



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:19 am BST

PDB ID : 1ZAJ
Title : Fructose-1,6-bisphosphate aldolase from rabbit muscle in complex with mannitol-1,6-bisphosphate, a competitive inhibitor
Authors : St-Jean, M.; Lafrance-Vanasse, J.; Liotard, B.; Sygusch, J.
Deposited on : 2005-04-06
Resolution : 1.89 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

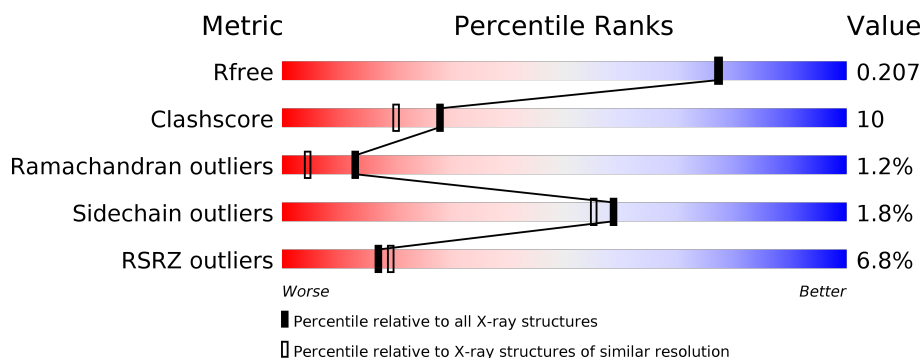
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>18%</div> </div> <div>•</div> </div>
1	B	363	<div> <div>5%</div> <div> <div></div> <div>82%</div> <div>17%</div> </div> <div>•</div> </div>
1	C	363	<div> <div>8%</div> <div> <div></div> <div>82%</div> <div>18%</div> </div> <div>•</div> </div>
1	D	363	<div> <div>8%</div> <div> <div></div> <div>81%</div> <div>18%</div> </div> <div>•</div> </div>

2 Entry composition [i](#)

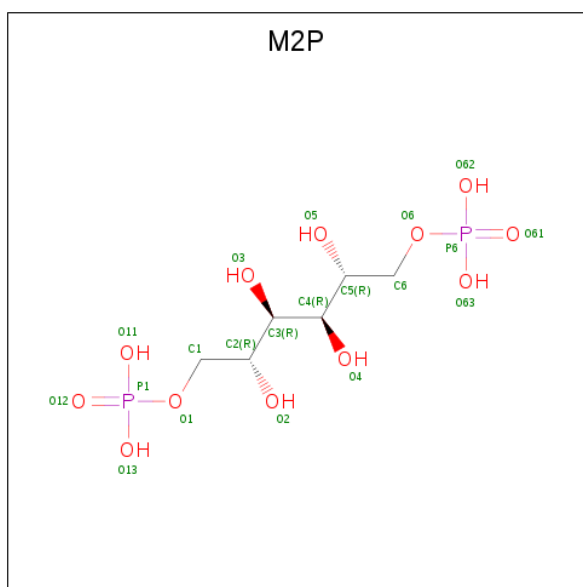
There are 3 unique types of molecules in this entry. The entry contains 13745 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructose-bisphosphate aldolase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	B	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	C	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			
1	D	363	Total	C	N	O	S	0	0	0
			2758	1733	489	525	11			

- 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	0
			20	6	12	2		
2	B	1	Total	C	O	P	0	0
			20	6	12	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	0
			20	6	12	2		
2	D	1	Total	C	O	P	0	0
			20	6	12	2		

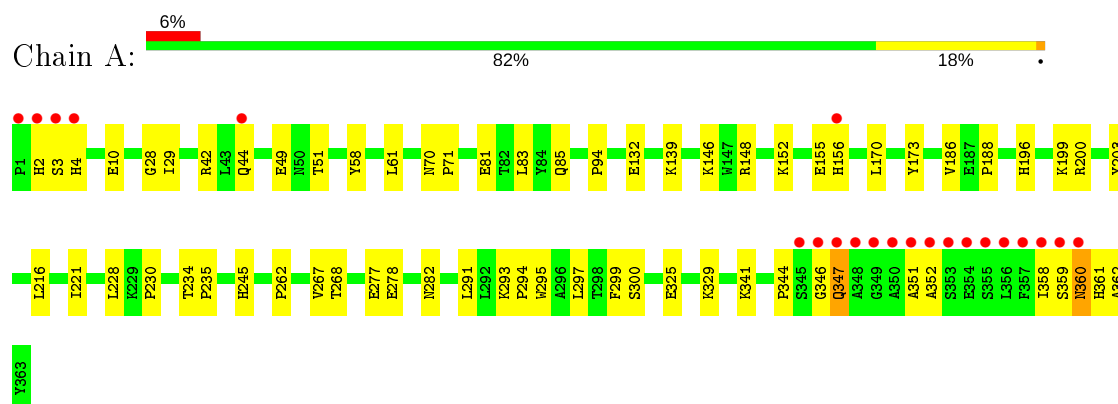
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	634	Total	O	0	0
			634	634		
3	B	691	Total	O	0	0
			691	691		
3	C	651	Total	O	0	0
			651	651		
3	D	657	Total	O	0	0
			657	657		

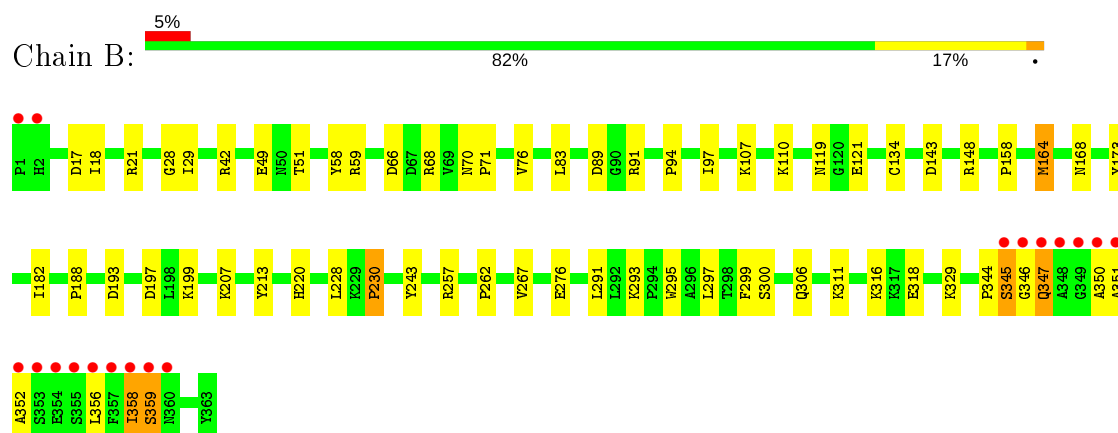
3 Residue-property plots [i](#)

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.

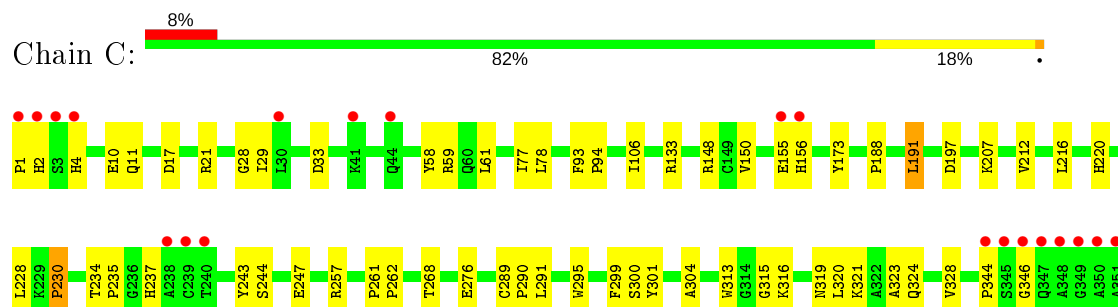
• Molecule 1: Fructose-bisphosphate aldolase A



• Molecule 1: Fructose-bisphosphate aldolase A

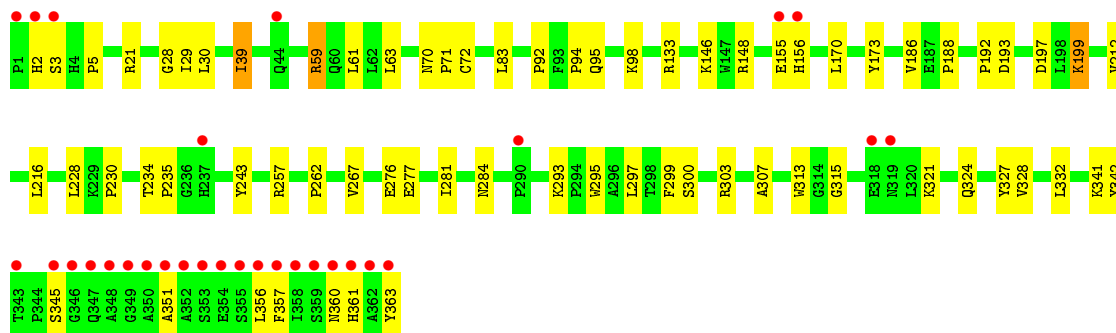
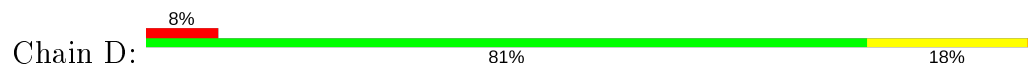


• Molecule 1: Fructose-bisphosphate aldolase A





• Molecule 1: Fructose-bisphosphate aldolase A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.04Å 103.33Å 84.36Å 90.00° 98.86° 90.00°	Depositor
Resolution (Å)	20.00 – 1.89 30.38 – 1.75	Depositor EDS
% Data completeness (in resolution range)	86.2 (20.00-1.89) 78.0 (30.38-1.75)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 1.75Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.167 , 0.204 0.171 , 0.207	Depositor DCC
R_{free} test set	5966 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 84.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13745	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.29	0/2812	0.57	0/3810
1	B	0.30	0/2812	0.58	0/3810
1	C	0.30	0/2812	0.58	0/3810
1	D	0.29	0/2812	0.57	0/3810
All	All	0.30	0/11248	0.57	0/15240

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.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	213	TYR	Sidechain

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	2758	0	2776	59	0
1	B	2758	0	2776	53	0
1	C	2758	0	2776	64	0
1	D	2758	0	2776	61	0
2	A	20	0	12	2	0
2	B	20	0	12	1	0
2	C	20	0	12	1	0
2	D	20	0	12	2	0
3	A	634	0	0	24	0
3	B	691	0	0	13	0
3	C	651	0	0	16	0
3	D	657	0	0	17	0
All	All	13745	0	11152	221	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 (221) 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:C:155:GLU:HG3	1:C:156:HIS:ND1	1.73	1.03
1:C:156:HIS:CD2	1:D:2:HIS:HD2	1.77	1.02
1:C:156:HIS:CD2	1:D:2:HIS:CD2	2.55	0.94
1:C:156:HIS:NE2	1:D:2:HIS:CD2	2.41	0.89
1:C:156:HIS:NE2	1:D:2:HIS:HD2	1.72	0.87
1:D:303:ARG:HB3	1:D:356:LEU:HD23	1.57	0.87
1:D:307:ALA:HB2	1:D:356:LEU:HD21	1.57	0.84
1:B:42:ARG:HE	1:B:42:ARG:HA	1.53	0.74
1:A:199:LYS:HE2	3:A:3094:HOH:O	1.87	0.73
1:D:228:LEU:HG	1:D:230:PRO:HD3	1.72	0.71
1:B:164:MET:HE1	1:B:168:ASN:HB2	1.71	0.70
1:B:49:GLU:HG2	1:B:51:THR:HG23	1.73	0.70
1:A:49:GLU:HG2	1:A:51:THR:HG23	1.74	0.69
1:A:200:ARG:NH2	1:D:2:HIS:HA	2.06	0.69
1:C:10:GLU:HG2	1:C:11:GLN:N	2.08	0.69
1:B:344:PRO:HG3	3:B:3572:HOH:O	1.92	0.68
1:A:360:ASN:HB3	3:A:3125:HOH:O	1.92	0.68
1:D:92:PRO:HD2	1:D:95:GLN:HE21	1.59	0.67
1:C:155:GLU:HG3	1:C:156:HIS:CE1	2.30	0.66
1:D:345:SER:HB2	3:D:3457:HOH:O	1.95	0.66
1:C:290:PRO:HG3	1:C:358:ILE:HD11	1.78	0.66
1:B:89:ASP:OD2	1:B:91:ARG:HD3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:HIS:HB2	3:D:3039:HOH:O	1.95	0.65
1:B:329:LYS:HE2	3:B:3044:HOH:O	1.97	0.65
1:D:98:LYS:HD2	3:D:3092:HOH:O	1.96	0.65
1:A:132:GLU:HG2	3:A:3221:HOH:O	1.97	0.63
1:A:228:LEU:HG	1:A:230:PRO:HD3	1.80	0.63
1:A:325:GLU:O	1:A:329:LYS:HG3	1.99	0.63
1:C:244:SER:OG	1:C:247:GLU:HG3	1.98	0.63
1:D:284:ASN:ND2	1:D:342:TYR:H	1.96	0.62
1:A:360:ASN:ND2	1:A:361:HIS:H	1.98	0.62
1:B:358:ILE:HG22	1:B:359:SER:H	1.64	0.61
1:D:148:ARG:HD2	2:D:3004:M2P:O4	2.00	0.61
1:C:289:CYS:SG	1:C:291:LEU:HD23	2.40	0.61
1:A:361:HIS:HA	3:A:3124:HOH:O	2.00	0.60
1:B:70:ASN:HB2	1:B:71:PRO:HD3	1.83	0.60
1:C:156:HIS:HE2	1:D:2:HIS:CD2	2.20	0.60
1:B:293:LYS:HG2	1:B:297:LEU:HD11	1.85	0.59
1:B:344:PRO:CG	3:B:3572:HOH:O	2.47	0.58
1:C:358:ILE:HG13	3:C:3100:HOH:O	2.04	0.58
1:A:268:THR:HB	1:A:300:SER:HB2	1.85	0.58
1:A:199:LYS:HG3	3:A:3434:HOH:O	2.04	0.57
1:A:70:ASN:HB2	1:A:71:PRO:HD3	1.86	0.57
1:B:291:LEU:O	1:B:293:LYS:HD3	2.04	0.57
1:A:325:GLU:HG3	1:A:329:LYS:HE3	1.88	0.56
1:C:228:LEU:HG	1:C:230:PRO:HD3	1.86	0.56
1:C:10:GLU:HB3	3:C:3637:HOH:O	2.06	0.55
1:D:39:ILE:HD13	1:D:39:ILE:O	2.06	0.55
1:A:245:HIS:HE1	3:A:3447:HOH:O	1.89	0.55
1:D:199:LYS:NZ	1:D:199:LYS:HB2	2.21	0.55
1:A:262:PRO:HG2	1:D:257:ARG:HA	1.88	0.55
1:D:70:ASN:HB2	1:D:71:PRO:HD3	1.89	0.55
1:D:293:LYS:HD2	1:D:297:LEU:HD12	1.89	0.55
1:C:324:GLN:O	1:C:328:VAL:HG23	2.07	0.54
1:B:164:MET:CE	1:B:168:ASN:HB2	2.38	0.54
1:B:267:VAL:HB	1:B:297:LEU:HD23	1.88	0.54
1:C:316:LYS:HD3	3:C:3563:HOH:O	2.06	0.54
1:A:245:HIS:CE1	3:A:3447:HOH:O	2.59	0.54
1:B:344:PRO:CD	3:B:3572:HOH:O	2.55	0.54
1:B:134:CYS:HB3	1:B:182:ILE:HD12	1.90	0.54
1:D:197:ASP:HB2	1:D:243:TYR:OH	2.07	0.54
1:A:4:HIS:NE2	1:B:119:ASN:HB2	2.23	0.53
1:A:278:GLU:HG2	3:A:3474:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:LYS:HD2	1:D:297:LEU:CD1	2.39	0.53
1:A:152:LYS:HE3	3:A:3547:HOH:O	2.09	0.52
1:A:146:LYS:NZ	2:A:3001:M2P:O4	2.42	0.52
1:A:3:SER:HB2	3:D:3264:HOH:O	2.08	0.52
1:A:29:ILE:HB	1:A:300:SER:HA	1.91	0.52
3:A:3090:HOH:O	1:D:3:SER:HB3	2.09	0.52
1:C:10:GLU:CG	1:C:11:GLN:N	2.72	0.52
1:D:192:PRO:HG2	1:D:357:PHE:HE1	1.73	0.52
1:D:28:GLY:HA3	1:D:299:PHE:CE1	2.45	0.52
1:C:10:GLU:HG2	1:C:11:GLN:H	1.71	0.52
1:D:361:HIS:HB3	3:D:3016:HOH:O	2.10	0.52
3:A:3311:HOH:O	1:B:164:MET:HG3	2.09	0.52
1:B:17:ASP:O	1:B:21:ARG:HG3	2.10	0.52
1:A:2:HIS:C	1:A:4:HIS:H	2.13	0.51
1:A:155:GLU:HG2	3:A:3463:HOH:O	2.10	0.51
1:B:228:LEU:HG	1:B:230:PRO:HD3	1.91	0.51
1:B:318:GLU:HG2	3:B:3287:HOH:O	2.10	0.51
1:C:28:GLY:HA3	1:C:299:PHE:CZ	2.46	0.51
1:B:352:ALA:HB2	3:B:3042:HOH:O	2.11	0.51
1:C:268:THR:HB	1:C:300:SER:HB2	1.93	0.50
1:D:351:ALA:HB1	3:D:3639:HOH:O	2.10	0.50
1:C:291:LEU:N	1:C:291:LEU:HD22	2.26	0.50
1:A:277:GLU:OE2	1:A:344:PRO:HB3	2.12	0.50
1:D:28:GLY:HA3	1:D:299:PHE:CZ	2.47	0.49
1:A:83:LEU:HD12	1:A:94:PRO:HG3	1.93	0.49
1:C:93:PHE:N	1:C:94:PRO:HD2	2.27	0.49
1:B:197:ASP:HB2	1:B:243:TYR:OH	2.13	0.49
1:A:42:ARG:CZ	1:A:42:ARG:HA	2.43	0.49
1:B:257:ARG:O	1:C:262:PRO:HD2	2.13	0.49
1:B:262:PRO:HG2	1:C:257:ARG:HA	1.95	0.49
1:D:276:GLU:CD	1:D:307:ALA:HB3	2.32	0.49
1:C:150:VAL:HG13	1:C:191:LEU:HD13	1.95	0.49
1:D:59:ARG:O	1:D:63:LEU:HG	2.13	0.49
1:C:21:ARG:NH2	3:C:3650:HOH:O	2.44	0.48
1:B:28:GLY:HA3	1:B:299:PHE:CZ	2.49	0.48
1:D:133:ARG:HD3	3:D:3401:HOH:O	2.14	0.48
1:A:216:LEU:HD22	1:A:221:ILE:HG13	1.95	0.48
1:C:2:HIS:HB2	3:C:3183:HOH:O	2.13	0.48
1:D:360:ASN:HB3	3:D:3635:HOH:O	2.12	0.48
1:C:29:ILE:HB	1:C:300:SER:HA	1.96	0.48
1:A:291:LEU:O	1:A:293:LYS:HD3	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:HIS:O	1:A:3:SER:HB3	2.14	0.48
1:B:148:ARG:HD2	2:B:3002:M2P:O4	2.14	0.47
1:B:121:GLU:OE2	1:B:158:PRO:HA	2.14	0.47
1:C:33:ASP:HB3	1:C:77:ILE:HG22	1.96	0.47
1:D:321:LYS:HG3	3:D:3449:HOH:O	2.13	0.47
1:B:42:ARG:HA	1:B:42:ARG:NE	2.25	0.47
1:A:200:ARG:HH12	1:A:203:TYR:HD2	1.61	0.47
1:C:1:PRO:N	1:D:156:HIS:HB3	2.29	0.47
1:D:29:ILE:HB	1:D:300:SER:HA	1.95	0.47
1:A:234:THR:HB	1:A:235:PRO:HD2	1.97	0.47
1:D:234:THR:HB	1:D:235:PRO:HD2	1.95	0.47
1:B:28:GLY:HA3	1:B:299:PHE:CE1	2.49	0.47
1:C:291:LEU:H	1:C:291:LEU:HD22	1.80	0.47
1:C:234:THR:HB	1:C:235:PRO:HD2	1.95	0.46
1:C:1:PRO:HG2	1:C:2:HIS:CD2	2.51	0.46
1:D:212:VAL:O	1:D:216:LEU:HG	2.16	0.46
1:C:301:TYR:HB3	1:C:304:ALA:HB3	1.97	0.46
1:B:164:MET:HE1	1:B:168:ASN:CB	2.42	0.46
1:A:347:GLN:HG3	3:A:3265:HOH:O	2.16	0.46
1:B:18:ILE:HD13	1:B:143:ASP:HB3	1.97	0.46
1:B:351:ALA:HB1	3:B:3355:HOH:O	2.14	0.46
1:D:341:LYS:HE3	3:D:3165:HOH:O	2.15	0.46
1:C:155:GLU:CD	3:C:3456:HOH:O	2.55	0.46
1:D:155:GLU:O	1:D:156:HIS:HB2	2.16	0.45
1:C:148:ARG:HD2	2:C:3003:M2P:O4	2.16	0.45
1:A:81:GLU:O	1:A:85:GLN:HG3	2.16	0.45
1:B:356:LEU:N	1:B:356:LEU:HD12	2.32	0.45
1:B:83:LEU:HD12	1:B:94:PRO:HG3	1.98	0.45
1:B:89:ASP:CG	1:B:91:ARG:HD3	2.36	0.45
1:B:76:VAL:HB	1:B:97:ILE:HD13	1.98	0.45
1:D:199:LYS:HD3	3:D:3566:HOH:O	2.16	0.45
1:D:146:LYS:NZ	2:D:3004:M2P:O4	2.46	0.45
1:A:196:HIS:HB2	1:A:200:ARG:HG2	1.98	0.45
1:A:2:HIS:HB3	3:A:3228:HOH:O	2.17	0.45
1:D:61:LEU:HD23	1:D:61:LEU:C	2.36	0.45
1:C:78:LEU:O	1:C:106:ILE:HD12	2.17	0.45
1:A:28:GLY:HA3	1:A:299:PHE:CZ	2.52	0.45
1:B:358:ILE:HG22	1:B:359:SER:N	2.29	0.45
1:B:29:ILE:HB	1:B:300:SER:HA	1.98	0.45
1:B:345:SER:HA	3:B:3234:HOH:O	2.17	0.45
1:C:360:ASN:HB2	3:C:3102:HOH:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:LEU:HD22	1:D:327:TYR:OH	2.17	0.44
1:A:267:VAL:HB	1:A:297:LEU:HD23	1.98	0.44
1:C:61:LEU:HD11	1:C:323:ALA:HB3	2.00	0.44
1:C:346:GLY:HA2	3:C:3236:HOH:O	2.17	0.44
1:D:92:PRO:HD2	1:D:95:GLN:NE2	2.28	0.44
1:D:72:CYS:SG	1:D:332:LEU:HD23	2.58	0.44
1:B:199:LYS:HG3	3:B:3224:HOH:O	2.18	0.44
1:D:193:ASP:OD1	1:D:360:ASN:HB2	2.17	0.44
1:B:329:LYS:HG2	3:B:3553:HOH:O	2.17	0.44
1:A:148:ARG:HD2	2:A:3001:M2P:O4	2.17	0.44
1:A:4:HIS:CE1	1:B:119:ASN:HB2	2.53	0.44
1:C:354:GLU:HB3	3:C:3594:HOH:O	2.18	0.43
1:D:360:ASN:ND2	3:D:3633:HOH:O	2.50	0.43
1:A:10:GLU:HG2	3:A:3305:HOH:O	2.18	0.43
1:A:42:ARG:NE	1:A:42:ARG:HA	2.32	0.43
1:C:2:HIS:CD2	1:C:2:HIS:N	2.84	0.43
1:C:58:TYR:O	1:C:61:LEU:HB3	2.18	0.43
1:C:197:ASP:HB2	1:C:243:TYR:OH	2.17	0.43
1:D:267:VAL:HB	1:D:297:LEU:HD23	2.01	0.43
1:C:61:LEU:C	1:C:61:LEU:HD23	2.39	0.43
1:B:207:LYS:NZ	1:C:220:HIS:HD2	2.17	0.43
1:B:316:LYS:HZ3	1:B:318:GLU:CG	2.32	0.43
1:C:156:HIS:HE1	3:C:3456:HOH:O	2.00	0.43
1:D:199:LYS:HE3	3:D:3264:HOH:O	2.17	0.43
3:A:3311:HOH:O	1:B:164:MET:CG	2.65	0.43
1:C:28:GLY:HA3	1:C:299:PHE:CE1	2.53	0.43
1:C:344:PRO:HA	3:C:3238:HOH:O	2.19	0.43
1:D:313:TRP:CZ2	1:D:315:GLY:HA2	2.54	0.43
1:A:3:SER:HA	3:D:3573:HOH:O	2.18	0.43
1:B:311:LYS:HE3	3:B:3690:HOH:O	2.18	0.43
1:A:44:GLN:HG2	3:A:3200:HOH:O	2.19	0.42
1:C:212:VAL:O	1:C:216:LEU:HG	2.18	0.42
1:C:316:LYS:HB2	1:C:319:ASN:ND2	2.34	0.42
1:D:277:GLU:O	1:D:281:ILE:HG13	2.19	0.42
1:B:66:ASP:OD2	1:B:68:ARG:NH2	2.39	0.42
1:A:362:ALA:HB2	3:D:3067:HOH:O	2.18	0.42
1:A:4:HIS:HA	3:A:3228:HOH:O	2.19	0.42
1:B:220:HIS:HD2	1:C:207:LYS:NZ	2.18	0.42
1:A:293:LYS:HG2	1:A:297:LEU:HD11	2.01	0.42
1:A:152:LYS:HD2	3:A:3064:HOH:O	2.18	0.42
1:D:324:GLN:O	1:D:328:VAL:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LYS:HE3	3:B:3126:HOH:O	2.19	0.42
1:B:276:GLU:HG3	3:B:3555:HOH:O	2.19	0.42
1:D:83:LEU:HD12	1:D:94:PRO:HG3	2.02	0.42
1:C:321:LYS:HA	1:C:321:LYS:HD2	1.91	0.42
1:D:313:TRP:CE2	1:D:315:GLY:HA2	2.54	0.42
1:A:245:HIS:HD2	1:A:282:ASN:OD1	2.02	0.41
1:A:347:GLN:CD	1:A:347:GLN:H	2.22	0.41
1:C:207:LYS:HE2	3:C:3103:HOH:O	2.19	0.41
1:A:139:LYS:HD2	3:A:3156:HOH:O	2.18	0.41
1:A:156:HIS:N	3:A:3083:HOH:O	2.44	0.41
1:A:170:LEU:HD22	1:A:186:VAL:HG13	2.02	0.41
1:A:44:GLN:CD	3:A:3233:HOH:O	2.58	0.41
1:A:58:TYR:O	1:A:61:LEU:HB3	2.20	0.41
1:B:58:TYR:OH	1:B:306:GLN:HB3	2.20	0.41
1:C:320:LEU:O	1:C:324:GLN:HG3	2.20	0.41
1:D:356:LEU:HG	3:D:3224:HOH:O	2.19	0.41
1:B:346:GLY:O	1:B:347:GLN:HB2	2.20	0.41
1:D:276:GLU:OE2	1:D:307:ALA:HB3	2.19	0.41
1:D:170:LEU:HD22	1:D:186:VAL:HG13	2.02	0.41
3:A:3424:HOH:O	1:B:110:LYS:HE3	2.21	0.41
1:A:341:LYS:HE3	3:A:3521:HOH:O	2.19	0.41
1:A:61:LEU:HD23	1:A:61:LEU:C	2.41	0.41
1:A:294:PRO:HG3	1:D:262:PRO:CG	2.50	0.41
1:D:284:ASN:HD21	1:D:342:TYR:H	1.64	0.41
1:C:276:GLU:HG3	3:C:3476:HOH:O	2.20	0.41
1:C:313:TRP:CZ2	1:C:315:GLY:HA2	2.56	0.41
1:C:133:ARG:HD3	3:C:3383:HOH:O	2.20	0.41
1:C:17:ASP:O	1:C:21:ARG:HG3	2.21	0.41
1:C:61:LEU:HD11	1:C:323:ALA:CB	2.51	0.41
1:C:237:HIS:HB3	3:C:3450:HOH:O	2.20	0.41
1:C:1:PRO:H3	1:D:156:HIS:HB3	1.86	0.41
1:A:293:LYS:HE2	1:A:293:LYS:HB2	1.90	0.40
1:D:21:ARG:NH1	3:D:3426:HOH:O	2.53	0.40
1:C:1:PRO:HG2	3:C:3259:HOH:O	2.21	0.40
1:C:261:PRO:HA	1:C:262:PRO:HD3	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	361/363 (99%)	333 (92%)	21 (6%)	7 (2%)	8	1
1	B	361/363 (99%)	339 (94%)	16 (4%)	6 (2%)	9	2
1	C	361/363 (99%)	342 (95%)	16 (4%)	3 (1%)	19	9
1	D	361/363 (99%)	339 (94%)	20 (6%)	2 (1%)	25	15
All	All	1444/1452 (99%)	1353 (94%)	73 (5%)	18 (1%)	13	4

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	SER
1	B	347	GLN
1	A	346	GLY
1	C	356	LEU
1	B	350	ALA
1	B	359	SER
1	D	5	PRO
1	A	347	GLN
1	A	352	ALA
1	C	4	HIS
1	D	188	PRO
1	A	351	ALA
1	A	359	SER
1	B	188	PRO
1	A	188	PRO
1	B	358	ILE
1	C	188	PRO
1	A	358	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	291/291 (100%)	288 (99%)	3 (1%)	76	76
1	B	291/291 (100%)	284 (98%)	7 (2%)	49	43
1	C	291/291 (100%)	286 (98%)	5 (2%)	60	57
1	D	291/291 (100%)	285 (98%)	6 (2%)	53	48
All	All	1164/1164 (100%)	1143 (98%)	21 (2%)	59	55

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	TYR
1	A	295	TRP
1	A	360	ASN
1	B	59	ARG
1	B	107	LYS
1	B	164	MET
1	B	173	TYR
1	B	193	ASP
1	B	230	PRO
1	B	295	TRP
1	C	59	ARG
1	C	173	TYR
1	C	191	LEU
1	C	230	PRO
1	C	295	TRP
1	D	39	ILE
1	D	59	ARG
1	D	173	TYR
1	D	199	LYS
1	D	295	TRP
1	D	363	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	HIS
1	A	95	GLN
1	A	180	ASN
1	A	241	GLN
1	A	245	HIS
1	A	360	ASN
1	A	361	HIS
1	B	136	GLN
1	B	220	HIS
1	B	237	HIS
1	B	319	ASN
1	C	54	ASN
1	C	95	GLN
1	C	220	HIS
1	C	241	GLN
1	C	245	HIS
1	D	2	HIS
1	D	54	ASN
1	D	85	GLN
1	D	95	GLN
1	D	180	ASN
1	D	284	ASN
1	D	360	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	M2P	A	3001	-	19,19,19	1.19	1 (5%)	28,28,28	0.82	1 (3%)
2	M2P	B	3002	-	19,19,19	1.18	1 (5%)	28,28,28	0.81	1 (3%)
2	M2P	C	3003	-	19,19,19	1.18	1 (5%)	28,28,28	0.80	1 (3%)
2	M2P	D	3004	-	19,19,19	1.19	1 (5%)	28,28,28	0.79	2 (7%)

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	-	-	4/24/24/24	-
2	M2P	B	3002	-	-	5/24/24/24	-
2	M2P	C	3003	-	-	8/24/24/24	-
2	M2P	D	3004	-	-	4/24/24/24	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	3001	M2P	P1-O12	3.41	1.61	1.50
2	D	3004	M2P	P1-O12	3.38	1.61	1.50
2	C	3003	M2P	P1-O12	3.38	1.61	1.50
2	B	3002	M2P	P1-O12	3.37	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3002	M2P	O11-P1-O1	2.22	112.64	106.73
2	C	3003	M2P	O11-P1-O1	2.22	112.64	106.73
2	A	3001	M2P	O11-P1-O1	2.15	112.47	106.73
2	D	3004	M2P	O11-P1-O1	2.15	112.45	106.73
2	D	3004	M2P	O6-P6-O61	2.05	112.21	106.47

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	M2P	O2-C2-C3-C4
2	A	3001	M2P	O2-C2-C3-O3
2	B	3002	M2P	C1-C2-C3-C4
2	B	3002	M2P	O2-C2-C3-C4
2	B	3002	M2P	C1-C2-C3-O3
2	B	3002	M2P	O2-C2-C3-O3
2	C	3003	M2P	C1-C2-C3-C4
2	C	3003	M2P	O2-C2-C3-C4
2	C	3003	M2P	C1-C2-C3-O3
2	C	3003	M2P	O2-C2-C3-O3
2	C	3003	M2P	C1-O1-P1-O12
2	D	3004	M2P	C1-C2-C3-C4
2	D	3004	M2P	O2-C2-C3-C4
2	D	3004	M2P	C1-C2-C3-O3
2	D	3004	M2P	O2-C2-C3-O3
2	A	3001	M2P	C1-C2-C3-O3
2	A	3001	M2P	C1-C2-C3-C4
2	C	3003	M2P	C6-O6-P6-O61
2	B	3002	M2P	C6-O6-P6-O63
2	C	3003	M2P	C1-O1-P1-O13
2	C	3003	M2P	C6-O6-P6-O63

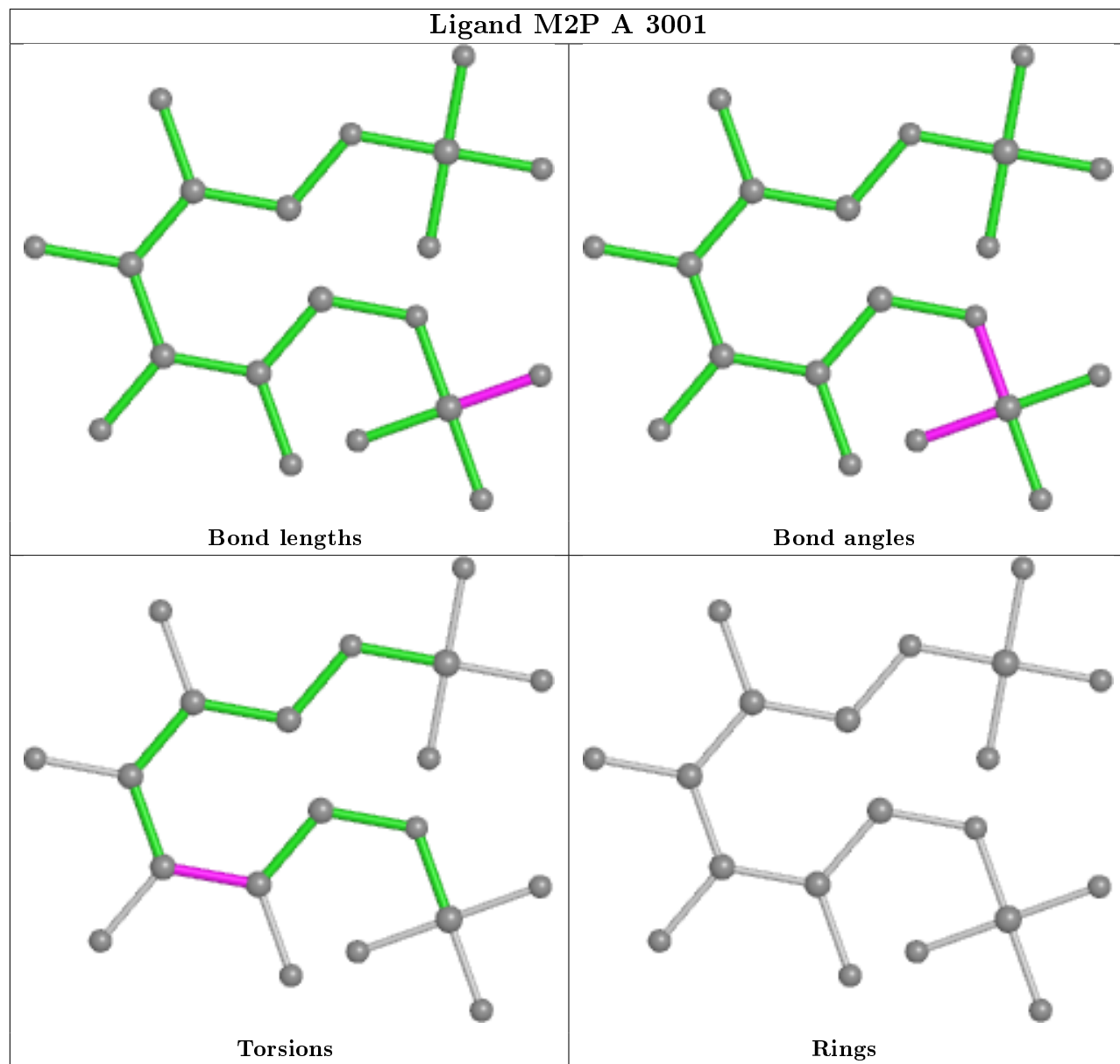
There are no ring outliers.

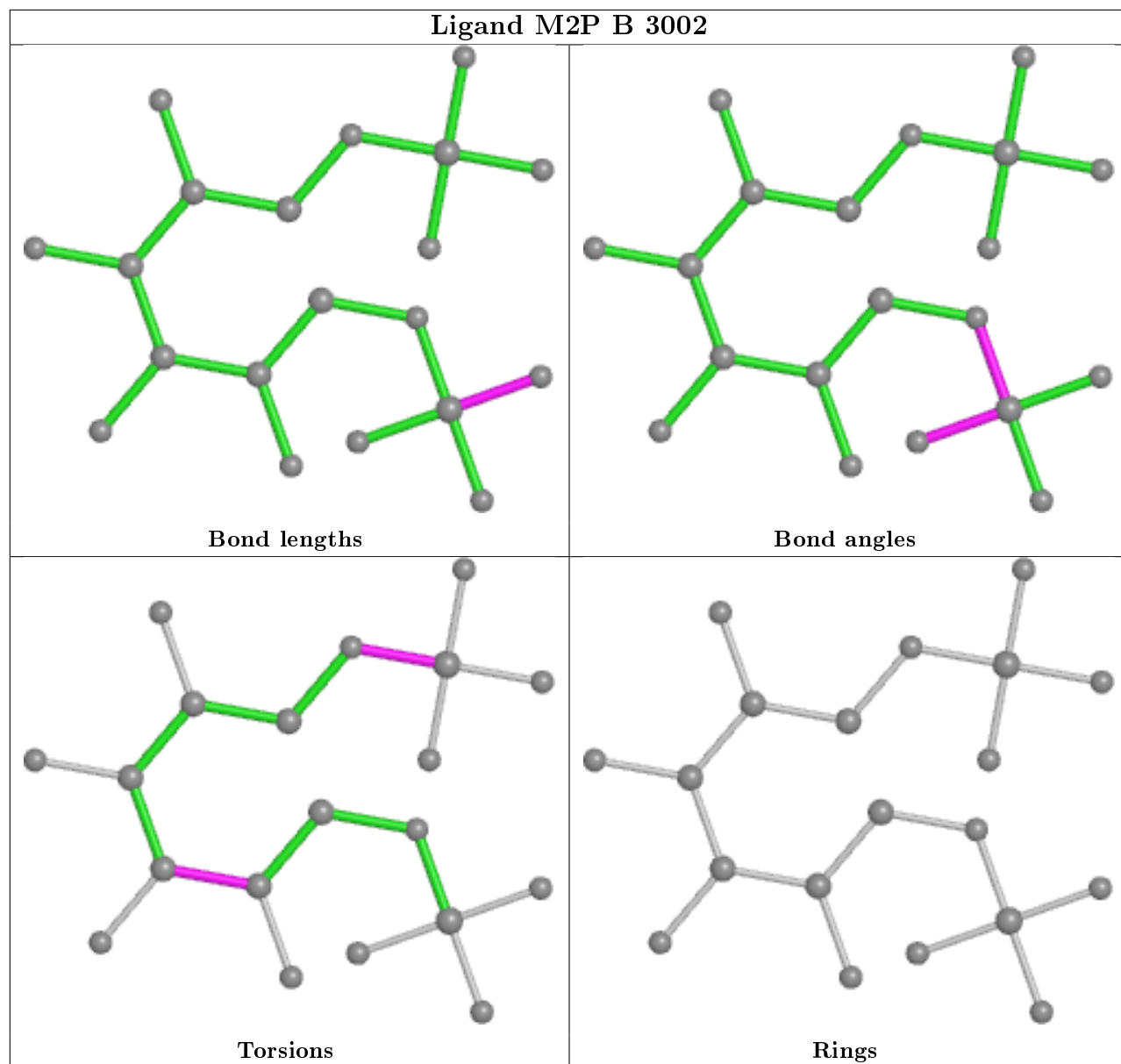
4 monomers are involved in 6 short contacts:

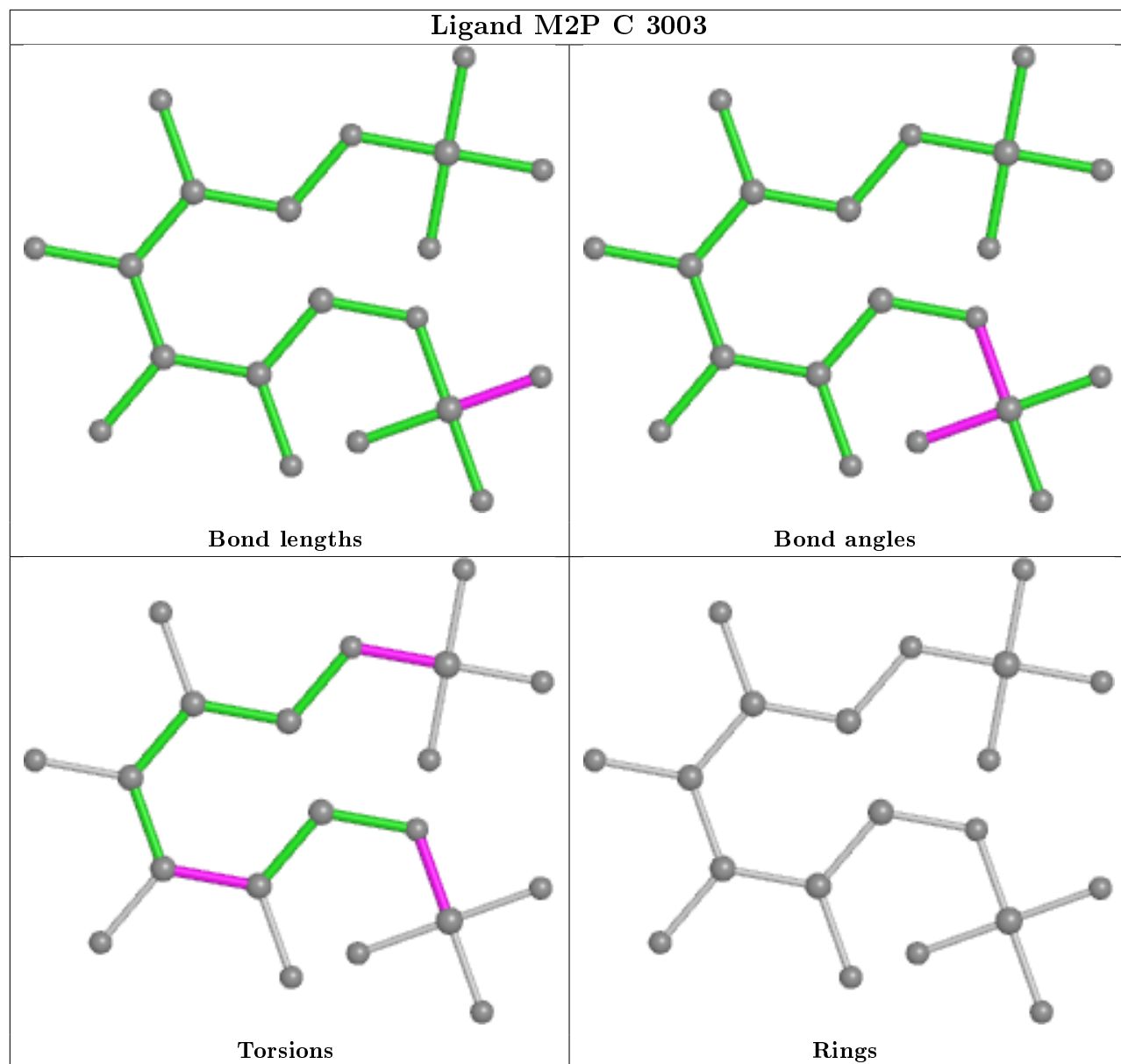
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3001	M2P	2	0
2	B	3002	M2P	1	0
2	C	3003	M2P	1	0
2	D	3004	M2P	2	0

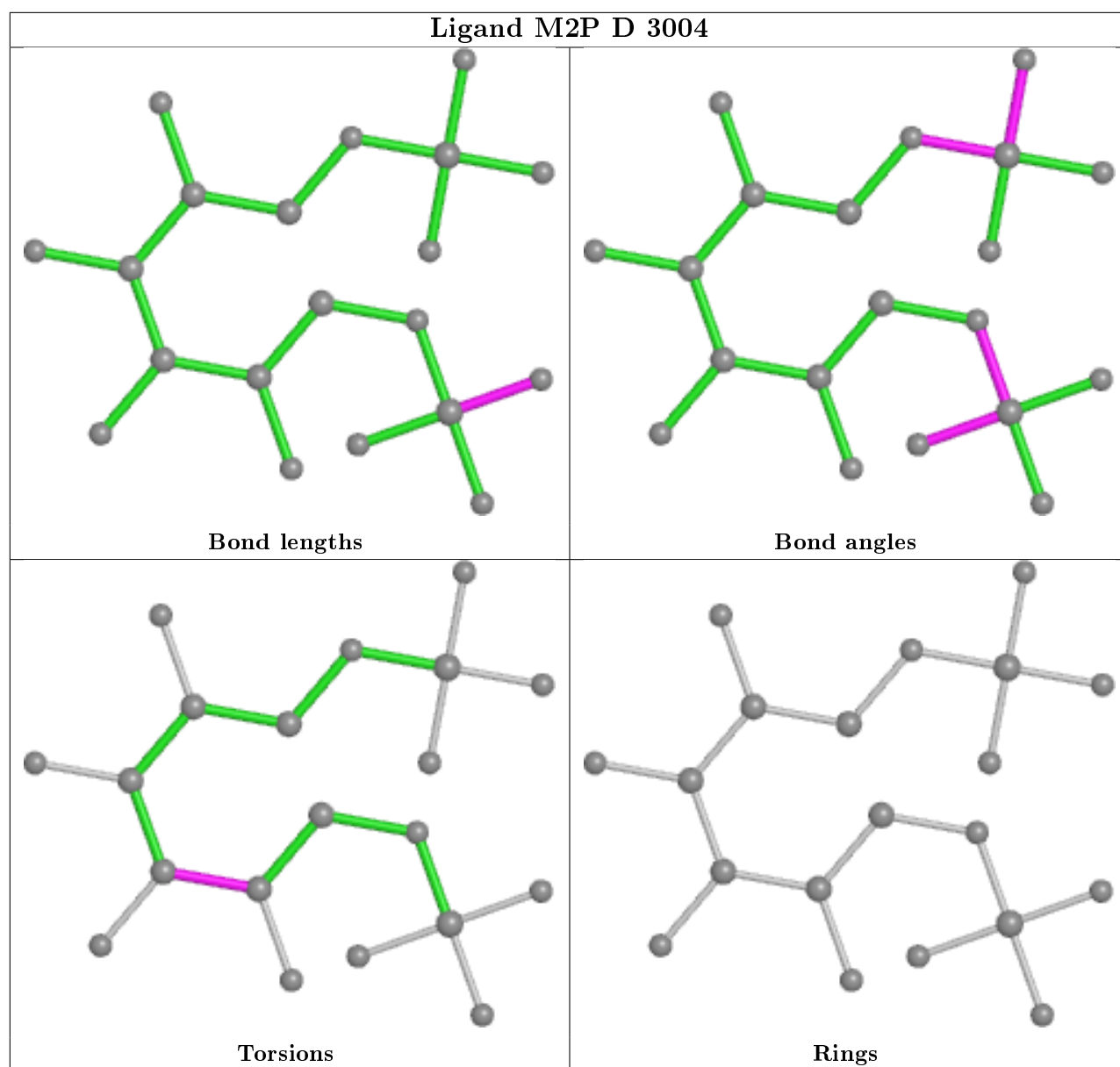
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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(Å ²)	Q<0.9
1	A	363/363 (100%)	0.23	22 (6%) 21 24	7, 16, 55, 90	15 (4%)
1	B	363/363 (100%)	0.17	18 (4%) 28 32	7, 14, 57, 87	15 (4%)
1	C	363/363 (100%)	0.25	29 (7%) 12 13	7, 16, 53, 89	15 (4%)
1	D	363/363 (100%)	0.23	30 (8%) 11 13	8, 19, 69, 105	3 (0%)
All	All	1452/1452 (100%)	0.22	99 (6%) 17 19	7, 16, 60, 105	48 (3%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	GLY	24.8
1	C	357	PHE	20.5
1	B	346	GLY	20.3
1	A	346	GLY	18.2
1	A	356	LEU	17.8
1	C	356	LEU	17.0
1	B	358	ILE	16.6
1	C	351	ALA	15.7
1	A	352	ALA	15.7
1	A	353	SER	14.6
1	A	351	ALA	14.6
1	B	351	ALA	13.5
1	A	348	ALA	13.4
1	C	1	PRO	12.2
1	A	347	GLN	11.9
1	B	357	PHE	11.7
1	B	359	SER	11.6
1	A	350	ALA	10.7
1	A	355	SER	10.6
1	A	345	SER	10.4
1	B	355	SER	10.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	352	ALA	10.3
1	B	356	LEU	10.1
1	D	363	TYR	9.5
1	D	348	ALA	8.9
1	D	361	HIS	8.9
1	A	357	PHE	8.8
1	B	348	ALA	8.7
1	C	350	ALA	8.5
1	A	358	ILE	8.2
1	B	353	SER	8.2
1	A	2	HIS	8.0
1	C	349	GLY	7.8
1	A	354	GLU	7.7
1	C	354	GLU	7.7
1	B	352	ALA	7.5
1	B	347	GLN	7.5
1	C	353	SER	7.4
1	C	348	ALA	7.2
1	C	355	SER	7.0
1	A	349	GLY	7.0
1	C	346	GLY	6.8
1	D	360	ASN	6.6
1	B	350	ALA	6.6
1	D	350	ALA	6.5
1	C	4	HIS	6.3
1	A	359	SER	6.3
1	D	351	ALA	6.0
1	A	1	PRO	5.8
1	C	358	ILE	5.6
1	A	360	ASN	5.3
1	D	362	ALA	5.0
1	C	2	HIS	5.0
1	D	359	SER	5.0
1	B	2	HIS	4.8
1	B	1	PRO	4.8
1	D	347	GLN	4.7
1	B	345	SER	4.7
1	C	156	HIS	4.6
1	C	359	SER	4.5
1	D	356	LEU	4.4
1	D	2	HIS	4.3
1	D	346	GLY	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	344	PRO	4.2
1	D	353	SER	4.2
1	A	4	HIS	4.2
1	C	3	SER	4.1
1	D	1	PRO	4.1
1	C	347	GLN	4.1
1	C	345	SER	4.0
1	D	352	ALA	4.0
1	B	354	GLU	4.0
1	D	355	SER	3.9
1	D	345	SER	3.8
1	A	3	SER	3.8
1	D	358	ILE	3.5
1	D	357	PHE	3.4
1	D	156	HIS	3.4
1	D	44	GLN	3.2
1	C	155	GLU	3.2
1	D	354	GLU	3.1
1	D	349	GLY	3.1
1	D	318	GLU	3.0
1	C	240	THR	3.0
1	C	238	ALA	3.0
1	A	156	HIS	2.8
1	D	155	GLU	2.7
1	B	360	ASN	2.6
1	D	237	HIS	2.6
1	D	319	ASN	2.5
1	C	44	GLN	2.4
1	D	3	SER	2.3
1	C	41	LYS	2.3
1	C	30	LEU	2.1
1	C	239	CYS	2.1
1	D	343	THR	2.1
1	A	44	GLN	2.1
1	D	290	PRO	2.1
1	C	360	ASN	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 [i](#)

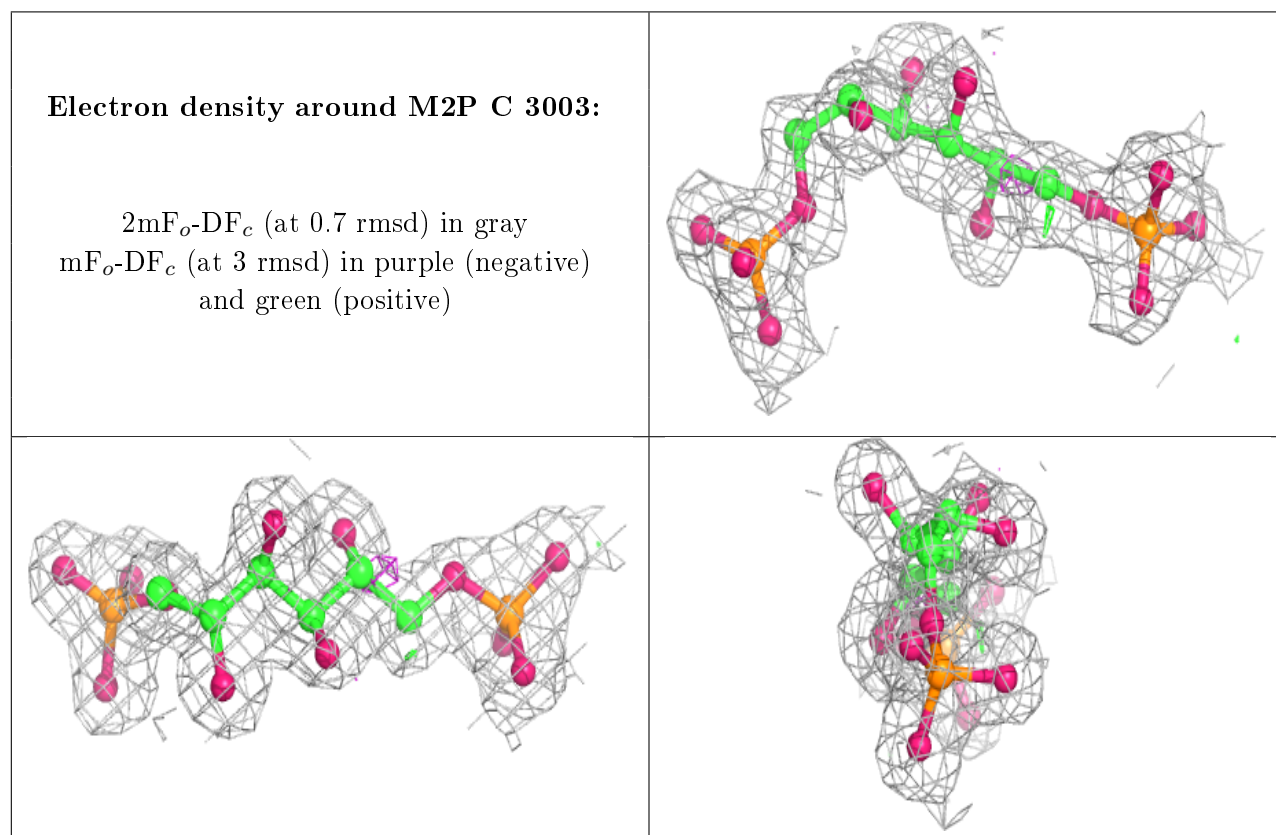
There are no carbohydrates in this entry.

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, 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.

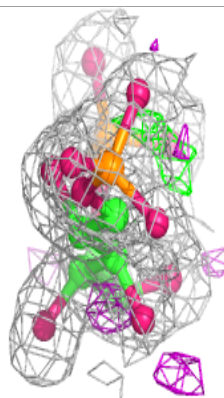
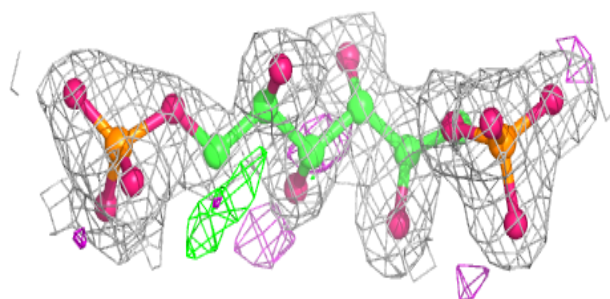
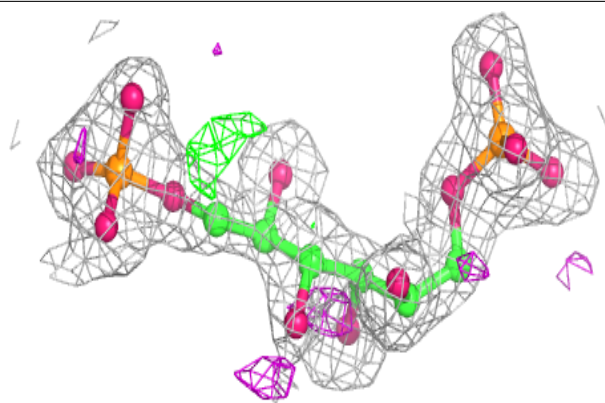
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	M2P	C	3003	20/20	0.95	0.10	16,23,29,29	0
2	M2P	D	3004	20/20	0.95	0.10	22,27,32,32	0
2	M2P	A	3001	20/20	0.96	0.09	15,21,29,31	0
2	M2P	B	3002	20/20	0.97	0.09	14,19,23,24	0

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.

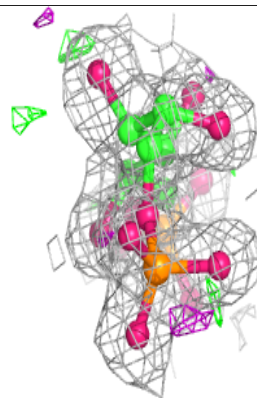
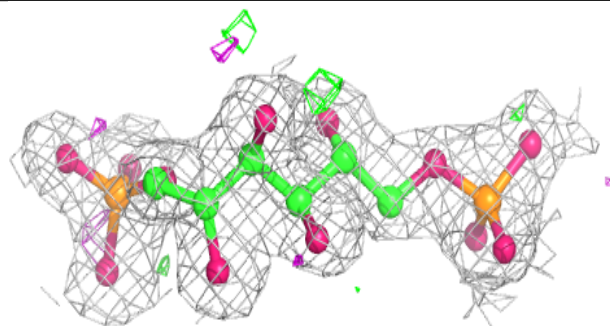
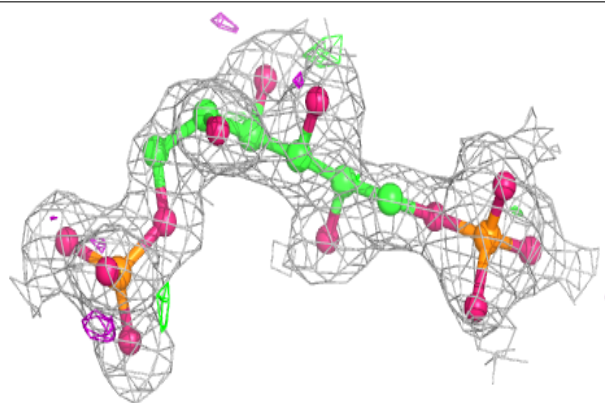


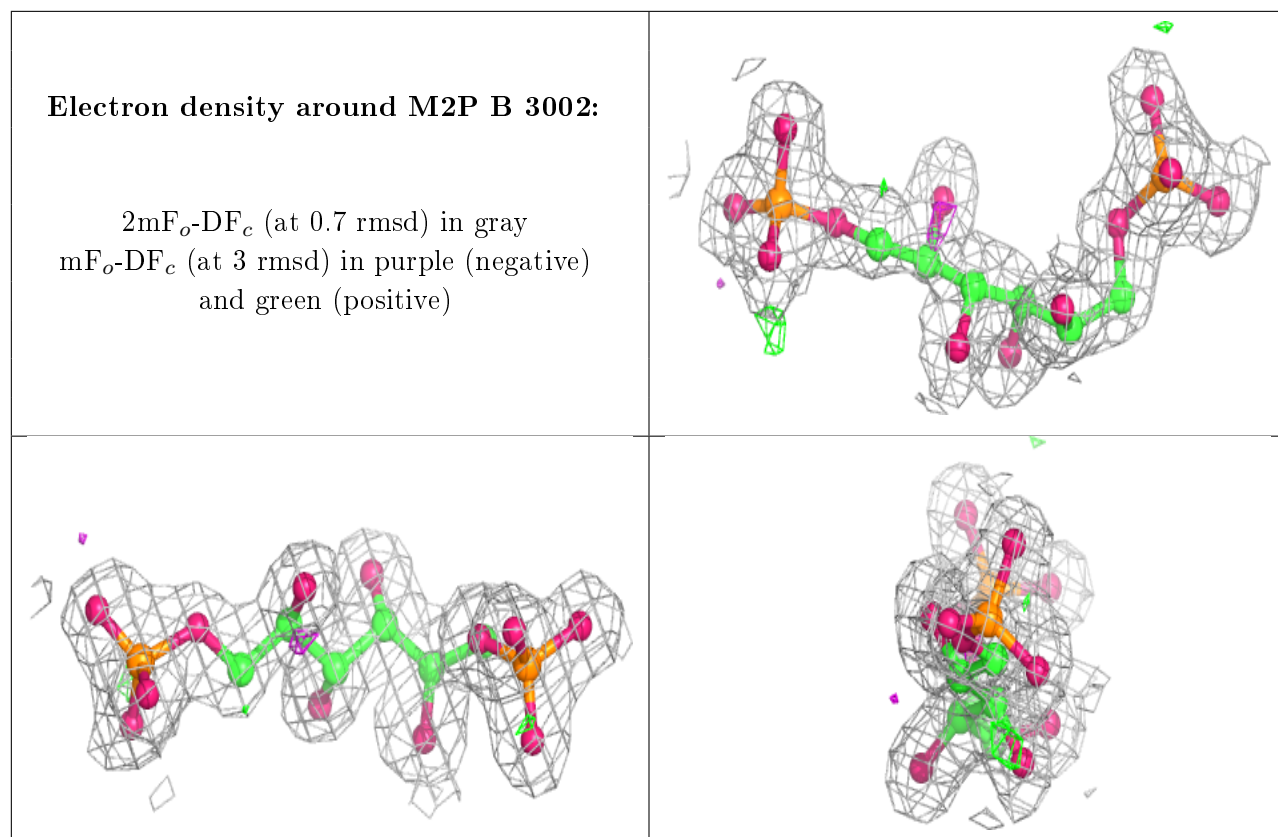
Electron density around M2P D 3004:

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

**Electron density around M2P A 3001:**

$2mF_o-DF_c$ (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.