



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:27 AM GMT

PDB ID : 3IHY
Title : Human PIK3C3 crystal structure
Authors : Siponen, M.I.; Tresaugues, L.; Arrowsmith, C.H.; Berglund, H.; Bountra, C.; Collins, R.; Edwards, A.M.; Flodin, S.; Flores, A.; Graslund, S.; Hammarstrom, M.; Johansson, A.; Johansson, I.; Karlberg, T.; Kotenyova, T.; Kotzsch, A.; Kragh Nielsen, T.; Moche, M.; Nyman, T.; Persson, C.; Roos, A.K.; Sagemark, J.; Schueler, H.; Schutz, P.; Thorsell, A.G.; Van Den Berg, S.; Weigelt, J.; Welin, M.; Wisniewska, M.; Nordlund, P.; Structural Genomics Consortium (SGC)
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
<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

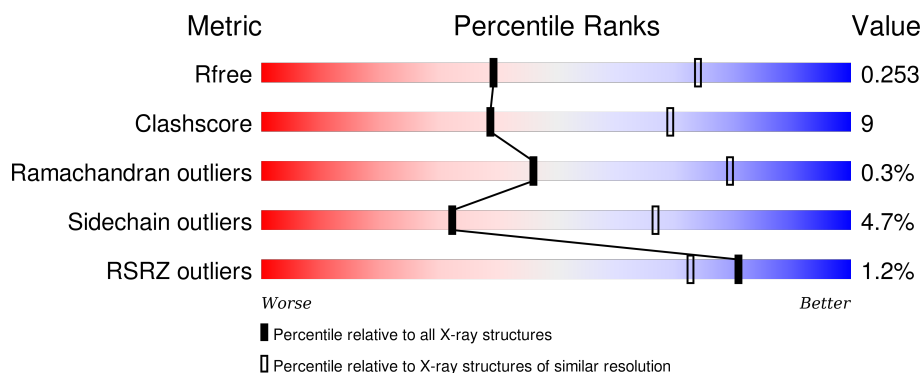
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	600	<div> <div>72%</div> <div>16%</div> <div>•</div> <div>11%</div> </div>
1	B	600	<div> <div>73%</div> <div>15%</div> <div>•</div> <div>11%</div> </div>
1	C	600	<div> <div>67%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
1	D	600	<div> <div>3%</div> <div>66%</div> <div>22%</div> <div>•</div> <div>12%</div> </div>
1	E	600	<div> <div>71%</div> <div>16%</div> <div>•</div> <div>11%</div> </div>

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

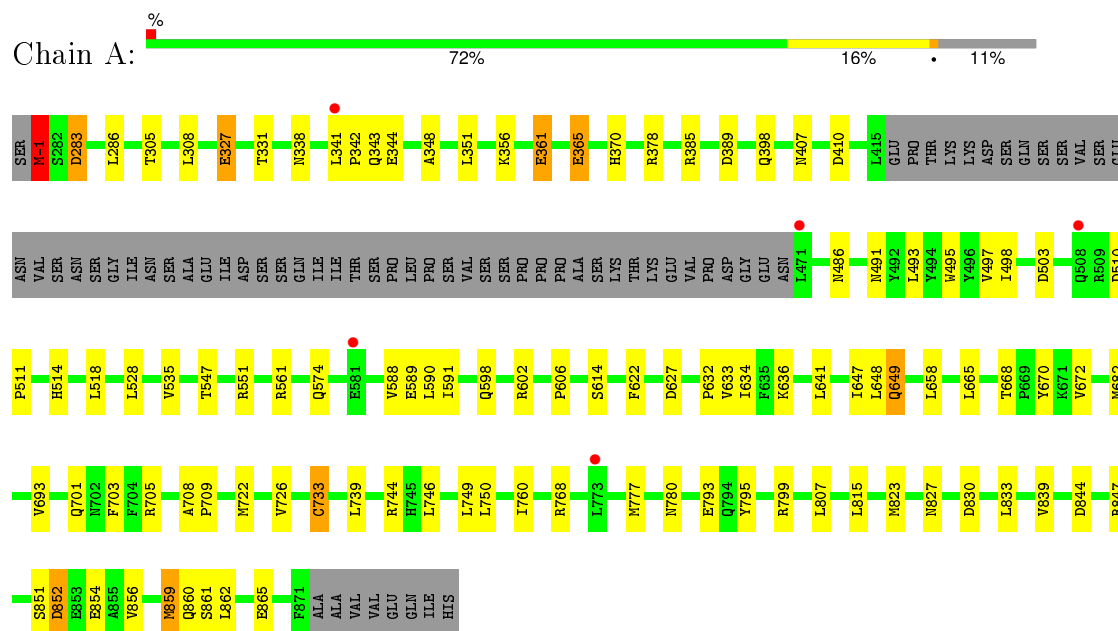
- Molecule 2 is water.

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

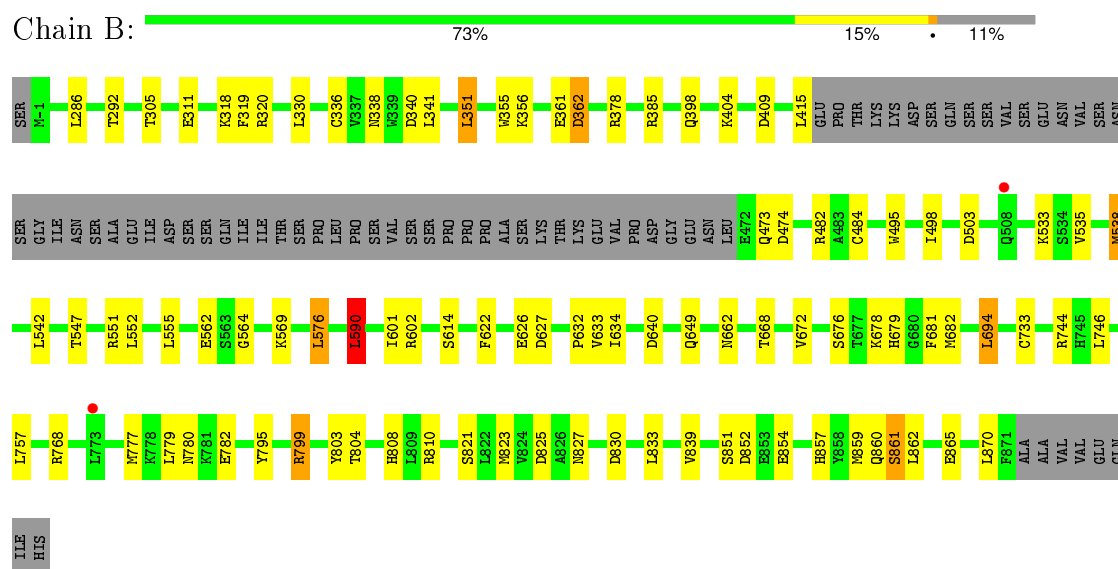
3 Residue-property plots

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

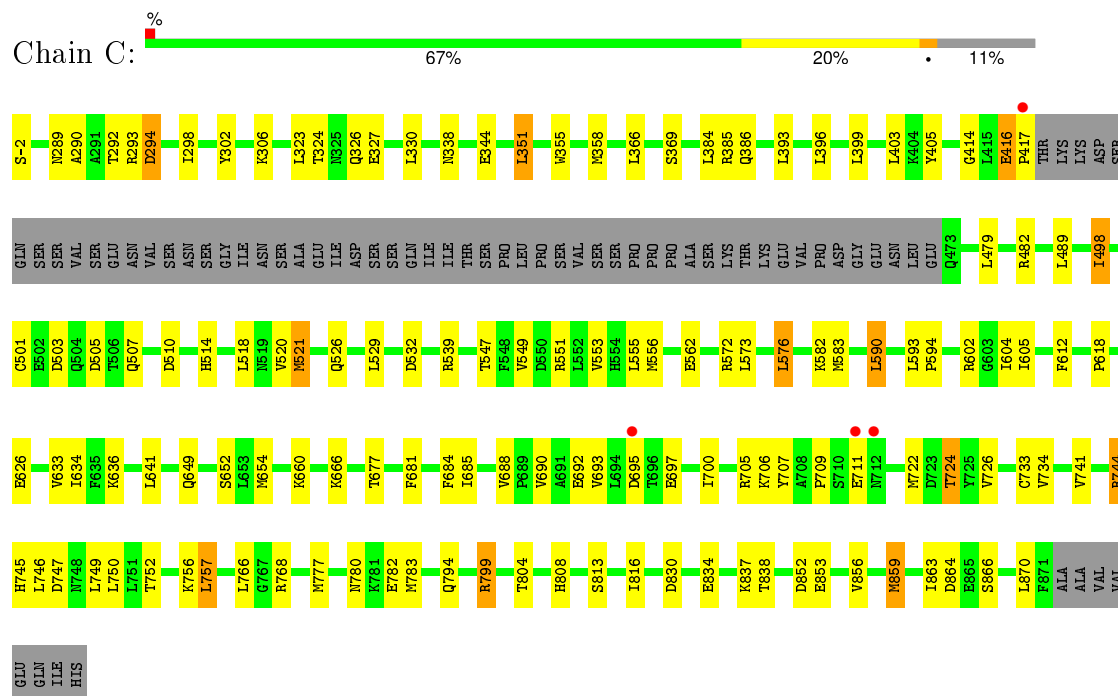
- Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3



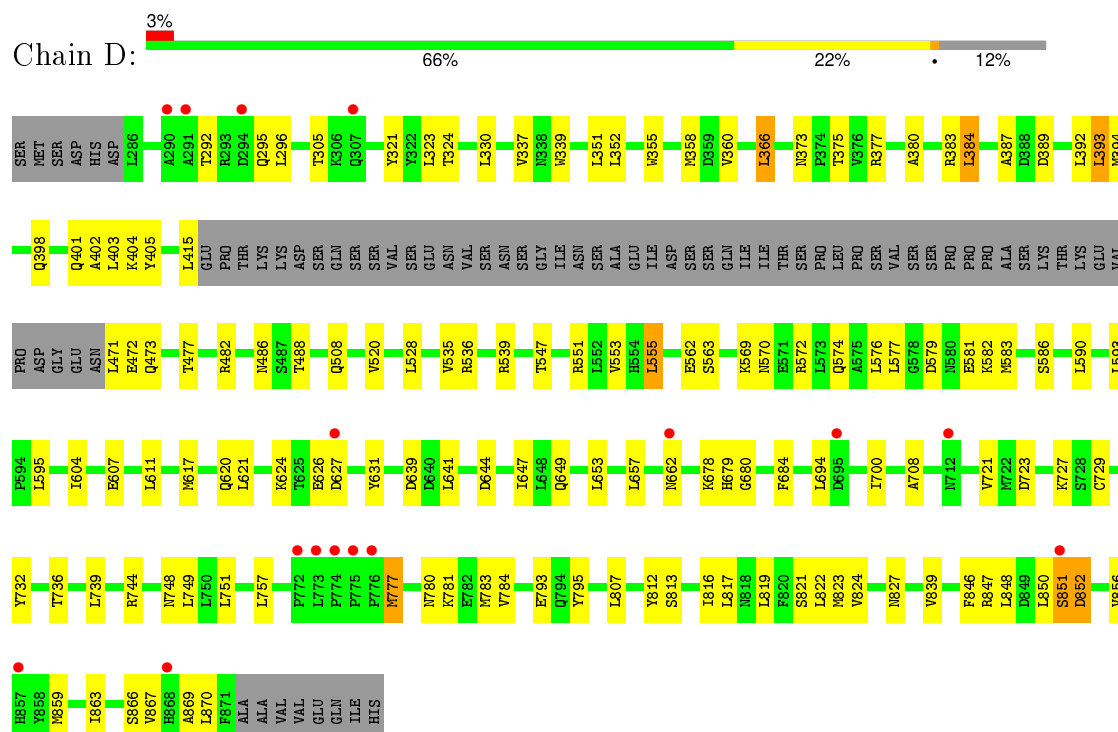
- Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3



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

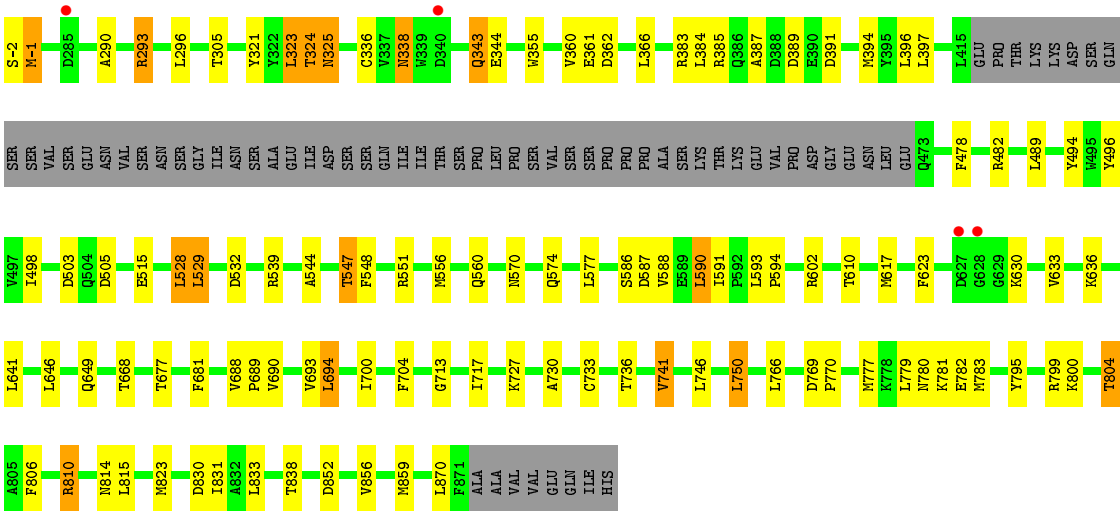


- Molecule 1: Phosphatidylinositol 3-kinase catalytic subunit type 3



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





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 19.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.84-2.80) 88.8 (19.83-2.80)	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 0.190 , 0.253	Depositor DCC
R_{free} test set	4076 reflections (5.29%)	DCC
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 , 38.7	EDS
Estimated twinning fraction	0.058 for -h,k,-k-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 81167 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.72	2/4428 (0.0%)	0.75	1/5985 (0.0%)
1	B	0.71	1/4423 (0.0%)	0.80	5/5975 (0.1%)
1	C	0.65	1/4430 (0.0%)	0.73	2/5990 (0.0%)
1	D	0.59	0/4387	0.69	1/5930 (0.0%)
1	E	0.67	2/4425 (0.0%)	0.74	1/5978 (0.0%)
All	All	0.67	6/22093 (0.0%)	0.74	10/29858 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	-1	MET	C-N	8.73	1.54	1.34
1	A	733	CYS	CB-SG	-5.95	1.72	1.81
1	E	336	CYS	CB-SG	-5.43	1.73	1.81
1	E	515	GLU	CG-CD	5.43	1.60	1.51
1	B	336	CYS	CB-SG	-5.21	1.73	1.81
1	C	733	CYS	CB-SG	-5.14	1.73	1.81

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	482	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	482	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	C	482	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	415	LEU	CA-CB-CG	5.71	128.43	115.30
1	A	-1	MET	C-N-CA	-5.41	108.16	121.70
1	C	482	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	E	528	LEU	CA-CB-CG	5.30	127.49	115.30
1	B	474	ASP	CB-CG-OD1	5.28	123.05	118.30
1	B	640	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	799	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	74	0
1	B	4339	0	4376	53	0
1	C	4344	0	4370	93	0
1	D	4303	0	4348	83	0
1	E	4340	0	4390	89	0
2	B	1	0	0	0	0
All	All	21670	0	21864	390	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 9.

All (390) 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:C:547:THR:HG22	1:C:551:ARG:NH1	1.67	1.08
1:D:749:LEU:HD21	1:D:783:MET:HE1	1.32	1.08
1:C:852:ASP:O	1:C:856:VAL:HG23	1.63	0.99
1:E:736:THR:HG22	1:E:741:VAL:HG11	1.47	0.96
1:C:734:VAL:HG22	1:C:859:MET:HE3	1.48	0.95
1:D:749:LEU:HD21	1:D:783:MET:CE	2.01	0.91
1:A:398:GLN:OE1	1:A:823:MET:HE1	1.70	0.91
1:A:398:GLN:HG3	1:A:823:MET:CE	2.02	0.90
1:D:398:GLN:HG3	1:D:823:MET:HE2	1.54	0.90
1:E:733:CYS:SG	1:E:777:MET:HE2	2.15	0.86
1:D:851:SER:O	1:D:852:ASP:HB2	1.74	0.86
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:A:398:GLN:HG3	1:A:823:MET:HE2	1.58	0.83
1:D:398:GLN:HG3	1:D:823:MET:CE	2.09	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:LEU:HD23	1:C:358:MET:HE2	1.61	0.82
1:D:851:SER:O	1:D:852:ASP:CB	2.28	0.82
1:B:398:GLN:HG3	1:B:823:MET:HE2	1.61	0.81
1:B:768:ARG:HD3	1:B:830:ASP:OD1	1.80	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:C:330:LEU:HD23	1:C:358:MET:CE	2.14	0.76
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:E:547:THR:HG23	1:E:551:ARG:NH1	2.03	0.74
1:D:360:VAL:HG11	1:D:387:ALA:HB2	1.69	0.74
1:C:358:MET:HE1	1:C:366:LEU:HD11	1.69	0.74
1:B:633:VAL:HG11	1:B:681:PHE:HD1	1.54	0.73
1:B:398:GLN:OE1	1:B:823:MET:HE1	1.89	0.73
1:C:749:LEU:HD21	1:C:783:MET:HE2	1.70	0.73
1:C:734:VAL:HG22	1:C:859:MET:CE	2.17	0.73
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:E:577:LEU:O	1:E:586:SER:OG	2.10	0.70
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:E:733:CYS:SG	1:E:777:MET:HE1	2.33	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:C:555:LEU:HD23	1:C:555:LEU:C	2.14	0.67
1:E:547:THR:HG22	1:E:551:ARG:HH12	1.58	0.67
1:A:851:SER:OG	1:A:854:GLU:OE1	2.05	0.67
1:C:358:MET:CE	1:C:366:LEU:HD11	2.25	0.67
1:A:861:SER:O	1:A:865:GLU:HG3	1.94	0.67
1:D:732:TYR:O	1:D:736:THR:HG23	1.94	0.67
1:A:859:MET:HE2	1:A:862:LEU:HD12	1.75	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:398:GLN:CG	1:D:823:MET:HE2	2.28	0.63
1:D:859:MET:HE2	1:D:863:ILE:HD11	1.81	0.63
1:D:863:ILE:O	1:D:867:VAL:HG23	1.98	0.63
1:C:582:LYS:HG3	1:C:583:MET:HE3	1.81	0.62
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: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:E:736:THR:CG2	1:E:741:VAL:HG11	2.28	0.60
1:A:398:GLN:HG3	1:A:823:MET:HE1	1.82	0.59
1:C:393:LEU:HD12	1:C:393:LEU:O	2.01	0.59
1:A:-1:MET:N	1:A:-1:MET:HE2	2.16	0.59
1:E:529:LEU:HD22	1:E:539:ARG:CD	2.31	0.59
1:A:746:LEU:HD21	1:A:780:ASN:ND2	2.18	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:646:LEU:HD13	1:E:823:MET:CE	2.33	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:636:LYS:HD2	1:E:641:LEU:HD21	1.84	0.58
1:E:570:ASN:O	1:E:574:GLN:HG3	2.03	0.58
1:C:746:LEU:HD21	1:C:780:ASN:HD21	1.69	0.58
1:E:852:ASP:O	1:E:856:VAL:HG23	2.04	0.57
1:E:795:TYR:CE2	1:E:799:ARG:HD2	2.40	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:D:780:ASN:HB3	1:D:783:MET:CE	2.35	0.56
1:A:398:GLN:CG	1:A:823:MET:CE	2.82	0.56
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:E:396:LEU:HD22	1:E:489:LEU:HD23	1.88	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:D:292:THR:HA	1:D:295:GLN:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:570:ASN:HD21	1:E:610:THR:HG23	1.71	0.56
1:C:324:THR:HG22	1:C:355:TRP:CE3	2.41	0.55
1:A:361:GLU:HB2	1:A:815:LEU:HD13	1.87	0.55
1:C:521:MET:CE	1:C:521:MET:HA	2.35	0.55
1:C:399:LEU:HD13	1:C:479:LEU:HD21	1.88	0.55
1:E:529:LEU:CD2	1:E:539:ARG:NE	2.69	0.55
1:C:666:LYS:HG3	1:C:724:THR:HG23	1.88	0.55
1:B:362:ASP:N	1:B:362:ASP:OD2	2.38	0.55
1:A:305:THR:HG21	1:A:839:VAL:HG11	1.87	0.55
1:E:588:VAL:HG22	1:E:602:ARG:O	2.06	0.55
1:D:393:LEU:HD11	1:D:488:THR:HG22	1.88	0.55
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:E:556:MET:O	1:E:560:GLN:HG3	2.07	0.55
1:D:377:ARG:O	1:D:380:ALA:HB3	2.07	0.55
1:B:564:GLY:O	1:B:569:LYS:NZ	2.40	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: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:834:GLU:OE1	1:C:837:LYS:HD3	2.08	0.54
1:C:654:MET:HE3	1:C:816:ILE:HD13	1.89	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:A:398:GLN:CD	1:A:823:MET:HE1	2.28	0.54
1:D:821:SER:O	1:D:824:VAL:HG13	2.07	0.54
1:C:414:GLY:O	1:C:526:GLN:NE2	2.41	0.54
1:C:396:LEU:HD22	1:C:489:LEU:HD23	1.88	0.54
1:D:708:ALA:CB	1:D:721:VAL:HG21	2.38	0.53
1:C:749:LEU:HD23	1:C:757:LEU:HD11	1.90	0.53
1:A:-1:MET:N	1:A:-1:MET:CE	2.71	0.53
1:C:804:THR:HG22	1:C:808:HIS:CD2	2.42	0.53
1:C:289:ASN:HB2	1:C:292:THR:HG23	1.90	0.53
1:E:736:THR:HG22	1:E:741:VAL:CG1	2.31	0.53
1:C:688:VAL:HG12	1:C:693:VAL:HG23	1.90	0.53
1:A:668:THR:O	1:A:668:THR:HG22	2.08	0.53
1:A:768:ARG:HD3	1:A:830:ASP:OD1	2.09	0.53
1:C:749:LEU:HD21	1:C:783:MET:HE3	1.90	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:D:847:ARG:NH2	1:D:850:LEU:HD21	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:MET:HG3	1:B:862:LEU:HB3	1.90	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
1:D:576:LEU:HD23	1:D:583:MET:SD	2.50	0.52
1:C:654:MET:CE	1:C:816:ILE:HD13	2.40	0.52
1:A:341:LEU:HD23	1:A:343:GLN:H	1.74	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: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:C:777:MET:HE1	1:C:863:ILE:HA	1.91	0.51
1:E:736:THR:HB	1:E:741:VAL:CG1	2.41	0.51
1:A:795:TYR:CE2	1:A:799:ARG:HD2	2.45	0.51
1:A:398:GLN:CG	1:A:823:MET:HE1	2.40	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:N	1:A:338:ASN:OD1	2.43	0.51
1:D:795:TYR:OH	1:D:867:VAL:HG21	2.11	0.51
1:A:807:LEU:HD11	1:A:856:VAL:CG2	2.41	0.51
1:A:636:LYS:HD2	1:A:641:LEU:HD21	1.92	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:290:ALA:HA	1:E:293:ARG:NH1	2.25	0.51
1:E:385:ARG:HG2	1:E:478:PHE:CE1	2.46	0.51
1:A:589:GLU:O	1:A:591:ILE:HG23	2.10	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:D:330:LEU:HD23	1:D:358:MET:HE2	1.93	0.50
1:E:529:LEU:CD2	1:E:539:ARG:CZ	2.87	0.50
1:A:344:GLU:O	1:A:348:ALA:N	2.42	0.50
1:D:321:TYR:O	1:D:324:THR:HG22	2.12	0.50
1:C:745:HIS:CE1	1:C:747:ASP:HB2	2.47	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:D:358:MET:O	1:D:383:ARG:NH1	2.44	0.50
1:E:360:VAL:HG22	1:E:383:ARG:O	2.11	0.50
1:D:553:VAL:HG21	1:D:679:HIS:CE1	2.46	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
1:A:768:ARG:HD2	1:A:833:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:HD13	1:B:355:TRP:CD2	2.46	0.50
1:E:532:ASP:OD1	1:E:532:ASP:C	2.50	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:C:551:ARG:HD2	1:C:583:MET:O	2.11	0.50
1:B:292:THR:HG21	1:B:319:PHE:CE2	2.47	0.50
1:D:780:ASN:HB3	1:D:783:MET:HE2	1.94	0.49
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:E:690:VAL:CG1	1:E:746:LEU:HD22	2.41	0.49
1:B:668:THR:HG22	1:B:668:THR:O	2.13	0.49
1:B:404:LYS:NZ	1:B:825:ASP:O	2.45	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:807:LEU:HD21	1:D:856:VAL:HG23	1.93	0.49
1:C:330:LEU:HD13	1:C:355:TRP:CD2	2.48	0.49
1:C:289:ASN:HD22	1:C:292:THR:HG23	1.76	0.49
1:C:384:LEU:C	1:C:386:GLN:H	2.16	0.49
1:E:544:ALA:HB1	1:E:591:ILE:HG21	1.94	0.49
1:D:586:SER:O	1:D:624:LYS:NZ	2.41	0.49
1:E:736:THR:CB	1:E:741:VAL:CG1	2.91	0.49
1:E:570:ASN:ND2	1:E:610:THR:HG23	2.26	0.49
1:B:851:SER:O	1:B:852:ASP:C	2.51	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:C:766:LEU:HD13	1:C:838:THR:HG23	1.94	0.49
1:E:646:LEU:HD13	1:E:823:MET:HE2	1.94	0.48
1:B:662:ASN:HD21	1:C:326:GLN:HG3	1.77	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:HG22	1:E:668:THR:O	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:555:LEU:HD12	1:D:583:MET:SD	2.54	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
1:D:473:GLN:NE2	1:D:477:THR:HG22	2.29	0.48
1:A:-1:MET:CA	1:A:-1:MET:HE2	2.44	0.48
1:B:552:LEU:HD12	1:B:555:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:VAL:HG11	1:E:387:ALA:HB2	1.95	0.48
1:A:407:ASN:HB3	1:A:410:ASP:OD2	2.14	0.48
1:D:547:THR:HG22	1:D:551:ARG:HH11	1.79	0.47
1:A:327:GLU:N	1:A:327:GLU:OE2	2.47	0.47
1:D:358:MET:HE3	1:D:366:LEU:HD21	1.96	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:E:387:ALA:O	1:E:482:ARG:NH2	2.46	0.47
1:D:590:LEU:HD23	1:D:626:GLU:HG3	1.96	0.47
1:A:574:GLN:HG2	1:A:606:PRO:O	2.13	0.47
1:B:804:THR:HG22	1:B:808:HIS:CE1	2.50	0.47
1:E:806:PHE:CG	1:E:859:MET:HE3	2.49	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:B:633:VAL:CG1	1:B:634:ILE:N	2.77	0.46
1:B:318:LYS:HD3	1:B:319:PHE:CE2	2.50	0.46
1:E:494:TYR:CE1	1:E:498:ILE:HG13	2.50	0.46
1:B:361:GLU:H	1:B:361:GLU:CD	2.19	0.46
1:C:562:GLU:HG2	1:C:572:ARG:NH1	2.24	0.46
1:D:389:ASP:CG	1:D:486:ASN:HD22	2.19	0.46
1:D:536:ARG:O	1:D:539:ARG:HB3	2.16	0.46
1:E:769:ASP:CG	1:E:770:PRO:HD2	2.36	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:C:692:GLU:HA	1:C:695:ASP:HB3	1.96	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:B:590:LEU:CD1	1:B:602:ARG:HG3	2.46	0.46
1:A:588:VAL:HG22	1:A:602:ARG:O	2.15	0.46
1:E:338:ASN:N	1:E:338:ASN:OD1	2.49	0.45
1:E:290:ALA:HA	1:E:293:ARG:HH11	1.81	0.45
1:D:330:LEU:HD21	1:D:352:LEU:CD1	2.46	0.45
1:C:330:LEU:HD23	1:C:358:MET:HE3	1.94	0.45
1:D:611:LEU:HD13	1:D:617:MET:HB3	1.97	0.45
1:B:803:TYR:OH	1:B:860:GLN:HG3	2.16	0.45
1:C:582:LYS:HG3	1:C:583:MET:HG2	1.98	0.45
1:C:289:ASN:HB2	1:C:292:THR:H	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:351:LEU:HD23	1:C:355:TRP:CZ3	2.52	0.45
1:A:851:SER:CB	1:A:854:GLU:OE1	2.65	0.45
1:E:646:LEU:HD13	1:E:823:MET:HE1	1.98	0.45
1:B:555:LEU:HD13	1:B:576:LEU:HB3	1.99	0.45
1:A:672:VAL:HG22	1:A:682:MET:HG3	1.98	0.45
1:D:398:GLN:OE1	1:D:823:MET:HE1	2.17	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:B:733:CYS:SG	1:B:777:MET:CE	3.04	0.45
1:B:757:LEU:C	1:B:757:LEU:HD23	2.37	0.45
1:D:813:SER:O	1:D:817:LEU:HG	2.17	0.45
1:D:296:LEU:HD22	1:D:323:LEU:HD11	1.99	0.45
1:C:572:ARG:HG2	1:C:576:LEU:HD22	1.98	0.45
1:C:369:SER:HB3	1:C:405:TYR:CE1	2.51	0.45
1:A:561:ARG:O	1:A:561:ARG:HG3	2.16	0.45
1:C:532:ASP:C	1:C:532:ASP:OD1	2.55	0.45
1:C:330:LEU:HD13	1:C:355:TRP:CG	2.51	0.45
1:D:859:MET:HE2	1:D:863:ILE:CD1	2.46	0.45
1:E:391:ASP:HA	1:E:394:MET:HE2	1.99	0.44
1:B:484:CYS:O	1:B:535:VAL:HG22	2.17	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:622:PHE:CE2	1:A:632:PRO:HB3	2.52	0.44
1:A:495:TRP:CE3	1:A:498:ILE:HD11	2.52	0.44
1:E:806:PHE:O	1:E:810:ARG:HG2	2.17	0.44
1:B:385:ARG:HH12	1:B:473:GLN:HB2	1.82	0.44
1:E:781:LYS:N	1:E:870:LEU:HD13	2.33	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:A:861:SER:O	1:A:865:GLU:CG	2.65	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:A:633:VAL:CG1	1:A:634:ILE:N	2.81	0.44
1:C:507:GLN:HG3	1:C:514:HIS:CD2	2.53	0.44
1:B:601:ILE:HD12	1:B:601:ILE:C	2.38	0.44
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:A:-1:MET:H1	1:A:-1:MET:CE	2.30	0.43
1:E:694:LEU:HD21	1:E:782:GLU:HG3	1.99	0.43
1:E:397:LEU:HD13	1:E:496:TYR:CE1	2.53	0.43
1:A:-1:MET:HB2	1:A:-1:MET:HE3	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:LEU:O	1:A:497:VAL:HG23	2.18	0.43
1:D:358:MET:CE	1:D:366:LEU:HD21	2.49	0.43
1:D:607:GLU:CD	1:D:607:GLU:H	2.22	0.43
1:C:636:LYS:HD2	1:C:641:LEU:HD21	2.00	0.43
1:E:736:THR:CG2	1:E:741:VAL:CG1	2.95	0.43
1:E:780:ASN:C	1:E:870:LEU:HD13	2.39	0.43
1:C:633:VAL:CG1	1:C:634:ILE:N	2.81	0.43
1:C:290:ALA:HA	1:C:293:ARG:NH1	2.33	0.43
1:C:684:PHE:O	1:C:685:ILE:HD13	2.18	0.43
1:C:521:MET:HE3	1:C:521:MET:HA	2.01	0.43
1:A:733:CYS:SG	1:A:777:MET:CE	3.07	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:B:780:ASN:OD1	1:B:782:GLU:HG2	2.18	0.43
1:D:337:VAL:HG11	1:D:339:TRP:CZ3	2.54	0.43
1:B:733:CYS:SG	1:B:777:MET:HE1	2.58	0.43
1:B:338:ASN:OD1	1:B:340:ASP:N	2.50	0.43
1:E:-2:SER:O	1:E:-1:MET:HB2	2.18	0.43
1:A:510:ASP:N	1:A:511:PRO:HD3	2.34	0.43
1:C:633:VAL:HG11	1:C:681:PHE:CD1	2.54	0.42
1:C:294:ASP:O	1:C:298:ILE:HG12	2.19	0.42
1:A:514:HIS:NE2	1:A:518:LEU:HD11	2.34	0.42
1:D:373:ASN:O	1:D:377:ARG:HG2	2.19	0.42
1:B:777:MET:HE2	1:B:777:MET:HB3	1.71	0.42
1:E:713:GLY:HA3	1:E:717:ILE:O	2.18	0.42
1:B:555:LEU:CD1	1:B:576:LEU:HB3	2.50	0.42
1:A:598:GLN:CD	1:A:598:GLN:H	2.22	0.42
1:D:339:TRP:CE3	1:D:373:ASN:ND2	2.87	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
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: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:E:361:GLU:N	1:E:361:GLU:OE1	2.41	0.42
1:D:403:LEU:HD13	1:D:520:VAL:HG21	2.01	0.42
1:C:604:ILE:HG22	1:C:605:ILE:N	2.35	0.42
1:E:323:LEU:C	1:E:325:ASN:H	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-1:MET:H1	1:A:-1:MET:HE3	1.84	0.42
1:D:377:ARG:HH22	1:D:405:TYR:HB2	1.84	0.42
1:B:662:ASN:ND2	1:C:326:GLN:HG3	2.35	0.42
1:C:706:LYS:HD2	1:C:707:TYR:CZ	2.54	0.42
1:A:844:ASP:O	1:A:847:ARG:HD2	2.20	0.42
1:E:560:GLN:NE2	1:E:617:MET:HB2	2.35	0.41
1:E:296:LEU:HD22	1:E:323:LEU:HD21	2.02	0.41
1:B:398:GLN:NE2	1:B:398:GLN:H	2.19	0.41
1:C:744:ARG:HD2	1:C:744:ARG:N	2.34	0.41
1:C:612:PHE:HB2	1:C:618:PRO:HG2	2.02	0.41
1:A:389:ASP:CG	1:A:486:ASN:HD22	2.21	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:C:804:THR:HG22	1:C:808:HIS:HD2	1.86	0.41
1:B:498:ILE:HD12	1:B:498:ILE:HA	1.82	0.41
1:E:831:ILE:HG12	1:E:838:THR:HG21	2.02	0.41
1:E:779:LEU:HD23	1:E:783:MET:CE	2.50	0.41
1:E:547:THR:HG22	1:E:548:PHE:N	2.36	0.41
1:C:555:LEU:HD21	1:C:573:LEU:CD1	2.49	0.41
1:E:384:LEU:HA	1:E:384:LEU:HD23	1.89	0.41
1:B:547:THR:CG2	1:B:551:ARG:NH1	2.74	0.41
1:E:689:PRO:HA	1:E:750:LEU:HD12	2.03	0.41
1:C:555:LEU:HD23	1:C:556:MET:N	2.35	0.41
1:E:396:LEU:HD22	1:E:489:LEU:CD2	2.50	0.41
1:C:697:GLU:OE2	1:C:706:LYS:NZ	2.43	0.41
1:D:816:ILE:HD13	1:D:846:PHE:HZ	1.86	0.41
1:B:694:LEU:HD22	1:B:746:LEU:HD13	2.03	0.41
1:C:705:ARG:O	1:C:709:PRO:HB3	2.21	0.41
1:B:795:TYR:CE2	1:B:799:ARG:HD2	2.55	0.40
1:C:700:ILE:HD12	1:C:782:GLU:O	2.20	0.40
1:C:501:CYS:SG	1:C:518:LEU:HD23	2.62	0.40
1:A:648:LEU:HA	1:A:648:LEU:HD13	1.94	0.40
1:A:649:GLN:HB2	1:A:649:GLN:HE21	1.62	0.40
1:E:394:MET:O	1:E:649:GLN:NE2	2.54	0.40
1:D:577:LEU:O	1:D:586:SER:HB2	2.21	0.40
1:B:495:TRP:HA	1:B:498:ILE:HG22	2.04	0.40
1:E:593:LEU:HD12	1:E:594:PRO:HD2	2.03	0.40
1:C:498:ILE:HD13	1:C:498:ILE:HA	1.88	0.40
1:D:387:ALA:O	1:D:482:ARG:NH2	2.53	0.40
1:A:495:TRP:CZ3	1:A:498:ILE:HD11	2.56	0.40
1:E:806:PHE:O	1:E:810:ARG:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:866:SER:O	1:D:869:ALA:HB3	2.21	0.40
1:B:676:SER:HB3	1:B:679:HIS:CE1	2.57	0.40
1:A:708:ALA:N	1:A:709:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

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	532/600 (89%)	502 (94%)	28 (5%)	2 (0%)	39	74
1	B	530/600 (88%)	510 (96%)	19 (4%)	1 (0%)	52	84
1	C	533/600 (89%)	506 (95%)	24 (4%)	3 (1%)	30	65
1	D	527/600 (88%)	501 (95%)	24 (5%)	2 (0%)	39	74
1	E	531/600 (88%)	510 (96%)	21 (4%)	0	100	100
All	All	2653/3000 (88%)	2529 (95%)	116 (4%)	8 (0%)	46	79

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%)	466 (96%)	17 (4%)	43	77
1	B	483/543 (89%)	454 (94%)	29 (6%)	24	56
1	C	483/543 (89%)	459 (95%)	24 (5%)	30	64
1	D	478/543 (88%)	459 (96%)	19 (4%)	38	73
1	E	484/543 (89%)	459 (95%)	25 (5%)	29	62
All	All	2411/2715 (89%)	2297 (95%)	114 (5%)	32	67

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	MET
1	A	283	ASP
1	A	308	LEU
1	A	327	GLU
1	A	351	LEU
1	A	361	GLU
1	A	365	GLU
1	A	370	HIS
1	A	378	ARG
1	A	491	ASN
1	A	590	LEU
1	A	627	ASP
1	A	649	GLN
1	A	744	ARG
1	A	793	GLU
1	A	852	ASP
1	A	859	MET
1	B	286	LEU
1	B	311	GLU
1	B	341	LEU
1	B	351	LEU
1	B	356	LYS
1	B	362	ASP

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Mol	Chain	Res	Type
1	B	378	ARG
1	B	409	ASP
1	B	415	LEU
1	B	533	LYS
1	B	538	MET
1	B	562	GLU
1	B	576	LEU
1	B	590	LEU
1	B	614	SER
1	B	627	ASP
1	B	649	GLN
1	B	678	LYS
1	B	694	LEU
1	B	744	ARG
1	B	779	LEU
1	B	810	ARG
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	416	GLU
1	C	498	ILE
1	C	505	ASP
1	C	510	ASP
1	C	521	MET
1	C	576	LEU
1	C	590	LEU
1	C	649	GLN
1	C	652	SER
1	C	660	LYS
1	C	724	THR
1	C	744	ARG
1	C	750	LEU

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Mol	Chain	Res	Type
1	C	757	LEU
1	C	799	ARG
1	C	813	SER
1	C	853	GLU
1	C	859	MET
1	D	351	LEU
1	D	355	TRP
1	D	366	LEU
1	D	384	LEU
1	D	393	LEU
1	D	472	GLU
1	D	508	GLN
1	D	555	LEU
1	D	563	SER
1	D	595	LEU
1	D	639	ASP
1	D	644	ASP
1	D	649	GLN
1	D	678	LYS
1	D	694	LEU
1	D	777	MET
1	D	793	GLU
1	D	827	ASN
1	D	851	SER
1	E	-1	MET
1	E	293	ARG
1	E	305	THR
1	E	323	LEU
1	E	324	THR
1	E	325	ASN
1	E	338	ASN
1	E	343	GLN
1	E	355	TRP
1	E	362	ASP
1	E	366	LEU
1	E	505	ASP
1	E	528	LEU
1	E	529	LEU
1	E	547	THR
1	E	587	ASP
1	E	590	LEU
1	E	694	LEU

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Mol	Chain	Res	Type
1	E	741	VAL
1	E	750	LEU
1	E	804	THR
1	E	810	ARG
1	E	814	ASN
1	E	830	ASP
1	E	833	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.40	5 (0%) 85 79	19, 35, 54, 67	0
1	B	535/600 (89%)	-0.44	2 (0%) 93 90	18, 31, 47, 55	0
1	C	537/600 (89%)	-0.34	4 (0%) 89 84	20, 38, 54, 66	0
1	D	531/600 (88%)	-0.05	16 (3%) 54 41	35, 54, 70, 83	0
1	E	535/600 (89%)	-0.35	4 (0%) 89 84	21, 36, 50, 64	0
All	All	2674/3000 (89%)	-0.31	31 (1%) 81 73	18, 38, 63, 83	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	712	ASN	4.4
1	D	773	LEU	3.8
1	D	772	PRO	3.7
1	D	307	GLN	3.5
1	D	868	HIS	3.3
1	B	773	LEU	3.1
1	D	290	ALA	3.0
1	D	627	ASP	3.0
1	C	711	GLU	2.9
1	D	695	ASP	2.8
1	E	340	ASP	2.8
1	E	627	ASP	2.8
1	A	341	LEU	2.8
1	A	581	GLU	2.6
1	D	857	HIS	2.5
1	E	628	GLY	2.5
1	D	291	ALA	2.4
1	C	695	ASP	2.3
1	D	774	PRO	2.3
1	E	285	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	776	PRO	2.3
1	C	712	ASN	2.1
1	D	294	ASP	2.1
1	A	471	LEU	2.1
1	A	508	GLN	2.1
1	D	775	PRO	2.1
1	D	662	ASN	2.1
1	A	773	LEU	2.0
1	B	508	GLN	2.0
1	C	417	PRO	2.0
1	D	851	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.