



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:24 am BST

PDB ID : 1DJY  
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM  
RAT COMPLEXED WITH INOSITOL-2,4,5-TRISPHOSPHATE  
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.  
Deposited on : 1996-08-24  
Resolution : 2.80 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](mailto: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.

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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

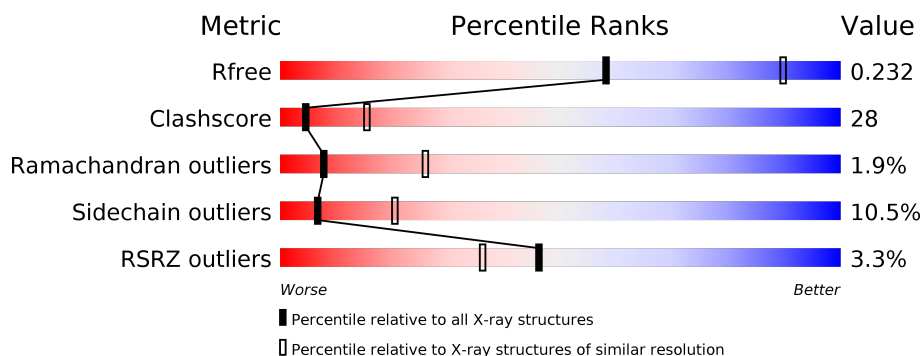
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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>44%</div> <div>33%</div> <div>• •</div> <div>18%</div> </div> </div>
1	B	624	<div> <div>2%</div> <div> <div></div> <div>45%</div> <div>38%</div> <div>6%</div> <div>•</div> <div>10%</div> </div> </div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8986 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	102	0	0
			4057	2565	709	761	22			
1	B	561	Total	C	N	O	S	125	0	0
			4465	2818	776	847	24			

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

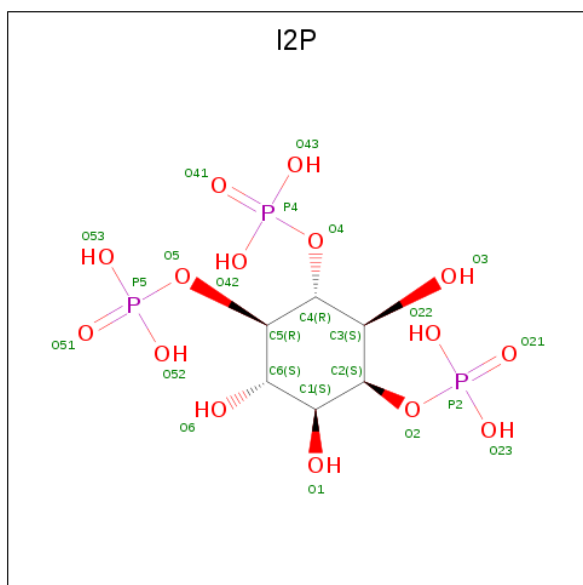
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).



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-2,4,5-TRIPHOSPHATE (three-letter code: I2P) (formula:  $C_6H_{15}O_{15}P_3$ ).

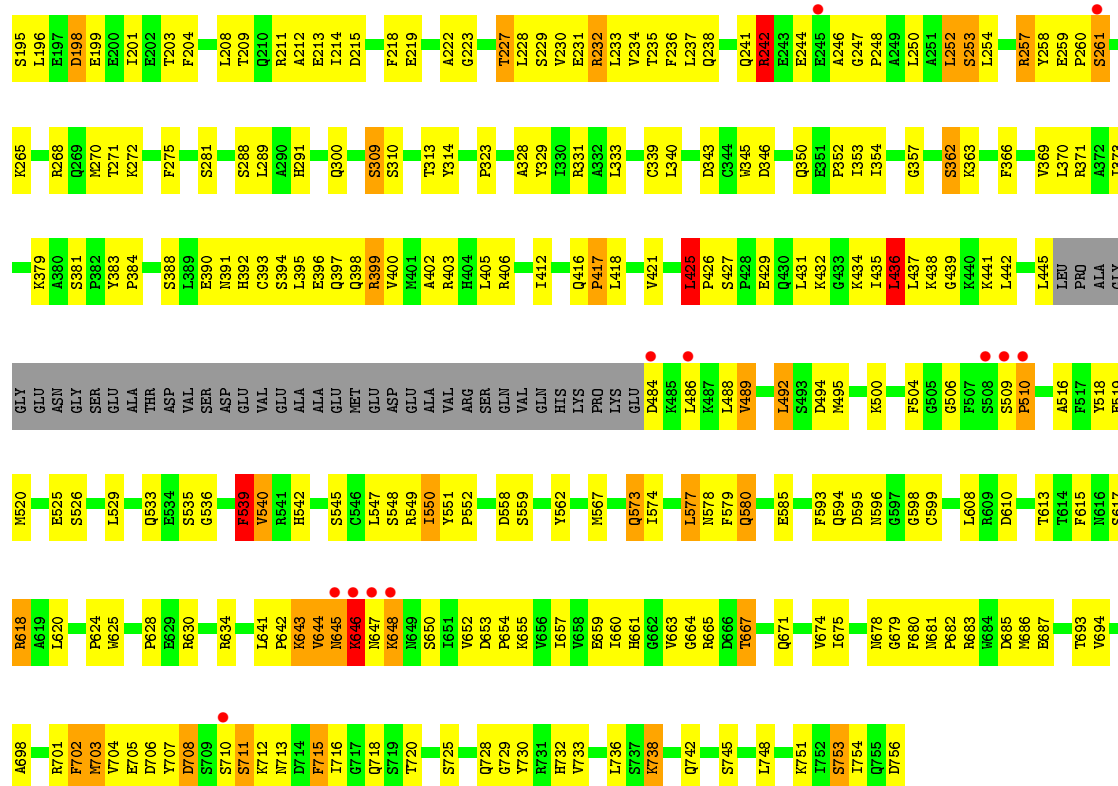


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			24	6	15	3		
4	B	1	Total	C	O	P	0	0
			24	6	15	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	190	Total	O	0	0
			190	190		
5	B	212	Total	O	0	0
			212	212		





## 4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	397.13Å 397.13Å 397.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.80 24.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.9 (10.00-2.80) 90.2 (24.68-2.80)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 2.80Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.210 , 0.260 0.194 , 0.232	Depositor DCC
$R_{free}$ test set	2285 reflections (3.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 93.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8986	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: I2P, 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	1.18	21/4152 (0.5%)	1.09	17/5624 (0.3%)
1	B	0.97	8/4565 (0.2%)	0.94	9/6174 (0.1%)
All	All	1.08	29/8717 (0.3%)	1.01	26/11798 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	257	ARG	CZ-NH1	25.41	1.66	1.33
1	A	581	THR	CA-CB	17.47	1.98	1.53
1	A	581	THR	N-CA	11.13	1.68	1.46
1	A	581	THR	CA-C	-10.44	1.25	1.52
1	A	257	ARG	CZ-NH2	9.73	1.45	1.33
1	A	366	PHE	CG-CD1	-8.93	1.25	1.38
1	B	366	PHE	CE1-CZ	-8.28	1.21	1.37
1	A	257	ARG	NE-CZ	8.24	1.43	1.33
1	A	702	PHE	CE2-CZ	-7.91	1.22	1.37
1	A	366	PHE	CE2-CZ	-7.91	1.22	1.37
1	A	366	PHE	CG-CD2	-7.90	1.26	1.38
1	A	366	PHE	CE1-CZ	-7.68	1.22	1.37
1	B	366	PHE	CE2-CZ	-7.47	1.23	1.37
1	A	702	PHE	CG-CD1	-7.37	1.27	1.38
1	B	702	PHE	CE1-CZ	-7.29	1.23	1.37
1	B	366	PHE	CG-CD2	-7.23	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	702	PHE	CG-CD2	-7.22	1.27	1.38
1	A	581	THR	C-O	-7.03	1.09	1.23
1	B	366	PHE	CG-CD1	-6.90	1.28	1.38
1	A	582	PRO	CG-CD	-6.09	1.30	1.50
1	B	708	ASP	C-O	5.70	1.34	1.23
1	A	702	PHE	CE1-CZ	-5.70	1.26	1.37
1	A	257	ARG	CD-NE	5.65	1.56	1.46
1	A	515	GLN	CD-NE2	5.61	1.46	1.32
1	B	702	PHE	CG-CD1	-5.54	1.30	1.38
1	A	282	ALA	CA-CB	-5.53	1.40	1.52
1	A	372	ALA	CA-CB	-5.36	1.41	1.52
1	A	515	GLN	CD-OE1	5.33	1.35	1.24
1	A	702	PHE	CG-CD2	-5.30	1.30	1.38

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ARG	NE-CZ-NH2	-24.78	107.91	120.30
1	A	257	ARG	NE-CZ-NH1	14.55	127.58	120.30
1	A	581	THR	CA-C-O	-13.98	90.74	120.10
1	A	211	ARG	NE-CZ-NH2	-10.69	114.96	120.30
1	A	257	ARG	CD-NE-CZ	-9.44	110.38	123.60
1	A	580	GLN	C-N-CA	9.37	145.11	121.70
1	A	581	THR	CA-C-N	8.43	140.69	117.10
1	B	436	LEU	CB-CG-CD1	-8.26	96.96	111.00
1	A	247	GLY	C-N-CD	-7.32	104.50	120.60
1	B	436	LEU	CB-CG-CD2	-7.22	98.73	111.00
1	B	425	LEU	CA-CB-CG	6.78	130.89	115.30
1	A	228	LEU	CB-CG-CD1	-6.11	100.61	111.00
1	B	577	LEU	CA-CB-CG	6.07	129.25	115.30
1	B	257	ARG	CG-CD-NE	5.81	124.00	111.80
1	A	399	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	582	PRO	N-CD-CG	5.67	111.71	103.20
1	B	399	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	252	LEU	CB-CG-CD1	-5.55	101.56	111.00
1	A	581	THR	C-N-CD	5.23	139.38	128.40
1	B	715	PHE	CB-CG-CD2	-5.22	117.15	120.80
1	B	703	MET	CG-SD-CE	-5.18	91.91	100.20
1	A	582	PRO	CA-N-CD	-5.13	104.31	111.50
1	B	247	GLY	C-N-CD	-5.12	109.33	120.60
1	A	211	ARG	NH1-CZ-NH2	5.04	124.94	119.40
1	A	202	GLU	N-CA-C	-5.03	97.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	GLY	N-CA-C	-5.00	100.60	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	581	THR	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	GLN	Mainchain
1	A	742	GLN	Sidechain

## 5.2 Too-close contacts [i](#)

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	199	1
1	B	4465	0	4375	273	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	24	0	9	0	0
4	B	24	0	8	1	0
5	A	190	0	0	15	0
5	B	212	0	0	16	0
All	All	8986	0	8370	467	1

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 28.

All (467) 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:581:THR:N	1:A:581:THR:CA	1.68	1.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:THR:CB	1:A:581:THR:CA	1.98	1.39
1:B:728:GLN:NE2	1:B:754:ILE:H	1.53	1.06
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.38	1.03
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.45	0.99
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.47	0.95
1:A:582:PRO:N	5:A:915:HOH:O	1.98	0.95
1:A:241:GLN:HE22	1:A:730:TYR:H	1.16	0.94
1:B:643:LYS:NZ	1:B:646:LYS:HG2	1.84	0.91
1:B:728:GLN:HE21	1:B:754:ILE:H	0.94	0.91
1:A:516:ALA:HB3	1:A:519:GLU:HG3	1.54	0.89
1:B:438:LYS:HE3	1:B:520:MET:HE2	1.55	0.86
1:B:708:ASP:O	5:B:968:HOH:O	1.94	0.86
1:B:728:GLN:HE21	1:B:754:ILE:N	1.72	0.85
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.57	0.85
1:A:573:GLN:H	1:A:573:GLN:HE21	1.23	0.84
1:A:573:GLN:H	1:A:573:GLN:NE2	1.75	0.83
1:A:238:GLN:HG3	1:A:246:ALA:CB	2.08	0.83
1:A:418:LEU:HB2	1:A:421:VAL:HG21	1.61	0.83
1:A:613:THR:HG22	1:A:615:PHE:H	1.45	0.81
1:B:196:LEU:HB3	1:B:201:ILE:CD1	2.12	0.79
1:A:436:LEU:N	1:A:436:LEU:HD23	1.98	0.78
1:A:581:THR:HG23	5:A:915:HOH:O	1.83	0.78
1:A:253:SER:HB2	1:A:257:ARG:HH21	1.49	0.78
1:A:548:SER:H	1:A:573:GLN:NE2	1.82	0.78
1:B:618:ARG:HG2	1:B:618:ARG:HH11	1.47	0.78
1:B:436:LEU:N	1:B:436:LEU:HD23	1.98	0.77
1:B:196:LEU:HB3	1:B:201:ILE:HD11	1.65	0.77
1:A:550:ILE:HG21	1:A:567:MET:CE	2.14	0.77
1:B:646:LYS:N	1:B:646:LYS:HD2	1.99	0.76
1:B:509:SER:HB3	1:B:510:PRO:HD3	1.67	0.76
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.65	0.76
1:A:582:PRO:CD	5:A:915:HOH:O	2.34	0.76
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.15	0.74
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.69	0.74
1:B:442:LEU:HD21	1:B:488:LEU:HB2	1.69	0.73
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.24	0.73
1:A:323:PRO:HA	1:A:362:SER:HB3	1.70	0.72
1:A:405:LEU:HD13	1:A:437:LEU:HD11	1.71	0.72
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.24	0.72
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.24	0.72
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ILE:HG21	1:A:567:MET:HE3	1.72	0.72
1:B:644:VAL:HG23	1:B:645:ASN:H	1.55	0.72
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.24	0.71
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.72	0.70
1:B:161:ASN:OD1	1:B:164:GLU:HG3	1.92	0.70
1:A:551:TYR:HB2	1:A:552:PRO:HD2	1.74	0.70
1:B:551:TYR:HB2	1:B:552:PRO:HD2	1.73	0.70
1:A:418:LEU:CB	1:A:421:VAL:HG21	2.20	0.70
1:A:582:PRO:HD2	5:A:915:HOH:O	1.90	0.70
1:B:323:PRO:HA	1:B:362:SER:HB3	1.74	0.69
1:B:643:LYS:HE3	1:B:646:LYS:CB	2.22	0.69
1:B:398:GLN:HB2	1:B:489:VAL:HG21	1.73	0.69
1:B:438:LYS:HE3	1:B:520:MET:CE	2.22	0.69
1:A:395:LEU:O	1:A:399:ARG:HG3	1.94	0.68
1:A:217:ALA:O	1:A:220:GLU:HG3	1.92	0.68
1:B:184:ILE:HG22	1:B:204:PHE:CD2	2.27	0.68
1:B:516:ALA:HB3	1:B:519:GLU:HG3	1.75	0.67
1:B:231:GLU:CD	1:B:231:GLU:H	1.98	0.67
1:B:172:LEU:O	1:B:174:ILE:N	2.28	0.67
1:B:630:ARG:HG2	5:B:765:HOH:O	1.94	0.67
1:B:646:LYS:HD2	1:B:646:LYS:H	1.58	0.67
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.30	0.67
1:B:402:ALA:HB2	1:B:492:LEU:HD12	1.76	0.66
1:A:331:ARG:HD2	5:A:908:HOH:O	1.93	0.66
1:A:398:GLN:HB2	1:A:489:VAL:HG21	1.77	0.66
1:B:222:ALA:HB2	1:B:228:LEU:HD23	1.77	0.66
1:B:536:GLY:O	1:B:540:VAL:HG23	1.96	0.66
1:A:507:PHE:HE1	1:A:542:HIS:HD1	1.44	0.66
1:A:287:PHE:CZ	1:A:594:GLN:HB3	2.30	0.66
1:B:163:LYS:O	1:B:166:LYS:HB2	1.96	0.66
1:B:166:LYS:HE3	1:B:178:ASP:CG	2.16	0.66
1:B:509:SER:HB2	5:B:918:HOH:O	1.96	0.66
1:B:166:LYS:HE3	1:B:178:ASP:OD2	1.97	0.65
1:A:703:MET:CE	1:A:715:PHE:HD1	2.10	0.65
1:B:648:LYS:NZ	1:B:650:SER:HB2	2.10	0.65
1:A:252:LEU:O	1:A:256:GLU:HG3	1.96	0.65
1:B:406:ARG:HG3	1:B:495:MET:HE1	1.78	0.65
1:B:548:SER:H	1:B:573:GLN:NE2	1.93	0.65
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.25	0.65
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.26	0.65
1:B:703:MET:HE3	1:B:715:PHE:HD2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:THR:O	1:A:207:MET:N	2.30	0.65
1:B:313:THR:HB	1:B:329:TYR:CE1	2.32	0.64
1:B:643:LYS:HZ1	1:B:646:LYS:HG2	1.59	0.64
1:A:536:GLY:O	1:A:540:VAL:HG23	1.97	0.64
1:B:729:GLY:O	1:B:751:LYS:HA	1.98	0.64
1:B:405:LEU:HD13	1:B:437:LEU:HD11	1.80	0.64
1:A:346:ASP:HA	1:A:397:GLN:OE1	1.97	0.64
1:B:429:GLU:OE1	1:B:432:LYS:HE2	1.98	0.64
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.27	0.64
1:B:733:VAL:HB	1:B:748:LEU:HB2	1.79	0.64
1:B:533:GLN:OE1	1:B:618:ARG:NH1	2.30	0.64
1:B:648:LYS:HZ2	1:B:650:SER:HB2	1.61	0.64
1:B:703:MET:CE	1:B:715:PHE:HD2	2.11	0.64
1:A:200:GLU:N	1:A:203:THR:H	1.96	0.63
1:A:703:MET:HE3	1:A:715:PHE:HD1	1.62	0.63
1:A:219:GLU:O	1:A:223:GLY:N	2.32	0.63
1:B:578:ASN:HB3	1:B:580:GLN:OE1	1.98	0.63
1:B:438:LYS:HD2	1:B:520:MET:HE1	1.80	0.63
1:B:190:HIS:O	1:B:192:GLN:HG2	1.99	0.63
1:B:160:MET:HA	1:B:164:GLU:OE1	1.98	0.63
1:A:238:GLN:HG3	1:A:246:ALA:HB3	1.80	0.63
1:A:670:ARG:HD3	5:A:758:HOH:O	2.00	0.62
1:B:418:LEU:HB2	1:B:421:VAL:CG2	2.28	0.62
1:B:261:SER:O	1:B:265:LYS:HB2	1.99	0.62
1:B:259:GLU:OE1	1:B:271:THR:N	2.28	0.62
1:B:425:LEU:HD12	1:B:426:PRO:HD2	1.81	0.62
1:A:729:GLY:O	1:A:751:LYS:HA	2.00	0.62
1:B:241:GLN:HE22	1:B:730:TYR:H	1.48	0.62
1:B:406:ARG:HG3	1:B:495:MET:CE	2.30	0.62
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.35	0.61
1:A:550:ILE:HG21	1:A:567:MET:HE2	1.82	0.61
1:A:539:PHE:O	1:A:542:HIS:N	2.33	0.61
1:A:539:PHE:O	1:A:542:HIS:HB3	1.99	0.61
1:A:252:LEU:HB3	1:A:256:GLU:OE2	2.01	0.61
1:A:406:ARG:HG3	1:A:495:MET:CE	2.30	0.61
1:B:573:GLN:H	1:B:573:GLN:NE2	1.98	0.61
1:B:618:ARG:HG2	1:B:618:ARG:NH1	2.13	0.61
1:B:431:LEU:HD22	1:B:436:LEU:HD21	1.83	0.60
1:B:707:TYR:HA	1:B:713:ASN:OD1	2.01	0.60
1:B:728:GLN:NE2	1:B:754:ILE:N	2.36	0.60
1:B:643:LYS:CE	1:B:646:LYS:HG2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LEU:O	1:B:174:ILE:HG13	2.01	0.60
1:A:368:ASP:OD1	1:A:371:ARG:NH2	2.32	0.59
1:A:525:GLU:O	1:A:529:LEU:HG	2.02	0.59
1:B:253:SER:O	1:B:257:ARG:HB2	2.02	0.59
1:A:225:ALA:HA	5:A:871:HOH:O	2.01	0.59
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.85	0.59
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.68	0.59
1:A:613:THR:HG22	1:A:615:PHE:N	2.17	0.59
1:A:744:PRO:HG2	5:A:894:HOH:O	2.01	0.59
1:B:643:LYS:HE3	1:B:646:LYS:HB2	1.84	0.59
1:B:509:SER:HB3	1:B:510:PRO:CD	2.31	0.59
1:B:713:ASN:OD1	5:B:968:HOH:O	2.16	0.59
1:A:520:MET:CE	1:A:549:ARG:HB2	2.33	0.59
1:A:230:VAL:HG12	1:A:231:GLU:N	2.18	0.59
1:B:388:SER:HA	1:B:438:LYS:HB3	1.85	0.59
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.38	0.58
1:B:539:PHE:O	1:B:542:HIS:HB3	2.04	0.58
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.39	0.58
1:A:316:LEU:HD23	1:A:328:ALA:HB2	1.86	0.58
1:A:642:PRO:HD2	1:A:716:ILE:HG23	1.85	0.58
1:A:253:SER:O	1:A:257:ARG:HB2	2.04	0.58
1:B:196:LEU:HD13	1:B:201:ILE:HD13	1.86	0.58
1:A:371:ARG:O	1:A:374:ARG:HB3	2.04	0.57
1:A:756:ASP:OD1	1:A:756:ASP:N	2.36	0.57
1:A:686:MET:HG3	1:A:687:GLU:N	2.17	0.57
1:B:164:GLU:O	1:B:167:ASP:HB2	2.04	0.57
1:B:595:ASP:OD1	1:B:596:ASN:N	2.35	0.57
1:B:711:SER:OG	1:B:712:LYS:N	2.37	0.57
1:A:595:ASP:OD1	1:A:596:ASN:N	2.37	0.57
1:B:399:ARG:O	1:B:403:ARG:HG3	2.05	0.57
1:A:261:SER:O	1:A:265:LYS:HB2	2.05	0.57
1:B:196:LEU:HB3	1:B:201:ILE:HD13	1.85	0.56
1:B:230:VAL:HG12	1:B:231:GLU:N	2.20	0.56
1:A:491:GLU:HG2	5:A:938:HOH:O	2.06	0.56
1:A:200:GLU:O	1:A:204:PHE:N	2.34	0.56
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.05	0.56
1:B:398:GLN:HB2	1:B:489:VAL:CG2	2.34	0.56
1:A:733:VAL:HB	1:A:748:LEU:HB2	1.87	0.56
1:A:406:ARG:HG3	1:A:495:MET:HE1	1.87	0.56
1:B:198:ASP:O	1:B:201:ILE:N	2.38	0.56
1:B:573:GLN:H	1:B:573:GLN:HE21	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:GLU:C	1:B:716:ILE:HD12	2.27	0.56
1:B:643:LYS:HZ2	1:B:646:LYS:HG2	1.70	0.55
1:A:593:PHE:O	1:A:598:GLY:HA2	2.06	0.55
1:B:211:ARG:NE	1:B:213:GLU:OE2	2.35	0.55
1:B:558:ASP:O	1:B:559:SER:HB2	2.06	0.55
1:B:525:GLU:O	1:B:529:LEU:HG	2.06	0.55
1:B:642:PRO:HD2	1:B:716:ILE:HG23	1.88	0.55
1:B:250:LEU:O	1:B:254:LEU:HG	2.06	0.55
1:A:394:SER:O	1:A:398:GLN:HG3	2.07	0.54
1:B:208:LEU:HD23	1:B:209:THR:HG23	1.89	0.54
1:A:706:ASP:HB3	1:A:714:ASP:HB2	1.89	0.54
1:B:702:PHE:O	1:B:718:GLN:HA	2.07	0.54
1:A:391:ASN:HD21	1:A:398:GLN:CD	2.11	0.54
1:A:581:THR:CA	1:A:581:THR:H	2.06	0.54
1:B:391:ASN:HD21	1:B:398:GLN:CD	2.10	0.54
1:B:703:MET:HE1	5:B:825:HOH:O	2.07	0.54
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.40	0.54
1:A:381:SER:HB2	1:A:599:CYS:HA	1.90	0.54
1:B:379:LYS:HE2	5:B:881:HOH:O	2.08	0.54
1:B:418:LEU:HB2	1:B:421:VAL:HG21	1.89	0.54
1:B:234:VAL:O	1:B:238:GLN:HG3	2.08	0.54
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.38	0.54
1:A:384:PRO:HG3	1:A:431:LEU:CB	2.38	0.54
1:A:573:GLN:NE2	1:A:573:GLN:N	2.51	0.54
1:B:309:SER:HB3	1:B:339:CYS:HB3	1.89	0.54
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.29	0.54
1:B:643:LYS:HE3	1:B:646:LYS:CG	2.37	0.54
1:A:503:HIS:HA	5:A:799:HOH:O	2.08	0.54
1:B:704:VAL:O	1:B:716:ILE:HB	2.08	0.54
1:B:610:ASP:O	1:B:613:THR:OG1	2.25	0.53
4:B:1:I2P:O1	4:B:1:I2P:O21	2.26	0.53
1:B:394:SER:O	1:B:398:GLN:HG3	2.08	0.53
1:B:654:PRO:HD2	1:B:675:ILE:O	2.07	0.53
1:B:442:LEU:CD2	1:B:488:LEU:HB2	2.37	0.53
1:A:204:PHE:O	1:A:207:MET:N	2.34	0.53
1:B:395:LEU:O	1:B:399:ARG:HG3	2.09	0.53
1:B:738:LYS:HB3	1:B:738:LYS:NZ	2.24	0.53
1:B:657:ILE:HD13	1:B:671:GLN:HB3	1.91	0.53
1:B:550:ILE:HG21	1:B:567:MET:HE3	1.90	0.52
1:A:204:PHE:O	1:A:208:LEU:N	2.34	0.52
1:B:593:PHE:O	1:B:598:GLY:HA2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.40	0.52
1:A:652:VAL:HG12	1:A:653:ASP:N	2.25	0.52
1:B:412:ILE:CG2	1:B:435:ILE:HG13	2.39	0.52
1:A:622:GLN:CA	1:B:445:LEU:HD13	2.40	0.52
1:A:238:GLN:HG3	1:A:246:ALA:HB1	1.91	0.52
1:B:182:ARG:O	1:B:185:PHE:HB3	2.09	0.52
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.39	0.52
1:B:599:CYS:HA	5:B:839:HOH:O	2.09	0.52
1:B:161:ASN:H	1:B:164:GLU:CD	2.13	0.52
1:B:160:MET:O	1:B:196:LEU:N	2.43	0.52
1:B:418:LEU:HB2	1:B:421:VAL:HG23	1.90	0.52
1:B:300:GLN:O	1:B:427:SER:HA	2.10	0.52
1:A:440:LYS:HA	5:A:936:HOH:O	2.09	0.51
1:B:213:GLU:HG2	1:B:214:ILE:N	2.26	0.51
1:B:383:TYR:CD2	1:B:599:CYS:HB2	2.45	0.51
1:A:227:THR:HG22	1:A:270:MET:O	2.10	0.51
1:A:551:TYR:HB2	1:A:552:PRO:CD	2.39	0.51
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.92	0.51
1:A:738:LYS:HB3	1:A:738:LYS:NZ	2.25	0.51
1:A:222:ALA:HB2	1:A:228:LEU:HD23	1.92	0.51
1:B:728:GLN:HG2	1:B:753:SER:HA	1.91	0.51
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	2.99	0.51
1:A:398:GLN:HB3	1:A:492:LEU:HD12	1.92	0.51
1:B:218:PHE:CE1	1:B:272:LYS:HA	2.46	0.51
1:B:383:TYR:HD2	1:B:599:CYS:HB2	1.75	0.51
1:A:314:TYR:OH	1:A:343:ASP:OD2	2.30	0.51
1:A:626:TRP:CE2	1:B:445:LEU:HG	2.46	0.51
1:A:654:PRO:HG3	1:A:678:ASN:O	2.10	0.51
1:A:398:GLN:HB2	1:A:489:VAL:CG2	2.39	0.50
1:A:399:ARG:O	1:A:403:ARG:HG3	2.11	0.50
1:B:431:LEU:O	1:B:434:LYS:HB2	2.11	0.50
1:A:528:ALA:HB3	1:A:567:MET:HE1	1.93	0.50
1:A:558:ASP:O	1:A:559:SER:HB2	2.11	0.50
1:B:547:LEU:HD23	1:B:573:GLN:CG	2.40	0.50
1:A:680:PHE:CD2	1:A:681:ASN:ND2	2.80	0.50
1:B:244:GLU:C	1:B:246:ALA:H	2.14	0.50
1:B:644:VAL:HG23	1:B:645:ASN:N	2.25	0.50
1:A:675:ILE:HG12	1:A:684:TRP:NE1	2.27	0.50
1:B:346:ASP:OD1	1:B:393:CYS:HA	2.12	0.50
1:B:551:TYR:HB2	1:B:552:PRO:CD	2.42	0.50
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:680:PHE:CD2	1:B:681:ASN:ND2	2.80	0.50
1:B:708:ASP:N	1:B:713:ASN:OD1	2.38	0.50
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.93	0.49
1:A:504:PHE:HB3	1:A:527:ARG:NH2	2.26	0.49
1:B:617:SER:HA	1:B:620:LEU:HD21	1.94	0.49
1:B:384:PRO:HG3	1:B:431:LEU:HB2	1.94	0.49
1:A:492:LEU:O	1:A:495:MET:HB2	2.13	0.49
1:A:241:GLN:NE2	1:A:730:TYR:H	1.98	0.49
1:B:644:VAL:HB	1:B:645:ASN:ND2	2.27	0.49
1:B:259:GLU:OE1	1:B:270:MET:HA	2.12	0.49
1:B:643:LYS:HE3	1:B:646:LYS:HG2	1.94	0.49
1:A:324:SER:HB2	1:A:362:SER:O	2.13	0.49
1:B:229:SER:O	1:B:232:ARG:HB2	2.12	0.49
1:B:390:GLU:HG3	5:B:937:HOH:O	2.12	0.49
1:A:244:GLU:C	1:A:246:ALA:H	2.16	0.49
1:B:539:PHE:O	1:B:542:HIS:N	2.46	0.49
1:A:438:LYS:HD2	1:A:520:MET:HE1	1.95	0.48
1:A:549:ARG:C	1:A:550:ILE:HG12	2.33	0.48
1:B:222:ALA:HB2	1:B:228:LEU:CD2	2.43	0.48
1:B:350:GLN:HA	1:B:397:GLN:HE21	1.78	0.48
1:A:250:LEU:HA	1:A:253:SER:OG	2.12	0.48
1:A:617:SER:HA	1:A:620:LEU:HD21	1.95	0.48
1:A:732:HIS:HA	1:A:748:LEU:O	2.14	0.48
1:B:509:SER:HA	5:B:920:HOH:O	2.12	0.48
1:B:188:CYS:SG	1:B:204:PHE:HB2	2.54	0.48
1:B:357:GLY:HA3	5:B:897:HOH:O	2.13	0.48
1:A:665:ARG:HG2	5:A:833:HOH:O	2.13	0.48
1:B:659:GLU:OE1	1:B:701:ARG:HD3	2.14	0.48
1:A:622:GLN:HA	1:B:445:LEU:CD1	2.44	0.48
1:B:231:GLU:O	1:B:235:THR:OG1	2.30	0.48
1:A:222:ALA:HA	1:A:228:LEU:CD2	2.44	0.47
1:B:346:ASP:HA	1:B:397:GLN:OE1	2.14	0.47
1:A:626:TRP:CE3	1:B:445:LEU:HD21	2.50	0.47
1:B:313:THR:HG21	1:B:329:TYR:CD1	2.50	0.47
1:B:509:SER:N	1:B:510:PRO:HD2	2.30	0.47
1:B:617:SER:HB2	1:B:663:VAL:HG12	1.96	0.47
1:B:644:VAL:CG2	1:B:645:ASN:H	2.13	0.47
1:A:298:MET:O	1:A:429:GLU:HG2	2.15	0.47
1:A:617:SER:HB2	1:A:663:VAL:HG12	1.95	0.47
1:B:644:VAL:HG11	1:B:715:PHE:O	2.14	0.47
1:A:222:ALA:CB	1:A:228:LEU:HD23	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:HG12	1:A:235:THR:N	2.28	0.47
1:B:174:ILE:HG22	1:B:176:VAL:HG13	1.96	0.47
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.95	0.47
1:A:557:THR:N	5:A:808:HOH:O	2.48	0.47
1:A:730:TYR:C	1:A:731:ARG:HG2	2.35	0.47
1:B:188:CYS:SG	1:B:204:PHE:HA	2.55	0.47
1:B:353:ILE:HD12	1:B:363:LYS:HG2	1.97	0.47
1:B:732:HIS:HA	1:B:748:LEU:O	2.15	0.47
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.96	0.47
1:B:520:MET:HG3	1:B:547:LEU:O	2.15	0.47
1:B:736:LEU:HD23	1:B:742:GLN:HA	1.97	0.47
1:A:233:LEU:O	1:A:236:PHE:HB3	2.14	0.46
1:A:237:LEU:HD13	1:A:250:LEU:HD23	1.98	0.46
1:A:496:ILE:N	1:A:496:ILE:HD12	2.31	0.46
1:A:578:ASN:HB3	1:A:580:GLN:OE1	2.14	0.46
1:B:646:LYS:HG3	1:B:650:SER:HB3	1.95	0.46
1:A:429:GLU:OE1	1:A:432:LYS:HE2	2.15	0.46
1:A:653:ASP:HA	1:A:675:ILE:O	2.16	0.46
1:B:489:VAL:HG12	5:B:929:HOH:O	2.15	0.46
1:A:346:ASP:OD2	1:A:394:SER:HB3	2.15	0.46
1:A:393:CYS:CB	1:A:401:MET:HE3	2.45	0.46
1:A:415:ASP:O	1:A:416:GLN:HG2	2.15	0.46
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.48	0.46
1:A:289:LEU:O	1:A:289:LEU:HD12	2.15	0.46
1:B:333:LEU:HD21	1:B:340:LEU:HD11	1.98	0.46
1:B:613:THR:HG22	1:B:615:PHE:H	1.81	0.46
1:A:556:ARG:HG2	1:A:560:SER:OG	2.15	0.46
1:B:188:CYS:SG	1:B:203:THR:HG22	2.56	0.46
1:B:328:ALA:HB1	5:B:871:HOH:O	2.16	0.46
1:B:644:VAL:CG1	1:B:716:ILE:HA	2.45	0.46
1:A:222:ALA:HB2	1:A:228:LEU:CD2	2.45	0.46
1:B:509:SER:H	1:B:510:PRO:HD2	1.79	0.46
1:A:681:ASN:N	1:A:682:PRO:CD	2.79	0.46
1:A:694:VAL:HG12	1:A:694:VAL:O	2.15	0.46
1:B:314:TYR:HB3	1:B:329:TYR:CE2	2.51	0.45
1:B:613:THR:HG23	5:B:777:HOH:O	2.17	0.45
1:B:540:VAL:HG13	1:B:608:LEU:HD22	1.98	0.45
1:B:550:ILE:HG21	1:B:567:MET:CE	2.46	0.45
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.17	0.45
1:A:547:LEU:HD23	1:A:573:GLN:CG	2.43	0.45
1:A:562:TYR:O	1:A:585:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:ASP:O	1:B:354:ILE:HA	2.16	0.45
1:A:214:ILE:HD13	1:A:214:ILE:HA	1.79	0.45
1:B:233:LEU:O	1:B:236:PHE:HB3	2.16	0.45
1:B:259:GLU:OE2	1:B:260:PRO:HD2	2.17	0.45
1:B:391:ASN:OD1	1:B:393:CYS:HB2	2.17	0.45
1:B:396:GLU:O	1:B:399:ARG:HB2	2.16	0.45
1:B:643:LYS:HD3	1:B:643:LYS:HA	1.58	0.45
1:B:228:LEU:HB2	1:B:270:MET:HB3	1.98	0.45
1:B:580:GLN:HG3	1:B:580:GLN:H	1.27	0.45
1:A:200:GLU:N	1:A:203:THR:CB	2.80	0.45
1:A:520:MET:HG3	1:A:547:LEU:O	2.16	0.45
1:B:412:ILE:HG22	1:B:435:ILE:HG13	1.99	0.45
1:B:549:ARG:C	1:B:550:ILE:HG12	2.36	0.45
1:A:504:PHE:CZ	1:A:506:GLY:CA	2.98	0.45
1:B:441:LYS:HB2	1:B:500:LYS:HG3	1.99	0.45
1:A:438:LYS:HE3	1:A:520:MET:CE	2.47	0.44
1:B:196:LEU:CB	1:B:201:ILE:HD11	2.43	0.44
1:B:580:GLN:HG2	5:B:870:HOH:O	2.17	0.44
1:A:523:PHE:HB2	1:A:550:ILE:HD13	1.99	0.44
1:B:686:MET:HG3	1:B:687:GLU:N	2.32	0.44
1:A:314:TYR:CE1	1:A:315:LEU:HG	2.52	0.44
1:B:653:ASP:O	1:B:674:VAL:HG13	2.17	0.44
1:B:291:HIS:HD2	1:B:725:SER:OG	1.99	0.44
1:B:227:THR:HG22	1:B:270:MET:O	2.17	0.44
1:B:634:ARG:NH2	5:B:762:HOH:O	2.30	0.44
1:B:405:LEU:HA	1:B:405:LEU:HD23	1.74	0.44
1:B:369:VAL:O	1:B:373:ILE:HG13	2.18	0.44
1:B:549:ARG:HG3	1:B:574:ILE:HG22	2.00	0.44
1:B:664:GLY:O	1:B:667:THR:OG1	2.35	0.44
1:B:701:ARG:HD3	1:B:701:ARG:HH11	1.66	0.44
1:B:730:TYR:CE1	1:B:751:LYS:HD3	2.53	0.44
1:A:248:PRO:HD2	1:A:249:ALA:H	1.83	0.44
1:A:657:ILE:HD13	1:A:671:GLN:HB3	2.00	0.44
1:B:165:LEU:O	1:B:168:PHE:N	2.51	0.44
1:A:241:GLN:HE22	1:A:730:TYR:N	1.97	0.44
1:A:341:GLU:OE1	1:A:549:ARG:NH2	2.50	0.44
1:A:349:ASN:O	1:A:349:ASN:OD1	2.36	0.44
1:A:646:LYS:C	1:A:648:LYS:H	2.21	0.44
1:A:680:PHE:HD2	1:A:681:ASN:ND2	2.15	0.44
1:B:169:LEU:O	1:B:172:LEU:O	2.36	0.44
1:B:736:LEU:CD2	1:B:742:GLN:HG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:SER:OG	1:A:574:ILE:HG23	2.18	0.43
1:A:615:PHE:HA	5:A:839:HOH:O	2.18	0.43
1:B:533:GLN:HA	1:B:533:GLN:OE1	2.17	0.43
1:B:701:ARG:HE	1:B:718:GLN:HG3	1.83	0.43
1:A:291:HIS:HD2	1:A:725:SER:OG	2.01	0.43
1:A:504:PHE:CE2	1:A:506:GLY:HA2	2.52	0.43
1:B:253:SER:HB2	1:B:257:ARG:HH21	1.83	0.43
1:A:702:PHE:O	1:A:718:GLN:HA	2.18	0.43
1:B:654:PRO:HG3	1:B:678:ASN:O	2.18	0.43
1:B:660:ILE:O	1:B:667:THR:HA	2.19	0.43
1:B:641:LEU:N	1:B:679:GLY:O	2.48	0.43
1:B:628:PRO:HA	1:B:693:THR:HA	2.00	0.43
1:B:648:LYS:C	1:B:650:SER:H	2.22	0.43
1:A:701:ARG:HH21	1:A:718:GLN:HG3	1.83	0.43
1:B:160:MET:H	1:B:196:LEU:H	1.65	0.43
1:A:213:GLU:HG2	1:A:214:ILE:N	2.32	0.43
1:B:310:SER:HG	1:B:313:THR:HG1	1.67	0.43
1:A:300:GLN:O	1:A:305:TYR:HE1	2.02	0.43
1:B:258:TYR:O	1:B:260:PRO:HD3	2.18	0.43
1:B:183:LYS:O	1:B:187:GLU:HG3	2.19	0.43
1:B:738:LYS:CB	1:B:738:LYS:NZ	2.81	0.43
1:A:438:LYS:HA	1:A:499:CYS:HB2	2.01	0.43
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.49	0.43
1:B:645:ASN:O	1:B:647:ASN:N	2.52	0.43
1:A:405:LEU:HD23	1:A:405:LEU:HA	1.87	0.42
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.72	0.42
1:B:241:GLN:NE2	1:B:241:GLN:CA	2.83	0.42
1:B:345:TRP:CZ2	1:B:392:HIS:CD2	3.06	0.42
1:A:398:GLN:CB	1:A:489:VAL:CG2	2.96	0.42
1:B:176:VAL:CG2	1:B:181:ALA:HB2	2.49	0.42
1:B:442:LEU:HD21	1:B:488:LEU:CB	2.44	0.42
1:A:507:PHE:O	1:A:510:PRO:HD2	2.19	0.42
1:B:574:ILE:HG22	1:B:574:ILE:O	2.19	0.42
1:A:259:GLU:OE2	1:A:260:PRO:HD2	2.20	0.42
1:B:237:LEU:HD23	1:B:237:LEU:HA	1.77	0.42
1:B:388:SER:HB2	1:B:438:LYS:HD3	2.01	0.42
1:A:272:LYS:O	1:A:275:PHE:HB3	2.19	0.42
1:A:321:THR:HG22	1:A:360:PHE:HB2	2.01	0.42
1:A:426:PRO:HG2	1:A:431:LEU:CD1	2.32	0.42
1:A:689:GLU:OE2	1:B:494:ASP:OD2	2.37	0.42
1:B:562:TYR:O	1:B:585:GLU:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:694:VAL:O	1:B:694:VAL:HG12	2.19	0.42
1:A:556:ARG:HA	5:A:808:HOH:O	2.19	0.42
1:B:212:ALA:O	1:B:215:ASP:HB2	2.19	0.42
1:B:259:GLU:HA	1:B:260:PRO:HD2	1.88	0.42
1:A:393:CYS:SG	1:A:401:MET:CE	3.08	0.42
1:B:198:ASP:O	1:B:201:ILE:HB	2.20	0.42
1:B:241:GLN:N	1:B:241:GLN:HE21	2.17	0.42
1:B:549:ARG:HG3	1:B:574:ILE:CG2	2.50	0.42
1:A:314:TYR:HB3	1:A:329:TYR:CE2	2.55	0.41
1:A:354:ILE:HD12	1:A:369:VAL:HG21	2.02	0.41
1:A:393:CYS:HB2	1:A:401:MET:HE3	2.01	0.41
1:A:437:LEU:HD23	1:A:437:LEU:HA	1.63	0.41
1:B:238:GLN:O	1:B:242:ARG:HA	2.20	0.41
1:A:628:PRO:HA	1:A:693:THR:HA	2.01	0.41
1:B:313:THR:CG2	1:B:329:TYR:CD1	3.03	0.41
1:B:509:SER:N	1:B:510:PRO:CD	2.82	0.41
1:A:391:ASN:OD1	1:A:393:CYS:HB2	2.20	0.41
1:A:556:ARG:HH11	1:A:556:ARG:HG2	1.86	0.41
1:A:398:GLN:CB	1:A:489:VAL:HG21	2.48	0.41
1:A:703:MET:HE2	1:A:715:PHE:HD1	1.84	0.41
1:B:191:SER:OG	1:B:193:THR:HG23	2.20	0.41
1:B:370:LEU:CD1	1:B:405:LEU:HD23	2.50	0.41
1:B:208:LEU:HD23	1:B:209:THR:CG2	2.50	0.41
1:B:219:GLU:O	1:B:223:GLY:N	2.42	0.41
1:B:661:HIS:O	1:B:698:ALA:HA	2.21	0.41
1:B:178:ASP:O	1:B:182:ARG:N	2.51	0.41
1:B:188:CYS:SG	1:B:204:PHE:CA	3.09	0.41
1:B:214:ILE:HD13	1:B:214:ILE:HA	1.89	0.41
1:B:352:PRO:HD3	1:B:400:VAL:HG11	2.03	0.41
1:B:706:ASP:N	1:B:716:ILE:HD12	2.35	0.41
1:A:738:LYS:NZ	1:A:738:LYS:CB	2.83	0.41
1:B:248:PRO:O	1:B:252:LEU:HB2	2.21	0.41
1:A:654:PRO:HD2	1:A:675:ILE:O	2.21	0.41
1:A:536:GLY:HA3	1:A:616:ASN:ND2	2.36	0.41
1:B:701:ARG:HH21	1:B:718:GLN:HG3	1.86	0.41
1:A:438:LYS:HE3	1:A:520:MET:HE2	2.03	0.41
1:A:590:LEU:HA	1:A:590:LEU:HD23	1.79	0.41
1:A:728:GLN:HG2	1:A:753:SER:HA	2.02	0.41
1:B:166:LYS:NZ	1:B:178:ASP:HA	2.35	0.41
1:B:272:LYS:O	1:B:275:PHE:HB3	2.21	0.41
1:B:381:SER:HB2	1:B:599:CYS:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:PHE:CD1	1:B:272:LYS:HA	2.56	0.40
1:B:681:ASN:N	1:B:682:PRO:CD	2.83	0.40
1:A:259:GLU:O	1:A:265:LYS:HD2	2.21	0.40
1:A:516:ALA:CB	1:A:518:TYR:CZ	3.04	0.40
1:B:289:LEU:O	1:B:289:LEU:HD12	2.20	0.40
1:B:542:HIS:CD2	1:B:542:HIS:C	2.94	0.40
1:B:730:TYR:CZ	1:B:751:LYS:HD3	2.56	0.40
1:A:222:ALA:HA	1:A:228:LEU:HD23	2.03	0.40
1:B:164:GLU:H	1:B:164:GLU:HG3	1.67	0.40
1:B:258:TYR:CE1	1:B:281:SER:HB2	2.56	0.40
1:B:641:LEU:HD23	1:B:641:LEU:HA	1.80	0.40
1:B:352:PRO:HA	1:B:397:GLN:OE1	2.22	0.40
1:B:439:GLY:CA	5:B:935:HOH:O	2.69	0.40
1:A:396:GLU:O	1:A:399:ARG:HB2	2.21	0.40
1:B:516:ALA:CB	1:B:518:TYR:CZ	3.05	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:NE2	1:A:238:GLN:NE2[52_555]	2.03	0.17

## 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%)	461 (91%)	39 (8%)	9 (2%)	8	28
1	B	557/624 (89%)	495 (89%)	51 (9%)	11 (2%)	7	24
All	All	1066/1248 (85%)	956 (90%)	90 (8%)	20 (2%)	8	26

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	581	THR
1	A	645	ASN
1	A	710	SER
1	B	173	ASN
1	B	644	VAL
1	A	204	PHE
1	A	509	SER
1	A	540	VAL
1	B	540	VAL
1	B	646	LYS
1	A	539	PHE
1	B	645	ASN
1	A	579	PHE
1	B	198	ASP
1	B	242	ARG
1	A	514	GLY
1	B	288	SER
1	B	539	PHE
1	B	417	PRO
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	444/545 (82%)	401 (90%)	43 (10%)	8	24
1	B	492/545 (90%)	437 (89%)	55 (11%)	6	18
All	All	936/1090 (86%)	838 (90%)	98 (10%)	7	20

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LEU
1	A	210	GLN
1	A	216	ARG
1	A	220	GLU

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Mol	Chain	Res	Type
1	A	227	THR
1	A	232	ARG
1	A	234	VAL
1	A	242	ARG
1	A	253	SER
1	A	257	ARG
1	A	261	SER
1	A	309	SER
1	A	362	SER
1	A	424	SER
1	A	436	LEU
1	A	487	LYS
1	A	489	VAL
1	A	508	SER
1	A	513	SER
1	A	526	SER
1	A	535	SER
1	A	539	PHE
1	A	545	SER
1	A	563	SER
1	A	573	GLN
1	A	579	PHE
1	A	580	GLN
1	A	581	THR
1	A	594	GLN
1	A	643	LYS
1	A	646	LYS
1	A	648	LYS
1	A	655	LYS
1	A	665	ARG
1	A	667	THR
1	A	685	ASP
1	A	709	SER
1	A	727	LYS
1	A	738	LYS
1	A	742	GLN
1	A	745	SER
1	A	753	SER
1	A	756	ASP
1	B	158	ASN
1	B	159	LYS
1	B	162	PHE

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Mol	Chain	Res	Type
1	B	163	LYS
1	B	164	GLU
1	B	165	LEU
1	B	168	PHE
1	B	178	ASP
1	B	186	ARG
1	B	194	ASP
1	B	195	SER
1	B	199	GLU
1	B	227	THR
1	B	232	ARG
1	B	242	ARG
1	B	252	LEU
1	B	253	SER
1	B	261	SER
1	B	268	ARG
1	B	309	SER
1	B	331	ARG
1	B	362	SER
1	B	371	ARG
1	B	425	LEU
1	B	436	LEU
1	B	484	ASP
1	B	486	LEU
1	B	489	VAL
1	B	492	LEU
1	B	526	SER
1	B	535	SER
1	B	539	PHE
1	B	545	SER
1	B	550	ILE
1	B	573	GLN
1	B	577	LEU
1	B	579	PHE
1	B	580	GLN
1	B	594	GLN
1	B	618	ARG
1	B	643	LYS
1	B	646	LYS
1	B	648	LYS
1	B	652	VAL
1	B	655	LYS

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Mol	Chain	Res	Type
1	B	665	ARG
1	B	667	THR
1	B	683	ARG
1	B	685	ASP
1	B	710	SER
1	B	711	SER
1	B	738	LYS
1	B	745	SER
1	B	753	SER
1	B	756	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	241	GLN
1	A	291	HIS
1	A	349	ASN
1	A	573	GLN
1	A	594	GLN
1	A	639	GLN
1	A	645	ASN
1	A	718	GLN
1	A	734	HIS
1	B	241	GLN
1	B	291	HIS
1	B	515	GLN
1	B	542	HIS
1	B	573	GLN
1	B	594	GLN
1	B	639	GLN
1	B	645	ASN
1	B	718	GLN
1	B	728	GLN
1	B	734	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 6 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$
4	I2P	A	1	2	24,24,24	1.85	7 (29%)	36,39,39	2.21	11 (30%)
4	I2P	B	1	2	24,24,24	1.88	7 (29%)	36,39,39	2.05	13 (36%)
3	ACT	B	5	-	1,3,3	3.15	1 (100%)	0,3,3	0.00	-
3	ACT	A	5	-	1,3,3	2.82	1 (100%)	0,3,3	0.00	-

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	I2P	A	1	2	-	4/15/39/39	0/1/1/1
4	I2P	B	1	2	-	4/15/39/39	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	I2P	P5-O51	4.62	1.65	1.50
4	B	1	I2P	P5-O5	4.60	1.68	1.59
4	A	1	I2P	P5-O5	4.47	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	I2P	P5-O51	4.45	1.64	1.50
3	B	5	ACT	CH3-C	3.15	1.52	1.48
4	A	1	I2P	P4-O43	2.83	1.65	1.54
3	A	5	ACT	CH3-C	2.82	1.52	1.48
4	B	1	I2P	O1-C1	-2.79	1.36	1.43
4	B	1	I2P	C5-C4	2.56	1.57	1.52
4	A	1	I2P	P5-O53	2.47	1.64	1.54
4	A	1	I2P	P4-O41	2.47	1.58	1.50
4	A	1	I2P	P2-O21	2.46	1.58	1.50
4	B	1	I2P	P4-O41	2.42	1.58	1.50
4	A	1	I2P	P2-O22	2.34	1.63	1.54
4	B	1	I2P	P4-O43	2.10	1.62	1.54
4	B	1	I2P	P5-O53	2.06	1.62	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	I2P	C1-C6-C5	-5.48	97.16	109.68
4	A	1	I2P	O4-C4-C5	-5.22	96.37	108.69
4	A	1	I2P	O4-C4-C3	-5.03	96.97	108.66
4	A	1	I2P	O1-C1-C2	4.94	123.04	109.94
4	B	1	I2P	C1-C6-C5	-4.49	99.43	109.68
4	B	1	I2P	O1-C1-C6	-4.41	100.15	110.35
4	B	1	I2P	O4-C4-C5	-4.17	98.85	108.69
4	B	1	I2P	O2-P2-O21	-3.73	95.00	109.39
4	B	1	I2P	O23-P2-O21	-3.73	96.09	110.68
4	A	1	I2P	C3-C2-C1	-3.59	105.68	110.85
4	B	1	I2P	O23-P2-O2	2.91	119.03	105.99
4	A	1	I2P	O23-P2-O21	-2.84	99.55	110.68
4	A	1	I2P	O1-C1-C6	-2.70	104.10	110.35
4	B	1	I2P	O5-C5-C6	-2.69	102.42	108.66
4	A	1	I2P	O2-P2-O21	-2.60	99.35	109.39
4	B	1	I2P	O4-C4-C3	-2.55	102.72	108.66
4	B	1	I2P	O1-C1-C2	2.45	116.44	109.94
4	B	1	I2P	O22-P2-O21	2.43	120.19	110.68
4	A	1	I2P	O23-P2-O2	2.15	115.63	105.99
4	A	1	I2P	O42-P4-O41	-2.15	102.26	110.68
4	B	1	I2P	C6-C1-C2	2.14	114.57	109.68
4	B	1	I2P	C6-C5-C4	2.07	116.39	111.66
4	B	1	I2P	O3-C3-C2	-2.07	104.46	109.94
4	A	1	I2P	O5-P5-O51	2.06	117.33	109.39

There are no chirality outliers.

All (8) torsion outliers are listed below:

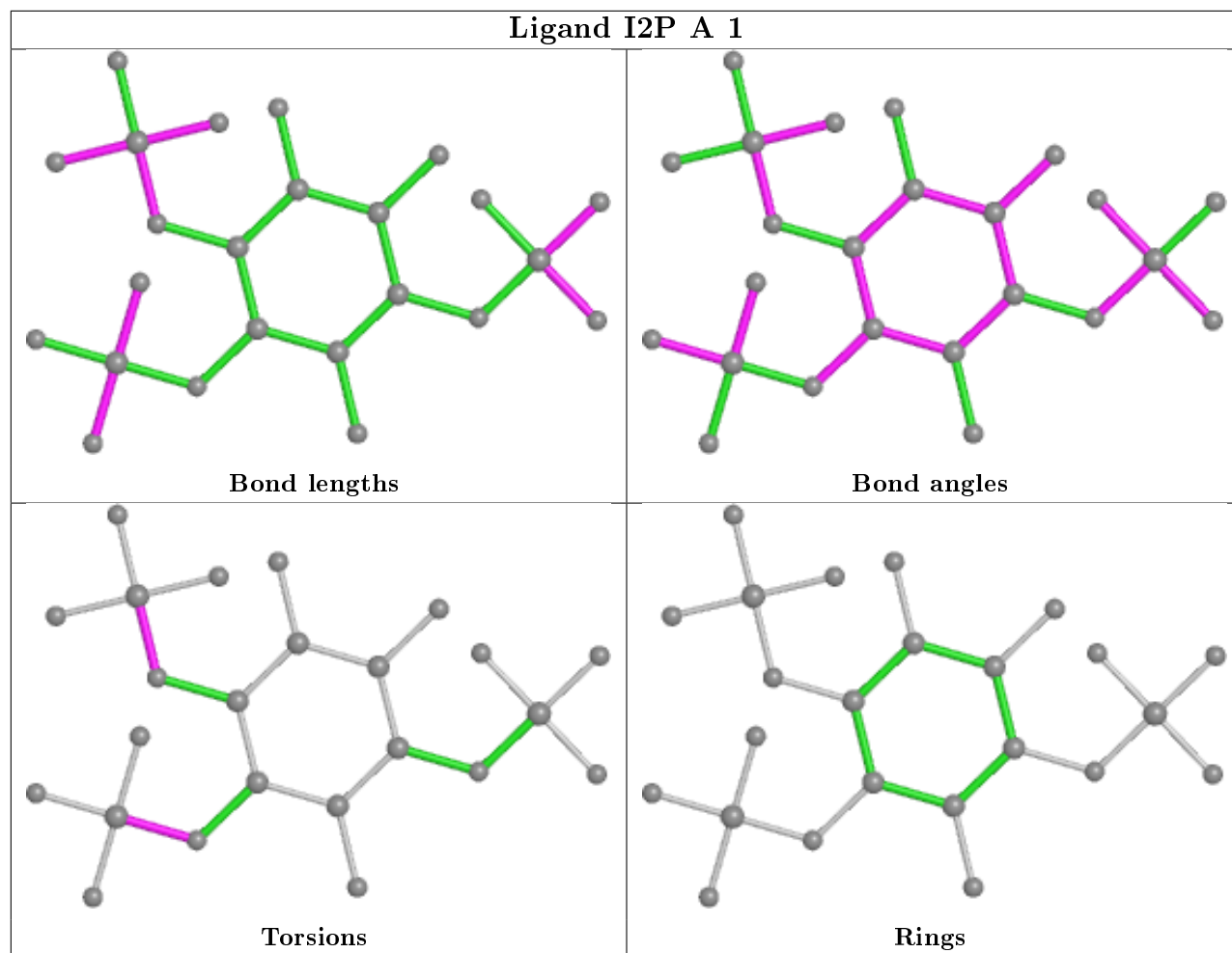
Mol	Chain	Res	Type	Atoms
4	A	1	I2P	C4-O4-P4-O41
4	A	1	I2P	C5-O5-P5-O52
4	B	1	I2P	C1-C2-O2-P2
4	A	1	I2P	C4-O4-P4-O42
4	A	1	I2P	C5-O5-P5-O53
4	B	1	I2P	C3-C2-O2-P2
4	B	1	I2P	C2-O2-P2-O22
4	B	1	I2P	C5-O5-P5-O53

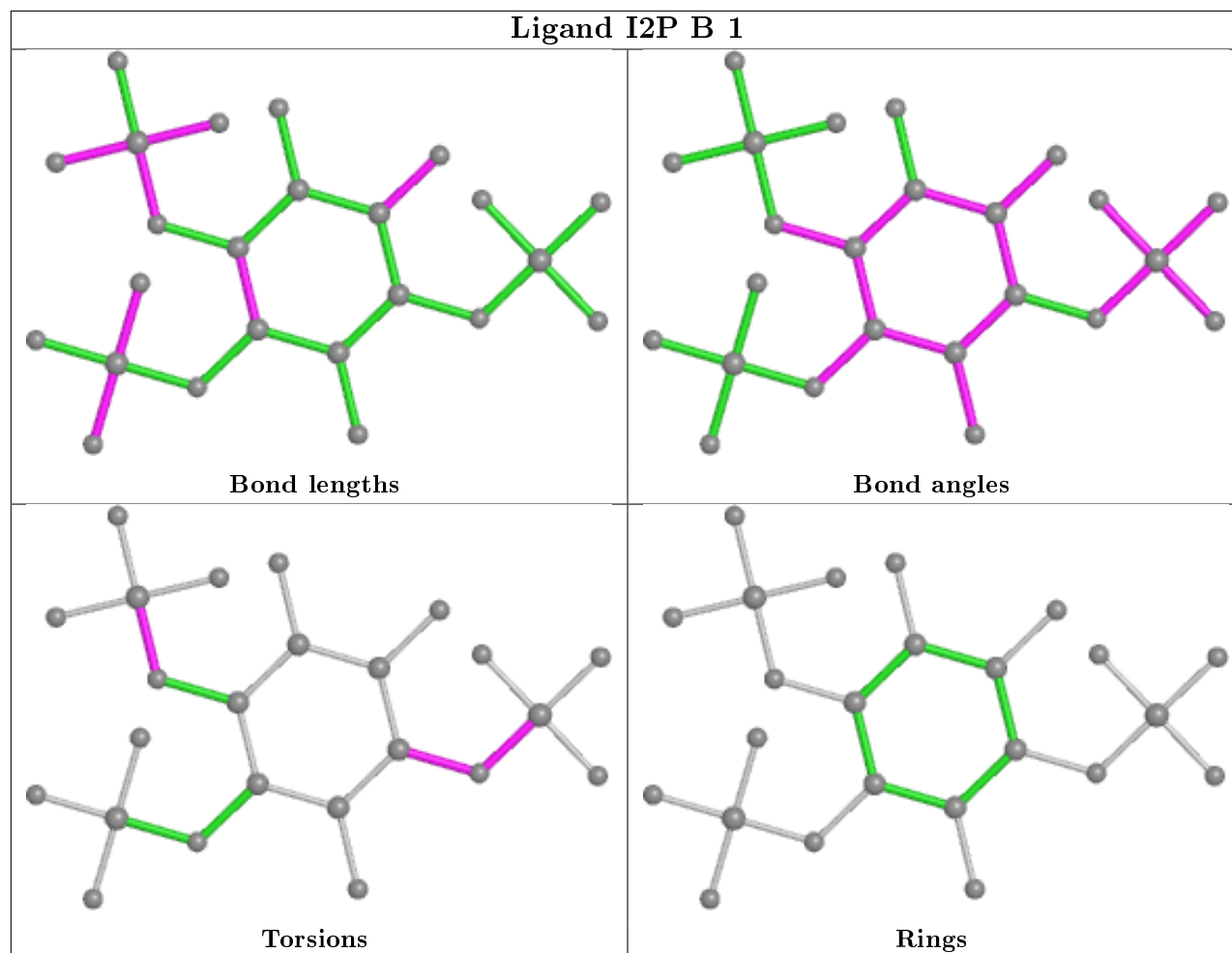
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	I2P	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	509/624 (81%)	-0.49	20 (3%)	39 29	5, 23, 78, 104	19 (3%)
1	B	556/624 (89%)	-0.44	15 (2%)	54 44	4, 24, 77, 112	21 (3%)
All	All	1065/1248 (85%)	-0.46	35 (3%)	46 36	4, 24, 78, 112	40 (3%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	ILE	8.4
1	A	202	GLU	7.0
1	B	510	PRO	6.9
1	A	510	PRO	6.7
1	A	205	TYR	6.2
1	A	509	SER	5.7
1	B	645	ASN	5.5
1	B	509	SER	5.5
1	A	647	ASN	5.0
1	A	203	THR	4.0
1	B	647	ASN	4.0
1	B	484	ASP	3.9
1	A	421	VAL	3.6
1	A	200	GLU	3.6
1	B	508	SER	3.5
1	A	420	GLY	3.2
1	B	648	LYS	3.2
1	A	645	ASN	3.1
1	B	261	SER	3.0
1	B	486	LEU	2.9
1	A	208	LEU	2.8
1	A	711	SER	2.6
1	B	160	MET	2.5
1	A	504	PHE	2.4

*Continued on next page...*



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Mol	Chain	Res	Type	RSRZ
1	A	505	GLY	2.4
1	B	710	SER	2.3
1	A	204	PHE	2.2
1	A	709	SER	2.2
1	B	245	GLU	2.2
1	B	646	LYS	2.2
1	B	161	ASN	2.1
1	A	508	SER	2.0
1	A	710	SER	2.0
1	B	173	ASN	2.0
1	A	503	HIS	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, 95<sup>th</sup> 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.

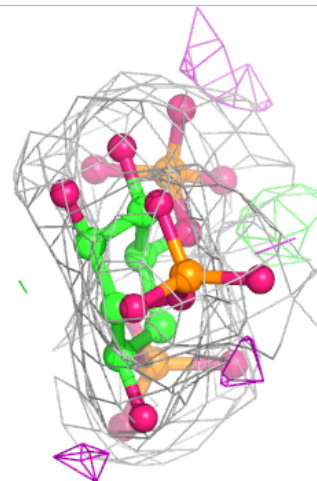
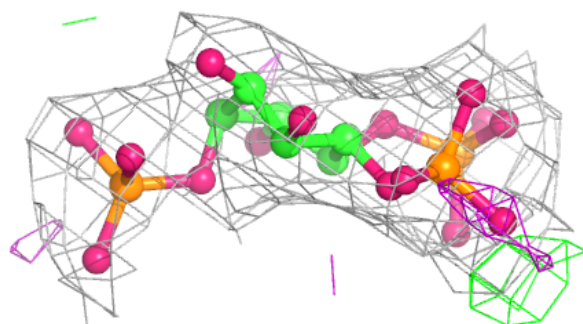
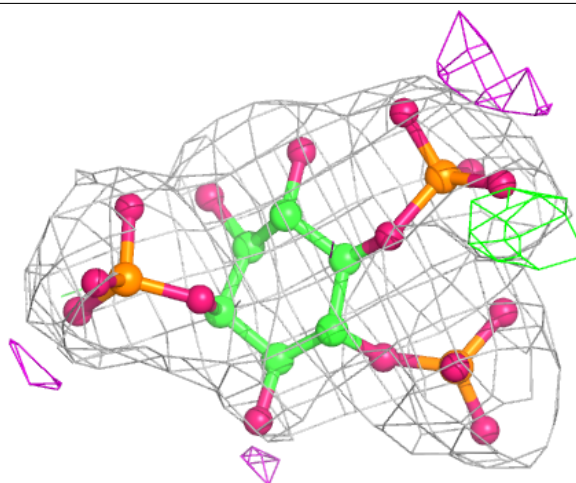
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	3	1/1	0.92	0.07	58,58,58,58	0
2	CA	A	4	1/1	0.94	0.07	89,89,89,89	0
2	CA	B	4	1/1	0.95	0.18	72,72,72,72	0
2	CA	B	3	1/1	0.96	0.06	68,68,68,68	0
4	I2P	A	1	24/24	0.97	0.12	16,29,61,63	0
4	I2P	B	1	24/24	0.98	0.10	12,26,41,45	0
2	CA	A	2	1/1	0.98	0.05	24,24,24,24	0
3	ACT	A	5	4/4	0.98	0.22	35,38,38,40	0
3	ACT	B	5	4/4	0.99	0.14	23,30,31,36	0
2	CA	B	2	1/1	0.99	0.06	13,13,13,13	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.

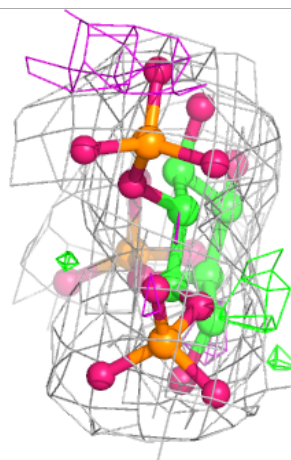
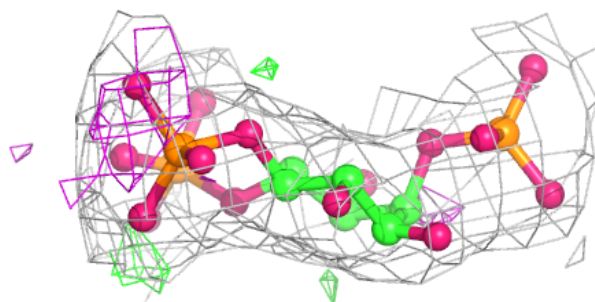
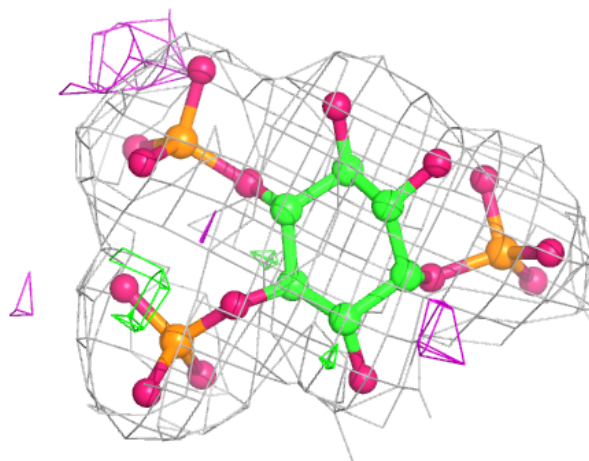
**Electron density around I2P A 1:**

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



**Electron density around I2P 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.