



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:31 PM UTC

PDB ID : 1DJI / pdb_00001dji
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

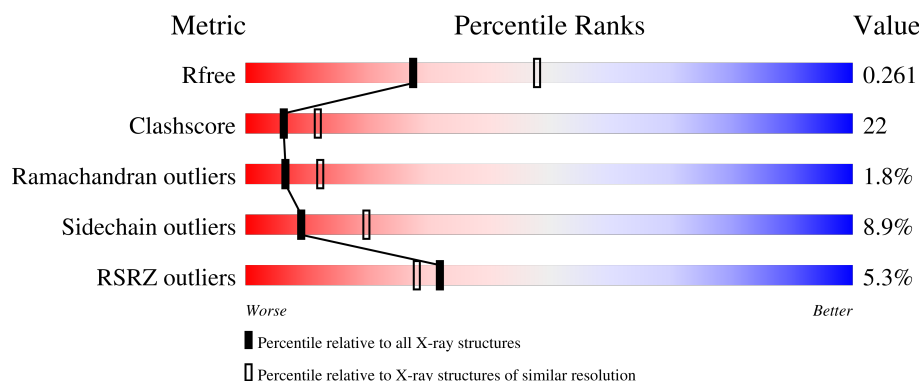
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	4% 51% 26% • • 18%
1	B	624	5% 53% 30% 6% 10%

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.

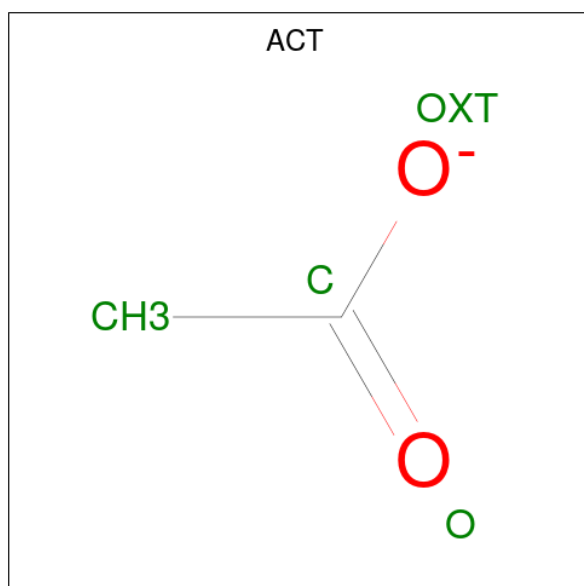
- Molecule 1 is a protein called PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

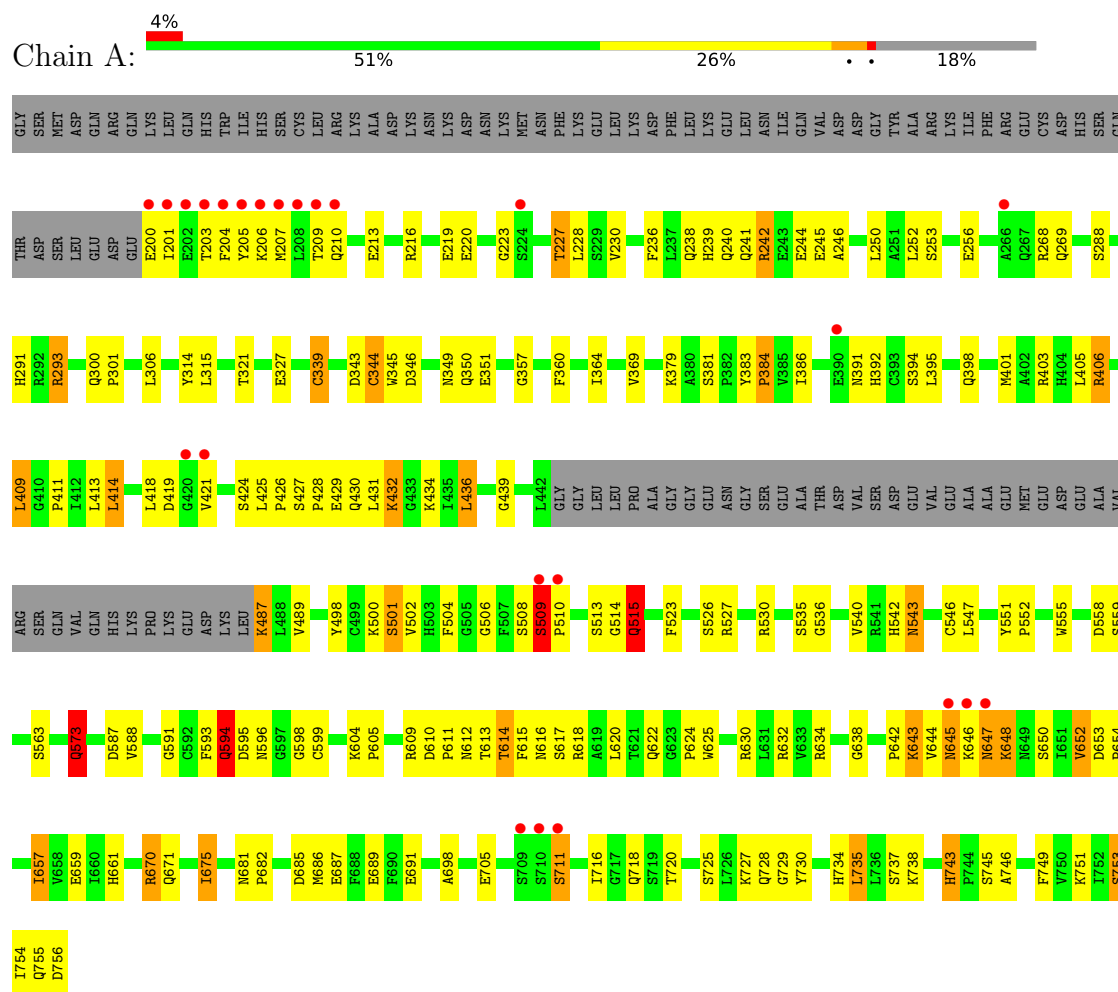
- Molecule 4 is water.

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

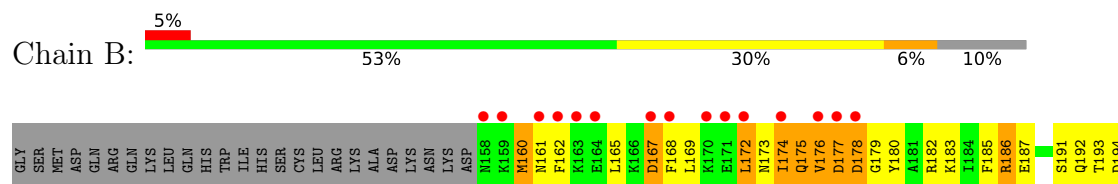
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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, α , β , γ	398.03Å 398.03Å 398.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (10.00-2.50) 95.8 (10.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.50Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.220 , 0.280 0.213 , 0.261	Depositor DCC
R_{free} test set	3908 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 122.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9403	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: ACT, CA

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	0.86	0/4165	1.11	16/5641 (0.3%)
1	B	0.90	4/4544 (0.1%)	1.13	26/6144 (0.4%)
All	All	0.88	4/8709 (0.0%)	1.12	42/11785 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	390	GLU	C-O	-7.95	1.13	1.24
1	B	167	ASP	N-CA	-6.09	1.39	1.46
1	B	573	GLN	CD-NE2	-5.12	1.22	1.33
1	B	702	PHE	CE1-CZ	-5.03	1.23	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	594	GLN	N-CA-C	-8.96	101.78	112.89
1	B	391	ASN	N-CA-C	8.93	129.82	110.80
1	B	226	GLU	N-CA-C	-8.76	102.60	113.20
1	A	594	GLN	N-CA-C	-8.24	102.67	112.89
1	A	711	SER	N-CA-C	7.87	118.37	108.45
1	B	306	LEU	N-CA-C	-7.65	97.11	109.96
1	B	180	TYR	N-CA-C	-7.36	103.20	111.07
1	A	344	CYS	N-CA-C	7.35	120.65	108.96
1	A	306	LEU	N-CA-C	-7.28	97.73	109.96
1	B	752	ILE	CA-C-N	-6.78	112.54	122.65
1	B	752	ILE	C-N-CA	-6.78	112.54	122.65
1	B	654	PRO	N-CA-C	6.76	122.14	111.38
1	B	245	GLU	N-CA-C	-6.64	105.58	113.21
1	A	614	THR	N-CA-C	-6.61	104.53	112.59
1	A	384	PRO	N-CA-C	6.34	121.16	111.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	509	SER	N-CA-C	6.17	123.44	109.81
1	A	425	LEU	N-CA-C	-5.95	101.63	110.20
1	B	167	ASP	CB-CA-C	-5.90	101.88	110.96
1	B	384	PRO	N-CA-C	5.84	120.38	111.15
1	B	265	LYS	N-CA-C	-5.79	104.65	110.97
1	A	245	GLU	N-CA-C	-5.79	106.44	112.93
1	B	258	TYR	N-CA-C	5.79	121.38	113.97
1	A	428	PRO	N-CA-C	-5.69	105.62	113.53
1	B	179	GLY	N-CA-C	-5.69	105.90	115.62
1	A	391	ASN	N-CA-C	5.67	122.88	110.80
1	B	591	GLY	N-CA-C	-5.67	105.63	112.49
1	A	591	GLY	N-CA-C	-5.58	105.75	112.49
1	A	515	GLN	N-CA-C	5.57	122.67	110.80
1	A	735	LEU	N-CA-C	5.55	118.50	110.28
1	B	651	ILE	N-CA-C	5.54	120.87	109.34
1	B	515	GLN	N-CA-C	5.52	122.56	110.80
1	B	723	TRP	N-CA-C	5.45	120.36	111.37
1	B	392	HIS	N-CA-C	-5.33	105.05	112.30
1	B	673	ALA	N-CA-C	-5.27	103.65	110.19
1	A	573	GLN	N-CA-C	5.27	119.78	112.45
1	B	743	HIS	C-N-CD	-5.19	103.72	125.00
1	A	743	HIS	C-N-CD	-5.18	103.78	125.00
1	B	375	ASP	N-CA-C	5.17	117.82	111.82
1	A	675	ILE	N-CA-C	-5.14	101.05	108.71
1	B	344	CYS	N-CA-C	5.14	118.00	109.46
1	B	651	ILE	CB-CA-C	-5.12	102.89	111.29
1	B	497	ILE	N-CA-C	5.09	116.27	111.48

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	166	0
1	B	4445	0	4353	205	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	26	0
All	All	9403	0	8353	365	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 (365) 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:HE21	1:B:573:GLN:N	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:A:543:ASN:HD22	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:N	1:B:177:ASP:OD1	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
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:B:743:HIS:NE2	4:B:1089:HOH:O	2.29	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:335:LYS:NZ	4:B:896:HOH:O	2.29	0.65
1:B:573:GLN:HE21	1:B:573:GLN:H	0.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:B:350:GLN:NE2	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:643:LYS:C	1:B:643:LYS:HD2	2.16	0.63
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: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:439:GLY:C	1:B:501:SER:HB2	2.26	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:N	1:A:436:LEU:HD23	2.18	0.59
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:643:LYS:C	1:A:645:ASN:H	2.10	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:HA	1:A:327:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:241:GLN:C	1:A:242:ARG:HG2	2.29	0.56
1:B:436:LEU:HD23	1:B:436:LEU:N	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: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: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:439:GLY:C	1:A:501:SER:HB2	2.32	0.54
1:A:686:MET:HE3	1:A:687:GLU:O	2.07	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:191:SER:C	1:B:192:GLN:HG2	2.33	0.54
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.38	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:705:GLU:C	1:B:716:ILE:HD12	2.34	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:B:241:GLN:C	1:B:242:ARG:HG2	2.35	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:A:622:GLN:HB2	1:B:445:LEU:HD13	1.91	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: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:227:THR:HG21	1:A:269:GLN:CD	2.36	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:244:GLU:C	1:B:246:ALA:H	2.18	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
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:B:438:LYS:NZ	4:B:1054:HOH:O	2.43	0.50
1:B:515:GLN:NE2	1:B:542:HIS:CE1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:508:SER:OG	1:A:509:SER:N	2.36	0.49
1:A:551:TYR:HB2	1:A:552:PRO:HD2	1.95	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:HH11	1:B:293:ARG:CG	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:A:689:GLU:HB3	1:B:491:GLU:HG3	1.95	0.48
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.12	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:B:406:ARG:NH1	1:B:406:ARG:HG3	2.28	0.48
1:B:406:ARG:HH11	1:B:406:ARG:CG	2.26	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:NH1	1:B:293:ARG:HG3	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:NH1	1:A:406:ARG:HG3	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
1:A:509:SER:CB	1:A:510:PRO:HD3	2.43	0.48
1:A:652:VAL:C	1:A:654:PRO:HD3	2.39	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:A:242:ARG:HG3	1:A:728:GLN:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:ASP:O	1:A:559:SER:HB2	2.13	0.47
1:A:349:ASN:O	1:A:350:GLN:HB2	2.14	0.47
1:A:686:MET:HG3	1:A:687:GLU:N	2.27	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:B:632:ARG:HH22	1:B:755:GLN:CD	2.22	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:240:GLN:OE1	1:B:730:TYR:HE2	1.98	0.46
1:B:350:GLN:NE2	1:B:397:GLN:HE21	2.13	0.46
1:A:436:LEU:HD23	1:A:436:LEU:H	1.80	0.46
1:B:350:GLN:HA	1:B:350:GLN:HE21	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:225:ALA:C	1:B:227:THR:H	2.24	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: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:B:231:GLU:CD	1:B:231:GLU:H	2.24	0.46
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.50	0.46
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:172:LEU:C	1:B:174:ILE:H	2.25	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
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:A:643:LYS:C	1:A:645:ASN:N	2.75	0.45
1:B:728:GLN:HE21	1:B:753:SER:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NE2	1:B:350:GLN:CA	2.79	0.44
1:B:434:LYS:HA	1:B:434:LYS:HD2	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:B:227:THR:HG21	1:B:269:GLN:CD	2.42	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:288:SER:HB2	1:A:727:LYS:HD3	2.00	0.43
1:A:595:ASP:OD1	1:A:596:ASN:N	2.46	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:705:GLU:C	1:A:716:ILE:HD12	2.44	0.43
1:A:403:ARG:HD2	4:A:1147:HOH:O	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:GLN:NE2	1:A:542:HIS:HE1	2.16	0.42
1:A:573:GLN:CD	1:A:573:GLN:H	2.28	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:A:434:LYS:HD2	1:A:434:LYS:HA	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:HD3	1:A:487:LYS:HA	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:168:PHE:CD1	1:B:168:PHE:C	2.98	0.41
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:610:ASP:C	1:A:612:ASN:H	2.29	0.41
1:A:634:ARG:NH2	1:A:751:LYS:HD2	2.35	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: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:549:ARG:HA	1:B:574:ILE:O	2.21	0.41
1:A:293:ARG:NH1	1:A:293:ARG:HG3	2.36	0.41
1:A:594:GLN:O	1:A:594:GLN:HG3	2.21	0.41
1:B:293:ARG:NH1	1:B:293:ARG:CG	2.82	0.41
1:B:504:PHE:HD2	1:B:527:ARG:HH21	1.69	0.41
1:A:250:LEU:O	1:A:253:SER:OG	2.29	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:HG3	4:A:925:HOH:O	2.20	0.40
1:A:242:ARG:HH11	1:A:242:ARG:HD3	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:610:ASP:C	1:B:612:ASN:N	2.79	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 ⓘ

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%)	470 (92%)	31 (6%)	8 (2%)	7	14
1	B	553/624 (89%)	510 (92%)	32 (6%)	11 (2%)	6	10
All	All	1062/1248 (85%)	980 (92%)	63 (6%)	19 (2%)	6	12

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
1	B	176	VAL
1	B	178	ASP
1	B	391	ASN
1	B	515	GLN

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Mol	Chain	Res	Type
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%)	407 (91%)	41 (9%)	8	19
1	B	489/545 (90%)	447 (91%)	42 (9%)	10	21
All	All	937/1090 (86%)	854 (91%)	83 (9%)	9	20

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	THR
1	A	207	MET
1	A	209	THR
1	A	227	THR
1	A	242	ARG
1	A	244	GLU
1	A	293	ARG
1	A	339	CYS
1	A	344	CYS
1	A	379	LYS
1	A	406	ARG
1	A	409	LEU

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Mol	Chain	Res	Type
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	530	ARG
1	A	535	SER
1	A	543	ASN
1	A	563	SER
1	A	573	GLN
1	A	594	GLN
1	A	643	LYS
1	A	648	LYS
1	A	650	SER
1	A	652	VAL
1	A	657	ILE
1	A	670	ARG
1	A	685	ASP
1	A	691	GLU
1	A	711	SER
1	A	738	LYS
1	A	745	SER
1	A	753	SER
1	B	160	MET
1	B	167	ASP
1	B	172	LEU
1	B	177	ASP
1	B	186	ARG
1	B	201	ILE
1	B	210	GLN
1	B	219	GLU
1	B	227	THR
1	B	242	ARG
1	B	244	GLU
1	B	293	ARG
1	B	350	GLN

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Mol	Chain	Res	Type
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	573	GLN
1	B	577	LEU
1	B	594	GLN
1	B	643	LYS
1	B	646	LYS
1	B	647	ASN
1	B	652	VAL
1	B	657	ILE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	241	GLN
1	A	291	HIS
1	A	349	ASN
1	A	515	GLN
1	A	542	HIS
1	A	543	ASN
1	A	639	GLN
1	A	661	HIS

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Mol	Chain	Res	Type
1	A	718	GLN
1	A	728	GLN
1	A	734	HIS
1	A	755	GLN
1	B	190	HIS
1	B	239	HIS
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	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 oligosaccharides 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	-	3,3,3	0.94	0	3,3,3	0.88	0
3	ACT	A	5	-	3,3,3	0.87	0	3,3,3	0.86	0

There are no bond length outliers.

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, 95th 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 ²)	Q<0.9
1	A	509/624 (81%)	-0.15	24 (4%)	36 32	17, 34, 87, 121	12 (2%)
1	B	554/624 (88%)	-0.11	32 (5%)	29 25	17, 35, 79, 114	19 (3%)
All	All	1063/1248 (85%)	-0.12	56 (5%)	32 28	17, 35, 80, 121	31 (2%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	206	LYS	7.7
1	B	176	VAL	6.9
1	A	203	THR	6.1
1	B	650	SER	5.9
1	A	510	PRO	5.5
1	A	202	GLU	4.7
1	A	201	ILE	4.5
1	A	645	ASN	4.5
1	A	647	ASN	4.3
1	A	509	SER	4.0
1	A	421	VAL	4.0
1	B	177	ASP	3.9
1	A	207	MET	3.7
1	B	171	GLU	3.5
1	B	711	SER	3.5
1	B	170	LYS	3.4
1	A	711	SER	3.4
1	B	158	ASN	3.3
1	A	205	TYR	3.3
1	A	209	THR	3.2
1	B	509	SER	3.1
1	B	508	SER	3.0
1	A	420	GLY	2.9
1	B	245	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	164	GLU	2.8
1	B	647	ASN	2.7
1	A	204	PHE	2.7
1	B	390	GLU	2.7
1	B	178	ASP	2.6
1	B	162	PHE	2.6
1	A	710	SER	2.6
1	A	266	ALA	2.5
1	A	200	GLU	2.5
1	B	174	ILE	2.4
1	A	709	SER	2.4
1	B	646	LYS	2.4
1	A	646	LYS	2.4
1	A	224	SER	2.3
1	B	163	LYS	2.3
1	B	709	SER	2.3
1	B	168	PHE	2.3
1	B	161	ASN	2.3
1	A	208	LEU	2.3
1	B	484	ASP	2.2
1	B	644	VAL	2.2
1	B	246	ALA	2.2
1	B	159	LYS	2.2
1	B	515	GLN	2.2
1	B	712	LYS	2.2
1	B	266	ALA	2.2
1	A	210	GLN	2.1
1	B	172	LEU	2.1
1	B	485	LYS	2.0
1	A	390	GLU	2.0
1	B	247	GLY	2.0
1	B	167	ASP	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
2	CA	A	3	1/1	0.76	0.10	67,67,67,67	1
2	CA	B	2	1/1	0.80	0.07	69,69,69,69	1
2	CA	A	1	1/1	0.84	0.13	53,53,53,53	1
2	CA	B	1	1/1	0.93	0.06	54,54,54,54	1
2	CA	B	3	1/1	0.97	0.08	57,57,57,57	1
3	ACT	A	5	4/4	0.97	0.04	25,31,32,36	0
2	CA	A	2	1/1	0.98	0.03	55,55,55,55	1
3	ACT	B	5	4/4	0.99	0.05	24,26,26,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.