



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 06:09 am BST

PDB ID : 1DJI  
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM  
RAT COMPLEXED WITH CALCIUM  
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.  
Deposited on : 1996-09-25  
Resolution : 2.50 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

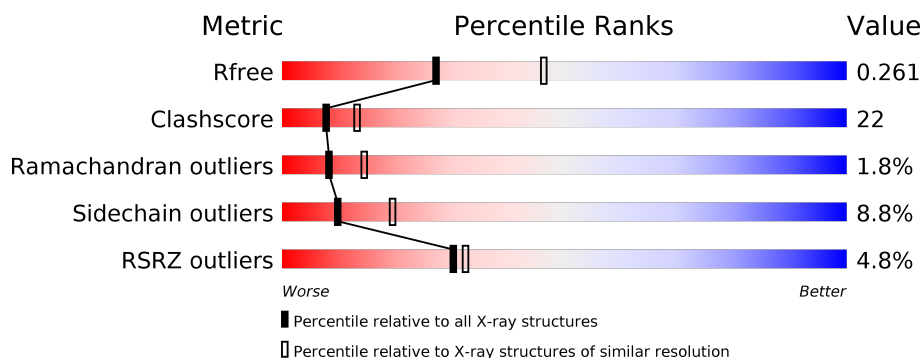
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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>4%</div> <div> <div></div> <div>52%</div> <div>26%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	624	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>28%</div> <div>5%</div> <div>10%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9403 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	67	0	0
			4070	2573	709	766	22			
1	B	559	Total	C	N	O	S	102	0	0
			4445	2807	771	843	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 4	C 2	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

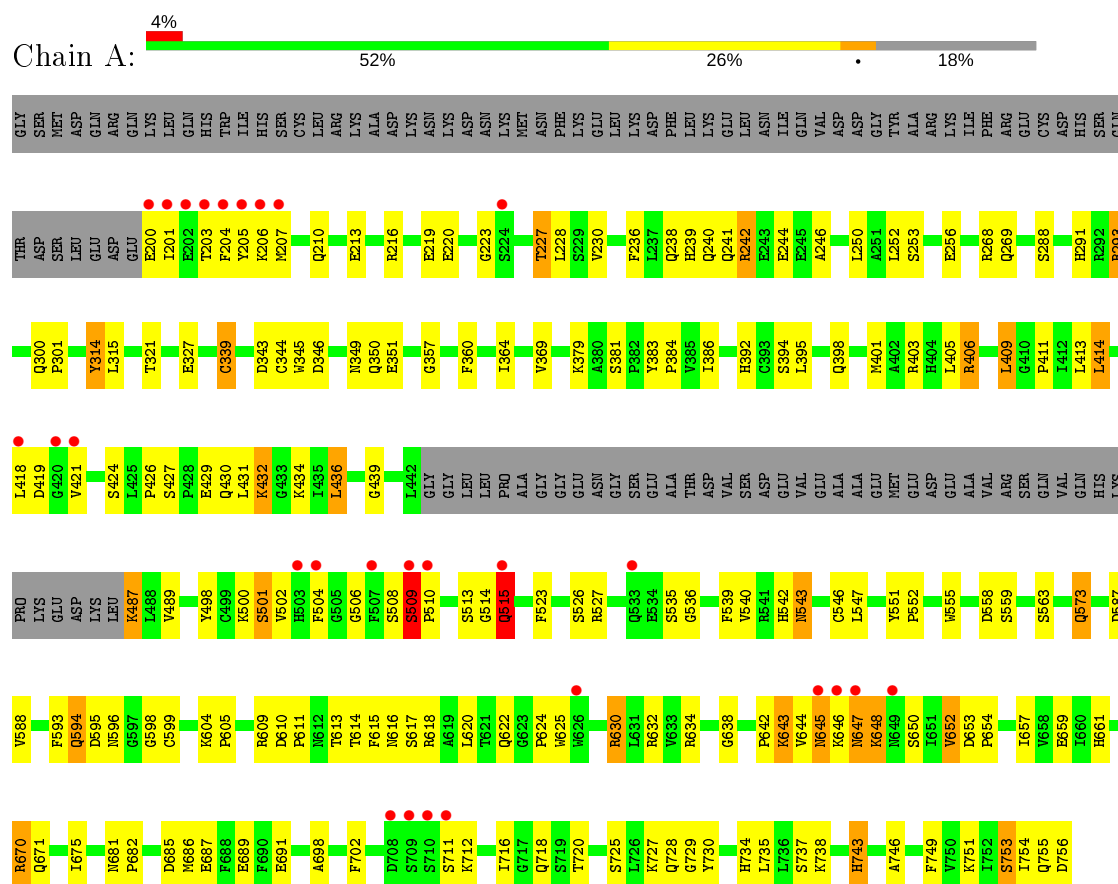
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	408	Total 408	O 408	0	0
4	B	466	Total 466	O 466	0	0

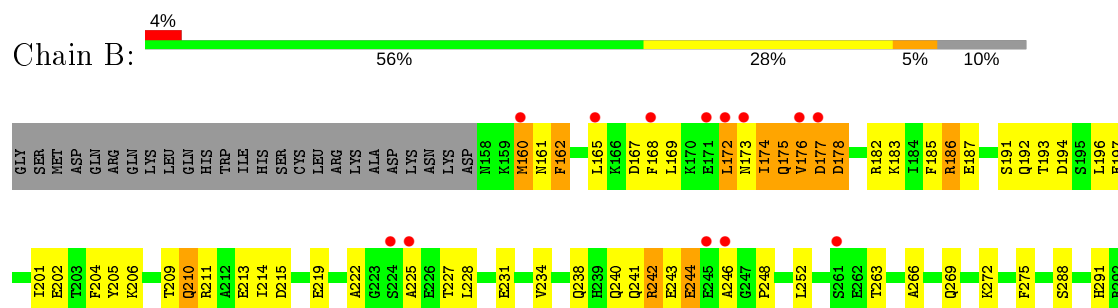
### 3 Residue-property plots

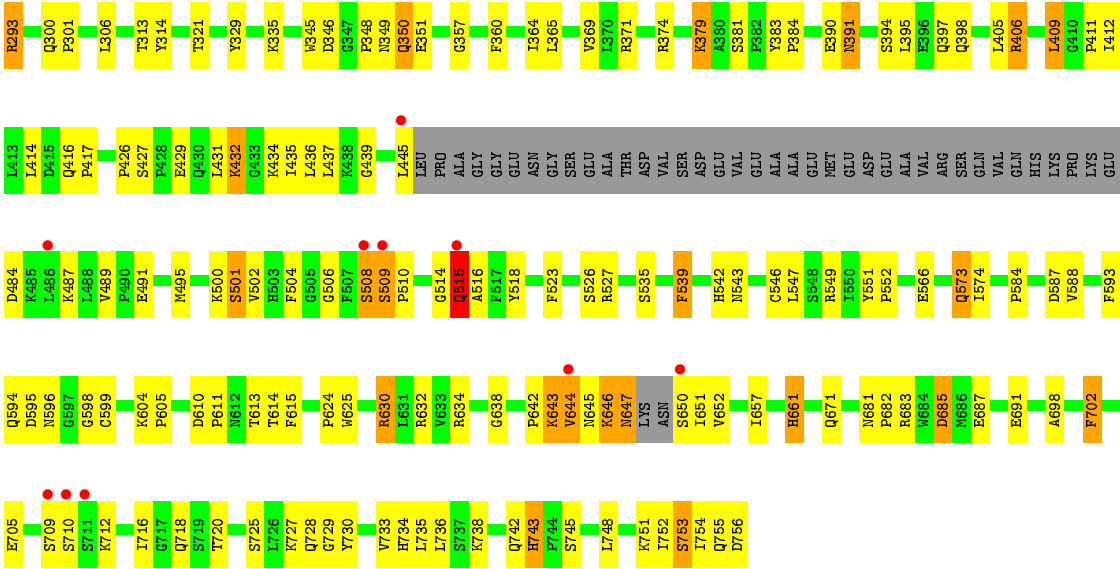
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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



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





## 4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	398.03 Å   398.03 Å   398.03 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	10.00 – 2.50 24.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (10.00-2.50) 97.5 (24.88-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.50 Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.220   ,   0.280 0.214   ,   0.261	Depositor DCC
$R_{free}$ test set	3908 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 109.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9403	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 1.61% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.70	8/4165 (0.2%)	0.79	1/5641 (0.0%)
1	B	0.74	7/4544 (0.2%)	0.81	3/6144 (0.0%)
All	All	0.72	15/8709 (0.2%)	0.80	4/11785 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	TYR	CE2-CZ	-8.73	1.27	1.38
1	A	314	TYR	CE1-CZ	-7.75	1.28	1.38
1	B	702	PHE	CE1-CZ	-7.26	1.23	1.37
1	B	314	TYR	CE1-CZ	-7.14	1.29	1.38
1	B	314	TYR	CG-CD2	-7.02	1.30	1.39
1	B	314	TYR	CG-CD1	-6.84	1.30	1.39
1	B	702	PHE	CG-CD2	-6.65	1.28	1.38
1	A	314	TYR	CE2-CZ	-6.23	1.30	1.38
1	A	702	PHE	CE1-CZ	-6.06	1.25	1.37
1	A	702	PHE	CG-CD1	-5.94	1.29	1.38
1	A	702	PHE	CE2-CZ	-5.83	1.26	1.37
1	A	314	TYR	CG-CD2	-5.66	1.31	1.39
1	A	314	TYR	CG-CD1	-5.42	1.32	1.39
1	A	702	PHE	CG-CD2	-5.08	1.31	1.38
1	B	390	GLU	C-O	-5.00	1.13	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	743	HIS	C-N-CD	-7.67	103.72	120.60
1	A	743	HIS	C-N-CD	-7.65	103.78	120.60
1	B	391	ASN	N-CA-C	6.97	129.82	111.00
1	B	306	LEU	N-CA-C	-5.14	97.11	111.00



There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4070	0	3994	162	0
1	B	4445	0	4353	201	0
2	A	3	0	0	1	0
2	B	3	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0
4	A	408	0	0	15	0
4	B	466	0	0	25	0
All	All	9403	0	8353	357	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 22.

All (357) 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)
2:A:2:CA:CA	4:A:778:HOH:O	1.19	1.16
1:B:573:GLN:N	1:B:573:GLN:HE21	1.46	1.13
1:B:613:THR:HG22	1:B:615:PHE:H	1.11	1.10
1:B:172:LEU:HB2	1:B:174:ILE:HG13	1.33	1.03
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.22	1.02
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.23	0.98
1:B:573:GLN:H	1:B:573:GLN:NE2	1.59	0.98
1:A:613:THR:HG22	1:A:615:PHE:H	1.27	0.95
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.53	0.89
1:B:630:ARG:HD2	1:B:755:GLN:HE21	1.37	0.87
1:B:365:LEU:HG	4:B:1044:HOH:O	1.75	0.86
1:A:238:GLN:HE21	1:A:246:ALA:HB3	1.41	0.84
1:B:504:PHE:HB3	1:B:527:ARG:NH2	1.93	0.84
1:B:728:GLN:NE2	1:B:754:ILE:H	1.76	0.84
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:HG2	1:A:246:ALA:CB	2.09	0.82
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.93	0.82
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.62	0.82
1:A:728:GLN:NE2	1:A:754:ILE:H	1.76	0.81
1:B:613:THR:HG22	1:B:615:PHE:N	1.95	0.81
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.16	0.80
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.64	0.79
1:B:241:GLN:HE22	1:B:730:TYR:H	1.30	0.79
1:A:241:GLN:HE22	1:A:730:TYR:H	1.31	0.79
1:B:172:LEU:HB2	1:B:174:ILE:CG1	2.14	0.77
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.66	0.77
1:B:162:PHE:CD1	1:B:165:LEU:HD23	2.21	0.76
1:B:202:GLU:O	1:B:206:LYS:HG3	1.86	0.75
1:A:613:THR:HG22	1:A:615:PHE:N	1.99	0.75
1:B:646:LYS:HG3	1:B:647:ASN:OD1	1.85	0.75
1:B:350:GLN:HG2	4:B:1205:HOH:O	1.87	0.75
1:B:630:ARG:CD	1:B:755:GLN:HE21	2.00	0.75
1:A:238:GLN:HG2	1:A:246:ALA:HB1	1.70	0.73
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.71	0.73
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.24	0.73
1:A:394:SER:O	1:A:398:GLN:HG3	1.90	0.72
1:B:185:PHE:CE1	1:B:196:LEU:HG	2.24	0.71
1:B:227:THR:CG2	1:B:269:GLN:HB3	2.21	0.71
1:B:573:GLN:N	1:B:573:GLN:NE2	2.26	0.71
1:A:543:ASN:HD22	1:A:543:ASN:N	1.88	0.70
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.73	0.70
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.20	0.70
1:B:162:PHE:CE1	1:B:165:LEU:HD23	2.26	0.70
1:B:196:LEU:HB3	1:B:201:ILE:HG12	1.73	0.70
1:A:418:LEU:HB2	1:A:421:VAL:CG2	2.21	0.70
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.73	0.69
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.28	0.68
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.23	0.67
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.25	0.67
1:A:643:LYS:CE	1:A:648:LYS:HA	2.25	0.67
1:A:268:ARG:NE	4:A:941:HOH:O	2.26	0.67
1:A:616:ASN:OD1	1:A:618:ARG:HB2	1.94	0.67
1:B:177:ASP:OD1	1:B:177:ASP:N	2.27	0.67
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.24	0.66
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.78	0.66
1:B:162:PHE:O	1:B:165:LEU:HB3	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.77	0.66
1:B:394:SER:O	1:B:398:GLN:HG3	1.96	0.66
1:B:588:VAL:HG21	1:B:661:HIS:HD2	1.60	0.66
1:B:588:VAL:HG21	1:B:661:HIS:CD2	2.31	0.65
1:B:186:ARG:HG2	4:B:861:HOH:O	1.96	0.65
1:B:752:ILE:N	4:B:770:HOH:O	2.29	0.65
1:B:227:THR:HG21	1:B:269:GLN:HB3	1.78	0.65
1:A:643:LYS:HE3	1:A:647:ASN:O	1.97	0.65
1:B:610:ASP:OD1	1:B:611:PRO:HD2	1.95	0.65
1:B:573:GLN:H	1:B:573:GLN:HE21	0.74	0.65
1:A:610:ASP:OD1	1:A:611:PRO:HD2	1.97	0.65
1:B:647:ASN:OD1	1:B:647:ASN:N	2.29	0.64
1:B:321:THR:HG22	1:B:360:PHE:HB2	1.80	0.64
1:B:350:GLN:NE2	1:B:350:GLN:HA	2.11	0.64
1:B:683:ARG:NH2	1:B:685:ASP:OD2	2.30	0.64
1:B:643:LYS:CE	1:B:646:LYS:HB3	2.27	0.64
1:A:238:GLN:HE21	1:A:246:ALA:CB	2.10	0.64
1:A:206:LYS:O	1:A:210:GLN:HB2	1.97	0.64
1:A:219:GLU:O	1:A:223:GLY:N	2.26	0.64
1:B:162:PHE:CZ	1:B:182:ARG:HB2	2.34	0.63
1:B:539:PHE:O	1:B:543:ASN:ND2	2.29	0.63
1:A:343:ASP:HB3	4:A:1132:HOH:O	1.99	0.62
1:A:418:LEU:HB2	1:A:421:VAL:HG21	1.80	0.62
1:B:335:LYS:NZ	4:B:896:HOH:O	2.29	0.62
1:B:644:VAL:HG23	1:B:645:ASN:H	1.63	0.62
1:A:201:ILE:O	1:A:205:TYR:HB2	1.98	0.62
1:B:500:LYS:HE3	4:B:1060:HOH:O	2.00	0.62
1:A:238:GLN:NE2	1:A:246:ALA:HB3	2.13	0.62
1:B:293:ARG:NH1	4:B:797:HOH:O	2.29	0.62
1:B:379:LYS:NZ	4:B:905:HOH:O	2.33	0.62
1:B:168:PHE:CE1	1:B:172:LEU:HD11	2.35	0.62
1:B:234:VAL:O	1:B:238:GLN:HG3	2.00	0.61
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.30	0.61
1:B:411:PRO:O	1:B:434:LYS:NZ	2.33	0.61
1:A:421:VAL:HG11	1:A:498:TYR:CE1	2.35	0.61
1:A:411:PRO:O	1:A:434:LYS:NZ	2.35	0.60
1:B:632:ARG:NE	4:B:773:HOH:O	2.30	0.60
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.32	0.60
1:A:542:HIS:HD2	1:A:543:ASN:ND2	1.99	0.59
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.32	0.59
1:A:436:LEU:HD23	1:A:436:LEU:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ALA:HA	1:B:228:LEU:HD23	1.84	0.59
1:B:436:LEU:H	1:B:436:LEU:HD23	1.68	0.59
1:A:405:LEU:O	1:A:409:LEU:HB2	2.02	0.59
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.32	0.58
1:B:429:GLU:OE1	1:B:432:LYS:HE3	2.03	0.58
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.03	0.58
1:B:211:ARG:HG3	4:B:844:HOH:O	2.04	0.58
1:B:742:GLN:NE2	4:B:822:HOH:O	2.35	0.58
1:A:241:GLN:HE22	1:A:730:TYR:N	2.02	0.57
1:B:178:ASP:OD1	1:B:178:ASP:N	2.37	0.57
1:B:300:GLN:O	1:B:427:SER:HA	2.03	0.57
1:A:236:PHE:HA	4:A:931:HOH:O	2.02	0.57
1:A:252:LEU:O	1:A:256:GLU:HG3	2.04	0.57
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.40	0.57
1:B:593:PHE:O	1:B:598:GLY:HA2	2.05	0.57
1:A:395:LEU:HD22	1:A:489:VAL:HG12	1.87	0.57
1:A:242:ARG:HG3	1:A:728:GLN:HB2	1.87	0.56
1:A:418:LEU:HD12	1:A:426:PRO:HB3	1.86	0.56
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.40	0.56
1:B:436:LEU:N	1:B:436:LEU:HD23	2.21	0.56
1:A:381:SER:HB2	1:A:599:CYS:HA	1.86	0.56
1:B:206:LYS:O	1:B:210:GLN:HB3	2.05	0.56
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.88	0.56
1:A:395:LEU:HD22	1:A:489:VAL:CG1	2.36	0.56
1:B:643:LYS:HD2	1:B:643:LYS:C	2.16	0.56
1:A:728:GLN:HE22	1:A:754:ILE:H	1.53	0.56
1:B:197:GLU:O	1:B:201:ILE:HG13	2.06	0.56
1:B:439:GLY:C	1:B:501:SER:HB2	2.26	0.55
1:B:595:ASP:OD1	1:B:596:ASN:N	2.38	0.55
1:A:429:GLU:OE1	1:A:432:LYS:HE3	2.07	0.55
1:A:509:SER:HB3	1:A:510:PRO:HD3	1.87	0.55
1:B:643:LYS:HE3	1:B:646:LYS:HB3	1.88	0.55
1:B:379:LYS:NZ	4:B:906:HOH:O	2.38	0.55
1:B:300:GLN:HB3	1:B:301:PRO:HD2	1.89	0.55
1:A:593:PHE:O	1:A:598:GLY:HA2	2.08	0.54
1:A:508:SER:OG	1:A:509:SER:N	2.36	0.54
1:A:643:LYS:C	1:A:645:ASN:H	2.10	0.54
1:A:737:SER:HA	4:A:1036:HOH:O	2.07	0.54
1:B:657:ILE:HD13	1:B:671:GLN:HB3	1.89	0.54
1:A:213:GLU:HG3	1:A:749:PHE:CD2	2.43	0.54
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:ARG:HD2	1:B:755:GLN:NE2	2.16	0.54
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.36	0.54
1:B:729:GLY:O	1:B:751:LYS:HA	2.08	0.54
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.41	0.53
1:B:644:VAL:CG2	1:B:645:ASN:H	2.17	0.53
1:B:248:PRO:O	1:B:252:LEU:HD12	2.08	0.53
1:B:416:GLN:HG2	1:B:417:PRO:HD2	1.90	0.53
1:B:735:LEU:O	1:B:743:HIS:HB2	2.08	0.53
1:B:238:GLN:HG2	1:B:246:ALA:HB3	1.89	0.53
1:B:431:LEU:O	1:B:434:LYS:HB2	2.09	0.53
1:A:555:TRP:N	4:A:1064:HOH:O	2.33	0.53
1:B:405:LEU:O	1:B:409:LEU:HB2	2.08	0.53
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.91	0.53
1:A:536:GLY:HA3	4:A:987:HOH:O	2.09	0.53
1:A:227:THR:HG21	1:A:269:GLN:OE1	2.10	0.52
1:A:643:LYS:HE3	1:A:648:LYS:HA	1.90	0.52
1:B:162:PHE:HA	1:B:165:LEU:HB3	1.91	0.52
1:A:241:GLN:C	1:A:242:ARG:HG2	2.29	0.52
1:A:406:ARG:HH11	1:A:406:ARG:CG	2.22	0.51
1:A:300:GLN:HB3	1:A:301:PRO:CD	2.40	0.51
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.44	0.51
1:B:172:LEU:N	1:B:172:LEU:HD23	2.26	0.51
1:A:638:GLY:O	1:A:681:ASN:HA	2.10	0.51
1:B:174:ILE:O	1:B:176:VAL:N	2.44	0.51
1:B:242:ARG:HD3	4:B:771:HOH:O	2.09	0.51
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.91	0.51
1:B:162:PHE:N	4:B:1152:HOH:O	2.19	0.51
1:B:227:THR:HG23	1:B:269:GLN:HB3	1.93	0.51
1:A:515:GLN:NE2	1:A:542:HIS:CE1	2.79	0.51
1:A:735:LEU:O	1:A:743:HIS:HB2	2.10	0.51
1:A:618:ARG:HG3	4:A:987:HOH:O	2.11	0.51
1:B:604:LYS:HB3	1:B:605:PRO:HD2	1.91	0.51
1:A:728:GLN:HE21	1:A:753:SER:HA	1.75	0.51
1:B:383:TYR:HD2	1:B:599:CYS:HB2	1.75	0.50
1:A:241:GLN:NE2	1:A:729:GLY:HA3	2.27	0.50
1:B:183:LYS:O	1:B:187:GLU:HG3	2.11	0.50
1:B:162:PHE:CE1	1:B:182:ARG:HA	2.46	0.50
1:A:622:GLN:CA	1:B:445:LEU:HD11	2.41	0.50
1:B:734:HIS:HE1	4:B:1123:HOH:O	1.95	0.50
1:A:200:GLU:O	1:A:204:PHE:N	2.43	0.50
1:A:542:HIS:CD2	1:A:543:ASN:ND2	2.79	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:THR:O	1:B:266:ALA:HB3	2.12	0.50
1:A:536:GLY:O	1:A:540:VAL:HG23	2.12	0.50
1:B:272:LYS:O	1:B:275:PHE:HB3	2.12	0.50
1:A:250:LEU:O	1:A:253:SER:OG	2.29	0.49
1:B:515:GLN:NE2	1:B:542:HIS:CE1	2.80	0.49
1:B:644:VAL:HG23	1:B:645:ASN:N	2.26	0.49
1:B:381:SER:HB2	1:B:599:CYS:HA	1.93	0.49
1:A:613:THR:HG22	1:A:614:THR:N	2.27	0.49
1:A:439:GLY:C	1:A:501:SER:HB2	2.32	0.49
1:A:604:LYS:HB3	1:A:605:PRO:HD2	1.94	0.49
1:A:421:VAL:HG11	1:A:498:TYR:CZ	2.47	0.49
1:A:551:TYR:HB2	1:A:552:PRO:HD2	1.95	0.49
1:B:191:SER:C	1:B:192:GLN:HG2	2.33	0.49
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.46	0.49
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.42	0.49
1:B:160:MET:HG2	1:B:161:ASN:N	2.26	0.49
1:B:293:ARG:CG	1:B:293:ARG:HH11	2.26	0.49
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.48	0.49
1:A:239:HIS:HD2	4:A:800:HOH:O	1.95	0.49
1:A:657:ILE:HD13	1:A:671:GLN:HB3	1.95	0.49
1:A:734:HIS:HE1	4:A:1042:HOH:O	1.95	0.49
1:B:191:SER:OG	1:B:193:THR:HG23	2.13	0.49
1:A:238:GLN:HG2	1:A:246:ALA:HB3	1.88	0.48
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.12	0.48
1:A:689:GLU:HB3	1:B:491:GLU:HG3	1.95	0.48
1:A:227:THR:HG21	1:A:269:GLN:HB3	1.94	0.48
1:A:547:LEU:HD23	1:A:573:GLN:CG	2.42	0.48
1:B:643:LYS:HE2	1:B:650:SER:O	2.13	0.48
1:A:686:MET:HG3	1:A:687:GLU:N	2.27	0.48
1:B:406:ARG:CG	1:B:406:ARG:HH11	2.26	0.48
1:B:406:ARG:NH1	1:B:406:ARG:HG3	2.28	0.48
1:A:543:ASN:ND2	1:A:543:ASN:N	2.60	0.48
1:B:547:LEU:HD23	1:B:573:GLN:CG	2.41	0.48
1:B:227:THR:HG21	1:B:269:GLN:OE1	2.13	0.48
1:B:293:ARG:HG3	1:B:293:ARG:NH1	2.29	0.48
1:B:348:PRO:HB2	1:B:349:ASN:ND2	2.28	0.48
1:B:288:SER:HB2	1:B:727:LYS:HD3	1.95	0.48
1:A:291:HIS:HD2	1:A:725:SER:OG	1.97	0.48
1:A:406:ARG:HG3	1:A:406:ARG:NH1	2.28	0.48
1:B:752:ILE:O	1:B:752:ILE:HG22	2.14	0.48
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:SER:CB	1:A:510:PRO:HD3	2.43	0.48
1:B:613:THR:HG22	1:B:614:THR:N	2.28	0.47
1:A:413:LEU:HD12	1:A:414:LEU:N	2.30	0.47
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.49	0.47
1:A:227:THR:HG23	1:A:269:GLN:HB3	1.96	0.47
1:A:346:ASP:OD2	1:A:394:SER:HB3	2.14	0.47
1:B:705:GLU:C	1:B:716:ILE:HD12	2.34	0.47
1:A:558:ASP:O	1:A:559:SER:HB2	2.13	0.47
1:A:242:ARG:HG3	1:A:728:GLN:CB	2.44	0.47
1:A:349:ASN:O	1:A:350:GLN:HB2	2.14	0.47
1:A:729:GLY:O	1:A:751:LYS:HA	2.15	0.47
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.29	0.47
1:A:220:GLU:HA	1:A:220:GLU:OE1	2.15	0.47
1:A:542:HIS:HD2	1:A:543:ASN:HD21	1.61	0.47
1:B:727:LYS:HE2	4:B:788:HOH:O	2.15	0.46
1:B:350:GLN:NE2	1:B:397:GLN:HE21	2.13	0.46
1:B:240:GLN:OE1	1:B:730:TYR:HE2	1.98	0.46
1:A:436:LEU:HD23	1:A:436:LEU:H	1.80	0.46
1:B:350:GLN:HE21	1:B:350:GLN:HA	1.81	0.46
1:B:412:ILE:CG2	1:B:435:ILE:HG13	2.46	0.46
1:B:162:PHE:HB2	4:B:1153:HOH:O	2.16	0.46
1:B:291:HIS:HD2	1:B:725:SER:HA	1.80	0.46
1:A:755:GLN:HG2	1:A:756:ASP:N	2.30	0.46
1:A:227:THR:HG21	1:A:269:GLN:CD	2.36	0.46
1:A:659:GLU:OE1	1:A:661:HIS:HE1	1.98	0.46
1:B:227:THR:CG2	1:B:228:LEU:N	2.79	0.46
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.50	0.46
1:B:244:GLU:C	1:B:246:ALA:H	2.18	0.45
1:B:365:LEU:CG	4:B:1044:HOH:O	2.49	0.45
1:A:653:ASP:HA	1:A:675:ILE:O	2.16	0.45
1:A:681:ASN:N	1:A:682:PRO:CD	2.79	0.45
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.40	0.45
1:B:643:LYS:NZ	1:B:646:LYS:CB	2.79	0.45
1:A:300:GLN:O	1:A:427:SER:HA	2.15	0.45
1:A:500:LYS:HE3	4:A:850:HOH:O	2.16	0.45
1:A:632:ARG:NH2	1:B:406:ARG:CZ	2.80	0.45
1:B:515:GLN:NE2	1:B:546:CYS:SG	2.90	0.45
1:A:227:THR:CG2	1:A:228:LEU:N	2.79	0.45
1:A:339:CYS:SG	1:A:386:ILE:HB	2.56	0.45
1:B:566:GLU:HB3	4:B:1084:HOH:O	2.17	0.45
1:B:604:LYS:HB3	1:B:605:PRO:CD	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.17	0.45
1:A:551:TYR:HB2	1:A:552:PRO:CD	2.46	0.45
1:A:587:ASP:HB3	1:A:718:GLN:NE2	2.31	0.45
1:B:728:GLN:HE21	1:B:753:SER:HA	1.80	0.45
1:A:727:LYS:HE2	4:A:947:HOH:O	2.16	0.45
1:A:406:ARG:CG	1:A:406:ARG:NH1	2.80	0.45
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.17	0.45
1:B:681:ASN:N	1:B:682:PRO:CD	2.80	0.45
1:B:186:ARG:HA	1:B:186:ARG:HD2	1.77	0.44
1:A:630:ARG:NH2	1:B:406:ARG:NH2	2.65	0.44
1:B:661:HIS:O	1:B:698:ALA:HA	2.17	0.44
1:A:509:SER:N	1:A:510:PRO:CD	2.80	0.44
1:B:213:GLU:HG2	1:B:214:ILE:N	2.30	0.44
1:B:350:GLN:CA	1:B:350:GLN:NE2	2.79	0.44
1:B:434:LYS:HD2	1:B:434:LYS:HA	1.67	0.44
1:B:551:TYR:HB2	1:B:552:PRO:CD	2.48	0.44
1:B:702:PHE:CE2	1:B:733:VAL:HG21	2.52	0.44
1:A:661:HIS:O	1:A:698:ALA:HA	2.18	0.44
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.48	0.44
1:A:421:VAL:CG1	1:A:498:TYR:CE1	3.01	0.44
1:A:504:PHE:CZ	1:A:506:GLY:CA	2.99	0.44
1:B:186:ARG:HG2	1:B:186:ARG:HH11	1.83	0.44
1:A:604:LYS:HB3	1:A:605:PRO:CD	2.47	0.44
1:B:508:SER:OG	1:B:509:SER:N	2.51	0.44
1:B:638:GLY:O	1:B:681:ASN:HA	2.18	0.43
1:A:238:GLN:NE2	1:A:246:ALA:O	2.51	0.43
1:A:595:ASP:OD1	1:A:596:ASN:N	2.46	0.43
1:A:288:SER:HB2	1:A:727:LYS:HD3	2.00	0.43
1:B:484:ASP:O	1:B:487:LYS:N	2.37	0.43
1:A:515:GLN:HE22	1:A:546:CYS:HB3	1.84	0.43
1:B:755:GLN:HG2	4:B:772:HOH:O	2.18	0.43
1:A:643:LYS:O	1:A:645:ASN:N	2.51	0.43
1:A:403:ARG:HD2	4:A:1147:HOH:O	2.19	0.43
1:A:652:VAL:C	1:A:654:PRO:HD3	2.39	0.43
1:A:743:HIS:HB3	1:A:746:ALA:HB3	2.00	0.43
1:B:426:PRO:HB2	1:B:431:LEU:HD11	1.98	0.43
1:A:314:TYR:CE1	1:A:315:LEU:HG	2.53	0.43
1:B:243:GLU:HB2	1:B:246:ALA:HB2	2.01	0.43
1:A:418:LEU:HD12	1:A:421:VAL:HG21	2.01	0.43
1:A:617:SER:HA	1:A:620:LEU:HD21	2.00	0.43
1:B:196:LEU:O	1:B:201:ILE:HD11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:PHE:N	1:B:523:PHE:CD1	2.87	0.42
1:B:729:GLY:N	4:B:770:HOH:O	2.49	0.42
1:A:418:LEU:CD1	1:A:430:GLN:HB3	2.49	0.42
1:A:515:GLN:NE2	1:A:542:HIS:HE1	2.16	0.42
1:B:437:LEU:HD12	1:B:495:MET:HB3	2.01	0.42
1:A:613:THR:CG2	1:A:615:PHE:H	2.14	0.42
1:B:395:LEU:HD22	1:B:489:VAL:CG1	2.50	0.42
1:B:165:LEU:HD11	1:B:204:PHE:CE2	2.54	0.42
1:B:632:ARG:HH22	1:B:755:GLN:CD	2.22	0.42
1:A:434:LYS:HA	1:A:434:LYS:HD2	1.68	0.42
1:B:173:ASN:O	1:B:175:GLN:N	2.51	0.42
1:B:371:ARG:O	1:B:374:ARG:HB3	2.20	0.42
1:A:487:LYS:HA	1:A:487:LYS:HD3	1.31	0.42
1:B:613:THR:HG23	4:B:950:HOH:O	2.20	0.42
1:B:702:PHE:CD2	1:B:733:VAL:HG21	2.55	0.42
1:A:588:VAL:HA	1:A:720:THR:HG21	2.02	0.42
1:B:346:ASP:HA	1:B:397:GLN:OE1	2.19	0.41
1:B:632:ARG:NH1	4:B:1164:HOH:O	2.30	0.41
1:B:162:PHE:CD1	1:B:165:LEU:CD2	2.99	0.41
1:B:215:ASP:OD1	1:B:272:LYS:NZ	2.36	0.41
1:B:160:MET:O	1:B:196:LEU:N	2.51	0.41
1:B:736:LEU:HD23	1:B:742:GLN:HA	2.02	0.41
1:A:240:GLN:OE1	1:A:730:TYR:HE2	2.04	0.41
1:A:523:PHE:CD1	1:A:523:PHE:N	2.88	0.41
1:A:609:ARG:HH11	1:A:609:ARG:HD2	1.73	0.41
1:A:634:ARG:NH2	1:A:751:LYS:HD2	2.35	0.41
1:B:225:ALA:C	1:B:227:THR:H	2.24	0.41
1:B:365:LEU:CD2	4:B:1044:HOH:O	2.69	0.41
1:A:398:GLN:O	1:A:401:MET:HB2	2.21	0.41
1:B:584:PRO:O	1:B:587:ASP:HB2	2.21	0.41
1:B:743:HIS:NE2	4:B:1089:HOH:O	2.29	0.41
1:A:230:VAL:HG23	1:A:268:ARG:O	2.21	0.41
1:A:504:PHE:HD2	1:A:527:ARG:HH21	1.68	0.41
1:B:165:LEU:HD11	1:B:204:PHE:CZ	2.55	0.41
1:B:222:ALA:HA	1:B:228:LEU:CD2	2.50	0.41
1:B:231:GLU:CD	1:B:231:GLU:H	2.24	0.41
1:B:549:ARG:HA	1:B:574:ILE:O	2.21	0.41
1:A:293:ARG:HG3	1:A:293:ARG:NH1	2.36	0.41
1:A:594:GLN:HG3	1:A:594:GLN:O	2.21	0.41
1:B:293:ARG:CG	1:B:293:ARG:NH1	2.82	0.41
1:B:504:PHE:HD2	1:B:527:ARG:HH21	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:TYR:CZ	1:B:209:THR:HG21	2.56	0.40
1:B:313:THR:HB	1:B:329:TYR:CE1	2.56	0.40
1:B:412:ILE:O	1:B:412:ILE:HG22	2.21	0.40
1:A:216:ARG:HG3	4:A:925:HOH:O	2.20	0.40
1:A:242:ARG:HD3	1:A:242:ARG:HH11	1.74	0.40
1:A:670:ARG:NH1	4:A:963:HOH:O	2.30	0.40
1:B:193:THR:O	1:B:194:ASP:HB2	2.21	0.40
1:A:547:LEU:HA	1:A:573:GLN:OE1	2.21	0.40
1:B:172:LEU:C	1:B:174:ILE:H	2.25	0.40
1:B:643:LYS:HZ2	1:B:646:LYS:HB2	1.86	0.40
1:B:643:LYS:HE3	1:B:646:LYS:CB	2.50	0.40
1:A:613:THR:HG21	1:A:615:PHE:HB2	2.03	0.40
1:B:183:LYS:O	1:B:186:ARG:HB2	2.21	0.40
1:B:733:VAL:HB	1:B:748:LEU:HB2	2.02	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%)	470 (92%)	31 (6%)	8 (2%)	9	17
1	B	553/624 (89%)	510 (92%)	32 (6%)	11 (2%)	7	12
All	All	1062/1248 (85%)	980 (92%)	63 (6%)	19 (2%)	8	14

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	SER
1	A	513	SER
1	A	515	GLN
1	B	175	GLN

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Mol	Chain	Res	Type
1	B	176	VAL
1	B	178	ASP
1	B	391	ASN
1	B	515	GLN
1	B	644	VAL
1	A	514	GLY
1	A	647	ASN
1	A	646	LYS
1	B	169	LEU
1	B	510	PRO
1	A	644	VAL
1	A	645	ASN
1	B	514	GLY
1	B	174	ILE
1	B	651	ILE

### 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%)	9	19
1	B	489/545 (90%)	447 (91%)	42 (9%)	10	20
All	All	937/1090 (86%)	855 (91%)	82 (9%)	10	19

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	THR
1	A	207	MET
1	A	227	THR
1	A	242	ARG
1	A	244	GLU
1	A	293	ARG
1	A	339	CYS
1	A	344	CYS

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Mol	Chain	Res	Type
1	A	379	LYS
1	A	406	ARG
1	A	409	LEU
1	A	414	LEU
1	A	419	ASP
1	A	424	SER
1	A	432	LYS
1	A	436	LEU
1	A	487	LYS
1	A	501	SER
1	A	502	VAL
1	A	509	SER
1	A	515	GLN
1	A	526	SER
1	A	535	SER
1	A	539	PHE
1	A	543	ASN
1	A	563	SER
1	A	573	GLN
1	A	594	GLN
1	A	630	ARG
1	A	643	LYS
1	A	648	LYS
1	A	650	SER
1	A	652	VAL
1	A	670	ARG
1	A	685	ASP
1	A	691	GLU
1	A	711	SER
1	A	712	LYS
1	A	738	LYS
1	A	753	SER
1	B	160	MET
1	B	162	PHE
1	B	167	ASP
1	B	172	LEU
1	B	177	ASP
1	B	186	ARG
1	B	210	GLN
1	B	219	GLU
1	B	242	ARG
1	B	244	GLU

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Mol	Chain	Res	Type
1	B	293	ARG
1	B	350	GLN
1	B	379	LYS
1	B	406	ARG
1	B	409	LEU
1	B	414	LEU
1	B	432	LYS
1	B	501	SER
1	B	502	VAL
1	B	508	SER
1	B	509	SER
1	B	515	GLN
1	B	526	SER
1	B	535	SER
1	B	539	PHE
1	B	573	GLN
1	B	594	GLN
1	B	630	ARG
1	B	643	LYS
1	B	646	LYS
1	B	647	ASN
1	B	652	VAL
1	B	661	HIS
1	B	685	ASP
1	B	691	GLU
1	B	709	SER
1	B	710	SER
1	B	712	LYS
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	241	GLN
1	A	291	HIS
1	A	515	GLN
1	A	542	HIS
1	A	543	ASN

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Mol	Chain	Res	Type
1	A	612	ASN
1	A	639	GLN
1	A	661	HIS
1	A	718	GLN
1	A	728	GLN
1	A	734	HIS
1	A	755	GLN
1	B	241	GLN
1	B	291	HIS
1	B	349	ASN
1	B	350	GLN
1	B	515	GLN
1	B	542	HIS
1	B	573	GLN
1	B	639	GLN
1	B	661	HIS
1	B	718	GLN
1	B	728	GLN
1	B	734	HIS
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, 6 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	ACT	B	5	-	1,3,3	2.64	1 (100%)	0,3,3	0.00	-
3	ACT	A	5	-	1,3,3	2.99	1 (100%)	0,3,3	0.00	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5	ACT	CH3-C	2.99	1.52	1.48
3	B	5	ACT	CH3-C	2.64	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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%)	-0.12	28 (5%)	25 26	18, 34, 89, 121	12 (2%)
1	B	554/624 (88%)	-0.18	23 (4%)	36 39	18, 36, 82, 114	19 (3%)
All	All	1063/1248 (85%)	-0.15	51 (4%)	30 32	18, 35, 85, 121	31 (2%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	THR	8.8
1	A	201	ILE	8.5
1	A	509	SER	8.1
1	A	510	PRO	7.9
1	A	202	GLU	7.5
1	A	204	PHE	7.0
1	B	509	SER	6.5
1	A	421	VAL	6.2
1	A	645	ASN	5.6
1	B	176	VAL	5.5
1	A	200	GLU	5.4
1	B	245	GLU	5.0
1	A	710	SER	5.0
1	B	508	SER	4.6
1	A	205	TYR	4.4
1	B	168	PHE	4.4
1	B	710	SER	4.3
1	B	486	LEU	4.2
1	B	246	ALA	3.6
1	A	711	SER	3.6
1	A	646	LYS	3.4
1	A	709	SER	3.4
1	B	160	MET	3.3
1	A	420	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	649	ASN	3.1
1	A	224	SER	3.1
1	A	206	LYS	3.0
1	B	711	SER	3.0
1	B	173	ASN	3.0
1	A	207	MET	2.9
1	B	650	SER	2.9
1	A	533	GLN	2.8
1	A	647	ASN	2.8
1	A	504	PHE	2.7
1	B	261	SER	2.6
1	B	224	SER	2.6
1	B	709	SER	2.6
1	B	644	VAL	2.5
1	A	515	GLN	2.4
1	B	172	LEU	2.4
1	B	515	GLN	2.4
1	B	171	GLU	2.4
1	B	225	ALA	2.3
1	B	445	LEU	2.3
1	B	165	LEU	2.2
1	A	626	TRP	2.2
1	A	418	LEU	2.2
1	A	507	PHE	2.2
1	B	177	ASP	2.1
1	A	708	ASP	2.1
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	B	2	1/1	0.71	0.11	69,69,69,69	1
2	CA	A	3	1/1	0.75	0.12	67,67,67,67	1
2	CA	A	1	1/1	0.88	0.27	53,53,53,53	1
2	CA	B	1	1/1	0.95	0.10	54,54,54,54	1
2	CA	A	2	1/1	0.97	0.04	55,55,55,55	1
2	CA	B	3	1/1	0.98	0.06	57,57,57,57	1
3	ACT	B	5	4/4	0.99	0.10	24,26,26,28	0
3	ACT	A	5	4/4	0.99	0.09	25,31,32,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.