WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2023 – 12:21 PM EDT

PDB ID	:	3W9F
Title	:	Crystal structure of the ankyrin repeat domain of chicken TRPV4 in complex with IP3
Authors	:	Itoh, Y.; Hamada-nakahara, S.; Suetsugu, S.
Deposited on	:	2013-04-04
Resolution	:	1.90 Å(reported)

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

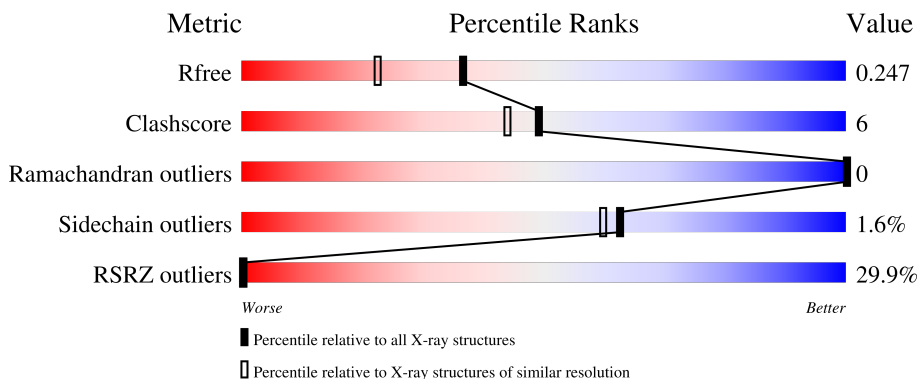|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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		0.247
Clashscore		6
Ramachandran outliers		0
Sidechain outliers		1.6%
RSRZ outliers		29.9%

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	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 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	260	10% 88% 10% ·
1	B	260	15% 85% 12% ·
1	C	260	32% 79% 16% · ·
1	D	260	58% 75% 20% · ·

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
2	I3P	D	2001	-	-	-	X

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 8642 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 Vanilloid receptor-related osmotically activated channel protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	8	0
			2058	1302	379	368	9			
1	B	255	Total	C	N	O	S	0	6	0
			2049	1296	376	368	9			
1	C	249	Total	C	N	O	S	0	1	0
			1989	1263	361	357	8			
1	D	249	Total	C	N	O	S	0	1	0
			1989	1261	365	355	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	MET	-	expression tag	UNP Q9DFS3
A	383	ALA	-	expression tag	UNP Q9DFS3
A	384	ALA	-	expression tag	UNP Q9DFS3
A	385	ALA	-	expression tag	UNP Q9DFS3
A	386	HIS	-	expression tag	UNP Q9DFS3
A	387	HIS	-	expression tag	UNP Q9DFS3
A	388	HIS	-	expression tag	UNP Q9DFS3
A	389	HIS	-	expression tag	UNP Q9DFS3
A	390	HIS	-	expression tag	UNP Q9DFS3
A	391	HIS	-	expression tag	UNP Q9DFS3
B	132	MET	-	expression tag	UNP Q9DFS3
B	383	ALA	-	expression tag	UNP Q9DFS3
B	384	ALA	-	expression tag	UNP Q9DFS3
B	385	ALA	-	expression tag	UNP Q9DFS3
B	386	HIS	-	expression tag	UNP Q9DFS3
B	387	HIS	-	expression tag	UNP Q9DFS3
B	388	HIS	-	expression tag	UNP Q9DFS3
B	389	HIS	-	expression tag	UNP Q9DFS3
B	390	HIS	-	expression tag	UNP Q9DFS3
B	391	HIS	-	expression tag	UNP Q9DFS3
C	132	MET	-	expression tag	UNP Q9DFS3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	383	ALA	-	expression tag	UNP Q9DFS3
C	384	ALA	-	expression tag	UNP Q9DFS3
C	385	ALA	-	expression tag	UNP Q9DFS3
C	386	HIS	-	expression tag	UNP Q9DFS3
C	387	HIS	-	expression tag	UNP Q9DFS3
C	388	HIS	-	expression tag	UNP Q9DFS3
C	389	HIS	-	expression tag	UNP Q9DFS3
C	390	HIS	-	expression tag	UNP Q9DFS3
C	391	HIS	-	expression tag	UNP Q9DFS3
D	132	MET	-	expression tag	UNP Q9DFS3
D	383	ALA	-	expression tag	UNP Q9DFS3
D	384	ALA	-	expression tag	UNP Q9DFS3
D	385	ALA	-	expression tag	UNP Q9DFS3
D	386	HIS	-	expression tag	UNP Q9DFS3
D	387	HIS	-	expression tag	UNP Q9DFS3
D	388	HIS	-	expression tag	UNP Q9DFS3
D	389	HIS	-	expression tag	UNP Q9DFS3
D	390	HIS	-	expression tag	UNP Q9DFS3
D	391	HIS	-	expression tag	UNP Q9DFS3

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula: $C_6H_{15}O_{15}P_3$).
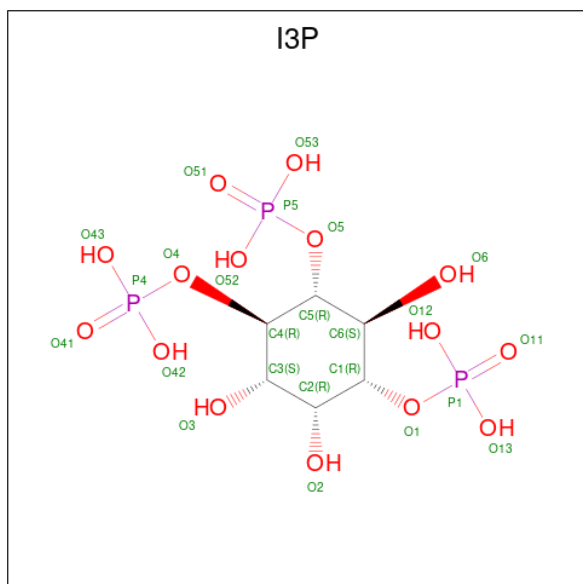
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			24	6	15	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total 24	C 6	O 15	P 3	0	0
2	C	1	Total 24	C 6	O 15	P 3	0	0
2	D	1	Total 24	C 6	O 15	P 3	0	0

- Molecule 3 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total 244	O 244	0	0
3	B	201	Total 201	O 201	0	0
3	C	15	Total 15	O 15	0	0
3	D	1	Total 1	O 1	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: Vanilloid receptor-related osmotically activated channel protein
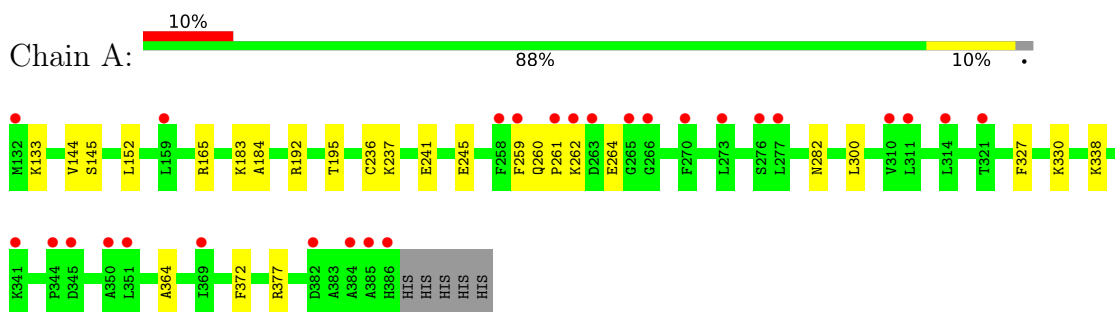
Chain A:

• Molecule 1: Vanilloid receptor-related osmotically activated channel protein

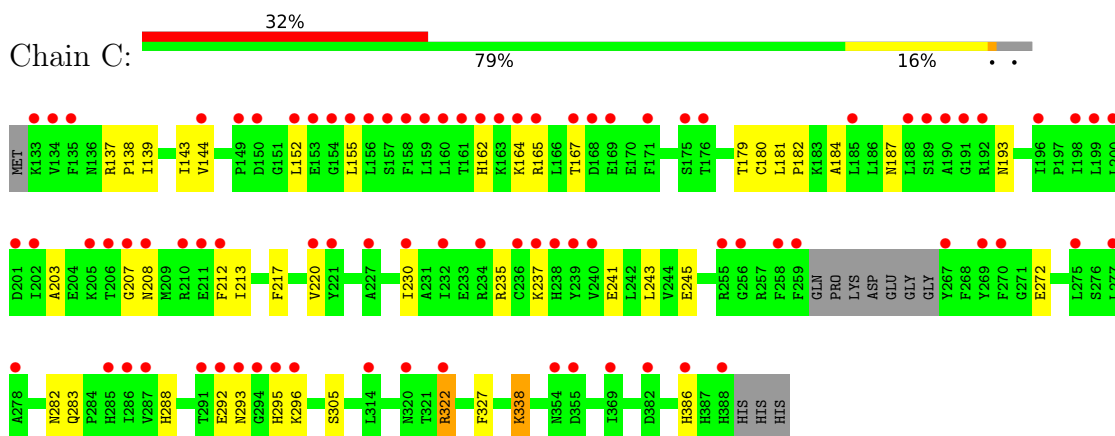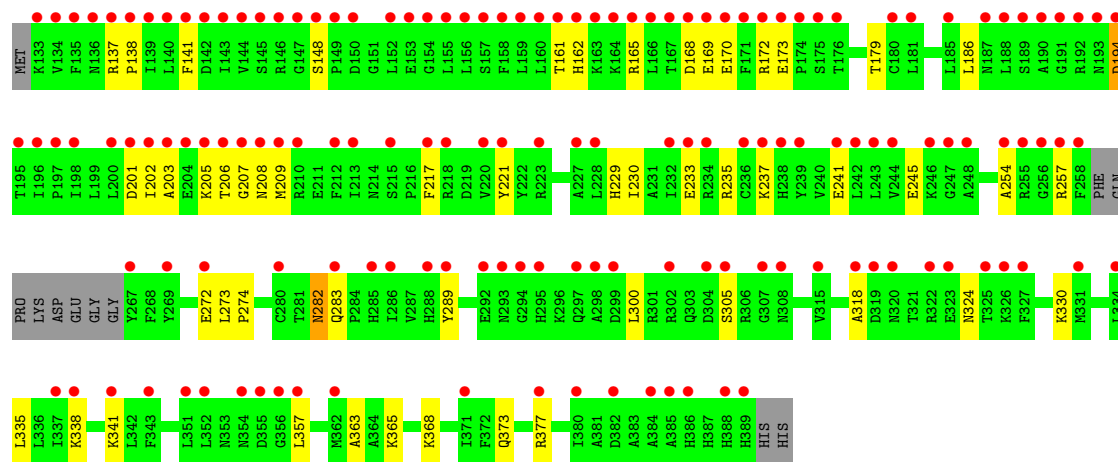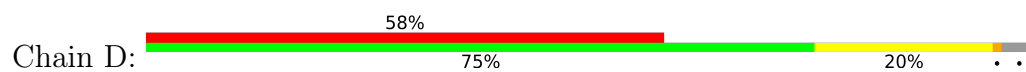Chain B:

• Molecule 1: Vanilloid receptor-related osmotically activated channel protein

Chain C:

• Molecule 1: Vanilloid receptor-related osmotically activated channel protein

Chain D:
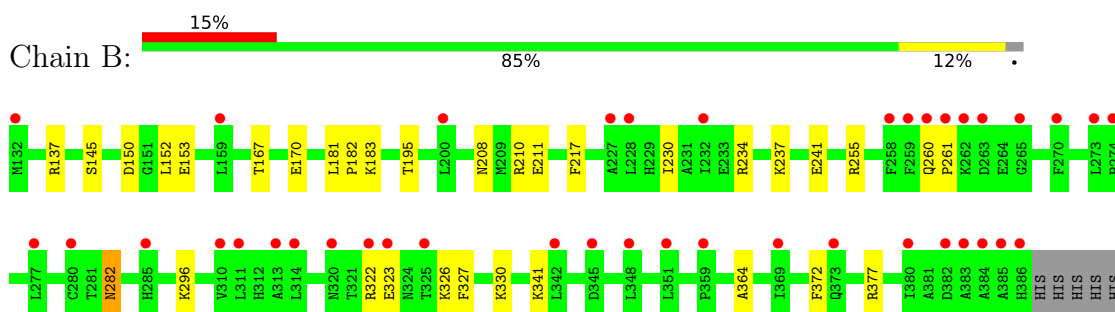
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.09Å 48.34Å 132.15Å 90.00° 101.44° 90.00°	Depositor
Resolution (Å)	32.81 – 1.90 32.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.7 (32.81-1.90) 92.8 (32.81-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.89Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.246 0.220 , 0.247	Depositor DCC
R_{free} test set	2054 reflections (2.04%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.534	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.2	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8642	wwPDB-VP
Average B, all atoms (Å^2)	64.0	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 67.07 % 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 5.4638e-06. 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: I3P

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	0.49	0/2139	0.63	0/2884
1	B	0.48	0/2120	0.65	0/2859
1	C	0.34	0/2034	0.58	0/2745
1	D	0.31	0/2035	0.60	0/2747
All	All	0.42	0/8328	0.62	0/11235

There are no bond length outliers.

There are no bond angle outliers.

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	2058	0	2096	17	0
1	B	2049	0	2080	21	0
1	C	1989	0	2008	24	0
1	D	1989	0	2007	37	0
2	A	24	0	9	1	0
2	B	24	0	9	2	0
2	C	24	0	9	0	0
2	D	24	0	9	3	0
3	A	244	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	201	0	0	5	0
3	C	15	0	0	0	0
3	D	1	0	0	0	0
All	All	8642	0	8227	97	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 6.

All (97) 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:D:172:ARG:HG2	1:D:179:THR:HG22	1.66	0.77
1:A:192[A]:ARG:NH1	3:A:2214:HOH:O	2.24	0.69
1:C:292[B]:GLU:OE1	1:C:338:LYS:NZ	2.26	0.69
1:D:330:LYS:NZ	2:D:2001:I3P:O13	2.26	0.68
1:A:377:ARG:NH2	3:A:2319:HOH:O	2.26	0.68
1:B:322:ARG:NH1	1:B:323:GLU:OE1	2.29	0.66
1:D:203:ALA:O	1:D:208:ASN:N	2.28	0.66
1:B:210:ARG:NH1	3:B:2258:HOH:O	2.25	0.65
1:D:237:LYS:NZ	2:D:2001:I3P:O51	2.26	0.65
1:D:201:ASP:OD2	1:D:205:LYS:NZ	2.20	0.65
1:B:377:ARG:NH2	3:B:2284:HOH:O	2.30	0.65
1:A:237:LYS:NZ	3:A:2295:HOH:O	2.29	0.63
1:D:221:TYR:O	1:D:257:ARG:N	2.32	0.61
1:C:322:ARG:HD3	1:D:165:ARG:HD2	1.84	0.60
1:B:330:LYS:NZ	2:B:2001:I3P:O13	2.35	0.59
1:C:144:VAL:HG21	1:C:180:CYS:HB2	1.84	0.57
1:C:288:HIS:O	1:C:292[B]:GLU:HG2	2.03	0.57
1:D:165:ARG:NH2	1:D:207:GLY:O	2.37	0.57
1:C:217:PHE:CZ	1:C:230:ILE:HD11	2.40	0.57
1:D:300:LEU:HD21	1:D:335:LEU:HD22	1.87	0.56
1:C:208:ASN:ND2	1:C:212:PHE:HB2	2.21	0.55
1:D:272:GLU:OE2	1:D:305:SER:OG	2.18	0.55
1:D:194:ASP:OD2	1:D:194:ASP:N	2.31	0.54
1:A:165[A]:ARG:NH2	1:C:386:HIS:HB3	2.23	0.54
1:C:245:GLU:HG2	1:C:295:HIS:NE2	2.23	0.54
1:A:152:LEU:HD11	1:A:195:THR:HB	1.88	0.53
1:D:169:GLU:HA	1:D:172:ARG:HE	1.73	0.53
1:C:144:VAL:HG13	1:C:184:ALA:HB2	1.90	0.53
1:D:237:LYS:O	1:D:241:GLU:HG3	2.09	0.53
1:D:202:ILE:O	1:D:206:THR:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:LYS:O	1:C:241:GLU:HG3	2.10	0.52
1:A:300:LEU:HD11	1:A:338:LYS:HG2	1.92	0.51
1:D:229:HIS:ND1	1:D:254:ALA:HB2	2.26	0.51
1:D:318:ALA:HA	1:D:324:ASN:OD1	2.10	0.51
1:D:373:GLN:O	1:D:377:ARG:HG3	2.10	0.51
1:D:363:ALA:O	1:D:368:LYS:N	2.41	0.51
1:C:203:ALA:O	1:C:208:ASN:N	2.44	0.51
1:D:282:ASN:ND2	2:D:2001:I3P:O12	2.39	0.50
1:A:330:LYS:NZ	2:A:2001:I3P:O13	2.39	0.49
1:D:229:HIS:CD2	1:D:274:PRO:HG3	2.47	0.49
1:B:322:ARG:CZ	1:B:326:LYS:HD2	2.43	0.49
1:C:152:LEU:HD22	1:C:155:LEU:HD22	1.93	0.49
1:C:293:ASN:ND2	1:C:296:LYS:O	2.36	0.49
1:A:260:GLN:HB3	1:A:261:PRO:HD2	1.95	0.49
1:B:364:ALA:HB2	1:B:372:PHE:CE1	2.47	0.48
1:B:217:PHE:CZ	1:B:230:ILE:HD11	2.49	0.47
1:A:364:ALA:HB2	1:A:372:PHE:CE1	2.49	0.47
1:C:181:LEU:HD21	1:C:243:LEU:HD21	1.97	0.46
1:B:145:SER:HB3	1:B:183:LYS:HE3	1.98	0.46
1:D:241:GLU:O	1:D:245:GLU:N	2.33	0.46
1:B:211:GLU:OE1	1:B:211:GLU:N	2.37	0.46
1:C:235:ARG:NH2	1:C:283:GLN:HG2	2.30	0.46
1:C:213:ILE:HG23	1:C:243:LEU:HD22	1.98	0.45
1:D:137:ARG:HB3	1:D:138:PRO:HD3	1.98	0.45
1:B:260:GLN:HB3	1:B:261:PRO:HD2	1.97	0.45
1:D:229:HIS:CE1	1:D:254:ALA:HB2	2.51	0.45
1:D:141:PHE:HE2	1:D:173:GLU:HB2	1.83	0.44
1:B:341:LYS:NZ	3:B:2231:HOH:O	2.51	0.44
1:C:187:ASN:O	1:C:193:ASN:ND2	2.50	0.44
1:C:272:GLU:OE2	1:C:305:SER:OG	2.26	0.44
1:D:233:GLU:HA	1:D:233:GLU:OE1	2.18	0.44
1:C:139:ILE:O	1:C:143:ILE:HG13	2.18	0.43
1:D:141:PHE:CE2	1:D:173:GLU:HB2	2.53	0.43
1:C:165:ARG:NH2	1:C:207:GLY:O	2.44	0.43
1:D:203:ALA:HB1	1:D:209:MET:HA	2.00	0.43
1:C:179:THR:O	1:C:182:PRO:HD2	2.19	0.43
1:A:259:PHE:N	1:A:264:GLU:OE1	2.40	0.43
1:A:144:VAL:HG13	1:A:184:ALA:HB2	2.01	0.42
1:D:168:ASP:HB3	1:D:170:GLU:HG2	2.00	0.42
1:D:338:LYS:O	1:D:341:LYS:HB3	2.18	0.42
1:D:217:PHE:HZ	1:D:230:ILE:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:HB3	1:A:183:LYS:HE3	2.02	0.42
1:D:235:ARG:NH2	1:D:283:GLN:HG2	2.34	0.42
1:A:133:LYS:HE2	3:A:2175:HOH:O	2.20	0.42
1:B:296:LYS:HE2	1:B:296:LYS:HB2	1.81	0.42
1:A:262:LYS:HD3	1:A:262:LYS:HA	1.89	0.41
1:B:255:ARG:NH1	3:B:2138:HOH:O	2.32	0.41
1:B:150:ASP:O	1:B:153:GLU:HG3	2.20	0.41
1:B:167:THR:HG23	1:B:208:ASN:HD21	1.85	0.41
1:C:162:HIS:HB3	1:C:164:LYS:NZ	2.35	0.41
1:D:357:LEU:HD11	1:D:365:LYS:HD3	2.02	0.41
1:A:237:LYS:O	1:A:241:GLU:HG3	2.20	0.41
1:B:282:ASN:ND2	2:B:2001:I3P:O12	2.53	0.41
1:D:186:LEU:HD23	1:D:186:LEU:HA	1.90	0.41
1:A:245:GLU:OE1	3:A:2185:HOH:O	2.22	0.41
1:B:237:LYS:O	1:B:241:GLU:HG3	2.20	0.41
1:D:137:ARG:HB2	1:D:170:GLU:O	2.21	0.41
1:B:181:LEU:HB3	1:B:182:PRO:HD3	2.03	0.41
1:C:144:VAL:HG11	1:C:180:CYS:O	2.20	0.41
1:D:241:GLU:HA	1:D:289:TYR:CE2	2.56	0.41
1:B:137:ARG:HB2	1:B:170:GLU:O	2.21	0.40
1:B:210:ARG:NH1	3:B:2265:HOH:O	2.46	0.40
1:D:273:LEU:HA	1:D:274:PRO:HD3	1.96	0.40
1:B:152:LEU:HD11	1:B:195:THR:HB	2.03	0.40
1:D:161:THR:HG22	1:D:162:HIS:ND1	2.37	0.40
1:A:236:CYS:HB3	3:A:2340:HOH:O	2.22	0.40
1:C:137:ARG:HB3	1:C:138:PRO:HD3	2.03	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	261/260 (100%)	255 (98%)	6 (2%)	0	100	100
1	B	259/260 (100%)	252 (97%)	7 (3%)	0	100	100
1	C	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
1	D	246/260 (95%)	238 (97%)	8 (3%)	0	100	100
All	All	1012/1040 (97%)	983 (97%)	29 (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	224/221 (101%)	222 (99%)	2 (1%)	78	79
1	B	222/221 (100%)	218 (98%)	4 (2%)	59	55
1	C	213/221 (96%)	207 (97%)	6 (3%)	43	36
1	D	213/221 (96%)	210 (99%)	3 (1%)	67	65
All	All	872/884 (99%)	857 (98%)	15 (2%)	62	57

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	A	327	PHE
1	B	234[A]	ARG
1	B	234[B]	ARG
1	B	282	ASN
1	B	327	PHE
1	C	167	THR
1	C	220	VAL
1	C	282	ASN
1	C	322	ARG
1	C	327	PHE
1	C	338	LYS
1	D	148	SER

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Mol	Chain	Res	Type
1	D	194	ASP
1	D	282	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	208	ASN
1	C	282	ASN
1	C	285	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 ⓘ

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	I3P	A	2001	-	24,24,24	0.94	0	36,39,39	0.69	0
2	I3P	C	2001	-	24,24,24	0.91	0	36,39,39	0.86	0
2	I3P	D	2001	-	24,24,24	0.89	0	36,39,39	0.74	0
2	I3P	B	2001	-	24,24,24	0.88	0	36,39,39	0.76	1 (2%)

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	I3P	A	2001	-	-	4/15/39/39	0/1/1/1
2	I3P	C	2001	-	-	0/15/39/39	0/1/1/1
2	I3P	D	2001	-	-	3/15/39/39	0/1/1/1
2	I3P	B	2001	-	-	1/15/39/39	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2001	I3P	C2-C3-C4	2.05	114.36	109.68

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	I3P	C4-O4-P4-O41
2	D	2001	I3P	C4-C5-O5-P5
2	D	2001	I3P	C6-C5-O5-P5
2	D	2001	I3P	C1-O1-P1-O11
2	A	2001	I3P	C4-O4-P4-O43
2	A	2001	I3P	C1-O1-P1-O12
2	A	2001	I3P	C1-O1-P1-O13
2	B	2001	I3P	C1-O1-P1-O13

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	I3P	1	0
2	D	2001	I3P	3	0
2	B	2001	I3P	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 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 I3P A 2001

Bond lengths

Bond angles

Torsions

Rings

Ligand I3P D 2001

Bond lengths

Bond angles

Torsions

Rings

Ligand I3P B 2001

Bond lengths

Bond angles

Torsions

Rings
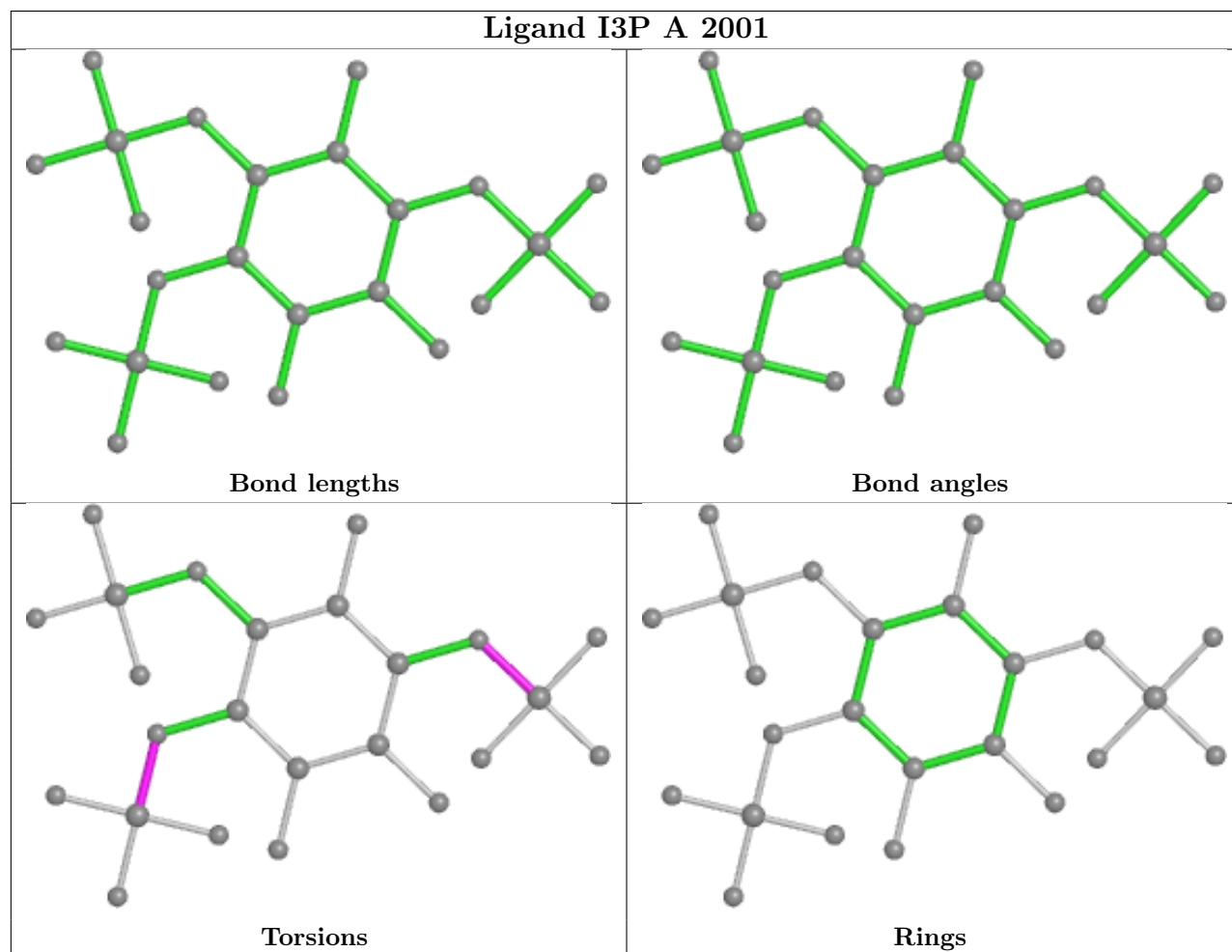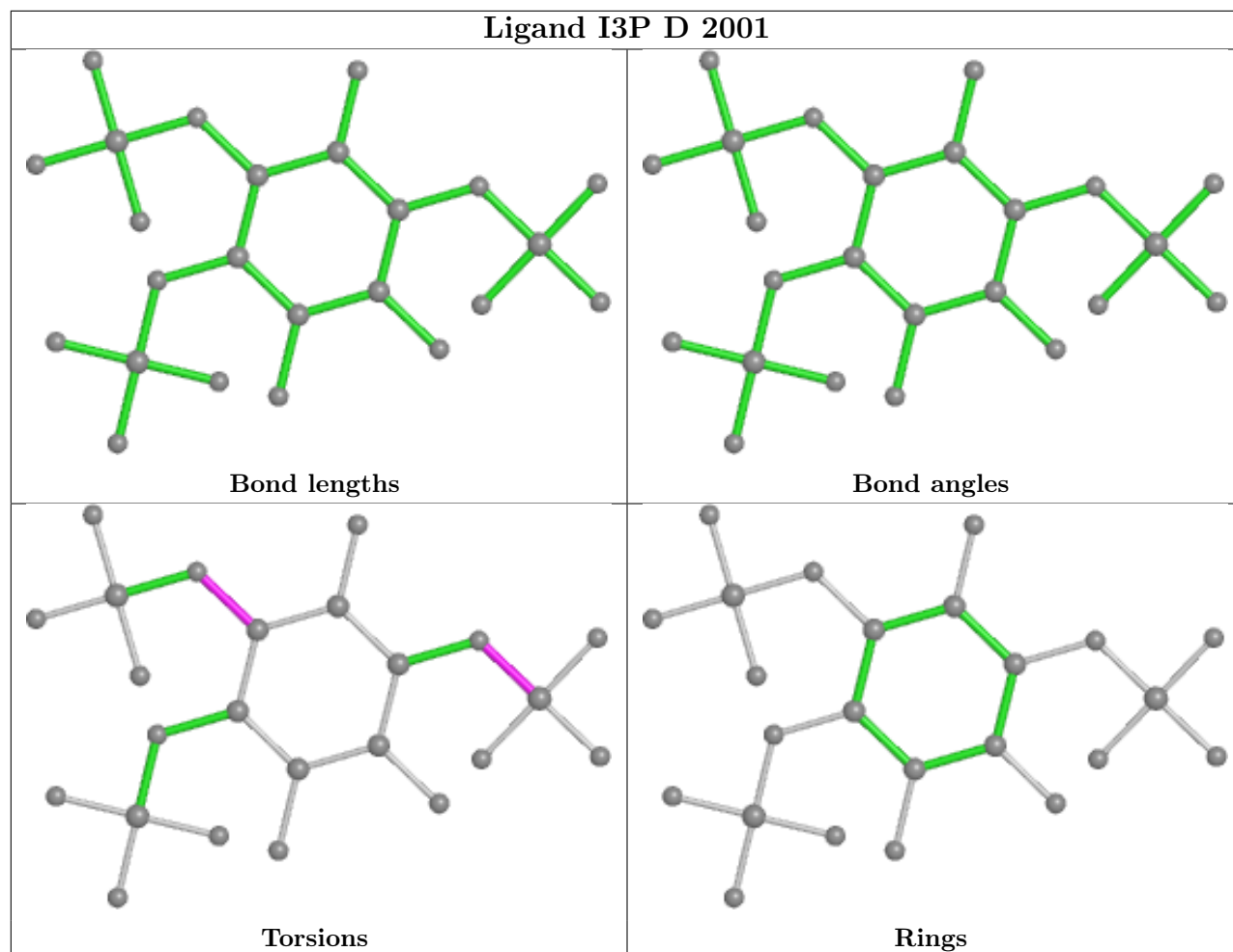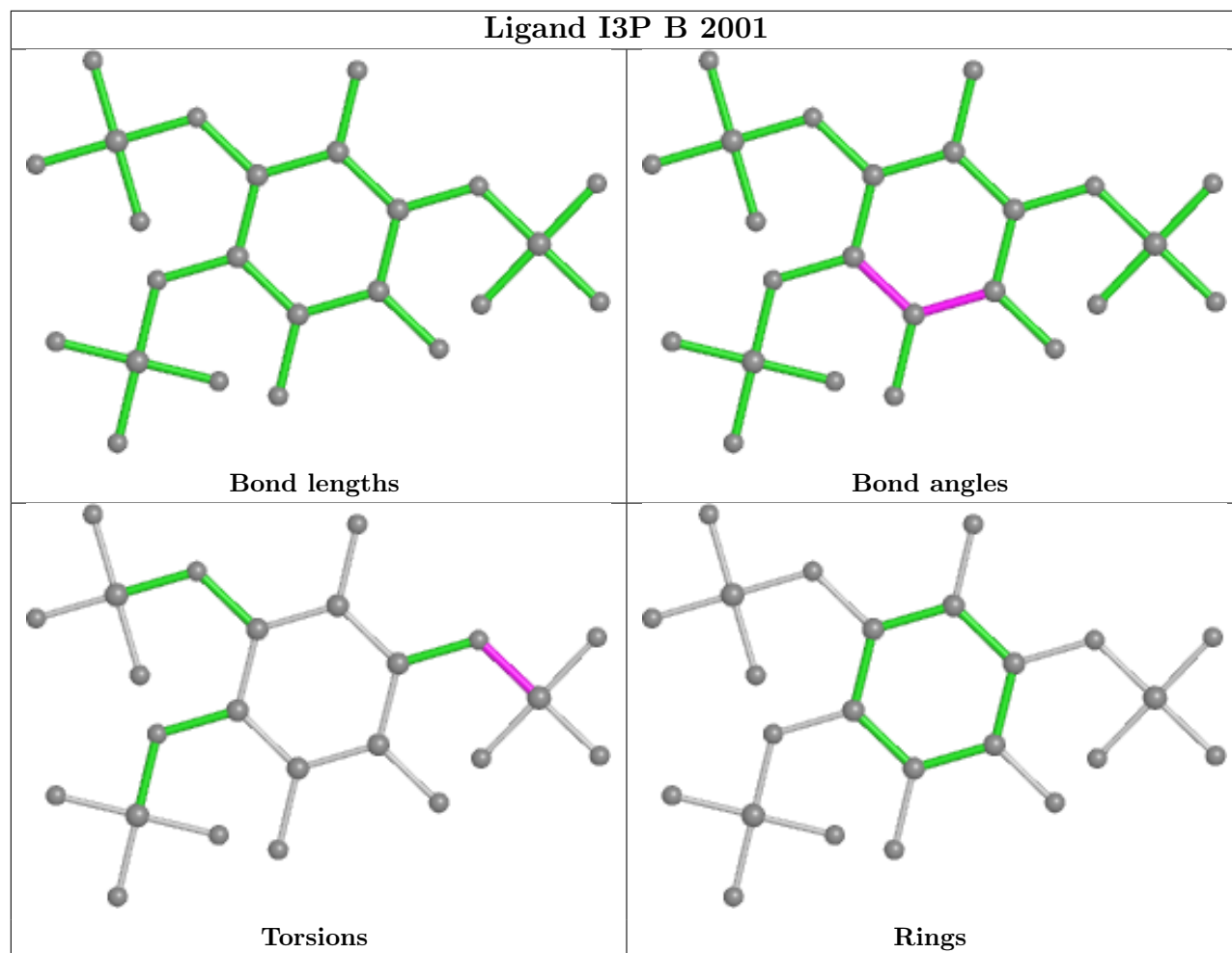
5.7 Other polymers ⓘ

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(Å^2)	Q<0.9
1	A	255/260 (98%)	0.65	27 (10%)	6	7	17, 29, 62, 98	0
1	B	255/260 (98%)	0.92	40 (15%)	2	2	19, 35, 84, 131	0
1	C	249/260 (95%)	1.72	84 (33%)	0	0	38, 78, 113, 161	0
1	D	249/260 (95%)	3.01	150 (60%)	0	0	62, 106, 140, 157	0
All	All	1008/1040 (96%)	1.56	301 (29%)	0	0	17, 61, 129, 161	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	139	ILE	13.9
1	D	157	SER	13.0
1	C	258	PHE	11.7
1	D	159	LEU	9.4
1	B	386	HIS	9.3
1	D	166	LEU	8.7
1	D	323	GLU	8.7
1	D	285	HIS	8.6
1	D	160	LEU	8.5
1	D	198	ILE	8.4
1	B	384	ALA	8.4
1	C	388	HIS	8.2
1	D	156	LEU	8.2
1	D	152	LEU	7.7
1	D	389	HIS	7.5
1	D	133	LYS	7.4
1	D	170	GLU	7.3
1	C	207	GLY	7.3
1	D	134	VAL	7.3
1	D	238	HIS	7.3
1	C	158	PHE	7.2

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Mol	Chain	Res	Type	RSRZ
1	D	161	THR	7.2
1	D	289	TYR	7.2
1	C	190	ALA	7.1
1	B	383	ALA	7.0
1	D	195	THR	7.0
1	D	171	PHE	6.8
1	B	132	MET	6.7
1	C	162	HIS	6.6
1	D	207	GLY	6.5
1	D	162	HIS	6.5
1	A	262	LYS	6.4
1	D	205	LYS	6.4
1	D	294	GLY	6.3
1	D	176	THR	6.3
1	D	155	LEU	6.3
1	C	259	PHE	6.1
1	D	167	THR	6.1
1	C	134	VAL	6.1
1	A	385	ALA	6.1
1	C	208	ASN	6.0
1	D	232	ILE	6.0
1	C	152	LEU	5.9
1	D	388	HIS	5.8
1	C	161	THR	5.8
1	D	189	SER	5.7
1	D	172	ARG	5.7
1	D	175	SER	5.6
1	C	163	LYS	5.6
1	D	295	HIS	5.5
1	D	292	GLU	5.5
1	C	155	LEU	5.4
1	D	286	ILE	5.4
1	D	192	ARG	5.4
1	D	190	ALA	5.3
1	D	298	ALA	5.3
1	A	386	HIS	5.3
1	B	261	PRO	5.3
1	A	261	PRO	5.1
1	C	192	ARG	5.1
1	C	196	ILE	5.1
1	B	322	ARG	4.9
1	D	164	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	191	GLY	4.8
1	D	385	ALA	4.8
1	D	153	GLU	4.8
1	D	213	ILE	4.7
1	D	193	ASN	4.7
1	D	158	PHE	4.7
1	D	150	ASP	4.7
1	D	188	LEU	4.7
1	D	144	VAL	4.7
1	D	196	ILE	4.7
1	C	160	LEU	4.6
1	D	221	TYR	4.6
1	B	262	LYS	4.6
1	D	201	ASP	4.6
1	D	149	PRO	4.6
1	C	159	LEU	4.6
1	C	295	HIS	4.6
1	D	197	PRO	4.6
1	D	305	SER	4.6
1	D	237	LYS	4.5
1	C	202	ILE	4.5
1	D	210	ARG	4.5
1	D	307	GLY	4.4
1	D	257	ARG	4.4
1	C	369	ILE	4.3
1	D	386	HIS	4.3
1	D	163	LYS	4.3
1	C	320	ASN	4.3
1	D	154	GLY	4.2
1	D	141	PHE	4.2
1	C	149	PRO	4.2
1	D	135	PHE	4.2
1	D	200	LEU	4.2
1	B	345	ASP	4.2
1	C	157	SER	4.2
1	C	188	LEU	4.1
1	D	239	TYR	4.1
1	D	212	PHE	4.1
1	C	164	LYS	4.1
1	D	256	GLY	4.1
1	D	185	LEU	4.0
1	B	258	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	357	LEU	4.0
1	C	165	ARG	4.0
1	B	385	ALA	3.9
1	D	337	ILE	3.9
1	C	167	THR	3.8
1	D	181	LEU	3.8
1	D	355	ASP	3.8
1	D	255	ARG	3.8
1	D	293	ASN	3.8
1	A	258	PHE	3.8
1	D	220	VAL	3.8
1	C	236	CYS	3.7
1	D	247	GLY	3.7
1	D	384	ALA	3.7
1	D	209	MET	3.7
1	A	310	VAL	3.7
1	D	174	PRO	3.7
1	D	140	LEU	3.7
1	D	283	GLN	3.7
1	C	355	ASP	3.7
1	C	210	ARG	3.6
1	D	187	ASN	3.6
1	C	205	LYS	3.6
1	D	297	GLN	3.6
1	D	338	LYS	3.6
1	C	221	TYR	3.6
1	D	169	GLU	3.6
1	D	223	ARG	3.6
1	D	142	ASP	3.5
1	C	294	GLY	3.5
1	D	136	ASN	3.5
1	D	267	TYR	3.5
1	A	266	GLY	3.5
1	D	351	LEU	3.4
1	C	354	ASN	3.4
1	A	384	ALA	3.4
1	B	310	VAL	3.4
1	A	345	ASP	3.4
1	C	296	LYS	3.3
1	C	256	GLY	3.3
1	D	148	SER	3.3
1	B	382	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	3.3
1	D	356	GLY	3.2
1	D	322	ARG	3.2
1	B	313	ALA	3.2
1	B	380	ILE	3.2
1	D	217	PHE	3.2
1	D	246	LYS	3.2
1	D	382	ASP	3.2
1	D	208	ASN	3.2
1	D	341	LYS	3.1
1	D	354	ASN	3.1
1	B	263	ASP	3.1
1	C	176	THR	3.1
1	D	258	PHE	3.1
1	C	234	ARG	3.1
1	A	265	GLY	3.1
1	A	344	PRO	3.1
1	B	320	ASN	3.1
1	D	254	ALA	3.1
1	C	322	ARG	3.1
1	C	239	TYR	3.1
1	C	201	ASP	3.0
1	C	285	HIS	3.0
1	B	351	LEU	3.0
1	C	171	PHE	3.0
1	C	240	VAL	3.0
1	D	194	ASP	3.0
1	B	270	PHE	3.0
1	D	343	PHE	3.0
1	D	165	ARG	3.0
1	B	260	GLN	3.0
1	C	291	THR	3.0
1	C	199	LEU	3.0
1	D	352	LEU	3.0
1	B	373	GLN	3.0
1	C	191	GLY	3.0
1	B	273	LEU	3.0
1	C	133	LYS	3.0
1	C	198	ILE	3.0
1	C	267	TYR	3.0
1	A	311	LEU	2.9
1	D	168	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	308	ASN	2.9
1	D	147	GLY	2.9
1	D	371	ILE	2.9
1	C	169	GLU	2.9
1	C	144	VAL	2.9
1	C	206	THR	2.9
1	D	233	GLU	2.9
1	A	273	LEU	2.8
1	D	280	CYS	2.8
1	D	334	LEU	2.8
1	D	206	THR	2.7
1	D	143	ILE	2.7
1	D	325	THR	2.7
1	D	327	PHE	2.7
1	D	315	VAL	2.7
1	D	146	ARG	2.7
1	D	138	PRO	2.7
1	C	275	LEU	2.7
1	B	259	PHE	2.7
1	B	277	LEU	2.7
1	D	318	ALA	2.6
1	C	269	TYR	2.6
1	C	200	LEU	2.6
1	D	248	ALA	2.6
1	C	150	ASP	2.6
1	D	319	ASP	2.6
1	C	277	LEU	2.6
1	D	244	VAL	2.6
1	D	236	CYS	2.6
1	B	325	THR	2.6
1	D	269	TYR	2.6
1	C	255	ARG	2.6
1	D	302	ARG	2.5
1	D	204	GLU	2.5
1	B	285	HIS	2.5
1	C	238	HIS	2.5
1	C	278	ALA	2.5
1	D	234	ARG	2.5
1	C	227	ALA	2.5
1	D	241	GLU	2.5
1	C	212	PHE	2.5
1	C	237	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	132	MET	2.5
1	B	311	LEU	2.5
1	D	243	LEU	2.5
1	D	215	SER	2.5
1	B	265	GLY	2.4
1	D	227	ALA	2.4
1	D	137	ARG	2.4
1	D	218	ARG	2.4
1	C	230	ILE	2.4
1	C	287	VAL	2.4
1	B	314	LEU	2.4
1	D	228	LEU	2.4
1	B	359	PRO	2.4
1	D	320	ASN	2.4
1	C	211	GLU	2.4
1	C	135	PHE	2.4
1	A	369	ILE	2.4
1	D	326	LYS	2.3
1	D	180	CYS	2.3
1	D	304	ASP	2.3
1	B	342	LEU	2.3
1	D	145	SER	2.3
1	A	350	ALA	2.3
1	B	227	ALA	2.3
1	D	242	LEU	2.3
1	D	202	ILE	2.3
1	D	362	MET	2.3
1	A	159	LEU	2.3
1	A	351	LEU	2.3
1	C	220	VAL	2.3
1	C	314	LEU	2.3
1	D	272	GLU	2.3
1	B	232	ILE	2.2
1	C	189	SER	2.2
1	C	293	ASN	2.2
1	C	286	ILE	2.2
1	A	263	ASP	2.2
1	C	382	ASP	2.2
1	C	153	GLU	2.2
1	D	173	GLU	2.2
1	D	288	HIS	2.2
1	A	259	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	280	CYS	2.2
1	D	331	MET	2.1
1	B	200	LEU	2.1
1	B	274	PRO	2.1
1	A	382	ASP	2.1
1	C	154	GLY	2.1
1	B	228	LEU	2.1
1	C	185	LEU	2.1
1	A	276	SER	2.1
1	C	175	SER	2.1
1	D	380	ILE	2.1
1	A	277[A]	LEU	2.1
1	C	168	ASP	2.1
1	A	270	PHE	2.1
1	C	270	PHE	2.1
1	D	377	ARG	2.1
1	D	203	ALA	2.1
1	C	232	ILE	2.1
1	A	314	LEU	2.1
1	A	321	THR	2.0
1	B	159	LEU	2.0
1	B	348	LEU	2.0
1	B	369	ILE	2.0
1	B	323	GLU	2.0
1	D	299	ASP	2.0
1	A	341	LYS	2.0
1	C	292[A]	GLU	2.0
1	C	386	HIS	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.
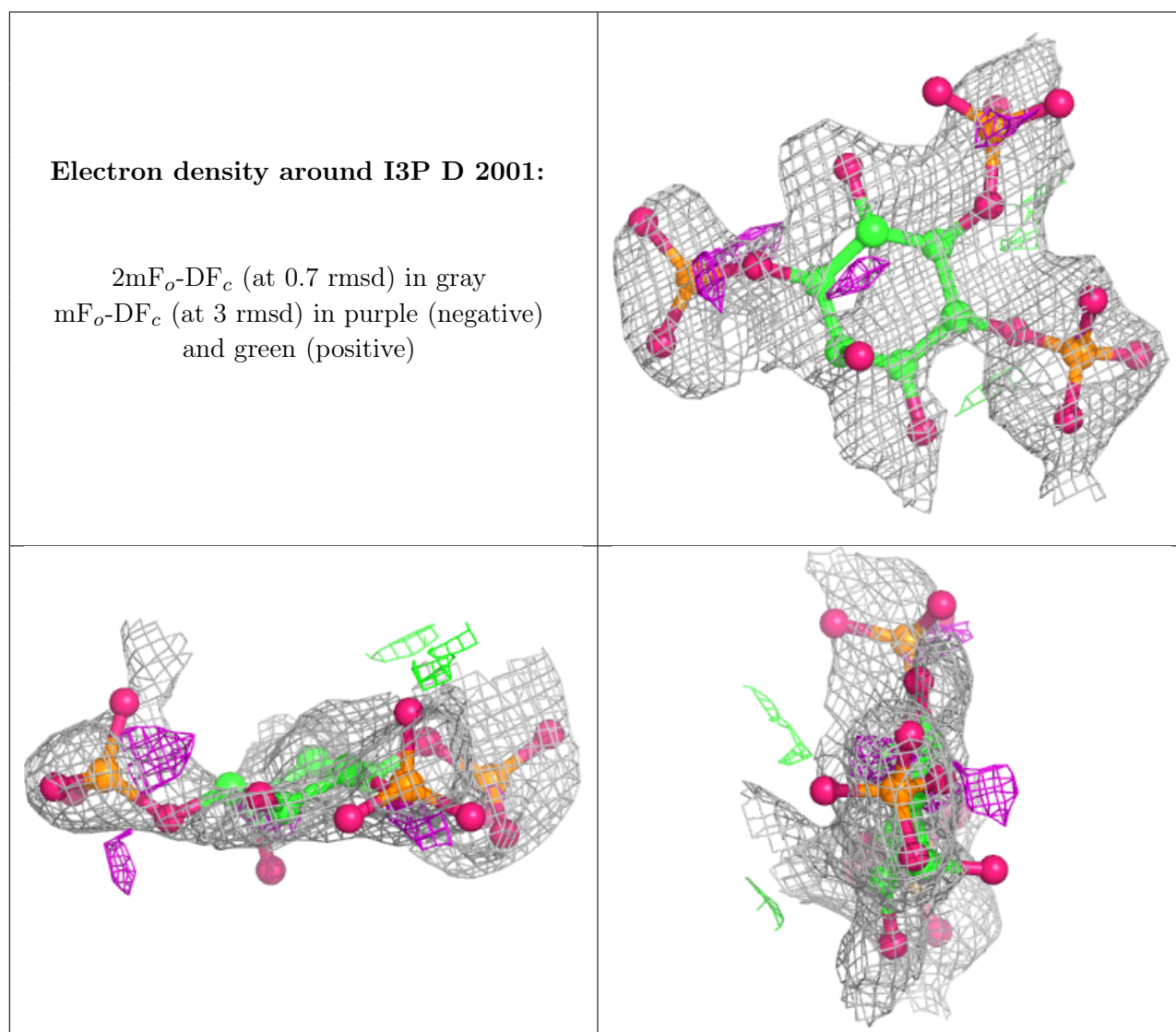
6.4   Ligands ⓘ

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.
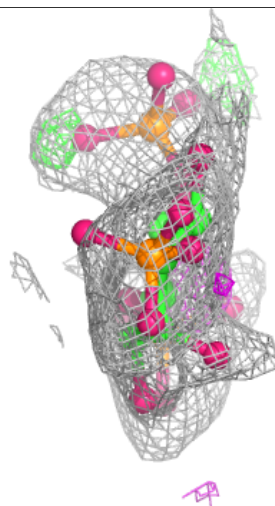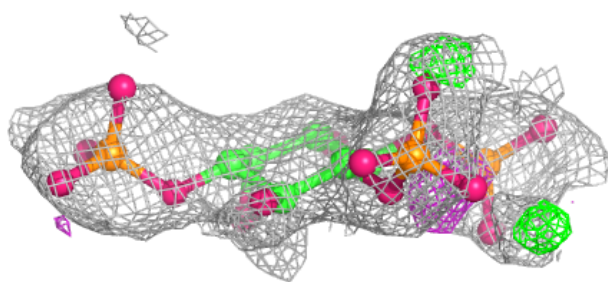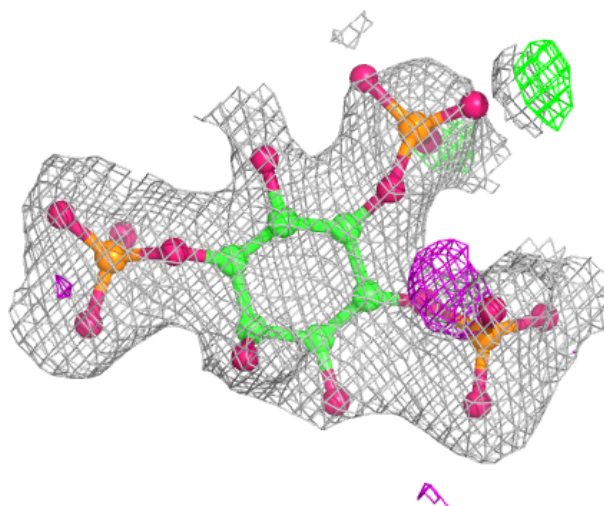
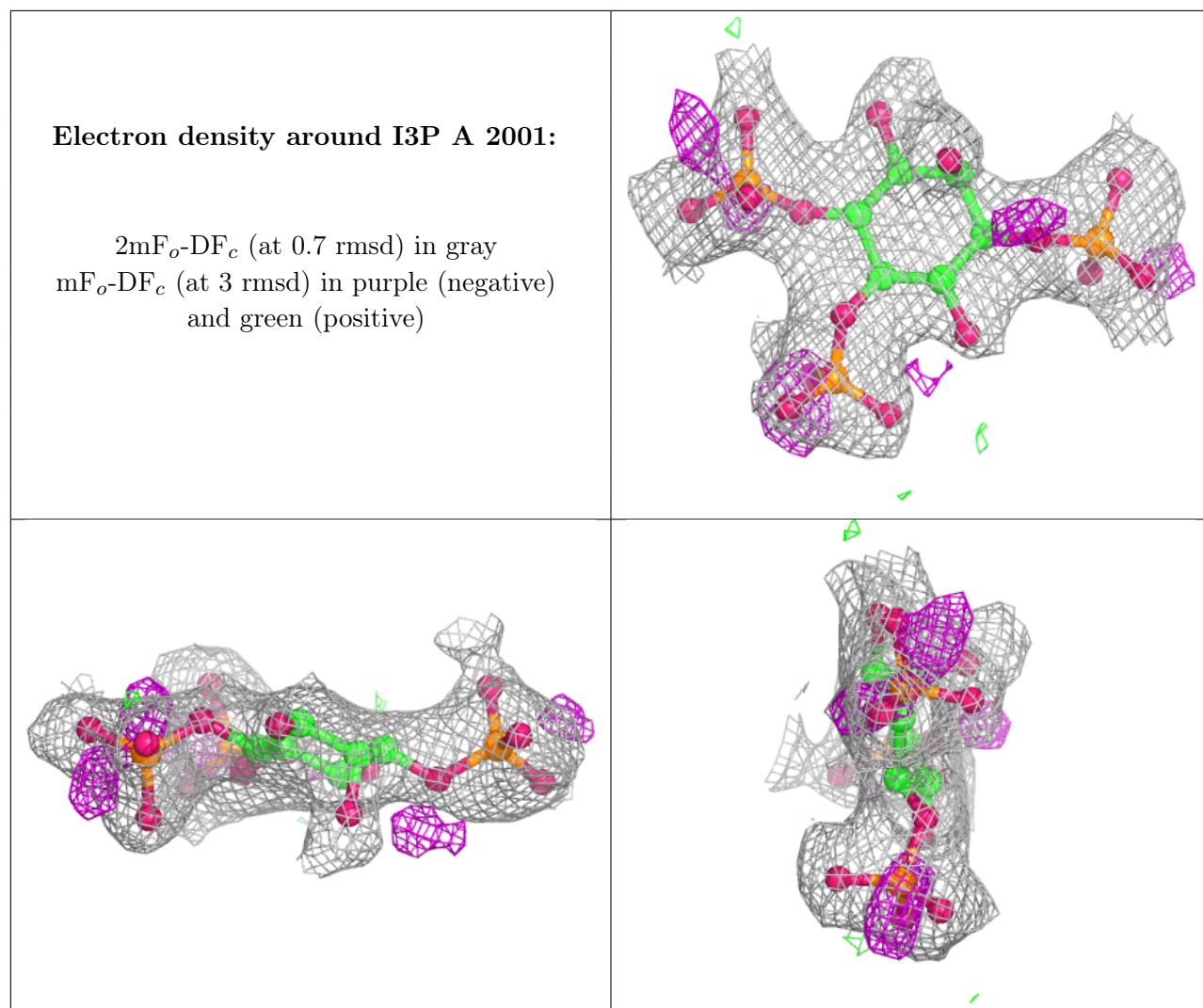| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	I3P	D	2001	24/24	0.65	0.43	87,95,120,121	0
2	I3P	B	2001	24/24	0.73	0.27	79,86,108,110	0
2	I3P	C	2001	24/24	0.86	0.23	68,79,94,96	0
2	I3P	A	2001	24/24	0.88	0.20	51,66,73,77	0

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 I3P D 2001:

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

Electron density around I3P B 2001:

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 I3P A 2001:

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

6.5　Other polymers ⓘ

There are no such residues in this entry.