



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:59 PM GMT

PDB ID : 1DJZ
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM
RAT COMPLEXED WITH INOSITOL-4,5-BISPHOSPHATE
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on : 1996-08-24
Resolution : 2.95 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) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

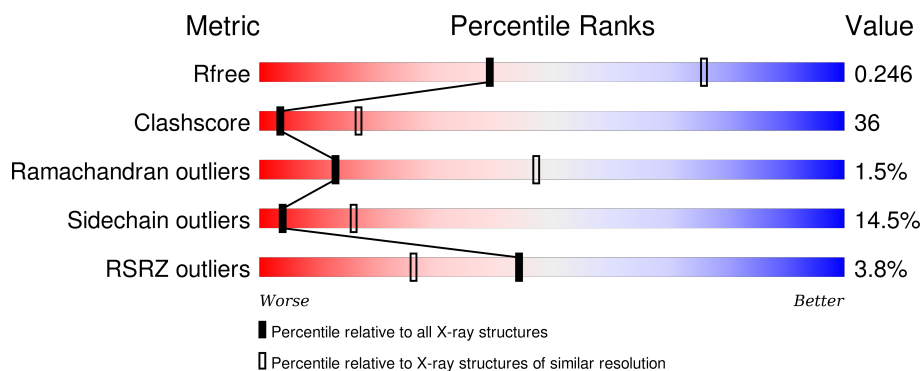
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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.

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
4	IP2	A	1	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8840 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.

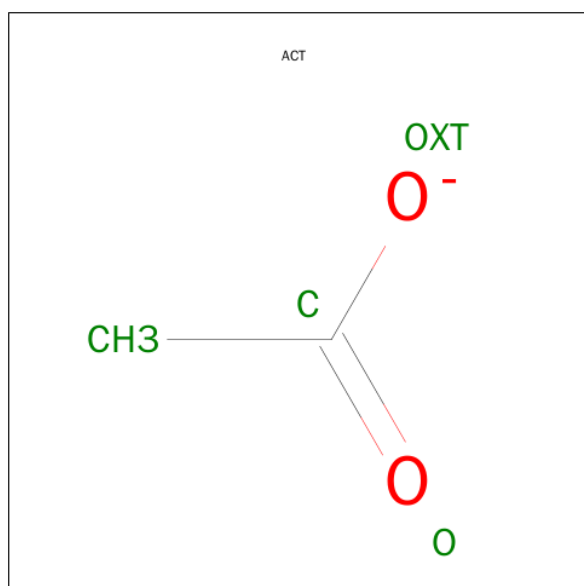
- Molecule 1 is a protein called PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	82	0	0
			4057	2565	709	761	22			
1	B	561	Total	C	N	O	S	109	0	0
			4465	2818	776	847	24			

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

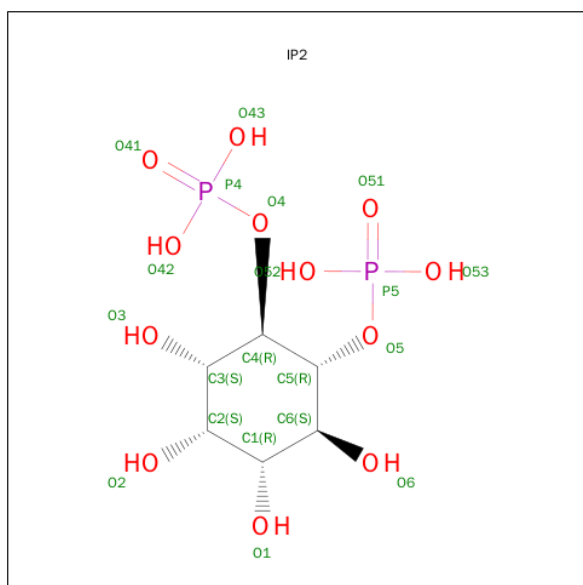
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 4 is D-MYO-INOSITOL-4,5-BISPHOSPHATE (three-letter code: IP2) (formula: $C_6H_{14}O_{12}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			20	6	12	2		
4	B	1	Total	C	O	P	0	0
			20	6	12	2		

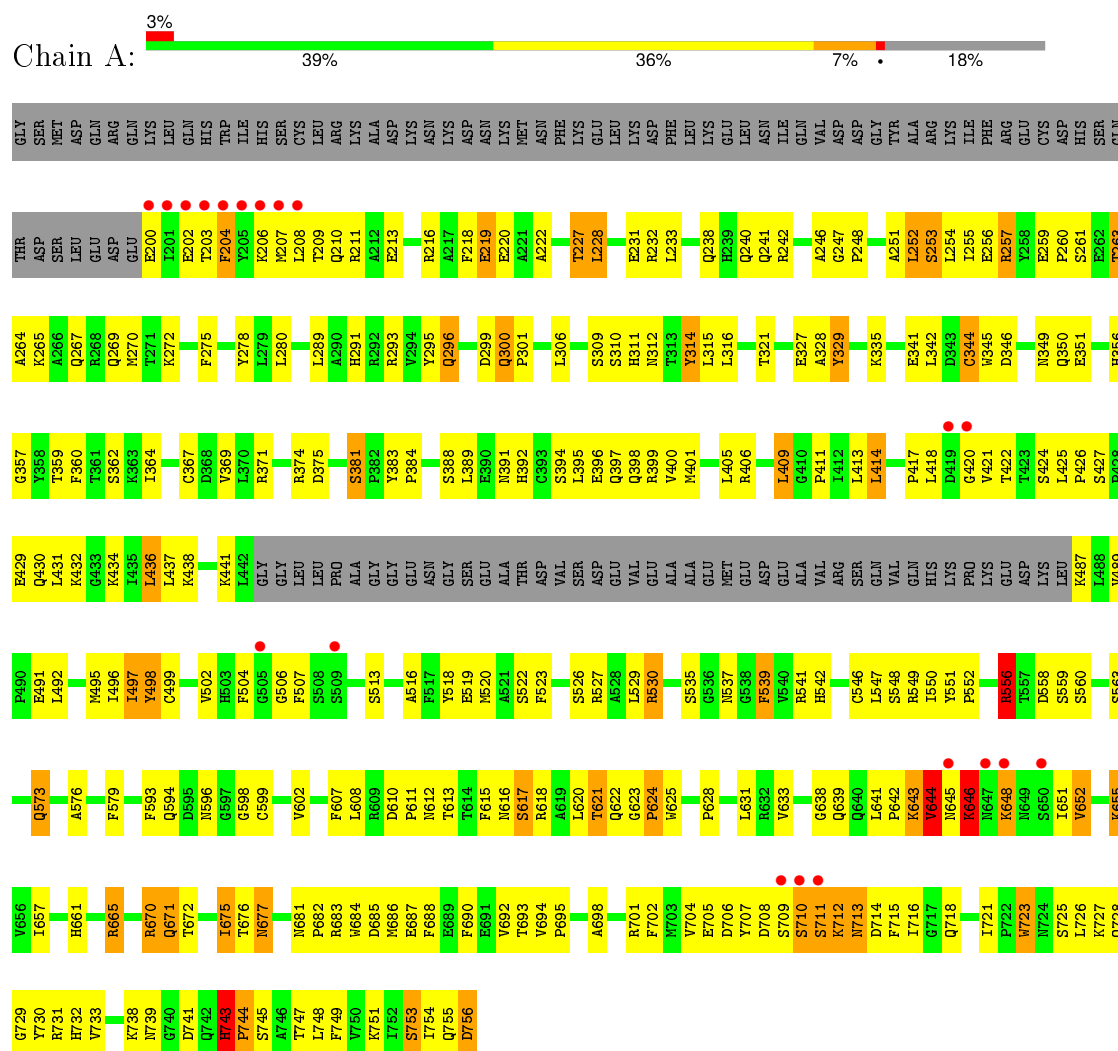
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		
5	B	141	Total	O	0	0
			141	141		

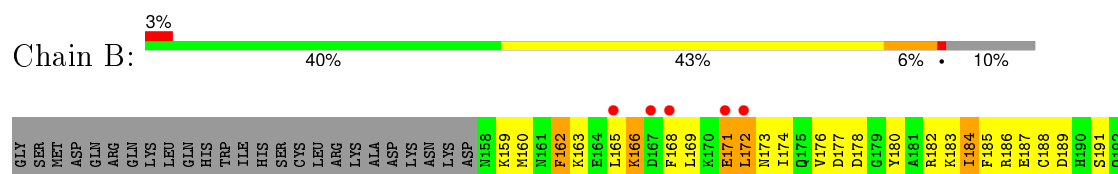
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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



Q728	P654	R556	E491	P426	P352	K265	T193
G729	R655	S560	L492	S427	I353	A266	D194
Y730	V656	N561	S493	L431	E356	R267	S195
R731	I657	D494	M495	I436	G357	Q268	L196
H732	V658	Y562	I496	K434	G357	Q269	E197
V733	E659	S563	I497	I435	V358	M270	D198
H734	T660	Q573	Y498	L436	T359	T271	E199
L735	H661	A576	C499	K438	S362	K272	E200
L736	R665	L577	K500	K439	K363	P275	E202
S737	Q671	N578	S501	K440	I364	L276	T203
K738	V674	D587	V502	K441	V369	M277	F204
N739	T675	L590	H503	I445	L370	L280	M207
G740	T676	F593	F504	LEU	R371	G284	Q210
D741	N677	Q594	G505	ALA	R374	F287	R211
H742	N678	D595	F507	ALA	D375	F287	A212
P744	N681	N596	S508	GLY	D376	E291	E213
T747	P682	G597	S509	GLY	A377	R292	I214
L748	V683	G598	T512	ASN	F378	R293	D215
F749	W684	C599	S513	GLY	K379	V294	F218
V750	W685	F607	G514	SER	Y383	Y295	F218
K751	W686	D610	Q515	GLU	P384	Q296	A221
I752	E687	N611	A516	ALA	S388	E297	A221
S753	V692	N612	F517	THR	L389	M298	T227
I754	T693	N613	Y518	ASP	L299	L228	L228
Q755	V694	T613	E519	VAL	E390	Q300	R232
D756	P695	G614	M520	SER	N391	P301	L233
	D696	T615	F523	ASP	H392	Y305	V234
	A698	F616	S524	GLU	C393	L306	T235
		N616	E525	VAL	S394	S309	L237
		R618	S526	GLU	L395	F236	F236
			S527	ALA	E396	S310	L237
			A528	ALA	Q397	Q238	H239
			L529	GLU	Q398	H311	H239
			R530	MET	R399	N312	Q240
			L531	GLU	V400	T313	Q241
			L532	ASP	M401	Y314	Q242
			Q533	GLU	L405	L315	E243
			W625	ALA	L406	L316	E244
			W626	VAL	R406	E245	E245
			R632	ARG	E327	A246	A246
			G638	SER	A328	G247	G247
			Q639	GLN	L409	Y329	A251
			P642	VAL	G410	I330	L252
			R645	GLN	P411	R331	L252
			K646	GLN	I412	A332	S253
			N647	HIS	I413	L354	L254
			K648	LYS	L414	T255	T255
			N649	PRO	P415	E256	E256
			S650	LYS	L418	L340	E256
			W651	GLU	P417	R341	Y258
			V652	D484	L418	L342	E259
			D653	L486	V421	W345	P260
				K487	T422	D346	S261
				L488	T423	Q350	T263
				W489	S424	E351	A264
				P490	L425		

4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	396.49 Å 396.49 Å 396.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.95 24.64 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.95) 94.2 (24.64-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.89 Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.212 , 0.270 0.192 , 0.246	Depositor DCC
R_{free} test set	2048 reflections (4.12%)	DCC
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 100.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 55725 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8840	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IP2, CA, ACT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.08	17/4152 (0.4%)	1.01	6/5624 (0.1%)
1	B	1.07	14/4565 (0.3%)	1.01	6/6174 (0.1%)
All	All	1.07	31/8717 (0.4%)	1.01	12/11798 (0.1%)

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	314	TYR	CE2-CZ	-11.14	1.24	1.38
1	A	329	TYR	CE2-CZ	-9.95	1.25	1.38
1	A	329	TYR	CG-CD1	-9.44	1.26	1.39
1	A	329	TYR	CE1-CZ	-8.93	1.26	1.38
1	B	498	TYR	CE1-CZ	-8.74	1.27	1.38
1	A	329	TYR	CG-CD2	-8.60	1.27	1.39
1	A	314	TYR	CE1-CZ	-8.53	1.27	1.38
1	B	314	TYR	CG-CD2	-8.45	1.28	1.39
1	A	314	TYR	CE2-CZ	-8.10	1.28	1.38
1	B	329	TYR	CE2-CZ	-8.09	1.28	1.38
1	B	314	TYR	CE1-CZ	-7.96	1.28	1.38
1	B	329	TYR	CG-CD1	-7.13	1.29	1.39
1	B	498	TYR	CG-CD2	-6.88	1.30	1.39
1	A	314	TYR	CG-CD2	-6.68	1.30	1.39
1	B	314	TYR	CG-CD1	-6.41	1.30	1.39
1	B	702	PHE	CE1-CZ	-6.32	1.25	1.37
1	B	498	TYR	CE2-CZ	-6.26	1.30	1.38
1	B	498	TYR	CG-CD1	-6.01	1.31	1.39
1	B	329	TYR	CE1-CZ	-5.97	1.30	1.38
1	A	702	PHE	CE2-CZ	-5.92	1.26	1.37
1	A	314	TYR	CG-CD1	-5.87	1.31	1.39
1	A	498	TYR	CE2-CZ	-5.82	1.30	1.38
1	A	702	PHE	CG-CD1	-5.81	1.30	1.38
1	A	498	TYR	CE1-CZ	-5.67	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	692	VAL	CA-CB	-5.58	1.43	1.54
1	B	329	TYR	CG-CD2	-5.54	1.31	1.39
1	A	702	PHE	CE1-CZ	-5.33	1.27	1.37
1	A	602	VAL	CB-CG1	-5.28	1.41	1.52
1	A	723	TRP	CB-CG	-5.22	1.40	1.50
1	A	498	TYR	CG-CD1	-5.08	1.32	1.39
1	A	702	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	743	HIS	C-N-CD	-14.12	89.52	120.60
1	A	743	HIS	C-N-CD	-14.12	89.54	120.60
1	B	247	GLY	C-N-CD	-7.20	104.77	120.60
1	A	247	GLY	C-N-CD	-6.97	105.26	120.60
1	A	644	VAL	CB-CA-C	5.94	122.68	111.40
1	A	556	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	645	ASN	N-CA-C	5.74	126.49	111.00
1	B	436	LEU	CB-CG-CD2	-5.53	101.61	111.00
1	A	670	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	B	654	PRO	N-CA-C	5.12	125.41	112.10
1	A	675	ILE	N-CA-C	-5.05	97.35	111.00
1	B	675	ILE	N-CA-C	-5.03	97.42	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4057	0	3972	290	0
1	B	4465	0	4375	313	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	4	0	3	0	0
3	B	4	0	3	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	9	3	0
4	B	20	0	9	4	0
5	A	125	0	0	4	0
5	B	141	0	0	19	0
All	All	8840	0	8371	595	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 36.

All (595) 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:196:LEU:HD22	1:B:200:GLU:HB3	1.28	1.14
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.23	1.01
1:B:728:GLN:NE2	1:B:754:ILE:H	1.59	1.00
1:A:548:SER:H	1:A:573:GLN:NE2	1.61	0.96
1:A:613:THR:HG22	1:A:615:PHE:H	1.28	0.95
1:B:401:MET:HE2	1:B:492:LEU:HD11	1.45	0.95
1:A:241:GLN:HE22	1:A:730:TYR:H	1.06	0.94
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.02	0.93
1:A:401:MET:HE2	1:A:492:LEU:HD11	1.48	0.92
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.55	0.89
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.55	0.89
1:B:548:SER:H	1:B:573:GLN:NE2	1.69	0.89
1:B:642:PRO:HG3	1:B:743:HIS:CD2	2.08	0.88
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.37	0.88
1:B:728:GLN:HE22	1:B:754:ILE:H	1.21	0.88
1:A:728:GLN:HE22	1:A:754:ILE:H	1.16	0.88
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.56	0.87
1:A:516:ALA:HB3	1:A:519:GLU:HG3	1.57	0.87
1:B:196:LEU:CD2	1:B:200:GLU:HB3	2.05	0.86
1:A:556:ARG:HH11	1:A:556:ARG:HG2	1.38	0.86
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.55	0.86
1:B:168:PHE:CE1	1:B:172:LEU:HD21	2.09	0.86
1:A:728:GLN:NE2	1:A:754:ILE:H	1.72	0.86
1:A:316:LEU:HD23	1:A:328:ALA:HB2	1.59	0.85
1:B:607:PHE:HE2	5:B:821:HOH:O	1.59	0.84
1:B:692:VAL:HG12	1:B:695:PRO:HD3	1.61	0.82
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.24	0.82
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.15	0.81
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.28	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:PRO:HG3	1:B:743:HIS:HD2	1.44	0.80
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.63	0.80
1:A:651:ILE:HD13	1:A:677:ASN:HD21	1.46	0.80
1:A:692:VAL:HG12	1:A:695:PRO:HD3	1.61	0.80
1:B:632:ARG:HH21	1:B:755:GLN:NE2	1.80	0.80
1:B:701:ARG:HE	1:B:718:GLN:NE2	1.79	0.79
1:B:530:ARG:HH11	1:B:530:ARG:HG3	1.45	0.79
1:A:573:GLN:H	1:A:573:GLN:NE2	1.82	0.78
1:A:420:GLY:O	1:A:422:THR:HG23	1.84	0.77
1:B:549:ARG:C	1:B:550:ILE:HD13	2.05	0.77
1:B:728:GLN:HE21	1:B:753:SER:HA	1.49	0.77
1:A:238:GLN:HG2	1:A:246:ALA:CB	2.16	0.76
1:B:196:LEU:HB3	1:B:201:ILE:CD1	2.15	0.76
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.68	0.76
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.21	0.75
1:B:234:VAL:O	1:B:238:GLN:HG3	1.86	0.75
1:B:221:ALA:HB1	1:B:228:LEU:HD21	1.68	0.74
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.99	0.74
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.15	0.74
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.03	0.74
1:B:174:ILE:HG22	1:B:176:VAL:HG23	1.68	0.74
1:B:436:LEU:N	1:B:436:LEU:HD23	2.01	0.73
1:B:241:GLN:HE22	1:B:730:TYR:H	1.35	0.73
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.18	0.73
1:B:573:GLN:H	1:B:573:GLN:NE2	1.87	0.73
1:A:438:LYS:HG3	1:A:499:CYS:HB3	1.70	0.73
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.69	0.72
1:B:316:LEU:HD23	1:B:328:ALA:HB2	1.71	0.72
1:B:203:THR:O	1:B:207:MET:HG3	1.89	0.72
1:A:394:SER:O	1:A:398:GLN:HG3	1.88	0.72
1:A:436:LEU:N	1:A:436:LEU:HD23	2.05	0.72
1:B:168:PHE:HE1	1:B:172:LEU:HD21	1.54	0.72
1:A:395:LEU:HD22	1:A:489:VAL:HG12	1.72	0.72
1:A:346:ASP:OD2	1:A:394:SER:HB3	1.90	0.71
1:B:259:GLU:OE2	1:B:260:PRO:HD2	1.90	0.71
1:A:520:MET:CE	1:A:549:ARG:HB2	2.21	0.71
1:A:350:GLN:OE1	1:A:396:GLU:HG3	1.90	0.71
1:B:551:TYR:HB2	1:B:552:PRO:HD2	1.73	0.71
1:A:311:HIS:NE2	4:A:1:IP2:H2	2.04	0.70
1:A:312:ASN:HB3	1:A:315:LEU:HD12	1.73	0.70
1:B:188:CYS:O	1:B:200:GLU:HG2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:728:GLN:NE2	1:B:754:ILE:N	2.38	0.70
1:A:203:THR:O	1:A:207:MET:HB2	1.92	0.70
1:B:730:TYR:CE1	1:B:751:LYS:HD3	2.27	0.70
1:A:417:PRO:HD3	1:A:497:ILE:HG13	1.73	0.70
1:B:504:PHE:HB3	1:B:527:ARG:NH2	2.07	0.70
1:B:701:ARG:NH2	1:B:718:GLN:HG3	2.05	0.70
1:B:184:ILE:HG22	1:B:204:PHE:CD1	2.27	0.69
1:A:651:ILE:HD13	1:A:677:ASN:ND2	2.07	0.69
1:B:520:MET:CE	1:B:549:ARG:HB2	2.22	0.69
1:B:425:LEU:HD12	5:B:767:HOH:O	1.91	0.69
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.28	0.69
1:B:174:ILE:CG2	1:B:176:VAL:HG23	2.22	0.69
1:A:675:ILE:HD13	1:A:684:TRP:NE1	2.07	0.69
1:A:548:SER:H	1:A:573:GLN:HE22	1.40	0.69
1:A:551:TYR:HB2	1:A:552:PRO:HD2	1.75	0.69
1:A:241:GLN:HE22	1:A:730:TYR:N	1.87	0.68
1:A:651:ILE:HD12	1:A:651:ILE:N	2.08	0.68
1:B:548:SER:H	1:B:573:GLN:HE22	1.40	0.68
1:B:701:ARG:NE	1:B:718:GLN:HE21	1.90	0.68
1:A:730:TYR:CE1	1:A:751:LYS:HD3	2.28	0.68
1:A:495:MET:O	1:A:497:ILE:HD13	1.93	0.68
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.23	0.68
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.76	0.68
1:B:346:ASP:OD2	1:B:394:SER:HB3	1.94	0.68
1:B:364:ILE:HD12	1:B:369:VAL:HG23	1.73	0.67
1:B:550:ILE:HD13	1:B:550:ILE:N	2.10	0.67
1:A:401:MET:CE	1:A:492:LEU:HD11	2.24	0.67
1:A:395:LEU:HD22	1:A:489:VAL:CG1	2.25	0.67
1:A:670:ARG:HD3	5:A:836:HOH:O	1.93	0.67
1:B:651:ILE:CG2	1:B:677:ASN:HA	2.25	0.66
1:A:356:HIS:ND1	1:A:359:THR:HG21	2.10	0.66
1:B:201:ILE:HD13	1:B:201:ILE:N	2.11	0.66
1:B:377:ALA:N	5:B:887:HOH:O	2.28	0.66
1:A:200:GLU:O	1:A:204:PHE:N	2.29	0.66
1:A:707:TYR:HA	1:A:713:ASN:OD1	1.96	0.66
1:B:342:LEU:HD12	1:B:342:LEU:N	2.12	0.65
1:A:426:PRO:HD3	1:A:498:TYR:CD2	2.31	0.65
1:A:549:ARG:NH1	4:A:1:IP2:O42	2.29	0.65
1:A:204:PHE:O	1:A:208:LEU:N	2.30	0.65
1:A:556:ARG:HG2	1:A:560:SER:OG	1.96	0.65
1:B:651:ILE:HG22	1:B:677:ASN:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:ARG:NH2	4:A:1:IP2:O3	2.29	0.65
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.26	0.65
1:A:272:LYS:O	1:A:275:PHE:HB3	1.96	0.65
1:B:728:GLN:NE2	1:B:753:SER:HA	2.11	0.65
1:A:617:SER:HA	1:A:620:LEU:HD21	1.79	0.64
1:A:238:GLN:HG2	1:A:246:ALA:HB1	1.78	0.64
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.80	0.64
1:A:497:ILE:HG22	1:A:498:TYR:CD1	2.32	0.64
1:B:549:ARG:HH22	4:B:1:IP2:C3	2.11	0.64
1:B:657:ILE:HD13	1:B:671:GLN:CB	2.28	0.64
1:B:189:ASP:HB3	5:B:845:HOH:O	1.96	0.64
1:B:491:GLU:OE1	1:B:491:GLU:N	2.29	0.63
1:B:516:ALA:HB3	1:B:519:GLU:HG3	1.79	0.63
1:B:696:ASP:HB2	5:B:821:HOH:O	1.97	0.63
1:A:335:LYS:HE2	5:A:841:HOH:O	1.98	0.63
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.33	0.63
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.34	0.63
1:B:645:ASN:ND2	1:B:647:ASN:O	2.31	0.63
1:B:516:ALA:HB1	1:B:518:TYR:CE2	2.34	0.63
1:A:316:LEU:CD2	1:A:328:ALA:HB2	2.29	0.62
1:B:721:ILE:HG21	1:B:726:LEU:HD13	1.80	0.62
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.28	0.62
1:B:379:LYS:HE2	5:B:833:HOH:O	1.99	0.62
1:A:216:ARG:NH2	1:A:683:ARG:HH22	1.96	0.62
1:A:384:PRO:HG3	1:A:431:LEU:CB	2.30	0.62
1:B:701:ARG:HH21	1:B:718:GLN:HG3	1.64	0.62
1:A:218:PHE:CE1	1:A:272:LYS:HA	2.35	0.62
1:B:353:ILE:HD12	1:B:363:LYS:HG2	1.81	0.62
1:A:701:ARG:NH2	1:A:718:GLN:HG3	2.15	0.62
1:A:222:ALA:HB2	1:A:228:LEU:HD23	1.82	0.62
1:B:509:SER:N	1:B:510:PRO:HD2	2.15	0.61
1:B:259:GLU:CD	1:B:260:PRO:HD2	2.20	0.61
1:A:701:ARG:HH21	1:A:718:GLN:HG3	1.65	0.61
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.30	0.61
1:A:207:MET:CE	1:A:210:GLN:HB3	2.30	0.61
1:B:267:GLN:O	1:B:269:GLN:HG3	2.01	0.61
1:A:728:GLN:NE2	1:A:754:ILE:N	2.47	0.61
1:B:196:LEU:HB3	1:B:201:ILE:HD11	1.80	0.61
1:B:515:GLN:HE21	1:B:542:HIS:HE1	1.49	0.60
1:A:672:THR:HG22	1:A:688:PHE:CZ	2.37	0.60
1:A:675:ILE:HD13	1:A:684:TRP:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.32	0.60
1:A:520:MET:HE3	1:A:549:ARG:CB	2.31	0.60
1:A:672:THR:HG22	1:A:688:PHE:HZ	1.66	0.60
1:B:376:TYR:N	5:B:887:HOH:O	2.34	0.60
1:A:711:SER:OG	1:A:712:LYS:N	2.33	0.60
1:B:657:ILE:HD13	1:B:671:GLN:HB3	1.84	0.59
1:B:327:GLU:OE2	1:B:331:ARG:HB2	2.02	0.59
1:A:364:ILE:HD12	1:A:369:VAL:HG23	1.82	0.59
1:A:616:ASN:OD1	1:A:618:ARG:HB2	2.02	0.59
1:A:259:GLU:OE1	1:A:270:MET:HA	2.02	0.59
1:B:401:MET:CE	1:B:492:LEU:HD11	2.28	0.59
1:A:730:TYR:CZ	1:A:751:LYS:HD3	2.38	0.59
1:A:395:LEU:O	1:A:399:ARG:HG3	2.03	0.59
1:B:515:GLN:NE2	1:B:542:HIS:HE1	2.01	0.59
1:A:573:GLN:H	1:A:573:GLN:HE21	1.51	0.59
1:B:183:LYS:HG2	1:B:184:ILE:HD13	1.84	0.59
1:A:739:ASN:HB2	1:A:741:ASP:OD2	2.02	0.59
1:B:184:ILE:N	1:B:184:ILE:HD13	2.16	0.58
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.33	0.58
1:A:504:PHE:HD2	1:A:527:ARG:NH2	2.01	0.58
1:B:421:VAL:HG11	1:B:426:PRO:HD3	1.84	0.58
1:A:263:THR:HG22	1:A:264:ALA:N	2.18	0.58
1:A:728:GLN:HE21	1:A:753:SER:HA	1.68	0.58
1:A:651:ILE:HG22	1:A:652:VAL:N	2.17	0.58
1:A:655:LYS:NZ	1:A:671:GLN:OE1	2.29	0.58
1:A:686:MET:HG3	1:A:687:GLU:N	2.17	0.58
1:A:623:GLY:HA3	1:A:625:TRP:CZ2	2.38	0.58
1:B:520:MET:HG3	1:B:547:LEU:O	2.04	0.58
1:A:502:VAL:HG21	1:A:519:GLU:HB3	1.86	0.58
1:B:341:GLU:C	1:B:342:LEU:HD12	2.24	0.58
1:A:723:TRP:N	5:A:823:HOH:O	2.37	0.58
1:B:300:GLN:O	1:B:427:SER:HA	2.05	0.57
1:B:705:GLU:C	1:B:716:ILE:HD12	2.25	0.57
1:A:216:ARG:HH21	1:A:683:ARG:NH2	1.99	0.57
1:A:617:SER:HB3	5:A:866:HOH:O	2.04	0.57
1:A:251:ALA:O	1:A:255:ILE:HG13	2.04	0.57
1:B:272:LYS:O	1:B:275:PHE:HB3	2.04	0.57
1:B:686:MET:HG3	1:B:687:GLU:N	2.19	0.57
1:A:216:ARG:HG3	1:A:216:ARG:HH11	1.68	0.57
1:B:729:GLY:O	1:B:751:LYS:HA	2.05	0.57
1:A:259:GLU:CD	1:A:260:PRO:HD2	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:551:TYR:HB2	1:B:552:PRO:CD	2.34	0.57
1:A:657:ILE:HD13	1:A:671:GLN:HB2	1.87	0.57
1:A:516:ALA:HB1	1:A:518:TYR:CE2	2.41	0.56
1:B:632:ARG:NH2	1:B:755:GLN:NE2	2.53	0.56
1:A:657:ILE:HD13	1:A:671:GLN:CB	2.34	0.56
1:B:549:ARG:O	1:B:550:ILE:HD13	2.04	0.56
1:B:172:LEU:O	1:B:174:ILE:N	2.38	0.56
1:B:197:GLU:O	1:B:201:ILE:HG12	2.05	0.56
1:A:341:GLU:C	1:A:342:LEU:HD12	2.25	0.56
1:B:549:ARG:HG2	1:B:549:ARG:NH1	2.20	0.56
1:B:218:PHE:CE1	1:B:272:LYS:HA	2.41	0.56
1:A:622:GLN:CB	1:B:445:LEU:HD13	2.33	0.56
1:A:593:PHE:O	1:A:598:GLY:HA2	2.06	0.56
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.06	0.56
1:A:289:LEU:O	1:A:289:LEU:HD12	2.05	0.56
1:A:398:GLN:O	1:A:401:MET:HB2	2.06	0.56
1:A:241:GLN:HB3	1:A:731:ARG:NH2	2.20	0.55
1:B:227:THR:HG21	1:B:269:GLN:CD	2.27	0.55
1:A:299:ASP:O	1:A:427:SER:HB3	2.06	0.55
1:B:730:TYR:CD1	1:B:751:LYS:HD3	2.41	0.55
1:A:253:SER:HB2	1:A:257:ARG:HH21	1.71	0.55
1:B:704:VAL:O	1:B:716:ILE:HB	2.06	0.55
1:A:491:GLU:N	1:A:491:GLU:OE1	2.36	0.55
1:A:549:ARG:NH1	1:A:549:ARG:HG2	2.20	0.55
1:A:621:THR:C	1:B:445:LEU:HD22	2.27	0.55
1:B:241:GLN:N	1:B:241:GLN:HE21	2.05	0.55
1:A:259:GLU:OE2	1:A:260:PRO:HD2	2.06	0.55
1:A:227:THR:HG21	1:A:269:GLN:CD	2.26	0.55
1:B:253:SER:HB2	1:B:257:ARG:HH21	1.72	0.55
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.35	0.54
1:B:384:PRO:HG3	1:B:431:LEU:HB2	1.89	0.54
1:B:327:GLU:OE2	1:B:331:ARG:HD2	2.07	0.54
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.37	0.54
1:B:393:CYS:N	5:B:871:HOH:O	2.41	0.54
1:A:756:ASP:OD1	1:A:756:ASP:N	2.40	0.54
1:B:409:LEU:HD13	1:B:409:LEU:N	2.23	0.54
1:B:184:ILE:HG22	1:B:204:PHE:CE1	2.43	0.54
1:B:418:LEU:HB2	1:B:421:VAL:HG21	1.90	0.54
1:B:213:GLU:HG2	1:B:214:ILE:N	2.22	0.54
1:B:296:GLN:HG3	1:B:596:ASN:ND2	2.23	0.54
1:B:645:ASN:C	1:B:647:ASN:H	2.10	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLN:HG3	1:A:596:ASN:CG	2.29	0.53
1:A:523:PHE:O	1:A:550:ILE:HA	2.07	0.53
1:B:418:LEU:HB2	1:B:421:VAL:CG2	2.37	0.53
1:A:715:PHE:CE2	1:A:718:GLN:HB2	2.43	0.53
1:B:556:ARG:HG2	1:B:556:ARG:HH11	1.71	0.53
1:A:280:LEU:HD23	1:A:732:HIS:CE1	2.43	0.53
1:A:291:HIS:HD2	1:A:725:SER:OG	1.91	0.53
1:B:657:ILE:HD13	1:B:671:GLN:HB2	1.91	0.53
1:A:607:PHE:CE2	1:A:625:TRP:HB3	2.43	0.53
1:B:556:ARG:HG2	1:B:560:SER:OG	2.08	0.53
1:A:383:TYR:HB3	1:A:384:PRO:CD	2.38	0.53
1:A:253:SER:HA	1:A:256:GLU:OE1	2.09	0.53
1:B:356:HIS:ND1	1:B:359:THR:HG21	2.24	0.53
1:B:311:HIS:CE1	1:B:312:ASN:HD22	2.26	0.53
1:A:643:LYS:O	1:A:645:ASN:N	2.41	0.53
1:B:507:PHE:O	1:B:510:PRO:HG2	2.09	0.52
1:B:607:PHE:CD2	1:B:625:TRP:HB3	2.45	0.52
1:A:651:ILE:HG21	1:A:677:ASN:C	2.30	0.52
1:B:525:GLU:O	1:B:529:LEU:HG	2.08	0.52
1:A:721:ILE:HG21	1:A:726:LEU:HD13	1.90	0.52
1:A:556:ARG:HG2	1:A:556:ARG:NH1	2.14	0.52
1:A:252:LEU:O	1:A:256:GLU:HG3	2.10	0.52
1:B:395:LEU:O	1:B:399:ARG:HG3	2.08	0.52
1:A:549:ARG:C	1:A:550:ILE:HD13	2.29	0.52
1:A:622:GLN:HA	1:B:445:LEU:HD11	1.91	0.52
1:A:607:PHE:CD2	1:A:625:TRP:HB3	2.44	0.52
1:B:683:ARG:NH2	1:B:685:ASP:OD2	2.43	0.52
1:B:523:PHE:O	1:B:550:ILE:HA	2.10	0.52
1:B:436:LEU:H	1:B:436:LEU:HD23	1.75	0.52
1:A:729:GLY:O	1:A:751:LYS:HA	2.10	0.52
1:B:438:LYS:HG3	1:B:499:CYS:HB3	1.92	0.52
1:A:367:CYS:HB2	1:A:371:ARG:NH2	2.25	0.52
1:A:441:LYS:HG3	1:A:496:ILE:HB	1.92	0.52
1:A:359:THR:C	1:A:360:PHE:HD1	2.14	0.51
1:B:346:ASP:OD1	1:B:393:CYS:HA	2.10	0.51
1:A:730:TYR:C	1:A:731:ARG:HG2	2.30	0.51
1:A:296:GLN:HG3	1:A:596:ASN:ND2	2.25	0.51
1:B:607:PHE:CE2	5:B:821:HOH:O	2.47	0.51
1:B:440:LYS:HA	5:B:770:HOH:O	2.09	0.51
1:A:360:PHE:CD1	1:A:360:PHE:N	2.79	0.51
1:A:300:GLN:O	1:A:427:SER:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:PHE:O	1:B:598:GLY:HA2	2.10	0.51
1:B:707:TYR:O	1:B:708:ASP:OD1	2.29	0.51
1:A:227:THR:HG21	1:A:269:GLN:OE1	2.11	0.51
1:B:639:GLN:HB2	1:B:747:THR:OG1	2.10	0.51
1:A:708:ASP:N	1:A:713:ASN:OD1	2.37	0.51
1:A:342:LEU:HD12	1:A:342:LEU:N	2.25	0.51
1:B:234:VAL:HG23	1:B:251:ALA:HB2	1.93	0.51
1:B:632:ARG:NE	5:B:815:HOH:O	2.24	0.51
1:A:504:PHE:CE1	1:A:507:PHE:CE1	2.99	0.51
1:B:180:TYR:CE1	1:B:184:ILE:HG12	2.45	0.51
1:B:169:LEU:O	1:B:172:LEU:O	2.29	0.50
1:B:350:GLN:HA	1:B:397:GLN:HE21	1.73	0.50
1:B:183:LYS:O	1:B:187:GLU:HG3	2.11	0.50
1:A:397:GLN:O	1:A:400:VAL:HB	2.11	0.50
1:A:706:ASP:HB3	1:A:714:ASP:HB2	1.93	0.50
1:B:549:ARG:NH2	4:B:1:IP2:O3	2.44	0.50
1:B:549:ARG:HG2	1:B:549:ARG:HH11	1.76	0.50
1:A:692:VAL:HG12	1:A:695:PRO:CD	2.35	0.50
1:B:240:GLN:HA	1:B:240:GLN:OE1	2.12	0.50
1:A:504:PHE:CZ	1:A:507:PHE:CE1	2.99	0.50
1:A:549:ARG:HG2	1:A:549:ARG:HH11	1.74	0.50
1:B:426:PRO:HB2	1:B:431:LEU:HD12	1.93	0.50
1:B:651:ILE:O	1:B:653:ASP:OD1	2.29	0.50
1:B:311:HIS:NE2	1:B:312:ASN:ND2	2.60	0.50
1:B:287:PHE:CE2	1:B:722:PRO:HD2	2.47	0.50
1:A:610:ASP:OD1	1:A:611:PRO:HD2	2.11	0.50
1:B:622:GLN:HG3	1:B:623:GLY:N	2.27	0.50
1:B:530:ARG:CG	1:B:530:ARG:HH11	2.19	0.50
1:B:259:GLU:OE1	1:B:270:MET:HA	2.12	0.50
1:B:398:GLN:O	1:B:401:MET:HB2	2.12	0.50
1:A:504:PHE:CD2	1:A:527:ARG:NH2	2.79	0.50
1:A:693:THR:C	1:A:695:PRO:HD2	2.31	0.50
1:A:222:ALA:HB2	1:A:228:LEU:CD2	2.41	0.50
1:B:391:ASN:HD21	1:B:398:GLN:CD	2.15	0.49
1:B:655:LYS:NZ	1:B:671:GLN:OE1	2.30	0.49
1:A:520:MET:HG3	1:A:547:LEU:O	2.12	0.49
1:A:551:TYR:HB2	1:A:552:PRO:CD	2.40	0.49
1:B:189:ASP:OD1	1:B:191:SER:OG	2.30	0.49
1:A:228:LEU:CD1	1:A:233:LEU:HA	2.42	0.49
1:A:405:LEU:HD23	1:A:409:LEU:CD2	2.42	0.49
1:A:497:ILE:CG2	1:A:498:TYR:CE1	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:HD13	1:A:409:LEU:N	2.27	0.49
1:B:263:THR:O	1:B:266:ALA:HB3	2.12	0.49
1:B:736:LEU:HD23	1:B:742:GLN:HA	1.92	0.49
1:A:537:ASN:ND2	1:A:613:THR:O	2.40	0.49
1:B:573:GLN:H	1:B:573:GLN:HE21	1.61	0.49
1:B:702:PHE:CD2	1:B:733:VAL:HG21	2.48	0.49
1:B:227:THR:HG21	1:B:269:GLN:OE1	2.12	0.49
1:B:411:PRO:O	1:B:434:LYS:NZ	2.45	0.49
1:A:426:PRO:HA	1:A:430:GLN:OE1	2.13	0.49
1:A:291:HIS:HA	1:A:295:TYR:CE2	2.48	0.49
1:A:241:GLN:NE2	1:A:729:GLY:HA3	2.28	0.48
1:A:218:PHE:CD1	1:A:272:LYS:HA	2.48	0.48
1:A:728:GLN:NE2	1:A:753:SER:HA	2.26	0.48
1:B:500:LYS:HE3	5:B:770:HOH:O	2.12	0.48
1:B:434:LYS:HA	1:B:434:LYS:HD2	1.66	0.48
1:B:261:SER:O	1:B:265:LYS:HB2	2.13	0.48
1:B:251:ALA:O	1:B:255:ILE:HG13	2.12	0.48
1:B:259:GLU:OE2	1:B:271:THR:HG23	2.13	0.48
1:A:371:ARG:O	1:A:374:ARG:HB3	2.13	0.48
1:A:622:GLN:HA	1:B:445:LEU:CD1	2.43	0.48
1:A:438:LYS:HA	1:A:499:CYS:HB2	1.94	0.48
1:A:356:HIS:HB3	1:A:359:THR:OG1	2.14	0.48
1:A:704:VAL:O	1:A:716:ILE:HB	2.13	0.48
1:B:509:SER:N	1:B:510:PRO:CD	2.76	0.48
1:A:755:GLN:HG2	1:A:756:ASP:N	2.22	0.48
1:B:395:LEU:HD22	1:B:489:VAL:CG1	2.43	0.48
1:A:507:PHE:CD1	1:A:542:HIS:ND1	2.81	0.48
1:B:221:ALA:CB	1:B:228:LEU:HD21	2.40	0.48
1:A:345:TRP:CZ2	1:A:357:GLY:HA3	2.48	0.48
1:B:533:GLN:OE1	1:B:618:ARG:NH1	2.47	0.48
1:B:504:PHE:HD2	1:B:527:ARG:NH2	2.11	0.48
1:B:701:ARG:CZ	1:B:718:GLN:HG3	2.44	0.48
1:B:418:LEU:HD12	1:B:426:PRO:HB3	1.95	0.48
1:A:360:PHE:HD1	1:A:360:PHE:N	2.12	0.48
1:A:639:GLN:HB2	1:A:747:THR:OG1	2.13	0.48
1:B:395:LEU:HD22	1:B:489:VAL:HG12	1.96	0.48
1:B:284:GLY:O	1:B:731:ARG:HB3	2.14	0.48
1:B:241:GLN:NE2	1:B:241:GLN:CA	2.76	0.48
1:B:549:ARG:NH1	4:B:1:IP2:O43	2.46	0.48
1:A:252:LEU:HD23	1:A:256:GLU:OE2	2.14	0.48
1:B:426:PRO:HG2	1:B:431:LEU:CD1	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:PHE:O	1:B:171:GLU:HB2	2.14	0.47
1:B:607:PHE:CE2	1:B:625:TRP:HB3	2.49	0.47
1:B:721:ILE:CG2	1:B:726:LEU:HD13	2.44	0.47
1:A:280:LEU:HD23	1:A:732:HIS:ND1	2.29	0.47
1:A:522:SER:HA	1:A:549:ARG:O	2.13	0.47
1:B:169:LEU:HA	1:B:172:LEU:HD12	1.95	0.47
1:A:202:GLU:O	1:A:206:LYS:N	2.29	0.47
1:A:622:GLN:CA	1:B:445:LEU:HD13	2.44	0.47
1:B:371:ARG:O	1:B:374:ARG:HB3	2.13	0.47
1:B:291:HIS:HD2	1:B:725:SER:OG	1.96	0.47
1:B:394:SER:O	1:B:398:GLN:HG3	2.14	0.47
1:B:162:PHE:O	1:B:165:LEU:HB3	2.14	0.47
1:A:743:HIS:HA	1:A:744:PRO:HD3	1.53	0.47
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.73	0.47
1:B:162:PHE:CZ	1:B:182:ARG:HA	2.50	0.47
1:A:705:GLU:C	1:A:716:ILE:HD12	2.35	0.47
1:B:162:PHE:CZ	1:B:182:ARG:HB2	2.49	0.47
1:B:651:ILE:O	1:B:651:ILE:HG22	2.13	0.47
1:A:712:LYS:HB3	1:A:713:ASN:H	1.28	0.47
1:B:610:ASP:OD1	1:B:611:PRO:HD2	2.13	0.47
1:A:351:GLU:HA	1:A:351:GLU:OE1	2.15	0.47
1:B:587:ASP:HB3	1:B:718:GLN:NE2	2.30	0.47
1:A:367:CYS:SG	1:A:371:ARG:NH2	2.88	0.47
1:A:623:GLY:HA3	1:A:625:TRP:CE2	2.50	0.47
1:A:530:ARG:CZ	1:A:530:ARG:HB2	2.30	0.47
1:A:391:ASN:HD21	1:A:398:GLN:CD	2.18	0.47
1:A:670:ARG:HG3	1:A:690:PHE:CZ	2.50	0.47
1:B:610:ASP:O	1:B:612:ASN:N	2.48	0.47
1:A:651:ILE:CD1	1:A:651:ILE:N	2.78	0.46
1:A:438:LYS:CG	1:A:499:CYS:HB3	2.43	0.46
1:A:200:GLU:O	1:A:203:THR:N	2.48	0.46
1:B:733:VAL:HB	1:B:748:LEU:HB2	1.97	0.46
1:A:227:THR:CG2	1:A:228:LEU:N	2.79	0.46
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.14	0.46
1:B:623:GLY:HA3	1:B:625:TRP:CZ2	2.50	0.46
1:A:497:ILE:CD1	1:A:497:ILE:N	2.78	0.46
1:B:294:VAL:HA	1:B:596:ASN:OD1	2.15	0.46
1:B:311:HIS:CE1	1:B:312:ASN:ND2	2.82	0.46
1:B:254:LEU:O	1:B:258:TYR:N	2.44	0.46
1:B:549:ARG:HH22	4:B:1:IP2:H3	1.81	0.46
1:B:509:SER:HB3	1:B:510:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:LEU:HD12	1:A:726:LEU:HA	1.46	0.46
1:B:280:LEU:HD23	1:B:732:HIS:ND1	2.31	0.46
1:B:384:PRO:HG3	1:B:431:LEU:CB	2.46	0.46
1:B:227:THR:CG2	1:B:269:GLN:HB3	2.46	0.46
1:A:497:ILE:CG2	1:A:498:TYR:CD1	2.98	0.46
1:A:248:PRO:O	1:A:252:LEU:HB2	2.16	0.46
1:A:381:SER:HB2	1:A:599:CYS:HA	1.97	0.46
1:A:693:THR:OG1	1:A:694:VAL:HG23	2.16	0.46
1:B:316:LEU:CD2	1:B:328:ALA:HB2	2.43	0.46
1:B:277:MET:HA	1:B:277:MET:CE	2.45	0.46
1:B:647:ASN:CG	1:B:648:LYS:H	2.20	0.46
1:A:548:SER:N	1:A:573:GLN:NE2	2.46	0.46
1:B:241:GLN:HA	1:B:241:GLN:NE2	2.31	0.46
1:B:259:GLU:OE1	1:B:271:THR:N	2.43	0.46
1:A:213:GLU:HG3	1:A:749:PHE:CD2	2.50	0.46
1:A:261:SER:O	1:A:265:LYS:HB2	2.16	0.46
1:A:492:LEU:HA	1:A:492:LEU:HD23	1.61	0.46
1:A:675:ILE:CD1	1:A:684:TRP:CD1	2.99	0.46
1:A:646:LYS:HD2	1:A:648:LYS:HE2	1.97	0.46
1:B:276:LEU:O	1:B:276:LEU:HD12	2.15	0.46
1:A:556:ARG:CG	1:A:556:ARG:HH11	2.18	0.46
1:A:694:VAL:N	1:A:695:PRO:HD2	2.30	0.46
1:A:507:PHE:CE1	1:A:542:HIS:ND1	2.79	0.45
1:B:270:MET:SD	1:B:275:PHE:HA	2.56	0.45
1:B:599:CYS:HA	5:B:771:HOH:O	2.16	0.45
1:A:548:SER:H	1:A:573:GLN:HE21	1.57	0.45
1:A:537:ASN:OD1	1:A:541:ARG:NE	2.41	0.45
1:A:516:ALA:CB	1:A:518:TYR:CZ	2.99	0.45
1:B:694:VAL:N	1:B:695:PRO:CD	2.79	0.45
1:A:539:PHE:O	1:A:542:HIS:HB3	2.16	0.45
1:A:311:HIS:HB2	1:A:576:ALA:HB1	1.97	0.45
1:B:702:PHE:O	1:B:718:GLN:HA	2.16	0.45
1:A:349:ASN:O	1:A:350:GLN:HB2	2.15	0.45
1:B:497:ILE:CD1	1:B:497:ILE:N	2.79	0.45
1:B:625:TRP:CD1	1:B:626:TRP:N	2.84	0.45
1:A:314:TYR:HB3	1:A:329:TYR:CE1	2.51	0.45
1:B:484:ASP:O	1:B:487:LYS:N	2.46	0.45
1:B:530:ARG:HG3	1:B:530:ARG:NH1	2.23	0.45
1:B:409:LEU:HD12	1:B:409:LEU:HA	1.52	0.45
1:B:743:HIS:HA	1:B:744:PRO:HD3	1.59	0.45
1:B:388:SER:HA	1:B:438:LYS:HB3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLU:OE1	1:B:396:GLU:HA	2.17	0.45
1:A:661:HIS:O	1:A:698:ALA:HA	2.17	0.45
1:A:396:GLU:HA	1:A:396:GLU:OE1	2.17	0.45
1:B:375:ASP:C	5:B:887:HOH:O	2.54	0.45
1:B:516:ALA:CB	1:B:518:TYR:CZ	3.00	0.45
1:A:291:HIS:HA	1:A:295:TYR:CD2	2.52	0.45
1:A:694:VAL:N	1:A:695:PRO:CD	2.79	0.45
1:B:227:THR:CG2	1:B:228:LEU:N	2.79	0.45
1:B:529:LEU:HD23	1:B:529:LEU:HA	1.74	0.45
1:B:661:HIS:O	1:B:698:ALA:HA	2.16	0.45
1:A:314:TYR:CE1	1:A:315:LEU:HG	2.52	0.45
1:B:162:PHE:CZ	1:B:182:ARG:CA	2.99	0.45
1:B:495:MET:O	1:B:497:ILE:HD13	2.16	0.45
1:A:240:GLN:HA	1:A:240:GLN:OE1	2.16	0.45
1:A:228:LEU:HD11	1:A:233:LEU:HA	1.99	0.44
1:B:305:TYR:CD1	1:B:305:TYR:N	2.84	0.44
1:A:426:PRO:HG3	1:A:498:TYR:CE2	2.52	0.44
1:A:426:PRO:HG2	1:A:431:LEU:HD11	1.98	0.44
1:A:314:TYR:CD1	1:A:315:LEU:HG	2.52	0.44
1:B:163:LYS:HA	1:B:166:LYS:HB2	1.99	0.44
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.52	0.44
1:A:228:LEU:CD1	1:A:233:LEU:CA	2.96	0.44
1:A:733:VAL:HB	1:A:748:LEU:HB2	2.00	0.44
1:B:561:ASN:OD1	1:B:578:ASN:N	2.30	0.44
1:A:529:LEU:HA	1:A:529:LEU:HD23	1.65	0.44
1:A:681:ASN:N	1:A:682:PRO:CD	2.80	0.44
1:A:227:THR:HG23	1:A:228:LEU:N	2.32	0.44
1:B:610:ASP:HA	1:B:611:PRO:HD3	1.54	0.44
1:A:694:VAL:HG12	1:A:694:VAL:O	2.17	0.44
1:B:165:LEU:CD1	1:B:204:PHE:CE2	3.00	0.44
1:A:715:PHE:HE2	1:A:718:GLN:HB2	1.81	0.44
1:A:657:ILE:HD13	1:A:671:GLN:HB3	1.99	0.44
1:B:212:ALA:O	1:B:215:ASP:HB2	2.18	0.44
1:A:542:HIS:CD2	1:A:546:CYS:HB2	2.52	0.44
1:B:184:ILE:HD12	1:B:184:ILE:HA	1.64	0.44
1:B:681:ASN:N	1:B:682:PRO:CD	2.81	0.44
1:B:675:ILE:HD13	1:B:684:TRP:CD1	2.52	0.44
1:A:622:GLN:HG3	1:A:623:GLY:N	2.32	0.44
1:B:244:GLU:C	1:B:246:ALA:H	2.20	0.44
1:A:241:GLN:HE21	1:A:241:GLN:N	2.15	0.43
1:A:651:ILE:CG2	1:A:652:VAL:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:ASN:OD1	1:B:541:ARG:NE	2.40	0.43
1:B:210:GLN:HE21	1:B:210:GLN:HB2	1.55	0.43
1:B:196:LEU:HB3	1:B:201:ILE:HD13	1.94	0.43
1:A:497:ILE:HG21	1:A:498:TYR:CE1	2.53	0.43
1:A:646:LYS:HA	1:A:646:LYS:HD3	1.46	0.43
1:A:405:LEU:HD23	1:A:409:LEU:HD22	1.99	0.43
1:A:301:PRO:HB3	1:A:425:LEU:O	2.18	0.43
1:A:645:ASN:O	1:A:646:LYS:O	2.35	0.43
1:A:706:ASP:N	1:A:714:ASP:O	2.38	0.43
1:B:659:GLU:OE1	1:B:701:ARG:HD3	2.18	0.43
1:A:651:ILE:CD1	1:A:677:ASN:HD21	2.24	0.43
1:A:497:ILE:HG22	1:A:498:TYR:CE1	2.54	0.43
1:B:613:THR:HG22	1:B:615:PHE:H	1.83	0.43
1:A:498:TYR:CD1	1:A:498:TYR:N	2.85	0.43
1:B:735:LEU:O	1:B:743:HIS:HB2	2.19	0.43
1:A:556:ARG:CG	1:A:556:ARG:NH1	2.79	0.43
1:B:397:GLN:O	1:B:400:VAL:HB	2.19	0.43
1:B:441:LYS:NZ	1:B:493:SER:O	2.51	0.43
1:B:734:HIS:HE1	5:B:777:HOH:O	2.00	0.43
1:B:701:ARG:HG3	1:B:720:THR:OG1	2.18	0.43
1:B:342:LEU:CD1	1:B:342:LEU:N	2.82	0.43
1:A:409:LEU:HA	1:A:409:LEU:HD12	1.66	0.43
1:B:233:LEU:O	1:B:236:PHE:HB3	2.19	0.43
1:B:542:HIS:CD2	1:B:542:HIS:C	2.92	0.42
1:B:441:LYS:HG3	1:B:496:ILE:HB	2.01	0.42
1:A:207:MET:SD	1:A:210:GLN:HB2	2.59	0.42
1:B:291:HIS:HA	1:B:295:TYR:CE2	2.55	0.42
1:B:654:PRO:HD2	1:B:675:ILE:O	2.20	0.42
1:B:556:ARG:HG2	1:B:556:ARG:NH1	2.34	0.42
1:B:739:ASN:HB2	1:B:741:ASP:OD2	2.19	0.42
1:A:496:ILE:HD13	1:A:496:ILE:N	2.34	0.42
1:B:675:ILE:HD13	1:B:684:TRP:NE1	2.34	0.42
1:B:412:ILE:O	1:B:412:ILE:HG22	2.18	0.42
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.78	0.42
1:A:432:LYS:HE3	1:A:432:LYS:HB3	1.91	0.42
1:A:504:PHE:CZ	1:A:506:GLY:CA	2.99	0.42
1:B:651:ILE:HA	1:B:651:ILE:HD13	1.59	0.42
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.08	0.42
1:A:429:GLU:OE1	1:A:432:LYS:HE2	2.18	0.42
1:A:306:LEU:HD23	1:A:306:LEU:HA	1.69	0.42
1:B:530:ARG:CG	1:B:530:ARG:NH1	2.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:VAL:HG21	1:B:519:GLU:HB3	2.00	0.42
1:A:405:LEU:HD13	1:A:437:LEU:HD11	2.01	0.42
1:A:628:PRO:HA	1:A:692:VAL:O	2.19	0.42
1:A:207:MET:HE3	1:A:210:GLN:HB3	1.99	0.42
1:B:182:ARG:O	1:B:185:PHE:HB3	2.20	0.42
1:B:191:SER:HB2	1:B:193:THR:HG23	2.01	0.42
1:A:610:ASP:HA	1:A:611:PRO:HD3	1.55	0.42
1:B:653:ASP:O	1:B:674:VAL:HG13	2.20	0.42
1:A:267:GLN:O	1:A:269:GLN:HG3	2.20	0.42
1:B:509:SER:H	1:B:510:PRO:HD2	1.83	0.42
1:A:558:ASP:O	1:A:559:SER:HB2	2.19	0.42
1:A:547:LEU:CD2	1:A:573:GLN:HG3	2.49	0.42
1:B:211:ARG:NE	1:B:213:GLU:OE2	2.47	0.42
1:A:608:LEU:HA	1:A:608:LEU:HD23	1.88	0.42
1:A:207:MET:SD	1:A:210:GLN:CB	3.09	0.41
1:B:162:PHE:HZ	1:B:182:ARG:HB2	1.85	0.41
1:A:638:GLY:O	1:A:681:ASN:HA	2.20	0.41
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.80	0.41
1:A:349:ASN:O	1:A:349:ASN:OD1	2.38	0.41
1:A:631:LEU:HG	1:A:633:VAL:HG23	2.02	0.41
1:A:573:GLN:N	1:A:573:GLN:NE2	2.61	0.41
1:B:311:HIS:CD2	1:B:312:ASN:HD22	2.37	0.41
1:A:371:ARG:O	1:A:375:ASP:N	2.47	0.41
1:B:497:ILE:HD12	1:B:497:ILE:N	2.36	0.41
1:B:176:VAL:HG12	1:B:177:ASP:N	2.36	0.41
1:B:732:HIS:NE2	1:B:749:PHE:CD1	2.89	0.41
1:B:342:LEU:HB2	1:B:389:LEU:HD23	2.01	0.41
1:A:344:CYS:O	1:A:392:HIS:HB2	2.19	0.41
1:A:411:PRO:O	1:A:434:LYS:NZ	2.52	0.41
1:A:651:ILE:CD1	1:A:677:ASN:ND2	2.80	0.41
1:A:426:PRO:HD3	1:A:498:TYR:CE2	2.55	0.41
1:B:333:LEU:HD21	1:B:340:LEU:HD11	2.02	0.41
1:B:169:LEU:O	1:B:172:LEU:HD12	2.21	0.41
1:A:651:ILE:HG21	1:A:677:ASN:O	2.20	0.41
1:A:665:ARG:HD3	1:A:693:THR:HG21	2.01	0.41
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.74	0.41
1:B:542:HIS:CD2	1:B:546:CYS:HB2	2.56	0.41
1:B:678:ASN:HA	5:B:879:HOH:O	2.20	0.41
1:A:652:VAL:HG23	1:A:652:VAL:H	1.53	0.41
1:B:162:PHE:CE1	1:B:182:ARG:HA	2.56	0.41
1:B:391:ASN:N	5:B:830:HOH:O	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:701:ARG:HD3	1:B:701:ARG:HH11	1.74	0.41
1:A:426:PRO:CG	1:A:498:TYR:CE2	3.04	0.41
1:B:162:PHE:HD1	1:B:162:PHE:HA	1.73	0.41
1:B:651:ILE:CG2	1:B:677:ASN:CA	2.98	0.41
1:A:228:LEU:CD1	1:A:233:LEU:N	2.84	0.41
1:B:311:HIS:HB2	1:B:576:ALA:HB1	2.02	0.41
1:B:739:ASN:ND2	5:B:890:HOH:O	2.53	0.41
1:A:413:LEU:HD12	1:A:414:LEU:H	1.86	0.41
1:B:405:LEU:HD13	1:B:437:LEU:HD11	2.02	0.41
1:A:216:ARG:NH1	1:A:216:ARG:HG3	2.34	0.41
1:B:730:TYR:CZ	1:B:751:LYS:HD3	2.56	0.41
1:A:425:LEU:HD23	1:A:498:TYR:HD2	1.86	0.41
1:B:492:LEU:HA	1:B:492:LEU:HD23	1.74	0.40
1:A:228:LEU:HD13	1:A:232:ARG:HB2	2.03	0.40
1:B:507:PHE:CZ	1:B:531:LEU:HD22	2.56	0.40
1:B:590:LEU:HD23	1:B:590:LEU:HA	1.78	0.40
1:A:709:SER:OG	1:A:710:SER:N	2.54	0.40
1:B:715:PHE:HB2	5:B:850:HOH:O	2.20	0.40
1:B:227:THR:HG21	1:B:269:GLN:HB3	2.04	0.40
1:A:321:THR:HG22	1:A:360:PHE:HB2	2.04	0.40
1:A:345:TRP:CE3	1:A:392:HIS:HB3	2.56	0.40
1:B:441:LYS:HE2	1:B:496:ILE:O	2.20	0.40
1:B:165:LEU:HD13	1:B:204:PHE:CE2	2.56	0.40
1:B:595:ASP:OD1	1:B:596:ASN:N	2.52	0.40
1:B:610:ASP:O	1:B:613:THR:OG1	2.35	0.40
1:B:198:ASP:O	1:B:201:ILE:N	2.47	0.40
1:A:622:GLN:CA	1:B:445:LEU:CD1	3.00	0.40
1:B:162:PHE:O	1:B:166:LYS:N	2.39	0.40
1:B:300:GLN:CB	1:B:301:PRO:CD	2.99	0.40
1:A:342:LEU:HB2	1:A:389:LEU:HD23	2.04	0.40
1:A:252:LEU:HD23	1:A:256:GLU:CD	2.42	0.40
1:B:254:LEU:HA	1:B:254:LEU:HD12	1.79	0.40
1:B:638:GLY:O	1:B:681:ASN:HA	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%)	449 (88%)	51 (10%)	9 (2%)	11	42
1	B	557/624 (89%)	485 (87%)	65 (12%)	7 (1%)	15	51
All	All	1066/1248 (85%)	934 (88%)	116 (11%)	16 (2%)	13	47

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	VAL
1	A	646	LYS
1	A	712	LYS
1	B	173	ASN
1	B	645	ASN
1	A	644	VAL
1	B	647	ASN
1	B	649	ASN
1	A	219	GLU
1	A	263	THR
1	B	512	THR
1	A	579	PHE
1	A	713	ASN
1	B	417	PRO
1	A	744	PRO
1	B	648	LYS

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%)	381 (86%)	63 (14%)	4	17
1	B	492/545 (90%)	419 (85%)	73 (15%)	4	15
All	All	936/1090 (86%)	800 (86%)	136 (14%)	4	16

All (136) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	PHE
1	A	209	THR
1	A	211	ARG
1	A	219	GLU
1	A	220	GLU
1	A	227	THR
1	A	228	LEU
1	A	231	GLU
1	A	242	ARG
1	A	252	LEU
1	A	253	SER
1	A	254	LEU
1	A	257	ARG
1	A	278	TYR
1	A	293	ARG
1	A	296	GLN
1	A	300	GLN
1	A	309	SER
1	A	310	SER
1	A	344	CYS
1	A	362	SER
1	A	381	SER
1	A	388	SER
1	A	406	ARG
1	A	409	LEU
1	A	414	LEU
1	A	418	LEU
1	A	424	SER
1	A	436	LEU
1	A	487	LYS
1	A	497	ILE
1	A	513	SER
1	A	526	SER
1	A	530	ARG
1	A	535	SER

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Mol	Chain	Res	Type
1	A	539	PHE
1	A	556	ARG
1	A	563	SER
1	A	573	GLN
1	A	594	GLN
1	A	612	ASN
1	A	617	SER
1	A	621	THR
1	A	624	PRO
1	A	643	LYS
1	A	644	VAL
1	A	646	LYS
1	A	648	LYS
1	A	652	VAL
1	A	655	LYS
1	A	665	ARG
1	A	671	GLN
1	A	676	THR
1	A	677	ASN
1	A	685	ASP
1	A	710	SER
1	A	711	SER
1	A	727	LYS
1	A	738	LYS
1	A	743	HIS
1	A	745	SER
1	A	753	SER
1	A	756	ASP
1	B	159	LYS
1	B	160	MET
1	B	162	PHE
1	B	166	LYS
1	B	171	GLU
1	B	172	LEU
1	B	178	ASP
1	B	184	ILE
1	B	186	ARG
1	B	194	ASP
1	B	210	GLN
1	B	211	ARG
1	B	227	THR
1	B	232	ARG

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Mol	Chain	Res	Type
1	B	238	GLN
1	B	242	ARG
1	B	253	SER
1	B	254	LEU
1	B	257	ARG
1	B	261	SER
1	B	262	GLU
1	B	263	THR
1	B	293	ARG
1	B	296	GLN
1	B	298	MET
1	B	300	GLN
1	B	309	SER
1	B	310	SER
1	B	327	GLU
1	B	331	ARG
1	B	362	SER
1	B	388	SER
1	B	406	ARG
1	B	409	LEU
1	B	414	LEU
1	B	423	THR
1	B	436	LEU
1	B	441	LYS
1	B	486	LEU
1	B	488	LEU
1	B	497	ILE
1	B	508	SER
1	B	526	SER
1	B	535	SER
1	B	539	PHE
1	B	563	SER
1	B	573	GLN
1	B	577	LEU
1	B	613	THR
1	B	614	THR
1	B	617	SER
1	B	621	THR
1	B	646	LYS
1	B	648	LYS
1	B	651	ILE
1	B	652	VAL

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Mol	Chain	Res	Type
1	B	655	LYS
1	B	659	GLU
1	B	665	ARG
1	B	671	GLN
1	B	676	THR
1	B	677	ASN
1	B	685	ASP
1	B	687	GLU
1	B	709	SER
1	B	710	SER
1	B	713	ASN
1	B	715	PHE
1	B	727	LYS
1	B	738	LYS
1	B	743	HIS
1	B	753	SER
1	B	755	GLN

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	241	GLN
1	A	291	HIS
1	A	312	ASN
1	A	349	ASN
1	A	573	GLN
1	A	639	GLN
1	A	645	ASN
1	A	718	GLN
1	A	728	GLN
1	A	743	HIS
1	B	210	GLN
1	B	241	GLN
1	B	291	HIS
1	B	312	ASN
1	B	349	ASN
1	B	515	GLN
1	B	542	HIS
1	B	573	GLN
1	B	639	GLN
1	B	718	GLN
1	B	728	GLN

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Mol	Chain	Res	Type
1	B	734	HIS
1	B	739	ASN
1	B	743	HIS
1	B	755	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	IP2	A	1	2	20,20,20	1.88	9 (45%)	28,32,32	1.83	9 (32%)
3	ACT	A	5	-	1,3,3	3.62	1 (100%)	0,3,3	0.00	-
4	IP2	B	1	2	20,20,20	1.88	7 (35%)	28,32,32	2.22	11 (39%)
3	ACT	B	5	-	1,3,3	3.97	1 (100%)	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IP2	A	1	2	-	0/10/34/34	0/1/1/1
3	ACT	A	5	-	-	0/0/0/0	0/0/0/0
4	IP2	B	1	2	-	0/10/34/34	0/1/1/1
3	ACT	B	5	-	-	0/0/0/0	0/0/0/0

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1	IP2	P4-O42	2.00	1.61	1.54
4	A	1	IP2	P5-O52	2.14	1.62	1.54
4	A	1	IP2	C6-C5	2.17	1.58	1.52
4	A	1	IP2	P4-O43	2.17	1.62	1.54
4	B	1	IP2	P4-O43	2.28	1.62	1.54
4	A	1	IP2	P5-O53	2.29	1.62	1.54
4	A	1	IP2	P4-O4	2.30	1.67	1.60
4	B	1	IP2	P4-O42	2.32	1.63	1.54
4	B	1	IP2	P5-O53	2.38	1.63	1.54
4	B	1	IP2	P5-O52	2.44	1.63	1.54
4	B	1	IP2	P4-O4	2.53	1.67	1.60
4	A	1	IP2	C5-C4	2.65	1.57	1.52
4	B	1	IP2	P5-O51	3.31	1.62	1.51
4	A	1	IP2	P4-O41	3.40	1.62	1.51
4	A	1	IP2	P5-O51	3.45	1.62	1.51
3	A	5	ACT	CH3-C	3.62	1.53	1.48
4	B	1	IP2	P4-O41	3.68	1.63	1.51
3	B	5	ACT	CH3-C	3.97	1.54	1.48

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	IP2	O1-C1-C2	-4.42	100.39	110.34
4	A	1	IP2	O2-C2-C1	-3.76	101.86	110.34
4	B	1	IP2	O2-C2-C1	-3.44	102.60	110.34
4	B	1	IP2	O3-C3-C2	-3.01	103.55	110.34
4	A	1	IP2	C3-C2-C1	-2.90	105.39	110.79
4	B	1	IP2	O3-C3-C4	-2.56	103.82	109.87
4	B	1	IP2	O5-C5-C4	-2.40	102.89	108.47
4	A	1	IP2	O3-C3-C2	2.16	115.21	110.34
4	A	1	IP2	O4-P4-O41	2.33	112.92	107.11
4	A	1	IP2	O4-C4-C3	2.33	113.48	108.38
4	A	1	IP2	O4-C4-C5	2.40	114.04	108.47
4	B	1	IP2	O4-C4-C3	2.54	113.93	108.38
4	B	1	IP2	C2-C3-C4	2.84	115.84	109.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1	IP2	C6-C5-C4	2.89	117.82	111.44
4	A	1	IP2	P4-O4-C4	3.07	128.93	121.56
4	A	1	IP2	C1-C6-C5	3.33	116.92	109.60
4	B	1	IP2	P5-O5-C5	3.38	129.67	121.56
4	B	1	IP2	P4-O4-C4	3.57	130.12	121.56
4	B	1	IP2	C1-C6-C5	3.97	118.32	109.60
4	B	1	IP2	C3-C2-C1	4.40	119.00	110.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	IP2	3	0
4	B	1	IP2	4	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, 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(Å²)	Q<0.9	
1	A	508/624 (81%)	-0.46	20 (3%)	43	25	4, 22, 82, 127	14 (2%)
1	B	558/624 (89%)	-0.39	21 (3%)	44	26	4, 23, 78, 118	23 (4%)
All	All	1066/1248 (85%)	-0.42	41 (3%)	44	26	4, 23, 81, 127	37 (3%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	509	SER	8.1
1	B	649	ASN	7.5
1	A	201	ILE	6.8
1	B	509	SER	6.2
1	B	514	GLY	5.8
1	A	202	GLU	5.7
1	B	510	PRO	5.5
1	A	203	THR	5.5
1	A	204	PHE	5.2
1	B	508	SER	4.8
1	A	200	GLU	4.3
1	A	647	ASN	4.0
1	A	710	SER	3.9
1	A	645	ASN	3.8
1	B	486	LEU	3.8
1	A	208	LEU	3.7
1	B	647	ASN	3.7
1	B	172	LEU	3.4
1	B	645	ASN	3.4
1	A	420	GLY	3.2
1	B	648	LYS	3.0
1	A	205	TYR	3.0
1	A	206	LYS	2.8
1	B	168	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	419	ASP	2.8
1	B	710	SER	2.8
1	A	648	LYS	2.7
1	B	515	GLN	2.5
1	B	165	LEU	2.5
1	A	207	MET	2.5
1	A	709	SER	2.4
1	B	709	SER	2.4
1	B	167	ASP	2.3
1	A	505	GLY	2.3
1	B	261	SER	2.2
1	B	171	GLU	2.2
1	A	650	SER	2.2
1	B	202	GLU	2.2
1	B	503	HIS	2.1
1	B	484	ASP	2.1
1	A	711	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
4	IP2	A	1	20/20	0.77	0.31	3.64	70,97,136,136	0
4	IP2	B	1	20/20	0.81	0.22	1.55	53,74,108,110	0
3	ACT	B	5	4/4	0.98	0.12	0.12	25,26,27,29	0
3	ACT	A	5	4/4	0.95	0.13	-0.02	36,38,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	CA	B	3	1/1	0.94	0.15	-0.64	74,74,74,74	0
2	CA	B	2	1/1	0.95	0.07	-2.70	37,37,37,37	0
2	CA	A	2	1/1	0.91	0.09	-	59,59,59,59	0
2	CA	A	3	1/1	0.78	0.12	-	66,66,66,66	0

6.5 Other polymers [i](#)

There are no such residues in this entry.