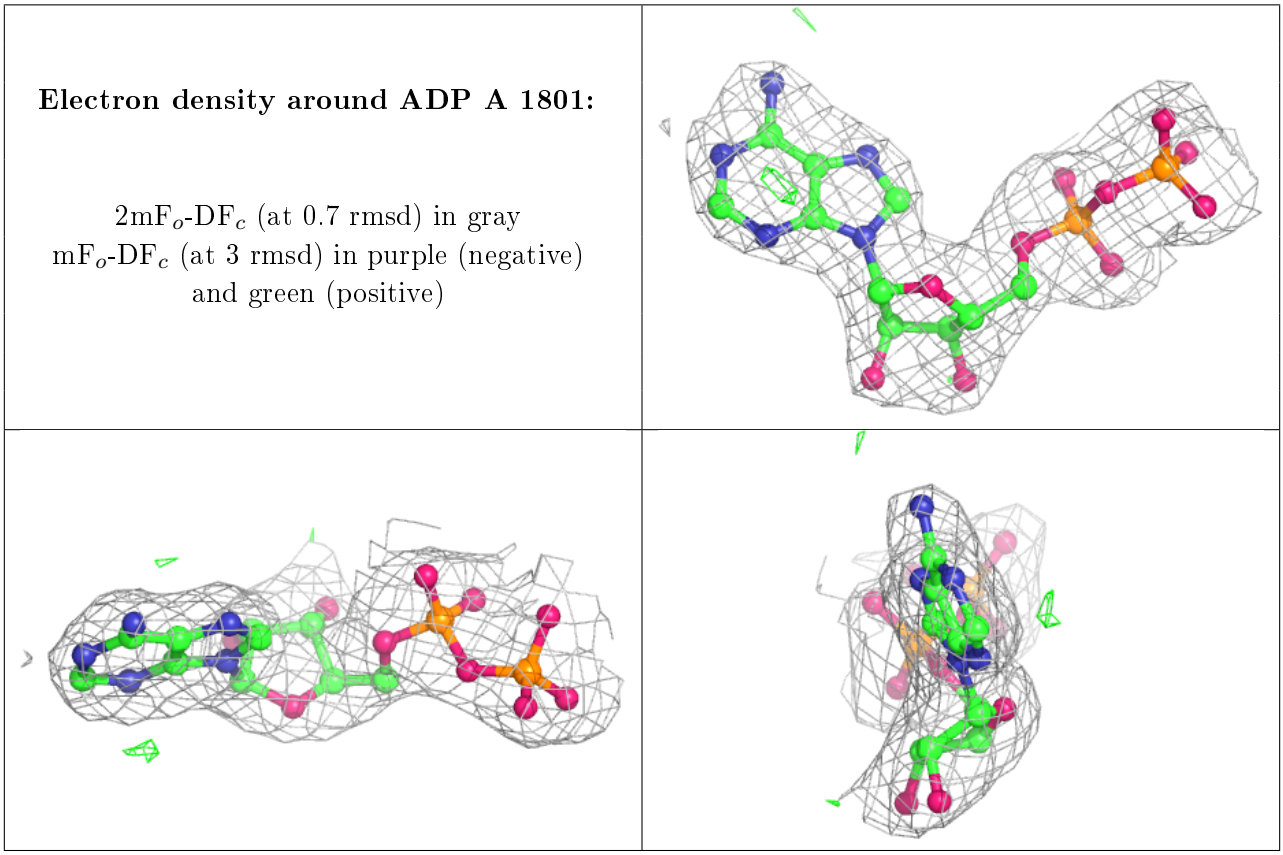
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	A	1011	1/1	0.79	0.19	57,57,57,57	0
5	MG	A	1001	1/1	0.91	0.07	40,40,40,40	0
4	ADP	A	1801	27/27	0.97	0.10	40,48,49,52	0

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 (i)

There are no such residues in this entry.