



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 02:21 am BST

PDB ID : 1DJH  
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM  
RAT COMPLEXED WITH BARIUM  
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.

---

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

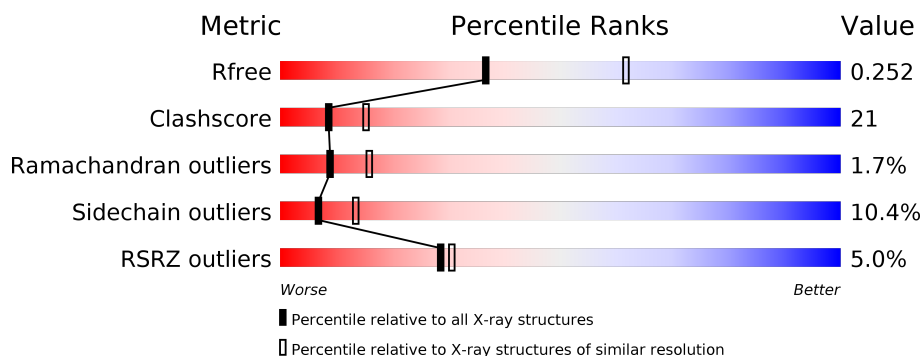
# 1 Overall quality at a glance

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>25%</div> <div>5%</div> <div>18%</div> </div> </div>
1	B	624	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>31%</div> <div>10%</div> </div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9257 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	70	0	0
			4057	2565	709	761	22			
1	B	559	Total	C	N	O	S	87	0	0
			4445	2807	771	843	24			

- Molecule 2 is BARIUM ION (three-letter code: BA) (formula: Ba).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Ba	0	0
			3	3		
2	A	3	Total	Ba	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 3	C 1	O 2	0	0
3	B	1	Total 4	C 2	O 2	0	0

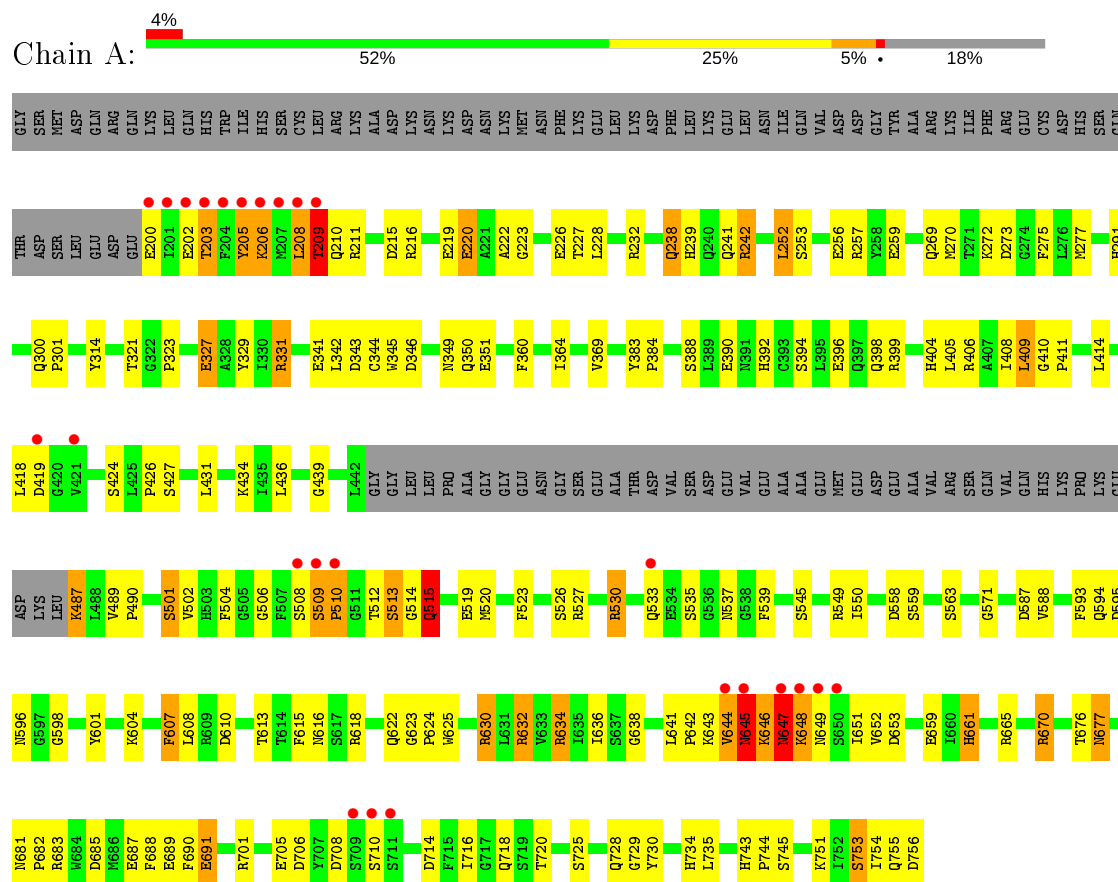
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	343	Total 343	O 343	0	0
4	B	399	Total 399	O 399	0	0

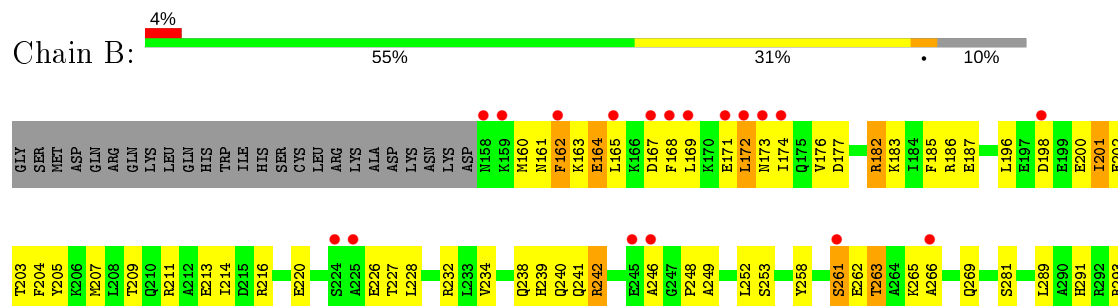
### 3 Residue-property plots

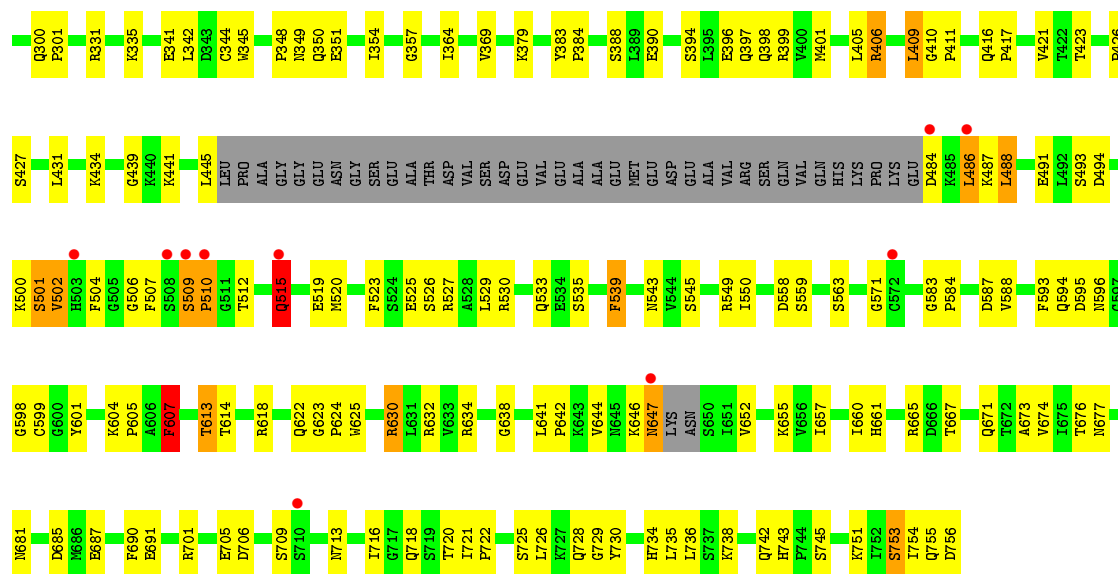
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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, $\alpha$ , $\beta$ , $\gamma$	398.25Å 398.25Å 398.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 24.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 99.6 (24.75-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 2.50Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.210 , 0.270 0.206 , 0.252	Depositor DCC
$R_{free}$ test set	3989 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 108.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9257	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 1.57% 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: BA, 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	0.77	13/4152 (0.3%)	0.82	5/5624 (0.1%)
1	B	0.76	11/4544 (0.2%)	0.81	4/6144 (0.1%)
All	All	0.77	24/8696 (0.3%)	0.81	9/11768 (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 (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	607	PHE	CE1-CZ	-8.15	1.21	1.37
1	A	601	TYR	CE2-CZ	-8.07	1.28	1.38
1	A	515	GLN	CB-CG	-7.81	1.31	1.52
1	B	601	TYR	CE1-CZ	-7.06	1.29	1.38
1	B	607	PHE	CE2-CZ	-6.78	1.24	1.37
1	B	607	PHE	CG-CD2	-6.47	1.29	1.38
1	A	690	PHE	CG-CD1	-6.43	1.29	1.38
1	A	601	TYR	CE1-CZ	-6.22	1.30	1.38
1	B	607	PHE	CG-CD1	-6.21	1.29	1.38
1	A	690	PHE	CE1-CZ	-6.21	1.25	1.37
1	A	690	PHE	CE2-CZ	-6.14	1.25	1.37
1	A	515	GLN	CG-CD	-6.09	1.37	1.51
1	A	601	TYR	CG-CD1	-6.07	1.31	1.39
1	B	601	TYR	CG-CD2	-6.04	1.31	1.39
1	B	690	PHE	CE2-CZ	-6.02	1.25	1.37
1	A	690	PHE	CG-CD2	-5.94	1.29	1.38

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	690	PHE	CE1-CZ	-5.89	1.26	1.37
1	A	607	PHE	CE2-CZ	-5.86	1.26	1.37
1	B	690	PHE	CG-CD1	-5.82	1.30	1.38
1	B	601	TYR	CG-CD1	-5.61	1.31	1.39
1	A	708	ASP	C-O	-5.56	1.12	1.23
1	B	601	TYR	CE2-CZ	-5.34	1.31	1.38
1	A	607	PHE	CE1-CZ	-5.26	1.27	1.37
1	A	601	TYR	CG-CD2	-5.04	1.32	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	GLN	N-CA-CB	-6.29	99.28	110.60
1	A	436	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	509	SER	N-CA-C	5.85	126.80	111.00
1	B	515	GLN	N-CA-C	5.70	126.40	111.00
1	A	515	GLN	CB-CG-CD	-5.56	97.14	111.60
1	B	390	GLU	N-CA-C	-5.15	97.11	111.00
1	B	510	PRO	N-CA-C	5.10	125.37	112.10
1	A	390	GLU	N-CA-C	-5.08	97.29	111.00
1	A	645	ASN	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	515	GLN	Sidechain
1	A	519	GLU	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	137	0
1	B	4445	0	4353	207	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	4	0	3	1	0
4	A	343	0	0	12	1
4	B	399	0	0	22	0
All	All	9257	0	8328	339	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 21.

All (339) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.41	1.01
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.23	1.00
1:B:673:ALA:HB1	4:B:1074:HOH:O	1.64	0.94
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.51	0.93
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.31	0.92
1:B:607:PHE:CD2	1:B:625:TRP:HB3	2.04	0.92
1:B:348:PRO:HB2	1:B:349:ASN:ND2	1.86	0.90
1:B:646:LYS:HE3	1:B:647:ASN:HD21	1.36	0.89
1:A:241:GLN:HE22	1:A:730:TYR:H	1.19	0.89
1:B:630:ARG:HD2	1:B:755:GLN:NE2	1.87	0.88
1:B:227:THR:HG21	1:B:269:GLN:HB3	1.55	0.88
1:B:161:ASN:H	1:B:164:GLU:HG3	1.39	0.87
1:B:486:LEU:H	1:B:486:LEU:HD12	1.41	0.86
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.07	0.85
1:B:172:LEU:HD12	1:B:174:ILE:HD12	1.58	0.84
1:B:227:THR:CG2	1:B:269:GLN:HB3	2.07	0.84
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.24	0.82
1:B:241:GLN:HE22	1:B:730:TYR:H	1.27	0.82
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.93	0.82
1:B:172:LEU:HB2	1:B:174:ILE:HG13	1.62	0.82
1:A:509:SER:HB3	1:A:510:PRO:HD3	1.61	0.81
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.09	0.81
1:B:630:ARG:HD2	1:B:755:GLN:HE21	1.45	0.81
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.15	0.81
1:A:520:MET:CE	1:A:549:ARG:HB2	2.12	0.80
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.61	0.79
1:B:162:PHE:CD1	1:B:165:LEU:HD23	2.16	0.79
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.65	0.79
1:B:504:PHE:HB3	1:B:527:ARG:NH2	1.98	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:THR:O	1:B:207:MET:HG3	1.83	0.78
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.65	0.78
1:B:728:GLN:NE2	1:B:754:ILE:H	1.82	0.78
1:B:520:MET:CE	1:B:549:ARG:HB2	2.15	0.77
1:B:607:PHE:CE2	1:B:625:TRP:HB3	2.21	0.74
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.17	0.74
1:B:605:PRO:HB2	1:B:607:PHE:CE1	2.23	0.74
1:A:227:THR:HG21	1:A:269:GLN:HB3	1.70	0.73
1:B:605:PRO:HB2	1:B:607:PHE:HE1	1.51	0.73
1:A:227:THR:HG21	1:A:269:GLN:OE1	1.89	0.73
1:B:227:THR:HG21	1:B:269:GLN:OE1	1.89	0.72
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.24	0.72
1:A:730:TYR:CE1	1:A:751:LYS:HD2	2.25	0.71
1:A:728:GLN:NE2	1:A:754:ILE:H	1.88	0.71
1:B:162:PHE:CE1	1:B:165:LEU:HD23	2.25	0.71
1:B:234:VAL:O	1:B:238:GLN:HG3	1.90	0.71
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.21	0.71
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.21	0.70
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.74	0.69
1:B:646:LYS:CE	1:B:647:ASN:HD21	2.05	0.68
1:B:632:ARG:NH2	4:B:767:HOH:O	2.27	0.68
1:B:730:TYR:CE1	1:B:751:LYS:HD2	2.28	0.67
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.77	0.67
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.77	0.66
1:A:607:PHE:CD2	1:A:625:TRP:HB3	2.30	0.66
1:A:651:ILE:HD12	1:A:677:ASN:ND2	2.09	0.66
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.77	0.66
1:A:394:SER:O	1:A:398:GLN:HG3	1.95	0.66
1:B:164:GLU:O	1:B:167:ASP:HB3	1.95	0.65
1:A:206:LYS:O	1:A:210:GLN:HB2	1.96	0.65
1:A:646:LYS:O	1:A:648:LYS:N	2.29	0.65
1:A:607:PHE:CE2	1:A:625:TRP:HB3	2.30	0.65
1:B:583:GLY:N	4:B:948:HOH:O	2.28	0.65
1:B:162:PHE:CE2	1:B:182:ARG:HG3	2.32	0.65
1:A:530:ARG:O	1:A:533:GLN:HB3	1.96	0.64
1:A:252:LEU:O	1:A:256:GLU:HG3	1.97	0.64
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.77	0.64
1:B:507:PHE:HB3	4:B:1111:HOH:O	1.97	0.64
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.32	0.64
1:A:508:SER:OG	1:A:509:SER:N	2.30	0.64
1:B:488:LEU:HD13	1:B:493:SER:HB2	1.80	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LEU:O	1:B:201:ILE:HD11	1.98	0.63
1:B:539:PHE:O	1:B:543:ASN:ND2	2.29	0.63
1:B:416:GLN:HG3	1:B:417:PRO:CD	2.25	0.63
1:B:588:VAL:HG21	1:B:661:HIS:HD2	1.62	0.63
1:B:632:ARG:NE	4:B:767:HOH:O	2.32	0.63
1:B:515:GLN:NE2	1:B:519:GLU:HB3	2.13	0.63
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.34	0.63
1:B:588:VAL:HG21	1:B:661:HIS:CD2	2.34	0.62
1:A:645:ASN:O	1:A:646:LYS:HB3	1.98	0.62
1:A:220:GLU:HG3	4:A:805:HOH:O	2.00	0.62
1:B:605:PRO:CB	1:B:607:PHE:HE1	2.13	0.62
1:B:728:GLN:HE21	1:B:753:SER:HA	1.64	0.62
1:B:646:LYS:HG3	1:B:647:ASN:H	1.65	0.62
1:B:165:LEU:HD11	1:B:204:PHE:CE2	2.35	0.61
1:B:168:PHE:O	1:B:171:GLU:HB3	1.99	0.61
1:A:241:GLN:HE22	1:A:730:TYR:N	1.93	0.61
1:B:238:GLN:HG2	1:B:246:ALA:HB3	1.82	0.61
1:B:348:PRO:HB2	1:B:349:ASN:HD22	1.63	0.61
1:B:162:PHE:O	1:B:165:LEU:HB3	2.01	0.61
1:B:379:LYS:NZ	4:B:1003:HOH:O	2.33	0.61
1:B:673:ALA:CB	4:B:1074:HOH:O	2.35	0.61
1:B:335:LYS:NZ	4:B:963:HOH:O	2.34	0.60
1:A:670:ARG:HD3	4:A:1055:HOH:O	2.00	0.60
1:B:394:SER:O	1:B:398:GLN:HG3	2.01	0.60
1:B:533:GLN:OE1	1:B:618:ARG:NH1	2.33	0.60
1:A:643:LYS:C	1:A:645:ASN:H	2.04	0.60
1:A:647:ASN:O	1:A:649:ASN:N	2.35	0.59
1:A:588:VAL:HG21	1:A:661:HIS:CD2	2.37	0.59
1:B:169:LEU:HD13	1:B:176:VAL:HG22	1.84	0.59
1:B:673:ALA:CA	4:B:1074:HOH:O	2.50	0.59
1:B:249:ALA:N	4:B:1100:HOH:O	2.35	0.59
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.33	0.59
1:B:607:PHE:H	1:B:607:PHE:HD1	1.49	0.59
1:A:202:GLU:O	1:A:206:LYS:HB2	2.03	0.58
1:A:202:GLU:O	1:A:206:LYS:N	2.37	0.58
1:A:504:PHE:HD2	1:A:527:ARG:NH2	2.00	0.58
1:B:169:LEU:HD13	1:B:176:VAL:CG2	2.33	0.58
1:B:595:ASP:OD1	1:B:596:ASN:N	2.35	0.58
1:B:439:GLY:C	1:B:501:SER:HB2	2.23	0.58
1:A:219:GLU:O	1:A:223:GLY:N	2.32	0.58
1:A:239:HIS:O	1:A:242:ARG:NH1	2.37	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:PHE:O	1:A:598:GLY:HA2	2.04	0.58
1:A:755:GLN:HG2	1:A:756:ASP:N	2.18	0.58
1:B:549:ARG:C	1:B:550:ILE:HD13	2.25	0.57
1:B:183:LYS:O	1:B:187:GLU:HG3	2.05	0.57
1:A:200:GLU:HA	1:A:203:THR:CB	2.35	0.57
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.37	0.57
1:B:593:PHE:O	1:B:598:GLY:HA2	2.05	0.57
1:A:291:HIS:HD2	1:A:725:SER:OG	1.88	0.57
1:A:216:ARG:O	1:A:219:GLU:HB2	2.05	0.57
1:B:504:PHE:HD2	1:B:527:ARG:NH2	2.04	0.56
1:A:216:ARG:HG3	1:A:216:ARG:HH11	1.69	0.56
1:B:300:GLN:O	1:B:427:SER:HA	2.04	0.56
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.39	0.56
1:B:161:ASN:OD1	1:B:164:GLU:HG2	2.06	0.55
1:B:736:LEU:HD23	1:B:742:GLN:HA	1.87	0.55
1:B:753:SER:HB2	4:B:770:HOH:O	2.05	0.55
1:B:502:VAL:HG21	1:B:519:GLU:HG2	1.88	0.55
1:A:343:ASP:HB3	4:A:978:HOH:O	2.06	0.55
1:A:509:SER:CB	1:A:510:PRO:HD3	2.35	0.55
1:A:327:GLU:HG3	1:A:331:ARG:HD2	1.89	0.55
1:B:162:PHE:HD1	1:B:165:LEU:HD23	1.69	0.55
1:B:263:THR:O	1:B:266:ALA:HB3	2.07	0.55
1:B:588:VAL:CG2	1:B:661:HIS:HD2	2.20	0.55
1:B:182:ARG:O	1:B:185:PHE:HB3	2.07	0.54
1:B:706:ASP:O	1:B:713:ASN:HB3	2.07	0.54
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.90	0.54
1:B:607:PHE:HD1	1:B:607:PHE:N	2.05	0.54
1:A:300:GLN:O	1:A:427:SER:HA	2.07	0.54
1:A:735:LEU:O	1:A:743:HIS:HB2	2.08	0.54
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.23	0.54
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.56	0.54
1:B:530:ARG:O	1:B:533:GLN:HB3	2.08	0.53
1:B:632:ARG:CZ	4:B:767:HOH:O	2.56	0.53
1:B:172:LEU:CD1	1:B:174:ILE:HD12	2.34	0.53
1:B:196:LEU:HB3	1:B:201:ILE:CD1	2.38	0.53
1:B:735:LEU:O	1:B:743:HIS:HB2	2.08	0.53
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.38	0.53
1:A:691:GLU:HG2	4:A:1060:HOH:O	2.08	0.53
1:B:622:GLN:HG3	1:B:623:GLY:N	2.23	0.53
1:B:196:LEU:HB3	1:B:201:ILE:HD13	1.90	0.53
1:B:216:ARG:O	1:B:220:GLU:HG3	2.09	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:GLY:O	1:B:681:ASN:HA	2.08	0.53
1:B:196:LEU:HD22	1:B:200:GLU:HB3	1.90	0.53
1:B:185:PHE:CE1	1:B:196:LEU:HG	2.44	0.53
1:A:643:LYS:O	1:A:645:ASN:N	2.42	0.52
1:A:622:GLN:OE1	1:B:445:LEU:HD11	2.09	0.52
1:B:607:PHE:CD1	1:B:607:PHE:N	2.77	0.52
1:A:252:LEU:HD23	1:A:256:GLU:OE2	2.10	0.52
1:B:205:TYR:O	1:B:209:THR:HG23	2.10	0.52
1:A:439:GLY:C	1:A:501:SER:HB2	2.30	0.52
1:A:588:VAL:HG21	1:A:661:HIS:HD2	1.75	0.51
1:B:705:GLU:C	1:B:716:ILE:HD12	2.30	0.51
1:A:644:VAL:O	1:A:645:ASN:HB2	2.10	0.51
1:B:239:HIS:O	1:B:242:ARG:NH1	2.43	0.51
1:B:342:LEU:HD12	1:B:342:LEU:N	2.26	0.51
1:B:607:PHE:HB2	1:B:613:THR:HG21	1.92	0.51
1:B:291:HIS:HD2	1:B:725:SER:OG	1.93	0.51
1:A:346:ASP:OD2	1:A:394:SER:HB3	2.11	0.51
1:B:674:VAL:N	4:B:1074:HOH:O	2.31	0.51
1:A:504:PHE:CD2	1:A:527:ARG:NH2	2.79	0.50
1:A:689:GLU:OE2	1:B:494:ASP:OD2	2.30	0.50
1:B:172:LEU:HB2	1:B:174:ILE:CG1	2.39	0.50
1:B:411:PRO:O	1:B:434:LYS:NZ	2.43	0.50
1:A:607:PHE:CE1	1:A:608:LEU:HG	2.46	0.50
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.42	0.50
1:A:405:LEU:O	1:A:409:LEU:HB2	2.10	0.50
1:B:533:GLN:HA	1:B:533:GLN:OE1	2.12	0.50
1:B:216:ARG:HG2	4:B:762:HOH:O	2.10	0.50
3:B:5:ACT:O	4:B:948:HOH:O	2.20	0.50
1:B:500:LYS:HE3	4:B:858:HOH:O	2.11	0.49
1:A:241:GLN:C	1:A:242:ARG:HG2	2.31	0.49
1:B:734:HIS:HE1	4:B:1025:HOH:O	1.96	0.49
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.77	0.49
1:B:657:ILE:HD13	1:B:671:GLN:CB	2.43	0.49
1:A:730:TYR:CZ	1:A:751:LYS:HD2	2.46	0.49
1:B:354:ILE:HD12	1:B:369:VAL:HG21	1.95	0.49
1:A:205:TYR:O	1:A:208:LEU:HB2	2.13	0.49
1:A:607:PHE:CE2	1:A:625:TRP:CB	2.96	0.49
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.48	0.48
1:A:638:GLY:O	1:A:681:ASN:HA	2.13	0.48
1:B:196:LEU:HA	1:B:196:LEU:HD23	1.60	0.48
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.48	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:HIS:HD2	4:A:793:HOH:O	1.96	0.48
1:A:241:GLN:NE2	1:A:729:GLY:HA3	2.28	0.48
1:A:200:GLU:C	1:A:202:GLU:H	2.16	0.48
1:B:227:THR:HG23	1:B:269:GLN:HB3	1.95	0.48
1:B:502:VAL:HG11	1:B:515:GLN:OE1	2.13	0.48
1:B:701:ARG:HE	1:B:718:GLN:NE2	2.11	0.48
1:B:227:THR:CG2	1:B:228:LEU:N	2.76	0.48
1:B:227:THR:HG21	1:B:269:GLN:CB	2.36	0.48
1:B:383:TYR:HD2	1:B:599:CYS:HB2	1.77	0.48
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.14	0.48
1:A:705:GLU:C	1:A:716:ILE:HD12	2.35	0.47
1:B:238:GLN:CG	1:B:246:ALA:HB1	2.41	0.47
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.13	0.47
1:B:607:PHE:CE2	1:B:625:TRP:CB	2.93	0.47
1:B:539:PHE:CD1	1:B:543:ASN:ND2	2.78	0.47
1:A:206:LYS:HA	1:A:209:THR:OG1	2.14	0.47
1:A:242:ARG:HG3	1:A:728:GLN:HB2	1.96	0.47
1:B:515:GLN:HG3	4:B:885:HOH:O	2.13	0.47
1:B:300:GLN:HB3	1:B:301:PRO:HD2	1.96	0.47
1:B:515:GLN:NE2	1:B:519:GLU:CB	2.76	0.47
1:A:227:THR:CG2	1:A:228:LEU:N	2.77	0.47
1:B:165:LEU:HD11	1:B:204:PHE:CZ	2.49	0.47
1:A:533:GLN:HA	1:A:533:GLN:OE1	2.13	0.47
1:B:646:LYS:HE3	1:B:647:ASN:ND2	2.16	0.47
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.30	0.46
1:B:550:ILE:HD13	1:B:550:ILE:N	2.30	0.46
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.03	0.46
1:B:584:PRO:O	1:B:587:ASP:HB2	2.15	0.46
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.16	0.46
1:B:515:GLN:HE22	1:B:519:GLU:HB3	1.79	0.46
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.46	0.46
1:B:164:GLU:H	1:B:164:GLU:HG2	1.40	0.46
1:A:323:PRO:HD3	4:A:1091:HOH:O	2.15	0.46
1:A:558:ASP:O	1:A:559:SER:HB2	2.14	0.46
1:B:182:ARG:HD3	1:B:186:ARG:HD3	1.97	0.46
1:B:484:ASP:O	1:B:487:LYS:HB2	2.15	0.46
1:A:259:GLU:OE1	1:A:270:MET:HA	2.15	0.46
1:B:486:LEU:HD12	1:B:486:LEU:N	2.21	0.46
1:A:616:ASN:OD1	1:A:618:ARG:HB2	2.16	0.46
1:B:426:PRO:HB2	1:B:431:LEU:HD11	1.97	0.46
1:B:558:ASP:O	1:B:559:SER:HB2	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:588:VAL:CG2	1:B:661:HIS:CD2	2.98	0.46
1:B:587:ASP:HB3	1:B:718:GLN:NE2	2.31	0.46
1:B:571:GLY:HA2	1:B:604:LYS:HE3	1.99	0.45
1:A:434:LYS:HD2	1:A:434:LYS:HA	1.85	0.45
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.83	0.45
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.39	0.45
1:B:248:PRO:O	1:B:252:LEU:HD12	2.16	0.45
1:B:384:PRO:HG3	1:B:431:LEU:HB2	1.98	0.45
1:A:595:ASP:OD1	1:A:596:ASN:N	2.47	0.45
1:B:405:LEU:O	1:B:409:LEU:HB2	2.16	0.45
1:A:689:GLU:HB3	1:B:491:GLU:HG3	1.98	0.45
1:B:213:GLU:HG2	1:B:214:ILE:N	2.31	0.45
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.46	0.45
1:A:396:GLU:O	1:A:399:ARG:HB2	2.17	0.45
1:B:523:PHE:N	1:B:523:PHE:CD1	2.85	0.45
1:B:504:PHE:CD2	1:B:527:ARG:NH2	2.84	0.45
1:A:571:GLY:HA2	1:A:604:LYS:HE3	1.99	0.45
1:B:162:PHE:CE2	1:B:182:ARG:CG	2.99	0.45
1:B:350:GLN:NE2	1:B:397:GLN:HE21	2.15	0.44
1:B:500:LYS:NZ	4:B:854:HOH:O	2.49	0.44
1:B:396:GLU:O	1:B:399:ARG:HB2	2.18	0.44
1:A:273:ASP:O	1:A:277:MET:HG2	2.18	0.44
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.29	0.44
1:A:634:ARG:HG2	1:A:636:ILE:HG13	1.99	0.44
1:A:744:PRO:HG2	4:A:888:HOH:O	2.16	0.44
1:A:504:PHE:CZ	1:A:506:GLY:CA	2.99	0.44
1:B:655:LYS:NZ	1:B:671:GLN:OE1	2.42	0.44
1:A:706:ASP:HB3	1:A:714:ASP:HB2	1.99	0.44
1:B:410:GLY:HA3	1:B:411:PRO:HD2	1.80	0.44
1:B:549:ARG:O	1:B:550:ILE:HD13	2.18	0.44
1:A:653:ASP:OD1	1:A:677:ASN:N	2.33	0.44
1:B:421:VAL:HB	4:B:895:HOH:O	2.18	0.44
1:A:341:GLU:C	1:A:342:LEU:HD12	2.39	0.43
1:A:728:GLN:HE21	1:A:753:SER:HA	1.82	0.43
1:B:726:LEU:HA	1:B:726:LEU:HD12	1.80	0.43
1:A:681:ASN:N	1:A:682:PRO:CD	2.81	0.43
1:B:240:GLN:HA	1:B:240:GLN:OE1	2.18	0.43
1:B:525:GLU:O	1:B:529:LEU:HG	2.18	0.43
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.53	0.43
1:A:208:LEU:O	1:A:210:GLN:N	2.50	0.43
1:A:411:PRO:O	1:A:434:LYS:NZ	2.51	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:VAL:CG2	1:B:519:GLU:HG2	2.48	0.43
1:B:657:ILE:HD13	1:B:671:GLN:HB2	2.00	0.43
1:B:660:ILE:O	1:B:667:THR:HA	2.19	0.43
1:A:613:THR:HA	4:A:928:HOH:O	2.17	0.42
1:B:241:GLN:C	1:B:242:ARG:HG2	2.34	0.42
1:B:515:GLN:HE22	1:B:519:GLU:CB	2.32	0.42
1:A:253:SER:O	1:A:257:ARG:HB2	2.19	0.42
1:B:434:LYS:HD2	1:B:434:LYS:HA	1.84	0.42
1:A:208:LEU:HA	1:A:208:LEU:HD22	1.58	0.42
1:A:607:PHE:CD1	1:A:608:LEU:HG	2.53	0.42
1:B:738:LYS:HB2	4:B:947:HOH:O	2.19	0.42
1:A:215:ASP:OD1	1:A:272:LYS:NZ	2.40	0.42
1:A:404:HIS:O	1:A:408:ILE:HG13	2.19	0.42
1:A:630:ARG:HD3	4:A:757:HOH:O	2.19	0.42
1:B:261:SER:O	1:B:265:LYS:HB2	2.18	0.42
1:A:622:GLN:HG3	1:A:623:GLY:N	2.35	0.42
1:A:701:ARG:HH21	1:A:718:GLN:HG3	1.83	0.42
1:B:258:TYR:CE1	1:B:281:SER:HB2	2.54	0.42
1:A:349:ASN:O	1:A:349:ASN:ND2	2.53	0.42
1:A:426:PRO:HG2	1:A:431:LEU:HD11	2.02	0.42
1:A:659:GLU:OE1	1:A:661:HIS:HE1	2.02	0.42
1:A:587:ASP:HB3	1:A:718:GLN:NE2	2.34	0.42
1:B:344:CYS:SG	1:B:401:MET:CE	3.08	0.42
1:A:487:LYS:HA	1:A:487:LYS:HD3	1.37	0.42
1:B:167:ASP:HB3	1:B:168:PHE:H	1.74	0.42
1:B:211:ARG:HG3	4:B:794:HOH:O	2.18	0.42
1:B:341:GLU:C	1:B:342:LEU:HD12	2.39	0.42
1:A:238:GLN:HG3	4:A:764:HOH:O	2.19	0.42
1:A:489:VAL:HA	1:A:490:PRO:HD3	1.88	0.42
1:A:342:LEU:HD12	1:A:342:LEU:N	2.35	0.41
1:A:537:ASN:N	4:A:924:HOH:O	2.52	0.41
1:A:734:HIS:HE1	4:A:884:HOH:O	2.03	0.41
1:B:441:LYS:NZ	1:B:493:SER:O	2.53	0.41
1:A:523:PHE:CD1	1:A:523:PHE:N	2.87	0.41
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.79	0.41
1:B:289:LEU:HD12	1:B:289:LEU:O	2.19	0.41
1:B:350:GLN:NE2	1:B:350:GLN:HA	2.34	0.41
1:B:641:LEU:HD23	1:B:641:LEU:HA	1.75	0.41
1:B:646:LYS:HA	1:B:646:LYS:HD2	1.79	0.41
1:B:348:PRO:HB2	1:B:349:ASN:HD21	1.78	0.41
1:A:300:GLN:HB3	1:A:301:PRO:CD	2.51	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LEU:HD22	1:B:200:GLU:CB	2.50	0.41
1:A:272:LYS:O	1:A:275:PHE:HB3	2.21	0.41
1:A:327:GLU:HG3	1:A:327:GLU:O	2.21	0.41
1:B:523:PHE:O	1:B:550:ILE:HA	2.20	0.41
1:B:729:GLY:O	1:B:751:LYS:HA	2.21	0.41
1:A:410:GLY:HA3	1:A:411:PRO:HD2	1.88	0.41
1:A:643:LYS:C	1:A:645:ASN:N	2.71	0.41
1:A:687:GLU:HG2	1:A:688:PHE:N	2.34	0.41
1:A:314:TYR:HB3	1:A:329:TYR:CE2	2.56	0.41
1:B:300:GLN:CB	1:B:301:PRO:CD	2.99	0.41
1:B:445:LEU:HD23	1:B:445:LEU:HA	1.88	0.41
1:B:594:GLN:HA	1:B:594:GLN:HE21	1.86	0.41
1:A:549:ARG:C	1:A:550:ILE:HD13	2.41	0.41
1:A:222:ALA:HA	1:A:228:LEU:HD23	2.03	0.41
1:A:632:ARG:NH2	1:B:406:ARG:CZ	2.84	0.40
1:B:409:LEU:HD12	1:B:409:LEU:HA	1.73	0.40
1:B:647:ASN:ND2	1:B:647:ASN:H	2.20	0.40
1:B:721:ILE:HA	1:B:722:PRO:HD3	1.94	0.40
1:B:647:ASN:ND2	1:B:647:ASN:N	2.69	0.40
1:B:657:ILE:HD13	1:B:671:GLN:HB3	2.04	0.40
1:A:613:THR:HG23	1:A:615:PHE:H	1.86	0.40
1:B:172:LEU:HD12	1:B:174:ILE:CD1	2.42	0.40
1:B:263:THR:O	1:B:266:ALA:N	2.55	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)
4:A:767:HOH:O	4:A:767:HOH:O[52_555]	1.74	0.46

## 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%)	468 (92%)	29 (6%)	12 (2%)	6	9
1	B	553/624 (89%)	506 (92%)	41 (7%)	6 (1%)	14	26
All	All	1062/1248 (85%)	974 (92%)	70 (7%)	18 (2%)	9	16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	SER
1	A	515	GLN
1	A	646	LYS
1	A	647	ASN
1	A	648	LYS
1	B	198	ASP
1	B	515	GLN
1	B	644	VAL
1	A	203	THR
1	A	510	PRO
1	A	513	SER
1	A	514	GLY
1	A	644	VAL
1	A	209	THR
1	B	512	THR
1	A	205	TYR
1	B	163	LYS
1	B	510	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/545 (82%)	395 (89%)	49 (11%)	6	12
1	B	489/545 (90%)	441 (90%)	48 (10%)	8	15
All	All	933/1090 (86%)	836 (90%)	97 (10%)	7	13

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

Mol	Chain	Res	Type
1	A	206	LYS
1	A	208	LEU
1	A	209	THR
1	A	211	ARG
1	A	220	GLU
1	A	226	GLU
1	A	232	ARG
1	A	238	GLN
1	A	242	ARG
1	A	252	LEU
1	A	327	GLU
1	A	331	ARG
1	A	344	CYS
1	A	350	GLN
1	A	388	SER
1	A	406	ARG
1	A	409	LEU
1	A	414	LEU
1	A	418	LEU
1	A	419	ASP
1	A	424	SER
1	A	487	LYS
1	A	501	SER
1	A	502	VAL
1	A	512	THR
1	A	513	SER
1	A	515	GLN
1	A	526	SER
1	A	530	ARG
1	A	535	SER
1	A	539	PHE
1	A	545	SER
1	A	563	SER
1	A	630	ARG
1	A	632	ARG
1	A	634	ARG
1	A	645	ASN
1	A	647	ASN
1	A	652	VAL
1	A	661	HIS
1	A	665	ARG
1	A	670	ARG
1	A	676	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	677	ASN
1	A	685	ASP
1	A	691	GLU
1	A	710	SER
1	A	745	SER
1	A	753	SER
1	B	160	MET
1	B	162	PHE
1	B	164	GLU
1	B	172	LEU
1	B	173	ASN
1	B	177	ASP
1	B	182	ARG
1	B	201	ILE
1	B	202	GLU
1	B	226	GLU
1	B	232	ARG
1	B	242	ARG
1	B	253	SER
1	B	261	SER
1	B	262	GLU
1	B	263	THR
1	B	293	ARG
1	B	331	ARG
1	B	388	SER
1	B	406	ARG
1	B	409	LEU
1	B	423	THR
1	B	486	LEU
1	B	488	LEU
1	B	501	SER
1	B	502	VAL
1	B	509	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	607	PHE
1	B	613	THR
1	B	614	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	630	ARG
1	B	647	ASN
1	B	652	VAL
1	B	665	ARG
1	B	676	THR
1	B	677	ASN
1	B	685	ASP
1	B	691	GLU
1	B	709	SER
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	HIS
1	A	241	GLN
1	A	291	HIS
1	A	349	ASN
1	A	392	HIS
1	A	543	ASN
1	A	594	GLN
1	A	639	GLN
1	A	661	HIS
1	A	718	GLN
1	A	728	GLN
1	A	734	HIS
1	B	241	GLN
1	B	291	HIS
1	B	349	ASN
1	B	350	GLN
1	B	392	HIS
1	B	515	GLN
1	B	594	GLN
1	B	639	GLN
1	B	647	ASN
1	B	661	HIS
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 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	3.01	1 (100%)	0,3,3	0.00	-
3	ACT	A	5	-	0,2,3	0.00	-	0,1,3	0.00	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	5	ACT	CH3-C	3.01	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5	ACT	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	509/624 (81%)	-0.13	25 (4%) 29 31	18, 34, 90, 124	11 (2%)
1	B	555/624 (88%)	-0.14	28 (5%) 28 30	18, 36, 87, 117	17 (3%)
All	All	1064/1248 (85%)	-0.14	53 (4%) 28 30	18, 35, 88, 124	28 (2%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	203	THR	8.7
1	A	510	PRO	8.6
1	B	510	PRO	8.5
1	A	201	ILE	8.2
1	A	509	SER	7.5
1	A	204	PHE	7.4
1	A	202	GLU	7.1
1	A	200	GLU	7.0
1	A	205	TYR	6.4
1	B	509	SER	6.4
1	A	645	ASN	5.7
1	A	647	ASN	5.7
1	B	168	PHE	5.5
1	A	207	MET	5.0
1	B	198	ASP	4.8
1	B	486	LEU	4.7
1	A	649	ASN	4.6
1	A	208	LEU	4.3
1	A	710	SER	4.2
1	B	515	GLN	4.1
1	A	644	VAL	3.8
1	B	169	LEU	3.8
1	A	711	SER	3.6
1	B	173	ASN	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	421	VAL	3.5
1	B	171	GLU	3.3
1	B	167	ASP	3.2
1	A	508	SER	3.2
1	B	647	ASN	3.2
1	B	165	LEU	3.1
1	B	508	SER	3.1
1	B	172	LEU	2.9
1	A	206	LYS	2.9
1	B	246	ALA	2.9
1	A	648	LYS	2.9
1	A	533	GLN	2.8
1	B	158	ASN	2.7
1	B	174	ILE	2.7
1	B	245	GLU	2.5
1	A	709	SER	2.5
1	B	224	SER	2.4
1	B	159	LYS	2.4
1	B	261	SER	2.2
1	B	266	ALA	2.2
1	B	503	HIS	2.2
1	B	572	CYS	2.2
1	B	225	ALA	2.1
1	A	650	SER	2.1
1	B	710	SER	2.1
1	B	162	PHE	2.1
1	A	419	ASP	2.1
1	B	484	ASP	2.0
1	A	209	THR	2.0

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

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

## 6.3 Carbohydrates ⓘ

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(Å <sup>2</sup> )	Q<0.9
2	BA	B	2	1/1	0.83	0.18	93,93,93,93	1
2	BA	B	3	1/1	0.86	0.10	86,86,86,86	1
2	BA	A	3	1/1	0.91	0.10	101,101,101,101	1
2	BA	A	1	1/1	0.91	0.07	71,71,71,71	1
3	ACT	A	5	3/4	0.95	0.13	36,36,36,38	0
2	BA	B	1	1/1	0.96	0.08	61,61,61,61	1
2	BA	A	2	1/1	0.98	0.15	99,99,99,99	1
3	ACT	B	5	4/4	0.99	0.16	25,27,27,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.