



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:09 AM UTC

PDB ID : 4IXH / pdb_00004ixh
Title : Crystal Structure of the Catalytic Domain of the Inosine Monophosphate Dehydrogenase from *Cryptosporidium parvum*
Authors : Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Kavitha, M.; Hedstrom, L.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2013-01-25
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

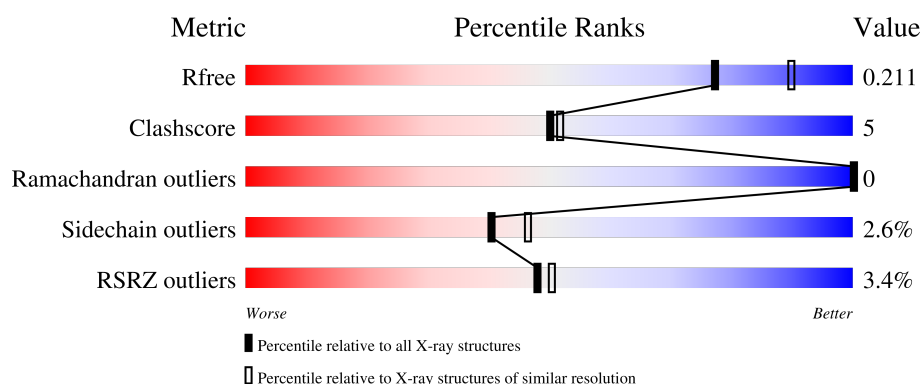
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	361	3% 81% 10% • 7%
1	B	361	3% 81% 10% • 7%
1	C	361	3% 80% 12% • 7%
1	D	361	4% 82% 9% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10776 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	6	0
			2532	1588	434	494	16			
1	B	334	Total	C	N	O	S	0	6	0
			2520	1583	431	491	15			
1	C	336	Total	C	N	O	S	0	4	0
			2516	1581	431	488	16			
1	D	334	Total	C	N	O	S	0	2	0
			2486	1563	424	484	15			

There are 24 discrepancies between the modelled and reference sequences:

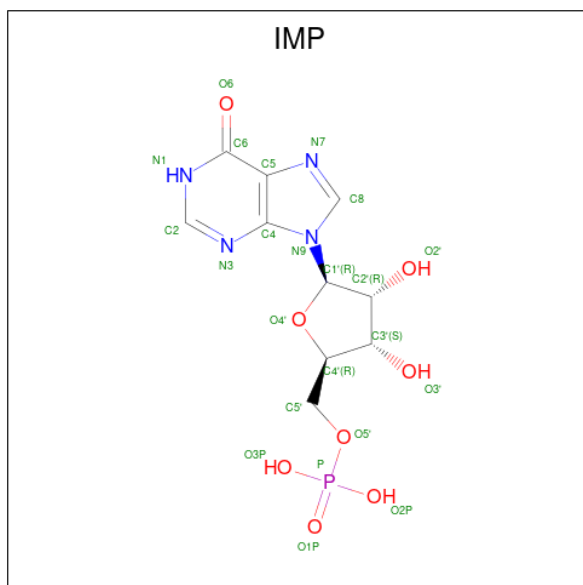
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8T6T2
A	-1	ASN	-	expression tag	UNP Q8T6T2
A	0	ALA	-	expression tag	UNP Q8T6T2
A	90	SER	-	linker	UNP Q8T6T2
A	91	GLY	-	linker	UNP Q8T6T2
A	92	GLY	-	linker	UNP Q8T6T2
B	-2	SER	-	expression tag	UNP Q8T6T2
B	-1	ASN	-	expression tag	UNP Q8T6T2
B	0	ALA	-	expression tag	UNP Q8T6T2
B	90	SER	-	linker	UNP Q8T6T2
B	91	GLY	-	linker	UNP Q8T6T2
B	92	GLY	-	linker	UNP Q8T6T2
C	-2	SER	-	expression tag	UNP Q8T6T2
C	-1	ASN	-	expression tag	UNP Q8T6T2
C	0	ALA	-	expression tag	UNP Q8T6T2
C	90	SER	-	linker	UNP Q8T6T2
C	91	GLY	-	linker	UNP Q8T6T2
C	92	GLY	-	linker	UNP Q8T6T2
D	-2	SER	-	expression tag	UNP Q8T6T2
D	-1	ASN	-	expression tag	UNP Q8T6T2
D	0	ALA	-	expression tag	UNP Q8T6T2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	90	SER	-	linker	UNP Q8T6T2
D	91	GLY	-	linker	UNP Q8T6T2
D	92	GLY	-	linker	UNP Q8T6T2

- Molecule 2 is INOSINIC ACID (CCD ID: IMP) (formula: $C_{10}H_{13}N_4O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	C	1	Total	C	N	O	P	0	0
			23	10	4	8	1		
2	D	1	Total	C	N	O	P	0	0
			23	10	4	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is (2S)-2-(naphthalen-1-yloxy)-N-[2-(pyridin-4-yl)-1,3-benzoxazol-5-yl]propanamide (CCD ID: Q21) (formula: C₂₅H₁₉N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 31	C 25	N 3	O 3	0	0
4	B	1	Total 31	C 25	N 3	O 3	0	0
4	B	1	Total 31	C 25	N 3	O 3	0	0
4	C	1	Total 31	C 25	N 3	O 3	0	0

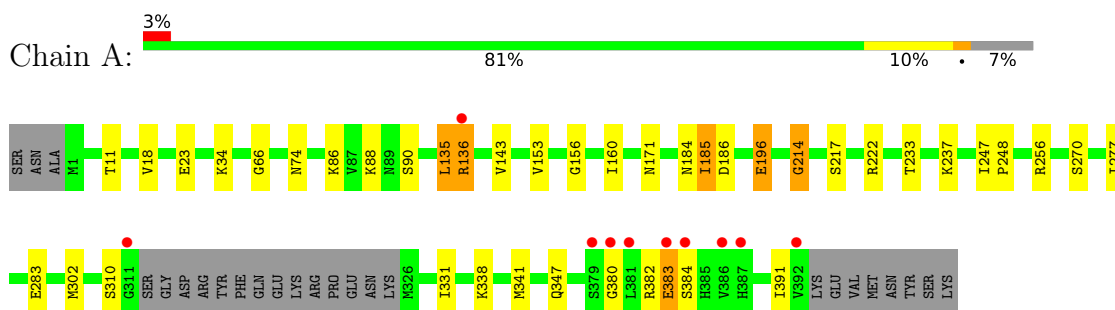
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	127	Total O 127 127	0	0
5	B	114	Total O 114 114	0	0
5	C	114	Total O 114 114	0	0
5	D	131	Total O 131 131	0	0

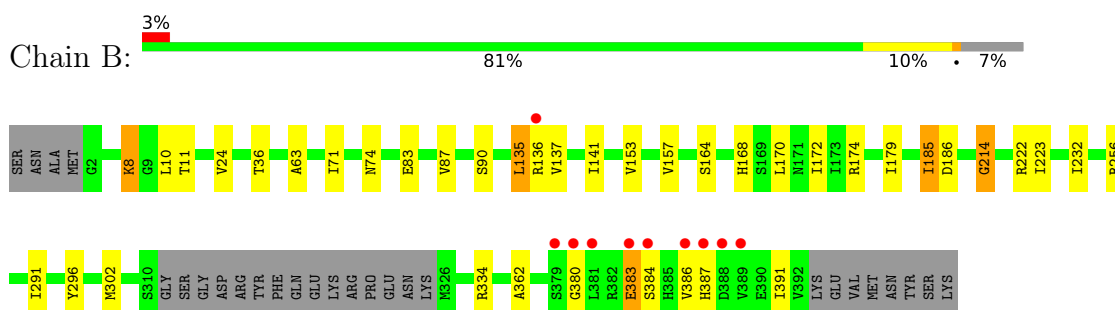
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

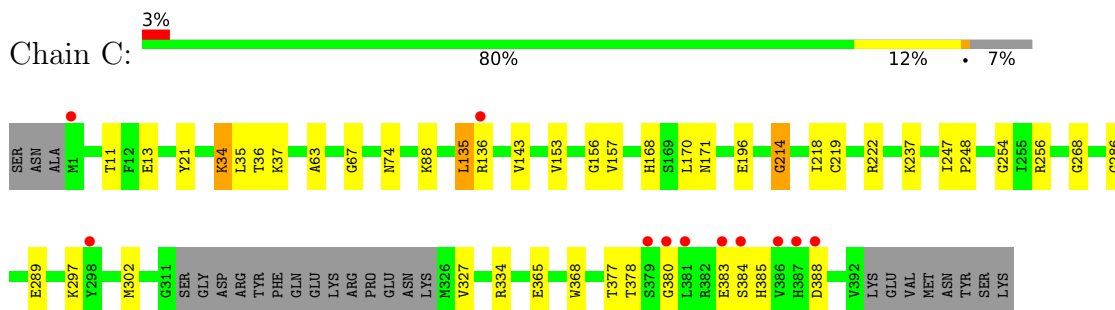
- Molecule 1: Inosine-5'-monophosphate dehydrogenase



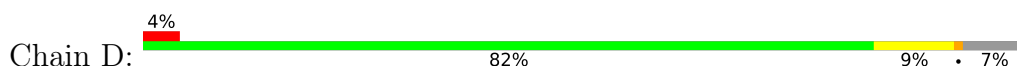
- Molecule 1: Inosine-5'-monophosphate dehydrogenase

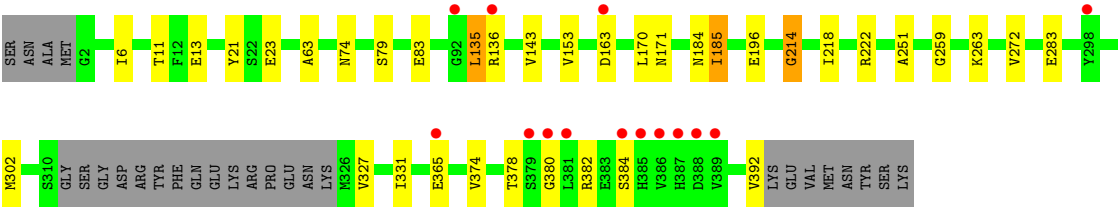


- Molecule 1: Inosine-5'-monophosphate dehydrogenase



- Molecule 1: Inosine-5'-monophosphate dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.19Å 92.02Å 92.14Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	35.52 – 2.10 35.52 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (35.52-2.10) 98.9 (35.52-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.10Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, R_{free}	0.162 , 0.210 0.163 , 0.211	Depositor DCC
R_{free} test set	4142 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	1.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10776	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IMP, EDO, Q21

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	0.48	0/2557	0.81	3/3440 (0.1%)
1	B	0.48	0/2545	0.83	3/3426 (0.1%)
1	C	0.46	0/2541	0.82	3/3419 (0.1%)
1	D	0.47	0/2511	0.85	3/3380 (0.1%)
All	All	0.47	0/10154	0.82	12/13665 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	214	GLY	CA-C-N	-6.05	113.99	120.47
1	D	214	GLY	C-N-CA	-6.05	113.99	120.47
1	B	214	GLY	N-CA-C	5.83	124.23	112.34
1	C	214	GLY	CA-C-N	-5.73	114.34	120.47
1	C	214	GLY	C-N-CA	-5.73	114.34	120.47
1	C	214	GLY	N-CA-C	5.68	123.92	112.34
1	B	214	GLY	CA-C-N	-5.55	114.05	120.04
1	B	214	GLY	C-N-CA	-5.55	114.05	120.04
1	A	214	GLY	CA-C-N	-5.27	114.35	120.04
1	A	214	GLY	C-N-CA	-5.27	114.35	120.04
1	D	214	GLY	N-CA-C	5.09	122.72	112.34
1	A	214	GLY	N-CA-C	5.06	122.67	112.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2532	0	2625	39	0
1	B	2520	0	2615	32	0
1	C	2516	0	2619	36	0
1	D	2486	0	2584	26	0
2	A	23	0	11	0	0
2	B	23	0	11	0	0
2	C	23	0	11	1	0
2	D	23	0	11	0	0
3	A	12	0	18	1	0
3	C	8	0	12	3	0
4	A	31	0	19	1	0
4	B	62	0	38	2	0
4	C	31	0	19	1	0
5	A	127	0	0	6	0
5	B	114	0	0	2	0
5	C	114	0	0	3	0
5	D	131	0	0	2	0
All	All	10776	0	10593	110	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 5.

All (110) 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:222:ARG:HD2	1:D:384:SER:HA	1.67	0.76
1:A:66:GLY:HA2	1:A:136[B]:ARG:HH21	1.57	0.68
1:A:222:ARG:HD2	1:B:384:SER:HA	1.75	0.67
1:B:222:ARG:HD2	1:C:384:SER:HA	1.73	0.67
1:D:74:ASN:HB2	1:D:302:MET:HE1	1.76	0.67
1:C:237:LYS:NZ	5:C:655:HOH:O	2.29	0.65
1:C:286:GLY:O	1:C:297:LYS:NZ	2.30	0.65
1:B:256[A]:ARG:NE	1:C:388:ASP:OD2	2.21	0.64
1:A:74:ASN:HB2	1:A:302:MET:HE1	1.79	0.63
1:D:143:VAL:HG21	1:D:171:ASN:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLY:HA2	1:D:11:THR:HG21	1.83	0.61
1:B:223:ILE:HD11	1:C:385:HIS:HA	1.82	0.61
1:A:153:VAL:HG22	1:A:185:ILE:HD12	1.83	0.60
1:A:384:SER:HA	1:D:222:ARG:HD2	1.83	0.60
1:B:74:ASN:HB2	1:B:302:MET:HE1	1.83	0.59
1:A:256:ARG:NH1	5:A:710:HOH:O	2.35	0.59
1:C:74:ASN:HB2	1:C:302:MET:HE1	1.84	0.59
1:A:160:ILE:HG12	1:A:185:ILE:HD13	1.85	0.58
1:A:338:LYS:NZ	5:A:664:HOH:O	2.37	0.58
1:B:11[A]:THR:HG21	1:C:380:GLY:HA2	1.86	0.58
1:A:331:ILE:HD13	1:B:391:ILE:HG12	1.86	0.58
1:C:143[A]:VAL:HG21	1:C:171:ASN:HB3	1.87	0.56
1:A:23:GLU:HG2	1:D:170:LEU:HB2	1.88	0.56
1:B:24:VAL:HG11	1:B:362:ALA:HB2	1.88	0.54
1:A:391:ILE:HG12	1:D:331:ILE:HD13	1.90	0.54
1:A:382:ARG:NH2	1:D:13:GLU:OE1	2.40	0.54
1:A:214:GLY:HA3	1:A:222:ARG:HE	1.72	0.54
1:A:237:LYS:HE3	5:A:707:HOH:O	2.07	0.54
1:A:11:THR:HG21	1:B:380:GLY:HA2	1.90	0.53
5:B:701:HOH:O	1:C:383:GLU:HG2	2.08	0.53
1:A:143:VAL:HG21	1:A:171[A]:ASN:HB3	1.92	0.52
1:B:36:THR:OG1	1:B:186:ASP:OD1	2.20	0.51
1:D:365:GLU:HG2	5:D:712:HOH:O	2.09	0.51
1:A:171[A]:ASN:ND2	5:A:680:HOH:O	2.42	0.51
1:B:87:VAL:HG11	1:B:137:VAL:HB	1.92	0.51
1:B:214:GLY:HA3	1:B:222:ARG:HE	1.76	0.51
1:C:334:ARG:HE	1:D:392:VAL:HG22	1.76	0.51
1:A:347[B]:GLN:HG2	1:D:327:VAL:HG21	1.93	0.51
1:C:63:ALA:HB1	1:C:135:LEU:HG	1.92	0.51
1:C:170:LEU:HB2	1:D:23:GLU:HG2	1.94	0.50
1:A:136[A]:ARG:NH1	5:A:667:HOH:O	2.45	0.50
1:D:153:VAL:HG22	1:D:185:ILE:HD12	1.94	0.49
1:C:88:LYS:HE3	1:C:156:GLY:O	2.12	0.49
1:C:254:GLY:O	1:C:256[A]:ARG:HD3	2.13	0.49
1:D:63:ALA:CB	1:D:135:LEU:HG	2.43	0.48
1:A:214:GLY:HA3	1:A:222:ARG:NE	2.29	0.48
1:B:214:GLY:HA3	1:B:222:ARG:NE	2.29	0.48
1:C:63:ALA:CB	1:C:135:LEU:HG	2.44	0.48
1:D:63:ALA:HB1	1:D:135:LEU:HG	1.95	0.48
1:A:18:VAL:HG21	1:D:6:ILE:HD11	1.96	0.47
1:C:378:THR:HG23	1:D:382:ARG:HH12	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LYS:HE3	1:A:156:GLY:O	2.14	0.47
1:B:291:ILE:HB	1:B:296:TYR:CE1	2.50	0.47
1:C:13:GLU:HG3	1:C:256[A]:ARG:NH2	2.30	0.46
1:A:383:GLU:HG2	5:D:719:HOH:O	2.16	0.46
1:C:219:CYS:SG	2:C:501:IMP:H2	2.56	0.46
1:C:35:LEU:HG	1:C:36:THR:HG23	1.98	0.45
1:B:136[B]:ARG:H	1:B:136[B]:ARG:HG3	1.49	0.45
1:B:334:ARG:HE	1:B:334:ARG:HB2	1.54	0.45
1:C:168:HIS:CE1	1:D:21:TYR:HB2	2.51	0.45
1:D:214:GLY:HA3	1:D:222:ARG:HE	1.81	0.45
1:C:34:LYS:H	3:C:504:EDO:H12	1.82	0.45
1:C:11:THR:HG21	1:D:380:GLY:HA2	1.98	0.45
1:D:214:GLY:HA3	1:D:222:ARG:NE	2.31	0.45
1:B:256[B]:ARG:NH1	5:B:693:HOH:O	2.34	0.45
1:C:13:GLU:OE1	1:C:256[B]:ARG:NH1	2.50	0.45
1:C:67:GLY:O	1:C:136[B]:ARG:NH1	2.50	0.44
1:B:90:SER:O	1:B:135:LEU:HD22	2.17	0.44
1:A:233:THR:HG22	1:A:237:LYS:HD3	1.99	0.44
1:C:368:TRP:CH2	3:C:504:EDO:H21	2.53	0.44
1:A:270:SER:OG	3:A:502:EDO:H11	2.17	0.44
1:B:8:LYS:HE2	1:C:377:THR:HG22	2.00	0.43
1:A:256:ARG:NH2	1:B:383:GLU:OE1	2.52	0.43
1:D:79:SER:O	1:D:83:GLU:HG2	2.18	0.43
1:A:74:ASN:HD21	1:A:310:SER:HB2	1.84	0.43
1:D:251:ALA:HB3	1:D:272:VAL:HG12	2.00	0.43
1:A:88:LYS:HD3	1:A:88:LYS:HA	1.80	0.43
1:A:34:LYS:HE2	1:A:34:LYS:HB3	1.89	0.42
1:B:141:ILE:HD11	1:B:179:ILE:HD11	2.01	0.42
4:A:504:Q21:O2	4:A:504:Q21:H15	2.19	0.42
1:C:143[B]:VAL:HG23	5:C:650:HOH:O	2.19	0.42
1:B:153:VAL:CG2	1:B:185:ILE:HG12	2.49	0.42
1:B:10:LEU:O	1:B:232:ILE:HB	2.20	0.42
1:D:259:GLY:O	1:D:263:LYS:HG3	2.20	0.42
1:C:268:GLY:HA2	3:C:503:EDO:H22	2.01	0.42
1:A:277:ILE:HG23	5:A:664:HOH:O	2.19	0.42
1:B:170:LEU:O	1:B:174:ARG:HG3	2.20	0.42
1:A:171[B]:ASN:ND2	4:B:501:Q21:H17	2.35	0.42
1:B:63:ALA:HB3	1:B:135:LEU:HG	2.02	0.42
1:C:256[A]:ARG:HE	1:C:256[A]:ARG:HB2	1.68	0.42
1:A:185:ILE:HG12	1:A:186:ASP:N	2.34	0.41
1:A:90:SER:O	1:A:135:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ILE:HA	1:A:248:PRO:HD3	1.85	0.41
1:C:153:VAL:HA	1:C:157:VAL:HG12	2.03	0.41
1:C:256[A]:ARG:NH1	5:C:684:HOH:O	2.50	0.41
1:C:214:GLY:HA3	1:C:222:ARG:HE	1.84	0.41
1:D:283:GLU:N	1:D:283:GLU:OE2	2.53	0.41
1:B:168:HIS:CE1	1:C:21:TYR:HB2	2.56	0.41
1:A:331:ILE:HG12	1:B:386:VAL:HG21	2.02	0.41
4:C:502:Q21:O2	4:C:502:Q21:H15	2.19	0.41
1:A:217:SER:HA	1:B:387:HIS:CE1	2.56	0.41
1:B:164:SER:HB2	1:B:172:ILE:HD11	2.02	0.41
1:A:283:GLU:CD	1:A:341:MET:HG2	2.45	0.41
1:B:63:ALA:CB	1:B:135:LEU:HG	2.50	0.41
1:B:71:ILE:HD13	1:B:83:GLU:HB3	2.02	0.41
1:C:247:ILE:HA	1:C:248:PRO:HD3	1.91	0.41
1:D:136[B]:ARG:HE	1:D:136[B]:ARG:HB2	1.75	0.41
1:A:196[A]:GLU:CD	1:A:196[A]:GLU:H	2.29	0.40
1:B:8:LYS:HE2	1:C:377:THR:CG2	2.52	0.40
4:B:503:Q21:O2	4:B:503:Q21:H15	2.21	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	338/361 (94%)	327 (97%)	11 (3%)	0	100	100
1	B	336/361 (93%)	324 (96%)	12 (4%)	0	100	100
1	C	336/361 (93%)	328 (98%)	8 (2%)	0	100	100
1	D	332/361 (92%)	324 (98%)	8 (2%)	0	100	100
All	All	1342/1444 (93%)	1303 (97%)	39 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	278/295 (94%)	269 (97%)	9 (3%)	34	38
1	B	277/295 (94%)	272 (98%)	5 (2%)	51	60
1	C	276/295 (94%)	268 (97%)	8 (3%)	37	42
1	D	273/295 (92%)	265 (97%)	8 (3%)	37	42
All	All	1104/1180 (94%)	1074 (97%)	30 (3%)	40	45

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	135	LEU
1	A	136[A]	ARG
1	A	136[B]	ARG
1	A	184	ASN
1	A	185	ILE
1	A	196[A]	GLU
1	A	196[B]	GLU
1	A	383	GLU
1	B	8	LYS
1	B	135	LEU
1	B	157	VAL
1	B	185	ILE
1	B	383	GLU
1	C	34	LYS
1	C	37	LYS
1	C	135	LEU
1	C	196	GLU
1	C	218	ILE
1	C	289	GLU
1	C	327	VAL
1	C	365	GLU
1	D	135	LEU
1	D	163	ASP

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Mol	Chain	Res	Type
1	D	184	ASN
1	D	185	ILE
1	D	196	GLU
1	D	218	ILE
1	D	374	VAL
1	D	378	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	B	56	HIS
1	B	168	HIS
1	B	387	HIS
1	C	144	ASN
1	D	168	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	IMP	D	501	-	25,25,25	1.08	2 (8%)	37,38,38	2.02	10 (27%)
3	EDO	C	504	-	3,3,3	0.43	0	2,2,2	0.40	0
4	Q21	C	502	-	35,35,35	1.44	5 (14%)	49,49,49	2.05	9 (18%)
3	EDO	A	503	-	3,3,3	0.34	0	2,2,2	0.41	0
2	IMP	B	502	-	25,25,25	1.06	1 (4%)	37,38,38	2.04	10 (27%)
4	Q21	A	504	-	35,35,35	1.39	4 (11%)	49,49,49	2.12	8 (16%)
4	Q21	B	501	-	35,35,35	1.41	4 (11%)	49,49,49	2.16	11 (22%)
4	Q21	B	503	-	35,35,35	1.41	4 (11%)	49,49,49	2.02	10 (20%)
3	EDO	A	505	-	3,3,3	0.55	0	2,2,2	0.09	0
2	IMP	A	501	-	25,25,25	1.00	1 (4%)	37,38,38	1.92	8 (21%)
3	EDO	A	502	-	3,3,3	0.46	0	2,2,2	0.39	0
2	IMP	C	501	-	25,25,25	0.99	1 (4%)	37,38,38	1.96	9 (24%)
3	EDO	C	503	-	3,3,3	0.52	0	2,2,2	0.06	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	IMP	D	501	-	-	0/10/26/26	0/3/3/3
3	EDO	C	504	-	-	1/1/1/1	-
4	Q21	C	502	-	-	0/16/16/16	0/5/5/5
3	EDO	A	503	-	-	1/1/1/1	-
2	IMP	B	502	-	-	0/10/26/26	0/3/3/3
4	Q21	A	504	-	-	0/16/16/16	0/5/5/5
4	Q21	B	501	-	-	0/16/16/16	0/5/5/5
4	Q21	B	503	-	-	0/16/16/16	0/5/5/5
3	EDO	A	505	-	-	1/1/1/1	-
2	IMP	A	501	-	-	0/10/26/26	0/3/3/3
3	EDO	A	502	-	-	0/1/1/1	-
2	IMP	C	501	-	-	0/10/26/26	0/3/3/3
3	EDO	C	503	-	-	1/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	502	Q21	O1-C7	-4.64	1.31	1.38
4	B	503	Q21	O1-C7	-4.32	1.31	1.38
2	D	501	IMP	C2-N3	4.30	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	IMP	C2-N3	4.20	1.37	1.30
4	B	501	Q21	O1-C7	-4.13	1.31	1.38
4	A	504	Q21	O1-C7	-3.99	1.32	1.38
4	B	501	Q21	C2-C1	-3.97	1.39	1.47
4	B	503	Q21	C2-C1	-3.94	1.39	1.47
4	A	504	Q21	C2-C1	-3.84	1.39	1.47
4	C	502	Q21	C2-C1	-3.81	1.39	1.47
2	C	501	IMP	C2-N3	3.78	1.37	1.30
2	A	501	IMP	C2-N3	3.73	1.37	1.30
4	A	504	Q21	C1-N1	3.05	1.37	1.30
4	B	503	Q21	C1-N1	3.04	1.37	1.30
4	C	502	Q21	C1-N1	2.98	1.37	1.30
4	B	501	Q21	C1-N1	2.89	1.37	1.30
4	B	501	Q21	C10-N3	-2.57	1.36	1.41
4	A	504	Q21	C10-N3	-2.46	1.36	1.41
4	C	502	Q21	C10-N3	-2.39	1.36	1.41
4	B	503	Q21	C10-N3	-2.28	1.37	1.41
4	C	502	Q21	C8-N1	-2.04	1.35	1.39
2	D	501	IMP	C5-N7	-2.01	1.35	1.39

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	501	Q21	O1-C1-N1	-7.24	106.39	115.10
4	A	504	Q21	O1-C1-N1	-7.11	106.53	115.10
4	C	502	Q21	O1-C1-N1	-7.00	106.67	115.10
4	B	503	Q21	O1-C1-N1	-6.88	106.82	115.10
4	B	501	Q21	O1-C7-C8	6.03	111.90	107.80
4	C	502	Q21	O1-C7-C8	5.91	111.81	107.80
4	A	504	Q21	O1-C7-C8	5.82	111.75	107.80
2	C	501	IMP	C5-C6-N1	5.54	118.75	110.78
2	B	502	IMP	C5-C6-N1	5.50	118.69	110.78
4	B	501	Q21	C8-N1-C1	5.46	110.46	104.53
2	D	501	IMP	C5-C6-N1	5.42	118.57	110.78
4	B	503	Q21	O1-C7-C8	5.32	111.41	107.80
4	A	504	Q21	C8-N1-C1	5.27	110.25	104.53
2	A	501	IMP	C5-C6-N1	5.18	118.23	110.78
4	B	501	Q21	C7-C8-N1	-5.05	103.92	108.60
4	A	504	Q21	C7-C8-N1	-4.92	104.04	108.60
4	C	502	Q21	C8-N1-C1	4.86	109.80	104.53
2	B	502	IMP	C2-N3-C4	4.73	119.85	111.53
2	D	501	IMP	C2-N3-C4	4.66	119.73	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	503	Q21	C8-N1-C1	4.64	109.57	104.53
2	D	501	IMP	C5-C4-N3	-4.56	120.56	127.27
4	C	502	Q21	C7-C8-N1	-4.50	104.43	108.60
2	C	501	IMP	C2-N3-C4	4.48	119.41	111.53
2	B	502	IMP	C5-C4-N3	-4.44	120.74	127.27
2	A	501	IMP	N1-C2-N3	-4.42	120.41	125.50
2	B	502	IMP	N1-C2-N3	-4.42	120.41	125.50
2	C	501	IMP	N1-C2-N3	-4.30	120.55	125.50
4	B	503	Q21	C7-C8-N1	-4.27	104.64	108.60
2	A	501	IMP	C2-N3-C4	4.26	119.02	111.53
2	C	501	IMP	C5-C4-N3	-4.19	121.09	127.27
4	A	504	Q21	O1-C1-C2	4.17	127.61	118.30
4	B	501	Q21	O1-C1-C2	4.15	127.58	118.30
2	D	501	IMP	N1-C2-N3	-4.10	120.78	125.50
4	C	502	Q21	O1-C1-C2	4.07	127.39	118.30
4	B	503	Q21	O1-C1-C2	3.68	126.53	118.30
2	A	501	IMP	C5-C4-N3	-3.67	121.87	127.27
2	D	501	IMP	C2-N1-C6	-3.50	120.29	125.09
4	B	503	Q21	C7-O1-C1	3.41	107.56	104.06
2	B	502	IMP	C2-N1-C6	-3.34	120.52	125.09
4	A	504	Q21	C7-O1-C1	3.28	107.42	104.06
4	B	501	Q21	C7-O1-C1	3.20	107.34	104.06
4	C	502	Q21	C7-O1-C1	3.15	107.28	104.06
2	B	502	IMP	N9-C8-N7	-3.10	107.65	113.40
2	C	501	IMP	C2-N1-C6	-3.08	120.87	125.09
2	B	502	IMP	C8-N7-C5	3.05	109.70	104.26
2	A	501	IMP	N9-C8-N7	-2.98	107.88	113.40
4	B	501	Q21	C9-C8-N1	2.95	135.67	129.31
4	B	503	Q21	C9-C8-N1	2.93	135.61	129.31
4	B	503	Q21	O3-C16-C21	2.90	119.88	114.62
2	D	501	IMP	N9-C8-N7	-2.90	108.03	113.40
2	D	501	IMP	C8-N7-C5	2.89	109.40	104.26
4	A	504	Q21	C9-C8-N1	2.87	135.50	129.31
4	C	502	Q21	C9-C8-N1	2.85	135.46	129.31
2	C	501	IMP	N9-C8-N7	-2.84	108.14	113.40
2	A	501	IMP	C8-N7-C5	2.78	109.20	104.26
2	C	501	IMP	C8-N7-C5	2.72	109.11	104.26
4	B	501	Q21	O3-C16-C21	2.69	119.50	114.62
2	A	501	IMP	C2-N1-C6	-2.68	121.41	125.09
4	A	504	Q21	O3-C16-C21	2.48	119.11	114.62
4	C	502	Q21	O3-C16-C21	2.47	119.09	114.62
2	D	501	IMP	O6-C6-C5	-2.44	120.09	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	IMP	O6-C6-C5	-2.37	120.27	126.53
4	B	503	Q21	O3-C16-C17	-2.32	120.42	124.58
2	B	502	IMP	C4-C5-N7	-2.26	107.09	110.67
2	D	501	IMP	C4-C5-N7	-2.21	107.16	110.67
4	B	501	Q21	O3-C16-C17	-2.20	120.65	124.58
2	A	501	IMP	C4-C5-N7	-2.20	107.19	110.67
4	B	501	Q21	C5-N2-C4	2.18	121.85	116.86
4	B	503	Q21	C5-N2-C4	2.06	121.58	116.86
2	D	501	IMP	N9-C4-N3	2.06	131.59	126.90
2	C	501	IMP	C4-C5-N7	-2.06	107.41	110.67
2	C	501	IMP	O6-C6-C5	-2.05	121.13	126.53
2	B	502	IMP	N9-C4-N3	2.05	131.56	126.90
4	B	501	Q21	C6-C5-N2	-2.02	120.15	123.60
4	C	502	Q21	O3-C16-C17	-2.02	120.98	124.58

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	EDO	O1-C1-C2-O2
3	C	504	EDO	O1-C1-C2-O2
3	C	503	EDO	O1-C1-C2-O2
3	A	505	EDO	O1-C1-C2-O2

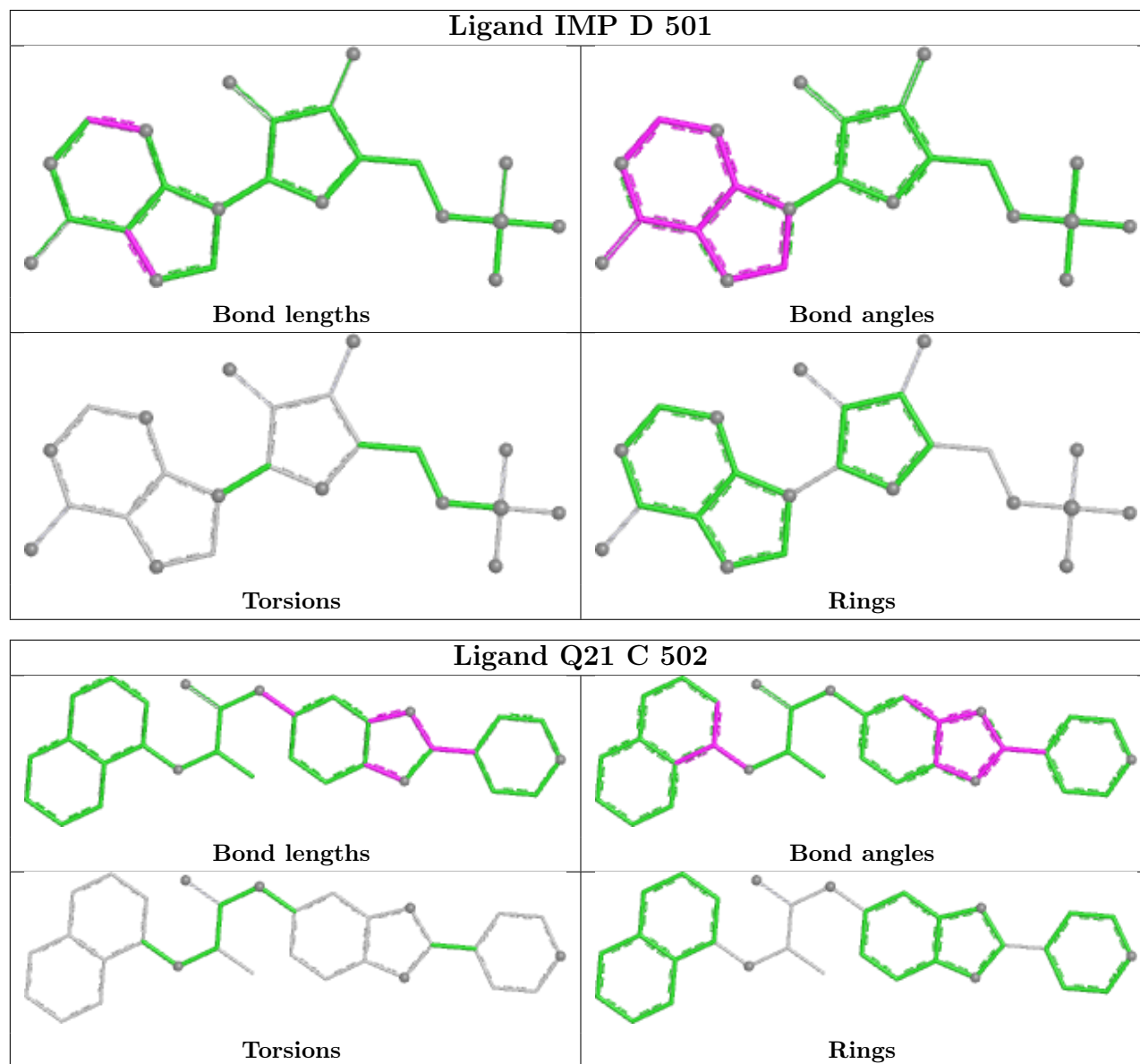
There are no ring outliers.

8 monomers are involved in 9 short contacts:

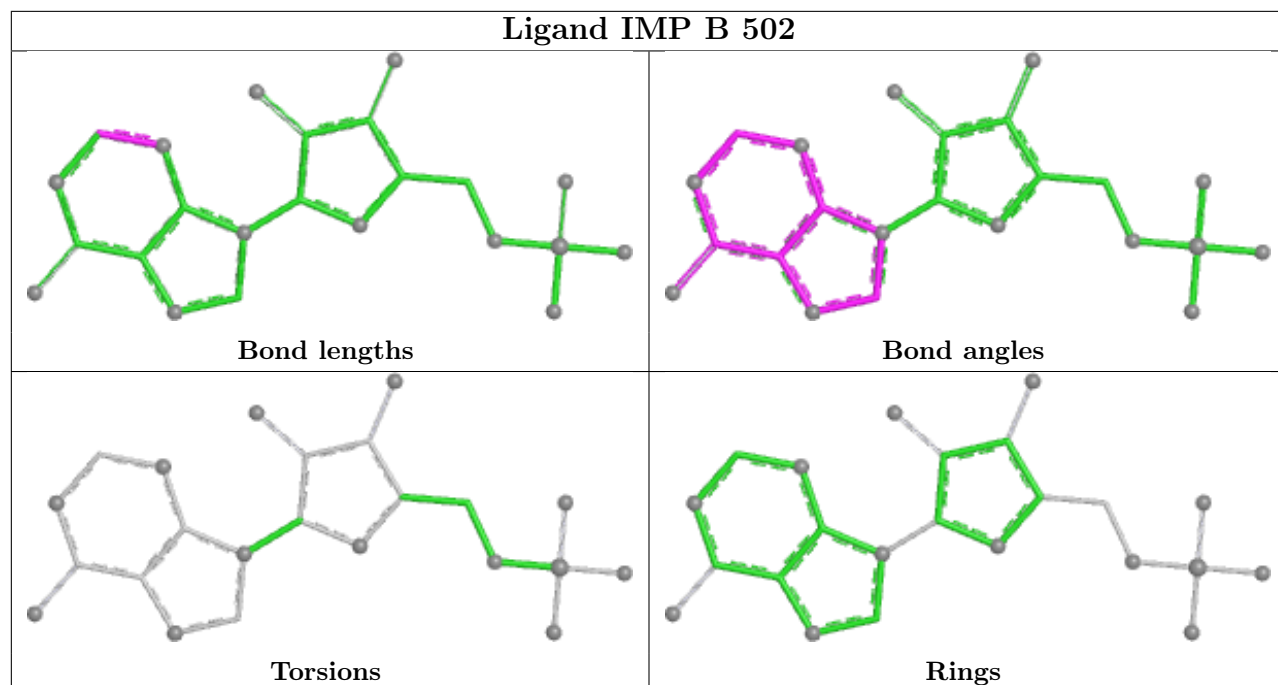
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	504	EDO	2	0
4	C	502	Q21	1	0
4	A	504	Q21	1	0
4	B	501	Q21	1	0
4	B	503	Q21	1	0
3	A	502	EDO	1	0
2	C	501	IMP	1	0
3	C	503	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

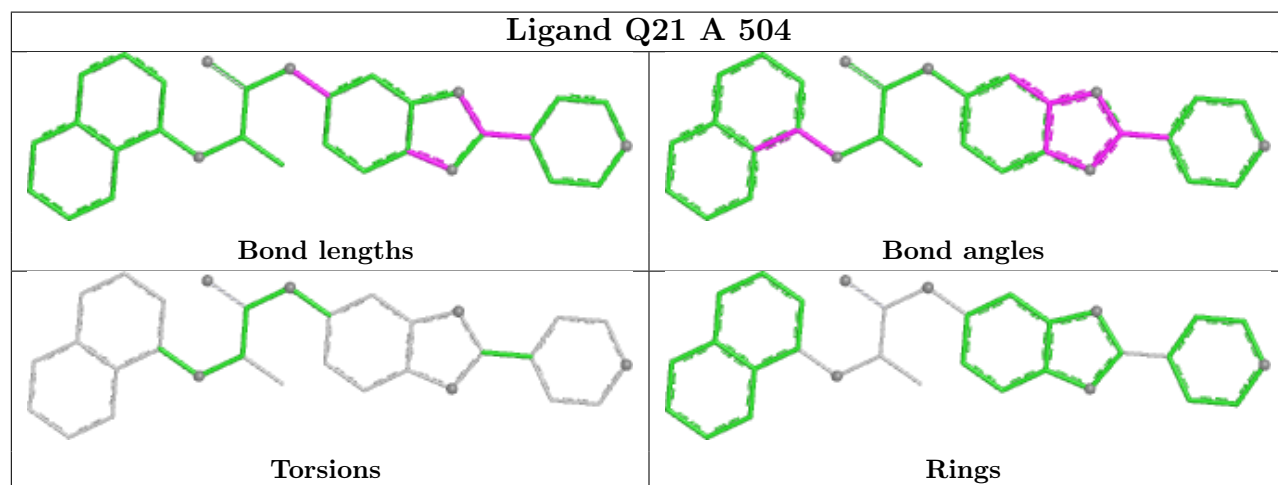
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



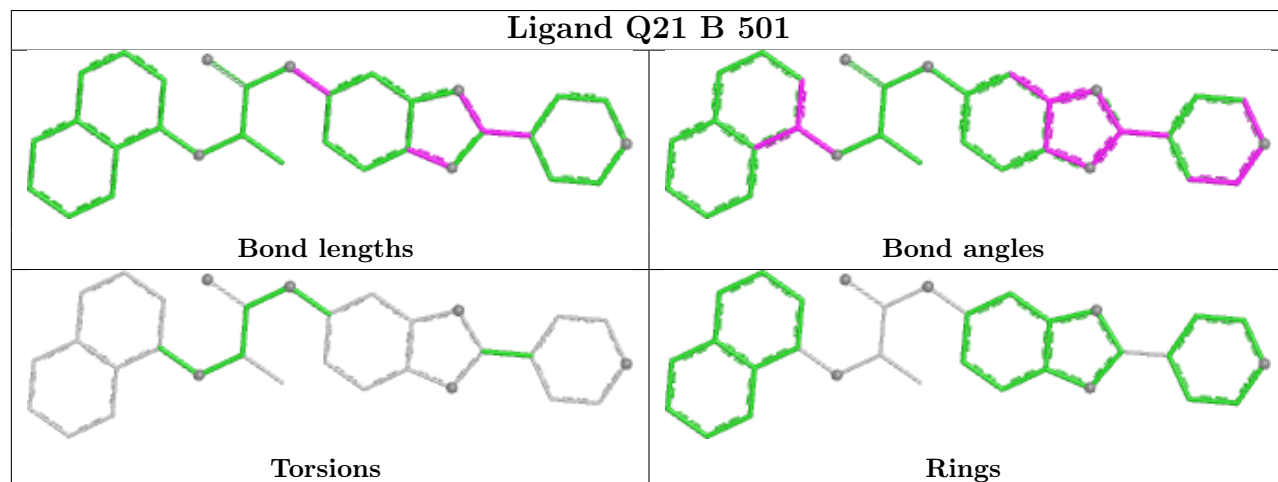
Ligand IMP B 502



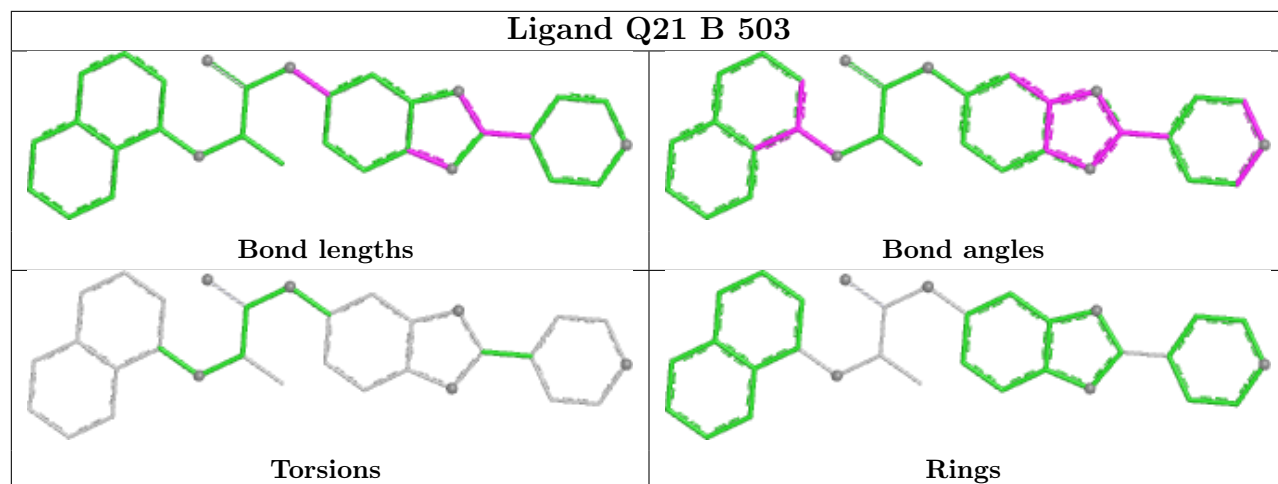
Ligand Q21 A 504



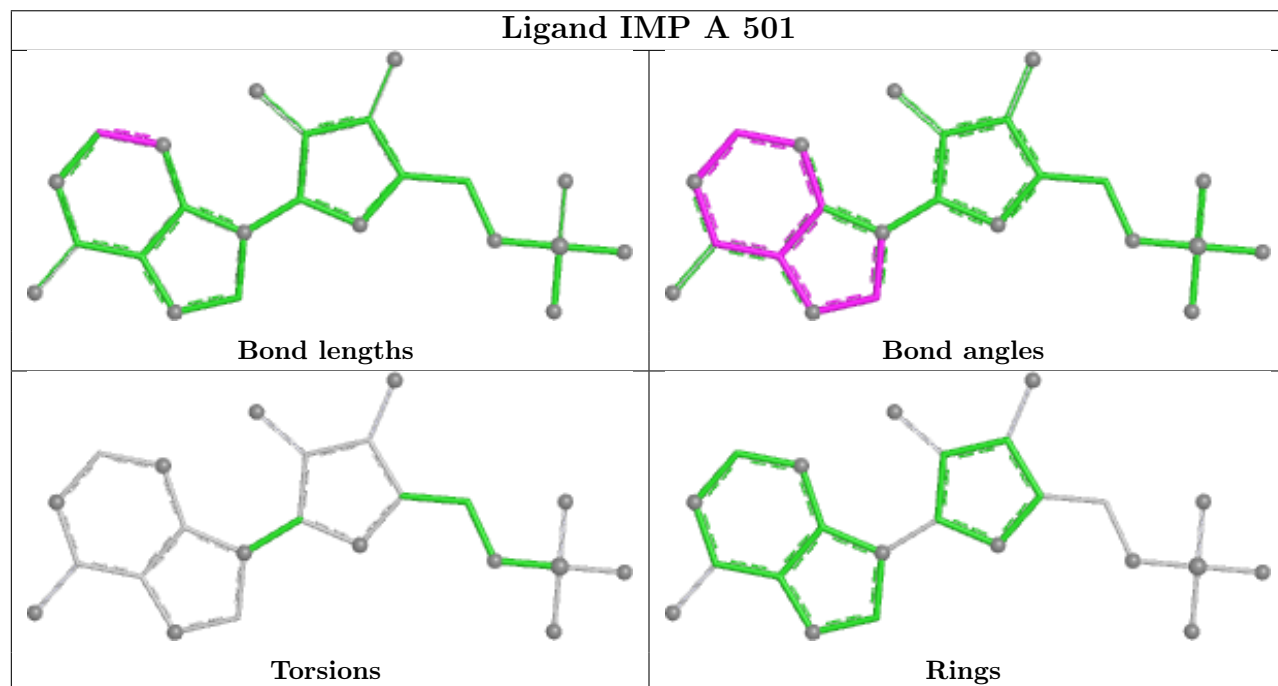
Ligand Q21 B 501

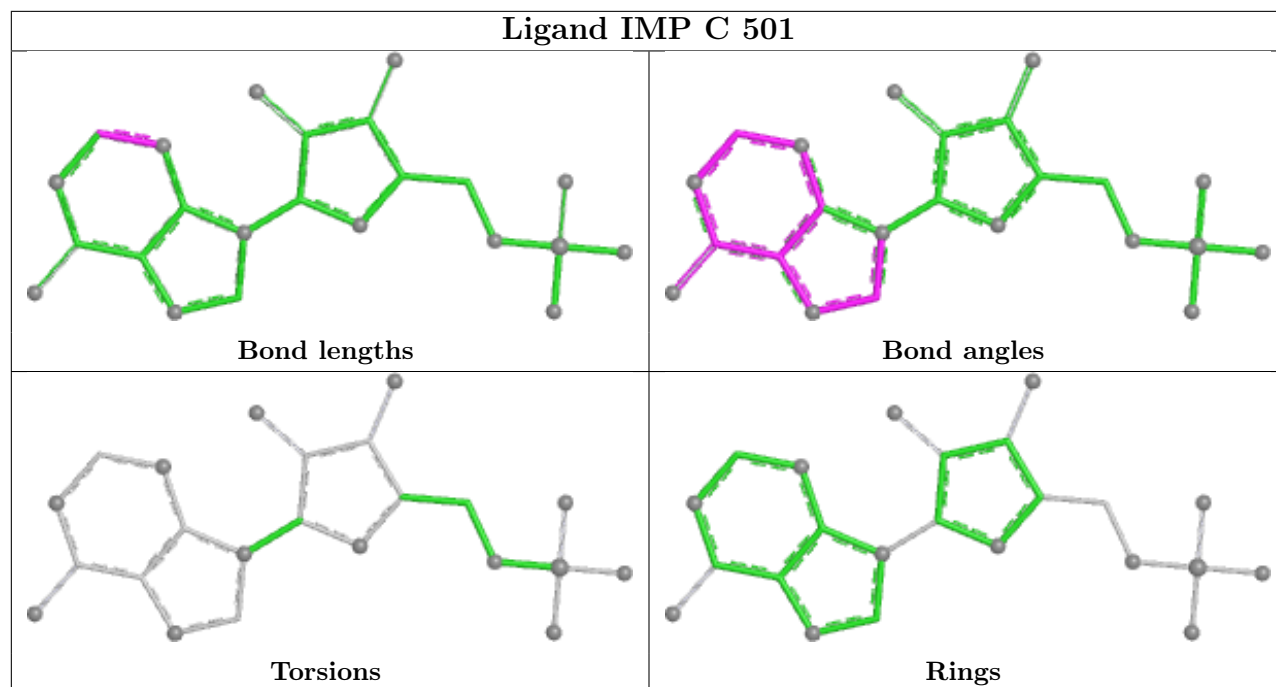


Ligand Q21 B 503



Ligand IMP A 501





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	336/361 (93%)	-0.22	10 (2%)	52	55	9, 31, 69, 100	9 (2%)
1	B	334/361 (92%)	-0.15	10 (2%)	52	55	11, 33, 65, 96	12 (3%)
1	C	336/361 (93%)	-0.22	11 (3%)	49	51	14, 33, 66, 103	11 (3%)
1	D	334/361 (92%)	-0.18	14 (4%)	40	42	14, 33, 69, 90	9 (2%)
All	All	1340/1444 (92%)	-0.19	45 (3%)	48	50	9, 32, 67, 103	41 (3%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	383	GLU	3.8
1	B	387	HIS	3.5
1	A	386	VAL	3.4
1	C	381	LEU	3.3
1	D	380	GLY	3.3
1	D	386	VAL	3.2
1	A	387	HIS	3.2
1	D	381	LEU	3.1
1	D	388	ASP	3.0
1	B	388	ASP	3.0
1	C	379	SER	2.8
1	C	386	VAL	2.8
1	D	379	SER	2.8
1	B	380	GLY	2.8
1	A	381	LEU	2.7
1	A	383	GLU	2.7
1	A	379	SER	2.7
1	C	383	GLU	2.6
1	A	392	VAL	2.6
1	C	388	ASP	2.6
1	D	163	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	384	SER	2.6
1	B	381	LEU	2.6
1	A	380	GLY	2.5
1	D	387	HIS	2.5
1	D	298	TYR	2.4
1	D	384	SER	2.4
1	C	136[A]	ARG	2.4
1	B	136[A]	ARG	2.4
1	A	136[A]	ARG	2.4
1	B	386	VAL	2.3
1	D	389	VAL	2.3
1	B	384	SER	2.3
1	D	92	GLY	2.2
1	D	385	HIS	2.2
1	D	136[A]	ARG	2.2
1	A	311	GLY	2.2
1	B	389	VAL	2.1
1	C	1	MET	2.1
1	B	379	SER	2.1
1	D	365	GLU	2.0
1	C	384	SER	2.0
1	C	387	HIS	2.0
1	C	380	GLY	2.0
1	C	298	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

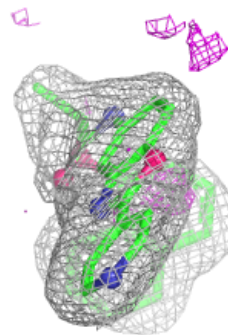
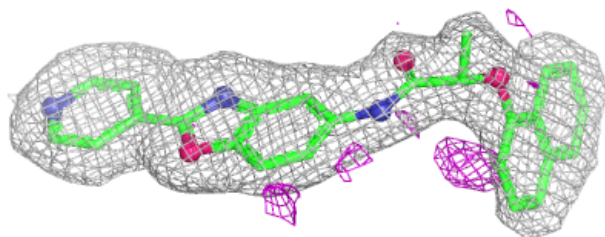
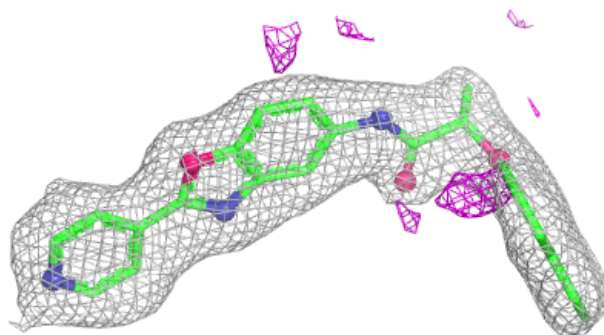
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	502	4/4	0.70	0.19	33,38,40,44	0
3	EDO	A	503	4/4	0.76	0.22	40,47,54,61	0
3	EDO	A	505	4/4	0.78	0.16	43,44,55,58	0
3	EDO	C	504	4/4	0.82	0.15	40,40,45,48	0
3	EDO	C	503	4/4	0.89	0.11	45,49,50,52	0
4	Q21	B	501	31/31	0.94	0.08	18,26,42,45	0
4	Q21	B	503	31/31	0.94	0.07	22,34,50,56	0
4	Q21	A	504	31/31	0.95	0.07	16,29,49,52	0
4	Q21	C	502	31/31	0.95	0.07	24,35,41,48	0
2	IMP	A	501	23/23	0.97	0.05	14,22,32,34	0
2	IMP	B	502	23/23	0.98	0.04	16,23,28,33	0
2	IMP	C	501	23/23	0.98	0.05	14,26,30,32	0
2	IMP	D	501	23/23	0.98	0.05	20,27,31,32	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.

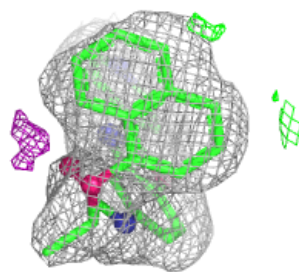
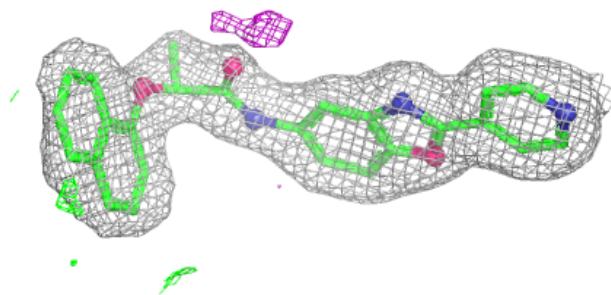
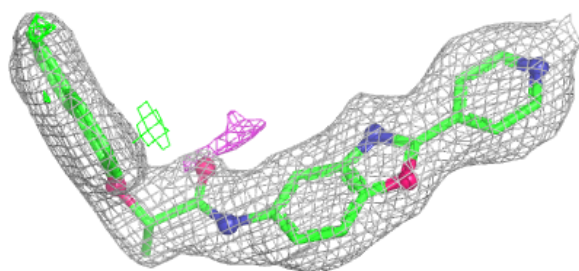
Electron density around Q21 B 501:

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

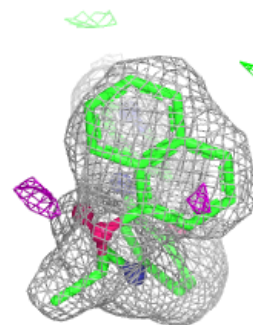
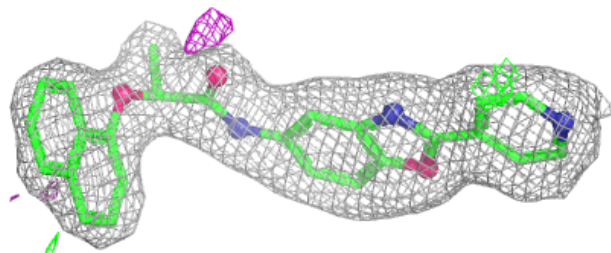
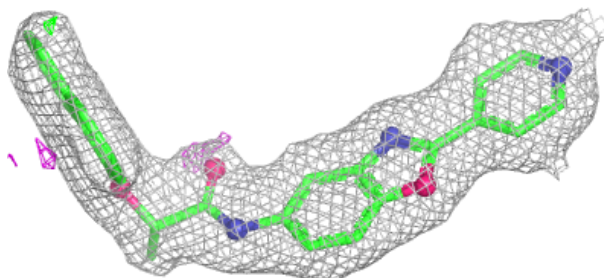


Electron density around Q21 B 503:

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

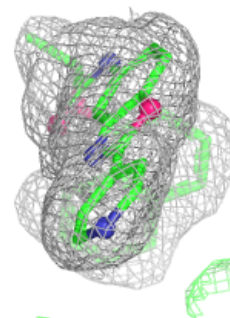
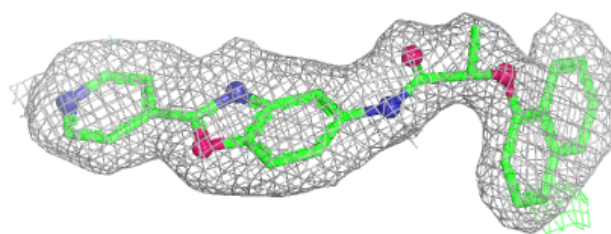
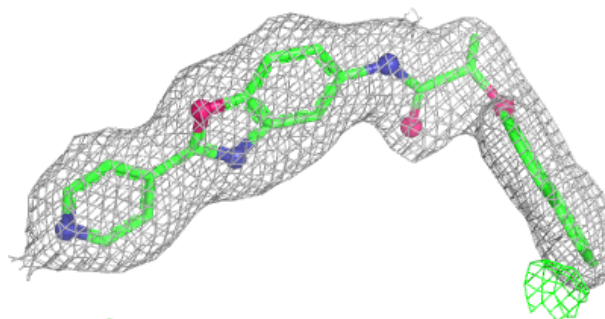
**Electron density around Q21 A 504:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

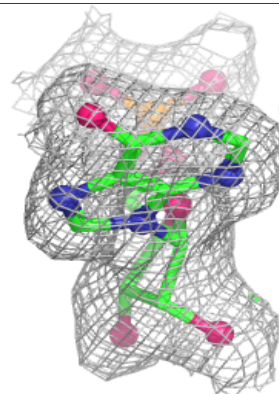
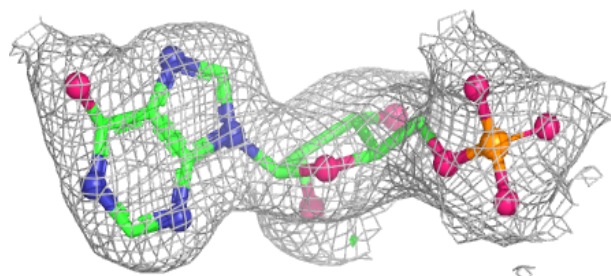
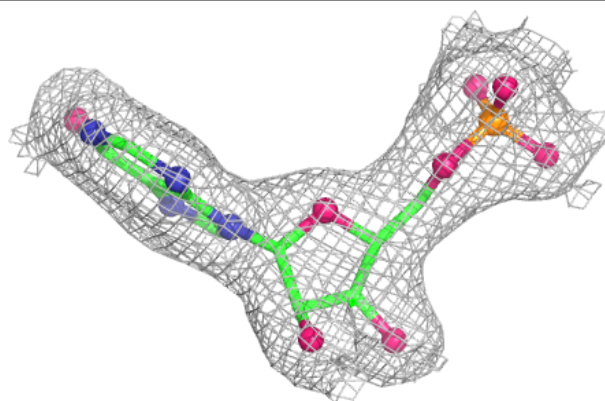


Electron density around Q21 C 502:

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

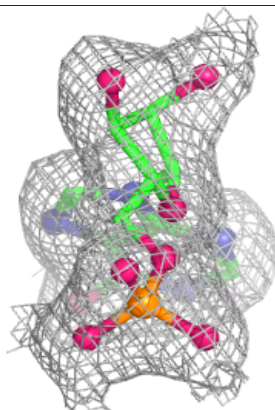
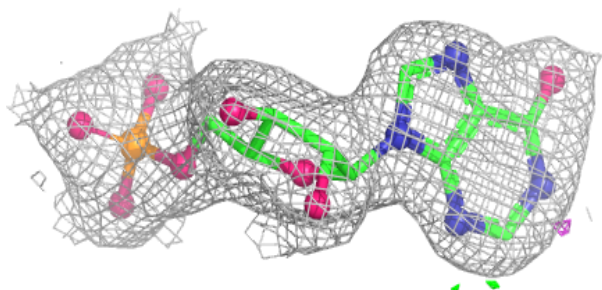
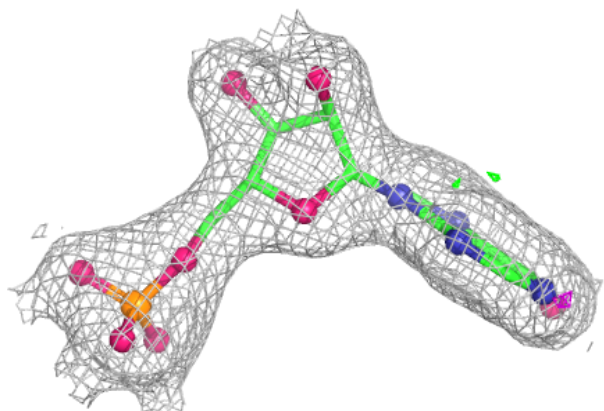
**Electron density around IMP A 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

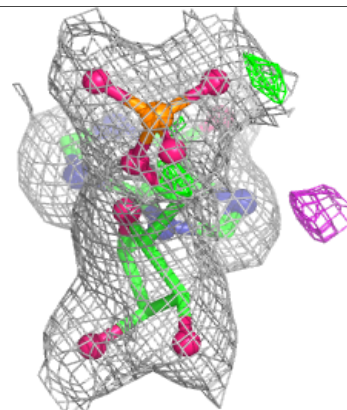
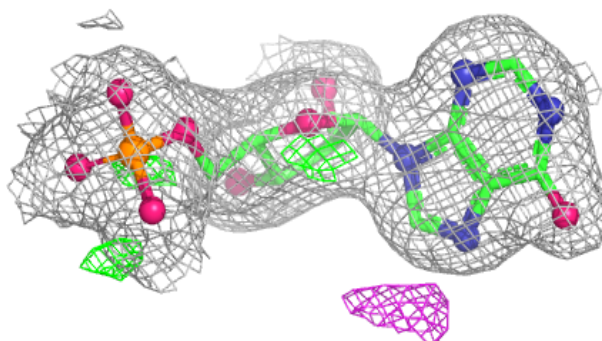
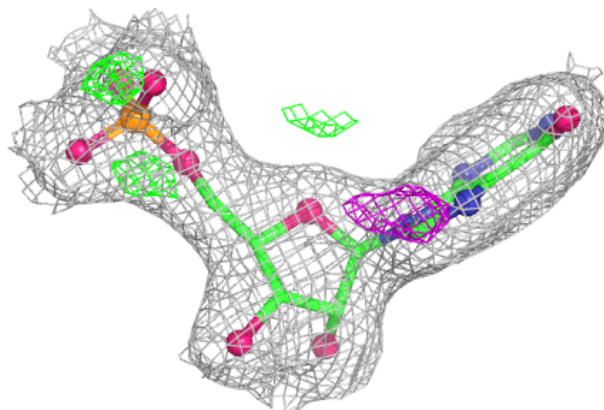


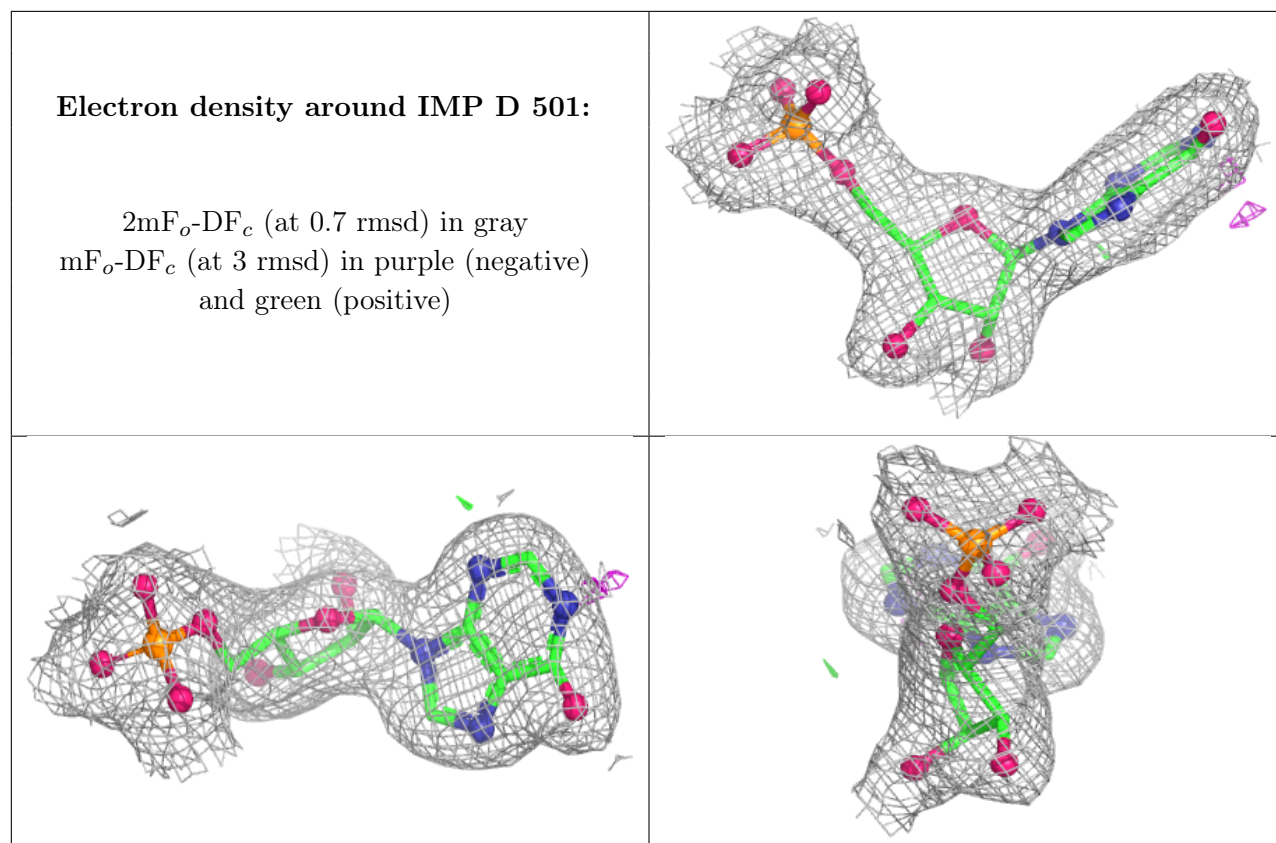
Electron density around IMP B 502:

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

**Electron density around IMP C 501:**

$2mF_o-DF_c$ (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.