



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:34 pm BST

PDB ID : 1DJW  
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM  
RAT COMPLEXED WITH INOSITOL-2-METHYLENE-1,2-CYCLIC-MON  
OPHOSPHONATE  
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.  
Deposited on : 1996-08-24  
Resolution : 2.45 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  
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

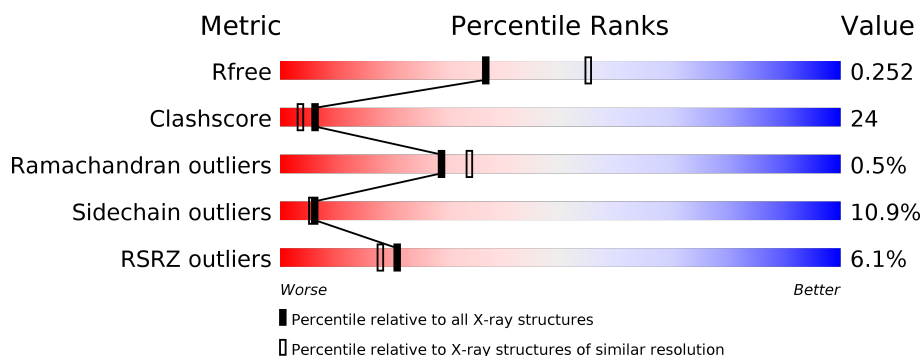
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	 6% 47% 31% • 18%
1	B	624	 4% 52% 34% • 10%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9318 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	89	0	0
			4057	2565	709	761	22			
1	B	561	Total	C	N	O	S	78	0	0
			4465	2818	776	847	24			

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

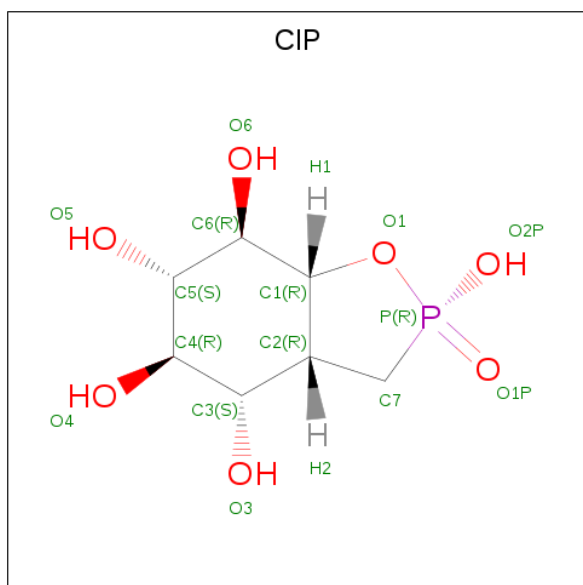
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ca	0	0
			3	3		
2	A	3	Total	Ca	0	0
			3	3		

- 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 INOSITOL-2-METHYLENE-1,2-CYCLIC-MONOPHOSPHATE (three-letter code: CIP) (formula:  $C_7H_{13}O_7P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			15	7	7	1		
4	B	1	Total	C	O	P	0	0
			15	7	7	1		

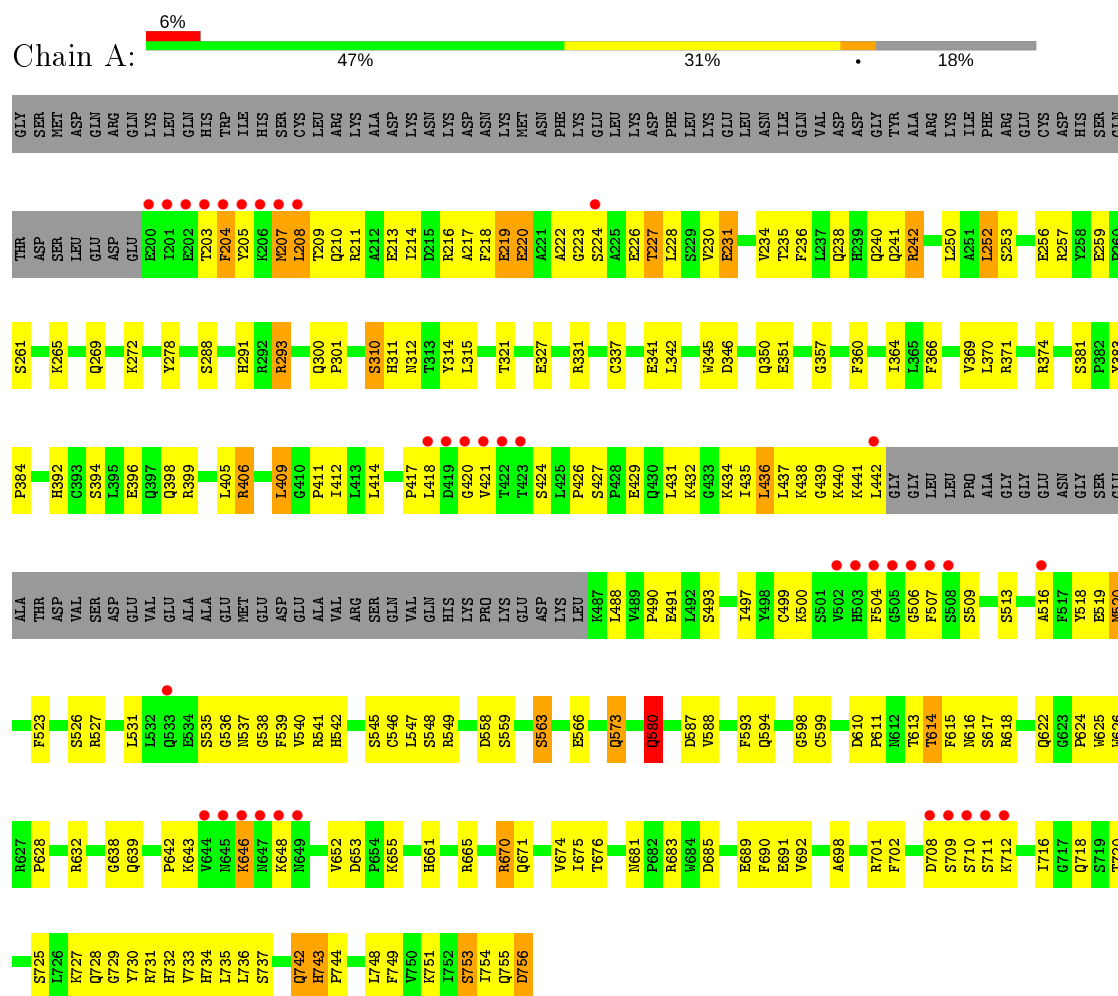
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	327	Total	O	0	0
			327	327		
5	B	425	Total	O	0	0
			425	425		

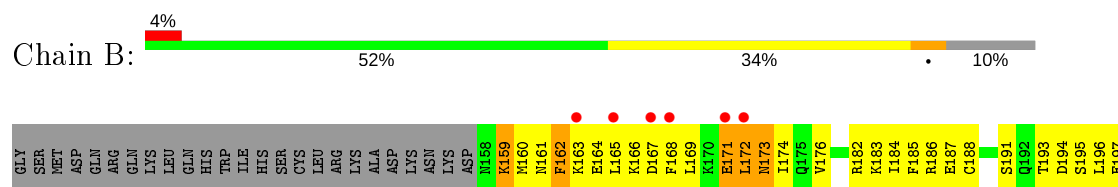
### 3 Residue-property plots

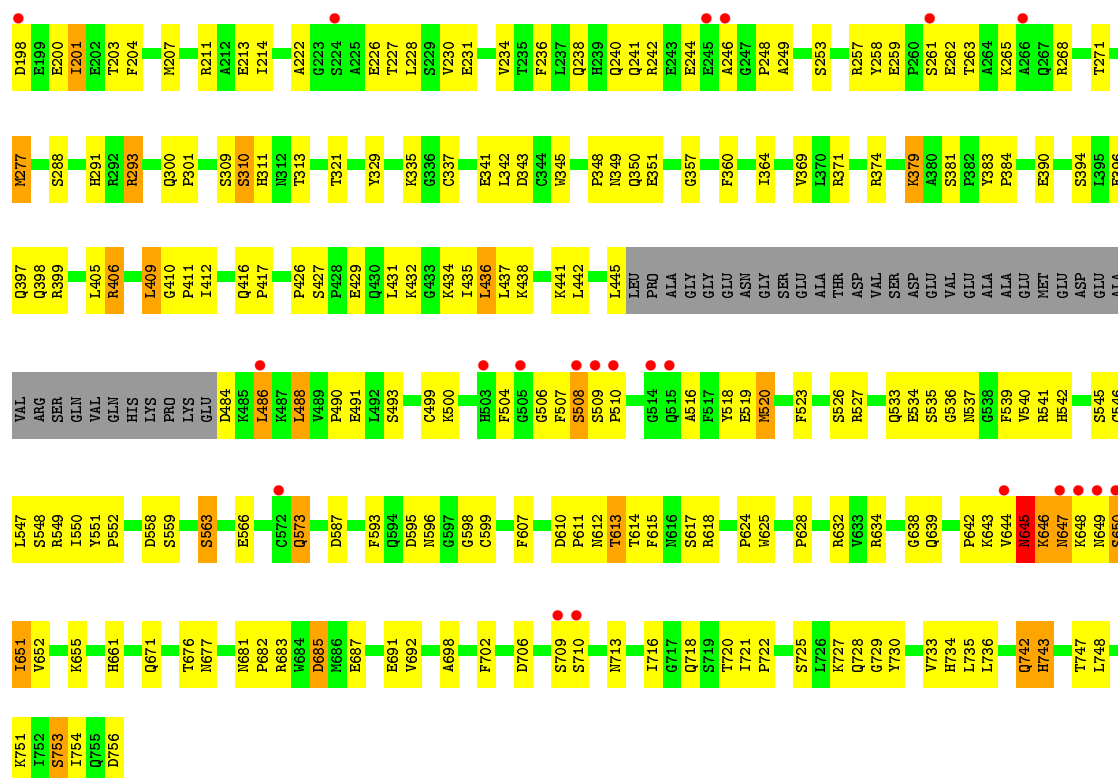
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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



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## 4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	397.03Å 397.03Å 397.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.45 24.81 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.0 (10.00-2.45) 98.0 (24.81-2.30)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.58 (at 2.31Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.217 , 0.270 0.209 , 0.252	Depositor DCC
$R_{free}$ test set	4692 reflections (4.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 94.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9318	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: CA, CIP, 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	0.75	6/4152 (0.1%)	0.81	3/5624 (0.1%)
1	B	0.68	4/4565 (0.1%)	0.80	3/6174 (0.0%)
All	All	0.72	10/8717 (0.1%)	0.80	6/11798 (0.1%)

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	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	GLU	CD-OE1	-12.22	1.12	1.25
1	A	702	PHE	CE2-CZ	-7.24	1.23	1.37
1	A	702	PHE	CG-CD1	-6.93	1.28	1.38
1	B	702	PHE	CE1-CZ	-6.55	1.25	1.37
1	A	702	PHE	CE1-CZ	-6.32	1.25	1.37
1	B	702	PHE	CE2-CZ	-6.05	1.25	1.37
1	B	702	PHE	CG-CD2	-5.71	1.30	1.38
1	A	626	TRP	CB-CG	-5.38	1.40	1.50
1	A	702	PHE	CG-CD2	-5.36	1.30	1.38
1	B	702	PHE	CG-CD1	-5.31	1.30	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	743	HIS	C-N-CD	-7.94	103.14	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	743	HIS	C-N-CD	-7.74	103.57	120.60
1	A	580	GLN	CB-CA-C	-6.63	97.14	110.40
1	B	645	ASN	N-CA-C	6.41	128.31	111.00
1	A	420	GLY	N-CA-C	-6.36	97.21	113.10
1	B	508	SER	N-CA-C	6.03	127.27	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	238	GLN	Sidechain
1	A	580	GLN	Sidechain

## 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	177	1
1	B	4465	0	4375	232	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	15	0	12	4	0
4	B	15	0	12	4	0
5	A	327	0	0	25	1
5	B	425	0	0	19	0
All	All	9318	0	8377	403	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 24.

All (403) 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:504:PHE:HB3	1:A:527:ARG:HH22	1.18	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.20	1.01
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.45	0.97
1:B:644:VAL:HG23	1:B:645:ASN:H	1.29	0.96
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.09	0.86
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.03	0.86
1:A:613:THR:HG22	1:A:615:PHE:H	1.40	0.86
1:B:348:PRO:HB2	1:B:349:ASN:ND2	1.91	0.86
1:B:728:GLN:NE2	1:B:754:ILE:H	1.73	0.86
1:B:486:LEU:H	1:B:486:LEU:HD12	1.42	0.85
1:A:537:ASN:HB3	5:A:797:HOH:O	1.76	0.85
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.94	0.83
1:B:504:PHE:HB3	1:B:527:ARG:NH2	1.94	0.83
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.60	0.82
1:B:548:SER:H	1:B:573:GLN:NE2	1.76	0.82
1:A:548:SER:H	1:A:573:GLN:NE2	1.77	0.81
1:A:439:GLY:HA2	5:A:1083:HOH:O	1.80	0.80
1:A:728:GLN:NE2	1:A:754:ILE:H	1.81	0.78
1:A:241:GLN:HE22	1:A:730:TYR:H	1.30	0.78
1:B:168:PHE:CE1	1:B:172:LEU:HD21	2.19	0.78
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.19	0.78
1:A:350:GLN:OE1	1:A:396:GLU:HG3	1.84	0.77
1:B:509:SER:HB2	5:B:1131:HOH:O	1.83	0.77
1:A:670:ARG:HD3	5:A:830:HOH:O	1.85	0.77
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.66	0.75
1:A:516:ALA:HB3	1:A:519:GLU:HG3	1.68	0.75
1:A:646:LYS:HA	1:A:646:LYS:CE	2.17	0.74
1:B:643:LYS:HE3	1:B:645:ASN:CB	2.18	0.74
1:A:573:GLN:H	1:A:573:GLN:NE2	1.87	0.73
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.24	0.73
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.69	0.73
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.71	0.72
1:B:162:PHE:CZ	1:B:182:ARG:HB2	2.24	0.72
1:B:736:LEU:HD23	1:B:742:GLN:HA	1.69	0.72
1:B:643:LYS:HE3	1:B:645:ASN:HB2	1.70	0.72
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.24	0.72
1:A:394:SER:O	1:A:398:GLN:HG3	1.89	0.72
1:B:436:LEU:N	1:B:436:LEU:HD23	2.05	0.71
1:B:436:LEU:H	1:B:436:LEU:HD23	1.55	0.71
1:B:573:GLN:H	1:B:573:GLN:NE2	1.89	0.71
1:A:547:LEU:HD23	1:A:573:GLN:HG2	1.73	0.71
1:A:547:LEU:HD23	1:A:573:GLN:CG	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ARG:HG3	5:B:1015:HOH:O	1.91	0.70
1:B:234:VAL:O	1:B:238:GLN:HG3	1.91	0.70
1:B:165:LEU:HD11	1:B:204:PHE:CZ	2.27	0.70
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.22	0.69
1:A:436:LEU:N	1:A:436:LEU:HD23	2.06	0.69
1:B:162:PHE:CD1	1:B:165:LEU:HD23	2.27	0.69
1:B:438:LYS:HA	5:B:957:HOH:O	1.93	0.68
1:B:196:LEU:HD22	1:B:200:GLU:HB3	1.75	0.68
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.75	0.68
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.40	0.68
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.75	0.68
1:B:162:PHE:O	1:B:165:LEU:HB3	1.94	0.68
1:B:222:ALA:HB2	1:B:228:LEU:HD23	1.77	0.67
1:B:429:GLU:OE1	1:B:432:LYS:HE2	1.94	0.67
1:B:405:LEU:HD13	1:B:437:LEU:HD11	1.77	0.67
1:B:172:LEU:O	1:B:174:ILE:HG13	1.95	0.66
1:B:172:LEU:HD12	1:B:174:ILE:HD12	1.75	0.66
1:A:536:GLY:O	1:A:540:VAL:HG23	1.95	0.66
1:B:241:GLN:HE22	1:B:730:TYR:H	1.44	0.66
1:A:341:GLU:OE2	1:A:549:ARG:NH2	2.29	0.65
1:A:429:GLU:OE1	1:A:432:LYS:HE2	1.95	0.65
1:B:335:LYS:NZ	5:B:867:HOH:O	2.29	0.65
1:A:742:GLN:NE2	5:A:846:HOH:O	2.30	0.65
1:B:645:ASN:ND2	1:B:647:ASN:O	2.30	0.65
1:B:643:LYS:HE2	1:B:650:SER:HA	1.78	0.65
1:A:573:GLN:H	1:A:573:GLN:HE21	1.44	0.65
1:B:191:SER:HB2	1:B:193:THR:HG23	1.76	0.65
1:B:394:SER:O	1:B:398:GLN:HG3	1.96	0.65
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.32	0.64
1:B:183:LYS:O	1:B:187:GLU:HG3	1.98	0.64
1:A:646:LYS:HA	1:A:646:LYS:NZ	2.13	0.64
1:A:436:LEU:H	1:A:436:LEU:HD23	1.62	0.64
1:B:184:ILE:HG22	1:B:204:PHE:CD1	2.33	0.64
1:B:438:LYS:HG3	1:B:520:MET:HE3	1.80	0.64
1:A:217:ALA:O	1:A:220:GLU:HG3	1.98	0.63
1:B:165:LEU:HD11	1:B:204:PHE:CE2	2.33	0.63
1:A:203:THR:O	1:A:207:MET:HB2	1.98	0.63
1:B:547:LEU:HD23	1:B:573:GLN:CG	2.28	0.63
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.34	0.63
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.34	0.63
1:A:616:ASN:OD1	1:A:618:ARG:HB2	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:683:ARG:HD2	5:B:946:HOH:O	1.98	0.63
1:B:341:GLU:OE2	1:B:549:ARG:NH2	2.32	0.62
1:B:728:GLN:HE21	1:B:753:SER:HA	1.64	0.62
1:A:236:PHE:N	5:A:959:HOH:O	2.19	0.62
1:A:219:GLU:O	1:A:223:GLY:N	2.29	0.62
1:A:507:PHE:HE1	1:A:542:HIS:HD1	1.46	0.62
1:B:197:GLU:O	1:B:201:ILE:HG12	2.00	0.62
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.29	0.62
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.29	0.62
1:B:161:ASN:N	1:B:164:GLU:OE1	2.30	0.62
1:B:516:ALA:HB3	1:B:519:GLU:HG3	1.81	0.62
1:A:203:THR:O	1:A:207:MET:N	2.33	0.61
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.33	0.61
1:A:756:ASP:OD1	1:A:756:ASP:N	2.33	0.61
1:A:242:ARG:HD2	5:A:890:HOH:O	2.01	0.61
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.34	0.61
1:A:346:ASP:OD2	1:A:394:SER:HB3	2.01	0.60
1:A:438:LYS:HG3	1:A:520:MET:HE3	1.82	0.60
1:B:222:ALA:CB	1:B:228:LEU:HD23	2.31	0.60
1:A:371:ARG:NE	5:A:864:HOH:O	2.29	0.60
1:B:168:PHE:CE1	1:B:172:LEU:HD11	2.37	0.59
1:B:168:PHE:CD1	1:B:172:LEU:HD21	2.37	0.59
1:B:504:PHE:HD2	1:B:527:ARG:NH2	2.00	0.59
1:A:291:HIS:HE1	5:A:971:HOH:O	1.85	0.59
1:A:670:ARG:HG3	1:A:690:PHE:CZ	2.38	0.59
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.37	0.59
1:B:646:LYS:O	1:B:646:LYS:HG2	2.03	0.59
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.38	0.59
1:B:643:LYS:HE2	1:B:650:SER:CA	2.33	0.59
1:A:504:PHE:HD2	1:A:527:ARG:NH2	1.99	0.59
1:A:235:THR:N	5:A:959:HOH:O	2.35	0.58
1:A:227:THR:HG21	1:A:269:GLN:OE1	2.03	0.58
1:A:547:LEU:CD2	1:A:573:GLN:HG2	2.33	0.58
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.32	0.58
1:B:644:VAL:CG2	1:B:645:ASN:H	2.08	0.58
1:A:412:ILE:HD12	1:A:412:ILE:H	1.68	0.58
1:B:258:TYR:HB3	1:B:277:MET:HB3	1.84	0.58
1:B:411:PRO:O	1:B:434:LYS:NZ	2.36	0.58
1:A:311:HIS:NE2	4:A:1:CIP:H72	2.19	0.58
1:B:185:PHE:CE1	1:B:196:LEU:HG	2.39	0.58
1:A:542:HIS:CD2	1:A:546:CYS:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.85	0.58
1:B:490:PRO:HD2	1:B:491:GLU:OE1	2.03	0.58
1:B:533:GLN:OE1	1:B:618:ARG:NH1	2.37	0.58
1:B:542:HIS:CD2	1:B:546:CYS:HB2	2.39	0.58
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.03	0.57
1:A:490:PRO:HD2	1:A:491:GLU:OE1	2.04	0.57
1:A:405:LEU:HD13	1:A:437:LEU:HD11	1.86	0.57
1:A:381:SER:HB2	1:A:599:CYS:HA	1.86	0.57
1:B:162:PHE:CE1	1:B:165:LEU:HD23	2.40	0.57
4:B:1:CIP:O2P	4:B:1:CIP:H6	2.05	0.57
1:B:644:VAL:HG23	1:B:645:ASN:N	2.11	0.57
1:A:252:LEU:O	1:A:256:GLU:HG3	2.05	0.56
1:B:311:HIS:NE2	4:B:1:CIP:H72	2.20	0.56
1:A:613:THR:HG22	1:A:615:PHE:N	2.17	0.56
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.87	0.56
1:A:442:LEU:HG	1:A:488:LEU:HD23	1.87	0.56
1:B:412:ILE:CG2	1:B:435:ILE:HG13	2.35	0.56
1:A:411:PRO:O	1:A:434:LYS:NZ	2.39	0.56
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.06	0.56
1:B:486:LEU:HD12	1:B:486:LEU:N	2.13	0.56
1:A:728:GLN:HE21	1:A:753:SER:HA	1.71	0.56
1:B:293:ARG:NH1	5:B:834:HOH:O	2.30	0.55
1:B:573:GLN:H	1:B:573:GLN:HE21	1.53	0.55
1:B:643:LYS:HE2	1:B:650:SER:C	2.27	0.55
1:A:736:LEU:HD23	1:A:742:GLN:HA	1.88	0.55
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.21	0.55
1:B:509:SER:N	1:B:510:PRO:HD2	2.21	0.55
1:A:488:LEU:HD21	1:A:493:SER:HB2	1.89	0.55
1:B:261:SER:O	1:B:265:LYS:HB2	2.07	0.55
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.41	0.55
1:A:211:ARG:HD3	5:A:900:HOH:O	2.06	0.55
1:B:412:ILE:H	1:B:412:ILE:HD12	1.72	0.54
1:B:174:ILE:CG2	1:B:176:VAL:HG23	2.38	0.54
1:A:259:GLU:O	1:A:265:LYS:HD2	2.08	0.54
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.37	0.54
1:B:188:CYS:O	1:B:200:GLU:HG2	2.08	0.54
1:A:618:ARG:HG3	5:A:817:HOH:O	2.08	0.54
1:B:172:LEU:O	1:B:174:ILE:N	2.40	0.54
1:B:191:SER:CB	1:B:193:THR:HG23	2.38	0.54
1:B:203:THR:O	1:B:207:MET:HG3	2.08	0.54
1:A:548:SER:H	1:A:573:GLN:HE22	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:LEU:HG	1:B:488:LEU:HD13	1.89	0.54
1:B:613:THR:HB	1:B:615:PHE:H	1.73	0.54
1:B:736:LEU:CD2	1:B:742:GLN:HA	2.38	0.53
1:B:438:LYS:HG3	1:B:520:MET:CE	2.39	0.53
1:B:632:ARG:HD2	5:B:932:HOH:O	2.08	0.53
1:A:291:HIS:HD2	1:A:725:SER:OG	1.92	0.53
1:B:643:LYS:HD2	1:B:645:ASN:HB2	1.90	0.53
1:A:610:ASP:OD1	1:A:611:PRO:HD2	2.09	0.53
1:A:638:GLY:O	1:A:681:ASN:HA	2.09	0.52
1:B:379:LYS:NZ	5:B:866:HOH:O	2.38	0.52
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.34	0.52
1:B:271:THR:HB	5:B:1174:HOH:O	2.08	0.52
1:B:735:LEU:O	1:B:743:HIS:HB2	2.09	0.52
1:B:549:ARG:C	1:B:550:ILE:HD13	2.30	0.52
1:A:341:GLU:C	1:A:342:LEU:HD12	2.30	0.52
1:B:507:PHE:O	1:B:510:PRO:HG2	2.10	0.52
1:B:542:HIS:HD2	1:B:546:CYS:HB2	1.73	0.52
1:B:241:GLN:N	1:B:241:GLN:HE21	2.08	0.52
1:B:441:LYS:HB3	1:B:500:LYS:HE3	1.92	0.52
1:B:548:SER:H	1:B:573:GLN:HE22	1.56	0.52
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.09	0.51
1:B:638:GLY:O	1:B:681:ASN:HA	2.10	0.51
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.11	0.51
1:A:593:PHE:O	1:A:598:GLY:HA2	2.10	0.51
1:B:751:LYS:NZ	5:B:995:HOH:O	2.39	0.51
1:A:504:PHE:CD2	1:A:527:ARG:NH2	2.79	0.51
1:B:593:PHE:O	1:B:598:GLY:HA2	2.10	0.51
1:B:168:PHE:HE1	1:B:172:LEU:HD21	1.73	0.51
1:B:321:THR:HG22	1:B:360:PHE:HB2	1.91	0.51
1:B:259:GLU:O	1:B:265:LYS:HD2	2.11	0.51
1:A:737:SER:HA	5:A:818:HOH:O	2.11	0.51
1:B:313:THR:HB	1:B:329:TYR:CE1	2.45	0.51
1:B:486:LEU:H	1:B:486:LEU:CD1	2.10	0.51
1:B:643:LYS:CE	1:B:645:ASN:HB2	2.37	0.51
1:A:204:PHE:O	1:A:207:MET:N	2.38	0.50
1:A:536:GLY:HA3	5:A:817:HOH:O	2.11	0.50
1:B:341:GLU:CD	1:B:549:ARG:HH22	2.15	0.50
1:A:311:HIS:NE2	4:A:1:CIP:H2	2.27	0.50
1:B:230:VAL:O	1:B:234:VAL:HG23	2.11	0.50
1:A:734:HIS:HE1	5:A:761:HOH:O	1.92	0.50
1:B:549:ARG:O	1:B:550:ILE:HD13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:C	1:B:342:LEU:HD12	2.32	0.50
1:A:504:PHE:CE1	1:A:507:PHE:CE1	2.99	0.50
1:A:504:PHE:CZ	1:A:507:PHE:CE1	3.00	0.49
1:B:504:PHE:CD2	1:B:527:ARG:NH2	2.79	0.49
1:B:648:LYS:O	1:B:649:ASN:OD1	2.29	0.49
1:A:655:LYS:NZ	1:A:671:GLN:OE1	2.35	0.49
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.94	0.49
1:B:563:SER:O	1:B:566:GLU:HG2	2.13	0.49
1:B:547:LEU:HD23	1:B:573:GLN:HG2	1.93	0.49
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.95	0.49
1:B:729:GLY:O	1:B:751:LYS:HA	2.13	0.49
1:B:172:LEU:HD12	1:B:174:ILE:CD1	2.42	0.49
1:B:162:PHE:CE1	1:B:182:ARG:HA	2.48	0.49
1:B:405:LEU:O	1:B:409:LEU:HB2	2.12	0.49
1:A:227:THR:HG23	1:A:269:GLN:HB3	1.93	0.49
1:A:412:ILE:HD12	1:A:412:ILE:N	2.28	0.49
1:B:248:PRO:HD2	1:B:249:ALA:H	1.78	0.49
1:A:241:GLN:NE2	1:A:729:GLY:HA3	2.28	0.49
1:B:222:ALA:HB2	1:B:228:LEU:CD2	2.42	0.49
1:B:291:HIS:HD2	1:B:725:SER:OG	1.96	0.48
1:B:198:ASP:HA	1:B:201:ILE:HG13	1.95	0.48
1:B:240:GLN:HA	1:B:240:GLN:OE1	2.13	0.48
1:B:162:PHE:CE2	1:B:166:LYS:NZ	2.80	0.48
1:B:547:LEU:CD2	1:B:573:GLN:HG2	2.44	0.48
1:A:405:LEU:O	1:A:409:LEU:HB2	2.14	0.48
1:A:222:ALA:HA	1:A:228:LEU:HD23	1.93	0.48
1:A:235:THR:HB	5:A:959:HOH:O	2.14	0.48
1:B:169:LEU:O	1:B:172:LEU:O	2.32	0.48
1:A:213:GLU:HG3	1:A:749:PHE:CD2	2.48	0.47
1:B:509:SER:N	1:B:510:PRO:CD	2.77	0.47
1:A:204:PHE:C	1:A:207:MET:H	2.16	0.47
1:B:381:SER:HB2	1:B:599:CYS:HA	1.95	0.47
1:A:300:GLN:HB3	1:A:301:PRO:CD	2.44	0.47
1:B:238:GLN:CG	1:B:246:ALA:HB1	2.32	0.47
1:A:222:ALA:HA	1:A:228:LEU:CD2	2.44	0.47
1:B:159:LYS:HA	1:B:196:LEU:O	2.13	0.47
1:B:288:SER:HB2	1:B:727:LYS:HD3	1.95	0.47
1:A:227:THR:HG21	1:A:269:GLN:CD	2.34	0.47
1:A:735:LEU:O	1:A:743:HIS:HB2	2.13	0.47
1:B:383:TYR:HD2	1:B:599:CYS:HB2	1.80	0.47
1:B:643:LYS:HE3	1:B:645:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:HIS:HA	1:A:341:GLU:OE2	2.14	0.47
1:B:371:ARG:O	1:B:374:ARG:HB3	2.15	0.47
1:A:441:LYS:HB3	1:A:500:LYS:HE3	1.95	0.47
1:B:587:ASP:HB3	1:B:718:GLN:NE2	2.30	0.47
1:A:537:ASN:OD1	1:A:541:ARG:NE	2.39	0.47
1:B:168:PHE:O	1:B:171:GLU:HB2	2.13	0.47
1:A:689:GLU:HB3	1:B:491:GLU:HG3	1.97	0.47
1:A:240:GLN:HA	1:A:240:GLN:OE1	2.14	0.47
1:A:253:SER:O	1:A:257:ARG:HB2	2.15	0.47
1:A:406:ARG:HH11	1:A:406:ARG:CG	2.27	0.47
1:A:537:ASN:CA	5:A:797:HOH:O	2.63	0.46
1:A:558:ASP:O	1:A:559:SER:HB2	2.15	0.46
1:A:755:GLN:HG2	1:A:756:ASP:N	2.30	0.46
1:B:300:GLN:O	1:B:427:SER:HA	2.14	0.46
1:B:643:LYS:CD	1:B:645:ASN:HB2	2.45	0.46
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.45	0.46
1:B:558:ASP:O	1:B:559:SER:HB2	2.15	0.46
1:B:706:ASP:O	1:B:713:ASN:HB3	2.15	0.46
4:A:1:CIP:O2P	4:A:1:CIP:H6	2.14	0.46
1:A:622:GLN:HA	1:B:445:LEU:CD1	2.45	0.46
1:A:208:LEU:N	1:A:208:LEU:CD2	2.79	0.46
1:A:628:PRO:HA	1:A:692:VAL:O	2.15	0.46
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.46	0.46
1:B:537:ASN:OD1	1:B:541:ARG:NE	2.39	0.46
1:A:227:THR:CG2	1:A:228:LEU:N	2.79	0.45
1:B:516:ALA:CB	1:B:518:TYR:CZ	2.99	0.45
1:B:610:ASP:OD1	1:B:611:PRO:HD2	2.16	0.45
1:A:438:LYS:HG3	1:A:520:MET:CE	2.44	0.45
1:A:300:GLN:O	1:A:427:SER:HA	2.17	0.45
1:B:165:LEU:CD1	1:B:204:PHE:CE2	3.00	0.45
1:B:213:GLU:HG2	1:B:214:ILE:N	2.30	0.45
1:A:729:GLY:O	1:A:751:LYS:HA	2.17	0.45
1:B:342:LEU:HD12	1:B:342:LEU:N	2.31	0.45
1:B:499:CYS:HB2	5:B:957:HOH:O	2.17	0.45
1:B:733:VAL:HB	1:B:748:LEU:HB2	1.97	0.45
1:B:734:HIS:HE1	5:B:778:HOH:O	1.97	0.45
1:B:348:PRO:HD2	5:B:836:HOH:O	2.16	0.45
1:B:504:PHE:HD2	1:B:527:ARG:HH21	1.64	0.45
1:B:607:PHE:O	1:B:613:THR:HG21	2.16	0.45
4:B:1:CIP:O4	5:B:1016:HOH:O	2.21	0.45
1:A:252:LEU:HD23	1:A:256:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ALA:HA	1:B:228:LEU:CD2	2.46	0.45
1:B:628:PRO:HA	1:B:692:VAL:O	2.16	0.45
1:B:683:ARG:NH2	1:B:685:ASP:OD2	2.50	0.45
1:B:661:HIS:O	1:B:698:ALA:HA	2.17	0.45
1:A:488:LEU:CD2	1:A:493:SER:HB2	2.45	0.45
1:A:733:VAL:HB	1:A:748:LEU:HB2	1.98	0.45
1:A:293:ARG:NH1	5:A:917:HOH:O	2.50	0.44
1:A:371:ARG:O	1:A:374:ARG:HB3	2.16	0.44
1:A:507:PHE:CE1	1:A:542:HIS:ND1	2.79	0.44
1:A:516:ALA:CB	1:A:518:TYR:CZ	3.00	0.44
1:A:661:HIS:O	1:A:698:ALA:HA	2.18	0.44
1:B:390:GLU:OE1	4:B:1:CIP:O2P	2.35	0.44
1:A:613:THR:HG22	1:A:614:THR:N	2.32	0.44
1:B:174:ILE:HG22	1:B:176:VAL:HG23	1.99	0.44
1:B:310:SER:HB3	1:B:337:CYS:SG	2.56	0.44
1:B:541:ARG:HD2	5:B:1131:HOH:O	2.16	0.44
1:A:537:ASN:N	5:A:797:HOH:O	2.50	0.44
1:A:588:VAL:HA	1:A:720:THR:HG21	2.00	0.44
1:B:241:GLN:NE2	1:B:241:GLN:CA	2.80	0.44
1:A:288:SER:HB2	1:A:727:LYS:HD3	1.98	0.44
1:A:708:ASP:HB2	5:A:1043:HOH:O	2.17	0.44
1:A:241:GLN:HB3	1:A:731:ARG:NH2	2.32	0.44
1:B:634:ARG:NH2	5:B:1171:HOH:O	2.32	0.44
1:A:440:LYS:HA	5:A:982:HOH:O	2.18	0.44
1:A:610:ASP:HA	1:A:611:PRO:HD3	1.69	0.44
1:B:241:GLN:HA	1:B:241:GLN:NE2	2.33	0.44
1:A:261:SER:O	1:A:265:LYS:HB2	2.18	0.44
1:A:312:ASN:H	1:A:341:GLU:CD	2.21	0.44
1:A:417:PRO:HD3	1:A:497:ILE:HD12	1.99	0.44
1:B:222:ALA:CA	1:B:228:LEU:HD23	2.48	0.44
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.99	0.43
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.48	0.43
1:A:537:ASN:CB	5:A:797:HOH:O	2.49	0.43
1:B:536:GLY:O	1:B:540:VAL:HG23	2.17	0.43
1:B:542:HIS:C	1:B:542:HIS:CD2	2.92	0.43
1:B:416:GLN:HA	1:B:417:PRO:HD3	1.78	0.43
1:A:755:GLN:HG3	5:A:842:HOH:O	2.18	0.43
1:B:162:PHE:CD1	1:B:165:LEU:CD2	2.99	0.43
1:B:222:ALA:HA	1:B:228:LEU:HD23	2.00	0.43
1:A:499:CYS:HB3	1:A:520:MET:HE3	2.01	0.43
1:A:639:GLN:HG3	5:A:827:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LYS:NZ	1:B:493:SER:O	2.51	0.43
1:B:412:ILE:HG21	1:B:435:ILE:HG13	2.00	0.43
1:B:681:ASN:N	1:B:682:PRO:CD	2.82	0.43
1:B:244:GLU:C	1:B:246:ALA:H	2.21	0.43
1:A:412:ILE:CG2	1:A:435:ILE:HG13	2.49	0.43
1:B:542:HIS:HD2	1:B:542:HIS:O	2.02	0.43
1:B:651:ILE:HA	1:B:651:ILE:HD13	1.49	0.43
1:B:410:GLY:HA3	1:B:411:PRO:HD3	1.65	0.42
1:B:164:GLU:O	1:B:167:ASP:HB2	2.19	0.42
1:B:523:PHE:N	1:B:523:PHE:CD1	2.87	0.42
1:B:551:TYR:HB2	1:B:552:PRO:HD2	2.01	0.42
1:A:549:ARG:HH12	4:A:1:CIP:HO3	1.66	0.42
1:B:160:MET:O	1:B:195:SER:HA	2.19	0.42
1:B:409:LEU:HD12	1:B:409:LEU:HA	1.78	0.42
1:B:434:LYS:HD2	1:B:434:LYS:HA	1.84	0.42
1:A:622:GLN:CA	1:B:445:LEU:HD13	2.49	0.42
1:A:655:LYS:HD2	1:A:674:VAL:HG22	2.01	0.42
1:A:587:ASP:HB3	1:A:718:GLN:NE2	2.33	0.42
1:B:651:ILE:CG2	1:B:677:ASN:HA	2.50	0.42
1:A:622:GLN:CB	1:B:445:LEU:HD13	2.45	0.42
1:B:643:LYS:HE3	1:B:645:ASN:CG	2.39	0.42
1:A:211:ARG:O	1:A:214:ILE:HB	2.20	0.42
1:A:310:SER:HB3	1:A:337:CYS:SG	2.60	0.42
1:A:396:GLU:O	1:A:399:ARG:HB2	2.20	0.42
1:A:434:LYS:HA	1:A:434:LYS:HD2	1.81	0.42
1:B:379:LYS:NZ	5:B:1000:HOH:O	2.49	0.42
1:B:396:GLU:O	1:B:399:ARG:HB2	2.19	0.42
1:B:595:ASP:OD1	1:B:596:ASN:N	2.50	0.42
1:A:250:LEU:O	1:A:253:SER:OG	2.30	0.42
1:A:314:TYR:CE2	1:A:315:LEU:HG	2.54	0.42
1:B:646:LYS:O	1:B:647:ASN:HB3	2.20	0.42
1:A:732:HIS:HA	1:A:748:LEU:O	2.20	0.42
1:B:406:ARG:HH11	1:B:406:ARG:CG	2.32	0.42
1:B:412:ILE:N	1:B:412:ILE:HD12	2.35	0.42
1:B:610:ASP:HA	1:B:611:PRO:HD3	1.72	0.42
1:B:639:GLN:HB2	1:B:747:THR:OG1	2.19	0.42
1:A:342:LEU:HD12	1:A:342:LEU:N	2.35	0.41
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.08	0.41
1:A:563:SER:O	1:A:566:GLU:HG2	2.20	0.41
1:B:236:PHE:O	1:B:240:GLN:HB2	2.20	0.41
1:A:341:GLU:CD	1:A:549:ARG:HH22	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ARG:NH2	1:A:718:GLN:HG3	2.35	0.41
1:A:218:PHE:CG	1:A:272:LYS:HG3	2.55	0.41
1:B:412:ILE:O	1:B:412:ILE:HG22	2.19	0.41
1:B:551:TYR:HB2	1:B:552:PRO:CD	2.50	0.41
1:A:366:PHE:CE2	1:A:370:LEU:HD11	2.56	0.41
1:A:406:ARG:CG	1:A:406:ARG:NH1	2.83	0.41
1:A:538:GLY:N	5:A:797:HOH:O	2.53	0.41
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.44	0.41
1:B:610:ASP:O	1:B:612:ASN:N	2.53	0.41
1:B:646:LYS:HE3	1:B:646:LYS:HB3	1.36	0.41
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.86	0.41
1:A:622:GLN:CA	1:B:445:LEU:CD1	2.99	0.41
1:B:436:LEU:N	1:B:436:LEU:CD2	2.80	0.41
1:A:230:VAL:O	1:A:234:VAL:HG23	2.21	0.41
1:A:523:PHE:CD2	1:A:531:LEU:CD1	3.04	0.41
1:B:431:LEU:O	1:B:434:LYS:HB2	2.21	0.41
1:A:622:GLN:CB	1:B:445:LEU:CD1	2.99	0.41
1:B:348:PRO:HB2	1:B:349:ASN:HD21	1.79	0.40
1:B:510:PRO:HD2	5:B:920:HOH:O	2.21	0.40
1:A:504:PHE:CZ	1:A:506:GLY:CA	3.01	0.40
1:B:516:ALA:CB	1:B:518:TYR:CE2	2.99	0.40
1:B:721:ILE:HA	1:B:722:PRO:HD3	1.92	0.40
1:A:523:PHE:CE2	1:A:531:LEU:CD1	3.04	0.40
1:A:653:ASP:HA	1:A:675:ILE:O	2.22	0.40
1:B:253:SER:O	1:B:257:ARG:HB2	2.22	0.40
1:B:442:LEU:CD2	1:B:484:ASP:HB3	2.51	0.40
1:A:409:LEU:HA	1:A:409:LEU:HD12	1.89	0.40
1:A:670:ARG:HA	5:A:1048:HOH:O	2.22	0.40
1:B:174:ILE:CG2	1:B:176:VAL:CG2	3.00	0.40
1:B:343:ASP:HB3	5:B:774:HOH:O	2.21	0.40
1:B:499:CYS:HB3	1:B:520:MET:CE	2.51	0.40
1:B:499:CYS:HB3	1:B:520:MET:HE3	2.04	0.40
1:B:655:LYS:NZ	1:B:671:GLN:OE1	2.45	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:231:GLU:OE1	5:A:896:HOH:O[52_555]	2.18	0.02

## 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%)	472 (93%)	35 (7%)	2 (0%)	34	41
1	B	557/624 (89%)	511 (92%)	43 (8%)	3 (0%)	29	34
All	All	1066/1248 (85%)	983 (92%)	78 (7%)	5 (0%)	29	34

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173	ASN
1	B	645	ASN
1	B	647	ASN
1	A	421	VAL
1	A	744	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%)	392 (88%)	52 (12%)	5	4
1	B	492/545 (90%)	442 (90%)	50 (10%)	7	7
All	All	936/1090 (86%)	834 (89%)	102 (11%)	6	6

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

Mol	Chain	Res	Type
1	A	204	PHE

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Mol	Chain	Res	Type
1	A	205	TYR
1	A	207	MET
1	A	208	LEU
1	A	209	THR
1	A	210	GLN
1	A	219	GLU
1	A	220	GLU
1	A	224	SER
1	A	226	GLU
1	A	227	THR
1	A	242	ARG
1	A	252	LEU
1	A	278	TYR
1	A	293	ARG
1	A	310	SER
1	A	331	ARG
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	509	SER
1	A	513	SER
1	A	520	MET
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	580	GLN
1	A	614	THR
1	A	617	SER
1	A	632	ARG
1	A	643	LYS
1	A	646	LYS
1	A	648	LYS
1	A	652	VAL
1	A	665	ARG
1	A	670	ARG
1	A	676	THR

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Mol	Chain	Res	Type
1	A	685	ASP
1	A	691	GLU
1	A	709	SER
1	A	710	SER
1	A	711	SER
1	A	712	LYS
1	A	742	GLN
1	A	753	SER
1	A	756	ASP
1	B	159	LYS
1	B	162	PHE
1	B	163	LYS
1	B	171	GLU
1	B	172	LEU
1	B	173	ASN
1	B	186	ARG
1	B	194	ASP
1	B	201	ILE
1	B	226	GLU
1	B	227	THR
1	B	231	GLU
1	B	242	ARG
1	B	262	GLU
1	B	263	THR
1	B	268	ARG
1	B	277	MET
1	B	293	ARG
1	B	309	SER
1	B	310	SER
1	B	379	LYS
1	B	406	ARG
1	B	409	LEU
1	B	436	LEU
1	B	486	LEU
1	B	488	LEU
1	B	508	SER
1	B	520	MET
1	B	526	SER
1	B	534	GLU
1	B	535	SER
1	B	539	PHE
1	B	545	SER

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Mol	Chain	Res	Type
1	B	563	SER
1	B	573	GLN
1	B	613	THR
1	B	614	THR
1	B	617	SER
1	B	646	LYS
1	B	650	SER
1	B	651	ILE
1	B	652	VAL
1	B	676	THR
1	B	685	ASP
1	B	691	GLU
1	B	709	SER
1	B	710	SER
1	B	742	GLN
1	B	753	SER
1	B	756	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	291	HIS
1	A	573	GLN
1	A	639	GLN
1	A	645	ASN
1	A	718	GLN
1	A	728	GLN
1	A	734	HIS
1	B	210	GLN
1	B	241	GLN
1	B	291	HIS
1	B	349	ASN
1	B	515	GLN
1	B	573	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 [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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$
3	ACT	A	5	-	1,3,3	3.07	1 (100%)	0,3,3	0.00	-
4	CIP	B	1	2	14,16,16	1.95	3 (21%)	19,26,26	2.19	8 (42%)
3	ACT	B	5	-	1,3,3	2.64	1 (100%)	0,3,3	0.00	-
4	CIP	A	1	2	14,16,16	1.84	3 (21%)	19,26,26	2.06	9 (47%)

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	CIP	A	1	2	-	-	0/2/2/2
4	CIP	B	1	2	-	-	0/2/2/2

All (8) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	CIP	P-O1P	4.82	1.63	1.51
4	B	1	CIP	P-O1P	4.68	1.62	1.51
4	B	1	CIP	P-C7	-3.87	1.76	1.82
3	A	5	ACT	CH3-C	3.07	1.52	1.48
4	A	1	CIP	P-O2P	2.82	1.63	1.56
3	B	5	ACT	CH3-C	2.64	1.52	1.48
4	B	1	CIP	P-O2P	2.62	1.62	1.56
4	A	1	CIP	P-C7	-2.29	1.79	1.82

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	CIP	O4-C4-C3	-4.42	100.14	110.35
4	B	1	CIP	O1P-P-C7	4.19	118.86	109.12
4	B	1	CIP	O6-C6-C5	-3.38	102.53	110.35
4	A	1	CIP	O6-C6-C5	-3.33	102.65	110.35
4	B	1	CIP	C6-C5-C4	-3.30	105.06	110.82
4	A	1	CIP	O1P-P-C7	3.22	116.60	109.12
4	B	1	CIP	C3-C2-C1	3.04	115.80	111.67
4	A	1	CIP	O2P-P-C7	2.73	113.54	106.91
4	B	1	CIP	C2-C3-C4	2.63	115.26	110.74
4	A	1	CIP	C3-C2-C1	2.55	115.13	111.67
4	B	1	CIP	O2P-P-C7	2.52	113.03	106.91
4	A	1	CIP	O4-C4-C5	-2.44	104.72	110.35
4	B	1	CIP	P-O1-C1	-2.21	109.05	112.20
4	A	1	CIP	C5-C4-C3	-2.20	106.98	110.82
4	A	1	CIP	C2-C3-C4	2.20	114.52	110.74
4	B	1	CIP	O6-C6-C1	2.17	115.70	109.94
4	A	1	CIP	P-O1-C1	-2.08	109.24	112.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	CIP	4	0
4	A	1	CIP	4	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	507/624 (81%)	-0.11	37 (7%) 15 11	18, 36, 84, 115	14 (2%)
1	B	558/624 (89%)	-0.19	28 (5%) 28 26	18, 37, 79, 108	16 (2%)
All	All	1065/1248 (85%)	-0.15	65 (6%) 21 18	18, 36, 81, 115	30 (2%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	ILE	12.0
1	A	204	PHE	8.5
1	B	509	SER	8.4
1	A	203	THR	7.9
1	A	202	GLU	7.6
1	B	510	PRO	7.6
1	B	649	ASN	7.2
1	A	647	ASN	6.8
1	B	508	SER	6.6
1	A	208	LEU	6.3
1	B	648	LYS	5.8
1	A	644	VAL	5.7
1	A	710	SER	5.6
1	A	645	ASN	5.5
1	A	420	GLY	5.3
1	B	514	GLY	5.2
1	B	246	ALA	5.1
1	A	205	TYR	5.1
1	A	421	VAL	4.8
1	B	486	LEU	4.7
1	A	646	LYS	4.6
1	A	200	GLU	4.6
1	B	650	SER	4.4
1	B	172	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	207	MET	4.0
1	B	168	PHE	3.9
1	A	206	LYS	3.7
1	B	198	ASP	3.6
1	A	508	SER	3.5
1	A	711	SER	3.5
1	B	710	SER	3.5
1	B	245	GLU	3.5
1	A	505	GLY	3.4
1	A	503	HIS	3.3
1	A	419	ASP	3.3
1	A	709	SER	3.1
1	A	422	THR	3.0
1	A	423	THR	3.0
1	B	505	GLY	2.9
1	A	504	PHE	2.8
1	A	418	LEU	2.8
1	A	533	GLN	2.8
1	A	516	ALA	2.7
1	A	507	PHE	2.7
1	A	648	LYS	2.6
1	A	506	GLY	2.6
1	A	442	LEU	2.5
1	A	649	ASN	2.5
1	B	224	SER	2.5
1	B	165	LEU	2.4
1	B	503	HIS	2.3
1	B	266	ALA	2.3
1	A	502	VAL	2.3
1	B	163	LYS	2.2
1	B	261	SER	2.2
1	B	167	ASP	2.2
1	B	644	VAL	2.2
1	B	171	GLU	2.2
1	A	712	LYS	2.1
1	B	515	GLN	2.1
1	B	572	CYS	2.1
1	B	709	SER	2.1
1	A	224	SER	2.0
1	A	708	ASP	2.0
1	B	647	ASN	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
4	CIP	A	1	15/15	0.60	0.37	42,49,55,56	15
4	CIP	B	1	15/15	0.69	0.30	43,49,55,55	15
2	CA	B	3	1/1	0.73	0.09	54,54,54,54	1
2	CA	A	4	1/1	0.77	0.18	58,58,58,58	1
2	CA	A	3	1/1	0.85	0.08	56,56,56,56	1
2	CA	A	2	1/1	0.89	0.09	50,50,50,50	0
2	CA	B	4	1/1	0.93	0.09	59,59,59,59	1
3	ACT	A	5	4/4	0.96	0.10	35,37,38,41	0
2	CA	B	2	1/1	0.98	0.05	46,46,46,46	0
3	ACT	B	5	4/4	0.98	0.06	23,26,26,26	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.