



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:10 PM UTC

PDB ID : 3IHY / pdb_00003ihy
Title : Human PIK3C3 crystal structure
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Deposited on : 2009-07-31
Resolution : 2.80 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
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)

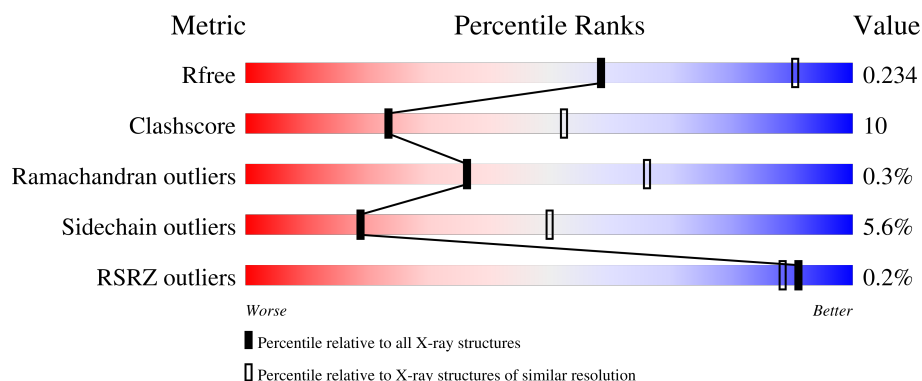
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	600	
1	B	600	
1	C	600	

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Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	D	600	% 64% 23% • 12%
1	E	600	69% 18% • 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21670 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 Phosphatidylinositol 3-kinase catalytic subunit type 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4343	2774	735	810	24			
1	B	535	Total	C	N	O	S	0	0	0
			4339	2771	735	809	24			
1	C	537	Total	C	N	O	S	0	0	0
			4344	2773	735	812	24			
1	D	531	Total	C	N	O	S	0	0	0
			4303	2752	728	800	23			
1	E	535	Total	C	N	O	S	0	0	0
			4340	2772	736	808	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8NEB9
A	-1	MET	-	expression tag	UNP Q8NEB9
B	-2	SER	-	expression tag	UNP Q8NEB9
B	-1	MET	-	expression tag	UNP Q8NEB9
C	-2	SER	-	expression tag	UNP Q8NEB9
C	-1	MET	-	expression tag	UNP Q8NEB9
D	280	SER	-	expression tag	UNP Q8NEB9
D	281	MET	-	expression tag	UNP Q8NEB9
E	-2	SER	-	expression tag	UNP Q8NEB9
E	-1	MET	-	expression tag	UNP Q8NEB9

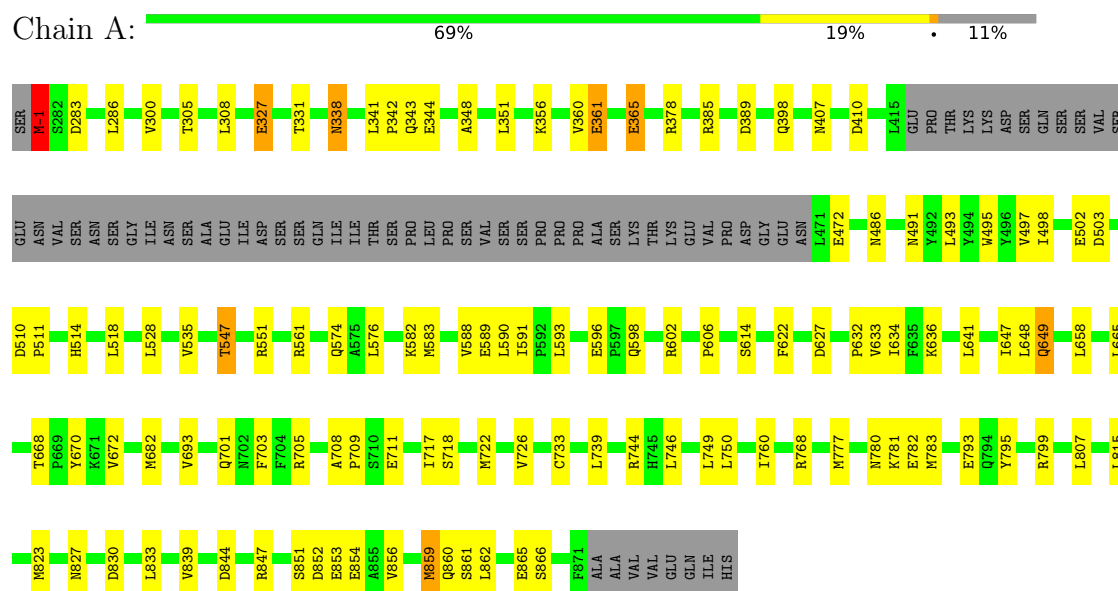
- Molecule 2 is water.

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

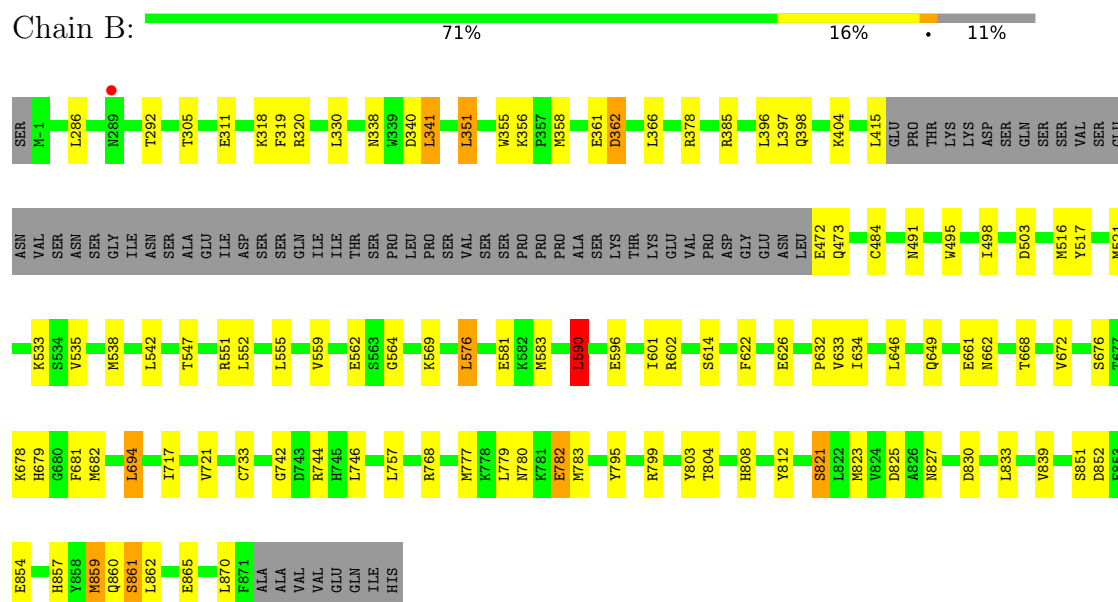
3 Residue-property plots

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

• Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3

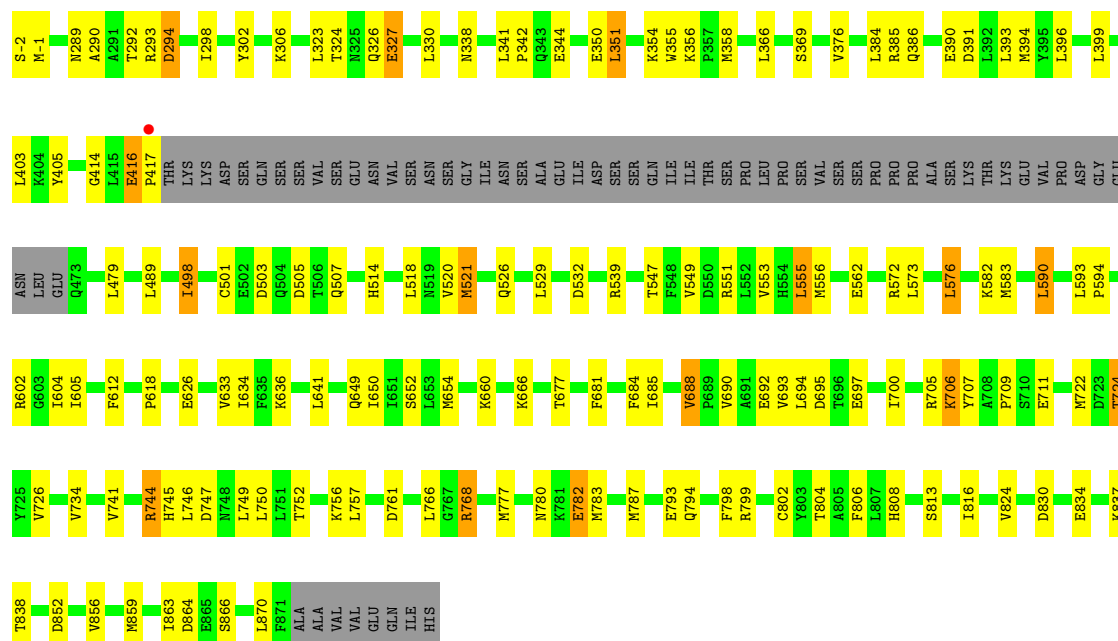


• Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3



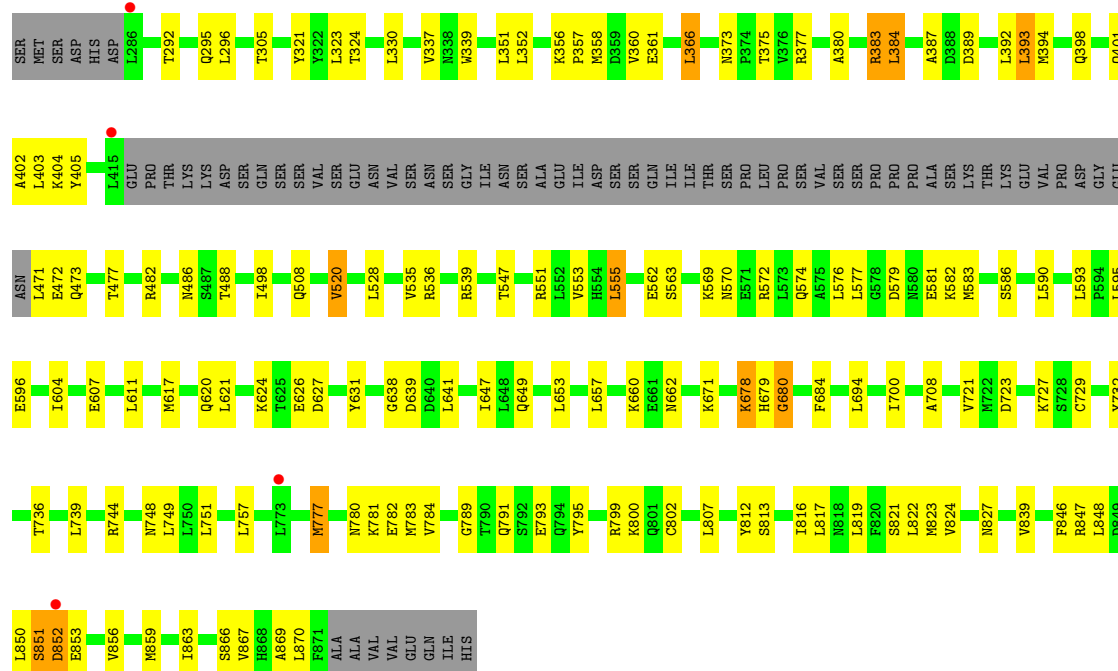
• Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3

Chain C:  65% 22% 10%



• Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3

Chain D:  64% 23% 12%



• Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3

Chain E:  69% 18% 11%

S-2	M-1	A290	R293	L296	T305	Y321	Y322	L323	T324	N326	N338	L341	P342	Q343	E344	K356	V360	E361	L366	N373	P374	R383	L384	R385	Q386	A387	D388	E389	E390	D391	M394	Y395	L396	L397	L415	GLU	PRO	THR	LYS	LYS	ASP	SER	GLN	SER	SER
VAL	SER	GLU	ASN	VAL	SER	ASN	SER	GLY	ILE	ASN	ALA	GLU	ILE	ASP	SER	SER	GLN	PRO	LEU	PRO	PRO	PRO	ALA	SER	LYS	THR	LYS	GLU	VAL	PRO	ASP	GLY	GLU	ASN	LEU	GLU	Q473	F478	R482	L489	L493	Y494	W495	Y496	V497
I498	D503	Q504	D505	R509	M521	L528	L529	D532	R539	A544	T547	P548	R551	M556	Q560	N570	Q574	A576	L576	L577	M583	N584	L585	S586	D587	V588	E589	L590	I591	P592	L593	P594	R602	T610	M617	F623	K630	V633							
K636	L641	L646	Q649	T668	V672	T677	F681	M682	V688	P689	V690	V693	L694	I700	F704	S710	E711	N712	C713	I717	K727	A730	C733	T736	V741	L746	L750	L766	D769	P770	M777	K778	L779	N780	K781	E782									
M783	Y795	R799	K800	T804	A805	F806	R810	N814	L815	N823	I831	A832	L833	T838	D852	V856	M859	L870	F871	ALA	ALA	VAL	VAL	GLU	GLN	ILE	HIS																		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	62.30Å 96.49Å 150.68Å 107.77° 91.75° 92.41°	Depositor
Resolution (Å)	19.84 – 2.80 19.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.84-2.80) 98.8 (19.84-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.187 , 0.255 (Not available) , 0.234	Depositor DCC
R_{free} test set	4076 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.058 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21670	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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 ⓘ

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	0.88	1/4428 (0.0%)	0.97	6/5985 (0.1%)
1	B	0.90	2/4423 (0.0%)	1.00	5/5975 (0.1%)
1	C	0.82	1/4430 (0.0%)	0.96	3/5990 (0.1%)
1	D	0.78	0/4387	0.95	5/5930 (0.1%)
1	E	0.84	0/4425	0.97	2/5978 (0.0%)
All	All	0.85	4/22093 (0.0%)	0.97	21/29858 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-1	MET	C-N	13.63	1.54	1.33
1	B	717	ILE	C-O	-5.57	1.18	1.24
1	B	742	GLY	N-CA	5.45	1.48	1.44
1	C	-1	MET	C-N	5.27	1.40	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	-1	MET	CA-C-N	-9.27	108.16	122.62
1	A	-1	MET	C-N-CA	-9.27	108.16	122.62
1	D	596	GLU	CA-C-N	7.19	127.19	119.28
1	D	596	GLU	C-N-CA	7.19	127.19	119.28
1	B	559	VAL	N-CA-C	6.15	116.27	110.30
1	E	-1	MET	O-C-N	-6.06	115.80	121.56
1	B	596	GLU	CA-C-N	5.84	125.54	119.82
1	B	596	GLU	C-N-CA	5.84	125.54	119.82
1	C	824	VAL	CB-CA-C	-5.53	103.59	112.16
1	D	520	VAL	N-CA-C	-5.46	105.00	110.30
1	D	680	GLY	N-CA-C	5.43	119.58	110.56
1	A	593	LEU	CA-C-N	-5.42	113.32	119.28
1	A	593	LEU	C-N-CA	-5.42	113.32	119.28
1	A	596	GLU	CA-C-N	5.36	125.17	119.28
1	A	596	GLU	C-N-CA	5.36	125.17	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	350	GLU	N-CA-C	-5.30	105.50	111.28
1	B	341	LEU	CA-C-N	5.19	125.49	119.47
1	B	341	LEU	C-N-CA	5.19	125.49	119.47
1	D	853	GLU	N-CA-C	-5.16	106.15	112.90
1	E	493	LEU	N-CA-C	-5.07	105.75	111.28
1	C	376	VAL	N-CA-C	-5.04	105.79	110.53

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	4343	0	4380	80	0
1	B	4339	0	4376	66	0
1	C	4344	0	4370	111	0
1	D	4303	0	4348	92	0
1	E	4340	0	4390	98	0
2	B	1	0	0	0	0
All	All	21670	0	21864	445	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 10.

All (445) 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:E:733:CYS:SG	1:E:777:MET:HE2	1.79	1.21
1:C:547:THR:HG22	1:C:551:ARG:NH1	1.67	1.08
1:D:398:GLN:HG3	1:D:823:MET:HE1	1.36	1.07
1:A:398:GLN:HG3	1:A:823:MET:HE1	1.36	1.06
1:D:749:LEU:HD21	1:D:783:MET:HE2	1.09	1.05
1:E:646:LEU:HD13	1:E:823:MET:HE2	1.40	1.03
1:C:330:LEU:HD23	1:C:358:MET:HE2	1.44	0.99
1:C:852:ASP:O	1:C:856:VAL:HG23	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:MET:N	1:A:-1:MET:HE2	1.77	0.98
1:D:780:ASN:HB3	1:D:783:MET:HE3	1.45	0.97
1:E:736:THR:HG22	1:E:741:VAL:HG11	1.47	0.96
1:A:-1:MET:HE2	1:A:-1:MET:H1	1.27	0.95
1:D:749:LEU:CD2	1:D:783:MET:HE2	1.98	0.93
1:A:398:GLN:HG3	1:A:823:MET:CE	2.02	0.90
1:A:398:GLN:CG	1:A:823:MET:HE1	2.02	0.89
1:A:-1:MET:HE2	1:A:-1:MET:CA	2.04	0.88
1:D:851:SER:O	1:D:852:ASP:HB2	1.74	0.86
1:D:749:LEU:HD21	1:D:783:MET:CE	2.01	0.86
1:B:733:CYS:SG	1:B:777:MET:HE1	2.17	0.84
1:E:733:CYS:SG	1:E:777:MET:CE	2.65	0.84
1:B:503:ASP:OD2	1:B:827:ASN:ND2	2.10	0.84
1:E:547:THR:CG2	1:E:551:ARG:HH12	1.91	0.84
1:A:503:ASP:OD2	1:A:827:ASN:ND2	2.11	0.83
1:B:547:THR:HG22	1:B:551:ARG:NH1	1.93	0.83
1:C:521:MET:HA	1:C:521:MET:HE3	1.60	0.83
1:D:398:GLN:HG3	1:D:823:MET:CE	2.09	0.82
1:D:851:SER:O	1:D:852:ASP:CB	2.28	0.82
1:D:398:GLN:CG	1:D:823:MET:HE1	2.10	0.81
1:B:768:ARG:HD3	1:B:830:ASP:OD1	1.80	0.81
1:C:734:VAL:HG22	1:C:859:MET:HE1	1.62	0.81
1:C:547:THR:HG22	1:C:551:ARG:HH12	1.48	0.79
1:A:547:THR:HG22	1:A:551:ARG:NH1	1.98	0.78
1:B:672:VAL:HG22	1:B:682:MET:HG3	1.66	0.78
1:A:658:LEU:HD13	1:A:665:LEU:HD12	1.67	0.77
1:B:398:GLN:OE1	1:B:823:MET:HE1	1.85	0.76
1:C:330:LEU:HD23	1:C:358:MET:CE	2.14	0.76
1:A:398:GLN:OE1	1:A:823:MET:HE1	1.85	0.75
1:D:305:THR:HG21	1:D:839:VAL:HG11	1.68	0.75
1:C:547:THR:CG2	1:C:551:ARG:NH1	2.47	0.75
1:E:529:LEU:HD21	1:E:539:ARG:CZ	2.17	0.75
1:C:749:LEU:HD21	1:C:783:MET:CE	2.17	0.74
1:D:360:VAL:HG11	1:D:387:ALA:HB2	1.69	0.74
1:E:547:THR:HG23	1:E:551:ARG:NH1	2.03	0.74
1:C:734:VAL:HG22	1:C:859:MET:CE	2.17	0.74
1:B:576:LEU:HG	1:B:583:MET:HE3	1.68	0.73
1:B:633:VAL:HG11	1:B:681:PHE:HD1	1.54	0.73
1:B:780:ASN:HB2	1:B:783:MET:HE3	1.69	0.73
1:D:394:MET:HE3	1:D:653:LEU:HD11	1.69	0.72
1:C:555:LEU:C	1:C:555:LEU:HD23	2.14	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:641:LEU:HD12	1:D:680:GLY:HA3	1.71	0.72
1:C:562:GLU:HG2	1:C:572:ARG:HH11	1.54	0.72
1:B:547:THR:HG22	1:B:551:ARG:HH11	1.54	0.72
1:C:749:LEU:HD21	1:C:783:MET:HE2	1.72	0.71
1:E:577:LEU:O	1:E:586:SER:OG	2.10	0.70
1:A:398:GLN:CD	1:A:823:MET:HE1	2.16	0.69
1:B:398:GLN:HG3	1:B:823:MET:HE1	1.74	0.69
1:E:672:VAL:HG22	1:E:682:MET:HE2	1.74	0.69
1:D:781:LYS:HG3	1:D:870:LEU:HD22	1.72	0.69
1:A:547:THR:HG22	1:A:551:ARG:HH12	1.58	0.69
1:C:590:LEU:HD21	1:C:626:GLU:HG3	1.75	0.68
1:E:397:LEU:HD23	1:E:649:GLN:OE1	1.94	0.68
1:A:851:SER:OG	1:A:854:GLU:OE1	2.05	0.67
1:E:547:THR:HG22	1:E:551:ARG:HH12	1.58	0.67
1:A:859:MET:HE2	1:A:862:LEU:HD12	1.75	0.67
1:D:780:ASN:CB	1:D:783:MET:HE3	2.22	0.67
1:A:861:SER:O	1:A:865:GLU:HG3	1.94	0.67
1:C:358:MET:CE	1:C:366:LEU:HD11	2.25	0.67
1:D:732:TYR:O	1:D:736:THR:HG23	1.94	0.67
1:C:654:MET:HE2	1:C:816:ILE:HD13	1.78	0.66
1:E:547:THR:CG2	1:E:551:ARG:NH1	2.59	0.66
1:D:292:THR:HA	1:D:295:GLN:HG3	1.78	0.65
1:D:802:CYS:HB3	1:D:859:MET:HE2	1.79	0.65
1:A:547:THR:CG2	1:A:551:ARG:NH1	2.61	0.64
1:E:503:ASP:HA	1:E:677:THR:HG21	1.80	0.64
1:A:283:ASP:HA	1:A:286:LEU:HD13	1.78	0.64
1:A:-1:MET:CA	1:A:-1:MET:CE	2.75	0.64
1:E:338:ASN:OD1	1:E:344:GLU:OE1	2.15	0.64
1:D:562:GLU:O	1:D:569:LYS:NZ	2.31	0.63
1:D:863:ILE:O	1:D:867:VAL:HG23	1.98	0.63
1:B:646:LEU:HD11	1:B:823:MET:HE3	1.81	0.63
1:A:780:ASN:HB3	1:A:783:MET:HE3	1.80	0.63
1:C:547:THR:CG2	1:C:551:ARG:HH12	2.11	0.62
1:C:416:GLU:N	1:C:417:PRO:HD2	2.14	0.62
1:B:768:ARG:CD	1:B:830:ASP:OD1	2.47	0.62
1:E:780:ASN:HB2	1:E:783:MET:HE3	1.82	0.61
1:C:503:ASP:HA	1:C:677:THR:HG21	1.81	0.61
1:C:690:VAL:HG12	1:C:746:LEU:HD13	1.81	0.61
1:D:330:LEU:HD23	1:D:358:MET:HE2	1.82	0.60
1:E:736:THR:CG2	1:E:741:VAL:HG11	2.28	0.60
1:E:806:PHE:CG	1:E:859:MET:HE3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:859:MET:HE3	1:D:863:ILE:HG13	1.83	0.59
1:C:393:LEU:HD12	1:C:393:LEU:O	2.01	0.59
1:A:746:LEU:HD21	1:A:780:ASN:ND2	2.18	0.59
1:E:529:LEU:HD22	1:E:539:ARG:CD	2.31	0.59
1:D:572:ARG:NH1	1:D:576:LEU:HD11	2.17	0.59
1:E:690:VAL:HG11	1:E:746:LEU:HD22	1.85	0.59
1:E:321:TYR:O	1:E:324:THR:HB	2.03	0.58
1:B:398:GLN:HG3	1:B:823:MET:CE	2.33	0.58
1:C:555:LEU:HD21	1:C:573:LEU:HD13	1.86	0.58
1:E:570:ASN:O	1:E:574:GLN:HG3	2.03	0.58
1:E:636:LYS:HD2	1:E:641:LEU:HD21	1.84	0.58
1:C:746:LEU:HD21	1:C:780:ASN:HD21	1.69	0.58
1:E:672:VAL:CG2	1:E:682:MET:HE2	2.34	0.57
1:E:795:TYR:CE2	1:E:799:ARG:HD2	2.40	0.57
1:E:852:ASP:O	1:E:856:VAL:HG23	2.04	0.57
1:C:547:THR:HG22	1:C:551:ARG:HH11	1.65	0.57
1:D:570:ASN:O	1:D:574:GLN:HG3	2.04	0.57
1:E:736:THR:HB	1:E:741:VAL:HG13	1.87	0.57
1:E:590:LEU:HD13	1:E:602:ARG:NH1	2.20	0.56
1:B:633:VAL:HG12	1:B:634:ILE:N	2.19	0.56
1:C:633:VAL:HG11	1:C:681:PHE:HD1	1.71	0.56
1:B:780:ASN:CB	1:B:783:MET:HE3	2.36	0.56
1:D:394:MET:HE3	1:D:653:LEU:CD1	2.33	0.56
1:B:320:ARG:HD2	1:B:351:LEU:HD13	1.88	0.56
1:C:403:LEU:HD13	1:C:520:VAL:HG21	1.87	0.56
1:E:396:LEU:HD22	1:E:489:LEU:HD23	1.88	0.56
1:E:391:ASP:OD1	1:E:394:MET:HE2	2.06	0.56
1:B:859:MET:HE3	1:B:859:MET:HA	1.88	0.56
1:D:292:THR:HA	1:D:295:GLN:CG	2.35	0.56
1:D:358:MET:HE1	1:D:366:LEU:HD21	1.87	0.56
1:E:570:ASN:HD21	1:E:610:THR:HG23	1.71	0.56
1:A:361:GLU:HB2	1:A:815:LEU:HD13	1.87	0.55
1:C:324:THR:HG22	1:C:355:TRP:CE3	2.41	0.55
1:B:398:GLN:CD	1:B:823:MET:HE1	2.31	0.55
1:C:399:LEU:HD13	1:C:479:LEU:HD21	1.88	0.55
1:A:305:THR:HG21	1:A:839:VAL:HG11	1.87	0.55
1:B:362:ASP:OD2	1:B:362:ASP:N	2.38	0.55
1:C:666:LYS:HG3	1:C:724:THR:HG23	1.88	0.55
1:E:529:LEU:CD2	1:E:539:ARG:NE	2.69	0.55
1:D:393:LEU:HD11	1:D:488:THR:HG22	1.88	0.55
1:E:588:VAL:HG22	1:E:602:ARG:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:729:CYS:SG	1:D:757:LEU:HD13	2.46	0.55
1:D:620:GLN:NE2	1:D:684:PHE:CE1	2.75	0.55
1:C:802:CYS:HB3	1:C:859:MET:HE3	1.89	0.55
1:C:806:PHE:HB2	1:C:859:MET:HE2	1.88	0.55
1:D:377:ARG:O	1:D:380:ALA:HB3	2.07	0.55
1:E:556:MET:O	1:E:560:GLN:HG3	2.07	0.55
1:B:564:GLY:O	1:B:569:LYS:NZ	2.40	0.55
1:C:358:MET:HE1	1:C:366:LEU:HD11	1.89	0.55
1:B:398:GLN:CG	1:B:823:MET:HE1	2.36	0.55
1:D:579:ASP:OD1	1:D:581:GLU:HG2	2.07	0.55
1:B:622:PHE:CE2	1:B:632:PRO:HB3	2.42	0.54
1:E:532:ASP:C	1:E:532:ASP:OD1	2.50	0.54
1:D:528:LEU:O	1:D:535:VAL:HG12	2.08	0.54
1:A:852:ASP:O	1:A:856:VAL:HG23	2.07	0.54
1:C:749:LEU:HD21	1:C:783:MET:HE3	1.88	0.54
1:C:834:GLU:OE1	1:C:837:LYS:HD3	2.08	0.54
1:B:305:THR:HG21	1:B:839:VAL:HG11	1.90	0.54
1:C:593:LEU:HD12	1:C:594:PRO:HD2	1.89	0.54
1:D:821:SER:O	1:D:824:VAL:HG13	2.07	0.54
1:C:384:LEU:C	1:C:386:GLN:H	2.16	0.54
1:C:396:LEU:HD22	1:C:489:LEU:HD23	1.88	0.54
1:C:414:GLY:O	1:C:526:GLN:NE2	2.41	0.54
1:A:576:LEU:HD22	1:A:583:MET:HE3	1.89	0.53
1:B:851:SER:O	1:B:852:ASP:C	2.51	0.53
1:D:708:ALA:CB	1:D:721:VAL:HG21	2.38	0.53
1:C:289:ASN:HB2	1:C:292:THR:HG23	1.90	0.53
1:C:749:LEU:HD23	1:C:757:LEU:HD11	1.90	0.53
1:C:804:THR:HG22	1:C:808:HIS:CD2	2.42	0.53
1:E:576:LEU:HD22	1:E:583:MET:HE2	1.91	0.53
1:E:736:THR:HG22	1:E:741:VAL:CG1	2.31	0.53
1:B:521:MET:HE3	1:B:521:MET:HA	1.89	0.53
1:C:688:VAL:HG12	1:C:693:VAL:HG23	1.90	0.53
1:A:668:THR:HG22	1:A:668:THR:O	2.08	0.53
1:A:-1:MET:H1	1:A:-1:MET:CE	2.10	0.53
1:A:768:ARG:HD3	1:A:830:ASP:OD1	2.09	0.53
1:D:657:LEU:HD22	1:D:812:TYR:CE1	2.43	0.53
1:A:746:LEU:HD21	1:A:780:ASN:HD21	1.74	0.52
1:B:777:MET:HG3	1:B:862:LEU:HB3	1.90	0.52
1:D:847:ARG:NH2	1:D:850:LEU:HD21	2.24	0.52
1:D:590:LEU:HD12	1:D:590:LEU:H	1.74	0.52
1:A:327:GLU:HB3	1:A:356:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:650:ILE:CG2	1:C:654:MET:HE3	2.40	0.52
1:A:341:LEU:HD23	1:A:343:GLN:H	1.74	0.52
1:C:654:MET:CE	1:C:816:ILE:HD13	2.40	0.52
1:D:576:LEU:HD23	1:D:583:MET:SD	2.50	0.52
1:D:398:GLN:NE2	1:D:819:LEU:HD22	2.25	0.52
1:E:633:VAL:HG11	1:E:681:PHE:HD1	1.75	0.52
1:C:358:MET:HE3	1:C:366:LEU:HD11	1.91	0.52
1:D:723:ASP:OD2	1:D:727:LYS:NZ	2.31	0.52
1:D:647:ILE:HD12	1:D:739:LEU:HD13	1.91	0.51
1:A:795:TYR:CE2	1:A:799:ARG:HD2	2.45	0.51
1:E:521:MET:HE3	1:E:521:MET:O	2.10	0.51
1:E:736:THR:HB	1:E:741:VAL:CG1	2.41	0.51
1:A:701:GLN:HB3	1:A:705:ARG:NH2	2.25	0.51
1:E:766:LEU:HD13	1:E:838:THR:HG23	1.93	0.51
1:A:338:ASN:OD1	1:A:338:ASN:N	2.43	0.51
1:A:636:LYS:HD2	1:A:641:LEU:HD21	1.92	0.51
1:A:807:LEU:HD11	1:A:856:VAL:CG2	2.41	0.51
1:D:795:TYR:OH	1:D:867:VAL:HG21	2.11	0.51
1:C:722:MET:O	1:C:726:VAL:HG23	2.11	0.51
1:E:704:PHE:HB3	1:E:717:ILE:CG2	2.41	0.51
1:A:341:LEU:HD23	1:A:342:PRO:HD2	1.93	0.51
1:E:769:ASP:CG	1:E:770:PRO:HD2	2.36	0.51
1:E:290:ALA:HA	1:E:293:ARG:NH1	2.25	0.51
1:A:589:GLU:O	1:A:591:ILE:HG23	2.10	0.51
1:E:385:ARG:HG2	1:E:478:PHE:CE1	2.46	0.51
1:E:623:PHE:O	1:E:630:LYS:HA	2.11	0.51
1:D:402:ALA:HB2	1:D:822:LEU:HD22	1.92	0.50
1:A:344:GLU:O	1:A:348:ALA:N	2.42	0.50
1:C:745:HIS:CE1	1:C:747:ASP:HB2	2.47	0.50
1:D:321:TYR:O	1:D:324:THR:HG22	2.12	0.50
1:E:529:LEU:CD2	1:E:539:ARG:CZ	2.87	0.50
1:A:547:THR:CG2	1:A:551:ARG:HH11	2.24	0.50
1:A:859:MET:CE	1:A:862:LEU:HD12	2.40	0.50
1:B:757:LEU:HD23	1:B:757:LEU:C	2.37	0.50
1:D:389:ASP:CG	1:D:486:ASN:HD22	2.19	0.50
1:B:361:GLU:CD	1:B:361:GLU:H	2.19	0.50
1:D:358:MET:O	1:D:383:ARG:NH1	2.44	0.50
1:D:553:VAL:HG21	1:D:679:HIS:CE1	2.46	0.50
1:E:360:VAL:HG22	1:E:383:ARG:O	2.11	0.50
1:E:529:LEU:HD22	1:E:539:ARG:NE	2.26	0.50
1:C:741:VAL:HG12	1:C:744:ARG:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:ARG:HD2	1:A:833:LEU:HD12	1.93	0.50
1:B:330:LEU:HD13	1:B:355:TRP:CD2	2.46	0.50
1:D:744:ARG:HH12	1:D:748:ASN:HB3	1.77	0.50
1:E:700:ILE:HD12	1:E:782:GLU:O	2.12	0.50
1:B:292:THR:HG21	1:B:319:PHE:CE2	2.47	0.50
1:C:551:ARG:HD2	1:C:583:MET:O	2.11	0.50
1:A:722:MET:O	1:A:726:VAL:HG23	2.12	0.49
1:C:799:ARG:NH2	1:C:864:ASP:OD1	2.41	0.49
1:E:704:PHE:HB3	1:E:717:ILE:HG23	1.94	0.49
1:B:404:LYS:NZ	1:B:825:ASP:O	2.45	0.49
1:B:668:THR:HG22	1:B:668:THR:O	2.13	0.49
1:C:302:TYR:CD2	1:C:306:LYS:HG2	2.47	0.49
1:D:394:MET:HB3	1:D:653:LEU:HD13	1.94	0.49
1:D:398:GLN:OE1	1:D:823:MET:HE1	2.13	0.49
1:E:690:VAL:CG1	1:E:746:LEU:HD22	2.41	0.49
1:C:532:ASP:C	1:C:532:ASP:OD1	2.55	0.49
1:D:807:LEU:HD21	1:D:856:VAL:HG23	1.93	0.49
1:C:697:GLU:OE2	1:C:706:LYS:NZ	2.43	0.49
1:C:330:LEU:HD13	1:C:355:TRP:CD2	2.48	0.49
1:D:638:GLY:O	1:D:678:LYS:NZ	2.41	0.49
1:C:289:ASN:HD22	1:C:292:THR:HG23	1.76	0.49
1:D:586:SER:O	1:D:624:LYS:NZ	2.41	0.49
1:E:544:ALA:HB1	1:E:591:ILE:HG21	1.94	0.49
1:E:570:ASN:ND2	1:E:610:THR:HG23	2.26	0.49
1:E:736:THR:CB	1:E:741:VAL:CG1	2.91	0.49
1:C:766:LEU:HD13	1:C:838:THR:HG23	1.94	0.49
1:D:582:LYS:HG3	1:D:583:MET:HG2	1.95	0.49
1:E:361:GLU:HB2	1:E:815:LEU:HD13	1.94	0.49
1:B:662:ASN:HD21	1:C:326:GLN:HG3	1.77	0.48
1:B:601:ILE:C	1:B:601:ILE:HD12	2.38	0.48
1:C:590:LEU:HD13	1:C:602:ARG:NH1	2.29	0.48
1:D:401:GLN:OE1	1:D:404:LYS:HE3	2.14	0.48
1:E:668:THR:O	1:E:668:THR:HG22	2.13	0.48
1:A:647:ILE:HD12	1:A:739:LEU:HD13	1.95	0.48
1:E:806:PHE:O	1:E:810:ARG:CG	2.62	0.48
1:C:746:LEU:HD21	1:C:780:ASN:ND2	2.28	0.48
1:D:473:GLN:NE2	1:D:477:THR:HG22	2.29	0.48
1:D:555:LEU:HD12	1:D:583:MET:SD	2.54	0.48
1:D:607:GLU:CD	1:D:607:GLU:H	2.22	0.48
1:D:813:SER:OG	1:D:848:LEU:HD21	2.14	0.48
1:E:800:LYS:O	1:E:804:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HD12	1:B:555:LEU:HD23	1.96	0.48
1:A:398:GLN:OE1	1:A:823:MET:CE	2.59	0.48
1:A:407:ASN:HB3	1:A:410:ASP:OD2	2.14	0.48
1:E:360:VAL:HG11	1:E:387:ALA:HB2	1.95	0.48
1:E:780:ASN:C	1:E:870:LEU:HD13	2.39	0.48
1:D:547:THR:HG22	1:D:551:ARG:HH11	1.79	0.47
1:A:327:GLU:OE2	1:A:327:GLU:N	2.47	0.47
1:C:866:SER:O	1:C:870:LEU:HG	2.13	0.47
1:D:375:THR:HG23	1:D:471:LEU:HD13	1.96	0.47
1:C:582:LYS:HE2	1:C:583:MET:HE3	1.96	0.47
1:E:387:ALA:O	1:E:482:ARG:NH2	2.46	0.47
1:A:574:GLN:HG2	1:A:606:PRO:O	2.13	0.47
1:D:590:LEU:HD23	1:D:626:GLU:HG3	1.96	0.47
1:B:804:THR:HG22	1:B:808:HIS:CE1	2.50	0.47
1:A:598:GLN:CD	1:A:598:GLN:H	2.22	0.47
1:C:583:MET:HE2	1:C:583:MET:HA	1.97	0.47
1:E:779:LEU:HD23	1:E:783:MET:HE1	1.96	0.47
1:E:688:VAL:HG12	1:E:693:VAL:HG23	1.97	0.47
1:B:590:LEU:HD21	1:B:626:GLU:HG3	1.96	0.47
1:E:323:LEU:C	1:E:325:ASN:H	2.23	0.47
1:B:318:LYS:HD3	1:B:319:PHE:CE2	2.50	0.46
1:B:633:VAL:CG1	1:B:634:ILE:N	2.77	0.46
1:C:521:MET:HA	1:C:521:MET:CE	2.35	0.46
1:E:494:TYR:CE1	1:E:498:ILE:HG13	2.50	0.46
1:A:389:ASP:CG	1:A:486:ASN:HD22	2.21	0.46
1:C:562:GLU:HG2	1:C:572:ARG:NH1	2.24	0.46
1:C:555:LEU:C	1:C:555:LEU:CD2	2.86	0.46
1:D:536:ARG:O	1:D:539:ARG:HB3	2.16	0.46
1:A:749:LEU:O	1:A:750:LEU:HD12	2.15	0.46
1:C:529:LEU:HD21	1:C:539:ARG:NH1	2.31	0.46
1:C:752:THR:OG1	1:C:756:LYS:HB2	2.14	0.46
1:A:733:CYS:SG	1:A:777:MET:HE3	2.56	0.46
1:B:358:MET:HE1	1:B:366:LEU:HD21	1.98	0.46
1:C:692:GLU:HA	1:C:695:ASP:HB3	1.96	0.46
1:A:582:LYS:HE2	1:A:583:MET:HE2	1.97	0.46
1:A:670:TYR:CE2	1:A:760:ILE:HG22	2.50	0.46
1:A:799:ARG:NH2	1:A:860:GLN:HG3	2.31	0.46
1:C:745:HIS:HE1	1:C:747:ASP:HB2	1.81	0.46
1:A:588:VAL:HG22	1:A:602:ARG:O	2.15	0.46
1:B:590:LEU:CD1	1:B:602:ARG:HG3	2.46	0.46
1:D:330:LEU:HD21	1:D:352:LEU:CD1	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:ALA:HA	1:E:293:ARG:HH11	1.81	0.45
1:E:338:ASN:OD1	1:E:338:ASN:N	2.49	0.45
1:B:803:TYR:OH	1:B:860:GLN:HG3	2.16	0.45
1:D:611:LEU:HD13	1:D:617:MET:HB3	1.97	0.45
1:C:289:ASN:HB2	1:C:292:THR:H	1.82	0.45
1:C:582:LYS:HG3	1:C:583:MET:HG2	1.98	0.45
1:D:604:ILE:HD13	1:D:621:LEU:HD13	1.99	0.45
1:B:857:HIS:O	1:B:861:SER:OG	2.33	0.45
1:A:672:VAL:HG22	1:A:682:MET:HG3	1.98	0.45
1:A:851:SER:CB	1:A:854:GLU:OE1	2.65	0.45
1:B:555:LEU:HD13	1:B:576:LEU:HB3	1.99	0.45
1:C:351:LEU:HD23	1:C:355:TRP:CZ3	2.52	0.45
1:D:777:MET:CE	1:D:863:ILE:HG12	2.47	0.45
1:E:795:TYR:CZ	1:E:799:ARG:HD2	2.52	0.45
1:D:296:LEU:HD22	1:D:323:LEU:HD11	1.99	0.45
1:D:813:SER:O	1:D:817:LEU:HG	2.17	0.45
1:A:561:ARG:O	1:A:561:ARG:HG3	2.16	0.45
1:C:369:SER:HB3	1:C:405:TYR:CE1	2.51	0.45
1:C:572:ARG:HG2	1:C:576:LEU:HD22	1.98	0.45
1:C:330:LEU:HD13	1:C:355:TRP:CG	2.51	0.45
1:C:777:MET:HE1	1:C:863:ILE:HA	1.98	0.45
1:D:398:GLN:CD	1:D:823:MET:HE1	2.42	0.45
1:B:484:CYS:O	1:B:535:VAL:HG22	2.17	0.44
1:D:789:GLY:C	1:D:791:GLN:H	2.25	0.44
1:C:768:ARG:NH1	1:C:830:ASP:OD1	2.50	0.44
1:D:547:THR:HG22	1:D:551:ARG:NH1	2.32	0.44
1:A:495:TRP:CE3	1:A:498:ILE:HD11	2.52	0.44
1:A:622:PHE:CE2	1:A:632:PRO:HB3	2.52	0.44
1:C:654:MET:HE2	1:C:816:ILE:CD1	2.46	0.44
1:E:391:ASP:HA	1:E:394:MET:HE2	2.00	0.44
1:B:385:ARG:HH12	1:B:473:GLN:HB2	1.82	0.44
1:E:806:PHE:O	1:E:810:ARG:HG2	2.17	0.44
1:B:538:MET:O	1:B:542:LEU:HG	2.17	0.44
1:C:549:VAL:O	1:C:553:VAL:HG23	2.18	0.44
1:E:781:LYS:N	1:E:870:LEU:HD13	2.33	0.44
1:A:861:SER:O	1:A:865:GLU:CG	2.65	0.44
1:B:821:SER:C	1:B:823:MET:H	2.26	0.44
1:A:633:VAL:CG1	1:A:634:ILE:N	2.81	0.44
1:A:795:TYR:CZ	1:A:799:ARG:HD2	2.52	0.44
1:E:389:ASP:OD1	1:E:482:ARG:NH1	2.50	0.44
1:C:507:GLN:HG3	1:C:514:HIS:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:627:ASP:OD2	1:D:627:ASP:N	2.42	0.44
1:E:750:LEU:N	1:E:750:LEU:CD1	2.80	0.43
1:E:782:GLU:H	1:E:782:GLU:CD	2.25	0.43
1:A:717:ILE:O	1:A:718:SER:C	2.60	0.43
1:B:646:LEU:CD1	1:B:823:MET:HE3	2.48	0.43
1:C:391:ASP:OD1	1:C:394:MET:HE2	2.18	0.43
1:E:694:LEU:HD21	1:E:782:GLU:HG3	1.99	0.43
1:A:493:LEU:O	1:A:497:VAL:HG23	2.18	0.43
1:C:768:ARG:HH11	1:C:830:ASP:CG	2.27	0.43
1:E:397:LEU:HD13	1:E:496:TYR:CE1	2.53	0.43
1:D:358:MET:CE	1:D:366:LEU:HD21	2.49	0.43
1:C:636:LYS:HD2	1:C:641:LEU:HD21	2.00	0.43
1:D:356:LYS:O	1:D:357:PRO:C	2.60	0.43
1:C:290:ALA:HA	1:C:293:ARG:NH1	2.33	0.43
1:C:633:VAL:CG1	1:C:634:ILE:N	2.81	0.43
1:C:684:PHE:O	1:C:685:ILE:HD13	2.18	0.43
1:E:736:THR:CG2	1:E:741:VAL:CG1	2.95	0.43
1:A:-1:MET:HE2	1:A:-1:MET:HA	1.95	0.43
1:A:733:CYS:SG	1:A:777:MET:CE	3.07	0.43
1:B:396:LEU:O	1:B:397:LEU:C	2.61	0.43
1:C:384:LEU:C	1:C:386:GLN:N	2.77	0.43
1:B:780:ASN:OD1	1:B:782:GLU:HG2	2.18	0.43
1:D:780:ASN:O	1:D:784:VAL:HG23	2.18	0.43
1:E:746:LEU:HD21	1:E:780:ASN:OD1	2.18	0.43
1:A:510:ASP:N	1:A:511:PRO:HD3	2.34	0.43
1:B:338:ASN:OD1	1:B:340:ASP:N	2.50	0.43
1:D:337:VAL:HG11	1:D:339:TRP:CZ3	2.54	0.43
1:E:-2:SER:O	1:E:-1:MET:HB2	2.18	0.43
1:A:514:HIS:NE2	1:A:518:LEU:HD11	2.34	0.42
1:A:749:LEU:HD21	1:A:783:MET:HE2	2.01	0.42
1:C:294:ASP:O	1:C:298:ILE:HG12	2.19	0.42
1:C:633:VAL:HG11	1:C:681:PHE:CD1	2.54	0.42
1:D:757:LEU:C	1:D:757:LEU:HD23	2.44	0.42
1:B:555:LEU:CD1	1:B:576:LEU:HB3	2.50	0.42
1:D:373:ASN:O	1:D:377:ARG:HG2	2.19	0.42
1:E:713:GLY:HA3	1:E:717:ILE:O	2.18	0.42
1:D:339:TRP:CE3	1:D:373:ASN:ND2	2.87	0.42
1:E:589:GLU:O	1:E:590:LEU:C	2.62	0.42
1:E:727:LYS:O	1:E:730:ALA:HB3	2.19	0.42
1:B:305:THR:HG21	1:B:839:VAL:CG1	2.50	0.42
1:D:384:LEU:HD22	1:D:392:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:LEU:HD22	1:A:535:VAL:HG13	2.02	0.42
1:A:693:VAL:HG13	1:A:703:PHE:HB2	2.02	0.42
1:C:761:ASP:OD1	1:C:761:ASP:C	2.62	0.42
1:C:330:LEU:CD2	1:C:358:MET:HE2	2.32	0.42
1:D:572:ARG:HG3	1:D:576:LEU:CD1	2.49	0.42
1:D:593:LEU:HD21	1:D:631:TYR:CE1	2.55	0.42
1:C:604:ILE:HG22	1:C:605:ILE:N	2.35	0.42
1:D:403:LEU:HD13	1:D:520:VAL:HG21	2.01	0.42
1:E:361:GLU:OE1	1:E:361:GLU:N	2.41	0.42
1:D:700:ILE:HG23	1:D:751:LEU:HD11	2.01	0.42
1:E:343:GLN:NE2	1:E:343:GLN:HA	2.34	0.42
1:A:844:ASP:O	1:A:847:ARG:HD2	2.20	0.42
1:B:662:ASN:ND2	1:C:326:GLN:HG3	2.35	0.42
1:C:695:ASP:OD1	1:C:695:ASP:C	2.63	0.42
1:C:706:LYS:HD2	1:C:707:TYR:CZ	2.54	0.42
1:D:377:ARG:HH22	1:D:405:TYR:HB2	1.84	0.42
1:E:296:LEU:HD22	1:E:323:LEU:HD21	2.02	0.41
1:E:560:GLN:NE2	1:E:617:MET:HB2	2.35	0.41
1:E:806:PHE:CD2	1:E:859:MET:HE3	2.54	0.41
1:B:398:GLN:H	1:B:398:GLN:NE2	2.19	0.41
1:B:516:MET:HE1	1:B:517:TYR:CZ	2.55	0.41
1:C:612:PHE:HB2	1:C:618:PRO:HG2	2.02	0.41
1:C:744:ARG:N	1:C:744:ARG:HD2	2.34	0.41
1:C:787:MET:HE1	1:C:798:PHE:CD1	2.55	0.41
1:C:794:GLN:OE1	1:C:794:GLN:N	2.49	0.41
1:A:331:THR:OG1	1:A:365:GLU:OE1	2.38	0.41
1:B:498:ILE:HD12	1:B:498:ILE:HA	1.82	0.41
1:C:734:VAL:HG22	1:C:859:MET:HE3	2.01	0.41
1:C:804:THR:HG22	1:C:808:HIS:HD2	1.86	0.41
1:A:859:MET:O	1:A:860:GLN:C	2.62	0.41
1:E:710:SER:O	1:E:711:GLU:C	2.63	0.41
1:E:779:LEU:HD23	1:E:783:MET:CE	2.50	0.41
1:E:831:ILE:HG12	1:E:838:THR:HG21	2.02	0.41
1:C:555:LEU:HD21	1:C:573:LEU:CD1	2.49	0.41
1:E:373:ASN:O	1:E:374:PRO:C	2.62	0.41
1:E:384:LEU:HD23	1:E:384:LEU:HA	1.89	0.41
1:B:338:ASN:OD1	1:B:338:ASN:C	2.62	0.41
1:B:547:THR:CG2	1:B:551:ARG:NH1	2.74	0.41
1:B:661:GLU:OE2	1:B:812:TYR:OH	2.39	0.41
1:E:689:PRO:HA	1:E:750:LEU:HD12	2.03	0.41
1:B:694:LEU:HD22	1:B:746:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:LEU:HD23	1:C:556:MET:N	2.35	0.41
1:C:582:LYS:HG3	1:C:583:MET:HE3	2.03	0.41
1:D:816:ILE:HD13	1:D:846:PHE:HZ	1.86	0.41
1:E:396:LEU:HD22	1:E:489:LEU:CD2	2.50	0.41
1:A:582:LYS:CG	1:A:583:MET:HE2	2.51	0.41
1:C:341:LEU:O	1:C:342:PRO:C	2.64	0.41
1:C:705:ARG:O	1:C:709:PRO:HB3	2.21	0.41
1:D:823:MET:HE2	1:D:823:MET:HB2	1.74	0.41
1:B:795:TYR:CE2	1:B:799:ARG:HD2	2.55	0.40
1:C:326:GLN:O	1:C:327:GLU:C	2.64	0.40
1:C:501:CYS:SG	1:C:518:LEU:HD23	2.62	0.40
1:C:700:ILE:HD12	1:C:782:GLU:O	2.20	0.40
1:A:648:LEU:HD13	1:A:648:LEU:HA	1.94	0.40
1:A:649:GLN:HE21	1:A:649:GLN:HB2	1.62	0.40
1:B:495:TRP:HA	1:B:498:ILE:HG22	2.04	0.40
1:C:498:ILE:HD13	1:C:498:ILE:HA	1.88	0.40
1:D:577:LEU:O	1:D:586:SER:HB2	2.21	0.40
1:E:394:MET:O	1:E:649:GLN:NE2	2.54	0.40
1:E:593:LEU:HD12	1:E:594:PRO:HD2	2.03	0.40
1:A:495:TRP:CZ3	1:A:498:ILE:HD11	2.56	0.40
1:D:387:ALA:O	1:D:482:ARG:NH2	2.53	0.40
1:E:547:THR:HG22	1:E:548:PHE:N	2.36	0.40
1:A:708:ALA:N	1:A:709:PRO:CD	2.84	0.40
1:B:676:SER:HB3	1:B:679:HIS:CE1	2.57	0.40
1:C:684:PHE:C	1:C:685:ILE:HD13	2.47	0.40
1:D:866:SER:O	1:D:869:ALA:HB3	2.21	0.40
1:E:806:PHE:O	1:E:810:ARG:HG3	2.20	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	532/600 (89%)	502 (94%)	28 (5%)	2 (0%)	30	60
1	B	530/600 (88%)	510 (96%)	19 (4%)	1 (0%)	43	72
1	C	533/600 (89%)	506 (95%)	24 (4%)	3 (1%)	21	51
1	D	527/600 (88%)	501 (95%)	24 (5%)	2 (0%)	30	60
1	E	531/600 (88%)	510 (96%)	21 (4%)	0	100	100
All	All	2653/3000 (88%)	2529 (95%)	116 (4%)	8 (0%)	36	66

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	385	ARG
1	A	614	SER
1	D	852	ASP
1	C	711	GLU
1	B	590	LEU
1	C	338	ASN
1	A	385	ARG
1	D	662	ASN

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	483/543 (89%)	458 (95%)	25 (5%)	21	53
1	B	483/543 (89%)	453 (94%)	30 (6%)	16	45
1	C	483/543 (89%)	454 (94%)	29 (6%)	17	47
1	D	478/543 (88%)	453 (95%)	25 (5%)	21	53
1	E	484/543 (89%)	458 (95%)	26 (5%)	20	51
All	All	2411/2715 (89%)	2276 (94%)	135 (6%)	19	50

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	300	VAL
1	A	308	LEU
1	A	327	GLU
1	A	338	ASN
1	A	351	LEU
1	A	360	VAL
1	A	361	GLU
1	A	365	GLU
1	A	378	ARG
1	A	472	GLU
1	A	491	ASN
1	A	502	GLU
1	A	547	THR
1	A	590	LEU
1	A	627	ASP
1	A	649	GLN
1	A	711	GLU
1	A	744	ARG
1	A	781	LYS
1	A	782	GLU
1	A	793	GLU
1	A	853	GLU
1	A	859	MET
1	A	866	SER
1	B	286	LEU
1	B	311	GLU
1	B	341	LEU
1	B	351	LEU
1	B	356	LYS
1	B	362	ASP
1	B	378	ARG
1	B	415	LEU
1	B	472	GLU
1	B	491	ASN
1	B	533	LYS
1	B	562	GLU
1	B	576	LEU
1	B	581	GLU
1	B	590	LEU
1	B	614	SER
1	B	649	GLN
1	B	678	LYS

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Mol	Chain	Res	Type
1	B	694	LEU
1	B	721	VAL
1	B	744	ARG
1	B	779	LEU
1	B	782	GLU
1	B	821	SER
1	B	833	LEU
1	B	854	GLU
1	B	859	MET
1	B	861	SER
1	B	865	GLU
1	B	870	LEU
1	C	-2	SER
1	C	294	ASP
1	C	323	LEU
1	C	327	GLU
1	C	344	GLU
1	C	351	LEU
1	C	354	LYS
1	C	356	LYS
1	C	390	GLU
1	C	416	GLU
1	C	498	ILE
1	C	505	ASP
1	C	521	MET
1	C	555	LEU
1	C	576	LEU
1	C	590	LEU
1	C	649	GLN
1	C	652	SER
1	C	660	LYS
1	C	688	VAL
1	C	694	LEU
1	C	706	LYS
1	C	724	THR
1	C	744	ARG
1	C	750	LEU
1	C	768	ARG
1	C	782	GLU
1	C	793	GLU
1	C	813	SER
1	D	351	LEU

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Mol	Chain	Res	Type
1	D	361	GLU
1	D	366	LEU
1	D	383	ARG
1	D	384	LEU
1	D	393	LEU
1	D	472	GLU
1	D	498	ILE
1	D	508	GLN
1	D	555	LEU
1	D	563	SER
1	D	595	LEU
1	D	639	ASP
1	D	649	GLN
1	D	660	LYS
1	D	671	LYS
1	D	678	LYS
1	D	694	LEU
1	D	777	MET
1	D	782	GLU
1	D	793	GLU
1	D	799	ARG
1	D	800	LYS
1	D	827	ASN
1	D	851	SER
1	E	-1	MET
1	E	305	THR
1	E	323	LEU
1	E	324	THR
1	E	325	ASN
1	E	338	ASN
1	E	341	LEU
1	E	343	GLN
1	E	356	LYS
1	E	366	LEU
1	E	505	ASP
1	E	509	ARG
1	E	528	LEU
1	E	529	LEU
1	E	547	THR
1	E	584	ASN
1	E	587	ASP
1	E	590	LEU

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Mol	Chain	Res	Type
1	E	694	LEU
1	E	741	VAL
1	E	750	LEU
1	E	782	GLU
1	E	804	THR
1	E	810	ARG
1	E	814	ASN
1	E	833	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	307	GLN
1	B	313	GLN
1	B	370	HIS
1	B	560	GLN
1	C	289	ASN
1	C	295	GLN
1	C	297	ASN
1	C	313	GLN
1	C	347	GLN
1	C	702	ASN
1	C	780	ASN
1	C	808	HIS
1	D	313	GLN
1	D	343	GLN
1	D	662	ASN
1	D	796	GLN
1	D	827	ASN
1	D	860	GLN
1	E	325	ASN
1	E	620	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	-1:MET	C	282:SER	N	3.19

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	536/600 (89%)	-0.51	0	100	100	19, 35, 54, 67	0
1	B	535/600 (89%)	-0.58	1 (0%)	91	88	18, 31, 47, 55	0
1	C	537/600 (89%)	-0.49	1 (0%)	91	88	20, 38, 54, 66	0
1	D	531/600 (88%)	-0.14	4 (0%)	82	75	35, 54, 70, 83	0
1	E	535/600 (89%)	-0.50	0	100	100	21, 36, 50, 64	0
All	All	2674/3000 (89%)	-0.44	6 (0%)	91	88	18, 38, 63, 83	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	415	LEU	3.0
1	D	852	ASP	2.7
1	D	286	LEU	2.6
1	C	417	PRO	2.6
1	B	289	ASN	2.5
1	D	773	LEU	2.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.