



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:59 PM GMT

PDB ID : 1DJG
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM
RAT COMPLEXED WITH LANTHANUM
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on : 1996-09-25
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

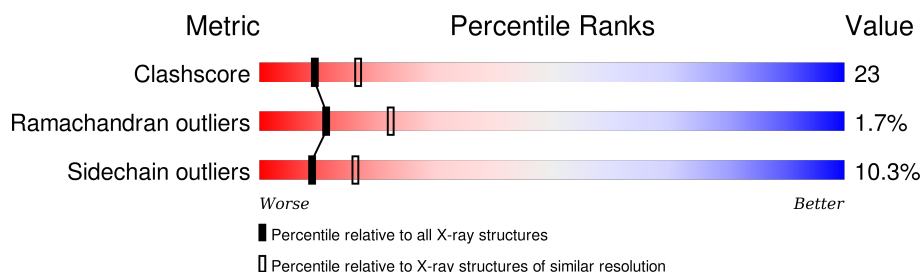
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	624	
1	B	624	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	A	5	-	-	X	-

2 Entry composition [i](#)

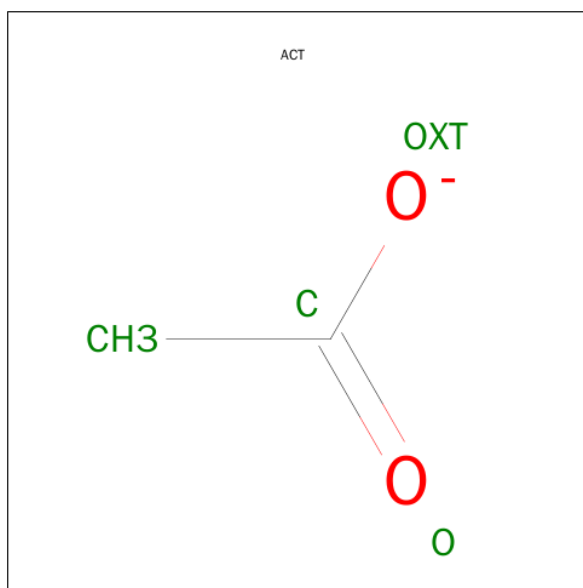
There are 4 unique types of molecules in this entry. The entry contains 9246 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	86	0	0
			4057	2565	709	761	22			
1	B	561	Total	C	N	O	S	101	0	0
			4465	2818	776	847	24			

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is LANTHANUM (III) ION (three-letter code: LA) (formula: La).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total 4	La 4	0	0
3	A	4	Total 4	La 4	0	0

- Molecule 4 is water.

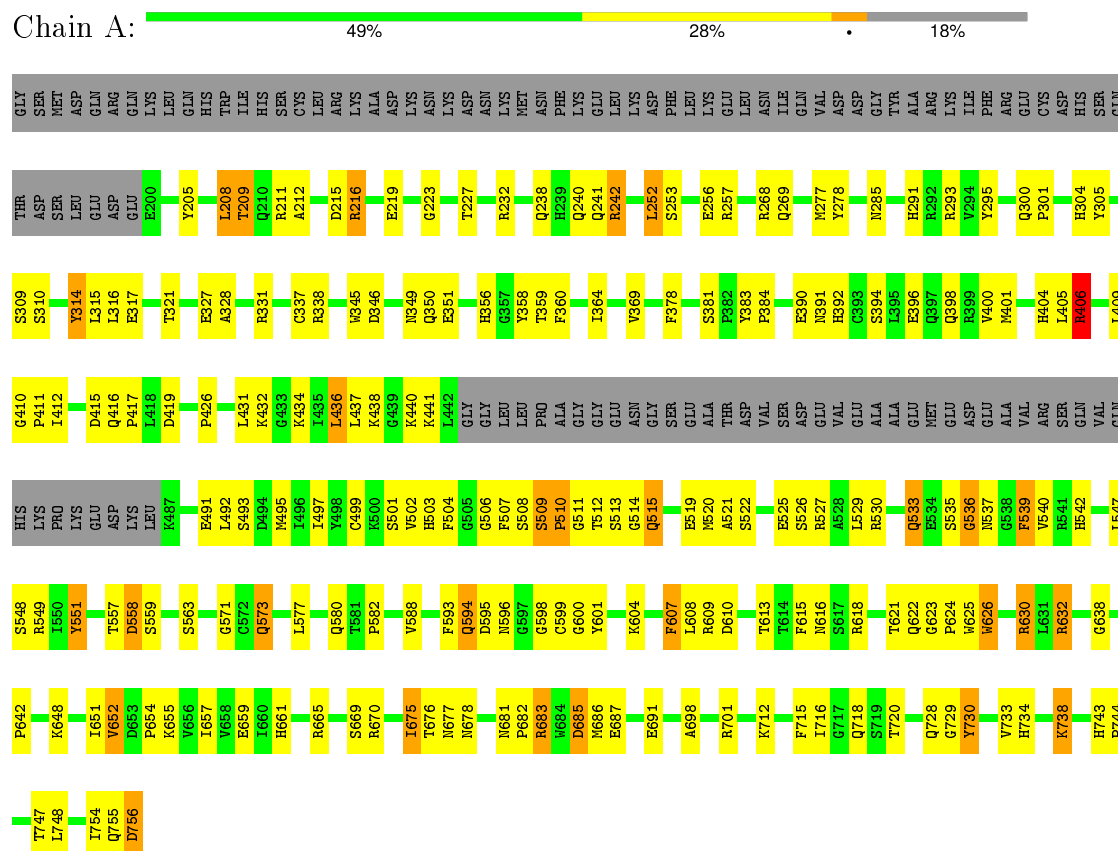
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	335	Total 335	O 335	0	0
4	B	373	Total 373	O 373	0	0

3 Residue-property plots

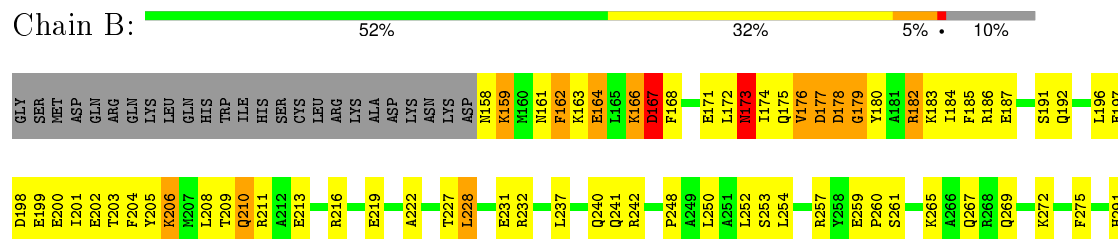
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

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



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



D559	D560	H661	R665	T675	N678	N681	F682	R683	N684	D685	M686	E687	E691	D696	L697	A698	R701	S709	S710	S711	K712	F715	L716	G717	Q718	S719	T720	Q728	G729	Y730	H734	L735	K738	H743	T747	K751	T752	S753	Q755	D756												
D558	S559	S563	E566	G571	G572	Q573	Q580	T581	P582	E583	F583	Q594	D595	N596	G597	C599	R604	P605	A606	F607	T613	T621	Q622	Q623	P624	L625	L630	L631	N632	N633	R634	L638	P642	K643	N647	K648	N649	S650	L651	V652	D653	P654	G655	V656	T657							
ARG	SER	GLN	VAL	GLN	HIS	LYS	PRO	LYS	GLU	D484	L488	L492	S493	L497	K500	S501	V502	H503	F504	G505	G506	S509	P510	G514	Q515	A516	F517	Y518	E519	N520	F523	S524	E525	S526	R527	A528	L529	Q533	E534	S535	G536	H537	G538	F539	L547	S548	Y551	P552				
L405	R406	L409	L412	D415	Q416	P417	L418	T421	T422	T423	S424	L425	P426	S427	L431	K432	L436	L437	C438	D439	K440	K441	L442	L445	LEU	PRO	ALA	GLY	GLY	GLU	ASN	GLY	SER	GLU	VAL	THR	ASP	VAL	SER	SER	GLU	VAL	GLU	ALA	ALA	GLU	MET	GLU	ASP	GLU	ALA	VAL
R292	R293	Q300	P301	H304	S309	S310	T313	Y314	L315	L316	Y329	I330	R331	C337	L342	D343	C344	H345	D346	R347	P348	N349	Q350	E351	C357	Y358	K378	K379	Y383	F384	S388	L389	E390	N391	H392	C393	S394	L395	E396	Q397	R398	M401										

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	397.92Å 397.92Å 397.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.5 (10.00-2.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.210 , 0.270	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9246	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

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: ACT, LA

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	0.98	29/4152 (0.7%)	0.88	4/5624 (0.1%)
1	B	1.00	31/4565 (0.7%)	0.90	8/6174 (0.1%)
All	All	0.99	60/8717 (0.7%)	0.89	12/11798 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	1	0
All	All	1	1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	730	TYR	CE2-CZ	-10.49	1.25	1.38
1	A	358	TYR	CE1-CZ	-9.51	1.26	1.38
1	A	314	TYR	CE2-CZ	-9.42	1.26	1.38
1	A	551	TYR	CE2-CZ	-9.34	1.26	1.38
1	B	314	TYR	CE1-CZ	-8.98	1.26	1.38
1	B	358	TYR	CE1-CZ	-8.89	1.26	1.38
1	B	730	TYR	CE1-CZ	-8.86	1.27	1.38
1	B	314	TYR	CE2-CZ	-8.76	1.27	1.38
1	B	551	TYR	CE1-CZ	-8.59	1.27	1.38
1	A	730	TYR	CE1-CZ	-8.37	1.27	1.38
1	B	730	TYR	CG-CD1	-8.33	1.28	1.39
1	B	715	PHE	CE1-CZ	-8.25	1.21	1.37
1	A	715	PHE	CE2-CZ	-8.23	1.21	1.37
1	B	358	TYR	CG-CD2	-8.14	1.28	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	TYR	CG-CD1	-7.88	1.28	1.39
1	B	607	PHE	CE2-CZ	-7.76	1.22	1.37
1	A	358	TYR	CG-CD2	-7.67	1.29	1.39
1	A	715	PHE	CG-CD1	-7.66	1.27	1.38
1	B	715	PHE	CE2-CZ	-7.62	1.22	1.37
1	A	607	PHE	CE2-CZ	-7.59	1.23	1.37
1	A	314	TYR	CG-CD1	-7.57	1.29	1.39
1	B	607	PHE	CE1-CZ	-7.49	1.23	1.37
1	A	551	TYR	CE1-CZ	-7.39	1.28	1.38
1	B	551	TYR	CG-CD2	-7.39	1.29	1.39
1	A	551	TYR	CG-CD1	-7.35	1.29	1.39
1	B	551	TYR	CE2-CZ	-7.19	1.29	1.38
1	B	378	PHE	CE1-CZ	-6.99	1.24	1.37
1	B	715	PHE	CG-CD1	-6.94	1.28	1.38
1	B	378	PHE	CE2-CZ	-6.79	1.24	1.37
1	B	730	TYR	CG-CD2	-6.72	1.30	1.39
1	B	358	TYR	CE2-CZ	-6.71	1.29	1.38
1	B	314	TYR	CG-CD2	-6.68	1.30	1.39
1	A	358	TYR	CG-CD1	-6.68	1.30	1.39
1	B	551	TYR	CG-CD1	-6.67	1.30	1.39
1	A	730	TYR	CG-CD2	-6.61	1.30	1.39
1	A	551	TYR	CG-CD2	-6.32	1.30	1.39
1	A	378	PHE	CE2-CZ	-6.30	1.25	1.37
1	B	159	LYS	C-O	-6.29	1.11	1.23
1	A	409	LEU	CG-CD1	-6.24	1.28	1.51
1	B	715	PHE	CG-CD2	-6.14	1.29	1.38
1	B	378	PHE	CG-CD2	-6.09	1.29	1.38
1	A	358	TYR	CE2-CZ	-6.03	1.30	1.38
1	A	607	PHE	CG-CD1	-5.98	1.29	1.38
1	B	409	LEU	CG-CD1	-5.88	1.30	1.51
1	A	730	TYR	CG-CD1	-5.85	1.31	1.39
1	B	607	PHE	CG-CD1	-5.79	1.30	1.38
1	A	378	PHE	CE1-CZ	-5.75	1.26	1.37
1	A	314	TYR	CE1-CZ	-5.75	1.31	1.38
1	A	730	TYR	CE2-CZ	-5.74	1.31	1.38
1	A	607	PHE	CE1-CZ	-5.57	1.26	1.37
1	A	715	PHE	CG-CD2	-5.55	1.30	1.38
1	B	378	PHE	CG-CD1	-5.54	1.30	1.38
1	B	607	PHE	CG-CD2	-5.45	1.30	1.38
1	B	409	LEU	CG-CD2	-5.40	1.31	1.51
1	A	715	PHE	CE1-CZ	-5.40	1.27	1.37
1	A	378	PHE	CG-CD2	-5.33	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	409	LEU	CG-CD2	-5.14	1.32	1.51
1	A	626	TRP	CB-CG	-5.06	1.41	1.50
1	B	358	TYR	CG-CD1	-5.06	1.32	1.39
1	A	607	PHE	CG-CD2	-5.05	1.31	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	393	CYS	CA-CB-SG	8.09	128.56	114.00
1	A	406	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	B	393	CYS	N-CA-C	6.06	127.35	111.00
1	A	509	SER	N-CA-C	5.79	126.63	111.00
1	B	173	ASN	CB-CA-C	5.50	121.39	110.40
1	B	179	GLY	N-CA-C	-5.39	99.62	113.10
1	B	510	PRO	N-CA-C	5.33	125.95	112.10
1	B	406	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	B	393	CYS	N-CA-CB	5.30	120.15	110.60
1	A	268	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	167	ASP	CB-CA-C	5.14	120.68	110.40
1	A	558	ASP	CB-CG-OD1	5.14	122.92	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	393	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	691	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	173	0
1	B	4465	0	4375	208	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	4	0	3	2	0
2	B	4	0	3	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	335	0	0	11	0
4	B	373	0	0	18	0
All	All	9246	0	8353	370	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 23.

All (370) 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:161:ASN:H	1:B:164:GLU:HG3	1.18	1.07
1:A:613:THR:HG22	1:A:615:PHE:H	1.23	1.02
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.24	1.01
1:B:438:LYS:HD2	1:B:520:MET:HE1	1.46	0.98
1:B:728:GLN:NE2	1:B:754:ILE:H	1.64	0.94
1:A:573:GLN:H	1:A:573:GLN:NE2	1.65	0.93
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.52	0.92
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.34	0.90
1:B:728:GLN:HE21	1:B:754:ILE:H	1.21	0.88
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.08	0.88
1:A:632:ARG:NH2	1:B:406:ARG:NH1	2.22	0.86
1:B:607:PHE:CD2	1:B:625:TRP:HB3	2.11	0.85
1:B:241:GLN:HE22	1:B:730:TYR:H	1.24	0.85
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.58	0.85
1:A:241:GLN:HE22	1:A:730:TYR:H	1.24	0.84
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.93	0.82
1:B:202:GLU:HB3	1:B:206:LYS:HE3	1.61	0.81
1:B:515:GLN:HB3	1:B:519:GLU:OE1	1.81	0.81
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.62	0.80
1:A:438:LYS:HD2	1:A:520:MET:HE1	1.61	0.79
1:A:573:GLN:H	1:A:573:GLN:HE21	1.27	0.79
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.18	0.79
1:A:738:LYS:HG3	2:A:5:ACT:H3	1.63	0.79
1:B:159:LYS:O	4:B:1060:HOH:O	2.00	0.79
1:A:216:ARG:HG3	1:A:216:ARG:HH11	1.47	0.78
1:B:202:GLU:HB3	1:B:206:LYS:CE	2.13	0.78
1:A:607:PHE:CD2	1:A:625:TRP:HB3	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:PHE:HB3	1:B:527:ARG:NH2	1.99	0.77
1:B:548:SER:H	1:B:573:GLN:NE2	1.81	0.77
1:B:573:GLN:H	1:B:573:GLN:NE2	1.83	0.76
1:A:390:GLU:HG2	1:A:392:HIS:CE1	2.21	0.75
1:B:605:PRO:HB2	1:B:607:PHE:CE1	2.22	0.75
1:A:394:SER:O	1:A:398:GLN:HG3	1.87	0.75
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.21	0.74
1:A:613:THR:CG2	1:A:615:PHE:H	2.01	0.74
1:A:548:SER:H	1:A:573:GLN:NE2	1.86	0.74
1:A:547:LEU:HD23	1:A:573:GLN:HG3	1.70	0.74
1:B:547:LEU:HD23	1:B:573:GLN:HG3	1.69	0.74
1:A:415:ASP:C	1:A:497:ILE:HD11	2.09	0.73
1:B:607:PHE:CE2	1:B:625:TRP:HB3	2.22	0.73
1:A:252:LEU:HD23	1:A:256:GLU:OE2	1.89	0.73
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.70	0.73
1:B:196:LEU:HD22	1:B:200:GLU:HB3	1.71	0.73
1:B:161:ASN:N	1:B:164:GLU:HG3	2.01	0.72
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.25	0.71
1:B:166:LYS:HE2	4:B:1099:HOH:O	1.89	0.71
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.73	0.70
1:B:438:LYS:HD2	1:B:520:MET:CE	2.22	0.70
1:B:202:GLU:HB3	1:B:206:LYS:HZ1	1.56	0.69
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.21	0.69
1:B:683:ARG:HD2	4:B:1003:HOH:O	1.93	0.68
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.23	0.68
1:A:616:ASN:OD1	1:A:618:ARG:HB2	1.94	0.68
1:B:728:GLN:HE21	1:B:754:ILE:N	1.92	0.68
1:B:755:GLN:HG2	4:B:1033:HOH:O	1.92	0.68
1:A:728:GLN:HE21	1:A:754:ILE:HB	1.57	0.68
1:B:202:GLU:HB3	1:B:206:LYS:NZ	2.09	0.68
1:B:401:MET:HE2	1:B:492:LEU:HD11	1.76	0.68
1:A:607:PHE:CE2	1:A:625:TRP:HB3	2.29	0.67
1:B:654:PRO:HD2	1:B:675:ILE:O	1.96	0.67
1:B:607:PHE:H	1:B:607:PHE:HD1	1.43	0.66
1:B:293:ARG:NH1	4:B:1000:HOH:O	2.28	0.66
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.25	0.66
1:A:252:LEU:O	1:A:256:GLU:HG3	1.95	0.66
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.30	0.65
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.07	0.65
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.79	0.65
1:B:174:ILE:O	1:B:176:VAL:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:HG3	1:B:417:PRO:CD	2.26	0.65
1:B:168:PHE:O	1:B:171:GLU:HB3	1.96	0.65
1:A:670:ARG:HD3	4:A:778:HOH:O	1.95	0.64
1:B:630:ARG:CD	1:B:755:GLN:HE21	2.11	0.64
1:B:524:SER:HA	1:B:551:TYR:CE1	2.31	0.64
1:A:728:GLN:NE2	1:A:754:ILE:HB	2.12	0.64
1:A:346:ASP:OD2	1:A:394:SER:HB3	1.98	0.64
1:A:285:ASN:ND2	1:A:734:HIS:HD2	1.96	0.63
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.32	0.63
1:B:415:ASP:C	1:B:497:ILE:HD11	2.18	0.63
1:B:593:PHE:O	1:B:598:GLY:HA2	1.98	0.63
1:B:196:LEU:HB3	1:B:201:ILE:HG12	1.81	0.63
1:A:208:LEU:HD23	1:A:208:LEU:N	2.14	0.62
1:A:219:GLU:O	1:A:223:GLY:N	2.29	0.62
1:B:622:GLN:HG3	1:B:623:GLY:N	2.14	0.62
1:A:317:GLU:O	1:A:580:GLN:NE2	2.32	0.62
1:A:515:GLN:HB3	1:A:519:GLU:OE1	1.99	0.61
1:B:504:PHE:HD2	1:B:527:ARG:NH2	1.98	0.61
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.81	0.61
1:B:162:PHE:CE2	1:B:182:ARG:HG2	2.35	0.61
1:B:594:GLN:HE21	1:B:594:GLN:HA	1.66	0.61
1:A:622:GLN:OE1	1:B:445:LEU:HD12	2.00	0.61
1:A:607:PHE:CE1	1:A:608:LEU:HG	2.35	0.61
1:A:593:PHE:O	1:A:598:GLY:HA2	2.01	0.60
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.34	0.60
1:A:504:PHE:HD2	1:A:527:ARG:NH2	1.98	0.60
1:B:391:ASN:N	4:B:766:HOH:O	2.27	0.60
1:A:316:LEU:HD23	1:A:328:ALA:HB2	1.83	0.59
1:B:730:TYR:CE1	1:B:751:LYS:HD2	2.36	0.58
1:B:711:SER:OG	1:B:712:LYS:N	2.32	0.58
1:A:507:PHE:CD1	1:A:542:HIS:HB2	2.38	0.58
1:A:416:GLN:N	1:A:497:ILE:HD11	2.18	0.58
1:B:683:ARG:NH1	4:B:994:HOH:O	2.32	0.58
1:B:583:GLY:HA3	4:B:911:HOH:O	2.02	0.58
1:A:291:HIS:CD2	1:A:295:TYR:CZ	2.91	0.58
1:A:349:ASN:O	1:A:349:ASN:ND2	2.37	0.58
1:B:696:ASP:HB2	4:B:768:HOH:O	2.04	0.58
1:B:642:PRO:HD2	1:B:716:ILE:HG23	1.85	0.58
1:B:418:LEU:HD12	1:B:426:PRO:HB3	1.86	0.57
1:B:248:PRO:O	1:B:252:LEU:HG	2.05	0.57
1:A:390:GLU:HG2	1:A:392:HIS:HE1	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:LYS:HE3	4:B:906:HOH:O	2.03	0.57
1:B:184:ILE:HG22	1:B:204:PHE:CD1	2.40	0.57
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.38	0.57
1:A:227:THR:HG21	1:A:269:GLN:OE1	2.05	0.57
1:B:183:LYS:O	1:B:187:GLU:HG3	2.05	0.56
1:A:417:PRO:HD3	1:A:497:ILE:HD13	1.86	0.56
1:B:630:ARG:HD2	1:B:755:GLN:HE21	1.69	0.56
1:A:622:GLN:CA	1:B:445:LEU:HD13	2.35	0.56
1:B:533:GLN:HA	1:B:533:GLN:OE1	2.06	0.56
1:A:632:ARG:HH22	1:B:406:ARG:NH1	2.02	0.56
1:B:346:ASP:OD2	1:B:394:SER:HB3	2.06	0.56
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.35	0.56
1:B:573:GLN:H	1:B:573:GLN:HE21	1.53	0.56
1:A:232:ARG:NH2	4:A:1066:HOH:O	2.38	0.56
1:B:634:ARG:CG	1:B:687:GLU:HB2	2.36	0.55
1:A:502:VAL:HG11	1:A:515:GLN:CD	2.26	0.55
1:B:595:ASP:OD1	1:B:596:ASN:N	2.38	0.55
1:A:683:ARG:NH2	1:A:685:ASP:OD2	2.40	0.55
1:B:605:PRO:HB2	1:B:607:PHE:HE1	1.69	0.55
1:B:734:HIS:ND1	1:B:747:THR:HG22	2.22	0.55
1:A:734:HIS:ND1	1:A:747:THR:HG22	2.20	0.55
1:A:356:HIS:HD1	1:A:359:THR:HG21	1.71	0.55
1:B:161:ASN:OD1	1:B:164:GLU:HG2	2.06	0.55
1:B:240:GLN:HA	1:B:240:GLN:OE1	2.07	0.55
1:B:394:SER:O	1:B:398:GLN:HG3	2.07	0.55
1:B:605:PRO:CB	1:B:607:PHE:HE1	2.20	0.54
1:A:241:GLN:HE22	1:A:730:TYR:N	1.98	0.54
1:B:632:ARG:HH22	1:B:755:GLN:NE2	2.06	0.54
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.73	0.54
1:B:222:ALA:C	1:B:232:ARG:HH11	2.11	0.54
1:B:205:TYR:O	1:B:208:LEU:HB3	2.08	0.54
1:B:197:GLU:O	1:B:201:ILE:HG13	2.08	0.54
1:B:379:LYS:HE2	4:B:891:HOH:O	2.06	0.54
1:B:202:GLU:CB	1:B:206:LYS:HE3	2.35	0.54
1:B:441:LYS:NZ	1:B:493:SER:O	2.41	0.54
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.88	0.53
1:B:426:PRO:HG2	1:B:431:LEU:CD1	2.34	0.53
1:A:738:LYS:HG3	2:A:5:ACT:CH3	2.35	0.53
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.38	0.53
1:A:595:ASP:OD1	1:A:596:ASN:N	2.38	0.53
1:A:626:TRP:CE3	1:B:445:LEU:HD21	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.08	0.53
1:B:681:ASN:HB2	4:B:922:HOH:O	2.07	0.53
1:B:211:ARG:NE	1:B:213:GLU:OE2	2.34	0.53
1:B:738:LYS:HD2	4:B:1100:HOH:O	2.09	0.53
1:A:533:GLN:HA	1:A:533:GLN:OE1	2.08	0.53
1:B:206:LYS:O	1:B:210:GLN:HB3	2.09	0.52
1:A:216:ARG:CG	1:A:216:ARG:HH11	2.21	0.52
1:A:652:VAL:CG1	1:A:716:ILE:HD11	2.40	0.52
1:A:240:GLN:HA	1:A:240:GLN:OE1	2.09	0.52
1:A:652:VAL:HG11	1:A:716:ILE:HD11	1.91	0.52
1:B:729:GLY:O	1:B:751:LYS:HA	2.09	0.52
1:A:504:PHE:CD2	1:A:527:ARG:NH2	2.78	0.52
1:A:345:TRP:CH2	1:A:392:HIS:CD2	2.98	0.52
1:B:196:LEU:HD22	1:B:200:GLU:CB	2.38	0.52
1:B:547:LEU:HD23	1:B:573:GLN:CG	2.37	0.52
1:B:630:ARG:HD2	1:B:755:GLN:NE2	2.25	0.52
1:B:638:GLY:O	1:B:681:ASN:HA	2.10	0.52
1:A:401:MET:HE2	1:A:492:LEU:HD11	1.92	0.52
1:A:638:GLY:O	1:A:681:ASN:HA	2.10	0.51
1:B:547:LEU:CD2	1:B:573:GLN:HG3	2.38	0.51
1:B:177:ASP:O	1:B:178:ASP:HB2	2.10	0.51
1:B:566:GLU:HB3	4:B:912:HOH:O	2.11	0.51
1:B:345:TRP:CZ2	1:B:392:HIS:CD2	2.99	0.51
1:A:539:PHE:O	1:A:542:HIS:HB3	2.10	0.51
1:B:728:GLN:NE2	1:B:754:ILE:N	2.46	0.51
1:A:547:LEU:HD23	1:A:573:GLN:CG	2.38	0.51
1:A:242:ARG:HG3	1:A:728:GLN:HB2	1.91	0.51
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.41	0.51
1:A:630:ARG:NH2	1:B:406:ARG:HH22	2.08	0.51
1:B:259:GLU:OE2	1:B:260:PRO:HD2	2.10	0.51
1:B:514:GLY:O	1:B:515:GLN:O	2.29	0.51
1:B:203:THR:N	1:B:206:LYS:HZ2	2.08	0.51
1:A:642:PRO:HD2	1:A:716:ILE:HG23	1.92	0.51
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.41	0.51
1:A:622:GLN:CB	1:B:445:LEU:HD13	2.41	0.50
1:B:582:PRO:HB3	1:B:738:LYS:HG2	1.92	0.50
1:B:261:SER:O	1:B:265:LYS:HB2	2.11	0.50
1:B:267:GLN:O	1:B:269:GLN:HG3	2.12	0.50
1:B:630:ARG:HD3	1:B:755:GLN:HE21	1.77	0.50
1:B:405:LEU:O	1:B:409:LEU:HB2	2.10	0.50
1:B:438:LYS:CD	1:B:520:MET:HE1	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:PHE:CD2	1:B:527:ARG:NH2	2.79	0.50
1:B:202:GLU:O	1:B:206:LYS:HG2	2.12	0.50
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.11	0.50
1:A:582:PRO:HB3	1:A:738:LYS:HG2	1.94	0.49
1:B:163:LYS:O	1:B:167:ASP:HB3	2.11	0.49
1:A:205:TYR:O	1:A:209:THR:OG1	2.27	0.49
1:A:551:TYR:N	1:A:551:TYR:CD1	2.80	0.49
1:B:686:MET:HG3	1:B:687:GLU:N	2.26	0.49
1:A:356:HIS:ND1	1:A:359:THR:HG21	2.26	0.49
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.26	0.49
1:A:535:SER:O	1:A:537:ASN:N	2.45	0.49
1:B:253:SER:O	1:B:257:ARG:HB2	2.12	0.49
1:B:202:GLU:CB	1:B:206:LYS:HZ1	2.21	0.49
1:A:659:GLU:OE1	1:A:661:HIS:HE1	1.95	0.49
1:A:613:THR:HG22	1:A:615:PHE:N	2.08	0.49
1:B:250:LEU:O	1:B:254:LEU:HG	2.12	0.49
1:B:607:PHE:CD1	1:B:607:PHE:N	2.78	0.49
1:A:652:VAL:HG11	1:A:716:ILE:CD1	2.43	0.49
1:A:622:GLN:HG3	1:A:623:GLY:N	2.27	0.49
1:B:390:GLU:HG2	1:B:392:HIS:NE2	2.27	0.49
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.42	0.49
1:B:661:HIS:O	1:B:698:ALA:HA	2.13	0.49
1:A:253:SER:O	1:A:257:ARG:HB2	2.13	0.49
1:A:607:PHE:CE2	1:A:625:TRP:CB	2.96	0.49
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.43	0.49
1:B:259:GLU:CD	1:B:260:PRO:HD2	2.33	0.49
1:B:730:TYR:CE1	1:B:751:LYS:CD	2.96	0.48
1:B:300:GLN:HB3	1:B:301:PRO:HD2	1.95	0.48
1:A:304:HIS:O	1:A:604:LYS:HB2	2.13	0.48
1:A:441:LYS:NZ	1:A:493:SER:O	2.46	0.48
1:A:391:ASN:HD21	1:A:398:GLN:CD	2.15	0.48
1:B:654:PRO:HG3	1:B:678:ASN:O	2.13	0.48
1:A:701:ARG:HH21	1:A:718:GLN:HG3	1.79	0.48
1:A:310:SER:HB3	1:A:337:CYS:SG	2.54	0.48
1:B:351:GLU:OE1	1:B:351:GLU:HA	2.12	0.48
1:B:395:LEU:HB2	4:B:1120:HOH:O	2.13	0.48
1:A:345:TRP:CZ2	1:A:392:HIS:CG	3.01	0.48
1:B:607:PHE:HD1	1:B:607:PHE:N	2.10	0.48
1:A:242:ARG:HB3	1:A:242:ARG:HE	1.42	0.48
1:B:701:ARG:HH21	1:B:718:GLN:HG3	1.78	0.48
1:A:558:ASP:O	1:A:559:SER:HB2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:GLN:HG2	1:A:756:ASP:N	2.28	0.47
1:B:313:THR:HB	1:B:329:TYR:CE1	2.48	0.47
1:B:416:GLN:N	1:B:497:ILE:HD11	2.29	0.47
1:A:622:GLN:HA	1:B:445:LEU:CD1	2.44	0.47
1:B:391:ASN:HD21	1:B:398:GLN:CD	2.18	0.47
1:A:676:THR:HG23	4:A:1077:HOH:O	2.15	0.47
1:A:686:MET:HB2	4:A:885:HOH:O	2.13	0.47
1:A:609:ARG:NH2	4:A:871:HOH:O	2.46	0.47
1:A:525:GLU:O	1:A:529:LEU:HG	2.14	0.47
1:B:571:GLY:HA2	1:B:604:LYS:HE3	1.97	0.47
1:B:504:PHE:HD2	1:B:527:ARG:HH21	1.62	0.47
1:B:548:SER:H	1:B:573:GLN:HE21	1.59	0.47
1:A:416:GLN:N	1:A:497:ILE:CD1	2.78	0.47
1:A:756:ASP:OD1	1:A:756:ASP:N	2.47	0.47
1:A:654:PRO:HD2	1:A:675:ILE:O	2.14	0.47
1:A:728:GLN:NE2	1:A:754:ILE:H	2.13	0.47
1:A:571:GLY:HA2	1:A:604:LYS:HE3	1.97	0.47
1:A:613:THR:HG21	1:A:615:PHE:HB3	1.96	0.47
1:B:345:TRP:CZ2	1:B:392:HIS:CG	3.03	0.47
1:B:524:SER:CA	1:B:551:TYR:CE1	2.98	0.46
1:A:502:VAL:CG1	1:A:503:HIS:N	2.78	0.46
1:B:205:TYR:O	1:B:209:THR:HG23	2.16	0.46
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.15	0.46
1:A:613:THR:CG2	1:A:615:PHE:HB3	2.46	0.46
1:A:400:VAL:HG12	1:A:404:HIS:CD2	2.50	0.46
1:B:607:PHE:CE2	1:B:625:TRP:CB	2.96	0.46
1:B:310:SER:HG	1:B:313:THR:HG1	1.58	0.46
1:B:416:GLN:N	1:B:497:ILE:CD1	2.79	0.46
1:B:701:ARG:NH2	1:B:718:GLN:HG3	2.31	0.46
1:A:651:ILE:HG21	1:A:677:ASN:C	2.37	0.46
1:A:701:ARG:NH2	1:A:718:GLN:HG3	2.30	0.45
1:A:314:TYR:CE1	1:A:315:LEU:HG	2.51	0.45
1:B:551:TYR:HB2	1:B:552:PRO:HD2	1.98	0.45
1:B:659:GLU:OE1	1:B:701:ARG:HD3	2.17	0.45
1:A:557:THR:HA	4:A:958:HOH:O	2.16	0.45
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.50	0.45
1:B:222:ALA:HB2	1:B:228:LEU:HD23	1.97	0.45
1:A:509:SER:N	1:A:510:PRO:HD2	2.32	0.45
1:B:342:LEU:HD12	1:B:342:LEU:N	2.30	0.45
1:B:605:PRO:HB2	1:B:607:PHE:CD1	2.52	0.45
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:HIS:O	1:B:604:LYS:HB2	2.16	0.45
1:B:735:LEU:O	1:B:743:HIS:HB2	2.16	0.45
1:A:412:ILE:O	1:A:412:ILE:HG22	2.16	0.45
1:A:300:GLN:HB3	1:A:301:PRO:CD	2.47	0.45
1:B:164:GLU:H	1:B:164:GLU:HG2	1.57	0.45
1:B:178:ASP:CG	1:B:179:GLY:H	2.18	0.45
1:A:438:LYS:CD	1:A:520:MET:HE1	2.39	0.45
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.63	0.45
1:B:172:LEU:O	1:B:174:ILE:HG13	2.17	0.45
1:A:507:PHE:CD1	1:A:542:HIS:CB	3.00	0.45
1:B:535:SER:O	1:B:537:ASN:N	2.49	0.45
1:A:405:LEU:HD13	1:A:437:LEU:HD11	1.97	0.45
1:B:605:PRO:CB	1:B:607:PHE:CE1	2.94	0.45
1:A:686:MET:HG3	1:A:687:GLU:N	2.30	0.45
1:B:436:LEU:HD23	1:B:436:LEU:N	2.32	0.45
1:A:573:GLN:N	1:A:573:GLN:NE2	2.48	0.44
1:B:191:SER:O	1:B:192:GLN:HB2	2.17	0.44
1:B:237:LEU:O	1:B:241:GLN:HB2	2.18	0.44
1:A:438:LYS:HE2	1:A:501:SER:OG	2.18	0.44
1:A:438:LYS:HA	1:A:499:CYS:HB2	2.00	0.44
1:A:607:PHE:CD1	1:A:608:LEU:HG	2.51	0.44
1:B:551:TYR:HB2	1:B:552:PRO:CD	2.47	0.44
1:A:630:ARG:HD3	4:A:981:HOH:O	2.18	0.44
1:B:582:PRO:HA	4:B:780:HOH:O	2.18	0.44
1:A:536:GLY:O	1:A:540:VAL:HG23	2.18	0.44
1:A:669:SER:C	1:A:670:ARG:HG2	2.38	0.44
1:B:558:ASP:O	1:B:559:SER:HB2	2.17	0.43
1:B:632:ARG:HH22	1:B:755:GLN:CD	2.20	0.43
1:A:491:GLU:HA	4:A:930:HOH:O	2.17	0.43
1:B:316:LEU:O	1:B:580:GLN:HG3	2.18	0.43
1:A:390:GLU:OE2	1:A:392:HIS:HE1	2.00	0.43
1:A:654:PRO:HG3	1:A:678:ASN:O	2.18	0.43
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.07	0.43
1:A:661:HIS:O	1:A:698:ALA:HA	2.19	0.43
1:A:291:HIS:CD2	1:A:295:TYR:CE1	3.07	0.43
1:A:300:GLN:HB3	1:A:301:PRO:HD2	2.01	0.43
1:B:412:ILE:O	1:B:412:ILE:HG22	2.18	0.43
1:A:681:ASN:N	1:A:682:PRO:CD	2.82	0.43
1:A:212:ALA:O	1:A:215:ASP:HB2	2.19	0.43
1:B:438:LYS:HE2	1:B:501:SER:OG	2.19	0.43
1:B:172:LEU:HB2	1:B:174:ILE:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:PHE:CE2	1:B:182:ARG:CG	3.01	0.43
1:B:405:LEU:HA	1:B:405:LEU:HD23	1.87	0.43
1:B:502:VAL:CG1	1:B:503:HIS:N	2.80	0.43
1:A:405:LEU:HA	1:A:405:LEU:HD23	1.90	0.42
1:B:199:GLU:O	1:B:202:GLU:N	2.49	0.42
1:B:185:PHE:CE1	1:B:196:LEU:HG	2.54	0.42
1:A:241:GLN:NE2	1:A:729:GLY:HA3	2.35	0.42
1:A:300:GLN:O	1:A:305:TYR:HE1	2.03	0.42
1:A:436:LEU:HD23	1:A:436:LEU:N	2.34	0.42
1:B:563:SER:O	1:B:566:GLU:HG2	2.20	0.42
1:A:316:LEU:CD2	1:A:328:ALA:HB2	2.47	0.42
1:B:272:LYS:O	1:B:275:PHE:HB3	2.19	0.42
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.19	0.42
1:A:607:PHE:HE1	1:A:608:LEU:HG	1.83	0.42
1:B:416:GLN:CA	1:B:497:ILE:CD1	2.97	0.42
1:A:588:VAL:HA	1:A:720:THR:HG21	2.02	0.42
1:A:743:HIS:HA	1:A:744:PRO:HD2	1.78	0.42
1:B:701:ARG:HD3	1:B:701:ARG:HH11	1.70	0.42
1:B:514:GLY:HA3	4:B:832:HOH:O	2.18	0.42
1:A:651:ILE:HG22	1:A:677:ASN:HA	2.02	0.42
1:A:410:GLY:HA3	1:A:411:PRO:HD3	1.74	0.41
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.43	0.41
1:B:630:ARG:CD	1:B:755:GLN:NE2	2.80	0.41
1:B:581:THR:HA	1:B:582:PRO:HD3	1.94	0.41
1:B:643:LYS:HA	1:B:643:LYS:HD2	1.65	0.41
1:B:388:SER:HA	1:B:438:LYS:HB3	2.02	0.41
1:A:351:GLU:HB2	4:A:973:HOH:O	2.21	0.41
1:A:338:ARG:HG3	1:A:601:TYR:CE1	2.56	0.41
1:A:622:GLN:HA	1:B:445:LEU:HD11	2.02	0.41
1:A:411:PRO:O	1:A:434:LYS:NZ	2.52	0.41
1:A:515:GLN:HE22	1:A:521:ALA:HB2	1.85	0.41
1:B:409:LEU:HD12	1:B:409:LEU:HA	1.88	0.41
1:B:383:TYR:HD2	1:B:599:CYS:HB2	1.86	0.41
1:B:211:ARG:HE	1:B:211:ARG:HB3	1.73	0.41
1:B:500:LYS:HE3	4:B:783:HOH:O	2.20	0.41
1:B:196:LEU:O	1:B:201:ILE:HD11	2.21	0.41
1:B:442:LEU:HD21	1:B:488:LEU:HB3	2.03	0.41
1:A:381:SER:HB2	1:A:599:CYS:HA	2.03	0.41
1:A:406:ARG:HE	1:A:495:MET:CE	2.34	0.41
1:A:600:GLY:HA2	4:A:779:HOH:O	2.20	0.41
1:B:421:VAL:HG12	1:B:424:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:GLU:O	1:B:529:LEU:HG	2.21	0.41
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.57	0.40
1:B:300:GLN:O	1:B:427:SER:HA	2.22	0.40
1:A:733:VAL:HB	1:A:748:LEU:HB2	2.04	0.40
1:B:344:CYS:O	1:B:392:HIS:HB2	2.20	0.40
1:B:390:GLU:HG2	1:B:392:HIS:CD2	2.57	0.40
1:B:216:ARG:HA	1:B:219:GLU:HG2	2.02	0.40
1:B:348:PRO:HB2	1:B:349:ASN:ND2	2.36	0.40
1:B:178:ASP:C	1:B:180:TYR:H	2.17	0.40
1:A:211:ARG:HG3	4:A:935:HOH:O	2.22	0.40
1:A:383:TYR:CB	1:A:384:PRO:HD2	2.45	0.40
1:A:502:VAL:CG1	1:A:515:GLN:NE2	2.85	0.40
1:B:523:PHE:N	1:B:523:PHE:CD1	2.90	0.40
1:B:310:SER:HB3	1:B:337:CYS:SG	2.62	0.40
1:A:522:SER:HA	1:A:549:ARG:O	2.21	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%)	471 (92%)	31 (6%)	7 (1%)	14	28
1	B	557/624 (89%)	511 (92%)	35 (6%)	11 (2%)	9	18
All	All	1066/1248 (85%)	982 (92%)	66 (6%)	18 (2%)	11	22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	GLN
1	B	175	GLN
1	B	176	VAL

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Mol	Chain	Res	Type
1	B	177	ASP
1	B	510	PRO
1	B	515	GLN
1	B	649	ASN
1	A	511	GLY
1	A	513	SER
1	A	536	GLY
1	B	173	ASN
1	B	178	ASP
1	B	198	ASP
1	B	536	GLY
1	A	514	GLY
1	A	648	LYS
1	A	510	PRO
1	B	514	GLY

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%)	404 (91%)	40 (9%)	12	23
1	B	492/545 (90%)	436 (89%)	56 (11%)	7	12
All	All	936/1090 (86%)	840 (90%)	96 (10%)	9	16

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	208	LEU
1	A	209	THR
1	A	216	ARG
1	A	238	GLN
1	A	242	ARG
1	A	252	LEU
1	A	277	MET
1	A	278	TYR

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Mol	Chain	Res	Type
1	A	293	ARG
1	A	309	SER
1	A	331	ARG
1	A	350	GLN
1	A	406	ARG
1	A	419	ASP
1	A	432	LYS
1	A	436	LEU
1	A	440	LYS
1	A	508	SER
1	A	512	THR
1	A	526	SER
1	A	530	ARG
1	A	533	GLN
1	A	539	PHE
1	A	563	SER
1	A	573	GLN
1	A	577	LEU
1	A	594	GLN
1	A	621	THR
1	A	630	ARG
1	A	632	ARG
1	A	652	VAL
1	A	655	LYS
1	A	657	ILE
1	A	665	ARG
1	A	675	ILE
1	A	683	ARG
1	A	685	ASP
1	A	712	LYS
1	A	738	LYS
1	A	756	ASP
1	B	158	ASN
1	B	162	PHE
1	B	164	GLU
1	B	166	LYS
1	B	167	ASP
1	B	173	ASN
1	B	182	ARG
1	B	186	ARG
1	B	206	LYS
1	B	210	GLN

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Mol	Chain	Res	Type
1	B	227	THR
1	B	228	LEU
1	B	231	GLU
1	B	242	ARG
1	B	291	HIS
1	B	293	ARG
1	B	309	SER
1	B	310	SER
1	B	331	ARG
1	B	406	ARG
1	B	409	LEU
1	B	416	GLN
1	B	423	THR
1	B	432	LYS
1	B	440	LYS
1	B	484	ASP
1	B	488	LEU
1	B	509	SER
1	B	515	GLN
1	B	526	SER
1	B	533	GLN
1	B	539	PHE
1	B	563	SER
1	B	573	GLN
1	B	594	GLN
1	B	607	PHE
1	B	613	THR
1	B	621	THR
1	B	630	ARG
1	B	643	LYS
1	B	647	ASN
1	B	648	LYS
1	B	650	SER
1	B	652	VAL
1	B	655	LYS
1	B	657	ILE
1	B	665	ARG
1	B	675	ILE
1	B	685	ASP
1	B	691	GLU
1	B	709	SER
1	B	710	SER

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Mol	Chain	Res	Type
1	B	711	SER
1	B	738	LYS
1	B	753	SER
1	B	756	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	349	ASN
1	A	392	HIS
1	A	515	GLN
1	A	573	GLN
1	A	594	GLN
1	A	661	HIS
1	A	718	GLN
1	A	734	HIS
1	B	241	GLN
1	B	291	HIS
1	B	349	ASN
1	B	573	GLN
1	B	594	GLN
1	B	661	HIS
1	B	718	GLN
1	B	728	GLN
1	B	755	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 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
2	ACT	A	5	-	1,3,3	2.31	1 (100%)	0,3,3	0.00	-
2	ACT	B	5	-	1,3,3	1.88	0	0,3,3	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	A	5	-	-	0/0/0/0	0/0/0/0
2	ACT	B	5	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	5	ACT	CH3-C	2.31	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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5	ACT	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.