



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:59 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

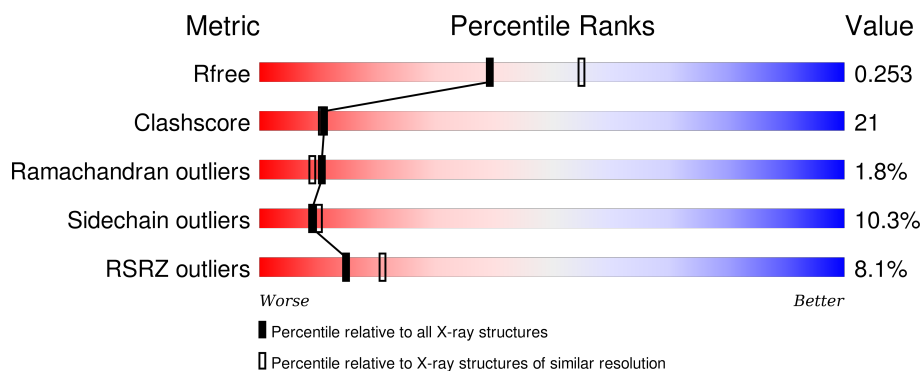
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	624	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	B	5	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9374 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

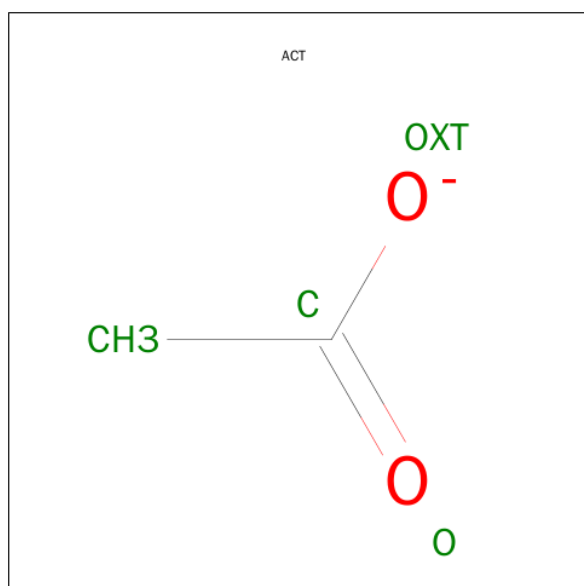
- Molecule 1 is a protein called PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

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

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

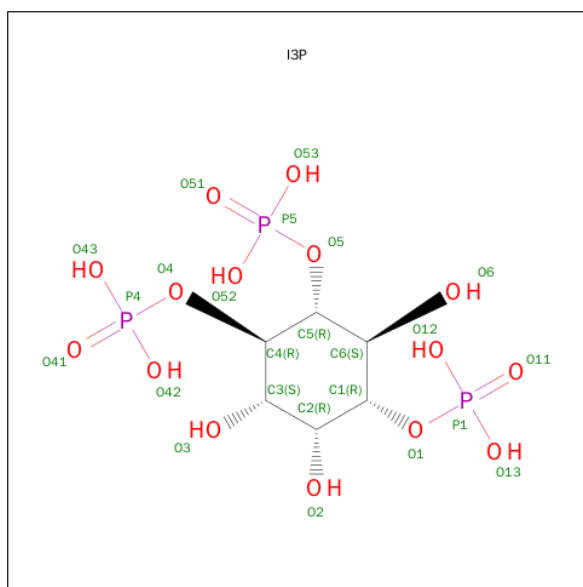
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: 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-1,4,5-TRIPHOSPHATE (three-letter code: I3P) (formula:  $C_6H_{15}O_{15}P_3$ ).



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

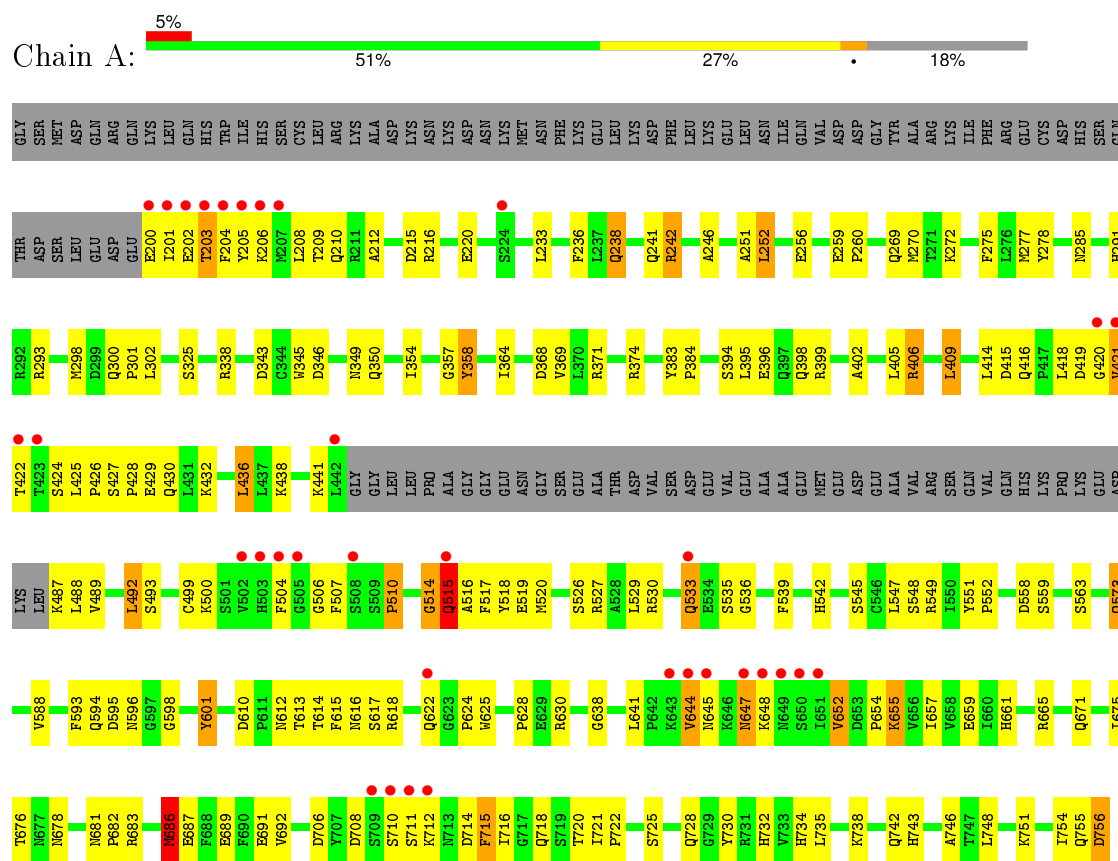
- Molecule 5 is water.

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

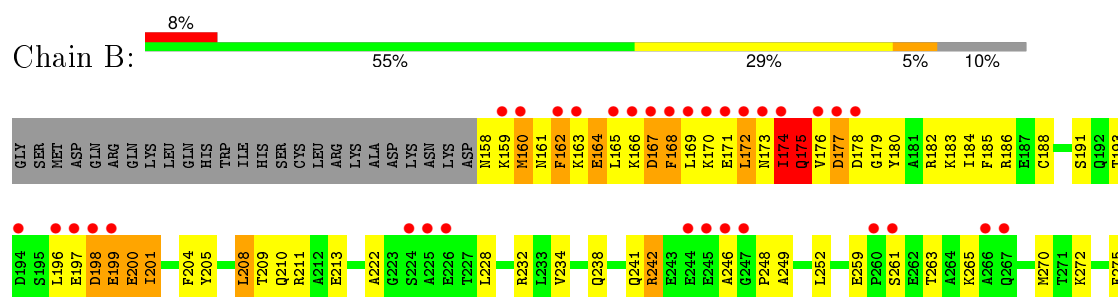
### 3 Residue-property plots

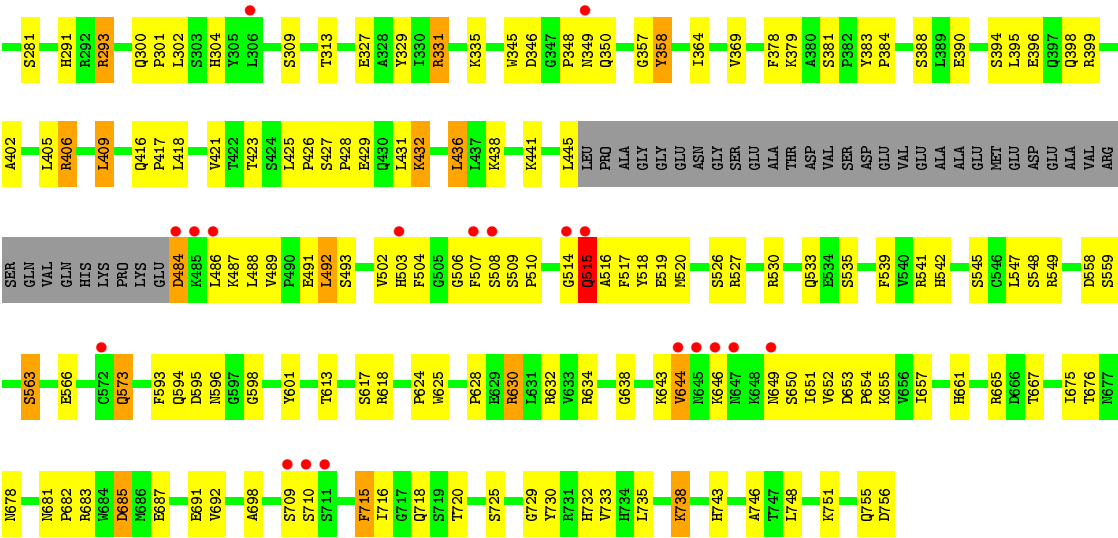
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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, $\alpha$ , $\beta$ , $\gamma$	397.54Å 397.54Å 397.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 24.70 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.4 (10.00-2.30) 95.9 (24.70-2.30)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.59 (at 2.31Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.220 , 0.270 0.212 , 0.253	Depositor DCC
$R_{free}$ test set	4609 reflections (4.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 97.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 113280 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

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

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, I3P, 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	0.80	10/4165 (0.2%)	0.82	2/5641 (0.0%)
1	B	0.79	8/4565 (0.2%)	0.81	0/6174
All	All	0.79	18/8730 (0.2%)	0.82	2/11815 (0.0%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	601	TYR	CE1-CZ	-8.23	1.27	1.38
1	A	715	PHE	CE1-CZ	-8.07	1.22	1.37
1	A	601	TYR	CE2-CZ	-7.60	1.28	1.38
1	A	601	TYR	CE1-CZ	-7.52	1.28	1.38
1	B	715	PHE	CE2-CZ	-7.52	1.23	1.37
1	B	601	TYR	CE2-CZ	-7.40	1.28	1.38
1	A	715	PHE	CG-CD2	-7.28	1.27	1.38
1	B	715	PHE	CE1-CZ	-7.14	1.23	1.37
1	A	358	TYR	CE1-CZ	-7.12	1.29	1.38
1	A	715	PHE	CE2-CZ	-7.10	1.23	1.37
1	A	601	TYR	CG-CD2	-7.04	1.30	1.39
1	B	601	TYR	CG-CD1	-7.02	1.30	1.39
1	B	601	TYR	CG-CD2	-7.01	1.30	1.39
1	A	601	TYR	CG-CD1	-7.01	1.30	1.39
1	A	715	PHE	CG-CD1	-6.97	1.28	1.38
1	B	715	PHE	CG-CD2	-6.88	1.28	1.38
1	B	715	PHE	CG-CD1	-6.12	1.29	1.38
1	A	358	TYR	CG-CD1	-5.98	1.31	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	514	GLY	N-CA-C	-7.40	94.60	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	686	MET	CG-SD-CE	6.48	110.57	100.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4070	0	3994	165	0
1	B	4465	0	4375	187	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	24	0	8	0	0
4	B	24	0	8	1	0
5	A	359	0	0	10	0
5	B	420	0	0	17	0
All	All	9374	0	8391	345	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (345) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:THR:HG22	1:A:615:PHE:H	1.04	1.10
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.16	1.05
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.21	1.04
1:B:169:LEU:HD12	1:B:176:VAL:HG13	1.07	1.03
1:A:200:GLU:N	1:A:203:THR:HG1	1.56	1.03
1:A:241:GLN:HE22	1:A:730:TYR:H	1.18	0.92
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.54	0.90
1:A:644:VAL:HG21	1:A:716:ILE:HG12	1.55	0.88
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.03	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:THR:HG22	1:A:615:PHE:N	1.88	0.87
1:A:573:GLN:H	1:A:573:GLN:HE21	1.18	0.87
1:B:504:PHE:HB3	1:B:527:ARG:NH2	1.91	0.85
1:A:418:LEU:HB2	1:A:421:VAL:HG21	1.57	0.84
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.59	0.84
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.57	0.84
1:A:520:MET:CE	1:A:549:ARG:HB2	2.08	0.84
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.58	0.83
1:B:515:GLN:HE21	1:B:542:HIS:HE1	1.26	0.82
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.93	0.82
1:A:216:ARG:HG3	1:A:216:ARG:HH11	1.45	0.81
1:B:520:MET:CE	1:B:549:ARG:HB2	2.10	0.81
1:A:573:GLN:H	1:A:573:GLN:NE2	1.78	0.80
1:B:208:LEU:HD23	1:B:209:THR:HG23	1.61	0.80
1:B:172:LEU:HD12	1:B:174:ILE:HG13	1.62	0.80
1:A:418:LEU:HB2	1:A:421:VAL:CG2	2.10	0.79
1:B:169:LEU:CD1	1:B:176:VAL:HG13	2.03	0.79
1:A:200:GLU:HA	1:A:203:THR:HB	1.64	0.79
1:B:208:LEU:HD23	1:B:209:THR:CG2	2.11	0.79
1:A:216:ARG:O	1:A:220:GLU:HG2	1.83	0.78
1:B:184:ILE:HG22	1:B:204:PHE:CE1	2.19	0.77
1:B:573:GLN:H	1:B:573:GLN:HE21	1.32	0.77
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.67	0.76
1:B:652:VAL:HG23	5:B:790:HOH:O	1.86	0.76
1:B:161:ASN:H	1:B:164:GLU:HG3	1.51	0.76
1:A:394:SER:O	1:A:398:GLN:HG3	1.86	0.75
1:B:394:SER:O	1:B:398:GLN:HG3	1.87	0.75
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.22	0.74
1:B:402:ALA:HB2	1:B:492:LEU:HD22	1.69	0.74
1:B:184:ILE:HG22	1:B:204:PHE:CD1	2.24	0.72
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.70	0.72
1:B:191:SER:HB2	1:B:193:THR:HG23	1.71	0.72
1:A:242:ARG:HD2	1:A:728:GLN:NE2	2.05	0.72
1:B:241:GLN:HE22	1:B:730:TYR:H	1.35	0.72
1:A:520:MET:HE2	1:A:549:ARG:HB2	1.74	0.70
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.73	0.70
1:B:520:MET:HE2	1:B:549:ARG:HB2	1.74	0.70
1:B:593:PHE:O	1:B:598:GLY:HA2	1.92	0.69
1:B:169:LEU:O	1:B:172:LEU:HD12	1.92	0.69
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.27	0.69
1:B:715:PHE:HB2	5:B:931:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:HD22	1:A:489:VAL:CG1	2.23	0.69
1:B:573:GLN:H	1:B:573:GLN:NE2	1.90	0.68
1:B:281:SER:HB2	5:B:854:HOH:O	1.93	0.68
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.75	0.68
1:B:178:ASP:O	1:B:180:TYR:N	2.27	0.68
1:B:172:LEU:CD1	1:B:174:ILE:HG13	2.23	0.68
1:A:622:GLN:OE1	1:B:445:LEU:HD12	1.94	0.67
1:B:515:GLN:NE2	1:B:542:HIS:HE1	1.92	0.67
1:A:421:VAL:HG11	1:A:426:PRO:HG3	1.75	0.67
1:A:346:ASP:OD2	1:A:394:SER:HB3	1.94	0.67
1:B:630:ARG:HD2	1:B:755:GLN:HE21	1.60	0.66
1:A:708:ASP:HB2	5:A:1000:HOH:O	1.95	0.66
1:B:160:MET:HB3	1:B:165:LEU:CD2	2.26	0.66
1:A:644:VAL:HG21	1:A:716:ILE:CG1	2.26	0.66
1:B:169:LEU:CB	1:B:176:VAL:HG22	2.27	0.65
1:B:242:ARG:NH1	5:B:1125:HOH:O	2.28	0.65
1:B:175:GLN:HG3	1:B:651:ILE:HD13	1.79	0.65
1:B:177:ASP:OD1	1:B:177:ASP:N	2.29	0.65
1:B:533:GLN:OE1	1:B:618:ARG:NH1	2.30	0.65
1:B:395:LEU:HD22	1:B:489:VAL:HG13	1.78	0.65
1:A:644:VAL:CG2	1:A:716:ILE:HG12	2.25	0.64
1:A:644:VAL:HG22	1:A:716:ILE:HG23	1.78	0.64
1:B:169:LEU:HB3	1:B:176:VAL:HG22	1.78	0.64
1:A:616:ASN:OD1	1:A:618:ARG:HB2	1.97	0.64
1:A:441:LYS:NZ	1:A:493:SER:O	2.30	0.64
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.25	0.64
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.09	0.64
1:A:395:LEU:HD22	1:A:489:VAL:HG13	1.79	0.64
1:B:161:ASN:H	1:B:164:GLU:CG	2.10	0.64
1:B:652:VAL:HG11	1:B:716:ILE:CD1	2.28	0.63
1:A:415:ASP:O	1:A:416:GLN:HG2	1.98	0.63
1:A:593:PHE:O	1:A:598:GLY:HA2	1.99	0.63
1:A:706:ASP:HB3	1:A:714:ASP:HB2	1.81	0.63
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.81	0.62
1:A:515:GLN:HB3	1:A:519:GLU:OE1	1.98	0.62
1:B:395:LEU:HD22	1:B:489:VAL:CG1	2.29	0.62
1:B:238:GLN:HG2	1:B:246:ALA:HB3	1.81	0.62
1:A:515:GLN:HE21	1:A:542:HIS:HE1	1.47	0.62
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.34	0.62
1:A:200:GLU:CA	1:A:203:THR:HB	2.30	0.62
1:B:484:ASP:O	1:B:488:LEU:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLU:HG3	5:A:971:HOH:O	2.00	0.62
1:A:743:HIS:HB3	1:A:746:ALA:HB3	1.82	0.61
1:B:515:GLN:HB3	1:B:519:GLU:OE1	1.99	0.61
1:B:300:GLN:OE1	1:B:304:HIS:HD2	1.84	0.61
1:A:269:GLN:NE2	5:A:907:HOH:O	2.29	0.61
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.34	0.61
1:B:196:LEU:HD22	1:B:200:GLU:HB2	1.82	0.61
1:A:200:GLU:O	1:A:204:PHE:HB3	2.00	0.60
1:A:241:GLN:HE22	1:A:730:TYR:N	1.94	0.60
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.30	0.60
1:A:515:GLN:HE21	1:A:542:HIS:CE1	2.19	0.60
1:B:516:ALA:HB1	1:B:518:TYR:CE1	2.36	0.60
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.02	0.60
1:B:441:LYS:NZ	1:B:493:SER:O	2.35	0.60
1:B:730:TYR:CE1	1:B:751:LYS:HD2	2.37	0.60
1:B:335:LYS:NZ	5:B:871:HOH:O	2.29	0.60
1:B:327:GLU:OE2	1:B:331:ARG:HD2	2.00	0.60
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.32	0.59
1:B:191:SER:CB	1:B:193:THR:HG23	2.31	0.59
1:B:683:ARG:NH2	1:B:685:ASP:OD2	2.35	0.59
1:B:234:VAL:O	1:B:238:GLN:HG3	2.02	0.59
1:A:515:GLN:NE2	1:A:542:HIS:HE1	2.01	0.59
1:A:730:TYR:CZ	1:A:751:LYS:HD2	2.38	0.59
1:A:441:LYS:HB3	1:A:500:LYS:HG3	1.84	0.58
1:B:249:ALA:HB3	5:B:1127:HOH:O	2.03	0.58
1:B:188:CYS:HB2	1:B:196:LEU:HD11	1.85	0.58
1:A:515:GLN:NE2	1:A:542:HIS:CE1	2.72	0.58
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.39	0.58
1:B:654:PRO:HD2	1:B:675:ILE:O	2.04	0.58
1:A:418:LEU:HD12	1:A:426:PRO:HB3	1.87	0.57
1:B:196:LEU:O	1:B:201:ILE:HD11	2.04	0.57
1:B:484:ASP:O	1:B:487:LYS:N	2.33	0.57
1:B:507:PHE:HB3	5:B:1092:HOH:O	2.04	0.57
1:B:175:GLN:OE1	1:B:175:GLN:HA	2.00	0.57
1:B:421:VAL:HG11	1:B:426:PRO:HD3	1.86	0.56
1:B:405:LEU:O	1:B:409:LEU:HB2	2.05	0.56
1:B:530:ARG:HH11	1:B:530:ARG:HG3	1.70	0.56
1:B:730:TYR:CZ	1:B:751:LYS:HD2	2.39	0.56
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.39	0.56
1:B:515:GLN:NE2	1:B:542:HIS:CE1	2.73	0.56
1:A:420:GLY:O	1:A:422:THR:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:ASN:HB3	5:A:1004:HOH:O	2.05	0.55
1:B:211:ARG:NE	1:B:213:GLU:OE2	2.33	0.55
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.41	0.55
1:A:536:GLY:HA3	5:A:788:HOH:O	2.06	0.55
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.41	0.55
1:B:346:ASP:OD2	1:B:394:SER:HB3	2.06	0.55
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.37	0.55
1:B:222:ALA:C	1:B:232:ARG:HH11	2.10	0.55
1:A:291:HIS:HD2	1:A:725:SER:OG	1.90	0.55
1:B:594:GLN:HE21	1:B:594:GLN:HA	1.70	0.55
1:A:742:GLN:NE2	5:A:858:HOH:O	2.39	0.55
1:B:300:GLN:O	1:B:427:SER:HA	2.06	0.54
1:B:667:THR:HG22	5:B:1161:HOH:O	2.07	0.54
1:A:613:THR:CG2	1:A:615:PHE:H	1.97	0.54
1:A:648:LYS:N	5:A:1004:HOH:O	2.41	0.54
1:B:272:LYS:O	1:B:275:PHE:HB3	2.08	0.54
1:A:638:GLY:O	1:A:681:ASN:HA	2.07	0.54
1:A:613:THR:HG22	1:A:614:THR:N	2.22	0.54
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.56	0.54
1:A:654:PRO:HD2	1:A:675:ILE:O	2.08	0.54
1:A:755:GLN:HG2	1:A:756:ASP:N	2.23	0.54
1:B:416:GLN:HG3	1:B:417:PRO:CD	2.34	0.53
1:A:202:GLU:O	1:A:205:TYR:HB3	2.07	0.53
1:B:291:HIS:HD2	1:B:725:SER:OG	1.91	0.53
1:A:402:ALA:HB2	1:A:492:LEU:HD22	1.90	0.53
1:B:649:ASN:O	1:B:651:ILE:HG12	2.08	0.53
1:A:735:LEU:O	1:A:743:HIS:HB2	2.09	0.53
1:A:420:GLY:O	1:A:422:THR:HG23	2.09	0.53
1:B:300:GLN:HB3	1:B:301:PRO:HD2	1.91	0.53
1:A:349:ASN:O	1:A:349:ASN:ND2	2.42	0.53
1:A:588:VAL:HA	1:A:720:THR:HG21	1.91	0.53
1:B:358:TYR:CD1	1:B:358:TYR:N	2.72	0.53
1:B:174:ILE:O	1:B:176:VAL:N	2.42	0.52
1:A:236:PHE:HA	5:A:974:HOH:O	2.10	0.52
1:B:248:PRO:O	1:B:252:LEU:HB2	2.10	0.52
1:A:252:LEU:O	1:A:256:GLU:HG3	2.09	0.52
1:A:200:GLU:N	1:A:203:THR:OG1	2.32	0.52
1:B:541:ARG:O	5:B:1094:HOH:O	2.19	0.52
1:A:573:GLN:N	1:A:573:GLN:NE2	2.53	0.52
1:B:390:GLU:HG3	5:B:1028:HOH:O	2.09	0.52
1:B:652:VAL:HG11	1:B:716:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:PRO:HB2	1:B:349:ASN:HD22	1.74	0.52
1:B:379:LYS:HE2	5:B:1062:HOH:O	2.09	0.52
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.36	0.52
1:B:514:GLY:O	1:B:515:GLN:O	2.28	0.52
1:A:300:GLN:O	1:A:427:SER:HA	2.10	0.51
1:A:238:GLN:NE2	1:A:246:ALA:HB3	2.26	0.51
1:A:396:GLU:O	1:A:399:ARG:HB2	2.10	0.51
1:B:425:LEU:HD21	1:B:517:PHE:O	2.10	0.51
1:B:743:HIS:HB3	1:B:746:ALA:HB3	1.93	0.51
1:B:594:GLN:NE2	1:B:594:GLN:HA	2.25	0.50
1:A:405:LEU:O	1:A:409:LEU:HB2	2.11	0.50
1:B:164:GLU:O	1:B:167:ASP:HB3	2.12	0.50
1:A:242:ARG:HG3	1:A:728:GLN:HB2	1.92	0.50
1:B:515:GLN:HB2	1:B:519:GLU:HB2	1.94	0.50
1:B:429:GLU:OE1	1:B:432:LYS:HE3	2.12	0.50
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.46	0.50
1:A:628:PRO:HA	1:A:692:VAL:O	2.11	0.50
1:A:618:ARG:HG3	5:A:788:HOH:O	2.12	0.49
1:A:730:TYR:CE1	1:A:751:LYS:HD2	2.46	0.49
1:A:547:LEU:HD23	1:A:573:GLN:CG	2.39	0.49
1:A:644:VAL:HG12	1:A:644:VAL:O	2.12	0.49
1:A:504:PHE:CE1	1:A:507:PHE:CE1	3.00	0.49
1:A:659:GLU:OE1	1:A:661:HIS:HE1	1.95	0.49
1:B:595:ASP:OD1	1:B:596:ASN:N	2.44	0.49
1:B:515:GLN:HE21	1:B:542:HIS:CE1	2.17	0.49
1:B:683:ARG:HD2	5:B:779:HOH:O	2.13	0.49
1:A:436:LEU:HD23	1:A:436:LEU:N	2.28	0.49
1:A:686:MET:HE2	1:A:687:GLU:O	2.13	0.49
1:B:652:VAL:HG12	1:B:653:ASP:N	2.26	0.49
1:B:638:GLY:O	1:B:681:ASN:HA	2.13	0.48
1:A:622:GLN:CA	1:B:445:LEU:HD11	2.40	0.48
1:A:644:VAL:CG1	1:A:714:ASP:HB3	2.43	0.48
1:B:197:GLU:O	1:B:201:ILE:HG12	2.12	0.48
1:B:348:PRO:HB2	1:B:349:ASN:ND2	2.27	0.48
1:B:630:ARG:HD2	1:B:755:GLN:NE2	2.26	0.48
1:B:514:GLY:HA3	5:B:1091:HOH:O	2.13	0.48
1:A:395:LEU:HD22	1:A:489:VAL:HG12	1.94	0.48
1:B:169:LEU:HB2	1:B:176:VAL:HG22	1.95	0.48
1:B:632:ARG:HH22	1:B:755:GLN:CD	2.16	0.48
1:B:738:LYS:HB2	5:B:875:HOH:O	2.14	0.48
1:B:161:ASN:N	1:B:164:GLU:HG3	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HD23	1:A:251:ALA:HB1	1.95	0.48
1:A:383:TYR:CB	1:A:384:PRO:HD2	2.37	0.47
1:A:425:LEU:HG	1:A:517:PHE:HD1	1.77	0.47
1:B:548:SER:H	1:B:573:GLN:NE2	2.12	0.47
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.44	0.47
1:A:414:LEU:HA	5:A:1043:HOH:O	2.13	0.47
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.44	0.47
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.96	0.47
1:A:488:LEU:HG	1:A:493:SER:HB2	1.95	0.47
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.49	0.47
1:B:735:LEU:O	1:B:743:HIS:HB2	2.14	0.47
1:B:349:ASN:O	1:B:350:GLN:HB2	2.14	0.47
1:B:161:ASN:O	1:B:164:GLU:HG2	2.14	0.47
1:B:436:LEU:N	1:B:436:LEU:HD23	2.29	0.47
1:B:628:PRO:HA	1:B:692:VAL:O	2.14	0.47
1:A:551:TYR:HB2	1:A:552:PRO:CD	2.44	0.47
1:A:302:LEU:HD23	1:A:428:PRO:HD3	1.97	0.47
1:A:418:LEU:HB2	1:A:421:VAL:HG23	1.95	0.47
1:B:259:GLU:OE1	1:B:270:MET:HA	2.15	0.47
1:A:300:GLN:HB3	1:A:301:PRO:HD2	1.97	0.47
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.80	0.47
1:B:261:SER:O	1:B:265:LYS:HB2	2.14	0.46
1:B:563:SER:O	1:B:566:GLU:HG2	2.16	0.46
1:B:632:ARG:NE	5:B:1123:HOH:O	2.46	0.46
1:B:198:ASP:O	1:B:201:ILE:HG13	2.15	0.46
1:B:652:VAL:CG1	1:B:716:ILE:HD11	2.46	0.46
1:B:228:LEU:CD2	1:B:232:ARG:HB3	2.45	0.46
1:A:396:GLU:OE1	1:A:399:ARG:NH1	2.47	0.46
1:A:285:ASN:ND2	1:A:734:HIS:HD2	2.14	0.46
1:A:644:VAL:HG21	1:A:716:ILE:CD1	2.45	0.46
1:A:681:ASN:N	1:A:682:PRO:CD	2.79	0.46
1:A:504:PHE:CZ	1:A:507:PHE:CE1	3.04	0.46
1:A:644:VAL:HG13	1:A:716:ILE:HA	1.98	0.46
1:B:302:LEU:HD23	1:B:428:PRO:HD3	1.98	0.46
1:B:652:VAL:HG11	1:B:716:ILE:HD13	1.98	0.45
1:B:313:THR:HB	1:B:329:TYR:CE1	2.51	0.45
1:A:206:LYS:O	1:A:210:GLN:HB2	2.17	0.45
1:A:242:ARG:CD	1:A:728:GLN:NE2	2.78	0.45
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.38	0.45
1:B:654:PRO:HG3	1:B:678:ASN:O	2.16	0.45
1:B:188:CYS:SG	1:B:204:PHE:HA	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ALA:CB	1:B:518:TYR:CE1	2.99	0.45
1:B:378:PHE:HA	1:B:381:SER:O	2.17	0.45
1:A:533:GLN:HA	1:A:533:GLN:OE1	2.17	0.45
1:B:199:GLU:HG2	1:B:200:GLU:N	2.33	0.44
1:B:191:SER:HB2	1:B:193:THR:CG2	2.43	0.44
1:A:728:GLN:NE2	1:A:754:ILE:H	2.15	0.44
1:B:162:PHE:N	5:B:1134:HOH:O	2.49	0.44
1:B:175:GLN:HB3	5:B:789:HOH:O	2.16	0.44
1:A:438:LYS:HA	1:A:499:CYS:HB2	1.98	0.44
4:B:1:I3P:O2	4:B:1:I3P:O11	2.36	0.44
1:A:613:THR:CG2	1:A:614:THR:N	2.80	0.44
1:B:184:ILE:CG2	1:B:204:PHE:CD1	2.99	0.44
1:A:398:GLN:O	1:A:492:LEU:HD23	2.18	0.44
1:A:548:SER:H	1:A:573:GLN:NE2	2.15	0.44
1:B:196:LEU:HA	1:B:196:LEU:HD23	1.63	0.44
1:B:558:ASP:O	1:B:559:SER:HB2	2.17	0.44
1:B:358:TYR:N	1:B:358:TYR:HD1	2.16	0.44
1:A:368:ASP:OD1	1:A:371:ARG:NH1	2.51	0.44
1:B:502:VAL:HG13	1:B:503:HIS:N	2.32	0.44
1:A:652:VAL:HG11	1:A:716:ILE:HD13	1.99	0.43
1:B:238:GLN:O	1:B:242:ARG:HA	2.17	0.43
1:B:178:ASP:O	1:B:180:TYR:HB3	2.18	0.43
1:A:298:MET:HB2	1:A:429:GLU:HG2	2.00	0.43
1:B:165:LEU:HG	1:B:185:PHE:CD1	2.52	0.43
1:A:338:ARG:HG3	1:A:601:TYR:CE1	2.53	0.43
1:B:163:LYS:O	1:B:167:ASP:HB2	2.19	0.43
1:B:533:GLN:HA	1:B:533:GLN:OE1	2.19	0.43
1:B:388:SER:HA	1:B:438:LYS:HB3	2.01	0.43
1:B:530:ARG:HH11	1:B:530:ARG:CG	2.32	0.43
1:A:409:LEU:HA	1:A:409:LEU:HD12	1.80	0.43
1:B:681:ASN:N	1:B:682:PRO:CD	2.80	0.43
1:B:547:LEU:HD23	1:B:573:GLN:CG	2.44	0.43
1:A:529:LEU:HA	1:A:529:LEU:HD23	1.85	0.43
1:A:595:ASP:OD1	1:A:596:ASN:N	2.47	0.43
1:A:272:LYS:O	1:A:275:PHE:HB3	2.18	0.43
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.54	0.43
1:A:504:PHE:CZ	1:A:506:GLY:CA	2.98	0.42
1:B:520:MET:HE2	1:B:549:ARG:CB	2.46	0.42
1:B:183:LYS:HG2	1:B:184:ILE:HD12	2.02	0.42
1:A:209:THR:HG22	1:A:209:THR:O	2.19	0.42
1:A:613:THR:HG21	1:A:615:PHE:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:GLN:HB2	1:A:519:GLU:HB2	2.01	0.42
1:B:162:PHE:HA	1:B:165:LEU:HB2	2.01	0.42
1:A:732:HIS:HA	1:A:748:LEU:O	2.18	0.42
1:A:652:VAL:HG11	1:A:716:ILE:CD1	2.50	0.42
1:B:445:LEU:HD23	1:B:445:LEU:HA	1.64	0.42
1:B:398:GLN:O	1:B:492:LEU:HD23	2.19	0.42
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.79	0.42
1:A:325:SER:HA	1:A:364:ILE:HG21	2.02	0.42
1:B:396:GLU:OE1	1:B:399:ARG:NH1	2.51	0.42
1:B:205:TYR:O	1:B:208:LEU:HB3	2.19	0.42
1:B:164:GLU:H	1:B:164:GLU:HG2	1.39	0.42
1:B:167:ASP:HB3	1:B:168:PHE:H	1.55	0.42
1:A:708:ASP:O	1:A:711:SER:O	2.38	0.42
1:A:654:PRO:HG3	1:A:678:ASN:O	2.19	0.42
1:A:260:PRO:HG3	1:A:277:MET:HE3	2.02	0.42
1:A:516:ALA:CB	1:A:518:TYR:CE2	3.02	0.41
1:B:661:HIS:O	1:B:698:ALA:HA	2.20	0.41
1:B:729:GLY:O	1:B:751:LYS:HA	2.20	0.41
1:A:558:ASP:O	1:A:559:SER:HB2	2.21	0.41
1:A:201:ILE:HG13	1:A:201:ILE:H	1.40	0.41
1:A:212:ALA:O	1:A:215:ASP:HB2	2.20	0.41
1:A:402:ALA:HB2	1:A:492:LEU:CD2	2.49	0.41
1:A:406:ARG:HH11	1:A:406:ARG:CG	2.33	0.41
1:A:241:GLN:NE2	1:A:730:TYR:H	2.01	0.41
1:A:300:GLN:HB3	1:A:301:PRO:CD	2.50	0.41
1:A:655:LYS:HE2	1:A:671:GLN:OE1	2.21	0.41
1:B:406:ARG:CG	1:B:406:ARG:HH11	2.34	0.41
1:B:504:PHE:CZ	1:B:506:GLY:CA	3.00	0.41
1:A:203:THR:HB	1:A:204:PHE:H	1.60	0.41
1:A:426:PRO:HA	1:A:430:GLN:OE1	2.20	0.41
1:B:418:LEU:HD12	1:B:426:PRO:HB3	2.03	0.41
1:A:371:ARG:O	1:A:374:ARG:HB3	2.20	0.41
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.50	0.41
1:A:644:VAL:HG12	1:A:714:ASP:HB3	2.03	0.41
1:B:573:GLN:N	1:B:573:GLN:NE2	2.63	0.41
1:A:343:ASP:O	1:A:354:ILE:HA	2.21	0.41
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.51	0.40
1:A:622:GLN:CB	1:B:445:LEU:CD1	3.00	0.40
1:A:357:GLY:C	1:A:358:TYR:CD1	2.95	0.40
1:A:594:GLN:NE2	1:A:594:GLN:HA	2.36	0.40
1:A:259:GLU:OE1	1:A:270:MET:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:GLN:CA	1:B:445:LEU:CD1	2.99	0.40
1:B:732:HIS:HA	1:B:748:LEU:O	2.21	0.40
1:B:293:ARG:HG3	1:B:293:ARG:NH1	2.36	0.40
1:A:689:GLU:HB3	1:B:491:GLU:HG3	2.03	0.40
1:A:644:VAL:HG13	1:A:715:PHE:O	2.22	0.40
1:B:733:VAL:HB	1:B:748:LEU:HB2	2.01	0.40
1:B:188:CYS:O	1:B:200:GLU:HB3	2.21	0.40
1:A:721:ILE:HA	1:A:722:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/624 (82%)	469 (92%)	33 (6%)	7 (1%)	14	13
1	B	557/624 (89%)	514 (92%)	31 (6%)	12 (2%)	8	6
All	All	1066/1248 (85%)	983 (92%)	64 (6%)	19 (2%)	11	9

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	A	644	VAL
1	B	179	GLY
1	B	198	ASP
1	B	509	SER
1	B	515	GLN
1	B	644	VAL
1	B	162	PHE
1	B	650	SER
1	A	203	THR

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Mol	Chain	Res	Type
1	B	167	ASP
1	A	647	ASN
1	B	175	GLN
1	A	510	PRO
1	B	168	PHE
1	A	421	VAL
1	A	514	GLY
1	B	174	ILE
1	B	510	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	448/545 (82%)	408 (91%)	40 (9%)	12	14
1	B	492/545 (90%)	435 (88%)	57 (12%)	7	7
All	All	940/1090 (86%)	843 (90%)	97 (10%)	9	10

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LEU
1	A	238	GLN
1	A	242	ARG
1	A	252	LEU
1	A	278	TYR
1	A	293	ARG
1	A	350	GLN
1	A	406	ARG
1	A	409	LEU
1	A	419	ASP
1	A	424	SER
1	A	432	LYS
1	A	436	LEU
1	A	487	LYS

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Mol	Chain	Res	Type
1	A	492	LEU
1	A	510	PRO
1	A	515	GLN
1	A	526	SER
1	A	530	ARG
1	A	533	GLN
1	A	535	SER
1	A	539	PHE
1	A	545	SER
1	A	563	SER
1	A	573	GLN
1	A	612	ASN
1	A	617	SER
1	A	630	ARG
1	A	645	ASN
1	A	652	VAL
1	A	655	LYS
1	A	657	ILE
1	A	665	ARG
1	A	676	THR
1	A	686	MET
1	A	691	GLU
1	A	710	SER
1	A	712	LYS
1	A	738	LYS
1	A	756	ASP
1	B	158	ASN
1	B	159	LYS
1	B	160	MET
1	B	164	GLU
1	B	166	LYS
1	B	170	LYS
1	B	171	GLU
1	B	172	LEU
1	B	173	ASN
1	B	174	ILE
1	B	175	GLN
1	B	177	ASP
1	B	182	ARG
1	B	186	ARG
1	B	199	GLU
1	B	200	GLU

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Mol	Chain	Res	Type
1	B	201	ILE
1	B	208	LEU
1	B	210	GLN
1	B	242	ARG
1	B	263	THR
1	B	293	ARG
1	B	309	SER
1	B	331	ARG
1	B	358	TYR
1	B	406	ARG
1	B	409	LEU
1	B	423	THR
1	B	432	LYS
1	B	436	LEU
1	B	484	ASP
1	B	486	LEU
1	B	492	LEU
1	B	508	SER
1	B	515	GLN
1	B	526	SER
1	B	535	SER
1	B	539	PHE
1	B	545	SER
1	B	563	SER
1	B	573	GLN
1	B	613	THR
1	B	617	SER
1	B	630	ARG
1	B	643	LYS
1	B	644	VAL
1	B	646	LYS
1	B	655	LYS
1	B	657	ILE
1	B	665	ARG
1	B	676	THR
1	B	685	ASP
1	B	691	GLU
1	B	709	SER
1	B	710	SER
1	B	738	LYS
1	B	756	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	291	HIS
1	A	349	ASN
1	A	515	GLN
1	A	542	HIS
1	A	573	GLN
1	A	594	GLN
1	A	639	GLN
1	A	645	ASN
1	A	661	HIS
1	A	718	GLN
1	A	728	GLN
1	B	241	GLN
1	B	291	HIS
1	B	304	HIS
1	B	349	ASN
1	B	515	GLN
1	B	542	HIS
1	B	573	GLN
1	B	594	GLN
1	B	639	GLN
1	B	718	GLN
1	B	755	GLN

### 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 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	$\# Z  > 2$
4	I3P	A	1	2	24,24,24	0.68	0	33,39,39	1.31	4 (12%)
3	ACT	A	5	-	1,3,3	2.44	1 (100%)	0,3,3	0.00	-
4	I3P	B	1	2	24,24,24	0.82	0	33,39,39	1.32	4 (12%)
3	ACT	B	5	-	1,3,3	2.62	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	I3P	A	1	2	-	0/15/39/39	0/1/1/1
3	ACT	A	5	-	-	0/0/0/0	0/0/0/0
4	I3P	B	1	2	-	0/15/39/39	0/1/1/1
3	ACT	B	5	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5	ACT	CH3-C	2.44	1.52	1.48
3	B	5	ACT	CH3-C	2.62	1.52	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	I3P	O1-C1-C6	-2.99	101.83	108.38
4	B	1	I3P	O1-C1-C6	-2.85	102.13	108.38
4	A	1	I3P	O5-C5-C6	-2.62	102.63	108.38
4	B	1	I3P	O6-C6-C1	-2.32	104.38	109.87
4	B	1	I3P	O13-P1-O11	-2.22	103.42	110.58
4	A	1	I3P	O4-P4-O41	2.34	112.96	107.11
4	B	1	I3P	O5-P5-O51	3.09	114.84	107.11
4	A	1	I3P	O5-P5-O51	3.36	115.51	107.11



There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	I3P	1	0

## 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	507/624 (81%)	0.03	34 (6%) 21 29	17, 34, 87, 122	13 (2%)
1	B	556/624 (89%)	0.16	52 (9%) 11 16	18, 36, 90, 118	21 (3%)
All	All	1063/1248 (85%)	0.10	86 (8%) 15 21	17, 35, 90, 122	34 (3%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	201	ILE	13.5
1	A	644	VAL	11.0
1	B	165	LEU	9.7
1	A	204	PHE	8.8
1	A	421	VAL	8.1
1	A	203	THR	7.8
1	A	202	GLU	6.8
1	A	200	GLU	6.7
1	B	514	GLY	6.3
1	B	508	SER	6.2
1	B	162	PHE	6.0
1	B	245	GLU	5.9
1	B	198	ASP	5.8
1	B	176	VAL	5.8
1	B	645	ASN	5.7
1	A	205	TYR	5.4
1	A	647	ASN	5.0
1	B	486	LEU	5.0
1	B	710	SER	4.9
1	A	420	GLY	4.9
1	B	649	ASN	4.6
1	A	645	ASN	4.5
1	A	710	SER	4.4
1	B	172	LEU	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	505	GLY	4.3
1	A	711	SER	4.2
1	B	173	ASN	4.2
1	B	167	ASP	4.1
1	A	504	PHE	4.1
1	B	174	ILE	3.9
1	A	648	LYS	3.9
1	A	503	HIS	3.9
1	A	515	GLN	3.7
1	B	261	SER	3.7
1	B	515	GLN	3.6
1	B	170	LYS	3.6
1	B	246	ALA	3.5
1	B	484	ASP	3.5
1	B	169	LEU	3.5
1	A	206	LYS	3.4
1	B	166	LYS	3.4
1	B	266	ALA	3.4
1	B	711	SER	3.3
1	B	485	LYS	3.3
1	A	709	SER	3.3
1	A	423	THR	3.3
1	A	643	LYS	3.2
1	B	171	GLU	3.2
1	B	199	GLU	3.1
1	B	572	CYS	3.1
1	A	712	LYS	3.0
1	B	178	ASP	2.9
1	B	647	ASN	2.8
1	A	207	MET	2.7
1	B	226	GLU	2.7
1	B	159	LYS	2.7
1	A	649	ASN	2.7
1	A	442	LEU	2.6
1	B	644	VAL	2.6
1	B	224	SER	2.6
1	B	709	SER	2.6
1	B	177	ASP	2.6
1	B	160	MET	2.5
1	B	267	GLN	2.5
1	B	163	LYS	2.5
1	B	646	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	503	HIS	2.4
1	A	622	GLN	2.4
1	B	168	PHE	2.4
1	A	224	SER	2.3
1	A	533	GLN	2.3
1	B	507	PHE	2.3
1	A	650	SER	2.3
1	B	197	GLU	2.3
1	B	194	ASP	2.3
1	A	502	VAL	2.3
1	A	508	SER	2.2
1	B	306	LEU	2.2
1	B	244	GLU	2.2
1	A	422	THR	2.2
1	B	225	ALA	2.2
1	B	247	GLY	2.2
1	B	196	LEU	2.1
1	A	651	ILE	2.1
1	B	349	ASN	2.0
1	B	260	PRO	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	ACT	B	5	4/4	0.97	0.16	2.40	32,32,33,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ACT	A	5	4/4	0.98	0.14	1.53	31,35,35,39	0
4	I3P	A	1	24/24	0.95	0.10	-0.20	33,55,133,150	0
4	I3P	B	1	24/24	0.97	0.08	-0.83	23,42,60,73	0
2	CA	B	2	1/1	0.96	0.06	-	43,43,43,43	0
2	CA	A	2	1/1	0.94	0.04	-	46,46,46,46	0
2	CA	B	3	1/1	0.96	0.11	-	71,71,71,71	0
2	CA	A	3	1/1	0.95	0.12	-	79,79,79,79	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.