



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:34 AM UTC

PDB ID : 3W9F / pdb_00003w9f
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)

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 ⓘ](#)) 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

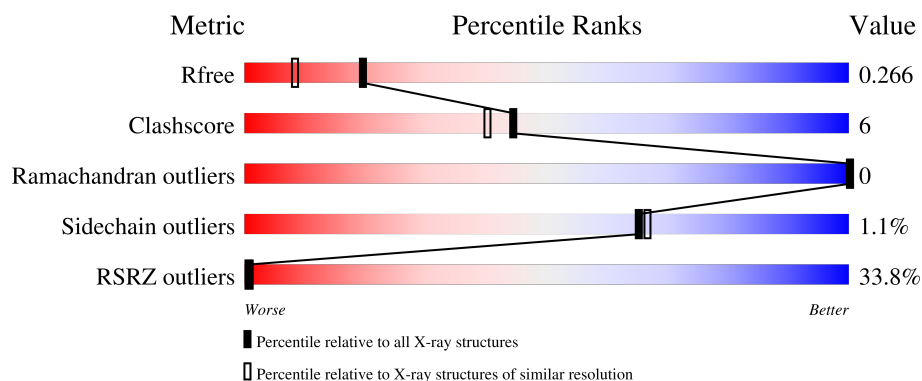
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 $\leq 5\%$. 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	260	5% 88% 10% .
1	B	260	14% 85% 12% .
1	C	260	40% 79% 16% ..
1	D	260	72% 73% 22% ..

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:

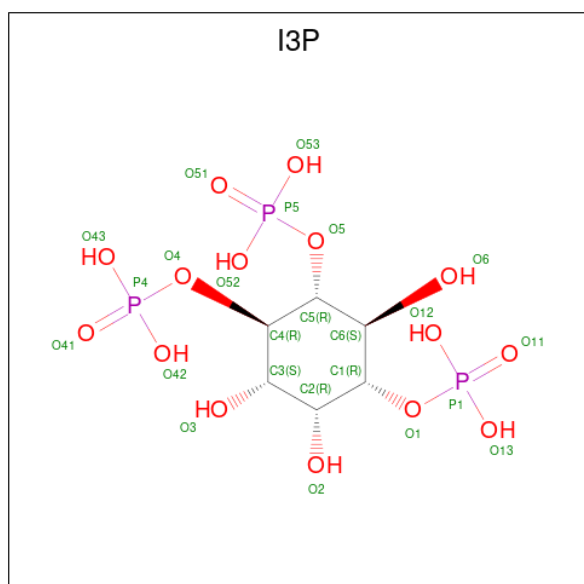
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	MET	-	expression tag	UNP Q9DFS3
A	383	ALA	-	expression tag	UNP Q9DFS3
A	384	ALA	-	expression tag	UNP Q9DFS3
A	385	ALA	-	expression tag	UNP Q9DFS3
A	386	HIS	-	expression tag	UNP Q9DFS3
A	387	HIS	-	expression tag	UNP Q9DFS3
A	388	HIS	-	expression tag	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 (CCD ID: 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	C	O	P	0	0
			24	6	15	3		
2	C	1	Total	C	O	P	0	0
			24	6	15	3		
2	D	1	Total	C	O	P	0	0
			24	6	15	3		

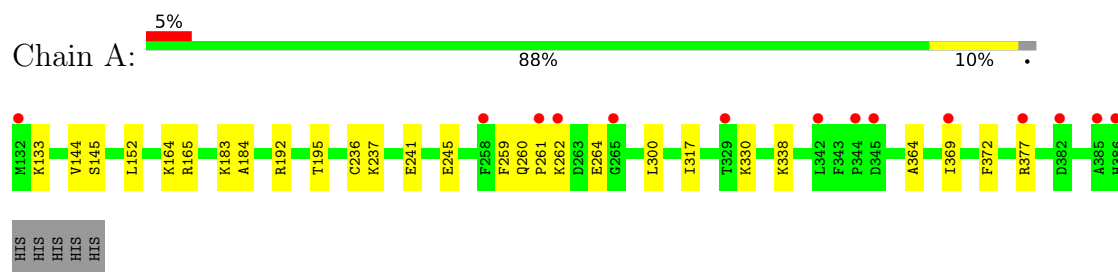
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	244	Total	O	0	0
			244	244		
3	B	201	Total	O	0	0
			201	201		
3	C	15	Total	O	0	0
			15	15		
3	D	1	Total	O	0	0
			1	1		

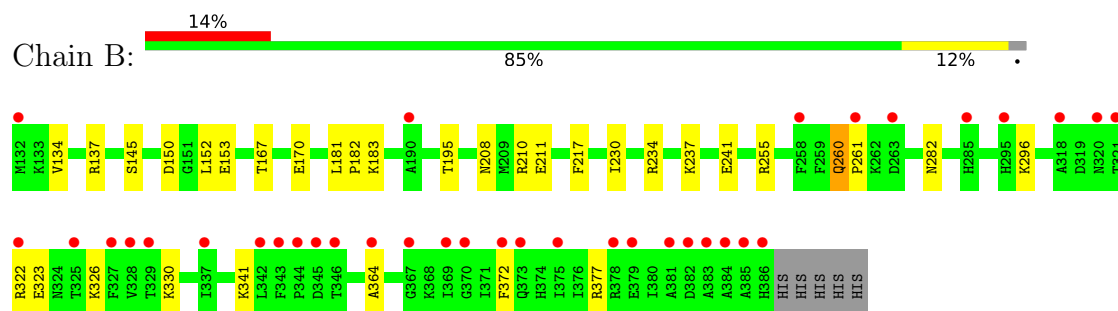
3 Residue-property plots [i](#)

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.

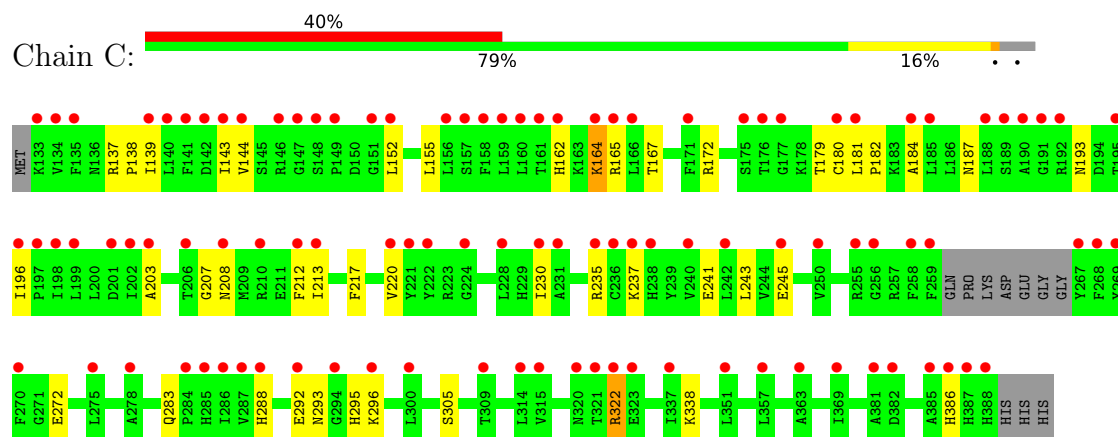
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



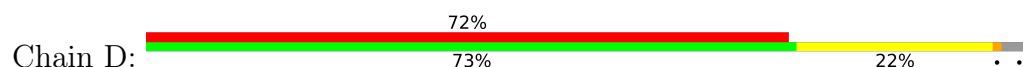
- Molecule 1: Vanilloid receptor-related osmotically activated channel protein



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



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





4 Data and refinement statistics

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) 93.1 (32.81-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.89Å)	Xtrriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.246 (Not available) , 0.266	Depositor DCC
R_{free} test set	2054 reflections (1.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.0	Xtrriage
Anisotropy	0.534	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8642	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtrriage'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.*

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: 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	0.62	0/2139	0.83	1/2884 (0.0%)
1	B	0.62	0/2120	0.88	2/2859 (0.1%)
1	C	0.45	1/2034 (0.0%)	0.88	1/2745 (0.0%)
1	D	0.42	0/2035	0.97	7/2747 (0.3%)
All	All	0.54	1/8328 (0.0%)	0.89	11/11235 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	196	ILE	CA-CB	5.33	1.57	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	322	ARG	N-CA-C	7.54	119.29	111.14
1	D	369	ILE	N-CA-C	6.70	117.40	110.36
1	D	283	GLN	CA-C-N	6.14	125.86	119.05
1	D	283	GLN	C-N-CA	6.14	125.86	119.05
1	B	260	GLN	CA-C-N	-5.73	113.85	119.64
1	B	260	GLN	C-N-CA	-5.73	113.85	119.64
1	D	388	HIS	N-CA-C	5.52	116.32	108.54
1	C	164	LYS	N-CA-C	5.44	118.13	109.81
1	D	158	PHE	N-CA-C	5.37	116.82	111.07
1	A	369	ILE	N-CA-C	5.17	115.38	110.42
1	D	369	ILE	CB-CA-C	-5.10	105.35	111.88

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	18	0
1	B	2049	0	2080	21	0
1	C	1989	0	2008	24	0
1	D	1989	0	2007	38	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	7	0
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	99	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 (99) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:164:LYS:NZ	3:A:2323:HOH:O	2.39	0.55
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
1:C:237:LYS:O	1:C:241:GLU:HG3	2.10	0.52
1:D:173:GLU:OE2	1:D:176:THR:OG1	2.28	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:A:183:LYS:NZ	3:A:2206:HOH:O	2.45	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:272:GLU:OE2	1:C:305:SER:OG	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	224/221 (101%)	223 (100%)	1 (0%)	84	87
1	B	222/221 (100%)	219 (99%)	3 (1%)	59	59
1	C	213/221 (96%)	209 (98%)	4 (2%)	50	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	213/221 (96%)	211 (99%)	2 (1%)	70	73
All	All	872/884 (99%)	862 (99%)	10 (1%)	65	67

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

Mol	Chain	Res	Type
1	A	317	ILE
1	B	134	VAL
1	B	234[A]	ARG
1	B	234[B]	ARG
1	C	167	THR
1	C	172	ARG
1	C	220	VAL
1	C	322	ARG
1	D	148	SER
1	D	194	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	208	ASN
1	B	282	ASN
1	C	282	ASN
1	D	282	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 oligosaccharides 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	D	2001	-	24,24,24	0.90	0	39,39,39	0.92	2 (5%)
2	I3P	C	2001	-	24,24,24	0.91	0	39,39,39	0.93	0
2	I3P	B	2001	-	24,24,24	0.90	0	39,39,39	0.82	1 (2%)
2	I3P	A	2001	-	24,24,24	0.96	0	39,39,39	0.74	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	I3P	D	2001	-	-	4/15/39/39	0/1/1/1
2	I3P	C	2001	-	-	0/15/39/39	0/1/1/1
2	I3P	B	2001	-	-	1/15/39/39	0/1/1/1
2	I3P	A	2001	-	-	1/15/39/39	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2001	I3P	P1-O1-C1	-2.36	117.14	123.43
2	B	2001	I3P	C2-C3-C4	2.06	114.36	109.68
2	D	2001	I3P	P4-O4-C4	-2.03	118.02	123.43

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	2001	I3P	C4-C5-O5-P5

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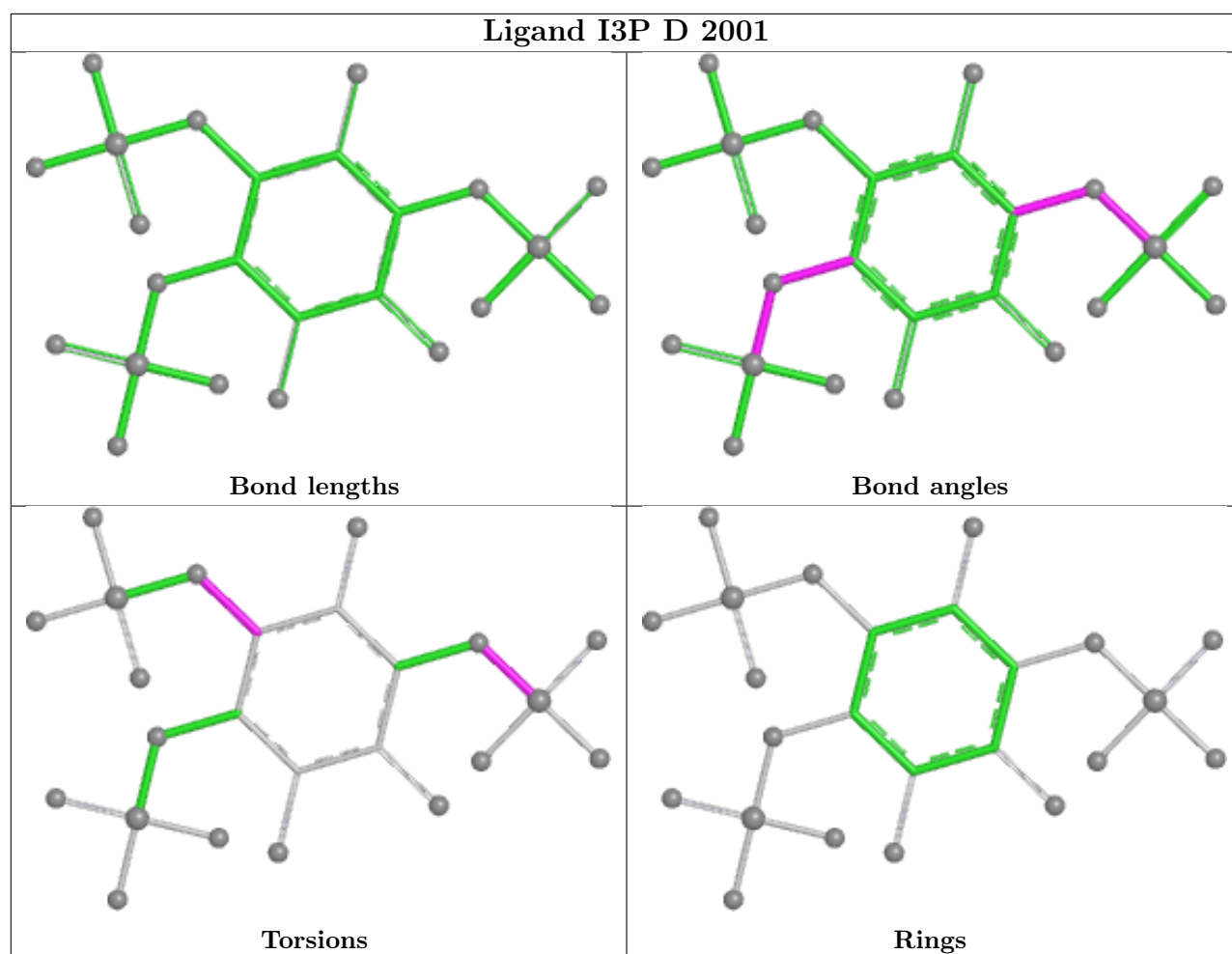
Mol	Chain	Res	Type	Atoms
2	D	2001	I3P	C6-C5-O5-P5
2	D	2001	I3P	C1-O1-P1-O11
2	B	2001	I3P	C1-O1-P1-O11
2	D	2001	I3P	C1-O1-P1-O13
2	A	2001	I3P	C4-O4-P4-O41

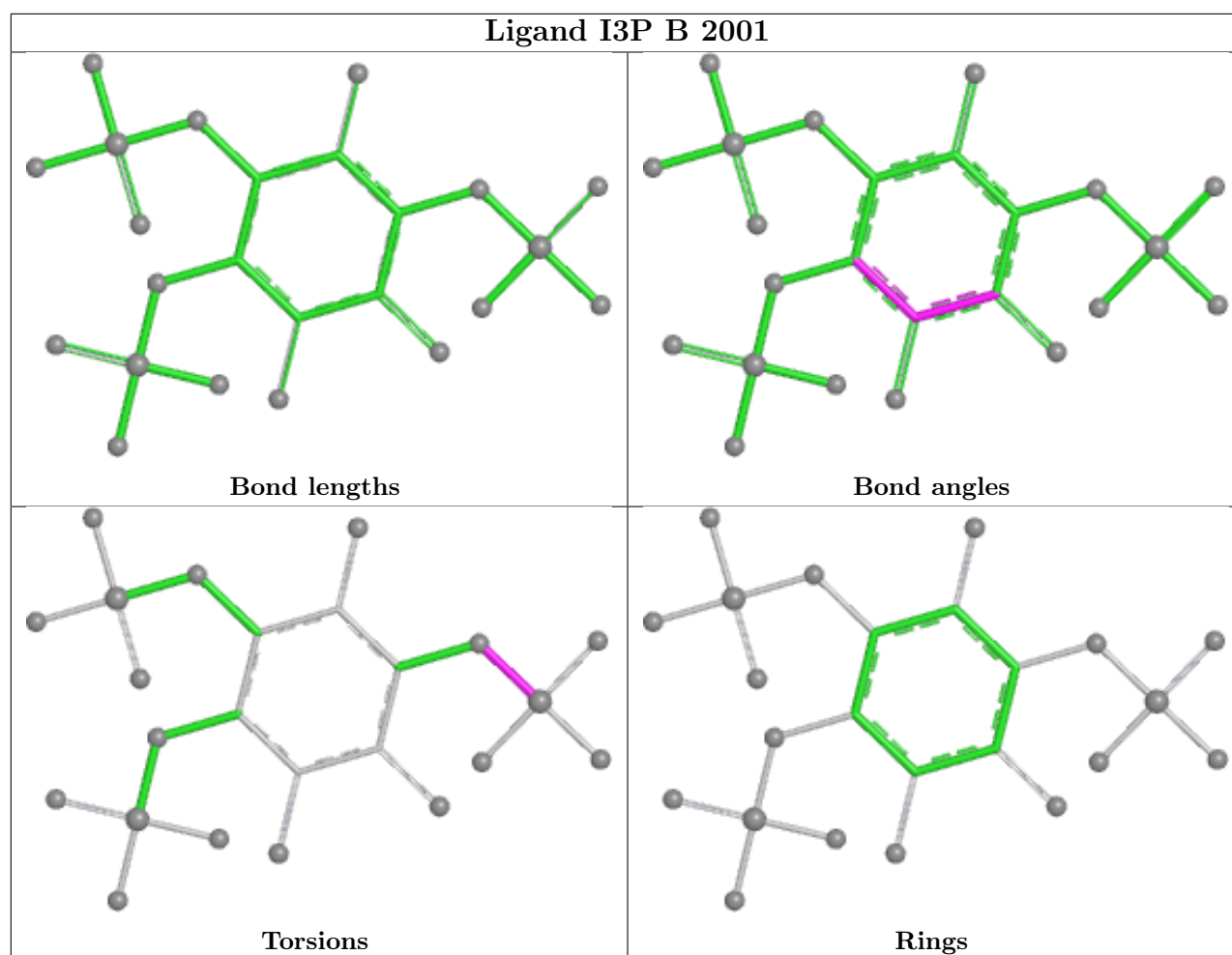
There are no ring outliers.

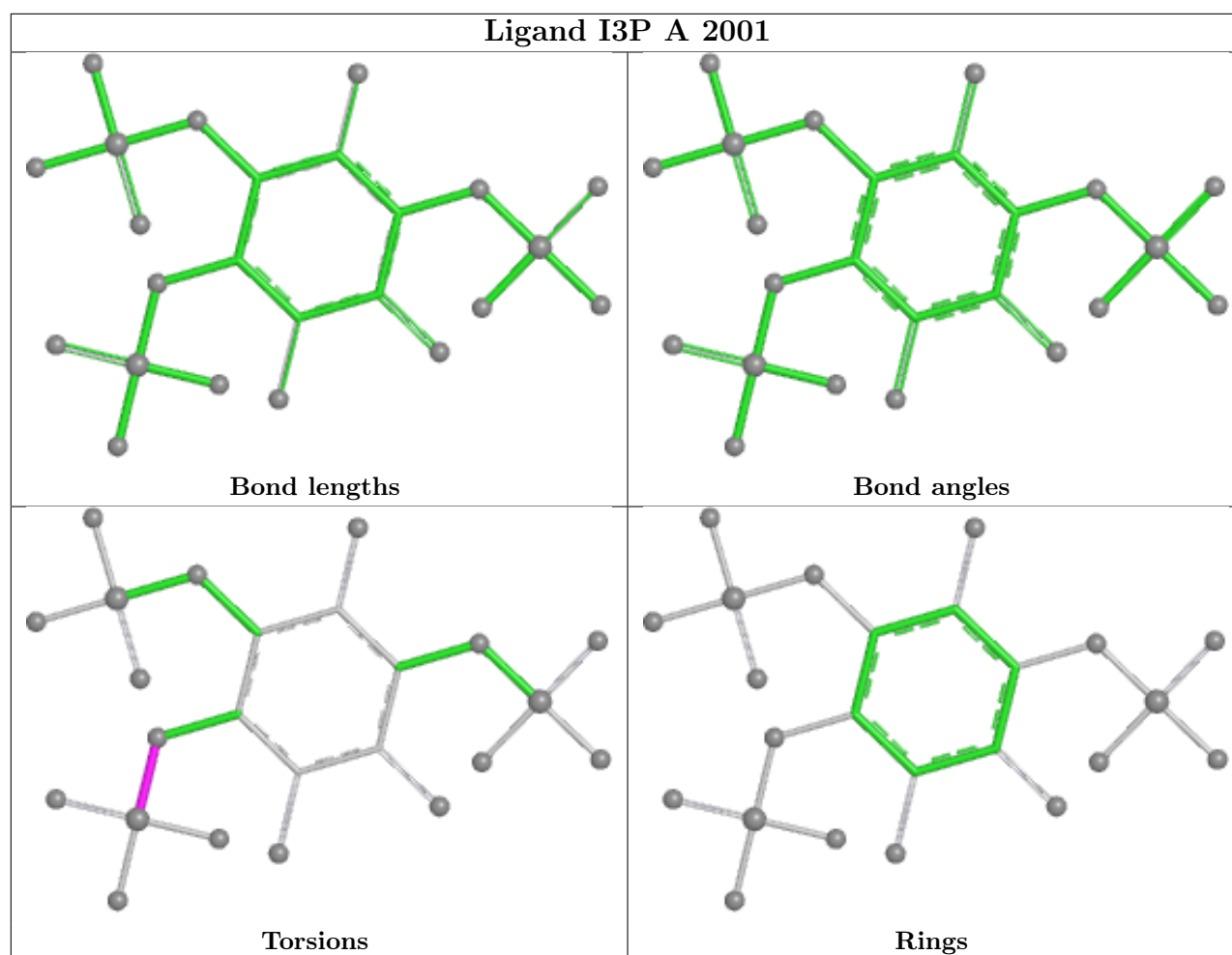
3 monomers are involved in 6 short contacts:

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







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	255/260 (98%)	0.17	14 (5%) 30 32	17, 27, 62, 98	8 (3%)
1	B	255/260 (98%)	0.59	36 (14%) 6 6	18, 34, 84, 131	6 (2%)
1	C	249/260 (95%)	1.90	103 (41%) 0 0	38, 78, 113, 161	1 (0%)
1	D	249/260 (95%)	2.78	188 (75%) 0 0	51, 106, 140, 157	1 (0%)
All	All	1008/1040 (96%)	1.35	341 (33%) 1 1	17, 60, 129, 161	16 (1%)

All (341) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	321	THR	6.4
1	D	195	THR	6.2
1	D	298	ALA	5.9
1	B	386	HIS	5.8
1	C	158	PHE	5.7
1	B	132	MET	5.7
1	C	258	PHE	5.5
1	D	286	ILE	5.4
1	D	369	ILE	5.4
1	C	236	CYS	5.3
1	B	384	ALA	5.2
1	B	385	ALA	5.1
1	D	267	TYR	5.1
1	D	364	ALA	4.9
1	D	256	GLY	4.9
1	D	220	VAL	4.9
1	D	213	ILE	4.9
1	D	166	LEU	4.9
1	D	258	PHE	4.9
1	D	233	GLU	4.8
1	C	166	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	256	GLY	4.8
1	C	171	PHE	4.7
1	D	175	SER	4.5
1	D	152	LEU	4.5
1	C	206	THR	4.5
1	D	386	HIS	4.4
1	D	177	GLY	4.4
1	D	231	ALA	4.3
1	D	351	LEU	4.3
1	D	357	LEU	4.3
1	D	176	THR	4.2
1	D	352	LEU	4.2
1	D	141	PHE	4.2
1	C	231	ALA	4.1
1	D	327	PHE	4.1
1	D	328	VAL	4.1
1	C	221	TYR	4.1
1	B	383	ALA	4.0
1	D	291	THR	4.0
1	D	325	THR	4.0
1	D	208	ASN	4.0
1	C	259	PHE	4.0
1	D	139	ILE	4.0
1	C	139	ILE	4.0
1	D	315	VAL	4.0
1	D	254	ALA	3.9
1	D	257	ARG	3.9
1	D	289	TYR	3.9
1	D	138	PRO	3.9
1	D	283	GLN	3.8
1	D	323	GLU	3.8
1	D	206	THR	3.8
1	D	193	ASN	3.8
1	D	221	TYR	3.8
1	D	196	ILE	3.8
1	D	334	LEU	3.7
1	B	373	GLN	3.7
1	D	329	THR	3.7
1	D	186	LEU	3.7
1	D	239	TYR	3.7
1	D	145	SER	3.7
1	D	142	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	198	ILE	3.7
1	D	144	VAL	3.7
1	D	342	LEU	3.7
1	C	267	TYR	3.7
1	C	188	LEU	3.6
1	D	156	LEU	3.6
1	D	157	SER	3.6
1	D	295	HIS	3.6
1	D	199	LEU	3.6
1	B	318	ALA	3.6
1	C	190	ALA	3.6
1	D	280	CYS	3.6
1	D	149	PRO	3.6
1	C	238	HIS	3.6
1	D	203	ALA	3.6
1	D	332	TYR	3.6
1	D	232	ILE	3.6
1	C	388	HIS	3.6
1	C	337	ILE	3.5
1	D	343	PHE	3.5
1	C	292[A]	GLU	3.5
1	B	285	HIS	3.5
1	D	284	PRO	3.5
1	D	372	PHE	3.5
1	D	246	LYS	3.5
1	C	195	THR	3.5
1	D	197	PRO	3.5
1	D	230	ILE	3.5
1	D	337	ILE	3.5
1	D	162	HIS	3.5
1	D	172	ARG	3.5
1	D	290	LEU	3.5
1	D	210	ARG	3.4
1	D	389	HIS	3.4
1	D	151	GLY	3.4
1	C	208	ASN	3.4
1	C	202	ILE	3.4
1	C	250	VAL	3.4
1	A	342	LEU	3.4
1	C	149	PRO	3.4
1	C	285	HIS	3.4
1	D	319	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	190	ALA	3.4
1	D	269	TYR	3.3
1	D	158	PHE	3.3
1	D	268	PHE	3.3
1	B	345	ASP	3.3
1	C	220	VAL	3.3
1	B	342	LEU	3.3
1	D	242	LEU	3.3
1	D	336	LEU	3.3
1	B	329	THR	3.3
1	D	171	PHE	3.3
1	D	134	VAL	3.3
1	D	388	HIS	3.3
1	C	181	LEU	3.3
1	B	344	PRO	3.3
1	C	198	ILE	3.2
1	D	385	ALA	3.2
1	D	243	LEU	3.2
1	D	281	THR	3.2
1	D	212	PHE	3.2
1	C	146	ARG	3.2
1	D	227	ALA	3.2
1	B	261	PRO	3.2
1	D	216	PRO	3.2
1	C	156	LEU	3.2
1	D	247	GLY	3.2
1	B	258	PHE	3.2
1	C	268	PHE	3.1
1	D	133	LYS	3.1
1	D	187	ASN	3.1
1	D	215	SER	3.1
1	D	371	ILE	3.1
1	D	135	PHE	3.1
1	D	161	THR	3.1
1	B	369	ILE	3.0
1	D	146	ARG	3.0
1	C	212	PHE	3.0
1	D	339	CYS	3.0
1	D	191	GLY	3.0
1	C	140	LEU	3.0
1	D	255	ARG	3.0
1	D	250	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	154	GLY	3.0
1	C	369	ILE	3.0
1	D	320	ASN	3.0
1	D	285	HIS	3.0
1	C	189	SER	3.0
1	B	381	ALA	3.0
1	D	248	ALA	3.0
1	C	147	GLY	2.9
1	C	135	PHE	2.9
1	D	308	ASN	2.9
1	C	203	ALA	2.9
1	D	318	ALA	2.9
1	C	162	HIS	2.9
1	B	337	ILE	2.9
1	C	363	ALA	2.9
1	D	236	CYS	2.9
1	C	159	LEU	2.9
1	C	351	LEU	2.9
1	D	307	GLY	2.9
1	D	229	HIS	2.9
1	D	238	HIS	2.9
1	D	184	ALA	2.9
1	C	199	LEU	2.9
1	D	188	LEU	2.9
1	D	207	GLY	2.9
1	D	214	ASN	2.8
1	C	386	HIS	2.8
1	A	262	LYS	2.8
1	C	164	LYS	2.8
1	C	157	SER	2.8
1	D	164	LYS	2.8
1	D	182	PRO	2.8
1	C	148	SER	2.8
1	D	202	ILE	2.8
1	D	360	LEU	2.8
1	D	316	ALA	2.8
1	C	320	ASN	2.8
1	D	163	LYS	2.8
1	D	368	LYS	2.8
1	C	284	PRO	2.8
1	D	174	PRO	2.8
1	A	385	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	343	PHE	2.7
1	D	205	LYS	2.7
1	C	357	LEU	2.7
1	A	369	ILE	2.7
1	D	148	SER	2.7
1	D	377	ARG	2.7
1	D	226	THR	2.7
1	C	177	GLY	2.7
1	D	224	GLY	2.7
1	D	252	ALA	2.6
1	D	355	ASP	2.6
1	D	137	ARG	2.6
1	C	141	PHE	2.6
1	A	261	PRO	2.6
1	D	228	LEU	2.6
1	A	132	MET	2.6
1	C	240	VAL	2.6
1	D	192	ARG	2.6
1	D	279	ALA	2.6
1	D	340	ALA	2.6
1	D	384	ALA	2.6
1	C	165	ARG	2.6
1	D	361	MET	2.6
1	A	345	ASP	2.6
1	B	367	GLY	2.6
1	C	144	VAL	2.6
1	D	383	ALA	2.6
1	D	185	LEU	2.6
1	C	196	ILE	2.6
1	C	176	THR	2.6
1	D	167	THR	2.5
1	C	275	LEU	2.5
1	C	294	GLY	2.5
1	C	184	ALA	2.5
1	C	134	VAL	2.5
1	C	245	GLU	2.5
1	B	263	ASP	2.5
1	D	240	VAL	2.5
1	C	296	LYS	2.5
1	B	322	ARG	2.4
1	C	222	TYR	2.4
1	C	255	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	235	ARG	2.4
1	D	362	MET	2.4
1	C	213	ILE	2.4
1	D	375	ILE	2.4
1	D	333	ASP	2.4
1	D	382	ASP	2.4
1	C	210	ARG	2.4
1	D	170	GLU	2.4
1	C	269	TYR	2.4
1	D	189	SER	2.4
1	B	372	PHE	2.4
1	D	217	PHE	2.4
1	C	382	ASP	2.4
1	A	329	THR	2.4
1	D	313	ALA	2.4
1	D	347	ASN	2.4
1	D	331	MET	2.4
1	D	160	LEU	2.4
1	C	161	THR	2.4
1	C	286	ILE	2.4
1	C	322	ARG	2.4
1	D	292	GLU	2.4
1	D	288	HIS	2.4
1	D	159	LEU	2.3
1	C	230	ILE	2.3
1	A	386	HIS	2.3
1	C	315	VAL	2.3
1	D	244	VAL	2.3
1	C	180	CYS	2.3
1	B	346	THR	2.3
1	D	143	ILE	2.3
1	C	191	GLY	2.3
1	B	378	ARG	2.3
1	C	287	VAL	2.3
1	C	185	LEU	2.3
1	C	387	HIS	2.3
1	D	293	ASN	2.3
1	D	344	PRO	2.3
1	A	377	ARG	2.3
1	C	224	GLY	2.3
1	D	147	GLY	2.3
1	D	150	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	237	LYS	2.3
1	D	348	LEU	2.3
1	D	294	GLY	2.2
1	D	363	ALA	2.2
1	B	328	VAL	2.2
1	D	183	LYS	2.2
1	B	325	THR	2.2
1	D	302	ARG	2.2
1	C	228	LEU	2.2
1	A	258	PHE	2.2
1	D	251	HIS	2.2
1	D	365	LYS	2.2
1	D	378	ARG	2.2
1	C	321	THR	2.2
1	C	160	LEU	2.2
1	D	155	LEU	2.2
1	D	225	GLN	2.2
1	A	382	ASP	2.2
1	B	370	GLY	2.2
1	C	175	SER	2.2
1	B	190	ALA	2.2
1	D	350	ALA	2.2
1	B	295[A]	HIS	2.2
1	B	320	ASN	2.2
1	D	178	LYS	2.2
1	D	312	HIS	2.2
1	C	192	ARG	2.2
1	B	382	ASP	2.2
1	D	273	LEU	2.2
1	D	367	GLY	2.2
1	C	197	PRO	2.2
1	C	235	ARG	2.2
1	D	223	ARG	2.2
1	D	330	LYS	2.2
1	D	297	GLN	2.1
1	D	299	ASP	2.1
1	D	381	ALA	2.1
1	C	201	ASP	2.1
1	D	249	ASP	2.1
1	B	321	THR	2.1
1	D	165	ARG	2.1
1	D	326	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	379	GLU	2.1
1	C	300	LEU	2.1
1	C	314	LEU	2.1
1	D	200	LEU	2.1
1	C	278	ALA	2.1
1	C	381	ALA	2.1
1	C	143	ILE	2.1
1	C	309	THR	2.1
1	C	151	GLY	2.1
1	D	209	MET	2.1
1	C	242	LEU	2.1
1	B	364	ALA	2.1
1	C	385	ALA	2.1
1	B	327	PHE	2.0
1	C	323	GLU	2.0
1	C	288	HIS	2.0
1	D	370	GLY	2.0
1	C	152	LEU	2.0
1	C	142	ASP	2.0
1	C	133	LYS	2.0
1	B	375	ILE	2.0
1	C	270	PHE	2.0
1	A	265	GLY	2.0
1	A	344	PRO	2.0
1	D	287	VAL	2.0
1	D	322	ARG	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](#)

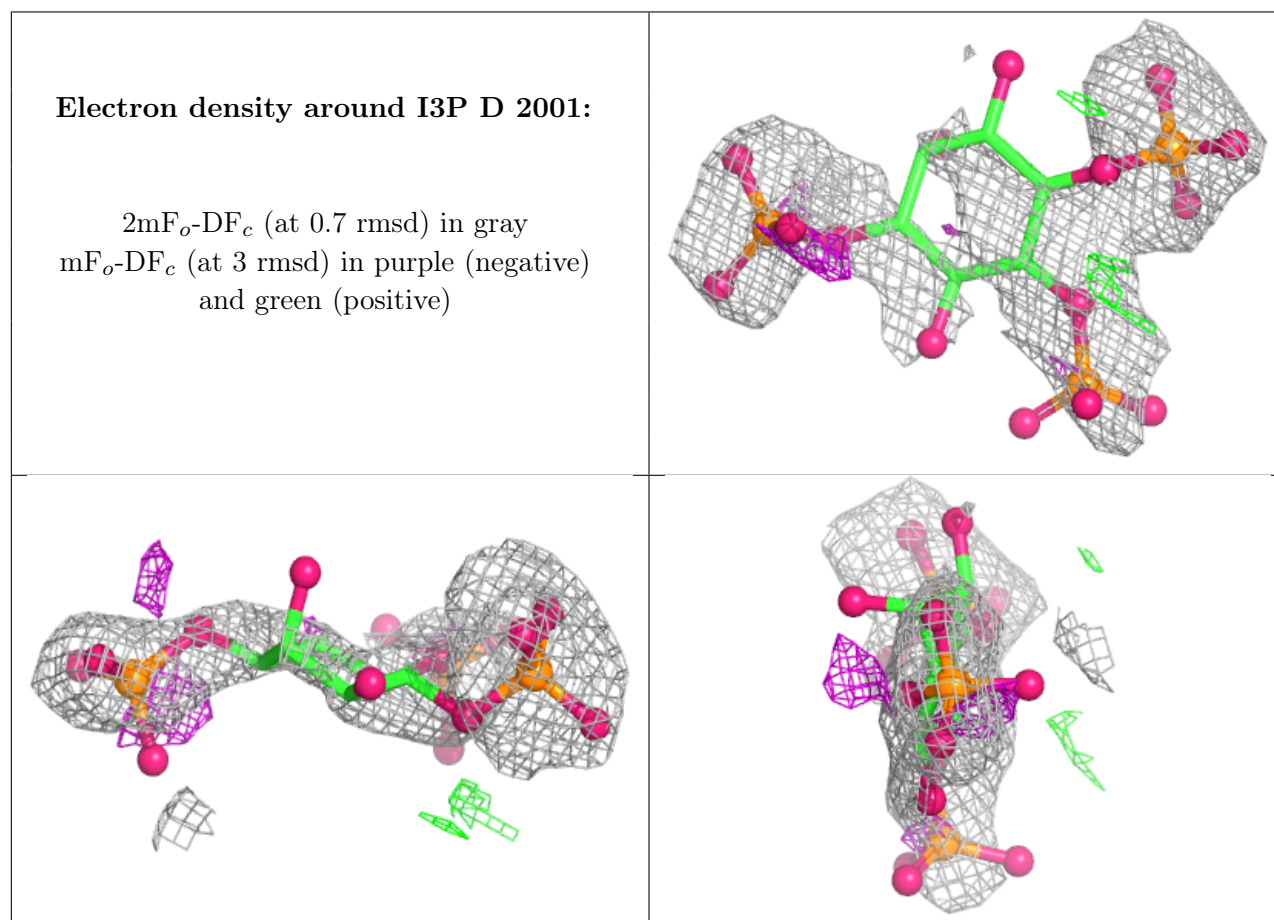
There are no oligosaccharides in this entry.

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.

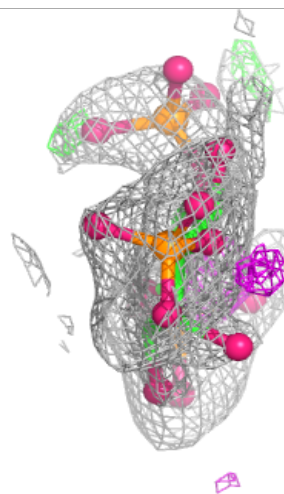
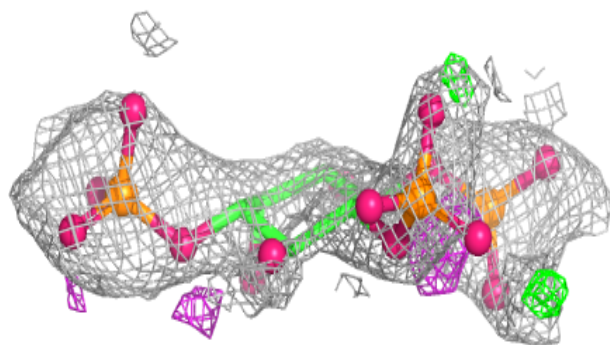
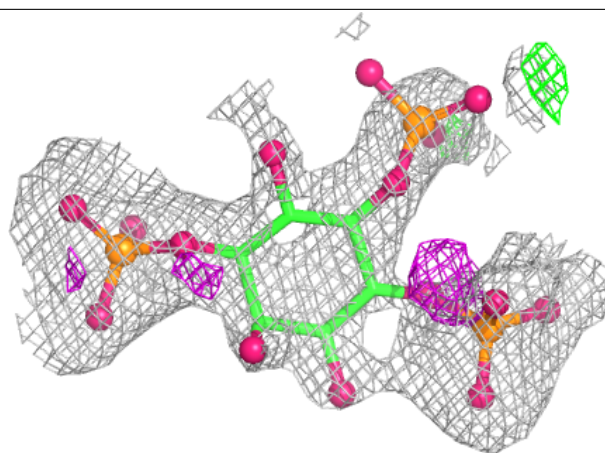
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	I3P	D	2001	24/24	0.65	0.15	87,95,120,121	0
2	I3P	B	2001	24/24	0.79	0.15	79,86,108,110	0
2	I3P	C	2001	24/24	0.84	0.14	68,79,94,96	0
2	I3P	A	2001	24/24	0.87	0.12	51,66,73,77	0

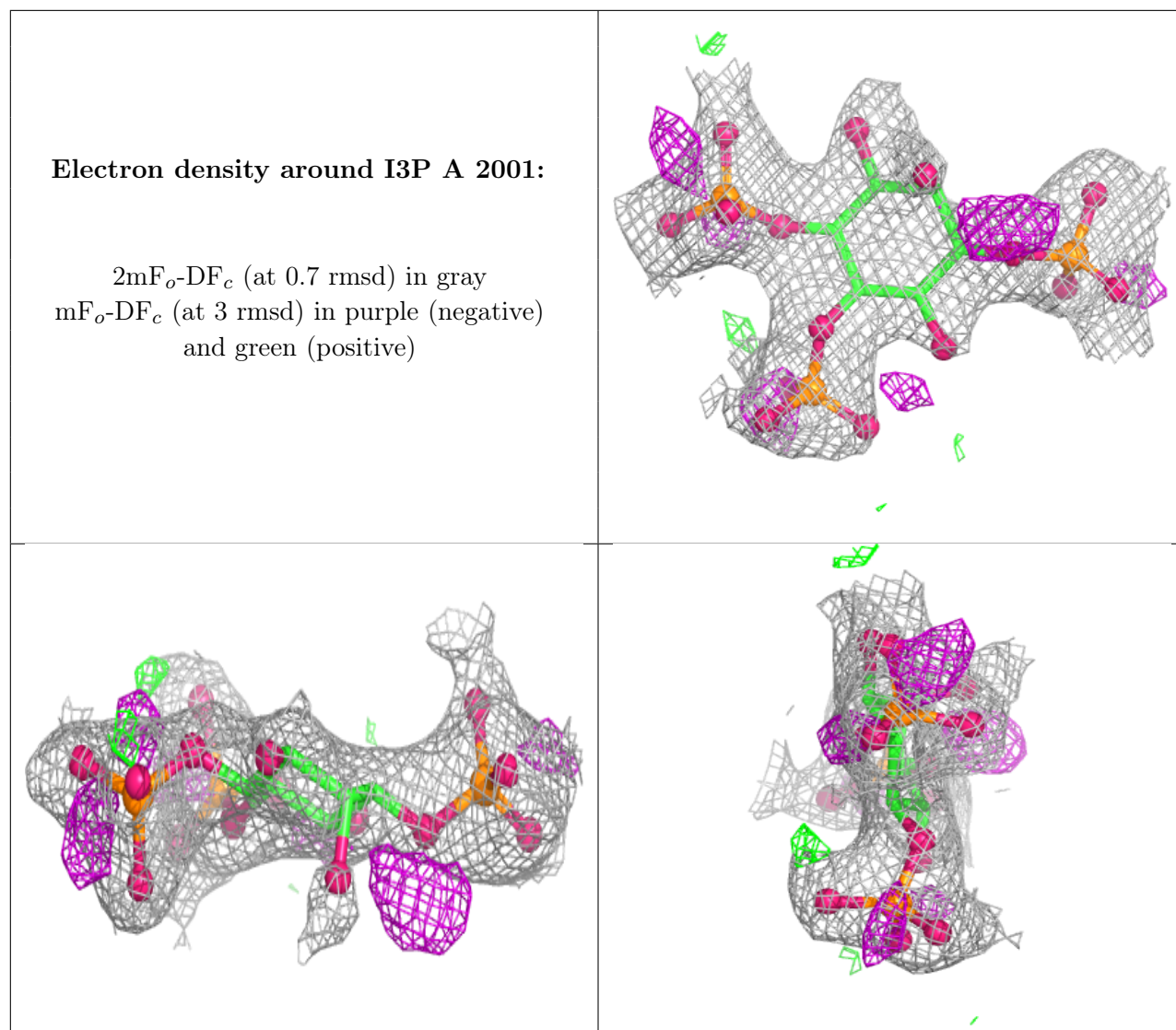
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around I3P 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.