Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 07:55 AM EDT

PDB ID	:	5F2L
Title	:	Tagatose-1,6-bisphosphate aldolase from Streptococcus pyogenes in complex with competitive inhibitor talitol-1,6-bisphosphate
Authors	:	LowKam, C.
Deposited on	:	2015-12-02
Resolution	:	1.75 Å(reported)

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

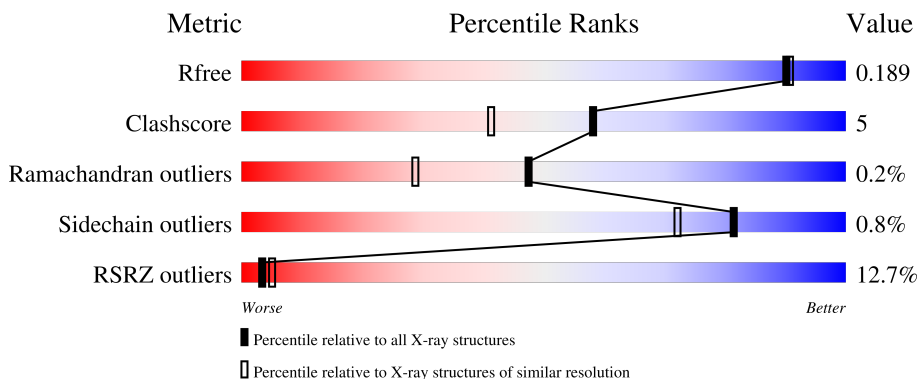|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.75 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	Percentile Ranks	Value
Rfree		0.189
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		0.8%
RSRZ outliers		12.7%

Worse   *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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	327	10% 94% · ·
1	B	327	6% 93% 6% ·
1	C	327	13% 90% 10%
1	D	327	21% 91% 8% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	B	403	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22115 atoms, of which 10292 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 Tagatose 1,6-diphosphate aldolase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	324	Total	C	H	N	O	S	0	9	0
			5153	1640	2565	426	513	9			
1	C	326	Total	C	H	N	O	S	0	5	0
			5166	1644	2575	427	511	9			
1	B	325	Total	C	H	N	O	S	0	15	0
			5217	1660	2597	432	519	9			
1	D	325	Total	C	H	N	O	S	0	2	0
			5119	1631	2552	423	504	9			

- Molecule 2 is D-MANNITOL-1,6-DIPHOSPHATE (three-letter code: M2P) (formula: $C_6H_{16}O_{12}P_2$).
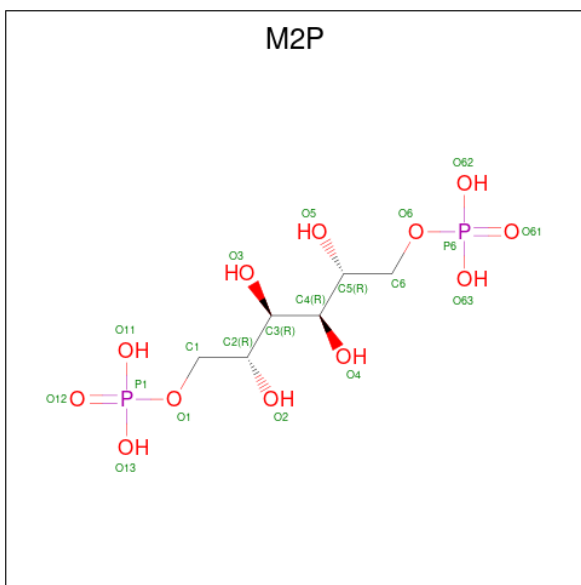
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	1
			40	12	24	4		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Ca 2	0	0
3	C	3	Total 3	Ca 3	0	0
3	B	2	Total 2	Ca 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).
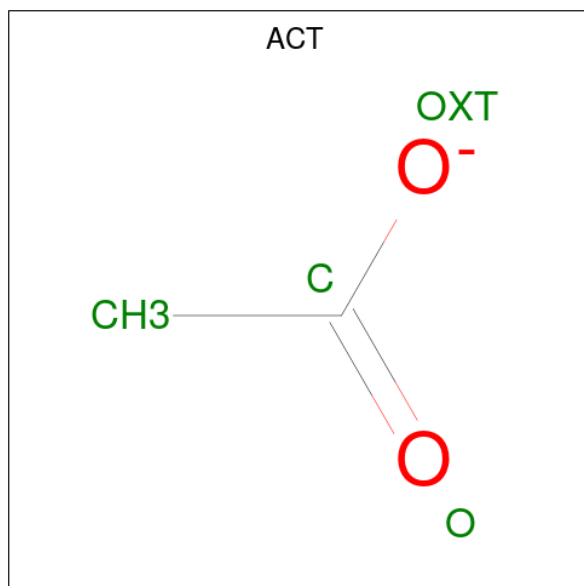
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total 7	C 2	H 3	O 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	446	Total O 446 446	0	0
6	C	267	Total O 267 267	0	0
6	B	448	Total O 448 448	0	0
6	D	242	Total O 242 242	0	0

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.

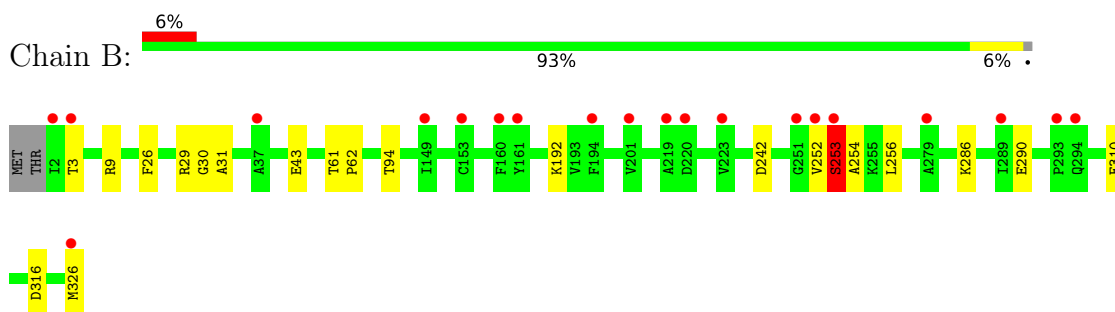- Molecule 1: Tagatose 1,6-diphosphate aldolase 2
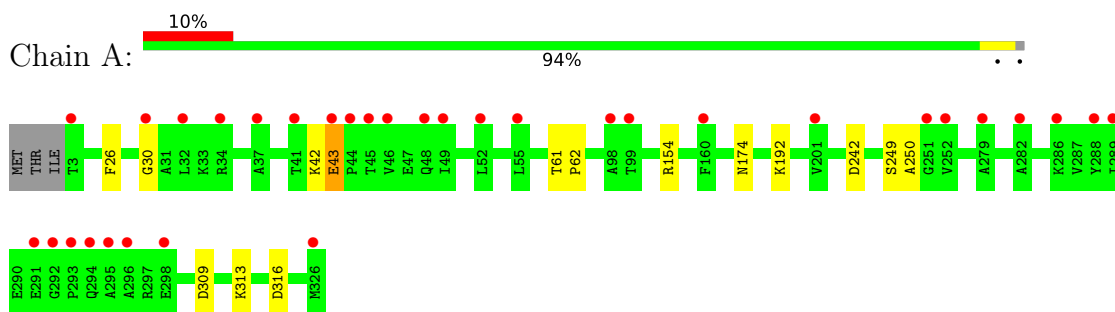
Chain A:

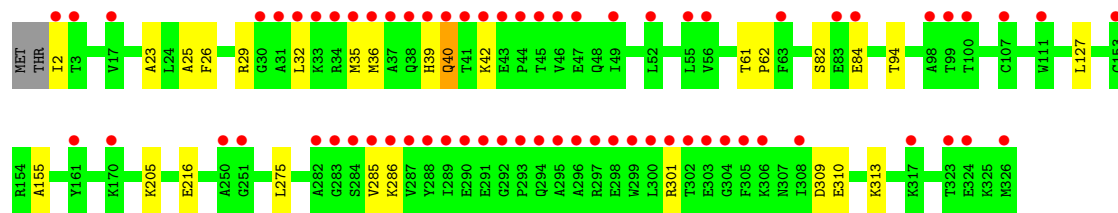

- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

Chain C:

- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

Chain B:

- Molecule 1: Tagatose 1,6-diphosphate aldolase 2

Chain D:
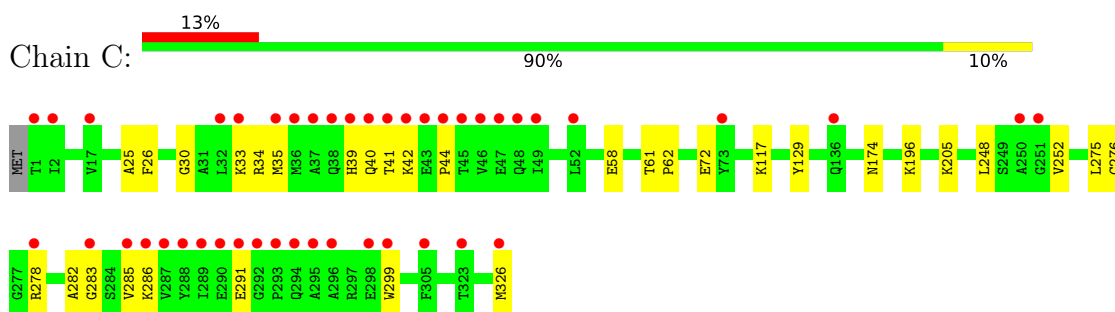
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.97Å 108.03Å 237.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.19 – 1.75 45.19 – 1.76	Depositor EDS
% Data completeness (in resolution range)	89.8 (45.19-1.75) 89.5 (45.19-1.76)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 1.76Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.163 , 0.189 0.170 , 0.189	Depositor DCC
R_{free} test set	2000 reflections (1.29%)	wwPDB-VP
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	22115	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.3946e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, ACT, CL, M2P

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	0.64	0/2659	0.59	0/3591
1	B	0.65	0/2692	0.64	1/3637 (0.0%)
1	C	0.56	0/2649	0.58	0/3576
1	D	0.48	0/2620	0.53	0/3536
All	All	0.59	0/10620	0.58	1/14340 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	43	GLU	C-N-CD	5.57	140.10	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	253[A]	SER	Mainchain

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	2588	2565	2535	13	0
1	B	2620	2597	2558	23	0
1	C	2591	2575	2560	35	1
1	D	2567	2552	2544	25	1
2	A	40	0	24	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
4	B	1	0	0	2	0
4	C	1	0	0	1	0
4	D	1	0	0	1	0
5	D	4	3	3	1	0
6	A	446	0	0	7	3
6	B	448	0	0	7	2
6	C	267	0	0	14	2
6	D	242	0	0	7	1
All	All	11823	10292	10224	100	5

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 5.

All (100) 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:42:LYS:HB2	6:A:3402:HOH:O	1.15	1.32
1:C:326:MET:CE	6:C:672:HOH:O	1.72	1.31
1:D:39:HIS:ND1	1:D:286:LYS:HD3	1.59	1.17
1:D:39:HIS:CE1	1:D:286:LYS:HD3	1.85	1.11
1:C:252:VAL:N	6:C:501:HOH:O	1.90	1.04
5:D:401:ACT:O	6:D:501:HOH:O	1.78	1.01
1:B:252[B]:VAL:HB	1:B:256:LEU:HD23	1.37	1.00
1:D:39:HIS:ND1	1:D:286:LYS:CD	2.29	0.95
1:D:286:LYS:NZ	6:D:502:HOH:O	2.01	0.92
1:B:252[B]:VAL:CB	1:B:256:LEU:HD23	1.99	0.92
1:C:41:THR:O	1:C:42:LYS:HG3	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:OE1	6:B:501:HOH:O	1.93	0.85
1:B:192:LYS:HE3	6:B:681:HOH:O	1.74	0.85
1:B:252[B]:VAL:CG1	1:B:256:LEU:HD23	2.07	0.84
1:C:39:HIS:CE1	1:C:286:LYS:HB3	2.11	0.84
1:C:39:HIS:HE1	1:C:286:LYS:HB3	1.43	0.83
1:C:205[B]:LYS:HG2	1:C:248:LEU:HD21	1.62	0.80
1:B:252[B]:VAL:O	1:B:253[B]:SER:CB	2.30	0.79
1:C:326:MET:HE3	6:C:672:HOH:O	1.50	0.78
1:B:242[B]:ASP:OD1	6:B:503:HOH:O	2.03	0.76
1:B:310:GLU:OE1	6:B:502:HOH:O	2.03	0.75
1:A:42:LYS:CB	6:A:3402:HOH:O	1.91	0.73
4:C:404:CL:CL	6:C:754:HOH:O	2.45	0.72
1:C:39:HIS:CE1	1:C:286:LYS:CB	2.72	0.71
1:B:31:ALA:N	4:B:403:CL:CL	2.59	0.71
1:C:196:LYS:HD2	6:C:731:HOH:O	1.92	0.70
1:B:252[B]:VAL:O	1:B:253[B]:SER:HB3	1.93	0.69
4:D:402:CL:CL	6:D:735:HOH:O	2.46	0.69
1:C:276:CYS:SG	6:C:755:HOH:O	2.51	0.69
1:C:39:HIS:HE1	1:C:286:LYS:CB	2.06	0.68
1:B:242[B]:ASP:OD1	6:B:504:HOH:O	2.12	0.66
1:C:291:GLU:OE2	6:C:502:HOH:O	2.13	0.66
1:C:205[B]:LYS:HG2	1:C:248:LEU:CD2	2.25	0.65
1:D:310:GLU:OE2	6:D:503:HOH:O	2.13	0.65
1:C:72[A]:GLU:OE2	6:C:503:HOH:O	2.14	0.64
1:A:242[B]:ASP:OD1	6:A:3101:HOH:O	2.15	0.64
1:D:32:LEU:O	1:D:36:MET:HG3	2.00	0.61
1:D:309:ASP:OD2	1:D:313:LYS:NZ	2.33	0.60
1:C:326:MET:HE1	6:C:672:HOH:O	1.67	0.60
1:D:25:ALA:HB2	1:D:275:LEU:HG	1.82	0.59
1:C:205[B]:LYS:HZ2	1:C:275:LEU:HD22	1.67	0.59
1:B:252[B]:VAL:HB	1:B:256:LEU:CD2	2.23	0.57
1:A:242[B]:ASP:OD1	6:A:3102:HOH:O	2.17	0.56
1:B:3:THR:O	6:B:505:HOH:O	2.18	0.56
1:B:9:ARG:NH2	1:B:326:MET:SD	2.74	0.56
1:C:30:GLY:O	1:C:34:ARG:HG3	2.06	0.56
1:C:35:MET:HE2	1:C:285:VAL:HG21	1.87	0.56
1:C:41:THR:O	1:C:42:LYS:CG	2.52	0.56
1:A:42:LYS:NZ	1:A:43:GLU:O	2.36	0.55
1:B:286:LYS:NZ	1:B:290:GLU:OE2	2.40	0.54
1:C:129:TYR:OH	6:C:504:HOH:O	2.18	0.54
1:C:25:ALA:HB2	1:C:275:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252[B]:VAL:CG1	1:B:256:LEU:CD2	2.82	0.54
1:B:252[B]:VAL:O	1:B:253[B]:SER:OG	2.27	0.53
1:D:2:ILE:N	6:D:511:HOH:O	2.42	0.53
1:C:196:LYS:CD	6:C:731:HOH:O	2.53	0.52
1:A:174[B]:ASN:ND2	6:A:3110:HOH:O	2.40	0.52
1:A:242[B]:ASP:OD2	6:A:3103:HOH:O	2.19	0.52
1:B:242[B]:ASP:OD2	6:B:506:HOH:O	2.19	0.52
1:B:252[B]:VAL:HG12	1:B:256:LEU:HD23	1.87	0.52
1:C:283:GLY:HA3	1:C:299:TRP:CZ2	2.45	0.51
1:D:301:ARG:NH2	6:D:510:HOH:O	2.40	0.51
1:D:23:ALA:HB3	1:D:275:LEU:HD12	1.92	0.51
1:C:39:HIS:ND1	1:C:286:LYS:HA	2.26	0.51
1:D:35:MET:HE2	1:D:285:VAL:HG11	1.94	0.50
1:A:30:GLY:N	2:A:3001[A]:M2P:O63	2.46	0.48
1:D:84:GLU:O	6:D:504:HOH:O	2.20	0.48
1:C:58:GLU:OE1	6:C:505:HOH:O	2.20	0.48
1:A:154:ARG:NH1	1:D:155:ALA:O	2.47	0.48
2:A:3001[A]:M2P:O5	2:A:3001[A]:M2P:O3	2.28	0.47
1:C:205[B]:LYS:HD2	1:C:275:LEU:HD22	1.95	0.47
1:D:40:GLN:NE2	1:D:42:LYS:HG3	2.30	0.47
1:C:33:LYS:HE3	1:C:44:PRO:HD2	1.96	0.46
1:B:30:GLY:N	4:B:403:CL:CL	2.85	0.46
1:C:205[B]:LYS:NZ	1:C:275:LEU:HD22	2.31	0.46
1:A:309:ASP:OD2	1:A:313:LYS:NZ	2.49	0.46
1:C:117:LYS:NZ	6:C:512:HOH:O	2.46	0.45
1:C:174[B]:ASN:ND2	6:C:515:HOH:O	2.49	0.45
1:D:82:SER:OG	1:D:84:GLU:OE1	2.34	0.45
1:C:61:THR:N	1:C:62:PRO:CD	2.81	0.44
1:D:29:ARG:CZ	1:D:94:THR:HG23	2.47	0.43
1:D:205[B]:LYS:HZ2	1:D:275:LEU:HD22	1.84	0.43
2:A:3001[A]:M2P:HO3	2:A:3001[A]:M2P:HO5	1.64	0.43
1:A:61:THR:N	1:A:62:PRO:CD	2.82	0.42
1:C:35:MET:CE	1:C:285:VAL:HG21	2.48	0.42
1:D:23:ALA:CB	1:D:275:LEU:HD12	2.48	0.42
1:D:205[B]:LYS:HZ2	1:D:275:LEU:CD2	2.32	0.42
1:A:192:LYS:HE3	6:A:3132:HOH:O	2.20	0.41
1:C:278:ARG:O	1:C:282:ALA:N	2.52	0.41
1:D:61:THR:N	1:D:62:PRO:CD	2.83	0.41
1:B:61:THR:N	1:B:62:PRO:CD	2.83	0.41
1:D:39:HIS:CG	1:D:286:LYS:CD	3.01	0.41
1:C:40:GLN:HE22	1:C:44:PRO:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ARG:CZ	1:D:94:THR:CG2	2.99	0.41
1:D:40:GLN:NE2	1:D:42:LYS:O	2.45	0.41
1:A:249:SER:O	1:A:250:ALA:HB3	2.21	0.41
1:D:127:LEU:C	1:D:127:LEU:HD23	2.41	0.41
1:C:25:ALA:HB2	1:C:275:LEU:CG	2.52	0.40
1:B:29:ARG:HB2	1:B:94:THR:HG21	2.03	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:3166:HOH:O	6:B:854:HOH:O[1_655]	1.98	0.22
6:C:709:HOH:O	6:D:654:HOH:O[2_565]	1.98	0.22
1:C:286:LYS:NZ	1:D:216:GLU:OE1[2_565]	2.11	0.09
6:A:3165:HOH:O	6:B:845:HOH:O[1_655]	2.15	0.05
6:A:3429:HOH:O	6:C:681:HOH:O[1_655]	2.17	0.03

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	331/327 (101%)	321 (97%)	10 (3%)	0	100	100
1	B	337/327 (103%)	318 (94%)	15 (4%)	4 (1%)	13	3
1	C	329/327 (101%)	316 (96%)	13 (4%)	0	100	100
1	D	325/327 (99%)	316 (97%)	9 (3%)	0	100	100
All	All	1322/1308 (101%)	1271 (96%)	47 (4%)	4 (0%)	47	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	253[A]	SER
1	B	253[B]	SER
1	B	254[A]	ALA
1	B	254[B]	ALA

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	278/274 (102%)	275 (99%)	3 (1%)	73	60
1	B	281/274 (103%)	277 (99%)	4 (1%)	67	52
1	C	277/274 (101%)	276 (100%)	1 (0%)	91	87
1	D	274/274 (100%)	272 (99%)	2 (1%)	84	75
All	All	1110/1096 (101%)	1100 (99%)	10 (1%)	81	67

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	PHE
1	A	43	GLU
1	A	316	ASP
1	C	26	PHE
1	B	26	PHE
1	B	253[A]	SER
1	B	253[B]	SER
1	B	316	ASP
1	D	26	PHE
1	D	40	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	39	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 10 are monoatomic - leaving 3 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	$\#|Z| > 2$
2	M2P	A	3001[B]	-	19,19,19	0.85	0	28,28,28	1.46	4 (14%)
5	ACT	D	401	-	3,3,3	0.94	0	3,3,3	1.86	2 (66%)
2	M2P	A	3001[A]	-	19,19,19	1.01	2 (10%)	28,28,28	0.80	1 (3%)

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
2	M2P	A	3001[B]	-	-	11/24/24/24	-
2	M2P	A	3001[A]	-	-	11/24/24/24	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001[A]	M2P	C3-C4	-2.24	1.48	1.53
2	A	3001[A]	M2P	O5-C5	-2.12	1.38	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001[B]	M2P	C5-C4-C3	-4.88	104.84	112.47
2	A	3001[B]	M2P	O2-C2-C3	-3.02	101.75	109.10
2	A	3001[B]	M2P	O3-C3-C4	2.64	115.63	109.47
2	A	3001[A]	M2P	C2-C3-C4	-2.39	108.73	112.47
5	D	401	ACT	OXT-C-O	-2.38	113.27	122.05
5	D	401	ACT	OXT-C-CH3	2.18	124.18	115.18
2	A	3001[B]	M2P	C2-C3-C4	-2.08	109.21	112.47

There are no chirality outliers.
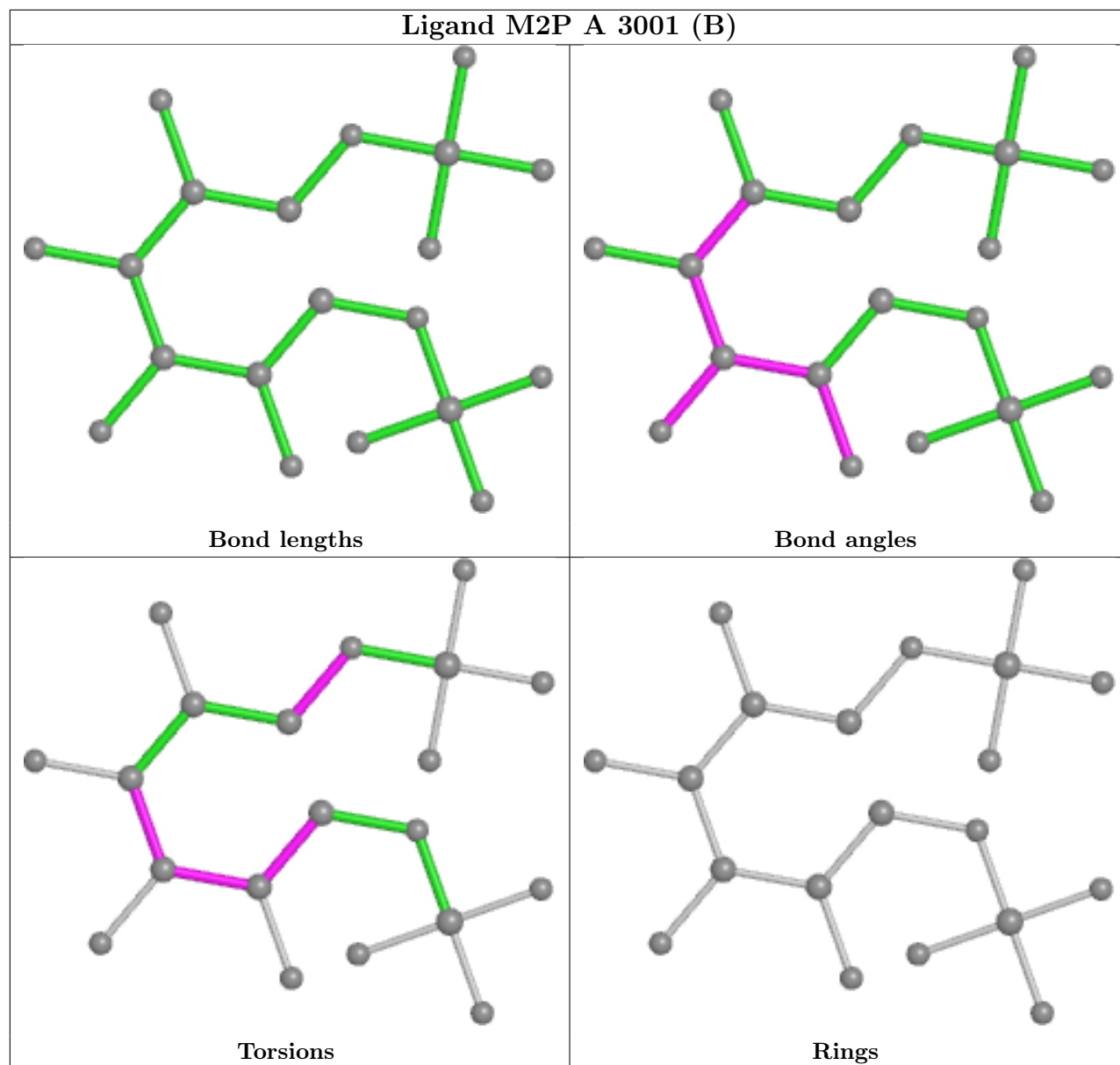
All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001[A]	M2P	C4-C5-C6-O6
2	A	3001[A]	M2P	O5-C5-C6-O6
2	A	3001[A]	M2P	C6-O6-P6-O62
2	A	3001[A]	M2P	C6-O6-P6-O63
2	A	3001[A]	M2P	C6-O6-P6-O61
2	A	3001[B]	M2P	O1-C1-C2-C3
2	A	3001[B]	M2P	O1-C1-C2-O2
2	A	3001[B]	M2P	C2-C3-C4-C5
2	A	3001[B]	M2P	O3-C3-C4-C5
2	A	3001[B]	M2P	C2-C3-C4-O4
2	A	3001[B]	M2P	C1-C2-C3-C4
2	A	3001[B]	M2P	O2-C2-C3-C4
2	A	3001[B]	M2P	C1-C2-C3-O3
2	A	3001[B]	M2P	O2-C2-C3-O3
2	A	3001[A]	M2P	O2-C2-C3-O3
2	A	3001[B]	M2P	O3-C3-C4-O4
2	A	3001[A]	M2P	C1-C2-C3-O3
2	A	3001[A]	M2P	C1-C2-C3-C4
2	A	3001[A]	M2P	O2-C2-C3-C4
2	A	3001[A]	M2P	C5-C6-O6-P6
2	A	3001[B]	M2P	C5-C6-O6-P6
2	A	3001[A]	M2P	C2-C1-O1-P1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	401	ACT	1	0
2	A	3001[A]	M2P	3	0

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

Ligand M2P A 3001 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand M2P A 3001 (A)

Bond lengths

Bond angles

Torsions

Rings
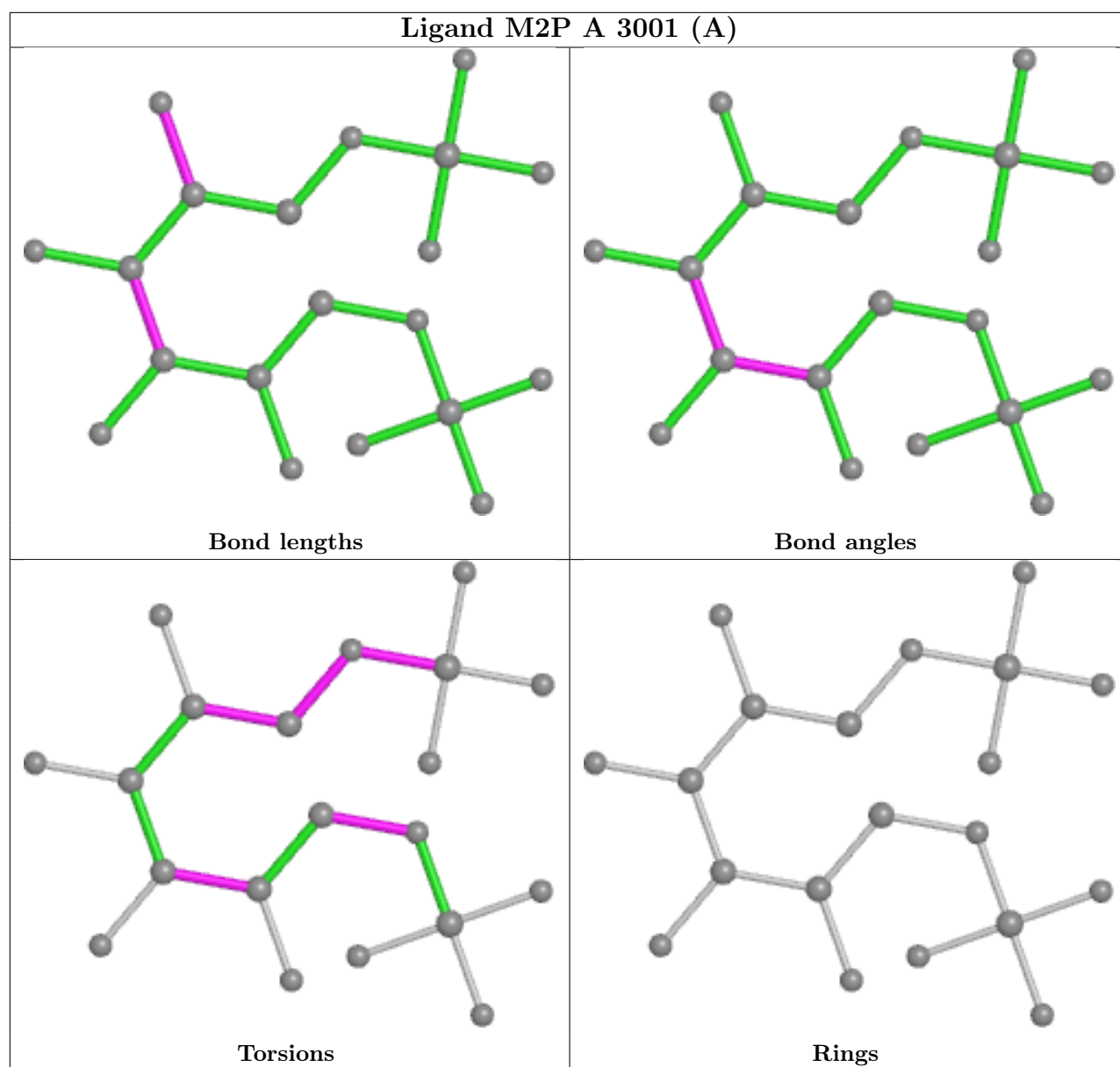
5.7 Other polymers ⓘ

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, 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(Å²)	Q<0.9
1	A	324/327 (99%)	0.54	33 (10%)	6	9	19, 29, 76, 120	0
1	B	325/327 (99%)	0.54	20 (6%)	20	26	18, 28, 62, 95	1 (0%)
1	C	326/327 (99%)	0.79	44 (13%)	3	4	21, 46, 93, 134	0
1	D	325/327 (99%)	1.12	68 (20%)	1	1	23, 47, 102, 131	0
All	All	1300/1308 (99%)	0.75	165 (12%)	3	5	18, 38, 89, 134	1 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2	ILE	11.2
1	D	37	ALA	10.4
1	C	41	THR	9.9
1	C	326	MET	9.7
1	C	289	ILE	9.2
1	A	296	ALA	7.7
1	C	288	TYR	7.4
1	D	49	ILE	7.4
1	A	295	ALA	7.3
1	D	289	ILE	7.1
1	D	39	HIS	6.6
1	D	293	PRO	6.6
1	C	37	ALA	6.5
1	D	299	TRP	6.4
1	D	295	ALA	6.3
1	D	288	TYR	6.3
1	D	326	MET	6.3
1	C	251	GLY	6.1
1	B	326	MET	6.1
1	D	287	VAL	6.0
1	A	293	PRO	6.0

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	RSRZ
1	D	44	PRO	6.0
1	A	37	ALA	5.9
1	A	326	MET	5.8
1	C	44	PRO	5.8
1	C	40	GLN	5.7
1	D	292	GLY	5.5
1	D	285	VAL	5.4
1	C	39	HIS	5.3
1	C	293	PRO	5.3
1	D	41	THR	5.2
1	D	42	LYS	5.2
1	D	38	GLN	5.2
1	C	42	LYS	5.1
1	D	45	THR	5.1
1	D	40	GLN	5.0
1	D	296	ALA	5.0
1	C	1	THR	5.0
1	A	49	ILE	4.9
1	C	292	GLY	4.6
1	B	252[A]	VAL	4.6
1	C	287	VAL	4.5
1	C	45	THR	4.4
1	C	299	TRP	4.4
1	D	286	LYS	4.3
1	C	46	VAL	4.3
1	D	251	GLY	4.3
1	D	98	ALA	4.2
1	B	293	PRO	4.2
1	A	289	ILE	4.1
1	B	294	GLN	4.0
1	B	289	ILE	4.0
1	C	48	GLN	3.9
1	B	253[A]	SER	3.9
1	D	43	GLU	3.8
1	D	290	GLU	3.8
1	D	36	MET	3.8
1	D	282	ALA	3.8
1	B	251[A]	GLY	3.8
1	A	44	PRO	3.8
1	D	34	ARG	3.8
1	D	30	GLY	3.8
1	D	294	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	295	ALA	3.8
1	C	290	GLU	3.8
1	C	38	GLN	3.7
1	D	305	PHE	3.7
1	C	32	LEU	3.7
1	D	84	GLU	3.6
1	B	3	THR	3.6
1	D	99	THR	3.6
1	A	41	THR	3.6
1	C	2	ILE	3.6
1	D	301	ARG	3.5
1	A	48	GLN	3.5
1	C	49	ILE	3.5
1	D	284	SER	3.4
1	C	47	GLU	3.4
1	A	292	GLY	3.4
1	B	153	CYS	3.4
1	A	294	GLN	3.4
1	A	43	GLU	3.4
1	C	43	GLU	3.4
1	C	286	LYS	3.3
1	C	52	LEU	3.3
1	D	170	LYS	3.3
1	B	219	ALA	3.3
1	D	46	VAL	3.3
1	D	31	ALA	3.3
1	D	3	THR	3.3
1	B	2	ILE	3.3
1	C	36	MET	3.2
1	D	283	GLY	3.2
1	A	46	VAL	3.2
1	C	285	VAL	3.2
1	D	297	ARG	3.2
1	D	63	PHE	3.2
1	C	294	GLN	3.2
1	C	296	ALA	3.1
1	C	33	LYS	3.1
1	C	323	THR	3.1
1	A	286	LYS	3.0
1	D	291	GLU	3.0
1	B	220	ASP	3.0
1	B	223	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	279	ALA	2.9
1	D	47	GLU	2.9
1	D	35	MET	2.9
1	D	33	LYS	2.9
1	D	55	LEU	2.9
1	D	100	THR	2.9
1	A	3	THR	2.8
1	D	250	ALA	2.8
1	D	52	LEU	2.8
1	A	45	THR	2.8
1	D	83	GLU	2.7
1	D	298	GLU	2.7
1	D	303	GLU	2.7
1	D	323	THR	2.7
1	D	308	ILE	2.6
1	A	98	ALA	2.6
1	D	17	VAL	2.6
1	C	136	GLN	2.6
1	D	324	GLU	2.5
1	D	306	LYS	2.5
1	C	250	ALA	2.5
1	A	52	LEU	2.5
1	C	291	GLU	2.5
1	B	279	ALA	2.5
1	A	291	GLU	2.5
1	A	99	THR	2.5
1	A	288	TYR	2.5
1	A	55	LEU	2.5
1	D	317	LYS	2.5
1	D	302	THR	2.4
1	A	282	ALA	2.4
1	D	32	LEU	2.4
1	A	34	ARG	2.4
1	B	37	ALA	2.4
1	D	300	LEU	2.4
1	C	305	PHE	2.4
1	D	304	GLY	2.4
1	D	107	CYS	2.3
1	B	160	PHE	2.3
1	B	201	VAL	2.3
1	A	32	LEU	2.3
1	A	30	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	56	VAL	2.2
1	A	160	PHE	2.2
1	B	149	ILE	2.2
1	B	194	PHE	2.2
1	C	298	GLU	2.2
1	D	153	CYS	2.2
1	A	298	GLU	2.1
1	C	283	GLY	2.1
1	B	161	TYR	2.1
1	D	161	TYR	2.1
1	C	17	VAL	2.1
1	C	278	ARG	2.1
1	C	35	MET	2.0
1	A	201	VAL	2.0
1	D	111	TRP	2.0
1	A	251	GLY	2.0
1	C	73	TYR	2.0
1	A	252	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.
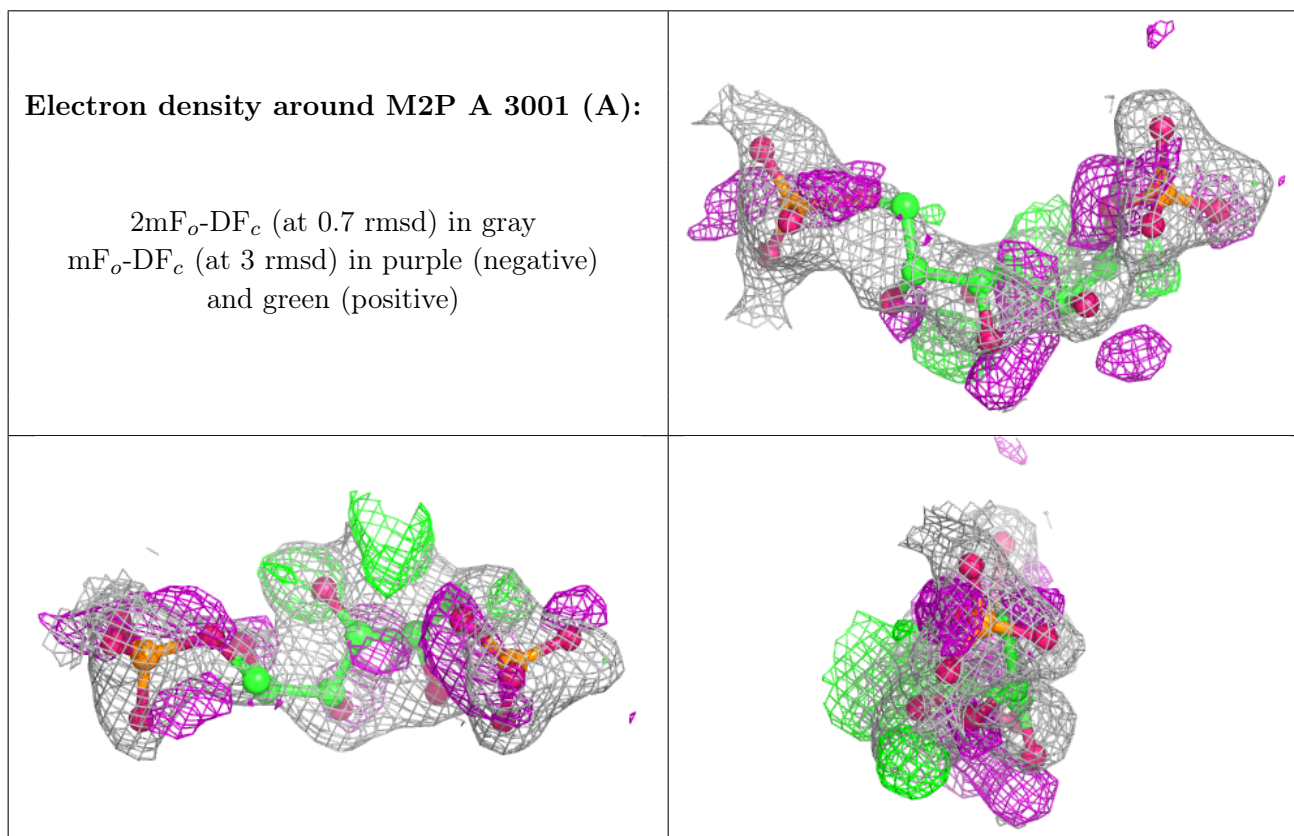
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ACT	D	401	4/4	0.61	0.28	40,48,57,64	0
4	CL	B	403	1/1	0.71	0.23	32,32,32,32	1
4	CL	C	404	1/1	0.75	0.11	75,75,75,75	0
3	CA	C	403	1/1	0.81	0.14	106,106,106,106	0
2	M2P	A	3001[A]	20/20	0.82	0.25	35,38,44,45	20

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	M2P	A	3001[B]	20/20	0.82	0.25	35,39,44,45	20
3	CA	C	402	1/1	0.83	0.14	86,86,86,86	0
4	CL	D	402	1/1	0.87	0.08	73,73,73,73	0
3	CA	C	401	1/1	0.95	0.07	38,38,38,38	0
3	CA	B	401	1/1	0.98	0.14	30,30,30,30	0
3	CA	A	3002	1/1	0.99	0.15	29,29,29,29	0
3	CA	B	402	1/1	0.99	0.05	41,41,41,41	0
3	CA	A	3003	1/1	1.00	0.06	39,39,39,39	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 M2P A 3001 (A):

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

Electron density around M2P A 3001 (B):

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

6.5 Other polymers ⓘ

There are no such residues in this entry.