



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:10 AM UTC

PDB ID : 1DJX / pdb_00001djx
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM
RAT COMPLEXED WITH INOSITOL-1,4,5-TRISPHOSPHATE
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on : 1996-08-24
Resolution : 2.30 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

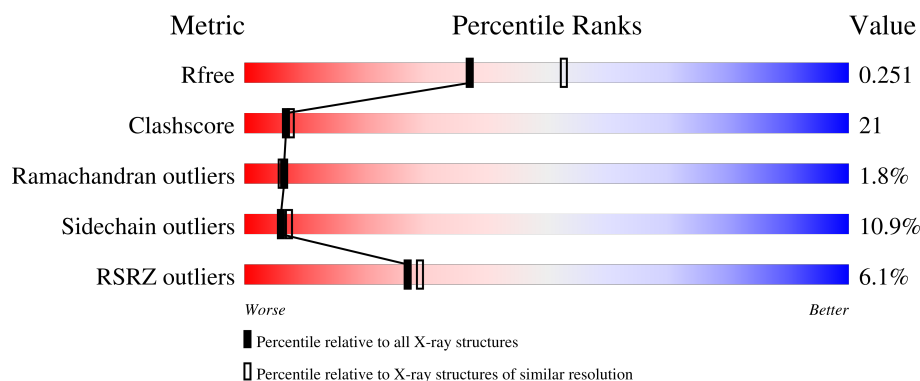
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	624	4% 51% 27% • 18%
1	B	624	7% 53% 30% 6% • 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9374 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 PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	87	0	0
			4070	2573	709	766	22			
1	B	561	Total	C	N	O	S	113	0	0
			4465	2818	776	847	24			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

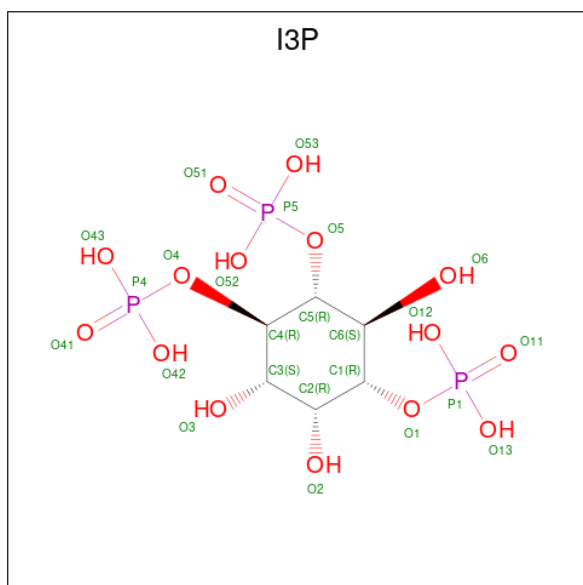
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

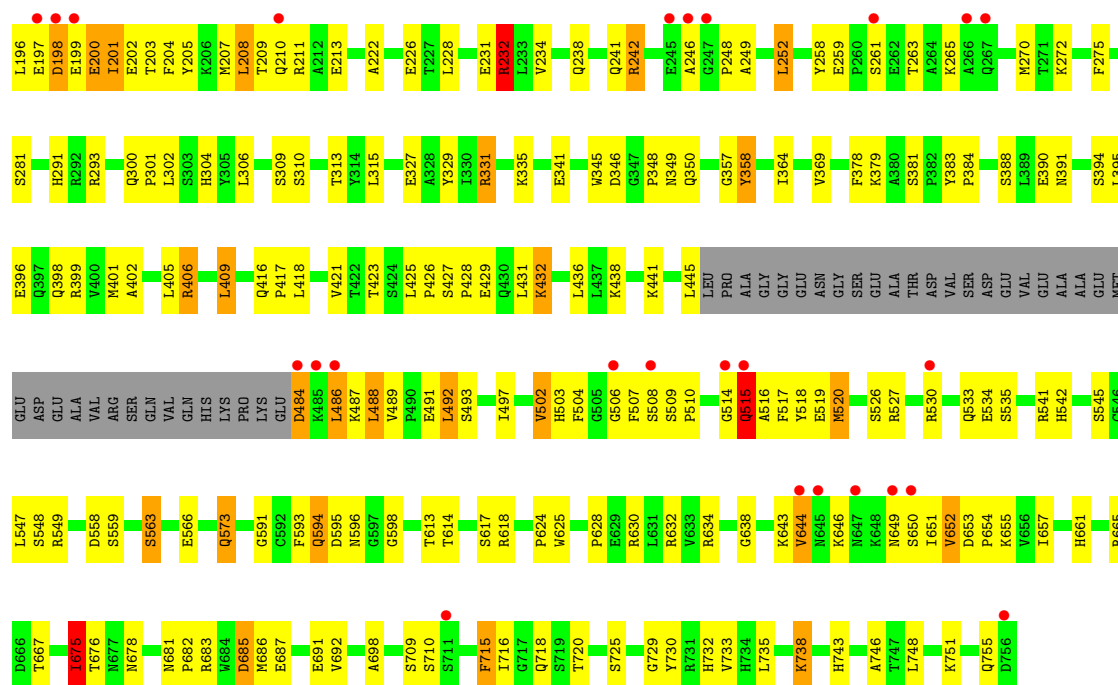
- Molecule 4 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: $C_6H_{15}O_{15}P_3$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	359	Total	O	0	0
			359	359		
5	B	420	Total	O	0	0
			420	420		



4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	397.54Å 397.54Å 397.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 10.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.4 (10.00-2.30) 94.5 (10.00-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.59 (at 2.31Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.220 , 0.270 0.212 , 0.251	Depositor DCC
R_{free} test set	4609 reflections (4.07%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 99.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9374	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.00	4/4165 (0.1%)	1.13	14/5641 (0.2%)
1	B	1.01	4/4565 (0.1%)	1.12	15/6174 (0.2%)
All	All	1.00	8/8730 (0.1%)	1.12	29/11815 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	520	MET	SD-CE	-11.55	1.50	1.79
1	A	520	MET	SD-CE	-8.59	1.58	1.79
1	B	686	MET	SD-CE	-7.65	1.60	1.79
1	A	715	PHE	CE1-CZ	-5.54	1.22	1.38
1	B	401	MET	SD-CE	-5.36	1.66	1.79
1	A	715	PHE	CG-CD2	-5.25	1.27	1.38
1	B	715	PHE	CE2-CZ	-5.20	1.23	1.38
1	A	715	PHE	CG-CD1	-5.03	1.28	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	594	GLN	N-CA-C	-9.46	101.16	112.89
1	B	594	GLN	N-CA-C	-8.76	101.20	112.23
1	A	497	ILE	CB-CA-C	-8.44	104.54	111.71
1	A	514	GLY	N-CA-C	-7.84	94.60	113.18
1	A	306	LEU	N-CA-C	-7.73	97.98	110.20
1	B	497	ILE	CB-CA-C	-6.72	106.00	111.71
1	B	614	THR	N-CA-C	-6.63	104.50	112.59
1	A	675	ILE	N-CA-C	-6.43	99.16	108.36
1	A	391	ASN	N-CA-C	6.41	118.73	108.41
1	B	675	ILE	N-CA-C	-5.92	99.34	107.99
1	B	232	ARG	N-CA-C	-5.92	104.91	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	SER	N-CA-C	5.86	121.51	113.77
1	B	226	GLU	N-CA-C	-5.85	105.73	112.92
1	B	180	TYR	N-CA-C	-5.77	98.51	110.80
1	B	486	LEU	N-CA-C	-5.75	105.93	113.17
1	B	306	LEU	N-CA-C	-5.71	100.37	109.96
1	A	384	PRO	N-CA-C	5.71	120.17	111.15
1	B	652	VAL	N-CA-C	5.37	118.26	109.78
1	A	258	TYR	N-CA-C	5.36	120.69	113.72
1	A	208	LEU	N-CA-C	-5.31	105.58	111.36
1	A	583	GLY	CA-C-N	5.25	125.06	119.28
1	A	583	GLY	C-N-CA	5.25	125.06	119.28
1	B	591	GLY	N-CA-C	-5.25	106.14	112.49
1	B	258	TYR	N-CA-C	5.22	120.50	113.72
1	A	711	SER	N-CA-C	5.18	117.41	109.95
1	A	418	LEU	N-CA-C	-5.12	103.64	110.55
1	B	534	GLU	N-CA-C	5.10	119.58	112.90
1	B	391	ASN	N-CA-C	5.06	117.01	108.96
1	B	315	LEU	N-CA-C	5.05	118.18	110.20

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	4070	0	3994	166	0
1	B	4465	0	4375	193	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	24	0	8	0	0
4	B	24	0	8	1	0
5	A	359	0	0	10	0
5	B	420	0	0	17	0
All	All	9374	0	8391	352	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 21.

All (352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:THR:HG22	1:A:615:PHE:H	1.04	1.10
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.16	1.05
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.21	1.04
1:A:200:GLU:N	1:A:203:THR:HG1	1.56	1.03
1:B:169:LEU:HD12	1:B:176:VAL:HG13	1.07	1.03
1:A:241:GLN:HE22	1:A:730:TYR:H	1.18	0.92
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.54	0.90
1:A:644:VAL:HG21	1:A:716:ILE:HG12	1.55	0.88
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.03	0.88
1:A:613:THR:HG22	1:A:615:PHE:N	1.88	0.87
1:A:573:GLN:H	1:A:573:GLN:HE21	1.18	0.87
1:B:504:PHE:HB3	1:B:527:ARG:NH2	1.91	0.85
1:A:418:LEU:HB2	1:A:421:VAL:HG21	1.57	0.84
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.59	0.84
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.57	0.84
1:A:520:MET:CE	1:A:549:ARG:HB2	2.08	0.84
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.58	0.83
1:B:515:GLN:HE21	1:B:542:HIS:HE1	1.26	0.82
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.93	0.82
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.45	0.81
1:B:520:MET:CE	1:B:549:ARG:HB2	2.10	0.81
1:A:573:GLN:H	1:A:573:GLN:NE2	1.78	0.80
1:B:208:LEU:HD23	1:B:209:THR:HG23	1.61	0.80
1:B:172:LEU:HD12	1:B:174:ILE:HG13	1.62	0.80
1:A:418:LEU:HB2	1:A:421:VAL:CG2	2.10	0.79
1:A:200:GLU:HA	1:A:203:THR:HB	1.64	0.79
1:B:169:LEU:CD1	1:B:176:VAL:HG13	2.03	0.79
1:B:208:LEU:HD23	1:B:209:THR:CG2	2.11	0.79
1:A:216:ARG:O	1:A:220:GLU:HG2	1.83	0.78
1:B:184:ILE:HG22	1:B:204:PHE:CE1	2.19	0.77
1:B:573:GLN:H	1:B:573:GLN:HE21	1.32	0.77
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.67	0.76
1:B:652:VAL:HG23	5:B:790:HOH:O	1.86	0.76
1:B:161:ASN:H	1:B:164:GLU:HG3	1.51	0.76
1:A:394:SER:O	1:A:398:GLN:HG3	1.86	0.75
1:B:394:SER:O	1:B:398:GLN:HG3	1.87	0.75
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.22	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:ALA:HB2	1:B:492:LEU:HD22	1.69	0.74
1:B:184:ILE:HG22	1:B:204:PHE:CD1	2.24	0.72
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.70	0.72
1:B:191:SER:HB2	1:B:193:THR:HG23	1.71	0.72
1:A:242:ARG:HD2	1:A:728:GLN:NE2	2.05	0.72
1:B:241:GLN:HE22	1:B:730:TYR:H	1.35	0.72
1:B:520:MET:HE2	1:B:549:ARG:HB2	1.72	0.71
1:A:520:MET:HE2	1:A:549:ARG:HB2	1.74	0.70
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.73	0.70
1:B:593:PHE:O	1:B:598:GLY:HA2	1.92	0.69
1:B:169:LEU:O	1:B:172:LEU:HD12	1.92	0.69
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.27	0.69
1:B:715:PHE:HB2	5:B:931:HOH:O	1.92	0.69
1:A:395:LEU:HD22	1:A:489:VAL:CG1	2.23	0.69
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.75	0.68
1:B:281:SER:HB2	5:B:854:HOH:O	1.93	0.68
1:B:573:GLN:H	1:B:573:GLN:NE2	1.90	0.68
1:B:178:ASP:O	1:B:180:TYR:N	2.27	0.68
1:B:172:LEU:CD1	1:B:174:ILE:HG13	2.23	0.68
1:A:622:GLN:OE1	1:B:445:LEU:HD12	1.94	0.67
1:B:515:GLN:NE2	1:B:542:HIS:HE1	1.92	0.67
1:A:421:VAL:HG11	1:A:426:PRO:HG3	1.75	0.67
1:A:346:ASP:OD2	1:A:394:SER:HB3	1.94	0.67
1:B:630:ARG:HD2	1:B:755:GLN:HE21	1.60	0.66
1:A:708:ASP:HB2	5:A:1000:HOH:O	1.95	0.66
1:B:160:MET:HB3	1:B:165:LEU:CD2	2.26	0.66
1:A:644:VAL:HG21	1:A:716:ILE:CG1	2.26	0.66
1:B:169:LEU:CB	1:B:176:VAL:HG22	2.27	0.65
1:B:242:ARG:NH1	5:B:1125:HOH:O	2.28	0.65
1:B:175:GLN:HG3	1:B:651:ILE:HD13	1.79	0.65
1:B:177:ASP:N	1:B:177:ASP:OD1	2.29	0.65
1:B:533:GLN:OE1	1:B:618:ARG:NH1	2.30	0.65
1:B:395:LEU:HD22	1:B:489:VAL:HG13	1.78	0.65
1:A:644:VAL:CG2	1:A:716:ILE:HG12	2.25	0.64
1:A:644:VAL:HG22	1:A:716:ILE:HG23	1.78	0.64
1:A:441:LYS:NZ	1:A:493:SER:O	2.30	0.64
1:A:616:ASN:OD1	1:A:618:ARG:HB2	1.97	0.64
1:B:169:LEU:HB3	1:B:176:VAL:HG22	1.78	0.64
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.25	0.64
1:A:216:ARG:HG3	1:A:216:ARG:NH1	2.09	0.64
1:A:395:LEU:HD22	1:A:489:VAL:HG13	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASN:H	1:B:164:GLU:CG	2.10	0.64
1:B:652:VAL:HG11	1:B:716:ILE:CD1	2.28	0.63
1:A:415:ASP:O	1:A:416:GLN:HG2	1.98	0.63
1:A:593:PHE:O	1:A:598:GLY:HA2	1.99	0.63
1:A:706:ASP:HB3	1:A:714:ASP:HB2	1.81	0.63
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.81	0.62
1:A:515:GLN:HB3	1:A:519:GLU:OE1	1.98	0.62
1:B:395:LEU:HD22	1:B:489:VAL:CG1	2.29	0.62
1:A:515:GLN:HE21	1:A:542:HIS:HE1	1.47	0.62
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.34	0.62
1:B:238:GLN:HG2	1:B:246:ALA:HB3	1.81	0.62
1:A:200:GLU:CA	1:A:203:THR:HB	2.30	0.62
1:B:484:ASP:O	1:B:488:LEU:N	2.31	0.62
1:A:220:GLU:HG3	5:A:971:HOH:O	2.00	0.62
1:A:743:HIS:HB3	1:A:746:ALA:HB3	1.82	0.61
1:B:515:GLN:HB3	1:B:519:GLU:OE1	1.99	0.61
1:B:300:GLN:OE1	1:B:304:HIS:HD2	1.84	0.61
1:A:269:GLN:NE2	5:A:907:HOH:O	2.29	0.61
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.34	0.61
1:B:196:LEU:HD22	1:B:200:GLU:HB2	1.82	0.61
1:A:200:GLU:O	1:A:204:PHE:HB3	2.00	0.60
1:A:241:GLN:HE22	1:A:730:TYR:N	1.94	0.60
1:A:515:GLN:HE21	1:A:542:HIS:CE1	2.19	0.60
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.30	0.60
1:B:516:ALA:HB1	1:B:518:TYR:CE1	2.36	0.60
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.02	0.60
1:B:441:LYS:NZ	1:B:493:SER:O	2.35	0.60
1:B:730:TYR:CE1	1:B:751:LYS:HD2	2.37	0.60
1:B:327:GLU:OE2	1:B:331:ARG:HD2	2.00	0.60
1:B:222:ALA:C	1:B:232:ARG:HH11	2.10	0.59
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.32	0.59
1:B:191:SER:CB	1:B:193:THR:HG23	2.31	0.59
1:B:683:ARG:NH2	1:B:685:ASP:OD2	2.35	0.59
1:A:515:GLN:NE2	1:A:542:HIS:HE1	2.01	0.59
1:B:234:VAL:O	1:B:238:GLN:HG3	2.02	0.59
1:A:730:TYR:CZ	1:A:751:LYS:HD2	2.38	0.59
1:A:441:LYS:HB3	1:A:500:LYS:HG3	1.84	0.58
1:B:249:ALA:HB3	5:B:1127:HOH:O	2.03	0.58
1:A:515:GLN:NE2	1:A:542:HIS:CE1	2.72	0.58
1:B:188:CYS:HB2	1:B:196:LEU:HD11	1.85	0.58
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:654:PRO:HD2	1:B:675:ILE:O	2.04	0.58
1:A:418:LEU:HD12	1:A:426:PRO:HB3	1.87	0.57
1:B:196:LEU:O	1:B:201:ILE:HD11	2.04	0.57
1:B:484:ASP:O	1:B:487:LYS:N	2.33	0.57
1:B:507:PHE:HB3	5:B:1092:HOH:O	2.04	0.57
1:B:175:GLN:HA	1:B:175:GLN:OE1	2.00	0.57
1:B:405:LEU:O	1:B:409:LEU:HB2	2.05	0.56
1:B:421:VAL:HG11	1:B:426:PRO:HD3	1.86	0.56
1:B:530:ARG:HG3	1:B:530:ARG:HH11	1.70	0.56
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.39	0.56
1:B:730:TYR:CZ	1:B:751:LYS:HD2	2.39	0.56
1:B:515:GLN:NE2	1:B:542:HIS:CE1	2.73	0.56
1:A:420:GLY:O	1:A:422:THR:N	2.39	0.56
1:A:647:ASN:HB3	5:A:1004:HOH:O	2.05	0.55
1:B:211:ARG:NE	1:B:213:GLU:OE2	2.33	0.55
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.41	0.55
1:A:536:GLY:HA3	5:A:788:HOH:O	2.06	0.55
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.41	0.55
1:B:346:ASP:OD2	1:B:394:SER:HB3	2.06	0.55
1:A:291:HIS:HD2	1:A:725:SER:OG	1.90	0.55
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.37	0.55
1:B:594:GLN:HA	1:B:594:GLN:HE21	1.70	0.55
1:A:742:GLN:NE2	5:A:858:HOH:O	2.39	0.55
1:B:300:GLN:O	1:B:427:SER:HA	2.06	0.54
1:B:667:THR:HG22	5:B:1161:HOH:O	2.07	0.54
1:A:613:THR:CG2	1:A:615:PHE:H	1.97	0.54
1:A:648:LYS:N	5:A:1004:HOH:O	2.41	0.54
1:B:272:LYS:O	1:B:275:PHE:HB3	2.08	0.54
1:A:638:GLY:O	1:A:681:ASN:HA	2.07	0.54
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.56	0.54
1:A:613:THR:HG22	1:A:614:THR:N	2.22	0.54
1:A:654:PRO:HD2	1:A:675:ILE:O	2.08	0.54
1:A:755:GLN:HG2	1:A:756:ASP:N	2.23	0.54
1:B:335:LYS:NZ	5:B:871:HOH:O	2.29	0.54
1:A:202:GLU:O	1:A:205:TYR:HB3	2.07	0.53
1:B:291:HIS:HD2	1:B:725:SER:OG	1.91	0.53
1:B:416:GLN:HG3	1:B:417:PRO:CD	2.34	0.53
1:A:402:ALA:HB2	1:A:492:LEU:HD22	1.90	0.53
1:B:649:ASN:O	1:B:651:ILE:HG12	2.08	0.53
1:A:420:GLY:O	1:A:422:THR:HG23	2.09	0.53
1:A:735:LEU:O	1:A:743:HIS:HB2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ASN:ND2	1:A:349:ASN:O	2.42	0.53
1:B:300:GLN:HB3	1:B:301:PRO:HD2	1.91	0.53
1:B:632:ARG:HH22	1:B:755:GLN:CD	2.16	0.53
1:A:588:VAL:HA	1:A:720:THR:HG21	1.91	0.53
1:B:358:TYR:CD1	1:B:358:TYR:N	2.72	0.53
1:B:174:ILE:O	1:B:176:VAL:N	2.42	0.52
1:A:236:PHE:HA	5:A:974:HOH:O	2.10	0.52
1:B:203:THR:CG2	1:B:207:MET:HE3	2.39	0.52
1:B:248:PRO:O	1:B:252:LEU:HB2	2.10	0.52
1:A:252:LEU:O	1:A:256:GLU:HG3	2.09	0.52
1:A:200:GLU:N	1:A:203:THR:OG1	2.32	0.52
1:B:541:ARG:O	5:B:1094:HOH:O	2.19	0.52
1:A:573:GLN:NE2	1:A:573:GLN:N	2.53	0.52
1:B:390:GLU:HG3	5:B:1028:HOH:O	2.09	0.52
1:B:652:VAL:HG11	1:B:716:ILE:HD11	1.91	0.52
1:B:348:PRO:HB2	1:B:349:ASN:HD22	1.74	0.52
1:B:379:LYS:HE2	5:B:1062:HOH:O	2.09	0.52
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.36	0.52
1:B:514:GLY:O	1:B:515:GLN:O	2.28	0.52
1:A:300:GLN:O	1:A:427:SER:HA	2.10	0.51
1:A:238:GLN:NE2	1:A:246:ALA:HB3	2.26	0.51
1:A:396:GLU:O	1:A:399:ARG:HB2	2.10	0.51
1:B:425:LEU:HD21	1:B:517:PHE:O	2.10	0.51
1:B:743:HIS:HB3	1:B:746:ALA:HB3	1.93	0.51
1:B:594:GLN:HA	1:B:594:GLN:NE2	2.25	0.50
1:A:405:LEU:O	1:A:409:LEU:HB2	2.11	0.50
1:A:242:ARG:HG3	1:A:728:GLN:HB2	1.92	0.50
1:B:164:GLU:O	1:B:167:ASP:HB3	2.12	0.50
1:B:429:GLU:OE1	1:B:432:LYS:HE3	2.12	0.50
1:B:515:GLN:HB2	1:B:519:GLU:HB2	1.94	0.50
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.46	0.50
1:A:628:PRO:HA	1:A:692:VAL:O	2.11	0.50
1:A:618:ARG:HG3	5:A:788:HOH:O	2.12	0.49
1:A:547:LEU:HD23	1:A:573:GLN:CG	2.39	0.49
1:A:730:TYR:CE1	1:A:751:LYS:HD2	2.46	0.49
1:A:644:VAL:HG12	1:A:644:VAL:O	2.12	0.49
1:A:504:PHE:CE1	1:A:507:PHE:CE1	3.00	0.49
1:A:659:GLU:OE1	1:A:661:HIS:HE1	1.95	0.49
1:B:595:ASP:OD1	1:B:596:ASN:N	2.44	0.49
1:B:515:GLN:HE21	1:B:542:HIS:CE1	2.17	0.49
1:A:436:LEU:N	1:A:436:LEU:HD23	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:ARG:HD2	5:B:779:HOH:O	2.13	0.49
1:B:652:VAL:HG12	1:B:653:ASP:N	2.26	0.49
1:B:638:GLY:O	1:B:681:ASN:HA	2.13	0.48
1:A:622:GLN:CA	1:B:445:LEU:HD11	2.40	0.48
1:A:644:VAL:CG1	1:A:714:ASP:HB3	2.43	0.48
1:B:197:GLU:O	1:B:201:ILE:HG12	2.12	0.48
1:B:203:THR:HG22	1:B:207:MET:HE3	1.96	0.48
1:B:348:PRO:HB2	1:B:349:ASN:ND2	2.27	0.48
1:B:630:ARG:HD2	1:B:755:GLN:NE2	2.26	0.48
1:A:395:LEU:HD22	1:A:489:VAL:HG12	1.94	0.48
1:B:514:GLY:HA3	5:B:1091:HOH:O	2.13	0.48
1:B:169:LEU:HB2	1:B:176:VAL:HG22	1.95	0.48
1:B:738:LYS:HB2	5:B:875:HOH:O	2.14	0.48
1:B:161:ASN:N	1:B:164:GLU:HG3	2.25	0.48
1:A:233:LEU:HD23	1:A:251:ALA:HB1	1.95	0.48
1:A:383:TYR:CB	1:A:384:PRO:HD2	2.37	0.47
1:A:425:LEU:HG	1:A:517:PHE:HD1	1.77	0.47
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.44	0.47
1:A:414:LEU:HA	5:A:1043:HOH:O	2.13	0.47
1:A:686:MET:HE2	1:A:687:GLU:O	2.14	0.47
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.44	0.47
1:B:548:SER:H	1:B:573:GLN:NE2	2.12	0.47
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.96	0.47
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.49	0.47
1:A:488:LEU:HG	1:A:493:SER:HB2	1.95	0.47
1:B:735:LEU:O	1:B:743:HIS:HB2	2.14	0.47
1:B:349:ASN:O	1:B:350:GLN:HB2	2.14	0.47
1:A:551:TYR:HB2	1:A:552:PRO:CD	2.44	0.47
1:B:161:ASN:O	1:B:164:GLU:HG2	2.14	0.47
1:B:436:LEU:N	1:B:436:LEU:HD23	2.29	0.47
1:B:628:PRO:HA	1:B:692:VAL:O	2.14	0.47
1:A:302:LEU:HD23	1:A:428:PRO:HD3	1.97	0.47
1:A:418:LEU:HB2	1:A:421:VAL:HG23	1.95	0.47
1:B:259:GLU:OE1	1:B:270:MET:HA	2.15	0.47
1:A:300:GLN:HB3	1:A:301:PRO:HD2	1.97	0.47
1:A:594:GLN:HA	1:A:594:GLN:HE21	1.80	0.47
1:B:261:SER:O	1:B:265:LYS:HB2	2.14	0.46
1:B:563:SER:O	1:B:566:GLU:HG2	2.16	0.46
1:B:632:ARG:NE	5:B:1123:HOH:O	2.46	0.46
1:A:285:ASN:ND2	1:A:734:HIS:HD2	2.14	0.46
1:A:396:GLU:OE1	1:A:399:ARG:NH1	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASP:O	1:B:201:ILE:HG13	2.15	0.46
1:B:228:LEU:CD2	1:B:232:ARG:HB3	2.45	0.46
1:B:652:VAL:CG1	1:B:716:ILE:HD11	2.46	0.46
1:A:644:VAL:HG21	1:A:716:ILE:CD1	2.45	0.46
1:A:681:ASN:N	1:A:682:PRO:CD	2.79	0.46
1:A:504:PHE:CZ	1:A:507:PHE:CE1	3.04	0.46
1:A:644:VAL:HG13	1:A:716:ILE:HA	1.98	0.46
1:B:302:LEU:HD23	1:B:428:PRO:HD3	1.98	0.46
1:A:357:GLY:C	1:A:358:TYR:CD1	2.95	0.45
1:B:652:VAL:HG11	1:B:716:ILE:HD13	1.98	0.45
1:A:206:LYS:O	1:A:210:GLN:HB2	2.17	0.45
1:B:313:THR:HB	1:B:329:TYR:CE1	2.51	0.45
1:A:242:ARG:CD	1:A:728:GLN:NE2	2.78	0.45
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.38	0.45
1:B:654:PRO:HG3	1:B:678:ASN:O	2.16	0.45
1:B:188:CYS:SG	1:B:204:PHE:HA	2.56	0.45
1:B:516:ALA:CB	1:B:518:TYR:CE1	2.99	0.45
1:A:533:GLN:OE1	1:A:533:GLN:HA	2.17	0.45
1:B:378:PHE:HA	1:B:381:SER:O	2.17	0.45
1:A:728:GLN:NE2	1:A:754:ILE:H	2.15	0.44
1:B:162:PHE:N	5:B:1134:HOH:O	2.49	0.44
1:B:191:SER:HB2	1:B:193:THR:CG2	2.43	0.44
1:A:438:LYS:HA	1:A:499:CYS:HB2	1.98	0.44
1:B:175:GLN:HB3	5:B:789:HOH:O	2.16	0.44
4:B:1:I3P:O11	4:B:1:I3P:O2	2.36	0.44
1:A:613:THR:CG2	1:A:614:THR:N	2.80	0.44
1:B:184:ILE:CG2	1:B:204:PHE:CD1	2.99	0.44
1:A:398:GLN:O	1:A:492:LEU:HD23	2.18	0.44
1:A:548:SER:H	1:A:573:GLN:NE2	2.15	0.44
1:B:196:LEU:HD23	1:B:196:LEU:HA	1.63	0.44
1:B:558:ASP:O	1:B:559:SER:HB2	2.17	0.44
1:B:358:TYR:N	1:B:358:TYR:HD1	2.16	0.44
1:A:368:ASP:OD1	1:A:371:ARG:NH1	2.51	0.44
1:B:502:VAL:HG13	1:B:503:HIS:N	2.32	0.44
1:A:652:VAL:HG11	1:A:716:ILE:HD13	1.99	0.43
1:B:238:GLN:O	1:B:242:ARG:HA	2.17	0.43
1:B:520:MET:HE2	1:B:549:ARG:CB	2.45	0.43
1:A:298:MET:HB2	1:A:429:GLU:HG2	2.00	0.43
1:B:178:ASP:O	1:B:180:TYR:HB3	2.18	0.43
1:B:165:LEU:HG	1:B:185:PHE:CD1	2.52	0.43
1:A:338:ARG:HG3	1:A:601:TYR:CE1	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:LYS:O	1:B:167:ASP:HB2	2.19	0.43
1:B:533:GLN:OE1	1:B:533:GLN:HA	2.19	0.43
1:B:388:SER:HA	1:B:438:LYS:HB3	2.01	0.43
1:A:409:LEU:HD12	1:A:409:LEU:HA	1.80	0.43
1:A:730:TYR:C	1:A:731:ARG:HG2	2.44	0.43
1:B:530:ARG:HH11	1:B:530:ARG:CG	2.32	0.43
1:B:681:ASN:N	1:B:682:PRO:CD	2.80	0.43
1:B:547:LEU:HD23	1:B:573:GLN:CG	2.44	0.43
1:A:272:LYS:O	1:A:275:PHE:HB3	2.18	0.43
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.85	0.43
1:A:595:ASP:OD1	1:A:596:ASN:N	2.47	0.43
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.54	0.43
1:A:504:PHE:CZ	1:A:506:GLY:CA	2.98	0.42
1:A:209:THR:O	1:A:209:THR:HG22	2.19	0.42
1:B:183:LYS:HG2	1:B:184:ILE:HD12	2.02	0.42
1:A:357:GLY:C	1:A:358:TYR:HD1	2.27	0.42
1:A:515:GLN:HB2	1:A:519:GLU:HB2	2.01	0.42
1:A:613:THR:HG21	1:A:615:PHE:HB3	2.01	0.42
1:A:732:HIS:HA	1:A:748:LEU:O	2.18	0.42
1:B:162:PHE:HA	1:B:165:LEU:HB2	2.01	0.42
1:A:652:VAL:HG11	1:A:716:ILE:CD1	2.50	0.42
1:B:445:LEU:HA	1:B:445:LEU:HD23	1.64	0.42
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.79	0.42
1:B:398:GLN:O	1:B:492:LEU:HD23	2.19	0.42
1:A:325:SER:HA	1:A:364:ILE:HG21	2.02	0.42
1:B:396:GLU:OE1	1:B:399:ARG:NH1	2.51	0.42
1:B:164:GLU:HG2	1:B:164:GLU:H	1.39	0.42
1:B:167:ASP:HB3	1:B:168:PHE:H	1.55	0.42
1:B:205:TYR:O	1:B:208:LEU:HB3	2.19	0.42
1:A:654:PRO:HG3	1:A:678:ASN:O	2.19	0.42
1:A:708:ASP:O	1:A:711:SER:O	2.38	0.42
1:A:516:ALA:CB	1:A:518:TYR:CE2	3.02	0.41
1:B:661:HIS:O	1:B:698:ALA:HA	2.20	0.41
1:A:201:ILE:H	1:A:201:ILE:HG13	1.40	0.41
1:A:212:ALA:O	1:A:215:ASP:HB2	2.20	0.41
1:A:558:ASP:O	1:A:559:SER:HB2	2.21	0.41
1:B:231:GLU:CD	1:B:231:GLU:H	2.28	0.41
1:B:729:GLY:O	1:B:751:LYS:HA	2.20	0.41
1:A:402:ALA:HB2	1:A:492:LEU:CD2	2.49	0.41
1:A:406:ARG:HH11	1:A:406:ARG:CG	2.33	0.41
1:A:241:GLN:NE2	1:A:730:TYR:H	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLN:HB3	1:A:301:PRO:CD	2.50	0.41
1:A:655:LYS:HE2	1:A:671:GLN:OE1	2.21	0.41
1:B:406:ARG:CG	1:B:406:ARG:HH11	2.34	0.41
1:B:165:LEU:C	1:B:167:ASP:N	2.78	0.41
1:B:310:SER:OG	1:B:313:THR:OG1	2.38	0.41
1:A:203:THR:HB	1:A:204:PHE:H	1.60	0.41
1:A:371:ARG:O	1:A:374:ARG:HB3	2.20	0.41
1:A:426:PRO:HA	1:A:430:GLN:OE1	2.20	0.41
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.50	0.41
1:B:418:LEU:HD12	1:B:426:PRO:HB3	2.03	0.41
1:B:504:PHE:CZ	1:B:506:GLY:CA	3.00	0.41
1:A:343:ASP:O	1:A:354:ILE:HA	2.21	0.41
1:A:644:VAL:HG12	1:A:714:ASP:HB3	2.03	0.41
1:B:329:TYR:OH	1:B:341:GLU:O	2.39	0.41
1:B:573:GLN:NE2	1:B:573:GLN:N	2.63	0.41
1:A:259:GLU:OE1	1:A:270:MET:HA	2.21	0.40
1:A:594:GLN:HA	1:A:594:GLN:NE2	2.36	0.40
1:A:622:GLN:CB	1:B:445:LEU:CD1	3.00	0.40
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.51	0.40
1:B:715:PHE:CD1	1:B:715:PHE:C	2.99	0.40
1:A:622:GLN:CA	1:B:445:LEU:CD1	2.99	0.40
1:A:689:GLU:HB3	1:B:491:GLU:HG3	2.03	0.40
1:B:293:ARG:NH1	1:B:293:ARG:HG3	2.36	0.40
1:B:732:HIS:HA	1:B:748:LEU:O	2.21	0.40
1:A:644:VAL:HG13	1:A:715:PHE:O	2.22	0.40
1:B:733:VAL:HB	1:B:748:LEU:HB2	2.01	0.40
1:A:721:ILE:HA	1:A:722:PRO:HD3	1.95	0.40
1:B:188:CYS:O	1:B:200:GLU:HB3	2.21	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	509/624 (82%)	469 (92%)	33 (6%)	7 (1%)	9	9
1	B	557/624 (89%)	514 (92%)	31 (6%)	12 (2%)	5	4
All	All	1066/1248 (85%)	983 (92%)	64 (6%)	19 (2%)	6	6

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	A	644	VAL
1	B	179	GLY
1	B	198	ASP
1	B	509	SER
1	B	515	GLN
1	B	644	VAL
1	B	162	PHE
1	B	650	SER
1	A	203	THR
1	B	167	ASP
1	A	647	ASN
1	B	175	GLN
1	A	510	PRO
1	B	168	PHE
1	A	421	VAL
1	A	514	GLY
1	B	174	ILE
1	B	510	PRO

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	448/545 (82%)	405 (90%)	43 (10%)	8	10
1	B	492/545 (90%)	433 (88%)	59 (12%)	5	5
All	All	940/1090 (86%)	838 (89%)	102 (11%)	6	7

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	208	LEU
1	A	216	ARG
1	A	238	GLN
1	A	242	ARG
1	A	252	LEU
1	A	350	GLN
1	A	406	ARG
1	A	409	LEU
1	A	419	ASP
1	A	424	SER
1	A	432	LYS
1	A	436	LEU
1	A	440	LYS
1	A	441	LYS
1	A	487	LYS
1	A	492	LEU
1	A	502	VAL
1	A	515	GLN
1	A	526	SER
1	A	530	ARG
1	A	533	GLN
1	A	535	SER
1	A	545	SER
1	A	563	SER
1	A	573	GLN
1	A	612	ASN
1	A	617	SER
1	A	630	ARG
1	A	644	VAL
1	A	645	ASN
1	A	652	VAL
1	A	655	LYS
1	A	657	ILE
1	A	665	ARG
1	A	675	ILE
1	A	676	THR
1	A	686	MET
1	A	691	GLU
1	A	710	SER
1	A	712	LYS
1	A	738	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	745	SER
1	B	159	LYS
1	B	160	MET
1	B	164	GLU
1	B	165	LEU
1	B	166	LYS
1	B	169	LEU
1	B	170	LYS
1	B	171	GLU
1	B	172	LEU
1	B	173	ASN
1	B	174	ILE
1	B	175	GLN
1	B	177	ASP
1	B	182	ARG
1	B	183	LYS
1	B	199	GLU
1	B	200	GLU
1	B	201	ILE
1	B	202	GLU
1	B	208	LEU
1	B	210	GLN
1	B	232	ARG
1	B	242	ARG
1	B	252	LEU
1	B	263	THR
1	B	309	SER
1	B	331	ARG
1	B	358	TYR
1	B	406	ARG
1	B	409	LEU
1	B	423	THR
1	B	432	LYS
1	B	484	ASP
1	B	486	LEU
1	B	488	LEU
1	B	492	LEU
1	B	502	VAL
1	B	508	SER
1	B	515	GLN
1	B	526	SER
1	B	535	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	545	SER
1	B	563	SER
1	B	573	GLN
1	B	613	THR
1	B	617	SER
1	B	643	LYS
1	B	644	VAL
1	B	646	LYS
1	B	655	LYS
1	B	657	ILE
1	B	665	ARG
1	B	675	ILE
1	B	676	THR
1	B	685	ASP
1	B	691	GLU
1	B	709	SER
1	B	710	SER
1	B	738	LYS

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

Mol	Chain	Res	Type
1	A	238	GLN
1	A	241	GLN
1	A	291	HIS
1	A	515	GLN
1	A	542	HIS
1	A	573	GLN
1	A	594	GLN
1	A	645	ASN
1	A	661	HIS
1	A	677	ASN
1	A	718	GLN
1	A	728	GLN
1	B	241	GLN
1	B	291	HIS
1	B	304	HIS
1	B	349	ASN
1	B	515	GLN
1	B	542	HIS
1	B	573	GLN
1	B	594	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	639	GLN
1	B	718	GLN
1	B	755	GLN

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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ACT	B	5	-	3,3,3	0.87	0	3,3,3	0.70	0
3	ACT	A	5	-	3,3,3	0.89	0	3,3,3	0.76	0
4	I3P	B	1	2	24,24,24	0.93	1 (4%)	39,39,39	1.20	3 (7%)
4	I3P	A	1	2	24,24,24	0.78	1 (4%)	39,39,39	1.17	3 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	I3P	A	1	2	-	4/15/39/39	0/1/1/1
4	I3P	B	1	2	-	2/15/39/39	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	I3P	P1-O1	-2.24	1.55	1.59
4	A	1	I3P	P1-O1	-2.01	1.56	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	I3P	O1-C1-C6	-3.26	101.83	108.73
4	B	1	I3P	O1-C1-C6	-3.12	102.13	108.73
4	A	1	I3P	O5-C5-C6	-2.88	102.63	108.73
4	B	1	I3P	O12-P1-O1	2.30	114.81	105.85
4	A	1	I3P	O12-P1-O1	2.27	114.69	105.85
4	B	1	I3P	O6-C6-C1	-2.17	104.38	109.94

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1	I3P	C2-C1-O1-P1
4	B	1	I3P	C2-C1-O1-P1
4	A	1	I3P	C6-C1-O1-P1
4	A	1	I3P	C4-O4-P4-O41
4	B	1	I3P	C6-C1-O1-P1
4	A	1	I3P	C4-O4-P4-O43

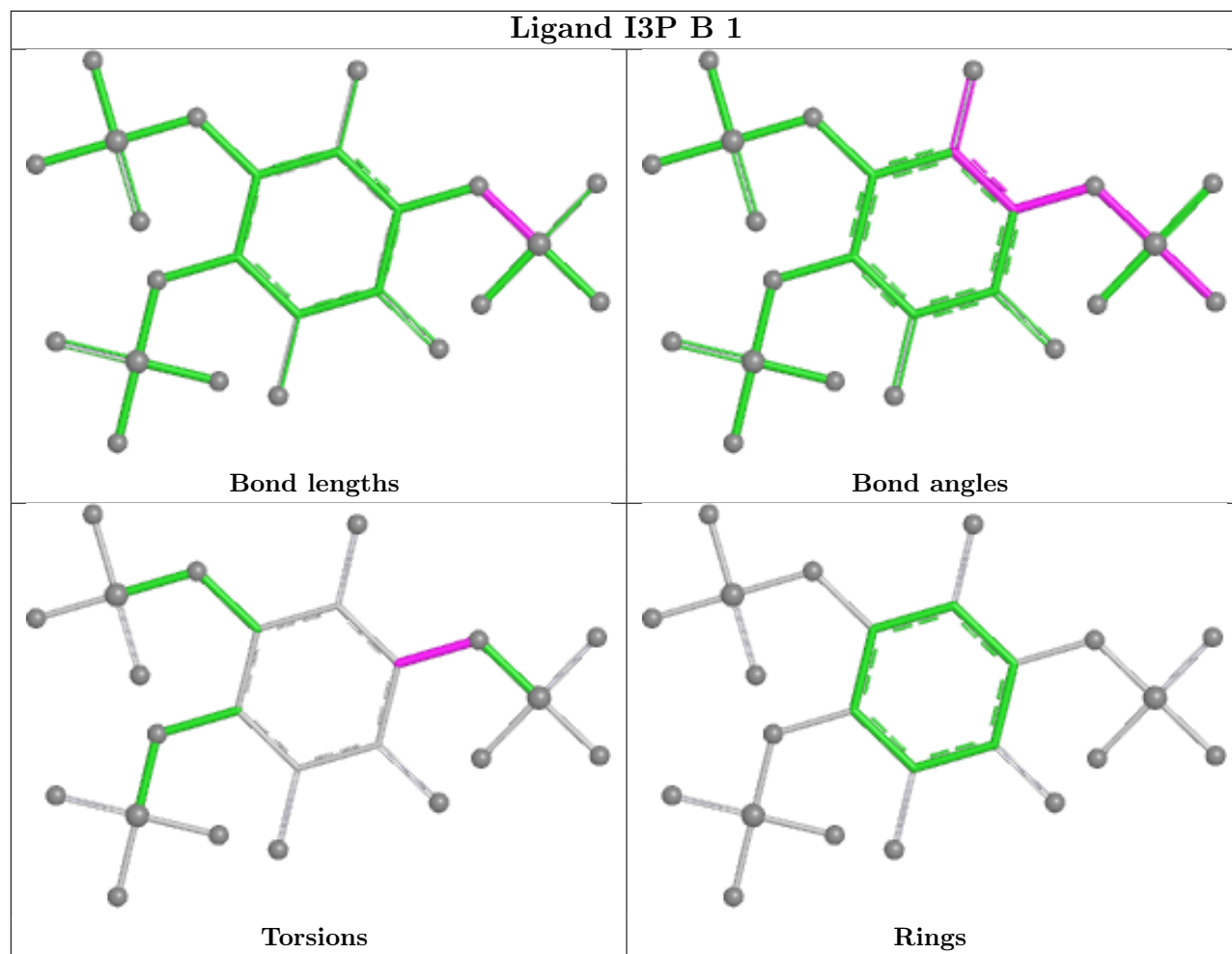
There are no ring outliers.

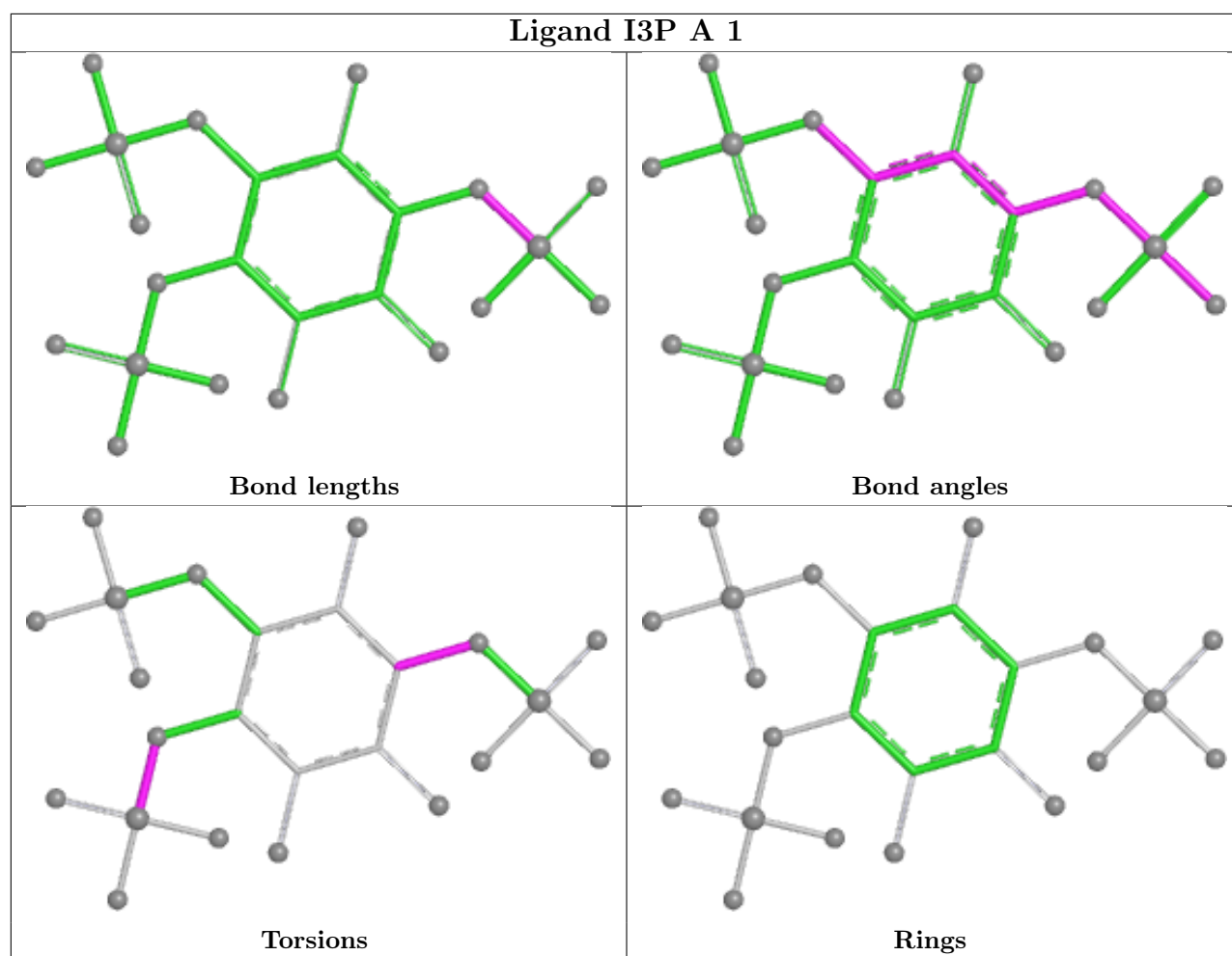
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	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	507/624 (81%)	-0.09	24 (4%)	36 38	16, 34, 82, 122	13 (2%)
1	B	556/624 (89%)	0.05	41 (7%)	20 22	16, 35, 86, 118	21 (3%)
All	All	1063/1248 (85%)	-0.02	65 (6%)	27 29	16, 35, 84, 122	34 (3%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	170	LYS	7.5
1	A	203	THR	6.6
1	A	201	ILE	6.4
1	A	644	VAL	6.2
1	B	176	VAL	5.8
1	A	206	LYS	5.5
1	A	200	GLU	5.3
1	B	177	ASP	5.2
1	B	645	ASN	5.1
1	A	202	GLU	4.7
1	B	514	GLY	4.3
1	B	173	ASN	4.2
1	B	171	GLU	4.2
1	B	649	ASN	4.1
1	B	178	ASP	4.1
1	B	165	LEU	4.1
1	B	162	PHE	4.0
1	B	167	ASP	3.8
1	B	161	ASN	3.8
1	B	484	ASP	3.7
1	A	205	TYR	3.7
1	B	179	GLY	3.6
1	A	421	VAL	3.6
1	A	207	MET	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	159	LYS	3.5
1	B	486	LEU	3.4
1	B	245	GLU	3.4
1	B	246	ALA	3.2
1	A	208	LEU	3.2
1	B	508	SER	3.1
1	B	266	ALA	3.1
1	B	485	LYS	3.1
1	A	645	ASN	3.0
1	A	204	PHE	2.9
1	A	515	GLN	2.9
1	B	644	VAL	2.9
1	A	647	ASN	2.8
1	B	711	SER	2.8
1	B	515	GLN	2.8
1	B	247	GLY	2.7
1	B	647	ASN	2.6
1	B	168	PHE	2.6
1	B	164	GLU	2.5
1	B	267	GLN	2.5
1	A	505	GLY	2.4
1	A	249	ALA	2.4
1	A	530	ARG	2.3
1	B	169	LEU	2.3
1	B	198	ASP	2.3
1	A	266	ALA	2.3
1	B	756	ASP	2.3
1	A	743	HIS	2.2
1	B	210	GLN	2.2
1	A	349	ASN	2.2
1	B	530	ARG	2.2
1	A	648	LYS	2.2
1	A	711	SER	2.2
1	B	506	GLY	2.2
1	B	197	GLU	2.1
1	B	199	GLU	2.1
1	A	209	THR	2.1
1	B	650	SER	2.0
1	A	756	ASP	2.0
1	B	160	MET	2.0
1	B	261	SER	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](#)

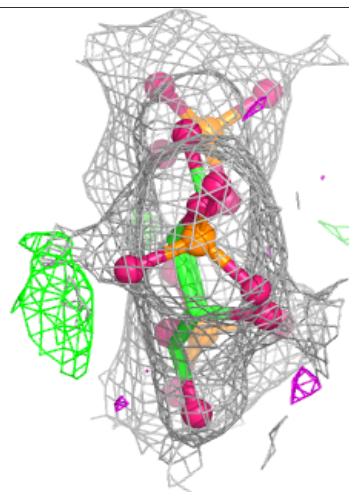
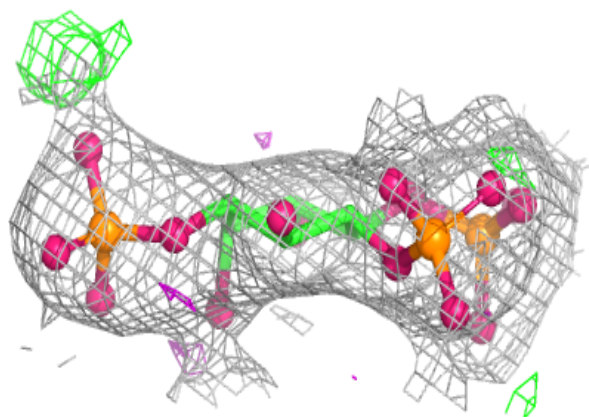
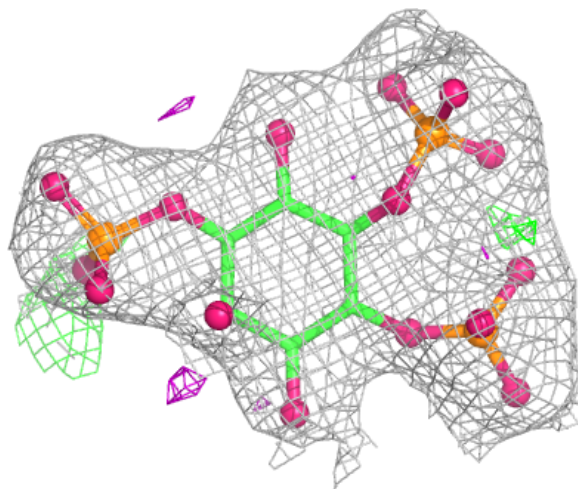
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

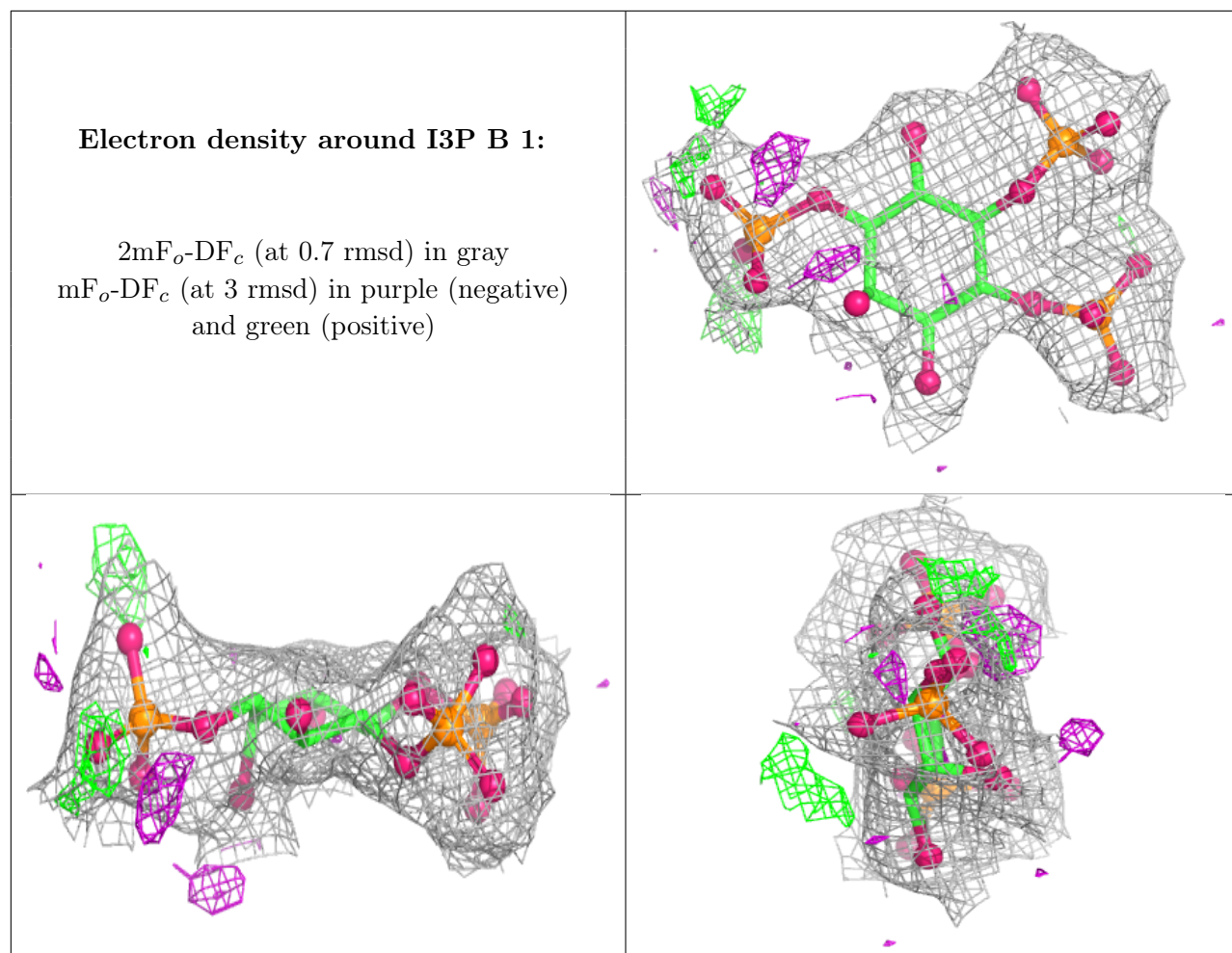
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	3	1/1	0.91	0.05	79,79,79,79	0
2	CA	A	2	1/1	0.94	0.06	46,46,46,46	0
4	I3P	A	1	24/24	0.95	0.09	33,55,133,150	0
2	CA	B	3	1/1	0.97	0.04	71,71,71,71	0
3	ACT	A	5	4/4	0.97	0.06	31,35,35,39	0
3	ACT	B	5	4/4	0.97	0.06	32,32,33,34	0
2	CA	B	2	1/1	0.97	0.04	43,43,43,43	0
4	I3P	B	1	24/24	0.97	0.06	23,42,60,73	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 A 1:

$2mF_o-DF_c$ (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.