



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 05:30 am BST

PDB ID : 1DJZ
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM
RAT COMPLEXED WITH INOSITOL-4,5-BISPHOSPHATE
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on : 1996-08-24
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

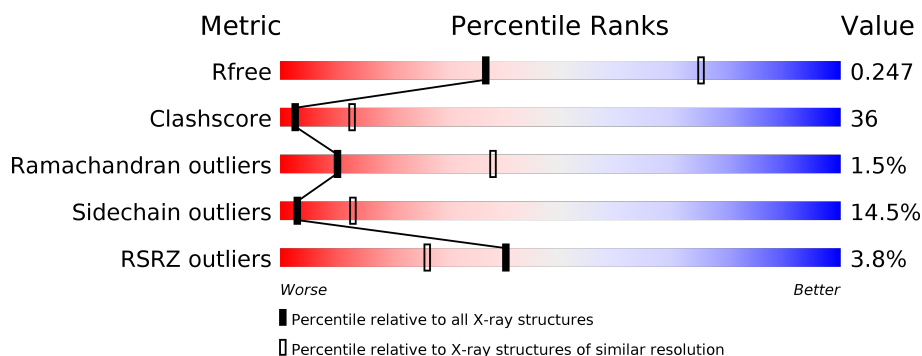
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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

Mol	Chain	Length	Quality of chain
1	A	624	<div> <div>3%</div> <div> <div></div> <div>39%</div> <div>36%</div> <div>7%</div> <div>18%</div> </div> </div>
1	B	624	<div> <div>3%</div> <div> <div></div> <div>40%</div> <div>43%</div> <div>6%</div> <div>10%</div> </div> </div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8840 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	82	0	0
			4057	2565	709	761	22			
1	B	561	Total	C	N	O	S	109	0	0
			4465	2818	776	847	24			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

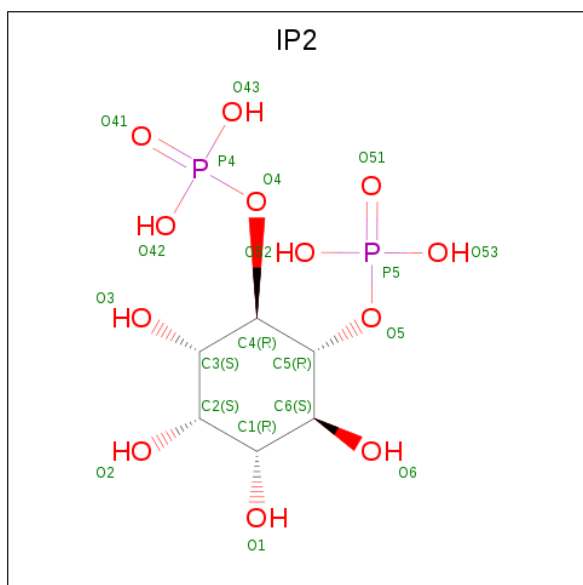
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ACETATE ION (three-letter code: 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-4,5-BISPHOSPHATE (three-letter code: IP2) (formula: $C_6H_{14}O_{12}P_2$).



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

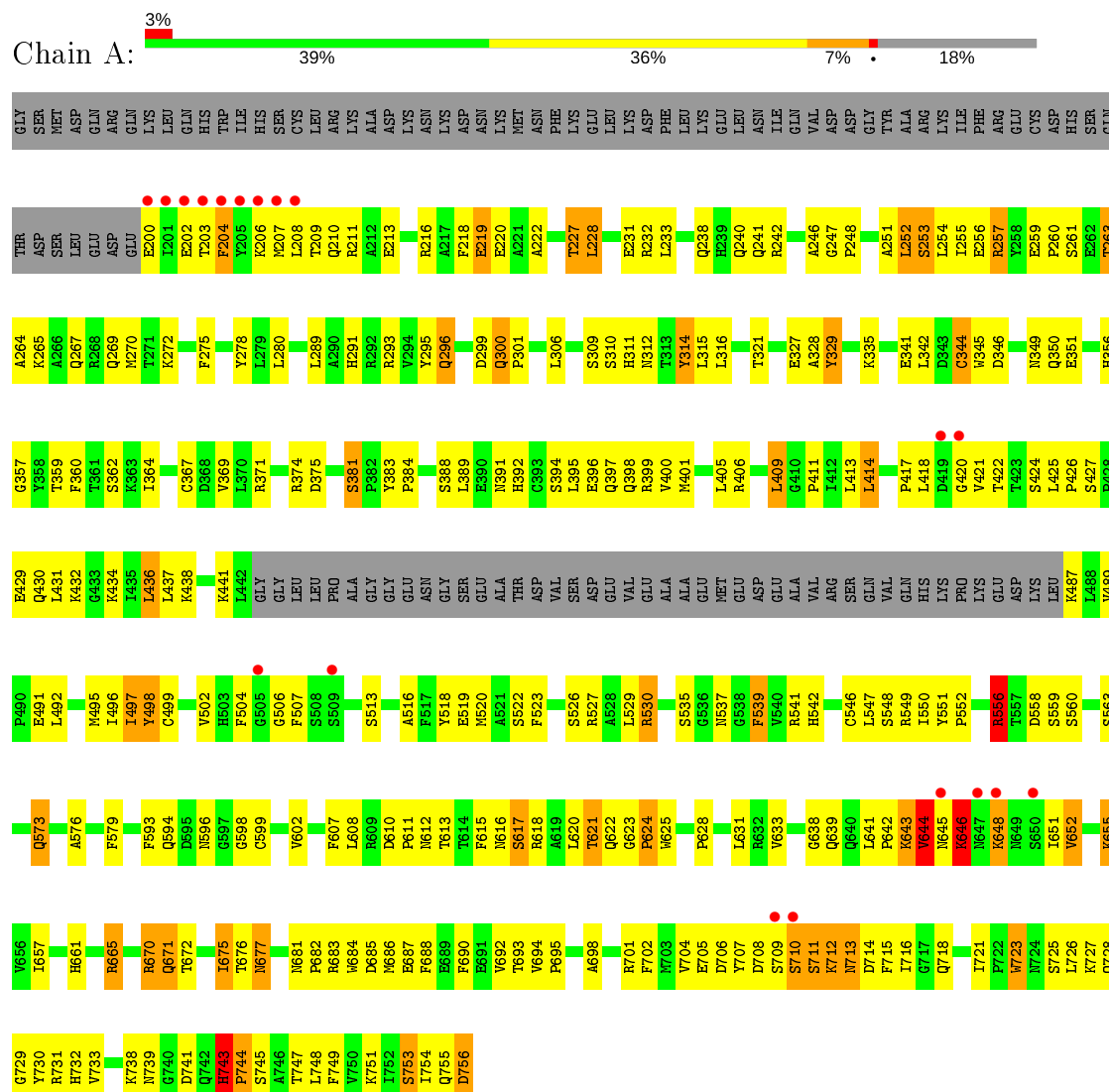
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	B	141	Total	O	0	0
			141	141		

3 Residue-property plots

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

• Molecule 1: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1



• Molecule 1: PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1





4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	396.49 Å 396.49 Å 396.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.95 24.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.95) 94.2 (24.64-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.89 Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.212 , 0.270 0.195 , 0.247	Depositor DCC
R_{free} test set	2048 reflections (3.68%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 100.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8840	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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: IP2, 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	1.08	17/4152 (0.4%)	1.01	6/5624 (0.1%)
1	B	1.07	14/4565 (0.3%)	1.01	6/6174 (0.1%)
All	All	1.07	31/8717 (0.4%)	1.01	12/11798 (0.1%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	TYR	CE2-CZ	-11.14	1.24	1.38
1	A	329	TYR	CE2-CZ	-9.95	1.25	1.38
1	A	329	TYR	CG-CD1	-9.44	1.26	1.39
1	A	329	TYR	CE1-CZ	-8.93	1.26	1.38
1	B	498	TYR	CE1-CZ	-8.74	1.27	1.38
1	A	329	TYR	CG-CD2	-8.60	1.27	1.39
1	A	314	TYR	CE1-CZ	-8.53	1.27	1.38
1	B	314	TYR	CG-CD2	-8.45	1.28	1.39
1	A	314	TYR	CE2-CZ	-8.10	1.28	1.38
1	B	329	TYR	CE2-CZ	-8.09	1.28	1.38
1	B	314	TYR	CE1-CZ	-7.96	1.28	1.38
1	B	329	TYR	CG-CD1	-7.13	1.29	1.39
1	B	498	TYR	CG-CD2	-6.88	1.30	1.39
1	A	314	TYR	CG-CD2	-6.68	1.30	1.39
1	B	314	TYR	CG-CD1	-6.41	1.30	1.39
1	B	702	PHE	CE1-CZ	-6.32	1.25	1.37
1	B	498	TYR	CE2-CZ	-6.26	1.30	1.38
1	B	498	TYR	CG-CD1	-6.01	1.31	1.39
1	B	329	TYR	CE1-CZ	-5.97	1.30	1.38
1	A	702	PHE	CE2-CZ	-5.92	1.26	1.37
1	A	314	TYR	CG-CD1	-5.87	1.31	1.39
1	A	498	TYR	CE2-CZ	-5.82	1.30	1.38
1	A	702	PHE	CG-CD1	-5.81	1.30	1.38
1	A	498	TYR	CE1-CZ	-5.67	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	692	VAL	CA-CB	-5.58	1.43	1.54
1	B	329	TYR	CG-CD2	-5.54	1.31	1.39
1	A	702	PHE	CE1-CZ	-5.33	1.27	1.37
1	A	602	VAL	CB-CG1	-5.28	1.41	1.52
1	A	723	TRP	CB-CG	-5.22	1.40	1.50
1	A	498	TYR	CG-CD1	-5.08	1.32	1.39
1	A	702	PHE	CG-CD2	-5.05	1.31	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	743	HIS	C-N-CD	-14.12	89.52	120.60
1	A	743	HIS	C-N-CD	-14.12	89.54	120.60
1	B	247	GLY	C-N-CD	-7.20	104.77	120.60
1	A	247	GLY	C-N-CD	-6.97	105.26	120.60
1	A	644	VAL	CB-CA-C	5.94	122.68	111.40
1	A	556	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	645	ASN	N-CA-C	5.74	126.49	111.00
1	B	436	LEU	CB-CG-CD2	-5.53	101.61	111.00
1	A	670	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	B	654	PRO	N-CA-C	5.12	125.41	112.10
1	A	675	ILE	N-CA-C	-5.05	97.35	111.00
1	B	675	ILE	N-CA-C	-5.03	97.42	111.00

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	4057	0	3972	290	0
1	B	4465	0	4375	313	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	9	3	0
4	B	20	0	9	4	0
5	A	125	0	0	4	0
5	B	141	0	0	19	0
All	All	8840	0	8371	595	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 36.

All (595) 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:B:196:LEU:HD22	1:B:200:GLU:HB3	1.28	1.14
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.23	1.01
1:B:728:GLN:NE2	1:B:754:ILE:H	1.59	1.00
1:A:548:SER:H	1:A:573:GLN:NE2	1.61	0.96
1:A:613:THR:HG22	1:A:615:PHE:H	1.28	0.95
1:B:401:MET:HE2	1:B:492:LEU:HD11	1.45	0.95
1:A:241:GLN:HE22	1:A:730:TYR:H	1.06	0.94
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.02	0.93
1:A:401:MET:HE2	1:A:492:LEU:HD11	1.48	0.92
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.55	0.89
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.55	0.89
1:B:548:SER:H	1:B:573:GLN:NE2	1.69	0.89
1:B:642:PRO:HG3	1:B:743:HIS:CD2	2.08	0.88
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.37	0.88
1:B:728:GLN:HE22	1:B:754:ILE:H	1.21	0.88
1:A:728:GLN:HE22	1:A:754:ILE:H	1.16	0.88
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.56	0.87
1:A:516:ALA:HB3	1:A:519:GLU:HG3	1.57	0.87
1:B:196:LEU:CD2	1:B:200:GLU:HB3	2.05	0.86
1:A:556:ARG:HH11	1:A:556:ARG:HG2	1.38	0.86
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.55	0.86
1:B:168:PHE:CE1	1:B:172:LEU:HD21	2.09	0.86
1:A:728:GLN:NE2	1:A:754:ILE:H	1.72	0.86
1:A:316:LEU:HD23	1:A:328:ALA:HB2	1.59	0.85
1:B:607:PHE:HE2	5:B:821:HOH:O	1.59	0.84
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.24	0.82
1:B:692:VAL:HG12	1:B:695:PRO:HD3	1.61	0.82
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.15	0.81
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:PRO:HG3	1:B:743:HIS:HD2	1.44	0.80
1:A:651:ILE:HD13	1:A:677:ASN:HD21	1.46	0.80
1:A:692:VAL:HG12	1:A:695:PRO:HD3	1.61	0.80
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.63	0.80
1:B:632:ARG:HH21	1:B:755:GLN:NE2	1.80	0.80
1:B:701:ARG:HE	1:B:718:GLN:NE2	1.79	0.79
1:B:530:ARG:HH11	1:B:530:ARG:HG3	1.45	0.79
1:A:573:GLN:H	1:A:573:GLN:NE2	1.82	0.78
1:A:420:GLY:O	1:A:422:THR:HG23	1.84	0.77
1:B:549:ARG:C	1:B:550:ILE:HD13	2.05	0.77
1:B:728:GLN:HE21	1:B:753:SER:HA	1.49	0.77
1:A:238:GLN:HG2	1:A:246:ALA:CB	2.16	0.76
1:B:196:LEU:HB3	1:B:201:ILE:CD1	2.15	0.76
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.68	0.76
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.21	0.75
1:B:234:VAL:O	1:B:238:GLN:HG3	1.86	0.75
1:B:221:ALA:HB1	1:B:228:LEU:HD21	1.68	0.74
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.99	0.74
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.15	0.74
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.03	0.74
1:B:174:ILE:HG22	1:B:176:VAL:HG23	1.68	0.74
1:B:436:LEU:N	1:B:436:LEU:HD23	2.01	0.73
1:B:241:GLN:HE22	1:B:730:TYR:H	1.35	0.73
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.18	0.73
1:B:573:GLN:H	1:B:573:GLN:NE2	1.87	0.73
1:A:438:LYS:HG3	1:A:499:CYS:HB3	1.70	0.73
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.69	0.72
1:B:316:LEU:HD23	1:B:328:ALA:HB2	1.71	0.72
1:B:203:THR:O	1:B:207:MET:HG3	1.89	0.72
1:A:394:SER:O	1:A:398:GLN:HG3	1.88	0.72
1:A:436:LEU:N	1:A:436:LEU:HD23	2.05	0.72
1:B:168:PHE:HE1	1:B:172:LEU:HD21	1.54	0.72
1:A:395:LEU:HD22	1:A:489:VAL:HG12	1.72	0.72
1:A:346:ASP:OD2	1:A:394:SER:HB3	1.90	0.71
1:B:259:GLU:OE2	1:B:260:PRO:HD2	1.90	0.71
1:A:520:MET:CE	1:A:549:ARG:HB2	2.21	0.71
1:A:350:GLN:OE1	1:A:396:GLU:HG3	1.90	0.71
1:B:551:TYR:HB2	1:B:552:PRO:HD2	1.73	0.71
1:A:311:HIS:NE2	4:A:1:IP2:H2	2.04	0.70
1:A:312:ASN:HB3	1:A:315:LEU:HD12	1.73	0.70
1:B:188:CYS:O	1:B:200:GLU:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:O	1:A:207:MET:HB2	1.92	0.70
1:B:728:GLN:NE2	1:B:754:ILE:N	2.38	0.70
1:A:417:PRO:HD3	1:A:497:ILE:HG13	1.73	0.70
1:B:730:TYR:CE1	1:B:751:LYS:HD3	2.27	0.70
1:B:504:PHE:HB3	1:B:527:ARG:NH2	2.07	0.70
1:B:701:ARG:NH2	1:B:718:GLN:HG3	2.05	0.70
1:B:184:ILE:HG22	1:B:204:PHE:CD1	2.27	0.69
1:A:651:ILE:HD13	1:A:677:ASN:ND2	2.07	0.69
1:B:520:MET:CE	1:B:549:ARG:HB2	2.22	0.69
1:B:425:LEU:HD12	5:B:767:HOH:O	1.91	0.69
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.28	0.69
1:A:675:ILE:HD13	1:A:684:TRP:NE1	2.07	0.69
1:B:174:ILE:CG2	1:B:176:VAL:HG23	2.22	0.69
1:A:551:TYR:HB2	1:A:552:PRO:HD2	1.75	0.69
1:A:548:SER:H	1:A:573:GLN:HE22	1.40	0.69
1:A:241:GLN:HE22	1:A:730:TYR:N	1.87	0.68
1:A:651:ILE:HD12	1:A:651:ILE:N	2.08	0.68
1:B:548:SER:H	1:B:573:GLN:HE22	1.40	0.68
1:B:701:ARG:NE	1:B:718:GLN:HE21	1.90	0.68
1:A:730:TYR:CE1	1:A:751:LYS:HD3	2.28	0.68
1:A:495:MET:O	1:A:497:ILE:HD13	1.93	0.68
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.23	0.68
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.76	0.68
1:B:346:ASP:OD2	1:B:394:SER:HB3	1.94	0.68
1:B:364:ILE:HD12	1:B:369:VAL:HG23	1.73	0.67
1:B:550:ILE:HD13	1:B:550:ILE:N	2.10	0.67
1:A:401:MET:CE	1:A:492:LEU:HD11	2.24	0.67
1:A:395:LEU:HD22	1:A:489:VAL:CG1	2.25	0.67
1:A:670:ARG:HD3	5:A:836:HOH:O	1.93	0.67
1:B:651:ILE:CG2	1:B:677:ASN:HA	2.25	0.66
1:A:356:HIS:ND1	1:A:359:THR:HG21	2.10	0.66
1:B:201:ILE:HD13	1:B:201:ILE:N	2.11	0.66
1:B:377:ALA:N	5:B:887:HOH:O	2.28	0.66
1:A:200:GLU:O	1:A:204:PHE:N	2.29	0.66
1:A:707:TYR:HA	1:A:713:ASN:OD1	1.96	0.66
1:B:342:LEU:HD12	1:B:342:LEU:N	2.12	0.65
1:A:426:PRO:HD3	1:A:498:TYR:CD2	2.31	0.65
1:A:204:PHE:O	1:A:208:LEU:N	2.30	0.65
1:A:549:ARG:NH1	4:A:1:IP2:O42	2.29	0.65
1:A:556:ARG:HG2	1:A:560:SER:OG	1.96	0.65
1:B:651:ILE:HG22	1:B:677:ASN:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:O	1:A:275:PHE:HB3	1.96	0.65
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.26	0.65
1:A:549:ARG:NH2	4:A:1:IP2:O3	2.29	0.65
1:B:728:GLN:NE2	1:B:753:SER:HA	2.11	0.65
1:A:617:SER:HA	1:A:620:LEU:HD21	1.79	0.64
1:A:238:GLN:HG2	1:A:246:ALA:HB1	1.78	0.64
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.80	0.64
1:A:497:ILE:HG22	1:A:498:TYR:CD1	2.32	0.64
1:B:549:ARG:HH22	4:B:1:IP2:C3	2.11	0.64
1:B:657:ILE:HD13	1:B:671:GLN:CB	2.28	0.64
1:B:189:ASP:HB3	5:B:845:HOH:O	1.96	0.64
1:B:491:GLU:OE1	1:B:491:GLU:N	2.29	0.63
1:B:516:ALA:HB3	1:B:519:GLU:HG3	1.79	0.63
1:A:335:LYS:HE2	5:A:841:HOH:O	1.98	0.63
1:B:696:ASP:HB2	5:B:821:HOH:O	1.97	0.63
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.33	0.63
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.34	0.63
1:B:645:ASN:ND2	1:B:647:ASN:O	2.31	0.63
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.34	0.63
1:A:316:LEU:CD2	1:A:328:ALA:HB2	2.29	0.62
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.28	0.62
1:B:721:ILE:HG21	1:B:726:LEU:HD13	1.80	0.62
1:B:379:LYS:HE2	5:B:833:HOH:O	1.99	0.62
1:A:384:PRO:HG3	1:A:431:LEU:CB	2.30	0.62
1:A:216:ARG:NH2	1:A:683:ARG:HH22	1.96	0.62
1:A:218:PHE:CE1	1:A:272:LYS:HA	2.35	0.62
1:B:701:ARG:HH21	1:B:718:GLN:HG3	1.64	0.62
1:B:353:ILE:HD12	1:B:363:LYS:HG2	1.81	0.62
1:A:701:ARG:NH2	1:A:718:GLN:HG3	2.15	0.62
1:A:222:ALA:HB2	1:A:228:LEU:HD23	1.82	0.62
1:B:509:SER:N	1:B:510:PRO:HD2	2.15	0.61
1:B:259:GLU:CD	1:B:260:PRO:HD2	2.20	0.61
1:A:701:ARG:HH21	1:A:718:GLN:HG3	1.65	0.61
1:A:207:MET:CE	1:A:210:GLN:HB3	2.30	0.61
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.30	0.61
1:B:267:GLN:O	1:B:269:GLN:HG3	2.01	0.61
1:A:728:GLN:NE2	1:A:754:ILE:N	2.47	0.61
1:B:196:LEU:HB3	1:B:201:ILE:HD11	1.80	0.61
1:A:672:THR:HG22	1:A:688:PHE:CZ	2.37	0.60
1:B:515:GLN:HE21	1:B:542:HIS:HE1	1.49	0.60
1:A:675:ILE:HD13	1:A:684:TRP:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.32	0.60
1:A:520:MET:HE3	1:A:549:ARG:CB	2.31	0.60
1:A:672:THR:HG22	1:A:688:PHE:HZ	1.66	0.60
1:A:711:SER:OG	1:A:712:LYS:N	2.33	0.60
1:B:376:TYR:N	5:B:887:HOH:O	2.34	0.60
1:B:657:ILE:HD13	1:B:671:GLN:HB3	1.84	0.59
1:B:327:GLU:OE2	1:B:331:ARG:HB2	2.02	0.59
1:A:364:ILE:HD12	1:A:369:VAL:HG23	1.82	0.59
1:A:259:GLU:OE1	1:A:270:MET:HA	2.02	0.59
1:A:616:ASN:OD1	1:A:618:ARG:HB2	2.02	0.59
1:A:395:LEU:O	1:A:399:ARG:HG3	2.03	0.59
1:A:730:TYR:CZ	1:A:751:LYS:HD3	2.38	0.59
1:B:401:MET:CE	1:B:492:LEU:HD11	2.28	0.59
1:B:515:GLN:NE2	1:B:542:HIS:HE1	2.01	0.59
1:A:573:GLN:H	1:A:573:GLN:HE21	1.51	0.59
1:A:739:ASN:HB2	1:A:741:ASP:OD2	2.02	0.59
1:B:183:LYS:HG2	1:B:184:ILE:HD13	1.84	0.59
1:B:184:ILE:N	1:B:184:ILE:HD13	2.16	0.58
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.33	0.58
1:A:263:THR:HG22	1:A:264:ALA:N	2.18	0.58
1:A:504:PHE:HD2	1:A:527:ARG:NH2	2.01	0.58
1:B:421:VAL:HG11	1:B:426:PRO:HD3	1.84	0.58
1:A:651:ILE:HG22	1:A:652:VAL:N	2.17	0.58
1:A:655:LYS:NZ	1:A:671:GLN:OE1	2.29	0.58
1:A:728:GLN:HE21	1:A:753:SER:HA	1.68	0.58
1:A:686:MET:HG3	1:A:687:GLU:N	2.17	0.58
1:A:623:GLY:HA3	1:A:625:TRP:CZ2	2.38	0.58
1:A:502:VAL:HG21	1:A:519:GLU:HB3	1.86	0.58
1:A:723:TRP:N	5:A:823:HOH:O	2.37	0.58
1:B:341:GLU:C	1:B:342:LEU:HD12	2.24	0.58
1:B:520:MET:HG3	1:B:547:LEU:O	2.04	0.58
1:B:300:GLN:O	1:B:427:SER:HA	2.05	0.57
1:A:216:ARG:HH21	1:A:683:ARG:NH2	1.99	0.57
1:A:251:ALA:O	1:A:255:ILE:HG13	2.04	0.57
1:A:617:SER:HB3	5:A:866:HOH:O	2.04	0.57
1:B:705:GLU:C	1:B:716:ILE:HD12	2.25	0.57
1:B:272:LYS:O	1:B:275:PHE:HB3	2.04	0.57
1:B:686:MET:HG3	1:B:687:GLU:N	2.19	0.57
1:A:216:ARG:HG3	1:A:216:ARG:HH11	1.68	0.57
1:A:259:GLU:CD	1:A:260:PRO:HD2	2.25	0.57
1:B:729:GLY:O	1:B:751:LYS:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:ILE:HD13	1:A:671:GLN:HB2	1.87	0.57
1:B:551:TYR:HB2	1:B:552:PRO:CD	2.34	0.57
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.41	0.56
1:A:657:ILE:HD13	1:A:671:GLN:CB	2.34	0.56
1:B:632:ARG:NH2	1:B:755:GLN:NE2	2.53	0.56
1:B:172:LEU:O	1:B:174:ILE:N	2.38	0.56
1:B:549:ARG:O	1:B:550:ILE:HD13	2.04	0.56
1:A:341:GLU:C	1:A:342:LEU:HD12	2.25	0.56
1:B:197:GLU:O	1:B:201:ILE:HG12	2.05	0.56
1:B:218:PHE:CE1	1:B:272:LYS:HA	2.41	0.56
1:B:549:ARG:HG2	1:B:549:ARG:NH1	2.20	0.56
1:A:289:LEU:O	1:A:289:LEU:HD12	2.05	0.56
1:A:327:GLU:HA	1:A:327:GLU:OE1	2.06	0.56
1:A:593:PHE:O	1:A:598:GLY:HA2	2.06	0.56
1:A:622:GLN:CB	1:B:445:LEU:HD13	2.33	0.56
1:A:398:GLN:O	1:A:401:MET:HB2	2.06	0.56
1:A:241:GLN:HB3	1:A:731:ARG:NH2	2.20	0.55
1:B:227:THR:HG21	1:B:269:GLN:CD	2.27	0.55
1:A:299:ASP:O	1:A:427:SER:HB3	2.06	0.55
1:B:730:TYR:CD1	1:B:751:LYS:HD3	2.41	0.55
1:A:253:SER:HB2	1:A:257:ARG:HH21	1.71	0.55
1:B:704:VAL:O	1:B:716:ILE:HB	2.06	0.55
1:A:491:GLU:N	1:A:491:GLU:OE1	2.36	0.55
1:A:259:GLU:OE2	1:A:260:PRO:HD2	2.06	0.55
1:A:549:ARG:NH1	1:A:549:ARG:HG2	2.20	0.55
1:B:241:GLN:N	1:B:241:GLN:HE21	2.05	0.55
1:A:621:THR:C	1:B:445:LEU:HD22	2.27	0.55
1:A:227:THR:HG21	1:A:269:GLN:CD	2.26	0.55
1:B:253:SER:HB2	1:B:257:ARG:HH21	1.72	0.55
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.35	0.54
1:B:327:GLU:OE2	1:B:331:ARG:HD2	2.07	0.54
1:B:384:PRO:HG3	1:B:431:LEU:HB2	1.89	0.54
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.37	0.54
1:A:756:ASP:OD1	1:A:756:ASP:N	2.40	0.54
1:B:393:CYS:N	5:B:871:HOH:O	2.41	0.54
1:B:409:LEU:HD13	1:B:409:LEU:N	2.23	0.54
1:B:184:ILE:HG22	1:B:204:PHE:CE1	2.43	0.54
1:B:213:GLU:HG2	1:B:214:ILE:N	2.22	0.54
1:B:418:LEU:HB2	1:B:421:VAL:HG21	1.90	0.54
1:B:296:GLN:HG3	1:B:596:ASN:ND2	2.23	0.54
1:A:296:GLN:HG3	1:A:596:ASN:CG	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:ASN:C	1:B:647:ASN:H	2.10	0.53
1:A:523:PHE:O	1:A:550:ILE:HA	2.07	0.53
1:A:715:PHE:CE2	1:A:718:GLN:HB2	2.43	0.53
1:B:418:LEU:HB2	1:B:421:VAL:CG2	2.37	0.53
1:B:556:ARG:HG2	1:B:556:ARG:HH11	1.71	0.53
1:A:291:HIS:HD2	1:A:725:SER:OG	1.91	0.53
1:A:280:LEU:HD23	1:A:732:HIS:CE1	2.43	0.53
1:B:657:ILE:HD13	1:B:671:GLN:HB2	1.91	0.53
1:A:607:PHE:CE2	1:A:625:TRP:HB3	2.43	0.53
1:B:556:ARG:HG2	1:B:560:SER:OG	2.08	0.53
1:A:253:SER:HA	1:A:256:GLU:OE1	2.09	0.53
1:A:383:TYR:HB3	1:A:384:PRO:CD	2.38	0.53
1:B:311:HIS:CE1	1:B:312:ASN:HD22	2.26	0.53
1:B:356:HIS:ND1	1:B:359:THR:HG21	2.24	0.53
1:A:643:LYS:O	1:A:645:ASN:N	2.41	0.53
1:B:507:PHE:O	1:B:510:PRO:HG2	2.09	0.52
1:A:651:ILE:HG21	1:A:677:ASN:C	2.30	0.52
1:A:721:ILE:HG21	1:A:726:LEU:HD13	1.90	0.52
1:B:525:GLU:O	1:B:529:LEU:HG	2.08	0.52
1:B:607:PHE:CD2	1:B:625:TRP:HB3	2.45	0.52
1:A:252:LEU:O	1:A:256:GLU:HG3	2.10	0.52
1:A:556:ARG:HG2	1:A:556:ARG:NH1	2.14	0.52
1:B:395:LEU:O	1:B:399:ARG:HG3	2.08	0.52
1:A:549:ARG:C	1:A:550:ILE:HD13	2.29	0.52
1:A:607:PHE:CD2	1:A:625:TRP:HB3	2.44	0.52
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.91	0.52
1:B:683:ARG:NH2	1:B:685:ASP:OD2	2.43	0.52
1:B:436:LEU:H	1:B:436:LEU:HD23	1.75	0.52
1:B:523:PHE:O	1:B:550:ILE:HA	2.10	0.52
1:A:729:GLY:O	1:A:751:LYS:HA	2.10	0.52
1:B:438:LYS:HG3	1:B:499:CYS:HB3	1.92	0.52
1:A:367:CYS:HB2	1:A:371:ARG:NH2	2.25	0.52
1:A:441:LYS:HG3	1:A:496:ILE:HB	1.92	0.52
1:A:359:THR:C	1:A:360:PHE:HD1	2.14	0.51
1:A:730:TYR:C	1:A:731:ARG:HG2	2.30	0.51
1:B:346:ASP:OD1	1:B:393:CYS:HA	2.10	0.51
1:A:296:GLN:HG3	1:A:596:ASN:ND2	2.25	0.51
1:B:440:LYS:HA	5:B:770:HOH:O	2.09	0.51
1:B:607:PHE:CE2	5:B:821:HOH:O	2.47	0.51
1:A:300:GLN:O	1:A:427:SER:HA	2.11	0.51
1:A:360:PHE:CD1	1:A:360:PHE:N	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:PHE:O	1:B:598:GLY:HA2	2.10	0.51
1:B:707:TYR:O	1:B:708:ASP:OD1	2.29	0.51
1:A:227:THR:HG21	1:A:269:GLN:OE1	2.11	0.51
1:B:639:GLN:HB2	1:B:747:THR:OG1	2.10	0.51
1:A:342:LEU:HD12	1:A:342:LEU:N	2.25	0.51
1:A:708:ASP:N	1:A:713:ASN:OD1	2.37	0.51
1:B:234:VAL:HG23	1:B:251:ALA:HB2	1.93	0.51
1:B:632:ARG:NE	5:B:815:HOH:O	2.24	0.51
1:A:504:PHE:CE1	1:A:507:PHE:CE1	2.99	0.51
1:B:180:TYR:CE1	1:B:184:ILE:HG12	2.45	0.51
1:A:397:GLN:O	1:A:400:VAL:HB	2.11	0.50
1:A:706:ASP:HB3	1:A:714:ASP:HB2	1.93	0.50
1:B:169:LEU:O	1:B:172:LEU:O	2.29	0.50
1:B:183:LYS:O	1:B:187:GLU:HG3	2.11	0.50
1:B:350:GLN:HA	1:B:397:GLN:HE21	1.73	0.50
1:B:549:ARG:NH2	4:B:1:IP2:O3	2.44	0.50
1:B:549:ARG:HG2	1:B:549:ARG:HH11	1.76	0.50
1:A:692:VAL:HG12	1:A:695:PRO:CD	2.35	0.50
1:B:240:GLN:HA	1:B:240:GLN:OE1	2.12	0.50
1:A:504:PHE:CZ	1:A:507:PHE:CE1	2.99	0.50
1:A:549:ARG:HG2	1:A:549:ARG:HH11	1.74	0.50
1:A:610:ASP:OD1	1:A:611:PRO:HD2	2.11	0.50
1:B:287:PHE:CE2	1:B:722:PRO:HD2	2.47	0.50
1:B:311:HIS:NE2	1:B:312:ASN:ND2	2.60	0.50
1:B:426:PRO:HB2	1:B:431:LEU:HD12	1.93	0.50
1:B:651:ILE:O	1:B:653:ASP:OD1	2.29	0.50
1:B:259:GLU:OE1	1:B:270:MET:HA	2.12	0.50
1:B:530:ARG:HH11	1:B:530:ARG:CG	2.19	0.50
1:B:622:GLN:HG3	1:B:623:GLY:N	2.27	0.50
1:B:398:GLN:O	1:B:401:MET:HB2	2.12	0.50
1:A:222:ALA:HB2	1:A:228:LEU:CD2	2.41	0.50
1:A:504:PHE:CD2	1:A:527:ARG:NH2	2.79	0.50
1:A:693:THR:C	1:A:695:PRO:HD2	2.31	0.50
1:B:391:ASN:HD21	1:B:398:GLN:CD	2.15	0.49
1:B:655:LYS:NZ	1:B:671:GLN:OE1	2.30	0.49
1:A:228:LEU:CD1	1:A:233:LEU:HA	2.42	0.49
1:A:405:LEU:HD23	1:A:409:LEU:CD2	2.42	0.49
1:A:520:MET:HG3	1:A:547:LEU:O	2.12	0.49
1:A:551:TYR:HB2	1:A:552:PRO:CD	2.40	0.49
1:B:189:ASP:OD1	1:B:191:SER:OG	2.30	0.49
1:A:409:LEU:N	1:A:409:LEU:HD13	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:ILE:CG2	1:A:498:TYR:CE1	2.96	0.49
1:B:263:THR:O	1:B:266:ALA:HB3	2.12	0.49
1:B:736:LEU:HD23	1:B:742:GLN:HA	1.92	0.49
1:A:537:ASN:ND2	1:A:613:THR:O	2.40	0.49
1:B:227:THR:HG21	1:B:269:GLN:OE1	2.12	0.49
1:B:411:PRO:O	1:B:434:LYS:NZ	2.45	0.49
1:B:573:GLN:H	1:B:573:GLN:HE21	1.61	0.49
1:B:702:PHE:CD2	1:B:733:VAL:HG21	2.48	0.49
1:A:426:PRO:HA	1:A:430:GLN:OE1	2.13	0.49
1:A:291:HIS:HA	1:A:295:TYR:CE2	2.48	0.49
1:A:218:PHE:CD1	1:A:272:LYS:HA	2.48	0.48
1:A:241:GLN:NE2	1:A:729:GLY:HA3	2.28	0.48
1:A:728:GLN:NE2	1:A:753:SER:HA	2.26	0.48
1:B:261:SER:O	1:B:265:LYS:HB2	2.13	0.48
1:B:434:LYS:HD2	1:B:434:LYS:HA	1.66	0.48
1:B:500:LYS:HE3	5:B:770:HOH:O	2.12	0.48
1:A:371:ARG:O	1:A:374:ARG:HB3	2.13	0.48
1:B:251:ALA:O	1:B:255:ILE:HG13	2.12	0.48
1:B:259:GLU:OE2	1:B:271:THR:HG23	2.13	0.48
1:A:356:HIS:HB3	1:A:359:THR:OG1	2.14	0.48
1:A:438:LYS:HA	1:A:499:CYS:HB2	1.94	0.48
1:A:704:VAL:O	1:A:716:ILE:HB	2.13	0.48
1:A:755:GLN:HG2	1:A:756:ASP:N	2.22	0.48
1:B:395:LEU:HD22	1:B:489:VAL:CG1	2.43	0.48
1:A:622:GLN:HA	1:B:445:LEU:CD1	2.43	0.48
1:B:509:SER:N	1:B:510:PRO:CD	2.76	0.48
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.48	0.48
1:A:507:PHE:CD1	1:A:542:HIS:ND1	2.81	0.48
1:B:221:ALA:CB	1:B:228:LEU:HD21	2.40	0.48
1:B:533:GLN:OE1	1:B:618:ARG:NH1	2.47	0.48
1:B:504:PHE:HD2	1:B:527:ARG:NH2	2.11	0.48
1:B:701:ARG:CZ	1:B:718:GLN:HG3	2.44	0.48
1:A:360:PHE:HD1	1:A:360:PHE:N	2.12	0.48
1:A:639:GLN:HB2	1:A:747:THR:OG1	2.13	0.48
1:B:418:LEU:HD12	1:B:426:PRO:HB3	1.95	0.48
1:B:395:LEU:HD22	1:B:489:VAL:HG12	1.96	0.48
1:B:284:GLY:O	1:B:731:ARG:HB3	2.14	0.48
1:B:241:GLN:NE2	1:B:241:GLN:CA	2.76	0.48
1:A:252:LEU:HD23	1:A:256:GLU:OE2	2.14	0.48
1:B:549:ARG:NH1	4:B:1:IP2:O43	2.46	0.48
1:A:280:LEU:HD23	1:A:732:HIS:ND1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PHE:O	1:B:171:GLU:HB2	2.14	0.47
1:B:426:PRO:HG2	1:B:431:LEU:CD1	2.37	0.47
1:B:607:PHE:CE2	1:B:625:TRP:HB3	2.49	0.47
1:B:721:ILE:CG2	1:B:726:LEU:HD13	2.44	0.47
1:A:202:GLU:O	1:A:206:LYS:N	2.29	0.47
1:A:522:SER:HA	1:A:549:ARG:O	2.13	0.47
1:B:169:LEU:HA	1:B:172:LEU:HD12	1.95	0.47
1:B:291:HIS:HD2	1:B:725:SER:OG	1.96	0.47
1:B:371:ARG:O	1:B:374:ARG:HB3	2.13	0.47
1:A:622:GLN:CA	1:B:445:LEU:HD13	2.44	0.47
1:A:743:HIS:HA	1:A:744:PRO:HD3	1.53	0.47
1:B:162:PHE:O	1:B:165:LEU:HB3	2.14	0.47
1:B:394:SER:O	1:B:398:GLN:HG3	2.14	0.47
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.73	0.47
1:B:162:PHE:CZ	1:B:182:ARG:HA	2.50	0.47
1:A:705:GLU:C	1:A:716:ILE:HD12	2.35	0.47
1:A:712:LYS:HB3	1:A:713:ASN:H	1.28	0.47
1:B:162:PHE:CZ	1:B:182:ARG:HB2	2.49	0.47
1:B:610:ASP:OD1	1:B:611:PRO:HD2	2.13	0.47
1:B:651:ILE:O	1:B:651:ILE:HG22	2.13	0.47
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.15	0.47
1:A:367:CYS:SG	1:A:371:ARG:NH2	2.88	0.47
1:B:587:ASP:HB3	1:B:718:GLN:NE2	2.30	0.47
1:A:530:ARG:CZ	1:A:530:ARG:HB2	2.30	0.47
1:A:623:GLY:HA3	1:A:625:TRP:CE2	2.50	0.47
1:A:391:ASN:HD21	1:A:398:GLN:CD	2.18	0.47
1:A:670:ARG:HG3	1:A:690:PHE:CZ	2.50	0.47
1:B:610:ASP:O	1:B:612:ASN:N	2.48	0.47
1:A:200:GLU:O	1:A:203:THR:N	2.48	0.46
1:A:438:LYS:CG	1:A:499:CYS:HB3	2.43	0.46
1:A:651:ILE:CD1	1:A:651:ILE:N	2.78	0.46
1:A:227:THR:CG2	1:A:228:LEU:N	2.79	0.46
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.14	0.46
1:B:733:VAL:HB	1:B:748:LEU:HB2	1.97	0.46
1:A:497:ILE:N	1:A:497:ILE:CD1	2.78	0.46
1:B:254:LEU:O	1:B:258:TYR:N	2.44	0.46
1:B:294:VAL:HA	1:B:596:ASN:OD1	2.15	0.46
1:B:311:HIS:CE1	1:B:312:ASN:ND2	2.82	0.46
1:B:623:GLY:HA3	1:B:625:TRP:CZ2	2.50	0.46
1:A:726:LEU:HA	1:A:726:LEU:HD12	1.46	0.46
1:B:509:SER:HB3	1:B:510:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ARG:HH22	4:B:1:IP2:H3	1.81	0.46
1:B:280:LEU:HD23	1:B:732:HIS:ND1	2.31	0.46
1:A:248:PRO:O	1:A:252:LEU:HB2	2.16	0.46
1:A:381:SER:HB2	1:A:599:CYS:HA	1.97	0.46
1:A:497:ILE:CG2	1:A:498:TYR:CD1	2.98	0.46
1:B:227:THR:CG2	1:B:269:GLN:HB3	2.46	0.46
1:B:384:PRO:HG3	1:B:431:LEU:CB	2.46	0.46
1:A:693:THR:OG1	1:A:694:VAL:HG23	2.16	0.46
1:B:277:MET:HA	1:B:277:MET:CE	2.45	0.46
1:B:316:LEU:CD2	1:B:328:ALA:HB2	2.43	0.46
1:B:647:ASN:CG	1:B:648:LYS:H	2.20	0.46
1:A:213:GLU:HG3	1:A:749:PHE:CD2	2.50	0.46
1:A:261:SER:O	1:A:265:LYS:HB2	2.16	0.46
1:A:548:SER:N	1:A:573:GLN:NE2	2.46	0.46
1:B:241:GLN:HA	1:B:241:GLN:NE2	2.31	0.46
1:B:259:GLU:OE1	1:B:271:THR:N	2.43	0.46
1:A:492:LEU:HA	1:A:492:LEU:HD23	1.61	0.46
1:A:646:LYS:HD2	1:A:648:LYS:HE2	1.97	0.46
1:A:675:ILE:CD1	1:A:684:TRP:CD1	2.99	0.46
1:B:276:LEU:O	1:B:276:LEU:HD12	2.15	0.46
1:A:556:ARG:CG	1:A:556:ARG:HH11	2.18	0.46
1:A:694:VAL:N	1:A:695:PRO:HD2	2.30	0.46
1:A:507:PHE:CE1	1:A:542:HIS:ND1	2.79	0.45
1:B:270:MET:SD	1:B:275:PHE:HA	2.56	0.45
1:B:599:CYS:HA	5:B:771:HOH:O	2.16	0.45
1:A:516:ALA:CB	1:A:518:TYR:CZ	2.99	0.45
1:A:537:ASN:OD1	1:A:541:ARG:NE	2.41	0.45
1:A:548:SER:H	1:A:573:GLN:HE21	1.57	0.45
1:B:694:VAL:N	1:B:695:PRO:CD	2.79	0.45
1:A:311:HIS:HB2	1:A:576:ALA:HB1	1.97	0.45
1:A:349:ASN:O	1:A:350:GLN:HB2	2.15	0.45
1:A:539:PHE:O	1:A:542:HIS:HB3	2.16	0.45
1:B:497:ILE:CD1	1:B:497:ILE:N	2.79	0.45
1:B:702:PHE:O	1:B:718:GLN:HA	2.16	0.45
1:A:314:TYR:HB3	1:A:329:TYR:CE1	2.51	0.45
1:B:484:ASP:O	1:B:487:LYS:N	2.46	0.45
1:B:625:TRP:CD1	1:B:626:TRP:N	2.84	0.45
1:B:409:LEU:HD12	1:B:409:LEU:HA	1.52	0.45
1:B:530:ARG:HG3	1:B:530:ARG:NH1	2.23	0.45
1:A:661:HIS:O	1:A:698:ALA:HA	2.17	0.45
1:B:396:GLU:OE1	1:B:396:GLU:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:SER:HA	1:B:438:LYS:HB3	1.99	0.45
1:B:743:HIS:HA	1:B:744:PRO:HD3	1.59	0.45
1:A:291:HIS:HA	1:A:295:TYR:CD2	2.52	0.45
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.17	0.45
1:B:375:ASP:C	5:B:887:HOH:O	2.54	0.45
1:B:516:ALA:CB	1:B:518:TYR:CZ	3.00	0.45
1:A:694:VAL:N	1:A:695:PRO:CD	2.79	0.45
1:B:227:THR:CG2	1:B:228:LEU:N	2.79	0.45
1:B:529:LEU:HD23	1:B:529:LEU:HA	1.74	0.45
1:B:661:HIS:O	1:B:698:ALA:HA	2.16	0.45
1:A:240:GLN:HA	1:A:240:GLN:OE1	2.16	0.45
1:A:314:TYR:CE1	1:A:315:LEU:HG	2.52	0.45
1:B:162:PHE:CZ	1:B:182:ARG:CA	2.99	0.45
1:B:495:MET:O	1:B:497:ILE:HD13	2.16	0.45
1:A:228:LEU:HD11	1:A:233:LEU:HA	1.99	0.44
1:B:305:TYR:CD1	1:B:305:TYR:N	2.84	0.44
1:A:314:TYR:CD1	1:A:315:LEU:HG	2.52	0.44
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.98	0.44
1:A:426:PRO:HG3	1:A:498:TYR:CE2	2.52	0.44
1:B:163:LYS:HA	1:B:166:LYS:HB2	1.99	0.44
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.52	0.44
1:A:228:LEU:CD1	1:A:233:LEU:CA	2.96	0.44
1:A:529:LEU:HA	1:A:529:LEU:HD23	1.65	0.44
1:A:681:ASN:N	1:A:682:PRO:CD	2.80	0.44
1:A:733:VAL:HB	1:A:748:LEU:HB2	2.00	0.44
1:B:561:ASN:OD1	1:B:578:ASN:N	2.30	0.44
1:A:227:THR:HG23	1:A:228:LEU:N	2.32	0.44
1:B:610:ASP:HA	1:B:611:PRO:HD3	1.54	0.44
1:A:694:VAL:HG12	1:A:694:VAL:O	2.17	0.44
1:A:657:ILE:HD13	1:A:671:GLN:HB3	1.99	0.44
1:A:715:PHE:HE2	1:A:718:GLN:HB2	1.81	0.44
1:B:165:LEU:CD1	1:B:204:PHE:CE2	3.00	0.44
1:B:212:ALA:O	1:B:215:ASP:HB2	2.18	0.44
1:A:542:HIS:CD2	1:A:546:CYS:HB2	2.52	0.44
1:B:184:ILE:HD12	1:B:184:ILE:HA	1.64	0.44
1:B:675:ILE:HD13	1:B:684:TRP:CD1	2.52	0.44
1:B:681:ASN:N	1:B:682:PRO:CD	2.81	0.44
1:A:622:GLN:HG3	1:A:623:GLY:N	2.32	0.44
1:B:244:GLU:C	1:B:246:ALA:H	2.20	0.44
1:A:241:GLN:HE21	1:A:241:GLN:N	2.15	0.43
1:A:651:ILE:CG2	1:A:652:VAL:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLN:HE21	1:B:210:GLN:HB2	1.55	0.43
1:B:537:ASN:OD1	1:B:541:ARG:NE	2.40	0.43
1:A:405:LEU:HD23	1:A:409:LEU:HD22	1.99	0.43
1:A:497:ILE:HG21	1:A:498:TYR:CE1	2.53	0.43
1:A:646:LYS:HA	1:A:646:LYS:HD3	1.46	0.43
1:B:196:LEU:HB3	1:B:201:ILE:HD13	1.94	0.43
1:A:301:PRO:HB3	1:A:425:LEU:O	2.18	0.43
1:A:645:ASN:O	1:A:646:LYS:O	2.35	0.43
1:A:706:ASP:N	1:A:714:ASP:O	2.38	0.43
1:A:497:ILE:HG22	1:A:498:TYR:CE1	2.54	0.43
1:A:651:ILE:CD1	1:A:677:ASN:HD21	2.24	0.43
1:B:613:THR:HG22	1:B:615:PHE:H	1.83	0.43
1:B:659:GLU:OE1	1:B:701:ARG:HD3	2.18	0.43
1:A:498:TYR:CD1	1:A:498:TYR:N	2.85	0.43
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.79	0.43
1:B:397:GLN:O	1:B:400:VAL:HB	2.19	0.43
1:B:441:LYS:NZ	1:B:493:SER:O	2.51	0.43
1:B:734:HIS:HE1	5:B:777:HOH:O	2.00	0.43
1:B:735:LEU:O	1:B:743:HIS:HB2	2.19	0.43
1:A:409:LEU:HA	1:A:409:LEU:HD12	1.66	0.43
1:B:233:LEU:O	1:B:236:PHE:HB3	2.19	0.43
1:B:342:LEU:CD1	1:B:342:LEU:N	2.82	0.43
1:B:701:ARG:HG3	1:B:720:THR:OG1	2.18	0.43
1:B:441:LYS:HG3	1:B:496:ILE:HB	2.01	0.42
1:B:542:HIS:CD2	1:B:542:HIS:C	2.92	0.42
1:A:207:MET:SD	1:A:210:GLN:HB2	2.59	0.42
1:B:291:HIS:HA	1:B:295:TYR:CE2	2.55	0.42
1:B:654:PRO:HD2	1:B:675:ILE:O	2.20	0.42
1:B:556:ARG:NH1	1:B:556:ARG:HG2	2.34	0.42
1:B:739:ASN:HB2	1:B:741:ASP:OD2	2.19	0.42
1:A:432:LYS:HE3	1:A:432:LYS:HB3	1.91	0.42
1:A:496:ILE:N	1:A:496:ILE:HD13	2.34	0.42
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.78	0.42
1:B:412:ILE:O	1:B:412:ILE:HG22	2.18	0.42
1:B:675:ILE:HD13	1:B:684:TRP:NE1	2.34	0.42
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.69	0.42
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.08	0.42
1:A:429:GLU:OE1	1:A:432:LYS:HE2	2.18	0.42
1:A:504:PHE:CZ	1:A:506:GLY:CA	2.99	0.42
1:B:651:ILE:HA	1:B:651:ILE:HD13	1.59	0.42
1:A:405:LEU:HD13	1:A:437:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:VAL:HG21	1:B:519:GLU:HB3	2.00	0.42
1:B:530:ARG:CG	1:B:530:ARG:NH1	2.80	0.42
1:A:207:MET:HE3	1:A:210:GLN:HB3	1.99	0.42
1:A:610:ASP:HA	1:A:611:PRO:HD3	1.55	0.42
1:A:628:PRO:HA	1:A:692:VAL:O	2.19	0.42
1:B:182:ARG:O	1:B:185:PHE:HB3	2.20	0.42
1:B:191:SER:HB2	1:B:193:THR:HG23	2.01	0.42
1:A:267:GLN:O	1:A:269:GLN:HG3	2.20	0.42
1:A:558:ASP:O	1:A:559:SER:HB2	2.19	0.42
1:B:509:SER:H	1:B:510:PRO:HD2	1.83	0.42
1:B:653:ASP:O	1:B:674:VAL:HG13	2.20	0.42
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.49	0.42
1:A:608:LEU:HA	1:A:608:LEU:HD23	1.88	0.42
1:B:211:ARG:NE	1:B:213:GLU:OE2	2.47	0.42
1:A:207:MET:SD	1:A:210:GLN:CB	3.09	0.41
1:A:638:GLY:O	1:A:681:ASN:HA	2.20	0.41
1:B:162:PHE:HZ	1:B:182:ARG:HB2	1.85	0.41
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.80	0.41
1:A:349:ASN:OD1	1:A:349:ASN:O	2.38	0.41
1:A:631:LEU:HG	1:A:633:VAL:HG23	2.02	0.41
1:A:371:ARG:O	1:A:375:ASP:N	2.47	0.41
1:A:573:GLN:N	1:A:573:GLN:NE2	2.61	0.41
1:B:311:HIS:CD2	1:B:312:ASN:HD22	2.37	0.41
1:B:497:ILE:HD12	1:B:497:ILE:N	2.36	0.41
1:B:176:VAL:HG12	1:B:177:ASP:N	2.36	0.41
1:B:732:HIS:NE2	1:B:749:PHE:CD1	2.89	0.41
1:A:344:CYS:O	1:A:392:HIS:HB2	2.19	0.41
1:A:411:PRO:O	1:A:434:LYS:NZ	2.52	0.41
1:B:342:LEU:HB2	1:B:389:LEU:HD23	2.01	0.41
1:A:426:PRO:HD3	1:A:498:TYR:CE2	2.55	0.41
1:A:651:ILE:CD1	1:A:677:ASN:ND2	2.80	0.41
1:B:333:LEU:HD21	1:B:340:LEU:HD11	2.02	0.41
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.74	0.41
1:A:651:ILE:HG21	1:A:677:ASN:O	2.20	0.41
1:A:665:ARG:HD3	1:A:693:THR:HG21	2.01	0.41
1:B:169:LEU:O	1:B:172:LEU:HD12	2.21	0.41
1:B:542:HIS:CD2	1:B:546:CYS:HB2	2.56	0.41
1:B:678:ASN:HA	5:B:879:HOH:O	2.20	0.41
1:A:652:VAL:H	1:A:652:VAL:HG23	1.53	0.41
1:B:162:PHE:CE1	1:B:182:ARG:HA	2.56	0.41
1:A:228:LEU:CD1	1:A:233:LEU:N	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:LEU:HD12	1:A:414:LEU:H	1.86	0.41
1:B:162:PHE:HD1	1:B:162:PHE:HA	1.73	0.41
1:B:311:HIS:HB2	1:B:576:ALA:HB1	2.02	0.41
1:B:405:LEU:HD13	1:B:437:LEU:HD11	2.02	0.41
1:B:651:ILE:CG2	1:B:677:ASN:CA	2.98	0.41
1:A:426:PRO:CG	1:A:498:TYR:CE2	3.04	0.41
1:B:391:ASN:N	5:B:830:HOH:O	2.40	0.41
1:B:701:ARG:HH11	1:B:701:ARG:HD3	1.74	0.41
1:B:739:ASN:ND2	5:B:890:HOH:O	2.53	0.41
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.34	0.41
1:A:425:LEU:HD23	1:A:498:TYR:HD2	1.86	0.41
1:B:730:TYR:CZ	1:B:751:LYS:HD3	2.56	0.41
1:A:228:LEU:HD13	1:A:232:ARG:HB2	2.03	0.40
1:A:709:SER:OG	1:A:710:SER:N	2.54	0.40
1:B:492:LEU:HA	1:B:492:LEU:HD23	1.74	0.40
1:B:507:PHE:CZ	1:B:531:LEU:HD22	2.56	0.40
1:B:590:LEU:HD23	1:B:590:LEU:HA	1.78	0.40
1:B:715:PHE:HB2	5:B:850:HOH:O	2.20	0.40
1:A:321:THR:HG22	1:A:360:PHE:HB2	2.04	0.40
1:A:345:TRP:CE3	1:A:392:HIS:HB3	2.56	0.40
1:B:227:THR:HG21	1:B:269:GLN:HB3	2.04	0.40
1:B:441:LYS:HE2	1:B:496:ILE:O	2.20	0.40
1:B:165:LEU:HD13	1:B:204:PHE:CE2	2.56	0.40
1:B:595:ASP:OD1	1:B:596:ASN:N	2.52	0.40
1:B:610:ASP:O	1:B:613:THR:OG1	2.35	0.40
1:A:252:LEU:HD23	1:A:256:GLU:CD	2.42	0.40
1:A:342:LEU:HB2	1:A:389:LEU:HD23	2.04	0.40
1:A:622:GLN:CA	1:B:445:LEU:CD1	3.00	0.40
1:B:162:PHE:O	1:B:166:LYS:N	2.39	0.40
1:B:198:ASP:O	1:B:201:ILE:N	2.47	0.40
1:B:300:GLN:CB	1:B:301:PRO:CD	2.99	0.40
1:B:254:LEU:HA	1:B:254:LEU:HD12	1.79	0.40
1:B:638:GLY:O	1:B:681:ASN:HA	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/624 (82%)	449 (88%)	51 (10%)	9 (2%)	8	33
1	B	557/624 (89%)	485 (87%)	65 (12%)	7 (1%)	12	41
All	All	1066/1248 (85%)	934 (88%)	116 (11%)	16 (2%)	10	38

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	VAL
1	A	646	LYS
1	A	712	LYS
1	B	173	ASN
1	B	645	ASN
1	A	644	VAL
1	B	647	ASN
1	B	649	ASN
1	A	219	GLU
1	A	263	THR
1	B	512	THR
1	A	579	PHE
1	A	713	ASN
1	B	417	PRO
1	A	744	PRO
1	B	648	LYS

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	444/545 (82%)	381 (86%)	63 (14%)	3	13
1	B	492/545 (90%)	419 (85%)	73 (15%)	3	12
All	All	936/1090 (86%)	800 (86%)	136 (14%)	3	13

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	PHE
1	A	209	THR
1	A	211	ARG
1	A	219	GLU
1	A	220	GLU
1	A	227	THR
1	A	228	LEU
1	A	231	GLU
1	A	242	ARG
1	A	252	LEU
1	A	253	SER
1	A	254	LEU
1	A	257	ARG
1	A	278	TYR
1	A	293	ARG
1	A	296	GLN
1	A	300	GLN
1	A	309	SER
1	A	310	SER
1	A	344	CYS
1	A	362	SER
1	A	381	SER
1	A	388	SER
1	A	406	ARG
1	A	409	LEU
1	A	414	LEU
1	A	418	LEU
1	A	424	SER
1	A	436	LEU
1	A	487	LYS
1	A	497	ILE
1	A	513	SER
1	A	526	SER
1	A	530	ARG
1	A	535	SER

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Mol	Chain	Res	Type
1	A	539	PHE
1	A	556	ARG
1	A	563	SER
1	A	573	GLN
1	A	594	GLN
1	A	612	ASN
1	A	617	SER
1	A	621	THR
1	A	624	PRO
1	A	643	LYS
1	A	644	VAL
1	A	646	LYS
1	A	648	LYS
1	A	652	VAL
1	A	655	LYS
1	A	665	ARG
1	A	671	GLN
1	A	676	THR
1	A	677	ASN
1	A	685	ASP
1	A	710	SER
1	A	711	SER
1	A	727	LYS
1	A	738	LYS
1	A	743	HIS
1	A	745	SER
1	A	753	SER
1	A	756	ASP
1	B	159	LYS
1	B	160	MET
1	B	162	PHE
1	B	166	LYS
1	B	171	GLU
1	B	172	LEU
1	B	178	ASP
1	B	184	ILE
1	B	186	ARG
1	B	194	ASP
1	B	210	GLN
1	B	211	ARG
1	B	227	THR
1	B	232	ARG

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Mol	Chain	Res	Type
1	B	238	GLN
1	B	242	ARG
1	B	253	SER
1	B	254	LEU
1	B	257	ARG
1	B	261	SER
1	B	262	GLU
1	B	263	THR
1	B	293	ARG
1	B	296	GLN
1	B	298	MET
1	B	300	GLN
1	B	309	SER
1	B	310	SER
1	B	327	GLU
1	B	331	ARG
1	B	362	SER
1	B	388	SER
1	B	406	ARG
1	B	409	LEU
1	B	414	LEU
1	B	423	THR
1	B	436	LEU
1	B	441	LYS
1	B	486	LEU
1	B	488	LEU
1	B	497	ILE
1	B	508	SER
1	B	526	SER
1	B	535	SER
1	B	539	PHE
1	B	563	SER
1	B	573	GLN
1	B	577	LEU
1	B	613	THR
1	B	614	THR
1	B	617	SER
1	B	621	THR
1	B	646	LYS
1	B	648	LYS
1	B	651	ILE
1	B	652	VAL

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Mol	Chain	Res	Type
1	B	655	LYS
1	B	659	GLU
1	B	665	ARG
1	B	671	GLN
1	B	676	THR
1	B	677	ASN
1	B	685	ASP
1	B	687	GLU
1	B	709	SER
1	B	710	SER
1	B	713	ASN
1	B	715	PHE
1	B	727	LYS
1	B	738	LYS
1	B	743	HIS
1	B	753	SER
1	B	755	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	291	HIS
1	A	312	ASN
1	A	349	ASN
1	A	573	GLN
1	A	639	GLN
1	A	645	ASN
1	A	718	GLN
1	A	728	GLN
1	A	743	HIS
1	B	210	GLN
1	B	241	GLN
1	B	291	HIS
1	B	312	ASN
1	B	349	ASN
1	B	515	GLN
1	B	542	HIS
1	B	573	GLN
1	B	639	GLN
1	B	718	GLN
1	B	728	GLN

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Mol	Chain	Res	Type
1	B	734	HIS
1	B	739	ASN
1	B	743	HIS
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 carbohydrates 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	A	5	-	1,3,3	3.99	1 (100%)	0,3,3	0.00	-
3	ACT	B	5	-	1,3,3	4.37	1 (100%)	0,3,3	0.00	-
4	IP2	B	1	2	20,20,20	2.11	8 (40%)	30,32,32	1.92	9 (30%)
4	IP2	A	1	2	20,20,20	2.10	7 (35%)	30,32,32	1.61	7 (23%)

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	IP2	B	1	2	-	1/10/34/34	0/1/1/1
4	IP2	A	1	2	-	1/10/34/34	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	IP2	P4-O4	4.43	1.67	1.59
3	B	5	ACT	CH3-C	4.37	1.54	1.48
4	A	1	IP2	P4-O4	4.06	1.67	1.59
3	A	5	ACT	CH3-C	3.99	1.53	1.48
4	B	1	IP2	P4-O41	3.95	1.63	1.50
4	A	1	IP2	P5-O51	3.72	1.62	1.50
4	A	1	IP2	P4-O41	3.66	1.62	1.50
4	B	1	IP2	P5-O51	3.56	1.62	1.50
4	A	1	IP2	C5-C4	2.73	1.57	1.52
4	B	1	IP2	P5-O5	2.51	1.64	1.59
4	A	1	IP2	P5-O5	2.37	1.63	1.59
4	A	1	IP2	C6-C5	2.31	1.58	1.52
4	B	1	IP2	P5-O52	2.24	1.63	1.54
4	B	1	IP2	P5-O53	2.19	1.63	1.54
4	B	1	IP2	P4-O42	2.13	1.63	1.54
4	A	1	IP2	P5-O53	2.10	1.62	1.54
4	B	1	IP2	P4-O43	2.09	1.62	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	IP2	C3-C2-C1	4.68	119.00	110.82
4	B	1	IP2	O1-C1-C2	-4.31	100.39	110.35
4	B	1	IP2	C1-C6-C5	3.79	118.32	109.68
4	A	1	IP2	O2-C2-C1	-3.67	101.86	110.35
4	B	1	IP2	O2-C2-C1	-3.35	102.60	110.35
4	A	1	IP2	C1-C6-C5	3.17	116.92	109.68
4	A	1	IP2	C3-C2-C1	-3.11	105.39	110.82
4	B	1	IP2	O3-C3-C2	-2.94	103.55	110.35
4	B	1	IP2	C2-C3-C4	2.70	115.84	109.68
4	A	1	IP2	C6-C5-C4	2.70	117.82	111.66
4	B	1	IP2	O5-C5-C4	-2.46	102.89	108.69
4	B	1	IP2	O3-C3-C4	-2.31	103.82	109.94
4	A	1	IP2	O4-C4-C5	2.27	114.04	108.69
4	B	1	IP2	O4-C4-C3	2.26	113.93	108.66
4	A	1	IP2	O3-C3-C2	2.10	115.21	110.35
4	A	1	IP2	O4-C4-C3	2.07	113.48	108.66

There are no chirality outliers.

All (2) torsion outliers are listed below:

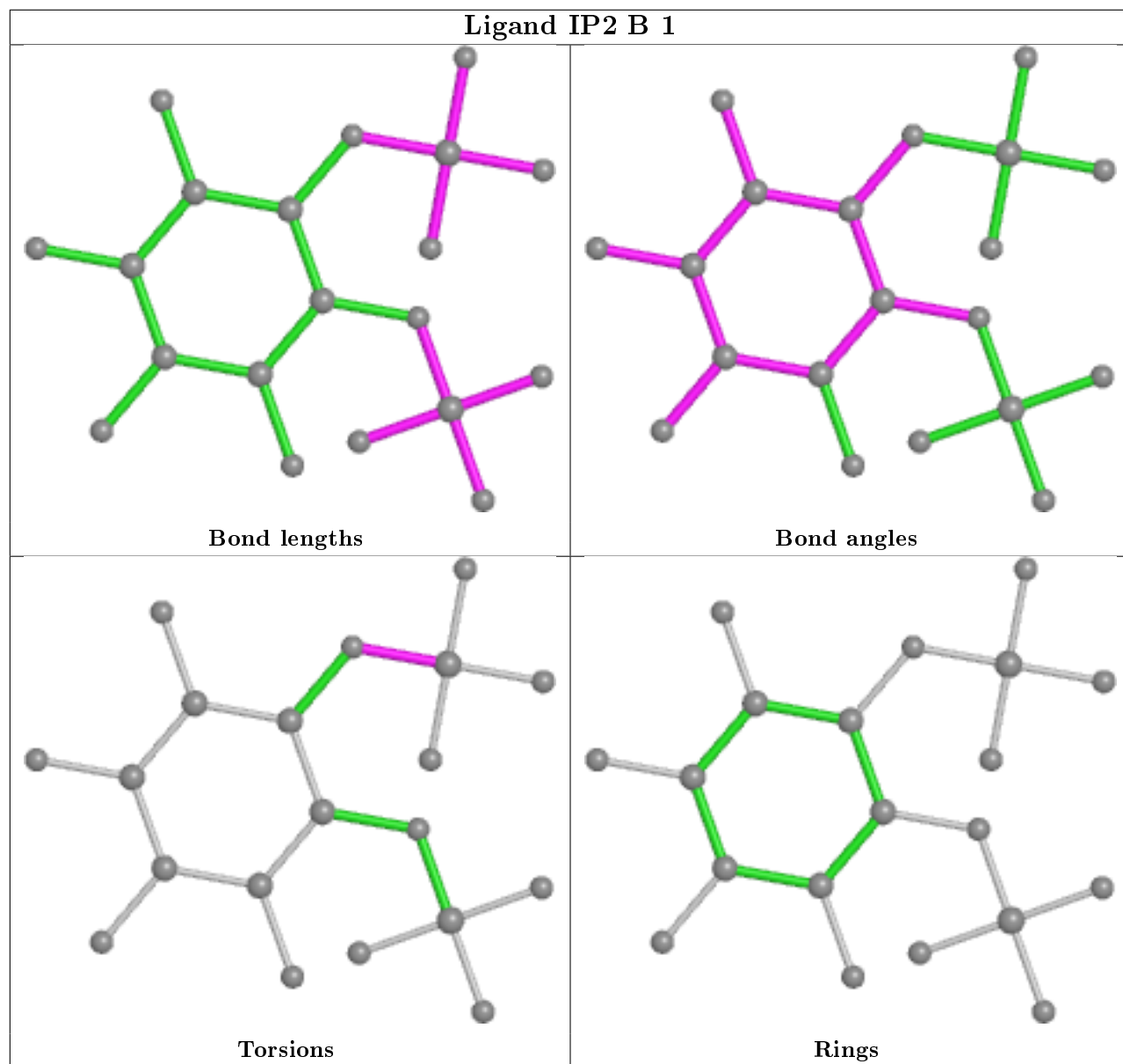
Mol	Chain	Res	Type	Atoms
4	B	1	IP2	C4-O4-P4-O41
4	A	1	IP2	C6-C5-O5-P5

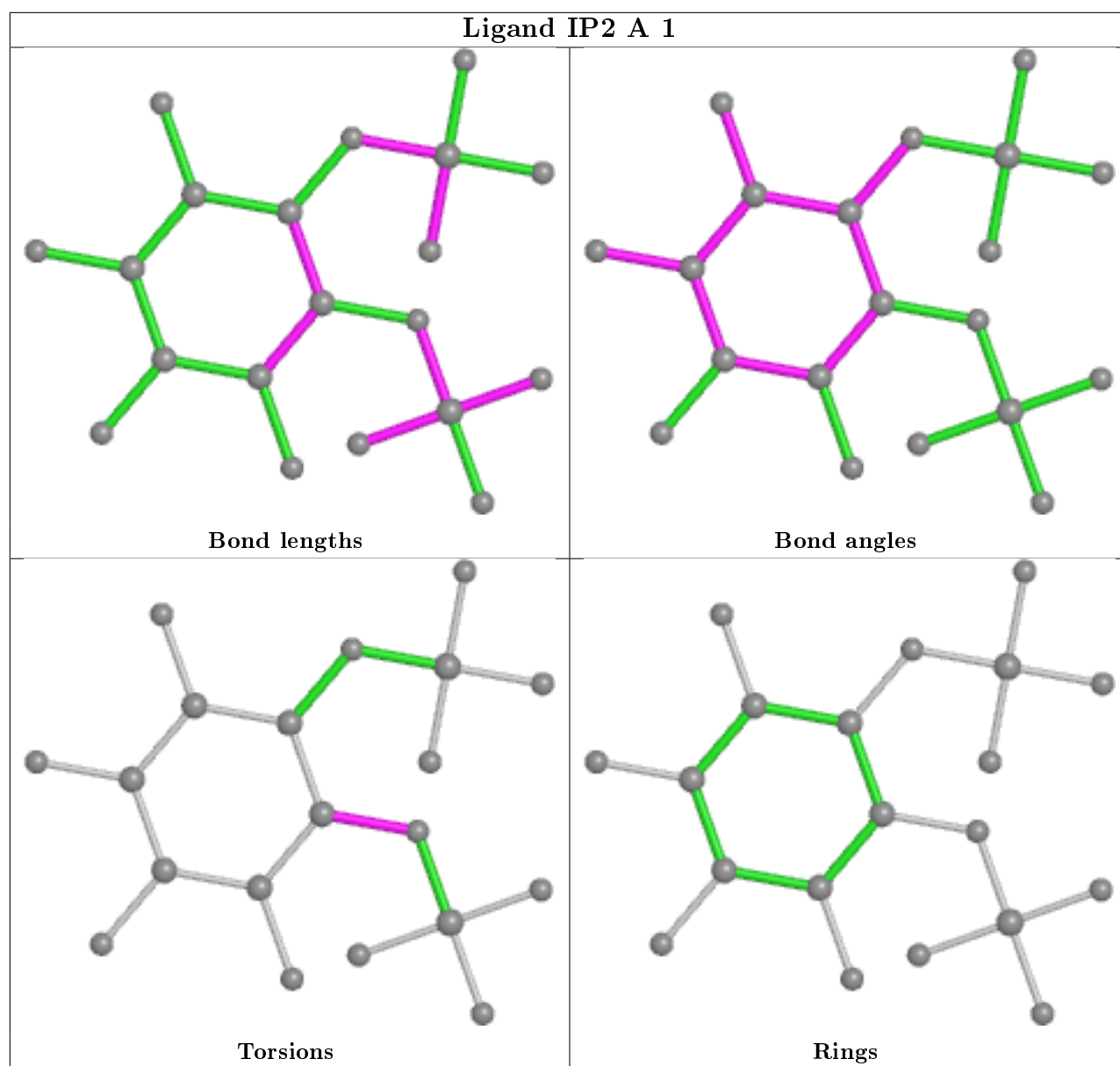
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	IP2	4	0
4	A	1	IP2	3	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	508/624 (81%)	-0.46	19 (3%)	41 27	4, 22, 82, 127	14 (2%)
1	B	558/624 (89%)	-0.40	21 (3%)	40 26	4, 23, 78, 118	23 (4%)
All	All	1066/1248 (85%)	-0.43	40 (3%)	40 26	4, 23, 81, 127	37 (3%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	SER	7.9
1	B	649	ASN	7.4
1	A	201	ILE	6.7
1	B	509	SER	6.0
1	B	514	GLY	5.7
1	A	202	GLU	5.6
1	B	510	PRO	5.4
1	A	203	THR	5.3
1	A	204	PHE	5.1
1	B	508	SER	4.7
1	A	200	GLU	4.3
1	A	647	ASN	3.9
1	A	710	SER	3.8
1	B	486	LEU	3.8
1	A	645	ASN	3.8
1	A	208	LEU	3.7
1	B	647	ASN	3.6
1	B	172	LEU	3.3
1	B	645	ASN	3.3
1	A	420	GLY	3.2
1	A	205	TYR	2.9
1	B	648	LYS	2.9
1	A	206	LYS	2.8
1	B	168	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	419	ASP	2.8
1	A	648	LYS	2.7
1	B	710	SER	2.7
1	B	165	LEU	2.4
1	B	515	GLN	2.4
1	A	207	MET	2.4
1	A	709	SER	2.3
1	B	709	SER	2.3
1	A	505	GLY	2.2
1	B	167	ASP	2.2
1	B	261	SER	2.2
1	B	171	GLU	2.1
1	A	650	SER	2.1
1	B	202	GLU	2.1
1	B	503	HIS	2.0
1	B	484	ASP	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	IP2	A	1	20/20	0.77	0.31	70,97,136,136	0
2	CA	A	3	1/1	0.78	0.12	66,66,66,66	0
4	IP2	B	1	20/20	0.81	0.22	53,74,108,110	0
2	CA	A	2	1/1	0.91	0.09	59,59,59,59	0
2	CA	B	3	1/1	0.95	0.15	74,74,74,74	0
3	ACT	A	5	4/4	0.95	0.13	36,38,38,39	0
2	CA	B	2	1/1	0.95	0.07	37,37,37,37	0

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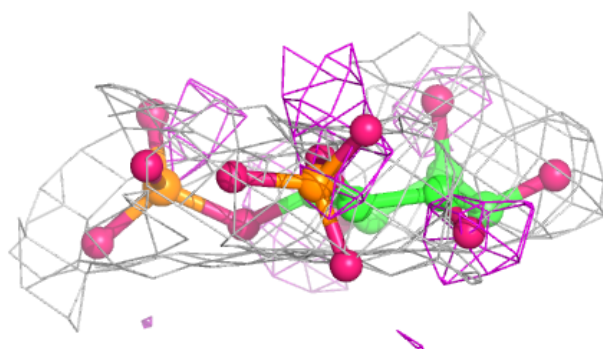
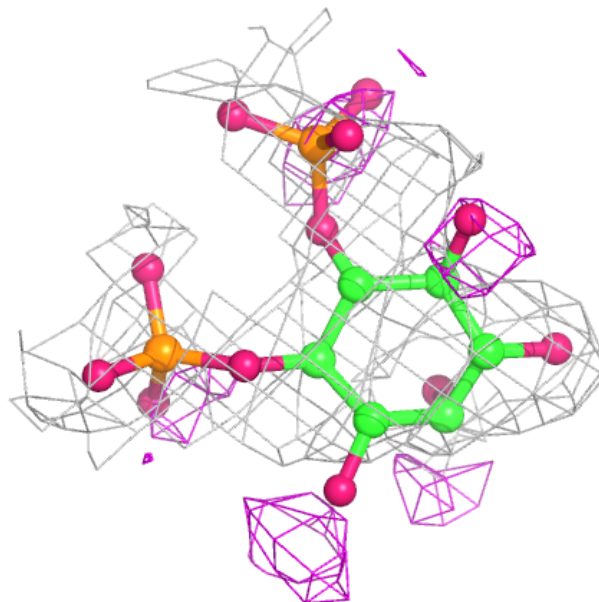
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ACT	B	5	4/4	0.98	0.12	25,26,27,29	0

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.

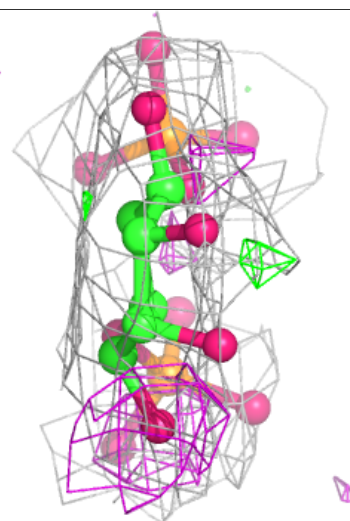
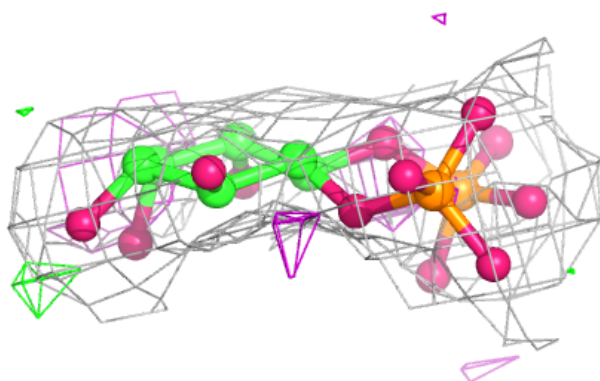
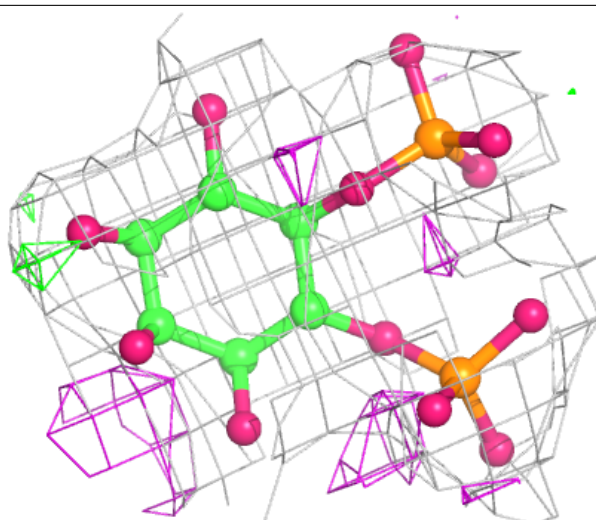
Electron density around IP2 A 1:

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



Electron density around IP2 B 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.