



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:24 PM UTC

PDB ID : 1DJH / pdb_00001djh
Title : PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C-DELTA1 FROM
RAT COMPLEXED WITH BARIUM
Authors : Essen, L.-O.; Perisic, O.; Williams, R.L.
Deposited on : 1996-09-25
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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

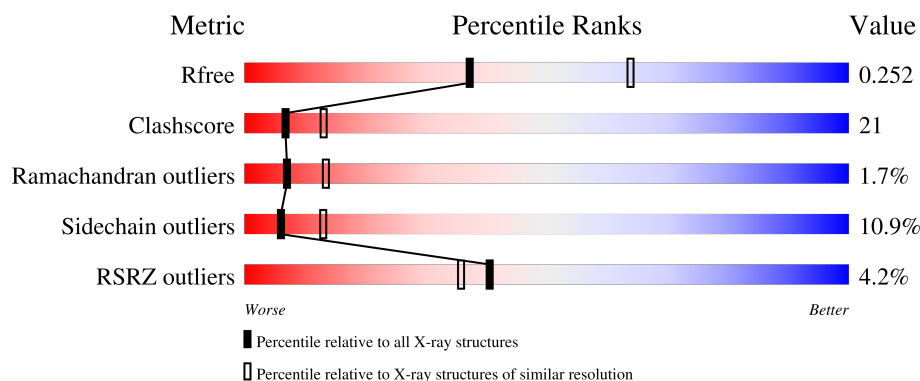
1 Overall quality at a glance

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% 50% 25% 6% • 18%
1	B	624	4% 54% 30% 5% • 10%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9257 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

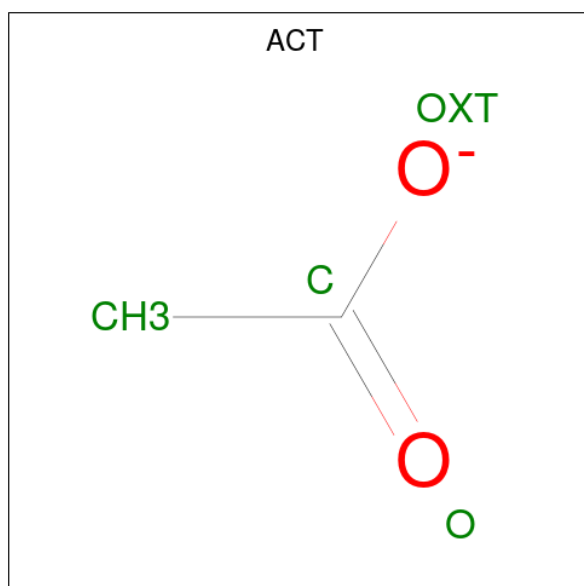
- Molecule 1 is a protein called PHOSPHOINOSITIDE-SPECIFIC PHOSPHOLIPASE C, ISOZYME DELTA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	70	0	0
			4057	2565	709	761	22			
1	B	559	Total	C	N	O	S	87	0	0
			4445	2807	771	843	24			

- Molecule 2 is BARIUM ION (CCD ID: BA) (formula: Ba).

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

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



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

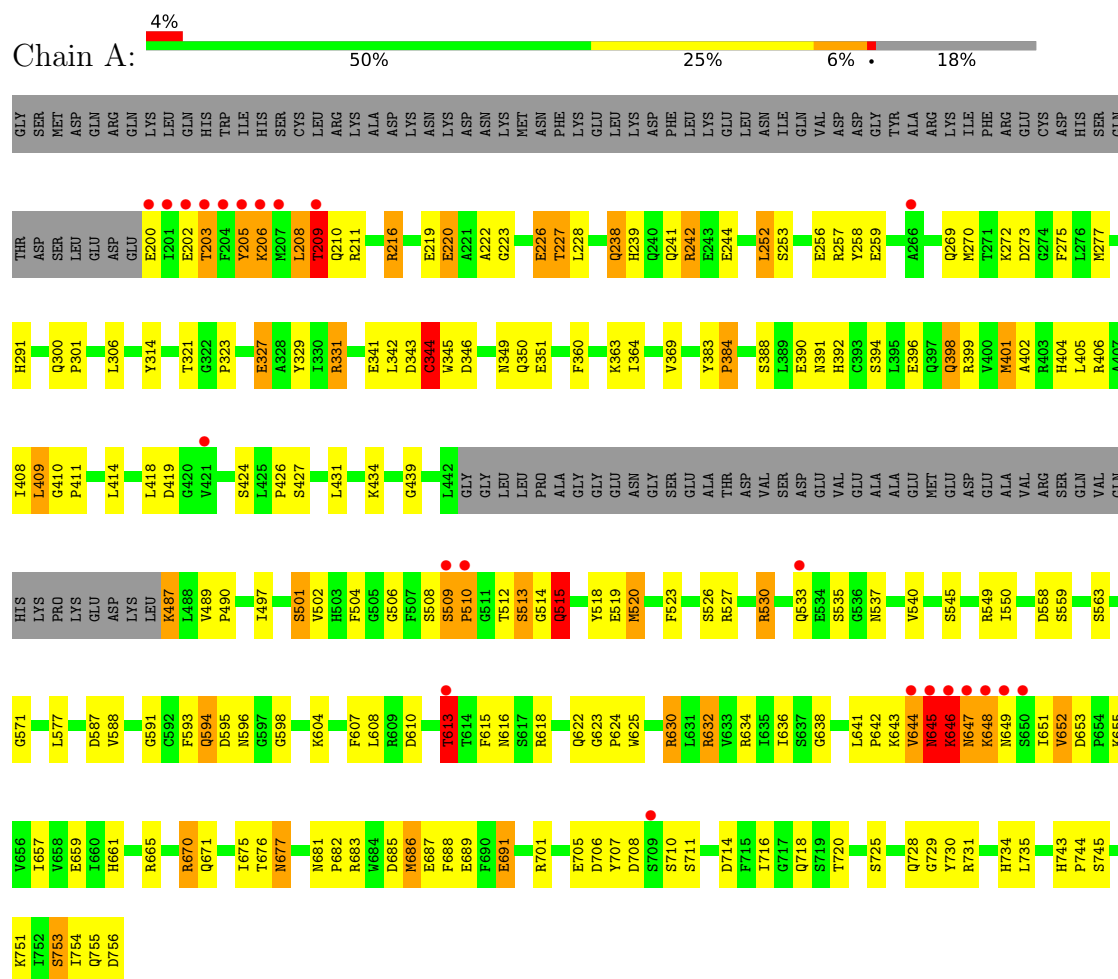
- Molecule 4 is water.

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

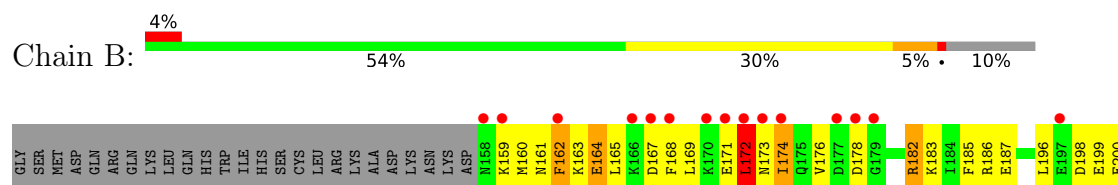
3 Residue-property plots

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



T676	G597	S501	L431	R331	I201
N677	G598	V502	K434	K335	E202
N681	C599	H503	F504	F204	T203
D685	K604	G505	G439	E341	Y205
N686	P605	F507	K440	L342	K206
E687	A606	S508	K441	M207	L208
E691	F607	S509	L445	D343	T209
E691	D610	P510	LEU	C344	Q210
R701	P611	G511	PRO	W345	R211
E705	N612	T512	ALA	P348	A212
D706	T613	Q515	GLY	N349	E213
S709	T614	G515	GLY	Q350	I214
S709	R618	E519	GLU	E351	D215
S710	Q622	M520	ASN	R216	R216
S711	G623	F523	GLY	I354	E220
K712	P624	S524	SER	G357	E226
N713	W625	E525	GLU	I364	T227
I716	R630	S526	THR	V369	L228
G717	L631	R527	ASP	K379	V234
Q718	R632	A528	VAL	S388	Q238
S719	V633	L529	SER	I389	H239
T720	R634	R530	ASP	E390	Q240
I721	G638	Q533	VAL	P384	Q241
P722	L641	E534	ALA	S388	R242
S725	P642	S535	ALA	E390	A246
L726	K643	F539	GLU	G247	G247
K727	V644	V540	MET	S394	P248
Q728	N645	N543	GLU	L395	A249
G729	K646	V544	ASP	E396	L252
Y730	N647	S545	ALA	Q397	S253
R731	LYS	N647	VAL	Q398	
H734	ASN	R549	ARG	R399	
L735	S650	I550	SER	V400	Y258
L736	I651	D558	GLN	M401	
S737	V652	S559	VAL	L405	S261
K738	D653	G571	GLN	R406	E262
Q742	P654	L577	HIS	L409	T263
H743	K655	G583	LYS	A264	A264
P744	V656	P584	PRO	K265	K265
S745	I657	D587	LYS	A266	A266
K751	I660	V588	GLU	P411	
L752	H661	G591	D484	Q269	
S753	R665	C592	K485	L414	Q269
L754	D666	F593	L486	D415	S281
Q755	T667	Q594	K487	Q416	
D756	Q671	D595	L488	P417	L289
	T672	N596	E491	V421	A290
	A673		L492	T422	H291
	V674		S493	T423	Q300
	I675		D494		P301
			K500	P426	L306
				S427	

4 Data and refinement statistics

Property	Value	Source
Space group	F 41 3 2	Depositor
Cell constants a, b, c, α , β , γ	398.25Å 398.25Å 398.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.50) 97.8 (10.00-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.50Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.210 , 0.270 0.206 , 0.252	Depositor DCC
R_{free} test set	3989 reflections (4.31%)	wwPDB-VP
Wilson B-factor (Å ²)	40.3	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 117.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9257	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: BA, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.95	8/4152 (0.2%)	1.13	22/5624 (0.4%)
1	B	0.95	3/4544 (0.1%)	1.12	24/6144 (0.4%)
All	All	0.95	11/8696 (0.1%)	1.12	46/11768 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	MET	SD-CE	-11.45	1.50	1.79
1	A	708	ASP	C-O	-9.86	1.12	1.23
1	B	520	MET	SD-CE	-7.57	1.60	1.79
1	A	401	MET	SD-CE	-7.19	1.61	1.79
1	A	515	GLN	CB-CG	-6.99	1.31	1.52
1	A	613	THR	N-CA	-6.21	1.38	1.46
1	A	515	GLN	CG-CD	-6.00	1.37	1.52
1	B	607	PHE	CE1-CZ	-5.59	1.21	1.38
1	A	520	MET	SD-CE	-5.46	1.65	1.79
1	A	686	MET	SD-CE	5.19	1.92	1.79
1	A	402	ALA	CA-CB	-5.19	1.45	1.53

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	515	GLN	CB-CG-CD	-9.09	97.14	112.60
1	B	226	GLU	N-CA-C	-8.03	103.06	113.17
1	B	509	SER	N-CA-C	7.69	126.80	109.81
1	A	613	THR	N-CA-C	7.56	121.30	109.96
1	B	515	GLN	N-CA-C	7.32	126.40	110.80
1	A	306	LEU	N-CA-C	-7.24	97.79	109.96
1	A	594	GLN	N-CA-C	-7.23	103.92	112.89
1	B	306	LEU	N-CA-C	-7.16	97.93	109.96
1	B	174	ILE	CB-CA-C	-6.98	102.91	111.08
1	B	594	GLN	N-CA-C	-6.95	104.28	112.89
1	A	675	ILE	N-CA-C	-6.91	98.48	108.36
1	B	265	LYS	N-CA-C	-6.64	103.73	110.97
1	A	515	GLN	N-CA-CB	-6.63	99.28	110.49
1	A	515	GLN	N-CA-C	6.42	124.47	110.80
1	A	390	GLU	N-CA-C	-6.38	97.29	108.20
1	A	645	ASN	N-CA-C	-6.28	97.42	110.80
1	A	344	CYS	N-CA-C	6.27	119.46	109.24
1	A	226	GLU	N-CA-C	-6.21	105.34	113.17
1	B	390	GLU	N-CA-C	-6.15	97.11	107.99
1	B	591	GLY	N-CA-C	-5.99	105.24	112.49
1	B	258	TYR	N-CA-C	5.88	121.49	113.97
1	A	591	GLY	N-CA-C	-5.84	105.42	112.49
1	A	497	ILE	CB-CA-C	-5.78	106.80	111.71
1	B	384	PRO	N-CA-C	5.67	120.11	111.15
1	B	654	PRO	N-CA-C	5.61	120.92	111.32
1	B	675	ILE	N-CA-C	-5.60	100.35	108.36
1	A	391	ASN	N-CA-C	5.55	117.69	108.20
1	B	178	ASP	N-CA-C	-5.51	103.64	110.41
1	A	398	GLN	N-CA-C	-5.47	105.32	111.28
1	B	486	LEU	N-CA-C	-5.37	106.50	113.16
1	B	520	MET	N-CA-C	5.37	117.16	108.41
1	B	172	LEU	N-CA-C	-5.34	106.54	112.57
1	A	707	TYR	N-CA-C	5.33	118.04	110.10
1	A	384	PRO	N-CA-C	5.24	119.43	111.15
1	A	258	TYR	N-CA-C	5.24	120.53	113.72
1	B	540	VAL	CB-CA-C	-5.22	105.02	111.70
1	B	202	GLU	N-CA-C	-5.20	105.30	110.97
1	B	344	CYS	N-CA-C	5.20	117.71	109.24
1	B	207	MET	N-CA-C	-5.13	105.81	111.71
1	A	540	VAL	CB-CA-C	-5.12	105.14	111.70
1	B	524	SER	N-CA-C	-5.12	103.64	110.55
1	B	644	VAL	N-CA-C	5.11	119.97	109.34
1	B	510	PRO	N-CA-C	5.10	125.37	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	646	LYS	N-CA-C	-5.08	99.99	110.80
1	A	711	SER	N-CA-C	5.03	114.89	108.24
1	A	497	ILE	N-CA-C	5.01	116.19	111.48

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	515	GLN	Sidechain
1	A	519	GLU	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4057	0	3972	144	0
1	B	4445	0	4353	213	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	3	0	0	0	0
3	B	4	0	3	1	0
4	A	343	0	0	12	1
4	B	399	0	0	22	0
All	All	9257	0	8328	352	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (352) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLN:HG3	1:B:417:PRO:HD2	1.41	1.01
1:A:504:PHE:HB3	1:A:527:ARG:HH22	1.23	1.00
1:B:673:ALA:HB1	4:B:1074:HOH:O	1.64	0.94
1:A:622:GLN:HB2	1:B:445:LEU:HD13	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:PHE:HB3	1:B:527:ARG:HH22	1.31	0.92
1:B:607:PHE:CD2	1:B:625:TRP:HB3	2.04	0.92
1:B:348:PRO:HB2	1:B:349:ASN:ND2	1.86	0.90
1:B:646:LYS:HE3	1:B:647:ASN:HD21	1.36	0.89
1:A:241:GLN:HE22	1:A:730:TYR:H	1.19	0.89
1:B:630:ARG:HD2	1:B:755:GLN:NE2	1.87	0.88
1:B:227:THR:HG21	1:B:269:GLN:HB3	1.55	0.88
1:B:161:ASN:H	1:B:164:GLU:HG3	1.39	0.87
1:B:486:LEU:H	1:B:486:LEU:HD12	1.41	0.86
1:B:238:GLN:HG2	1:B:246:ALA:CB	2.07	0.85
1:B:172:LEU:HD12	1:B:174:ILE:HD12	1.58	0.84
1:B:227:THR:CG2	1:B:269:GLN:HB3	2.07	0.84
1:A:216:ARG:HH21	1:A:683:ARG:HH22	1.24	0.82
1:B:241:GLN:HE22	1:B:730:TYR:H	1.27	0.82
1:A:504:PHE:HB3	1:A:527:ARG:NH2	1.93	0.82
1:B:172:LEU:HB2	1:B:174:ILE:HG13	1.62	0.82
1:A:509:SER:HB3	1:A:510:PRO:HD3	1.61	0.81
1:A:622:GLN:HB2	1:B:445:LEU:CD1	2.09	0.81
1:B:630:ARG:HD2	1:B:755:GLN:HE21	1.45	0.81
1:A:624:PRO:HD2	1:A:625:TRP:CE3	2.15	0.81
1:A:520:MET:HE3	1:A:549:ARG:HB2	1.62	0.80
1:A:520:MET:CE	1:A:549:ARG:HB2	2.12	0.80
1:B:383:TYR:HB3	1:B:384:PRO:HD2	1.61	0.79
1:B:162:PHE:CD1	1:B:165:LEU:HD23	2.16	0.79
1:B:504:PHE:HB3	1:B:527:ARG:NH2	1.98	0.79
1:B:203:THR:O	1:B:207:MET:HG3	1.83	0.78
1:B:238:GLN:HG2	1:B:246:ALA:HB1	1.65	0.78
1:B:728:GLN:NE2	1:B:754:ILE:H	1.82	0.78
1:B:520:MET:CE	1:B:549:ARG:HB2	2.15	0.77
1:B:607:PHE:CE2	1:B:625:TRP:HB3	2.21	0.74
1:A:227:THR:CG2	1:A:269:GLN:HB3	2.17	0.74
1:B:605:PRO:HB2	1:B:607:PHE:CE1	2.23	0.74
1:A:227:THR:HG21	1:A:269:GLN:HB3	1.70	0.73
1:B:605:PRO:HB2	1:B:607:PHE:HE1	1.51	0.73
1:A:227:THR:HG21	1:A:269:GLN:OE1	1.89	0.73
1:B:227:THR:HG21	1:B:269:GLN:OE1	1.89	0.72
1:A:504:PHE:CZ	1:A:506:GLY:HA2	2.24	0.72
1:A:730:TYR:CE1	1:A:751:LYS:HD2	2.25	0.71
1:A:728:GLN:NE2	1:A:754:ILE:H	1.88	0.71
1:B:162:PHE:CE1	1:B:165:LEU:HD23	2.25	0.71
1:B:520:MET:HE3	1:B:549:ARG:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:VAL:O	1:B:238:GLN:HG3	1.90	0.71
1:A:642:PRO:HD2	1:A:716:ILE:CG2	2.21	0.71
1:B:642:PRO:HD2	1:B:716:ILE:CG2	2.21	0.70
1:A:383:TYR:HB3	1:A:384:PRO:HD2	1.74	0.69
1:B:646:LYS:CE	1:B:647:ASN:HD21	2.05	0.68
1:B:632:ARG:NH2	4:B:767:HOH:O	2.27	0.68
1:B:730:TYR:CE1	1:B:751:LYS:HD2	2.28	0.67
1:A:321:THR:HG22	1:A:360:PHE:HB2	1.77	0.67
1:B:634:ARG:HG3	1:B:687:GLU:HB2	1.77	0.66
1:A:607:PHE:CD2	1:A:625:TRP:HB3	2.30	0.66
1:A:651:ILE:HD12	1:A:677:ASN:ND2	2.09	0.66
1:A:394:SER:O	1:A:398:GLN:HG3	1.95	0.66
1:B:164:GLU:O	1:B:167:ASP:HB3	1.95	0.65
1:A:206:LYS:O	1:A:210:GLN:HB2	1.96	0.65
1:A:646:LYS:O	1:A:648:LYS:N	2.29	0.65
1:A:607:PHE:CE2	1:A:625:TRP:HB3	2.30	0.65
1:A:643:LYS:C	1:A:645:ASN:H	2.04	0.65
1:B:583:GLY:N	4:B:948:HOH:O	2.28	0.65
1:B:162:PHE:CE2	1:B:182:ARG:HG3	2.32	0.65
1:A:530:ARG:O	1:A:533:GLN:HB3	1.96	0.64
1:A:252:LEU:O	1:A:256:GLU:HG3	1.97	0.64
1:B:426:PRO:HG2	1:B:431:LEU:HD11	1.77	0.64
1:B:507:PHE:HB3	4:B:1111:HOH:O	1.97	0.64
1:B:504:PHE:CZ	1:B:506:GLY:HA2	2.32	0.64
1:B:488:LEU:HD13	1:B:493:SER:HB2	1.80	0.64
1:B:196:LEU:O	1:B:201:ILE:HD11	1.98	0.63
1:B:539:PHE:O	1:B:543:ASN:ND2	2.29	0.63
1:B:416:GLN:HG3	1:B:417:PRO:CD	2.25	0.63
1:B:588:VAL:HG21	1:B:661:HIS:HD2	1.62	0.63
1:B:632:ARG:NE	4:B:767:HOH:O	2.32	0.63
1:B:515:GLN:NE2	1:B:519:GLU:HB3	2.13	0.63
1:B:624:PRO:HD2	1:B:625:TRP:CE3	2.34	0.63
1:B:439:GLY:C	1:B:501:SER:HB2	2.23	0.62
1:B:588:VAL:HG21	1:B:661:HIS:CD2	2.34	0.62
1:A:508:SER:OG	1:A:509:SER:N	2.30	0.62
1:A:645:ASN:O	1:A:646:LYS:HB3	1.98	0.62
1:A:220:GLU:HG3	4:A:805:HOH:O	2.00	0.62
1:B:549:ARG:C	1:B:550:ILE:HD13	2.25	0.62
1:B:605:PRO:CB	1:B:607:PHE:HE1	2.13	0.62
1:B:728:GLN:HE21	1:B:753:SER:HA	1.64	0.62
1:B:646:LYS:HG3	1:B:647:ASN:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:LEU:HD11	1:B:204:PHE:CE2	2.35	0.61
1:B:168:PHE:O	1:B:171:GLU:HB3	1.99	0.61
1:A:241:GLN:HE22	1:A:730:TYR:N	1.93	0.61
1:B:238:GLN:HG2	1:B:246:ALA:HB3	1.82	0.61
1:B:348:PRO:HB2	1:B:349:ASN:HD22	1.63	0.61
1:B:162:PHE:O	1:B:165:LEU:HB3	2.01	0.61
1:B:379:LYS:NZ	4:B:1003:HOH:O	2.33	0.61
1:B:673:ALA:CB	4:B:1074:HOH:O	2.35	0.61
1:B:335:LYS:NZ	4:B:963:HOH:O	2.34	0.60
1:A:670:ARG:HD3	4:A:1055:HOH:O	2.00	0.60
1:B:394:SER:O	1:B:398:GLN:HG3	2.01	0.60
1:B:533:GLN:OE1	1:B:618:ARG:NH1	2.33	0.60
1:A:647:ASN:O	1:A:649:ASN:N	2.35	0.59
1:A:588:VAL:HG21	1:A:661:HIS:CD2	2.37	0.59
1:B:169:LEU:HD13	1:B:176:VAL:HG22	1.84	0.59
1:B:673:ALA:CA	4:B:1074:HOH:O	2.50	0.59
1:B:249:ALA:N	4:B:1100:HOH:O	2.35	0.59
1:B:426:PRO:HB2	1:B:431:LEU:CD1	2.33	0.59
1:B:607:PHE:HD1	1:B:607:PHE:H	1.49	0.59
1:A:202:GLU:O	1:A:206:LYS:HB2	2.03	0.58
1:A:202:GLU:O	1:A:206:LYS:N	2.37	0.58
1:A:504:PHE:HD2	1:A:527:ARG:NH2	2.00	0.58
1:B:169:LEU:HD13	1:B:176:VAL:CG2	2.33	0.58
1:B:595:ASP:OD1	1:B:596:ASN:N	2.35	0.58
1:A:219:GLU:O	1:A:223:GLY:N	2.32	0.58
1:A:239:HIS:O	1:A:242:ARG:NH1	2.37	0.58
1:A:593:PHE:O	1:A:598:GLY:HA2	2.04	0.58
1:A:755:GLN:HG2	1:A:756:ASP:N	2.18	0.58
1:A:439:GLY:C	1:A:501:SER:HB2	2.30	0.57
1:B:183:LYS:O	1:B:187:GLU:HG3	2.05	0.57
1:A:200:GLU:HA	1:A:203:THR:CB	2.35	0.57
1:A:718:GLN:NE2	1:A:720:THR:OG1	2.37	0.57
1:B:593:PHE:O	1:B:598:GLY:HA2	2.05	0.57
1:A:291:HIS:HD2	1:A:725:SER:OG	1.88	0.57
1:A:216:ARG:O	1:A:219:GLU:HB2	2.05	0.57
1:B:705:GLU:C	1:B:716:ILE:HD12	2.30	0.56
1:B:344:CYS:CB	1:B:401:MET:HE3	2.35	0.56
1:B:504:PHE:HD2	1:B:527:ARG:NH2	2.04	0.56
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.69	0.56
1:B:300:GLN:O	1:B:427:SER:HA	2.04	0.56
1:B:718:GLN:NE2	1:B:720:THR:OG1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASN:OD1	1:B:164:GLU:HG2	2.06	0.55
1:B:736:LEU:HD23	1:B:742:GLN:HA	1.87	0.55
1:B:753:SER:HB2	4:B:770:HOH:O	2.05	0.55
1:B:502:VAL:HG21	1:B:519:GLU:HG2	1.88	0.55
1:A:343:ASP:HB3	4:A:978:HOH:O	2.06	0.55
1:A:509:SER:CB	1:A:510:PRO:HD3	2.35	0.55
1:A:327:GLU:HG3	1:A:331:ARG:HD2	1.89	0.55
1:A:686:MET:HE3	1:A:687:GLU:O	2.06	0.55
1:B:162:PHE:HD1	1:B:165:LEU:HD23	1.69	0.55
1:B:263:THR:O	1:B:266:ALA:HB3	2.07	0.55
1:B:588:VAL:CG2	1:B:661:HIS:HD2	2.20	0.55
1:B:182:ARG:O	1:B:185:PHE:HB3	2.07	0.54
1:B:706:ASP:O	1:B:713:ASN:HB3	2.07	0.54
1:A:384:PRO:HG3	1:A:431:LEU:HB2	1.90	0.54
1:B:607:PHE:HD1	1:B:607:PHE:N	2.05	0.54
1:A:200:GLU:C	1:A:202:GLU:H	2.16	0.54
1:A:241:GLN:C	1:A:242:ARG:HG2	2.31	0.54
1:A:300:GLN:O	1:A:427:SER:HA	2.07	0.54
1:A:735:LEU:O	1:A:743:HIS:HB2	2.08	0.54
1:B:350:GLN:HA	1:B:397:GLN:NE2	2.23	0.54
1:B:701:ARG:HE	1:B:718:GLN:HE21	1.56	0.54
1:B:530:ARG:O	1:B:533:GLN:HB3	2.08	0.53
1:B:632:ARG:CZ	4:B:767:HOH:O	2.56	0.53
1:B:172:LEU:CD1	1:B:174:ILE:HD12	2.34	0.53
1:B:196:LEU:HB3	1:B:201:ILE:CD1	2.38	0.53
1:B:735:LEU:O	1:B:743:HIS:HB2	2.08	0.53
1:A:364:ILE:HD12	1:A:369:VAL:CG2	2.38	0.53
1:A:691:GLU:HG2	4:A:1060:HOH:O	2.08	0.53
1:B:622:GLN:HG3	1:B:623:GLY:N	2.23	0.53
1:B:196:LEU:HB3	1:B:201:ILE:HD13	1.90	0.53
1:B:216:ARG:O	1:B:220:GLU:HG3	2.09	0.53
1:B:638:GLY:O	1:B:681:ASN:HA	2.08	0.53
1:B:196:LEU:HD22	1:B:200:GLU:HB3	1.90	0.53
1:B:185:PHE:CE1	1:B:196:LEU:HG	2.44	0.53
1:A:643:LYS:O	1:A:645:ASN:N	2.42	0.52
1:A:622:GLN:OE1	1:B:445:LEU:HD11	2.09	0.52
1:A:705:GLU:C	1:A:716:ILE:HD12	2.35	0.52
1:B:607:PHE:N	1:B:607:PHE:CD1	2.77	0.52
1:A:252:LEU:HD23	1:A:256:GLU:OE2	2.10	0.52
1:B:205:TYR:O	1:B:209:THR:HG23	2.10	0.52
1:A:588:VAL:HG21	1:A:661:HIS:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:HIS:O	1:B:242:ARG:NH1	2.43	0.51
1:A:644:VAL:O	1:A:645:ASN:HB2	2.10	0.51
1:B:342:LEU:HD12	1:B:342:LEU:N	2.26	0.51
1:B:607:PHE:HB2	1:B:613:THR:HG21	1.92	0.51
1:B:291:HIS:HD2	1:B:725:SER:OG	1.93	0.51
1:A:346:ASP:OD2	1:A:394:SER:HB3	2.11	0.51
1:B:674:VAL:N	4:B:1074:HOH:O	2.31	0.51
1:A:504:PHE:CD2	1:A:527:ARG:NH2	2.79	0.50
1:A:689:GLU:OE2	1:B:494:ASP:OD2	2.30	0.50
1:B:172:LEU:HB2	1:B:174:ILE:CG1	2.39	0.50
1:B:411:PRO:O	1:B:434:LYS:NZ	2.43	0.50
1:A:607:PHE:CE1	1:A:608:LEU:HG	2.46	0.50
1:B:300:GLN:HB3	1:B:301:PRO:CD	2.42	0.50
1:A:405:LEU:O	1:A:409:LEU:HB2	2.10	0.50
1:B:533:GLN:OE1	1:B:533:GLN:HA	2.12	0.50
1:B:216:ARG:HG2	4:B:762:HOH:O	2.10	0.50
3:B:5:ACT:O	4:B:948:HOH:O	2.20	0.50
1:B:500:LYS:HE3	4:B:858:HOH:O	2.11	0.49
1:B:734:HIS:HE1	4:B:1025:HOH:O	1.96	0.49
1:A:594:GLN:HA	1:A:594:GLN:HE21	1.77	0.49
1:B:657:ILE:HD13	1:B:671:GLN:CB	2.43	0.49
1:A:730:TYR:CZ	1:A:751:LYS:HD2	2.46	0.49
1:B:354:ILE:HD12	1:B:369:VAL:HG21	1.95	0.49
1:A:205:TYR:O	1:A:208:LEU:HB2	2.13	0.49
1:A:607:PHE:CE2	1:A:625:TRP:CB	2.96	0.49
1:A:624:PRO:HD2	1:A:625:TRP:CZ3	2.48	0.48
1:A:638:GLY:O	1:A:681:ASN:HA	2.13	0.48
1:B:196:LEU:HD23	1:B:196:LEU:HA	1.60	0.48
1:B:345:TRP:CZ2	1:B:357:GLY:HA3	2.48	0.48
1:A:239:HIS:HD2	4:A:793:HOH:O	1.96	0.48
1:A:241:GLN:NE2	1:A:729:GLY:HA3	2.28	0.48
1:B:227:THR:HG23	1:B:269:GLN:HB3	1.95	0.48
1:B:502:VAL:HG11	1:B:515:GLN:OE1	2.13	0.48
1:B:701:ARG:HE	1:B:718:GLN:NE2	2.11	0.48
1:B:227:THR:CG2	1:B:228:LEU:N	2.76	0.48
1:B:227:THR:HG21	1:B:269:GLN:CB	2.36	0.48
1:B:383:TYR:HD2	1:B:599:CYS:HB2	1.77	0.48
1:A:341:GLU:C	1:A:342:LEU:HD12	2.39	0.48
1:A:610:ASP:HB3	1:A:613:THR:OG1	2.14	0.48
1:A:643:LYS:C	1:A:645:ASN:N	2.71	0.47
1:B:341:GLU:C	1:B:342:LEU:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:GLN:CG	1:B:246:ALA:HB1	2.41	0.47
1:B:351:GLU:HA	1:B:351:GLU:OE1	2.13	0.47
1:B:607:PHE:CE2	1:B:625:TRP:CB	2.93	0.47
1:B:187:GLU:OE1	1:B:207:MET:HE1	2.14	0.47
1:B:539:PHE:CD1	1:B:543:ASN:ND2	2.78	0.47
1:A:206:LYS:HA	1:A:209:THR:OG1	2.14	0.47
1:A:242:ARG:HG3	1:A:728:GLN:HB2	1.96	0.47
1:B:515:GLN:HG3	4:B:885:HOH:O	2.13	0.47
1:A:344:CYS:CB	1:A:401:MET:HE3	2.44	0.47
1:B:300:GLN:HB3	1:B:301:PRO:HD2	1.96	0.47
1:B:515:GLN:NE2	1:B:519:GLU:CB	2.76	0.47
1:B:165:LEU:HD11	1:B:204:PHE:CZ	2.49	0.47
1:A:533:GLN:OE1	1:A:533:GLN:HA	2.13	0.47
1:B:241:GLN:C	1:B:242:ARG:HG2	2.34	0.47
1:B:646:LYS:HE3	1:B:647:ASN:ND2	2.16	0.47
1:A:216:ARG:HG3	1:A:216:ARG:NH1	2.30	0.46
1:A:345:TRP:CZ2	1:A:392:HIS:CD2	3.03	0.46
1:B:584:PRO:O	1:B:587:ASP:HB2	2.15	0.46
1:B:515:GLN:HE22	1:B:519:GLU:HB3	1.79	0.46
1:B:364:ILE:HD12	1:B:369:VAL:CG2	2.46	0.46
1:A:549:ARG:C	1:A:550:ILE:HD13	2.41	0.46
1:A:655:LYS:NZ	1:A:671:GLN:OE1	2.45	0.46
1:B:164:GLU:HG2	1:B:164:GLU:H	1.40	0.46
1:A:323:PRO:HD3	4:A:1091:HOH:O	2.15	0.46
1:A:558:ASP:O	1:A:559:SER:HB2	2.14	0.46
1:B:182:ARG:HD3	1:B:186:ARG:HD3	1.97	0.46
1:B:484:ASP:O	1:B:487:LYS:HB2	2.15	0.46
1:A:227:THR:CG2	1:A:228:LEU:N	2.77	0.46
1:A:259:GLU:OE1	1:A:270:MET:HA	2.15	0.46
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.16	0.46
1:B:486:LEU:HD12	1:B:486:LEU:N	2.21	0.46
1:A:616:ASN:OD1	1:A:618:ARG:HB2	2.16	0.46
1:B:426:PRO:HB2	1:B:431:LEU:HD11	1.97	0.46
1:B:558:ASP:O	1:B:559:SER:HB2	2.15	0.46
1:B:588:VAL:CG2	1:B:661:HIS:CD2	2.98	0.46
1:B:587:ASP:HB3	1:B:718:GLN:NE2	2.31	0.46
1:B:571:GLY:HA2	1:B:604:LYS:HE3	1.99	0.45
1:A:434:LYS:HA	1:A:434:LYS:HD2	1.85	0.45
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.83	0.45
1:B:383:TYR:HB3	1:B:384:PRO:CD	2.39	0.45
1:B:248:PRO:O	1:B:252:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:PRO:HG3	1:B:431:LEU:HB2	1.98	0.45
1:A:595:ASP:OD1	1:A:596:ASN:N	2.47	0.45
1:A:689:GLU:HB3	1:B:491:GLU:HG3	1.98	0.45
1:B:405:LEU:O	1:B:409:LEU:HB2	2.16	0.45
1:B:213:GLU:HG2	1:B:214:ILE:N	2.31	0.45
1:B:426:PRO:CG	1:B:431:LEU:HD11	2.46	0.45
1:A:396:GLU:O	1:A:399:ARG:HB2	2.17	0.45
1:B:504:PHE:CD2	1:B:527:ARG:NH2	2.84	0.45
1:B:523:PHE:N	1:B:523:PHE:CD1	2.85	0.45
1:A:571:GLY:HA2	1:A:604:LYS:HE3	1.99	0.45
1:B:162:PHE:CE2	1:B:182:ARG:CG	2.99	0.45
1:B:172:LEU:C	1:B:174:ILE:H	2.25	0.45
1:B:350:GLN:NE2	1:B:397:GLN:HE21	2.15	0.44
1:B:500:LYS:NZ	4:B:854:HOH:O	2.49	0.44
1:B:396:GLU:O	1:B:399:ARG:HB2	2.18	0.44
1:A:273:ASP:O	1:A:277:MET:HG2	2.18	0.44
1:B:416:GLN:CG	1:B:417:PRO:HD2	2.29	0.44
1:B:550:ILE:HD13	1:B:550:ILE:N	2.30	0.44
1:A:634:ARG:HG2	1:A:636:ILE:HG13	1.99	0.44
1:A:744:PRO:HG2	4:A:888:HOH:O	2.16	0.44
1:B:730:TYR:C	1:B:731:ARG:HG2	2.42	0.44
1:A:504:PHE:CZ	1:A:506:GLY:CA	2.99	0.44
1:B:655:LYS:NZ	1:B:671:GLN:OE1	2.42	0.44
1:A:706:ASP:HB3	1:A:714:ASP:HB2	1.99	0.44
1:B:410:GLY:HA3	1:B:411:PRO:HD2	1.80	0.44
1:B:549:ARG:O	1:B:550:ILE:HD13	2.18	0.44
1:A:653:ASP:OD1	1:A:677:ASN:N	2.33	0.44
1:B:421:VAL:HB	4:B:895:HOH:O	2.18	0.44
1:A:728:GLN:HE21	1:A:753:SER:HA	1.82	0.43
1:B:726:LEU:HD12	1:B:726:LEU:HA	1.80	0.43
1:A:681:ASN:N	1:A:682:PRO:CD	2.81	0.43
1:B:240:GLN:HA	1:B:240:GLN:OE1	2.18	0.43
1:B:525:GLU:O	1:B:529:LEU:HG	2.18	0.43
1:B:624:PRO:HD2	1:B:625:TRP:CZ3	2.53	0.43
1:A:208:LEU:O	1:A:210:GLN:N	2.50	0.43
1:A:411:PRO:O	1:A:434:LYS:NZ	2.51	0.43
1:B:502:VAL:CG2	1:B:519:GLU:HG2	2.48	0.43
1:B:657:ILE:HD13	1:B:671:GLN:HB2	2.00	0.43
1:B:660:ILE:O	1:B:667:THR:HA	2.19	0.43
1:A:613:THR:HA	4:A:928:HOH:O	2.17	0.42
1:B:515:GLN:HE22	1:B:519:GLU:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:SER:O	1:A:257:ARG:HB2	2.19	0.42
1:B:434:LYS:HA	1:B:434:LYS:HD2	1.84	0.42
1:A:208:LEU:HD22	1:A:208:LEU:HA	1.58	0.42
1:A:607:PHE:CD1	1:A:608:LEU:HG	2.53	0.42
1:A:730:TYR:C	1:A:731:ARG:HG2	2.44	0.42
1:B:738:LYS:HB2	4:B:947:HOH:O	2.19	0.42
1:A:404:HIS:O	1:A:408:ILE:HG13	2.19	0.42
1:A:630:ARG:HD3	4:A:757:HOH:O	2.19	0.42
1:B:261:SER:O	1:B:265:LYS:HB2	2.18	0.42
1:A:622:GLN:HG3	1:A:623:GLY:N	2.35	0.42
1:A:701:ARG:HH21	1:A:718:GLN:HG3	1.83	0.42
1:B:258:TYR:CE1	1:B:281:SER:HB2	2.54	0.42
1:A:349:ASN:ND2	1:A:349:ASN:O	2.53	0.42
1:A:426:PRO:HG2	1:A:431:LEU:HD11	2.02	0.42
1:A:587:ASP:HB3	1:A:718:GLN:NE2	2.34	0.42
1:A:659:GLU:OE1	1:A:661:HIS:HE1	2.02	0.42
1:B:344:CYS:SG	1:B:401:MET:CE	3.08	0.42
1:A:487:LYS:HA	1:A:487:LYS:HD3	1.37	0.42
1:B:167:ASP:HB3	1:B:168:PHE:H	1.74	0.42
1:B:211:ARG:HG3	4:B:794:HOH:O	2.18	0.42
1:A:238:GLN:HG3	4:A:764:HOH:O	2.19	0.42
1:B:652:VAL:HG12	1:B:706:ASP:CG	2.45	0.42
1:A:489:VAL:HA	1:A:490:PRO:HD3	1.88	0.42
1:A:342:LEU:HD12	1:A:342:LEU:N	2.35	0.41
1:A:537:ASN:N	4:A:924:HOH:O	2.52	0.41
1:A:734:HIS:HE1	4:A:884:HOH:O	2.03	0.41
1:B:441:LYS:NZ	1:B:493:SER:O	2.53	0.41
1:A:523:PHE:CD1	1:A:523:PHE:N	2.87	0.41
1:A:641:LEU:HA	1:A:641:LEU:HD23	1.79	0.41
1:B:289:LEU:O	1:B:289:LEU:HD12	2.19	0.41
1:B:350:GLN:HA	1:B:350:GLN:NE2	2.34	0.41
1:B:641:LEU:HD23	1:B:641:LEU:HA	1.75	0.41
1:B:646:LYS:HD2	1:B:646:LYS:HA	1.79	0.41
1:B:348:PRO:HB2	1:B:349:ASN:HD21	1.78	0.41
1:B:610:ASP:C	1:B:612:ASN:N	2.79	0.41
1:A:300:GLN:HB3	1:A:301:PRO:CD	2.51	0.41
1:A:652:VAL:HG12	1:A:706:ASP:CG	2.46	0.41
1:B:196:LEU:HD22	1:B:200:GLU:CB	2.50	0.41
1:A:272:LYS:O	1:A:275:PHE:HB3	2.21	0.41
1:A:327:GLU:HG3	1:A:327:GLU:O	2.21	0.41
1:A:363:LYS:C	1:A:364:ILE:HG23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:PHE:O	1:B:550:ILE:HA	2.20	0.41
1:B:729:GLY:O	1:B:751:LYS:HA	2.21	0.41
1:A:410:GLY:HA3	1:A:411:PRO:HD2	1.88	0.41
1:A:687:GLU:HG2	1:A:688:PHE:N	2.34	0.41
1:A:200:GLU:C	1:A:202:GLU:N	2.79	0.41
1:A:314:TYR:HB3	1:A:329:TYR:CE2	2.56	0.41
1:B:300:GLN:CB	1:B:301:PRO:CD	2.99	0.41
1:B:445:LEU:HA	1:B:445:LEU:HD23	1.88	0.41
1:B:594:GLN:HA	1:B:594:GLN:HE21	1.86	0.41
1:A:222:ALA:HA	1:A:228:LEU:HD23	2.03	0.41
1:A:632:ARG:NH2	1:B:406:ARG:CZ	2.84	0.40
1:B:409:LEU:HD12	1:B:409:LEU:HA	1.73	0.40
1:B:165:LEU:C	1:B:167:ASP:N	2.78	0.40
1:B:721:ILE:HA	1:B:722:PRO:HD3	1.94	0.40
1:A:518:TYR:CD1	1:A:518:TYR:C	2.99	0.40
1:B:647:ASN:ND2	1:B:647:ASN:N	2.69	0.40
1:B:657:ILE:HD13	1:B:671:GLN:HB3	2.04	0.40
1:A:613:THR:HG23	1:A:615:PHE:H	1.86	0.40
1:B:172:LEU:HD12	1:B:174:ILE:CD1	2.42	0.40
1:B:263:THR:O	1:B:266:ALA:N	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:767:HOH:O	4:A:767:HOH:O[52_555]	1.74	0.46

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	509/624 (82%)	468 (92%)	29 (6%)	12 (2%)	4 8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	553/624 (89%)	506 (92%)	41 (7%)	6 (1%)	11	22
All	All	1062/1248 (85%)	974 (92%)	70 (7%)	18 (2%)	7	13

All (18) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/545 (82%)	394 (89%)	50 (11%)	5	12
1	B	489/545 (90%)	437 (89%)	52 (11%)	6	14
All	All	933/1090 (86%)	831 (89%)	102 (11%)	6	13

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	LYS
1	A	208	LEU
1	A	209	THR
1	A	211	ARG
1	A	216	ARG
1	A	220	GLU
1	A	226	GLU
1	A	227	THR
1	A	238	GLN
1	A	242	ARG
1	A	244	GLU
1	A	252	LEU
1	A	327	GLU
1	A	331	ARG
1	A	344	CYS
1	A	350	GLN
1	A	388	SER
1	A	406	ARG
1	A	409	LEU
1	A	414	LEU
1	A	418	LEU
1	A	419	ASP
1	A	424	SER
1	A	487	LYS
1	A	501	SER
1	A	502	VAL
1	A	512	THR
1	A	513	SER
1	A	515	GLN
1	A	526	SER
1	A	530	ARG
1	A	535	SER
1	A	545	SER
1	A	563	SER
1	A	577	LEU
1	A	613	THR
1	A	630	ARG
1	A	632	ARG
1	A	645	ASN
1	A	652	VAL
1	A	657	ILE
1	A	665	ARG
1	A	670	ARG

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Mol	Chain	Res	Type
1	A	676	THR
1	A	677	ASN
1	A	685	ASP
1	A	691	GLU
1	A	710	SER
1	A	745	SER
1	A	753	SER
1	B	159	LYS
1	B	160	MET
1	B	162	PHE
1	B	164	GLU
1	B	172	LEU
1	B	173	ASN
1	B	182	ARG
1	B	199	GLU
1	B	201	ILE
1	B	202	GLU
1	B	226	GLU
1	B	227	THR
1	B	242	ARG
1	B	253	SER
1	B	261	SER
1	B	262	GLU
1	B	263	THR
1	B	331	ARG
1	B	344	CYS
1	B	388	SER
1	B	406	ARG
1	B	409	LEU
1	B	414	LEU
1	B	416	GLN
1	B	421	VAL
1	B	423	THR
1	B	486	LEU
1	B	488	LEU
1	B	501	SER
1	B	502	VAL
1	B	509	SER
1	B	515	GLN
1	B	526	SER
1	B	535	SER
1	B	545	SER

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Mol	Chain	Res	Type
1	B	577	LEU
1	B	607	PHE
1	B	613	THR
1	B	614	THR
1	B	647	ASN
1	B	651	ILE
1	B	652	VAL
1	B	657	ILE
1	B	665	ARG
1	B	676	THR
1	B	677	ASN
1	B	685	ASP
1	B	691	GLU
1	B	709	SER
1	B	745	SER
1	B	753	SER
1	B	756	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	GLN
1	A	239	HIS
1	A	241	GLN
1	A	291	HIS
1	A	349	ASN
1	A	392	HIS
1	A	543	ASN
1	A	594	GLN
1	A	639	GLN
1	A	640	GLN
1	A	661	HIS
1	A	718	GLN
1	A	728	GLN
1	A	734	HIS
1	B	241	GLN
1	B	291	HIS
1	B	349	ASN
1	B	350	GLN
1	B	392	HIS
1	B	515	GLN
1	B	594	GLN

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Mol	Chain	Res	Type
1	B	647	ASN
1	B	661	HIS
1	B	718	GLN
1	B	728	GLN
1	B	734	HIS
1	B	739	ASN
1	B	742	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	5	-	2,2,3	0.67	0	1,1,3	0.88	0
3	ACT	B	5	-	3,3,3	0.89	0	3,3,3	1.25	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.25	23 (4%)	38 33	17, 34, 83, 124	11 (2%)
1	B	555/624 (88%)	-0.22	22 (3%)	42 38	17, 35, 82, 117	17 (3%)
All	All	1064/1248 (85%)	-0.23	45 (4%)	40 36	17, 35, 83, 124	28 (2%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	PHE	6.2
1	A	203	THR	6.2
1	A	202	GLU	5.9
1	A	510	PRO	5.7
1	B	170	LYS	5.6
1	A	205	TYR	5.3
1	B	510	PRO	4.4
1	B	515	GLN	4.3
1	A	421	VAL	4.3
1	A	206	LYS	4.2
1	A	200	GLU	4.1
1	A	201	ILE	4.1
1	B	509	SER	3.9
1	A	648	LYS	3.8
1	A	509	SER	3.5
1	B	197	GLU	3.5
1	B	711	SER	3.2
1	A	645	ASN	3.2
1	B	159	LYS	3.2
1	A	647	ASN	3.1
1	B	158	ASN	3.1
1	A	207	MET	3.0
1	B	171	GLU	3.0
1	A	649	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	162	PHE	3.0
1	B	178	ASP	2.8
1	B	174	ILE	2.7
1	B	650	SER	2.6
1	A	644	VAL	2.6
1	B	179	GLY	2.6
1	B	266	ALA	2.5
1	B	168	PHE	2.5
1	A	209	THR	2.4
1	A	613	THR	2.4
1	A	533	GLN	2.4
1	B	167	ASP	2.3
1	A	650	SER	2.3
1	A	266	ALA	2.2
1	A	646	LYS	2.2
1	B	173	ASN	2.2
1	B	646	LYS	2.2
1	A	709	SER	2.2
1	B	166	LYS	2.2
1	B	177	ASP	2.2
1	B	172	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	BA	A	3	1/1	0.75	0.10	101,101,101,101	1
2	BA	B	3	1/1	0.87	0.09	86,86,86,86	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	BA	B	2	1/1	0.89	0.08	93,93,93,93	1
3	ACT	A	5	3/4	0.89	0.07	36,36,36,38	0
2	BA	A	2	1/1	0.90	0.07	99,99,99,99	1
2	BA	A	1	1/1	0.92	0.05	71,71,71,71	1
2	BA	B	1	1/1	0.95	0.03	61,61,61,61	1
3	ACT	B	5	4/4	0.99	0.05	25,27,27,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.