



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:09 AM UTC

PDB ID : 9FHG / pdb_00009fhg
Title : Crystallographic structure of AcrB V612N in LTO state
Authors : Lazarova, M.; Pos, K.M.
Deposited on : 2024-05-27
Resolution : 3.00 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

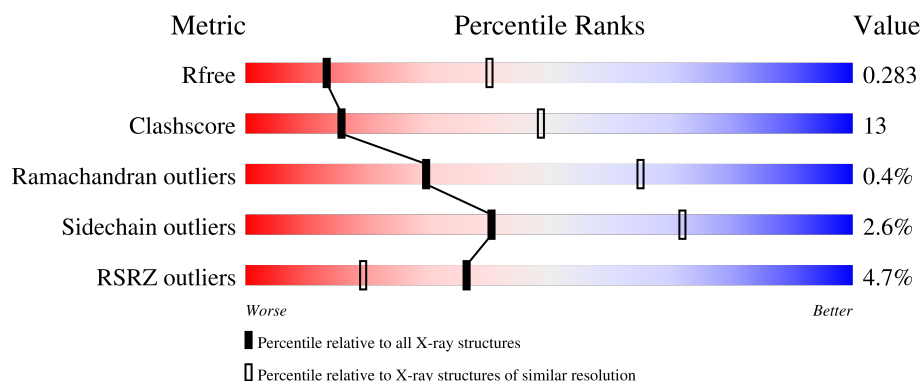
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	1057	 4% 70% 28% ..
1	B	1057	 5% 70% 27% .
1	C	1057	 6% 70% 27% ..
2	D	169	 2% 58% 34% . 8%
2	E	169	 3% 59% 31% . 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25972 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 Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1044	Total	C	N	O	S	0	0	0
			7944	5105	1316	1479	44			
1	B	1033	Total	C	N	O	S	0	0	0
			7850	5051	1296	1459	44			
1	C	1033	Total	C	N	O	S	0	0	0
			7850	5051	1296	1459	44			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	612	ASN	VAL	engineered mutation	UNP P31224
A	1050	LEU	-	expression tag	UNP P31224
A	1051	GLU	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression tag	UNP P31224
A	1057	HIS	-	expression tag	UNP P31224
B	612	ASN	VAL	engineered mutation	UNP P31224
B	1050	LEU	-	expression tag	UNP P31224
B	1051	GLU	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
B	1054	HIS	-	expression tag	UNP P31224
B	1055	HIS	-	expression tag	UNP P31224
B	1056	HIS	-	expression tag	UNP P31224
B	1057	HIS	-	expression tag	UNP P31224
C	612	ASN	VAL	engineered mutation	UNP P31224
C	1050	LEU	-	expression tag	UNP P31224
C	1051	GLU	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

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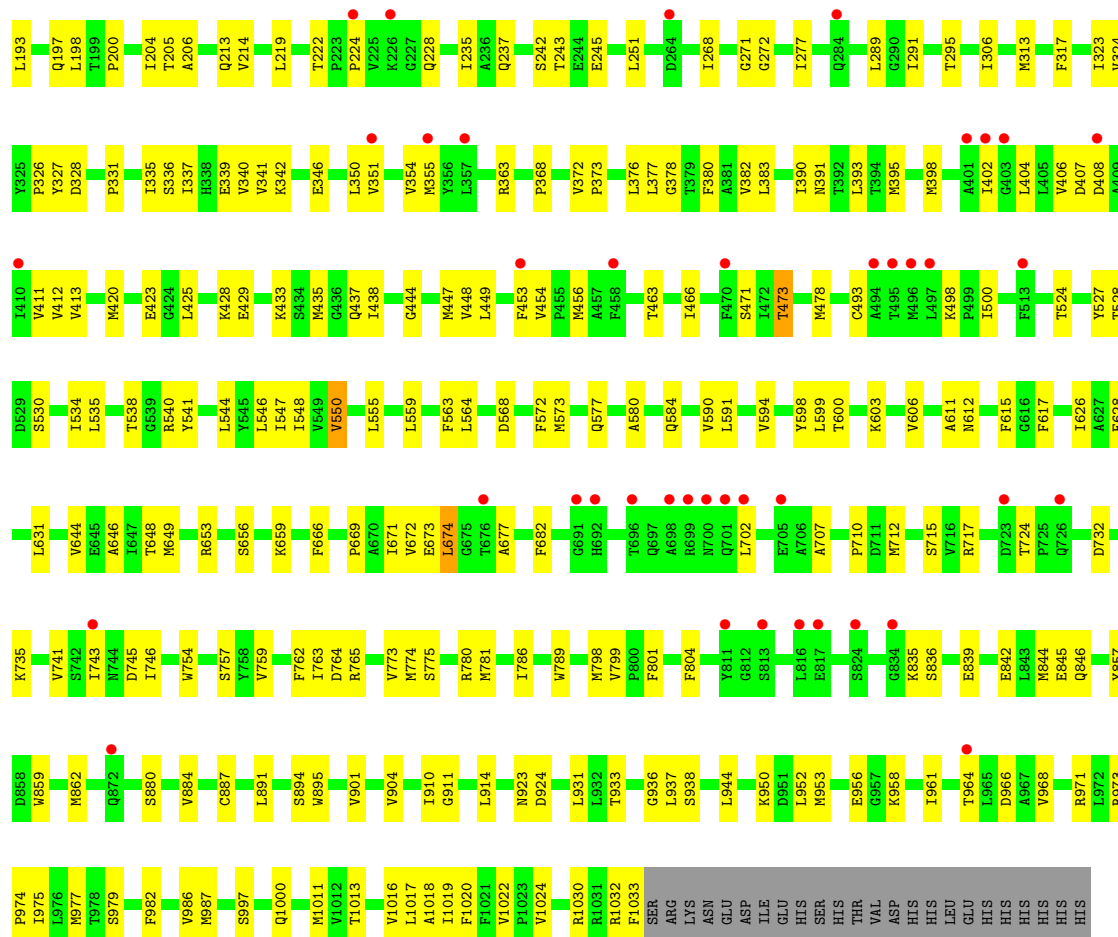
Chain	Residue	Modelled	Actual	Comment	Reference
C	1054	HIS	-	expression tag	UNP P31224
C	1055	HIS	-	expression tag	UNP P31224
C	1056	HIS	-	expression tag	UNP P31224
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is a protein called DARPIN.

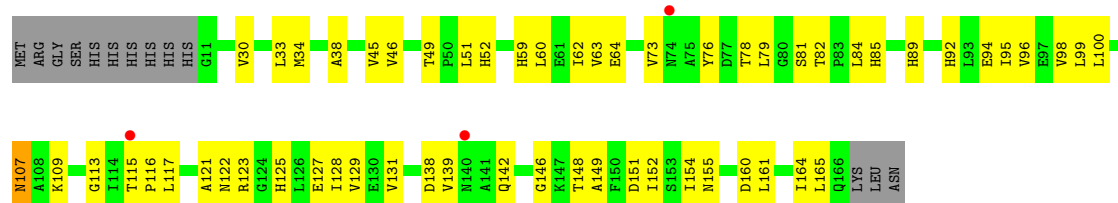
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	156	Total	C	N	O	S	0	0	0
			1177	741	206	229	1			
2	E	152	Total	C	N	O	S	0	0	0
			1151	726	202	222	1			

- Molecule 1: Multidrug efflux pump subunit AcrB

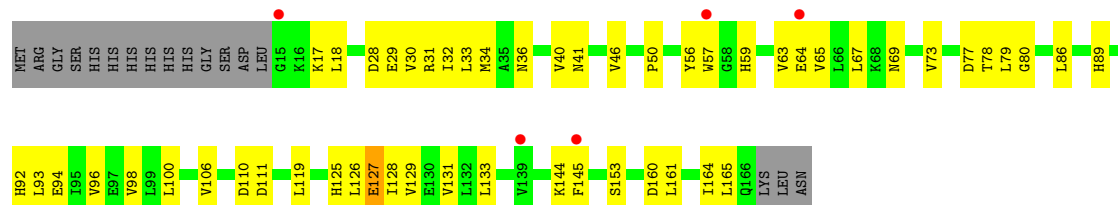




• Molecule 2: DARPIN



• Molecule 2: DARPIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	145.81Å 161.40Å 245.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.50 – 3.00 49.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.50-3.00) 99.7 (49.50-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.224 , 0.283 0.224 , 0.283	Depositor DCC
R_{free} test set	5794 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	75.9	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25972	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.43	1/8096 (0.0%)	0.65	1/10992 (0.0%)
1	B	0.44	1/8000 (0.0%)	0.64	1/10864 (0.0%)
1	C	0.41	1/8000 (0.0%)	0.63	0/10864
2	D	0.41	0/1196	0.64	0/1626
2	E	0.39	0/1170	0.61	0/1591
All	All	0.42	3/26462 (0.0%)	0.64	2/35937 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	426	PRO	CA-C	13.51	1.59	1.51
1	A	897	ILE	CA-CB	8.70	1.59	1.53
1	C	146	ASP	CA-C	5.67	1.60	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	426	PRO	O-C-N	10.69	126.22	121.31
1	A	461	GLY	N-CA-C	5.10	120.51	111.02

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	7944	0	8081	220	0
1	B	7850	0	7998	208	0
1	C	7850	0	7998	212	0
2	D	1177	0	1159	47	0
2	E	1151	0	1136	42	0
All	All	25972	0	26372	698	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 13.

All (698) 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)
2:E:153:SER:HB3	2:E:161:LEU:HD23	1.51	0.90
1:C:76:MET:HE3	1:C:95:GLU:HA	1.57	0.84
1:B:939:ALA:O	1:B:943:ILE:HG13	1.82	0.80
1:C:544:LEU:HA	1:C:547:ILE:HD12	1.64	0.78
1:C:15:ILE:O	1:C:19:ILE:HG13	1.82	0.78
1:C:659:LYS:HD3	1:C:659:LYS:H	1.50	0.77
1:A:149:MET:HE1	1:A:321:LEU:HD13	1.67	0.76
1:A:310:LEU:HA	1:A:313:MET:HE3	1.66	0.76
1:C:188:MET:HE1	1:C:200:PRO:HG3	1.67	0.76
2:D:63:VAL:HG21	2:D:95:ILE:HD13	1.66	0.75
1:B:973:ARG:HG2	1:B:977:MET:HE2	1.69	0.75
1:B:900:SER:HB3	1:B:1029:VAL:HG21	1.69	0.73
1:A:961:ILE:O	1:A:965:LEU:HD12	1.87	0.73
1:B:336:SER:HB3	1:B:395:MET:HE1	1.70	0.73
1:A:576:VAL:HG22	1:A:663:VAL:HG22	1.71	0.72
1:B:456:MET:HG2	1:B:467:TYR:HB3	1.71	0.72
1:C:57:VAL:HG21	1:C:86:GLY:HA2	1.71	0.72
1:C:324:VAL:HG23	1:C:326:PRO:HD3	1.71	0.71
1:C:428:LYS:HD2	1:C:429:GLU:H	1.56	0.71
1:C:901:VAL:O	1:C:904:VAL:HG12	1.90	0.71
1:C:979:SER:HA	1:C:1011:MET:HE2	1.71	0.71
1:C:950:LYS:HA	1:C:953:MET:HE2	1.71	0.70
1:C:355:MET:HE3	1:C:368:PRO:HG2	1.73	0.70
1:B:659:LYS:HE3	1:B:659:LYS:HA	1.74	0.69
1:C:200:PRO:O	1:C:204:ILE:HG13	1.92	0.69
2:D:115:THR:HG22	2:D:117:LEU:H	1.58	0.69
1:C:204:ILE:HG23	1:C:759:VAL:HG22	1.73	0.69
1:A:57:VAL:HG12	1:A:82:SER:HB3	1.75	0.68
1:A:445:ILE:HG22	1:A:449:LEU:CD1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:818:ARG:NH2	1:B:821:GLY:O	2.24	0.68
1:C:411:VAL:HG12	1:C:438:ILE:HD11	1.73	0.68
1:A:441:ALA:O	1:A:445:ILE:HD12	1.94	0.68
1:B:1025:PHE:O	1:B:1029:VAL:HG22	1.93	0.68
2:D:30:VAL:HG21	2:D:62:ILE:HG12	1.76	0.67
1:C:420:MET:HE3	1:C:500:ILE:HG12	1.76	0.66
2:D:34:MET:HE2	2:D:34:MET:HA	1.76	0.66
1:A:45:ILE:HD13	1:A:111:LEU:HD13	1.76	0.66
1:B:363:ARG:HH21	1:B:498:LYS:HE2	1.59	0.66
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.78	0.66
1:C:69:MET:HE1	1:C:107:VAL:HG13	1.77	0.66
1:B:875:SER:O	1:B:879:ILE:HD12	1.96	0.66
1:A:420:MET:HE2	1:A:500:ILE:HG13	1.77	0.66
1:A:347:ALA:HA	1:A:350:LEU:HD12	1.78	0.66
1:C:420:MET:HG2	1:C:500:ILE:HB	1.78	0.66
1:B:909:VAL:HG12	1:B:913:LEU:HD11	1.77	0.65
1:C:76:MET:HG3	1:C:95:GLU:HG3	1.78	0.65
1:C:673:GLU:N	1:C:673:GLU:OE1	2.25	0.65
1:A:16:ALA:O	1:A:20:MET:HG3	1.96	0.65
1:A:878:ALA:O	1:A:882:ILE:HG12	1.97	0.65
1:A:273:GLU:HG2	1:A:772:TYR:HE2	1.62	0.65
1:A:213:GLN:HG3	1:B:56:THR:HG23	1.77	0.64
1:B:341:VAL:O	1:B:345:VAL:HG23	1.97	0.64
1:B:335:ILE:HD13	1:B:995:ALA:HB1	1.78	0.64
2:D:154:ILE:HD12	2:D:155:ASN:N	2.12	0.64
1:A:509:LYS:O	1:A:514:GLY:HA3	1.97	0.64
1:A:361:ASN:O	1:A:365:THR:HG23	1.97	0.64
1:B:909:VAL:HG22	1:B:935:ILE:HD11	1.80	0.64
1:C:162:MET:HE1	1:C:323:ILE:HD11	1.80	0.64
1:C:342:LYS:O	1:C:346:GLU:HG3	1.99	0.63
1:C:669:PRO:HB2	1:C:862:MET:HE3	1.79	0.63
2:E:56:TYR:HB2	2:E:86:LEU:HD13	1.79	0.63
2:E:65:VAL:O	2:E:69:ASN:ND2	2.31	0.63
2:E:34:MET:HE2	2:E:34:MET:HA	1.79	0.63
1:A:532:GLY:CA	1:A:965:LEU:HD21	2.28	0.63
2:E:92:HIS:O	2:E:96:VAL:HG23	1.98	0.63
1:B:220:GLY:HA2	1:C:781:MET:CE	2.28	0.63
1:B:355:MET:HE1	1:B:413:VAL:HG11	1.80	0.63
1:C:775:SER:HB3	1:C:780:ARG:HD3	1.79	0.63
1:A:682:PHE:HE1	1:A:684:LEU:HD13	1.64	0.62
1:A:775:SER:HB3	1:A:780:ARG:HD3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:THR:O	1:C:528:THR:HG23	1.98	0.62
1:A:777:ALA:O	1:A:781:MET:HG2	2.00	0.62
2:D:127:GLU:O	2:D:131:VAL:HG23	2.00	0.62
1:B:16:ALA:O	1:B:20:MET:HG3	1.99	0.62
1:C:328:ASP:O	1:C:331:PRO:HD2	1.99	0.62
1:A:356:TYR:HA	1:A:365:THR:HG21	1.81	0.62
1:C:904:VAL:HG22	1:C:938:SER:HB2	1.81	0.62
2:D:96:VAL:HG21	2:D:128:ILE:HG12	1.81	0.62
1:C:958:LYS:NZ	1:C:966:ASP:OD2	2.28	0.61
1:B:997:SER:HA	1:B:1000:GLN:HE21	1.64	0.61
1:C:190:PRO:HB3	1:C:789:TRP:CE3	2.35	0.61
1:A:13:TRP:O	1:A:17:ILE:HG13	2.01	0.61
1:B:359:LEU:HD22	1:B:417:GLU:HG3	1.81	0.61
1:C:447:MET:SD	1:C:887:CYS:HB3	2.41	0.61
2:E:89:HIS:HB2	2:E:119:LEU:HD13	1.83	0.61
1:B:414:GLU:HG3	1:B:977:MET:HE1	1.82	0.61
1:C:103:ALA:O	1:C:107:VAL:HG23	2.00	0.61
1:A:420:MET:HE1	1:A:499:PRO:HA	1.82	0.60
1:B:650:ARG:HG3	1:B:650:ARG:HH11	1.66	0.60
1:A:1027:VAL:O	1:A:1031:ARG:HD3	2.00	0.60
2:E:56:TYR:HD1	2:E:57:TRP:HD1	1.48	0.60
1:B:441:ALA:O	1:B:445:ILE:HG13	2.02	0.60
2:D:161:LEU:O	2:D:165:LEU:HD12	2.01	0.60
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.66	0.60
1:B:395:MET:O	1:B:398:MET:HB2	2.01	0.60
1:C:535:LEU:HD13	1:C:961:ILE:HD12	1.84	0.60
1:A:893:GLU:O	1:A:893:GLU:HG3	2.02	0.60
1:C:398:MET:HG2	1:C:473:THR:HG21	1.83	0.60
1:C:1032:ARG:HD2	1:C:1033:PHE:CE1	2.37	0.60
1:B:961:ILE:H	1:B:961:ILE:HD12	1.65	0.59
1:C:702:LEU:HD11	1:C:844:MET:HE1	1.84	0.59
1:A:355:MET:HE2	1:A:355:MET:HA	1.84	0.59
2:D:96:VAL:HG12	2:D:100:LEU:HD11	1.83	0.59
2:E:93:LEU:HD13	2:E:128:ILE:HG13	1.84	0.59
1:B:223:PRO:HD2	1:C:780:ARG:HH22	1.67	0.59
1:B:248:LYS:HA	1:B:261:LEU:HD12	1.85	0.59
1:C:38:ILE:HD11	1:C:671:ILE:HD12	1.84	0.59
2:D:148:THR:O	2:D:151:ASP:N	2.36	0.59
2:E:29:GLU:HA	2:E:32:ILE:HG22	1.84	0.59
1:B:590:VAL:O	1:B:594:VAL:HG23	2.02	0.59
2:D:125:HIS:O	2:D:129:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:46:VAL:O	2:E:77:ASP:HB2	2.03	0.58
1:B:400:LEU:HG	1:B:929:VAL:HG12	1.85	0.58
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.85	0.58
1:A:809:TRP:CD1	2:E:79:LEU:HD12	2.38	0.58
1:A:1012:VAL:O	1:A:1016:VAL:HG22	2.03	0.58
1:C:33:ALA:O	1:C:337:ILE:HD11	2.04	0.58
1:C:165:ALA:HB3	1:C:313:MET:CE	2.33	0.58
1:B:879:ILE:O	1:B:883:VAL:HG23	2.04	0.58
1:A:843:LEU:HA	1:A:846:GLN:HG3	1.86	0.58
2:D:139:VAL:CG2	2:D:165:LEU:HD23	2.34	0.57
1:A:56:THR:HG23	1:C:213:GLN:HG3	1.86	0.57
1:A:59:ASP:HB3	1:C:763:ILE:HD11	1.85	0.57
1:B:1015:THR:O	1:B:1019:ILE:HG23	2.04	0.57
2:D:127:GLU:OE2	2:D:127:GLU:N	2.33	0.57
1:A:393:LEU:HD12	1:A:470:PHE:HE1	1.69	0.57
1:B:602:GLU:OE1	1:B:605:ASN:ND2	2.34	0.57
1:B:971:ARG:O	1:B:975:ILE:HG13	2.03	0.57
1:B:228:GLN:OE1	1:C:781:MET:HB3	2.04	0.57
1:C:341:VAL:HG22	1:C:395:MET:CE	2.34	0.57
2:E:46:VAL:C	2:E:78:THR:HG23	2.30	0.57
1:A:909:VAL:HG22	1:A:931:LEU:HD21	1.86	0.57
1:B:445:ILE:HG21	1:B:940:LYS:HG3	1.87	0.57
1:C:214:VAL:HG23	1:C:237:GLN:HB2	1.87	0.57
1:C:152:GLU:OE2	1:C:152:GLU:N	2.25	0.56
1:B:126:GLY:HA3	1:C:116:PRO:CB	2.36	0.56
1:C:717:ARG:HG2	1:C:717:ARG:HH11	1.71	0.56
1:A:261:LEU:N	1:A:264:ASP:OD2	2.32	0.56
1:C:186:ILE:HB	1:C:773:VAL:HG12	1.88	0.56
1:C:546:LEU:O	1:C:550:VAL:HG12	2.04	0.56
1:B:399:VAL:O	1:B:402:ILE:HG13	2.04	0.56
1:A:695:LEU:HG	1:A:825:MET:HE3	1.88	0.56
1:C:538:THR:HG22	1:C:1024:VAL:HG22	1.86	0.56
1:A:101:ASP:O	1:A:105:VAL:HG23	2.06	0.56
1:A:446:ALA:HB2	1:A:482:VAL:HG21	1.88	0.56
1:B:150:THR:O	1:B:154:ILE:HG13	2.06	0.56
1:B:646:ALA:HB1	1:B:650:ARG:HH12	1.71	0.56
1:A:687:GLN:HE21	1:A:856:GLY:HA3	1.71	0.56
1:C:682:PHE:HB2	1:C:859:TRP:CZ3	2.40	0.56
1:C:198:LEU:HD13	1:C:251:LEU:HD23	1.87	0.55
1:C:428:LYS:HD2	1:C:429:GLU:N	2.20	0.55
1:C:408:ASP:O	1:C:412:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:ASP:CG	1:B:792:ARG:HH22	2.12	0.55
1:C:341:VAL:HG22	1:C:395:MET:HE3	1.89	0.55
2:E:93:LEU:HD22	2:E:127:GLU:HB2	1.89	0.55
1:C:336:SER:O	1:C:340:VAL:HG23	2.06	0.55
1:C:764:ASP:OD1	1:C:765:ARG:NH1	2.38	0.55
1:A:370:ILE:HD12	1:A:370:ILE:N	2.20	0.55
1:A:57:VAL:CG1	1:A:88:VAL:HG22	2.37	0.55
1:C:145:THR:OG1	1:C:146:ASP:N	2.39	0.55
1:C:190:PRO:HB3	1:C:789:TRP:CZ3	2.41	0.55
1:C:393:LEU:HD13	1:C:466:ILE:HG23	1.89	0.55
1:C:712:MET:SD	1:C:835:LYS:HG2	2.47	0.55
1:A:495:THR:HG23	1:A:496:MET:HG2	1.89	0.55
1:B:523:SER:HA	1:B:526:HIS:HB2	1.89	0.55
1:B:989:LEU:HD22	1:B:1000:GLN:HB3	1.89	0.55
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.88	0.54
1:C:188:MET:HE1	1:C:200:PRO:CG	2.37	0.54
1:C:953:MET:HE1	1:C:1030:ARG:NH2	2.22	0.54
2:D:33:LEU:HD12	2:D:38:ALA:HB2	1.89	0.54
2:D:142:GLN:HB3	2:D:146:GLY:HA2	1.89	0.54
1:B:328:ASP:OD1	1:B:330:THR:OG1	2.23	0.54
1:A:361:ASN:HD22	1:A:364:ALA:H	1.55	0.54
1:C:376:LEU:HD22	1:C:398:MET:HE3	1.88	0.54
1:A:572:PHE:HE2	1:A:631:LEU:HD21	1.73	0.54
1:A:693:GLU:H	1:A:693:GLU:CD	2.14	0.54
1:B:982:PHE:O	1:B:986:VAL:HG12	2.08	0.54
1:C:4:PHE:O	1:C:8:ARG:HG3	2.07	0.54
1:C:836:SER:OG	1:C:839:GLU:HG3	2.08	0.54
1:B:445:ILE:O	1:B:449:LEU:HG	2.08	0.54
2:E:59:HIS:O	2:E:63:VAL:HG23	2.08	0.54
1:B:398:MET:HE2	1:B:473:THR:HG23	1.90	0.54
2:D:149:ALA:HA	2:D:152:ILE:HD13	1.90	0.53
1:B:898:PRO:O	1:B:902:MET:HG3	2.08	0.53
1:C:185:ARG:HH22	1:C:774:MET:CE	2.22	0.53
1:C:964:THR:O	1:C:968:VAL:HG23	2.08	0.53
2:E:30:VAL:O	2:E:34:MET:HG2	2.08	0.53
1:A:298:ASN:HB3	1:A:301:ASP:HB2	1.90	0.53
1:A:356:TYR:HD1	1:A:356:TYR:O	1.92	0.53
1:C:69:MET:CE	1:C:107:VAL:HG13	2.37	0.53
1:B:371:ALA:O	1:B:375:VAL:HG23	2.08	0.53
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.90	0.53
1:A:586:ARG:HG2	1:A:586:ARG:HH11	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:PHE:CZ	1:B:324:VAL:HG11	2.43	0.53
1:B:348:ILE:HG21	1:B:369:THR:HG23	1.91	0.53
1:B:393:LEU:HD12	1:B:470:PHE:CE2	2.44	0.53
1:B:80:SER:HB2	1:B:90:ILE:HG12	1.91	0.53
1:B:347:ALA:O	1:B:351:VAL:HG13	2.08	0.53
1:B:157:TYR:CZ	1:B:318:PRO:HD3	2.43	0.53
1:B:328:ASP:O	1:B:331:PRO:HD2	2.09	0.53
1:B:344:LEU:O	1:B:348:ILE:HD12	2.08	0.53
2:D:94:GLU:H	2:D:94:GLU:CD	2.16	0.53
1:A:1:MET:HB3	1:A:2:PRO:HD3	1.89	0.53
1:A:715:SER:HB2	1:A:830:GLN:HG3	1.90	0.53
1:B:138:MET:HE2	1:B:140:VAL:HG22	1.90	0.53
1:B:87:THR:HG21	1:B:620:ARG:HH21	1.74	0.53
1:A:361:ASN:ND2	1:A:364:ALA:H	2.07	0.52
1:B:416:VAL:HG21	1:B:431:THR:HG23	1.90	0.52
1:A:527:TYR:CD2	1:A:972:LEU:HD22	2.44	0.52
1:A:309:GLU:HG3	1:A:313:MET:HE2	1.92	0.52
1:A:427:PRO:O	1:A:431:THR:HG23	2.09	0.52
1:A:493:CYS:HA	1:A:497:LEU:HD23	1.90	0.52
1:C:653:ARG:O	1:C:656:SER:OG	2.23	0.52
1:C:746:ILE:HD13	1:C:804:PHE:CE1	2.45	0.52
1:A:617:PHE:CZ	1:A:666:PHE:HZ	2.27	0.52
1:A:836:SER:HB3	1:A:839:GLU:HG3	1.92	0.52
2:D:46:VAL:O	2:D:78:THR:OG1	2.25	0.52
2:E:34:MET:C	2:E:36:ASN:H	2.16	0.52
1:A:958:LYS:HD2	1:A:962:GLU:OE1	2.10	0.52
1:B:202:ASP:OD2	1:B:792:ARG:NH2	2.33	0.52
2:E:129:VAL:HG21	2:E:161:LEU:HD11	1.91	0.52
1:A:895:TRP:CE2	1:C:10:ILE:HG23	2.44	0.52
1:A:909:VAL:HG22	1:A:931:LEU:HD11	1.92	0.52
1:A:435:MET:HE2	1:A:490:PRO:HG3	1.91	0.52
1:A:733:GLN:O	1:A:737:GLN:HG3	2.10	0.52
1:A:888:LEU:CB	1:A:898:PRO:HB3	2.39	0.52
1:A:942:ALA:O	1:A:946:VAL:HG22	2.10	0.52
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.92	0.52
1:C:448:VAL:HG12	1:C:884:VAL:HG13	1.92	0.52
1:C:911:GLY:HA3	1:C:1013:THR:OG1	2.10	0.52
2:D:89:HIS:CD2	2:D:123:ARG:HD3	2.45	0.52
1:B:249:ILE:O	1:B:261:LEU:HD13	2.10	0.51
1:B:449:LEU:HB2	1:B:478:MET:SD	2.50	0.51
1:B:594:VAL:HG13	1:B:655:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:ALA:O	1:B:781:MET:HG2	2.10	0.51
1:B:809:TRP:NE1	2:D:79:LEU:HD12	2.24	0.51
1:C:997:SER:HA	1:C:1000:GLN:HB2	1.92	0.51
1:A:222:THR:HA	1:A:224:PRO:HD3	1.92	0.51
1:B:400:LEU:HD21	1:B:1003:VAL:HG22	1.91	0.51
1:B:527:TYR:O	1:B:531:VAL:HG23	2.10	0.51
2:E:160:ASP:O	2:E:164:ILE:HG13	2.09	0.51
1:A:505:HIS:HD1	1:A:521:GLU:CD	2.18	0.51
1:B:157:TYR:CE2	1:B:318:PRO:HD3	2.45	0.51
1:B:813:SER:OG	1:B:815:ARG:O	2.25	0.51
1:C:351:VAL:HG21	1:C:402:ILE:HG22	1.92	0.51
1:A:111:LEU:HG	1:A:115:MET:CE	2.40	0.51
1:A:186:ILE:HB	1:A:773:VAL:HG22	1.92	0.51
2:D:49:THR:O	2:D:52:HIS:HB2	2.10	0.51
1:A:395:MET:O	1:A:399:VAL:HG23	2.11	0.51
1:C:580:ALA:HB1	1:C:724:THR:HG22	1.92	0.51
1:C:674:LEU:HD12	1:C:674:LEU:H	1.76	0.51
1:A:975:ILE:HG22	1:A:976:LEU:HD22	1.93	0.51
1:B:456:MET:CG	1:B:467:TYR:HB3	2.39	0.51
1:B:605:ASN:O	1:B:632:LYS:HG3	2.11	0.51
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.93	0.51
1:A:909:VAL:HA	1:A:931:LEU:HD11	1.93	0.51
1:B:732:ASP:OD2	1:B:735:LYS:HB2	2.11	0.50
1:B:527:TYR:CE2	1:B:968:VAL:HG12	2.46	0.50
1:C:68:ASN:HD22	1:C:114:ALA:HB2	1.77	0.50
1:C:350:LEU:O	1:C:354:VAL:HG23	2.12	0.50
1:A:13:TRP:CZ2	1:A:492:LEU:HD11	2.47	0.50
1:A:370:ILE:HD12	1:A:370:ILE:H	1.77	0.50
1:A:671:ILE:O	1:A:674:LEU:HB3	2.12	0.50
1:C:600:THR:O	1:C:603:LYS:HE3	2.12	0.50
2:E:125:HIS:O	2:E:129:VAL:HG23	2.12	0.50
1:A:1021:PHE:HB3	1:A:1025:PHE:CZ	2.47	0.50
1:C:1:MET:HB3	1:C:2:PRO:HD3	1.94	0.50
1:C:104:GLN:C	1:C:104:GLN:OE1	2.55	0.50
1:A:350:LEU:HD22	1:A:984:LEU:HG	1.92	0.50
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.36	0.50
1:B:519:MET:O	1:B:522:LYS:HG2	2.11	0.50
2:E:127:GLU:O	2:E:131:VAL:HG23	2.12	0.50
1:B:278:ILE:HB	1:B:613:ASN:HB3	1.94	0.50
1:B:435:MET:O	1:B:439:GLN:HB3	2.12	0.50
1:C:407:ASP:O	1:C:411:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:59:HIS:O	2:D:63:VAL:HG23	2.12	0.50
2:D:107:ASN:HD21	2:D:138:ASP:H	1.59	0.50
1:A:10:ILE:HD13	1:B:895:TRP:CD1	2.47	0.50
1:A:684:LEU:O	1:A:824:SER:HA	2.12	0.50
1:C:453:PHE:O	1:C:456:MET:HG2	2.12	0.50
1:B:375:VAL:HG22	1:B:484:VAL:HG21	1.94	0.50
1:C:555:LEU:HD11	1:C:914:LEU:HD23	1.92	0.50
1:C:741:VAL:HG11	1:C:799:VAL:HG11	1.93	0.50
1:A:420:MET:CE	1:A:499:PRO:HA	2.42	0.49
1:A:111:LEU:HG	1:A:115:MET:HE1	1.95	0.49
1:A:680:PHE:CZ	1:A:829:GLY:HA3	2.48	0.49
1:A:350:LEU:O	1:A:354:VAL:HG23	2.13	0.49
1:B:269:GLU:HG3	1:B:270:LEU:O	2.13	0.49
1:B:5:PHE:CE2	1:B:487:ILE:HG12	2.47	0.49
1:B:38:ILE:HG23	1:B:465:ALA:HB3	1.94	0.49
1:C:449:LEU:HD12	1:C:478:MET:HE2	1.94	0.49
1:C:548:ILE:HG23	1:C:910:ILE:HD13	1.92	0.49
1:C:573:MET:CE	1:C:617:PHE:HZ	2.26	0.49
1:A:331:PRO:O	1:A:335:ILE:HG12	2.13	0.49
1:A:777:ALA:HB1	1:A:781:MET:HE3	1.94	0.49
1:B:445:ILE:HD13	1:B:940:LYS:CG	2.43	0.49
1:C:197:GLN:O	1:C:198:LEU:HD23	2.13	0.49
1:A:31:PRO:HG2	1:A:389:SER:HB2	1.93	0.49
1:A:360:GLN:NE2	1:A:517:ASN:OD1	2.32	0.49
1:A:393:LEU:HB3	1:A:470:PHE:CE1	2.48	0.49
1:A:879:ILE:HG21	1:C:25:LEU:HD11	1.95	0.49
1:A:57:VAL:HG13	1:A:88:VAL:HG22	1.95	0.49
1:A:532:GLY:HA2	1:A:965:LEU:HD21	1.95	0.49
1:B:534:ILE:HG23	1:B:541:TYR:CE2	2.48	0.49
1:B:897:ILE:N	1:B:898:PRO:HD2	2.27	0.49
1:C:754:TRP:CZ2	1:C:786:ILE:HD13	2.48	0.49
1:A:726:GLN:NE2	1:C:235:ILE:HG13	2.28	0.49
1:A:900:SER:OG	1:A:946:VAL:HG11	2.12	0.49
1:B:76:MET:HE2	1:B:94:PHE:O	2.12	0.49
1:C:159:ALA:HB3	1:C:181:GLN:HG3	1.94	0.49
1:B:375:VAL:O	1:B:379:THR:OG1	2.29	0.49
1:B:568:ASP:OD2	1:B:644:VAL:HG23	2.13	0.49
2:D:107:ASN:HD21	2:D:138:ASP:N	2.11	0.49
2:E:126:LEU:HD23	2:E:161:LEU:HD12	1.95	0.49
1:C:53:ASP:O	1:C:57:VAL:HG23	2.13	0.49
1:C:598:TYR:HB3	1:C:606:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:715:SER:O	1:C:717:ARG:NH1	2.46	0.49
2:D:89:HIS:NE2	2:D:123:ARG:HD3	2.28	0.49
2:E:64:GLU:HG2	2:E:98:VAL:HG11	1.94	0.49
1:B:647:ILE:HG13	1:B:650:ARG:NH2	2.27	0.48
1:C:205:THR:O	1:C:206:ALA:HB3	2.13	0.48
1:C:80:SER:HB3	1:C:90:ILE:HG12	1.95	0.48
1:B:702:LEU:HB2	1:B:851:LEU:HD11	1.95	0.48
1:C:590:VAL:O	1:C:594:VAL:HG23	2.13	0.48
1:C:735:LYS:HA	1:C:735:LYS:HD3	1.55	0.48
1:A:393:LEU:HD12	1:A:470:PHE:CE1	2.49	0.48
1:B:425:LEU:HD12	1:B:429:GLU:HB3	1.94	0.48
1:B:448:VAL:O	1:B:452:VAL:HG23	2.13	0.48
1:C:1016:VAL:HG12	1:C:1017:LEU:HD22	1.95	0.48
1:A:204:ILE:HG23	1:A:759:VAL:HG13	1.95	0.48
1:A:671:ILE:HG22	1:A:674:LEU:HB2	1.96	0.48
1:B:173:GLY:HA2	1:C:71:GLY:HA3	1.94	0.48
1:B:223:PRO:HD2	1:C:780:ARG:NH2	2.27	0.48
1:B:400:LEU:HB3	1:B:933:THR:HG21	1.96	0.48
2:D:139:VAL:HG23	2:D:165:LEU:HD23	1.95	0.48
1:A:586:ARG:O	1:A:590:VAL:HG23	2.14	0.48
1:A:843:LEU:HD13	1:A:846:GLN:HE21	1.77	0.48
1:B:879:ILE:HD12	1:B:879:ILE:H	1.79	0.48
1:C:527:TYR:CE2	1:C:968:VAL:HG12	2.49	0.48
1:C:540:ARG:HD3	1:C:540:ARG:N	2.27	0.48
2:E:153:SER:HB3	2:E:161:LEU:CD2	2.35	0.48
1:B:336:SER:CB	1:B:395:MET:HE1	2.41	0.48
1:B:775:SER:HB3	1:B:780:ARG:HD3	1.95	0.48
2:D:82:THR:O	2:D:85:HIS:HB2	2.14	0.48
2:D:121:ALA:HB2	2:D:149:ALA:HB1	1.96	0.48
1:A:682:PHE:HB2	1:A:859:TRP:CZ3	2.49	0.47
1:B:758:TYR:HB2	1:B:772:TYR:CE1	2.50	0.47
1:C:120:GLN:H	1:C:120:GLN:CD	2.22	0.47
1:A:13:TRP:CE2	1:A:492:LEU:HD11	2.49	0.47
1:B:706:ALA:CB	1:B:716:VAL:HG11	2.44	0.47
1:C:188:MET:HE3	1:C:193:LEU:HD11	1.96	0.47
1:C:291:ILE:HD13	1:C:306:ILE:HD13	1.96	0.47
2:E:28:ASP:N	2:E:28:ASP:OD1	2.47	0.47
1:B:492:LEU:HD22	1:B:496:MET:HE2	1.94	0.47
1:A:686:ASP:HB2	1:A:695:LEU:HD22	1.97	0.47
1:B:1018:ALA:O	1:B:1022:VAL:HG23	2.13	0.47
1:C:185:ARG:NH2	1:C:774:MET:HE3	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.39	0.47
1:A:562:SER:OG	1:A:924:ASP:HB3	2.14	0.47
1:B:220:GLY:HA2	1:C:781:MET:HE2	1.97	0.47
1:B:220:GLY:HA2	1:C:781:MET:HE1	1.96	0.47
1:C:185:ARG:HD3	1:C:272:GLY:O	2.15	0.47
2:D:84:LEU:HD11	2:D:96:VAL:HG13	1.97	0.47
1:A:144:ASN:ND2	1:A:149:MET:HB2	2.30	0.47
1:A:546:LEU:O	1:A:550:VAL:HG23	2.14	0.47
1:A:818:ARG:NH2	1:A:823:PRO:HD3	2.30	0.47
1:B:10:ILE:HD12	1:C:894:SER:N	2.29	0.47
1:B:293:LEU:HD13	1:B:299:ALA:HA	1.96	0.47
1:A:273:GLU:CD	1:A:770:LYS:HD2	2.40	0.47
1:B:78:MET:HG2	1:B:79:SER:N	2.29	0.47
1:C:674:LEU:HD12	1:C:674:LEU:N	2.30	0.47
1:B:367:ILE:HG12	1:B:496:MET:HE3	1.97	0.47
1:B:974:PRO:HA	1:B:977:MET:HE3	1.97	0.47
1:B:1003:VAL:O	1:B:1007:VAL:HG23	2.15	0.47
2:E:100:LEU:HD21	2:E:106:VAL:HG23	1.96	0.47
1:A:888:LEU:HB3	1:A:898:PRO:HB3	1.97	0.47
1:B:650:ARG:HG3	1:B:650:ARG:NH1	2.30	0.47
1:B:673:GLU:O	1:B:673:GLU:HG2	2.14	0.47
1:C:380:PHE:HA	1:C:383:LEU:HD12	1.97	0.46
1:C:842:GLU:O	1:C:846:GLN:HG3	2.16	0.46
1:A:578:LEU:HB2	1:A:623:ASN:HB2	1.97	0.46
1:A:1025:PHE:O	1:A:1029:VAL:HG23	2.15	0.46
1:B:62:THR:O	1:B:66:GLU:HG3	2.15	0.46
1:B:174:ASP:OD1	1:B:175:VAL:N	2.49	0.46
1:B:400:LEU:HD13	1:B:400:LEU:HA	1.78	0.46
1:A:230:LEU:HD11	1:B:809:TRP:CH2	2.50	0.46
1:A:563:PHE:O	1:A:925:VAL:HG23	2.16	0.46
1:A:226:LYS:HE2	1:B:585:GLU:OE2	2.14	0.46
1:A:23:GLY:HA3	1:A:377:LEU:O	2.15	0.46
1:A:762:PHE:CE2	1:A:764:ASP:HB2	2.51	0.46
1:B:620:ARG:NH1	1:B:620:ARG:HG3	2.31	0.46
1:C:534:ILE:HG23	1:C:541:TYR:CE1	2.50	0.46
1:A:129:VAL:C	1:A:130:GLU:HG2	2.41	0.46
1:A:190:PRO:HA	1:A:193:LEU:HB2	1.98	0.46
1:A:528:THR:HG21	1:A:969:ARG:HB3	1.97	0.46
1:B:527:TYR:HE2	1:B:968:VAL:HG12	1.81	0.46
2:D:60:LEU:O	2:D:64:GLU:HG3	2.16	0.46
2:D:160:ASP:O	2:D:164:ILE:HG13	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ILE:O	1:A:883:VAL:HG23	2.16	0.46
1:C:447:MET:CE	1:C:891:LEU:HD22	2.45	0.46
1:A:401:ALA:O	1:A:404:LEU:N	2.46	0.46
1:B:311:ALA:HA	1:B:314:GLU:HG3	1.98	0.46
1:B:893:GLU:O	1:B:893:GLU:HG3	2.15	0.46
1:C:183:ALA:N	1:C:271:GLY:O	2.33	0.46
1:C:933:THR:O	1:C:937:LEU:HG	2.15	0.46
1:A:342:LYS:HE3	1:A:346:GLU:OE2	2.16	0.46
1:A:347:ALA:HA	1:A:350:LEU:CD1	2.46	0.46
1:C:291:ILE:HG21	1:C:306:ILE:CD1	2.46	0.46
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.81	0.46
1:A:220:GLY:HA2	1:B:781:MET:SD	2.56	0.45
1:A:403:GLY:O	1:A:937:LEU:HD21	2.17	0.45
1:A:414:GLU:CD	1:A:974:PRO:HG3	2.40	0.45
1:A:859:TRP:CD1	1:A:867:ARG:HD2	2.51	0.45
1:A:965:LEU:O	1:A:969:ARG:HG2	2.16	0.45
1:B:108:GLN:HG3	1:C:112:GLN:HG3	1.98	0.45
1:B:185:ARG:NH2	1:B:774:MET:HE2	2.31	0.45
1:B:414:GLU:HG3	1:B:977:MET:CE	2.46	0.45
1:B:739:LEU:HD23	1:B:739:LEU:HA	1.79	0.45
1:C:327:TYR:CD2	1:C:628:PHE:HB3	2.51	0.45
1:C:378:GLY:O	1:C:382:VAL:HG23	2.16	0.45
2:E:17:LYS:HB3	2:E:33:LEU:HD11	1.97	0.45
2:E:144:LYS:HG2	2:E:145:PHE:CE1	2.51	0.45
1:B:255:GLN:H	1:B:255:GLN:CD	2.23	0.45
1:C:277:ILE:HG23	1:C:612:ASN:HD22	1.82	0.45
1:C:707:ALA:O	1:C:710:PRO:HD3	2.16	0.45
1:A:480:LEU:O	1:A:484:VAL:HG23	2.17	0.45
1:A:578:LEU:HB2	1:A:623:ASN:O	2.16	0.45
1:A:781:MET:HB3	1:C:228:GLN:OE1	2.16	0.45
2:D:51:LEU:HD11	2:D:63:VAL:HG13	1.98	0.45
1:A:987:MET:HB3	1:A:988:PRO:HD3	1.99	0.45
1:B:182:TYR:CD2	1:B:270:LEU:HD13	2.51	0.45
2:E:93:LEU:HD11	2:E:131:VAL:HG21	1.99	0.45
1:C:644:VAL:O	1:C:648:THR:HG23	2.17	0.45
1:C:659:LYS:H	1:C:659:LYS:CD	2.19	0.45
2:D:94:GLU:O	2:D:98:VAL:HG23	2.16	0.45
2:E:34:MET:C	2:E:36:ASN:N	2.75	0.45
1:A:326:PRO:HG3	1:A:610:PHE:CD2	2.52	0.45
2:E:96:VAL:HG21	2:E:128:ILE:HG12	1.99	0.45
1:A:318:PRO:HD2	1:A:321:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:ILE:O	1:A:449:LEU:HD12	2.17	0.45
1:A:636:ASP:N	1:A:636:ASP:OD1	2.50	0.45
1:B:584:GLN:N	1:B:622:GLN:HB3	2.31	0.45
1:C:411:VAL:HG12	1:C:438:ILE:CD1	2.43	0.45
1:C:185:ARG:HH22	1:C:774:MET:HE3	1.82	0.45
1:A:99:ASP:OD1	1:A:99:ASP:C	2.60	0.45
1:B:350:LEU:HA	1:B:350:LEU:HD23	1.64	0.45
1:B:652:THR:HG23	1:B:664:PHE:HB2	1.98	0.45
2:D:96:VAL:O	2:D:100:LEU:HD12	2.17	0.45
1:B:10:ILE:HD13	1:C:895:TRP:CD1	2.52	0.45
1:B:149:MET:HG3	1:B:154:ILE:HG12	1.98	0.45
1:B:340:VAL:HG23	1:B:399:VAL:HG23	1.99	0.45
1:B:445:ILE:HD13	1:B:940:LYS:HG3	1.99	0.45
1:B:809:TRP:CD1	2:D:79:LEU:HD12	2.52	0.45
1:C:21:LEU:HD23	1:C:21:LEU:HA	1.58	0.45
1:B:352:PHE:HE1	1:B:365:THR:OG1	1.99	0.44
1:A:619:GLY:O	1:A:624:THR:HG21	2.17	0.44
1:A:1003:VAL:O	1:A:1007:VAL:HG23	2.17	0.44
1:B:559:LEU:HD12	1:B:560:PRO:HD2	1.98	0.44
1:B:684:LEU:O	1:B:824:SER:HA	2.18	0.44
1:B:909:VAL:CG2	1:B:935:ILE:HD11	2.45	0.44
1:C:34:GLN:O	1:C:391:ASN:HB2	2.17	0.44
1:C:530:SER:O	1:C:534:ILE:HG13	2.17	0.44
2:E:79:LEU:HA	2:E:111:ASP:OD2	2.16	0.44
1:A:359:LEU:HB2	1:A:365:THR:HG22	1.99	0.44
1:A:572:PHE:CD2	1:A:644:VAL:HG13	2.52	0.44
1:A:758:TYR:CZ	1:A:770:LYS:HG2	2.53	0.44
1:A:913:LEU:HD23	1:A:913:LEU:HA	1.60	0.44
1:A:966:ASP:HA	1:A:969:ARG:HG2	1.99	0.44
1:B:835:LYS:HD2	1:B:835:LYS:N	2.31	0.44
1:B:988:PRO:HA	1:B:991:ILE:HG12	2.00	0.44
1:B:1024:VAL:O	1:B:1028:VAL:HG13	2.18	0.44
1:C:23:GLY:HA3	1:C:377:LEU:HB3	2.00	0.44
1:A:230:LEU:HD23	1:A:230:LEU:C	2.42	0.44
1:B:5:PHE:CD2	1:B:487:ILE:HG23	2.53	0.44
1:B:335:ILE:O	1:B:339:GLU:HG2	2.17	0.44
1:B:564:LEU:HD22	1:B:671:ILE:HG13	1.99	0.44
1:B:578:LEU:HD11	1:B:590:VAL:HG21	1.99	0.44
1:C:982:PHE:O	1:C:986:VAL:HG22	2.17	0.44
1:A:600:THR:O	1:A:603:LYS:HG3	2.18	0.44
1:B:405:LEU:HD11	1:B:477:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:573:MET:CE	1:C:617:PHE:CZ	3.00	0.44
1:A:345:VAL:O	1:A:349:ILE:HG12	2.18	0.44
1:A:586:ARG:NH2	1:A:660:ASP:O	2.50	0.44
1:A:686:ASP:HB3	1:A:823:PRO:HB2	1.99	0.44
1:B:685:ILE:HG22	1:B:687:GLN:HG2	1.98	0.44
1:B:1023:PRO:O	1:B:1027:VAL:HG23	2.18	0.44
1:C:646:ALA:HA	1:C:649:MET:HE3	1.99	0.44
1:B:653:ARG:O	1:B:656:SER:OG	2.35	0.44
1:C:599:LEU:HD23	1:C:599:LEU:HA	1.62	0.44
1:C:674:LEU:HB2	1:C:862:MET:HE2	1.99	0.44
1:C:973:ARG:O	1:C:977:MET:HG3	2.18	0.44
1:B:113:LEU:O	1:B:116:PRO:HD2	2.18	0.44
1:B:184:MET:HB3	1:B:771:VAL:HG22	1.99	0.44
1:B:871:ASN:O	1:B:874:PRO:HD2	2.18	0.44
1:B:894:SER:OG	1:B:897:ILE:HG13	2.17	0.44
1:B:952:LEU:HD23	1:B:952:LEU:HA	1.80	0.44
1:C:1032:ARG:O	1:C:1032:ARG:HD3	2.18	0.44
1:B:5:PHE:CE2	1:B:487:ILE:HG23	2.53	0.44
1:C:527:TYR:CE1	1:C:1019:ILE:HD12	2.53	0.44
2:D:33:LEU:HD12	2:D:38:ALA:CB	2.47	0.44
2:E:29:GLU:O	2:E:32:ILE:HG22	2.18	0.44
2:E:133:LEU:HD23	2:E:133:LEU:HA	1.80	0.44
1:A:196:PHE:HB2	1:A:198:LEU:HD23	2.00	0.43
1:A:234:ILE:C	1:A:235:ILE:HD13	2.42	0.43
1:A:464:GLY:O	1:A:468:ARG:HB2	2.17	0.43
1:A:507:GLU:OE1	1:A:507:GLU:N	2.45	0.43
1:A:621:GLY:O	1:A:624:THR:HG22	2.18	0.43
1:A:888:LEU:HB2	1:A:898:PRO:HB3	2.00	0.43
1:C:242:SER:OG	1:C:245:GLU:HG3	2.18	0.43
2:E:80:GLY:O	2:E:110:ASP:HA	2.18	0.43
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.50	0.43
1:C:745:ASP:OD1	1:C:745:ASP:N	2.50	0.43
1:C:801:PHE:HA	1:C:804:PHE:CZ	2.53	0.43
1:A:447:MET:HE2	1:A:447:MET:HB2	1.82	0.43
1:C:669:PRO:HD3	1:C:677:ALA:C	2.43	0.43
2:E:153:SER:CB	2:E:161:LEU:HD23	2.36	0.43
1:A:189:ASN:OD1	1:A:191:ASN:N	2.52	0.43
1:A:439:GLN:O	1:A:443:VAL:HG23	2.19	0.43
1:A:965:LEU:HA	1:A:968:VAL:HG22	2.01	0.43
1:B:524:THR:CG2	1:B:969:ARG:HG3	2.48	0.43
1:B:293:LEU:HG	1:B:297:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:VAL:HG22	1:C:323:ILE:HD13	2.00	0.43
1:C:762:PHE:CE2	1:C:764:ASP:HB2	2.53	0.43
1:A:192:GLU:HA	1:A:195:LYS:HB3	1.99	0.43
1:A:575:MET:HE3	1:A:575:MET:HB2	1.82	0.43
1:C:162:MET:HA	1:C:313:MET:HE2	2.01	0.43
1:B:195:LYS:HD3	1:B:196:PHE:CZ	2.54	0.43
1:B:458:PHE:HD1	1:B:458:PHE:N	2.17	0.43
1:C:732:ASP:OD2	1:C:735:LYS:HG2	2.18	0.43
1:C:880:SER:O	1:C:884:VAL:HG23	2.18	0.43
1:B:739:LEU:HD13	1:B:799:VAL:HG11	2.01	0.43
1:C:591:LEU:HD22	1:C:611:ALA:HB1	2.00	0.43
1:A:171:GLY:O	1:A:293:LEU:HD12	2.19	0.43
1:A:369:THR:O	1:A:373:PRO:HD2	2.19	0.43
1:A:445:ILE:HG22	1:A:449:LEU:HD11	2.00	0.43
1:A:573:MET:HE3	1:A:573:MET:HB2	1.68	0.43
1:B:303:ALA:HB2	1:B:330:THR:HG21	2.01	0.43
1:C:114:ALA:C	1:C:116:PRO:HD2	2.44	0.43
2:E:18:LEU:HD23	2:E:50:PRO:HG2	2.01	0.43
1:A:10:ILE:HG23	1:B:895:TRP:CZ2	2.54	0.43
1:A:277:ILE:HG23	1:A:612:ASN:OD1	2.19	0.43
1:A:669:PRO:HD2	1:A:672:VAL:HA	2.00	0.43
1:A:729:ILE:HD11	1:A:786:ILE:HD12	2.01	0.43
1:C:973:ARG:HB3	1:C:974:PRO:HD3	2.01	0.43
1:B:535:LEU:HD22	1:B:1027:VAL:HG21	2.01	0.42
1:B:719:ASN:HD22	1:B:826:GLU:CD	2.27	0.42
1:C:335:ILE:O	1:C:339:GLU:HG2	2.19	0.42
2:D:152:ILE:HD12	2:D:152:ILE:H	1.82	0.42
1:A:200:PRO:HG2	1:A:749:THR:HG23	2.01	0.42
1:A:559:LEU:HD11	1:A:922:THR:HA	2.01	0.42
1:B:126:GLY:HA3	1:C:116:PRO:HB2	2.00	0.42
1:B:259:ARG:HB3	1:B:261:LEU:CD2	2.49	0.42
1:B:703:LEU:HD11	1:B:718:PRO:HG3	2.01	0.42
1:B:905:VAL:O	1:B:909:VAL:HG23	2.19	0.42
1:B:932:LEU:HA	1:B:932:LEU:HD23	1.71	0.42
1:C:197:GLN:HA	1:C:798:MET:SD	2.58	0.42
1:C:572:PHE:CE2	1:C:631:LEU:HD21	2.54	0.42
2:D:92:HIS:O	2:D:96:VAL:HG23	2.19	0.42
2:D:148:THR:O	2:D:149:ALA:C	2.61	0.42
1:A:613:ASN:HD22	1:A:614:GLY:N	2.16	0.42
1:C:277:ILE:HG23	1:C:612:ASN:ND2	2.34	0.42
1:C:363:ARG:HD3	1:C:498:LYS:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:GLU:OE2	2:D:94:GLU:N	2.24	0.42
1:A:360:GLN:HE22	1:A:517:ASN:CG	2.23	0.42
1:C:617:PHE:HE2	1:C:666:PHE:HZ	1.67	0.42
2:D:122:ASN:HA	2:D:152:ILE:HG21	2.01	0.42
1:B:716:VAL:HA	1:B:828:LEU:O	2.19	0.42
1:C:32:VAL:HA	1:C:390:ILE:O	2.20	0.42
1:C:38:ILE:HG13	1:C:39:ALA:N	2.34	0.42
2:D:109:LYS:HB3	2:D:113:GLY:HA2	2.01	0.42
1:A:465:ALA:O	1:A:469:GLN:HG2	2.19	0.42
1:B:458:PHE:N	1:B:458:PHE:CD1	2.87	0.42
1:B:878:ALA:O	1:B:882:ILE:HD12	2.20	0.42
1:A:407:ASP:CG	1:A:978:THR:HG21	2.45	0.42
1:B:620:ARG:HG3	1:B:620:ARG:HH11	1.85	0.42
1:C:80:SER:CB	1:C:90:ILE:HG12	2.50	0.42
2:D:117:LEU:HD11	2:D:129:VAL:HG13	2.01	0.42
2:E:46:VAL:O	2:E:78:THR:HG23	2.19	0.42
1:B:459:PHE:O	1:B:464:GLY:HA3	2.19	0.42
1:B:709:HIS:N	1:B:710:PRO:HD3	2.35	0.42
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	2.02	0.42
1:C:155:SER:HB3	1:C:180:SER:O	2.20	0.42
1:C:944:LEU:O	1:C:971:ARG:HG3	2.19	0.42
1:A:228:GLN:OE1	1:A:229:GLN:NE2	2.52	0.42
1:A:895:TRP:CZ2	1:C:10:ILE:HG23	2.55	0.42
1:B:16:ALA:HB2	1:B:488:LEU:HD13	2.01	0.42
1:B:20:MET:HE2	1:B:20:MET:HB3	1.75	0.42
1:B:478:MET:O	1:B:478:MET:HG2	2.18	0.42
1:A:166:ILE:HG21	1:A:291:ILE:HD11	2.02	0.42
1:A:406:VAL:HG12	1:A:410:ILE:HD11	2.01	0.42
1:A:406:VAL:HG12	1:A:410:ILE:CD1	2.50	0.42
1:A:502:LYS:H	1:A:502:LYS:HG2	1.67	0.42
1:A:729:ILE:HG21	1:A:729:ILE:HD13	1.71	0.42
1:A:750:LEU:HB2	1:A:801:PHE:CZ	2.55	0.42
1:B:190:PRO:HB3	1:B:789:TRP:CE3	2.55	0.42
1:B:767:ARG:HG2	1:B:767:ARG:HH11	1.85	0.42
1:C:162:MET:HE3	1:C:317:PHE:CE1	2.55	0.42
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.84	0.42
1:C:449:LEU:HD23	1:C:936:GLY:HA3	2.02	0.41
1:A:429:GLU:N	1:A:429:GLU:OE2	2.53	0.41
1:A:456:MET:SD	1:A:467:TYR:HB3	2.60	0.41
1:A:695:LEU:HD12	1:A:695:LEU:O	2.21	0.41
1:A:891:LEU:HD23	1:A:892:TYR:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:VAL:HG13	1:B:480:LEU:HB2	2.01	0.41
1:C:372:VAL:HB	1:C:373:PRO:HD3	2.02	0.41
1:A:351:VAL:HG22	1:A:981:ALA:HB1	2.02	0.41
1:A:946:VAL:HG12	1:A:1026:PHE:HB2	2.01	0.41
1:B:1030:ARG:HD2	1:B:1030:ARG:HA	1.78	0.41
1:C:987:MET:HE3	1:C:987:MET:HB2	1.76	0.41
1:A:576:VAL:HG22	1:A:663:VAL:CG2	2.47	0.41
1:A:578:LEU:HD22	1:A:661:ALA:HB1	2.01	0.41
1:B:657:GLN:O	1:B:659:LYS:HD2	2.20	0.41
1:B:851:LEU:HD23	1:B:851:LEU:HA	1.83	0.41
1:C:102:ILE:O	1:C:106:GLN:HG3	2.21	0.41
1:C:423:GLU:OE1	1:C:425:LEU:HD11	2.20	0.41
1:C:444:GLY:O	1:C:448:VAL:HG22	2.20	0.41
1:C:555:LEU:HA	1:C:555:LEU:HD23	1.81	0.41
1:A:470:PHE:CE2	1:A:929:VAL:HG21	2.55	0.41
1:A:902:MET:O	1:A:905:VAL:HG23	2.20	0.41
1:A:996:GLY:O	1:A:1000:GLN:HG3	2.20	0.41
1:A:1038:GLU:CG	1:A:1039:ASP:H	2.33	0.41
1:B:375:VAL:HG13	1:B:480:LEU:CB	2.50	0.41
1:C:38:ILE:CD1	1:C:671:ILE:HD12	2.50	0.41
1:C:563:PHE:O	1:C:924:ASP:HB2	2.20	0.41
1:C:845:GLU:HG2	1:C:857:TYR:CE2	2.56	0.41
2:E:56:TYR:CD1	2:E:57:TRP:HD1	2.33	0.41
1:A:798:MET:HE3	1:A:798:MET:HB3	1.85	0.41
1:B:666:PHE:HD2	1:B:667:ASN:O	2.04	0.41
1:C:559:LEU:C	1:C:559:LEU:HD23	2.46	0.41
1:A:289:LEU:HA	1:A:289:LEU:HD23	1.84	0.41
1:B:49:TYR:C	1:B:49:TYR:CD1	2.99	0.41
1:B:733:GLN:OE1	1:B:743:ILE:HG21	2.21	0.41
1:C:243:THR:HB	1:C:268:ILE:HG22	2.02	0.41
1:C:534:ILE:HG23	1:C:541:TYR:CZ	2.56	0.41
1:C:944:LEU:HD23	1:C:944:LEU:HA	1.88	0.41
1:A:35:TYR:HD1	1:A:393:LEU:HD21	1.85	0.41
1:A:362:PHE:O	1:A:366:LEU:HG	2.21	0.41
1:A:445:ILE:HG22	1:A:449:LEU:HD12	2.01	0.41
1:A:527:TYR:CE2	1:A:968:VAL:HB	2.56	0.41
1:A:712:MET:HG2	1:A:843:LEU:HD23	2.03	0.41
1:C:175:VAL:HG12	1:C:289:LEU:HD22	2.03	0.41
1:C:559:LEU:HD22	1:C:923:ASN:HB2	2.02	0.41
1:C:1018:ALA:O	1:C:1022:VAL:HB	2.21	0.41
2:E:40:VAL:HG23	2:E:41:ASN:OD1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ASN:OD1	1:A:110:LYS:NZ	2.53	0.41
1:A:277:ILE:HA	1:A:613:ASN:O	2.21	0.41
1:A:445:ILE:O	1:A:448:VAL:HG22	2.21	0.41
1:A:692:HIS:N	1:A:693:GLU:OE2	2.54	0.41
1:A:844:MET:HA	1:A:844:MET:HE2	2.03	0.41
1:A:972:LEU:HD12	1:A:972:LEU:HA	1.72	0.41
1:B:524:THR:HG22	1:B:969:ARG:HG3	2.02	0.41
1:B:658:ILE:HG22	1:B:661:ALA:HB3	2.02	0.41
1:B:801:PHE:HA	1:B:804:PHE:CZ	2.56	0.41
1:C:2:PRO:HB3	1:C:435:MET:HE2	2.03	0.41
1:C:222:THR:HA	1:C:224:PRO:HD3	2.02	0.41
1:C:413:VAL:HG22	1:C:493:CYS:SG	2.61	0.41
1:C:573:MET:HE3	1:C:617:PHE:CZ	2.55	0.41
1:C:573:MET:HE1	1:C:617:PHE:HZ	1.85	0.41
1:C:1018:ALA:C	1:C:1020:PHE:H	2.28	0.41
2:D:73:VAL:HG23	2:D:99:LEU:HD22	2.02	0.41
1:A:156:ASP:OD1	1:A:769:LYS:NZ	2.53	0.41
1:B:154:ILE:O	1:B:158:VAL:HG23	2.20	0.41
1:B:566:ASP:OD1	1:B:566:ASP:N	2.54	0.41
1:C:134:SER:OG	1:C:673:GLU:O	2.39	0.41
1:C:175:VAL:CG1	1:C:289:LEU:HD22	2.51	0.41
1:C:743:ILE:HD12	1:C:743:ILE:H	1.86	0.41
1:A:412:VAL:O	1:A:416:VAL:HG23	2.22	0.40
1:A:445:ILE:HG13	1:A:943:ILE:HG21	2.03	0.40
1:B:459:PHE:HB2	1:B:464:GLY:HA2	2.03	0.40
1:B:762:PHE:CE2	1:B:764:ASP:HB2	2.55	0.40
1:C:433:LYS:HE2	1:C:437:GLN:NE2	2.36	0.40
1:C:615:PHE:CD1	1:C:615:PHE:C	2.99	0.40
2:D:115:THR:HG23	2:D:116:PRO:HD2	2.02	0.40
2:E:94:GLU:O	2:E:98:VAL:HG23	2.21	0.40
2:E:100:LEU:HD23	2:E:100:LEU:HA	1.93	0.40
1:A:366:LEU:O	1:A:370:ILE:HD12	2.21	0.40
1:A:450:SER:O	1:A:454:VAL:HG23	2.22	0.40
1:A:586:ARG:HG2	1:A:586:ARG:NH1	2.37	0.40
1:A:848:ALA:HA	1:A:851:LEU:CD2	2.52	0.40
1:C:33:ALA:O	1:C:391:ASN:HA	2.21	0.40
1:C:1032:ARG:HD2	1:C:1033:PHE:CD1	2.57	0.40
1:A:222:THR:HG22	1:A:224:PRO:HD3	2.03	0.40
1:A:914:LEU:HA	1:A:914:LEU:HD23	1.86	0.40
1:B:267:LYS:HA	1:B:267:LYS:HD3	1.84	0.40
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:LEU:HD21	1:C:937:LEU:HD21	2.04	0.40
2:E:67:LEU:HD22	2:E:73:VAL:HG12	2.03	0.40
1:A:10:ILE:HG13	1:B:893:GLU:OE2	2.21	0.40
1:A:281:PHE:O	1:A:284:GLN:HG2	2.20	0.40
1:A:528:THR:CG2	1:A:969:ARG:HB3	2.52	0.40
1:B:149:MET:HB2	1:B:153:ASP:CB	2.51	0.40
1:B:364:ALA:HA	1:B:497:LEU:HD21	2.02	0.40
1:C:568:ASP:OD2	1:C:644:VAL:HG23	2.21	0.40
1:C:952:LEU:HD23	1:C:952:LEU:HA	1.99	0.40
2:D:115:THR:HG22	2:D:117:LEU:N	2.30	0.40
1:B:882:ILE:O	1:B:886:LEU:HD23	2.22	0.40
1:C:101:ASP:O	1:C:105:VAL:HG23	2.21	0.40
2:D:96:VAL:HG12	2:D:100:LEU:CD1	2.51	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	1042/1057 (99%)	972 (93%)	63 (6%)	7 (1%)	18	53
1	B	1031/1057 (98%)	972 (94%)	57 (6%)	2 (0%)	43	76
1	C	1031/1057 (98%)	961 (93%)	67 (6%)	3 (0%)	36	70
2	D	154/169 (91%)	139 (90%)	15 (10%)	0	100	100
2	E	150/169 (89%)	137 (91%)	13 (9%)	0	100	100
All	All	3408/3509 (97%)	3181 (93%)	215 (6%)	12 (0%)	30	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	71	GLY

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Mol	Chain	Res	Type
1	A	126	GLY
1	A	678	THR
1	A	1037	ASN
1	A	388	PHE
1	A	738	ALA
1	A	787	GLY
1	B	674	LEU
1	C	146	ASP
1	B	820	ASN
1	A	367	ILE
1	C	295	THR

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	850/863 (98%)	828 (97%)	22 (3%)	40	72
1	B	839/863 (97%)	819 (98%)	20 (2%)	43	73
1	C	839/863 (97%)	816 (97%)	23 (3%)	39	71
2	D	120/132 (91%)	116 (97%)	4 (3%)	33	67
2	E	117/132 (89%)	114 (97%)	3 (3%)	40	72
All	All	2765/2853 (97%)	2693 (97%)	72 (3%)	40	72

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	SER
1	A	88	VAL
1	A	93	THR
1	A	238	THR
1	A	241	THR
1	A	270	LEU
1	A	276	ASP
1	A	405	LEU

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Mol	Chain	Res	Type
1	A	450	SER
1	A	492	LEU
1	A	552	MET
1	A	578	LEU
1	A	590	VAL
1	A	630	SER
1	A	636	ASP
1	A	801	PHE
1	A	851	LEU
1	A	865	GLN
1	A	990	VAL
1	A	1031	ARG
1	A	1038	GLU
1	A	1039	ASP
1	B	46	SER
1	B	48	SER
1	B	82	SER
1	B	88	VAL
1	B	128	SER
1	B	226	LYS
1	B	276	ASP
1	B	351	VAL
1	B	353	LEU
1	B	377	LEU
1	B	383	LEU
1	B	390	ILE
1	B	458	PHE
1	B	543	VAL
1	B	577	GLN
1	B	604	ASN
1	B	656	SER
1	B	914	LEU
1	B	947	GLU
1	B	966	ASP
1	C	46	SER
1	C	62	THR
1	C	82	SER
1	C	133	SER
1	C	134	SER
1	C	145	THR
1	C	177	LEU
1	C	181	GLN

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Mol	Chain	Res	Type
1	C	406	VAL
1	C	454	VAL
1	C	463	THR
1	C	471	SER
1	C	473	THR
1	C	550	VAL
1	C	564	LEU
1	C	577	GLN
1	C	584	GLN
1	C	626	ILE
1	C	672	VAL
1	C	674	LEU
1	C	757	SER
1	C	956	GLU
1	C	975	ILE
2	D	45	VAL
2	D	76	TYR
2	D	81	SER
2	D	107	ASN
2	E	31	ARG
2	E	127	GLU
2	E	165	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	124	GLN
1	A	144	ASN
1	A	191	ASN
1	A	194	ASN
1	A	254	ASN
1	A	361	ASN
1	A	439	GLN
1	A	596	HIS
1	A	613	ASN
1	A	687	GLN
1	A	797	GLN
1	A	846	GLN
1	A	872	GLN
1	B	161	ASN
1	B	191	ASN

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Mol	Chain	Res	Type
1	B	194	ASN
1	B	231	ASN
1	B	1000	GLN
1	C	34	GLN
1	C	151	GLN
1	C	194	ASN
1	C	229	GLN
1	C	526	HIS
1	C	577	GLN
1	C	605	ASN
1	C	612	ASN
1	C	642	ASN
1	C	871	ASN
1	C	872	GLN
2	D	102	ASN
2	D	107	ASN
2	D	142	GLN
2	E	142	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 ⓘ

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	1044/1057 (98%)	0.25	41 (3%)	43	24	47, 80, 115, 136	0
1	B	1033/1057 (97%)	0.27	52 (5%)	34	18	53, 79, 104, 121	0
1	C	1033/1057 (97%)	0.29	59 (5%)	29	15	49, 73, 94, 109	0
2	D	156/169 (92%)	0.12	3 (1%)	66	43	67, 80, 98, 108	0
2	E	152/169 (89%)	0.24	5 (3%)	49	28	71, 86, 107, 116	0
All	All	3418/3509 (97%)	0.26	160 (4%)	36	19	47, 77, 106, 136	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	618	ALA	6.3
1	B	284	GLN	6.0
1	B	407	ASP	5.5
1	A	537	SER	5.3
1	B	134	SER	5.1
1	A	541	TYR	5.1
1	B	670	ALA	4.9
1	B	671	ILE	4.8
1	B	615	PHE	4.7
1	B	574	THR	4.7
1	C	49	TYR	4.6
1	C	701	GLN	4.6
1	C	698	ALA	4.6
1	C	122	VAL	4.4
1	A	536	ARG	4.3
1	C	699	ARG	4.2
1	C	817	GLU	4.2
1	B	531	VAL	4.2
1	B	279	ALA	4.2
1	B	626	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	573	MET	4.1
1	B	628	PHE	4.1
1	B	617	PHE	4.1
1	C	816	LEU	4.1
1	A	873	ALA	4.1
1	A	123	GLN	3.9
1	C	48	SER	3.9
2	E	64	GLU	3.9
1	C	700	ASN	3.9
2	E	15	GLY	3.7
1	B	635	ALA	3.7
1	C	124	GLN	3.7
1	A	36	PRO	3.7
1	A	776	GLU	3.7
1	C	125	GLN	3.6
1	C	410	ILE	3.6
1	C	458	PHE	3.6
1	B	674	LEU	3.6
1	A	459	PHE	3.6
1	B	760	ASN	3.6
1	A	719	ASN	3.5
1	B	761	ASP	3.5
1	C	403	GLY	3.5
1	B	627	ALA	3.5
1	A	301	ASP	3.5
1	A	535	LEU	3.5
1	A	775	SER	3.5
1	B	629	VAL	3.4
1	B	854	GLY	3.4
1	C	813	SER	3.3
1	B	408	ASP	3.3
1	B	676	THR	3.3
2	D	140	ASN	3.3
1	B	610	PHE	3.3
1	C	692	HIS	3.3
1	C	676	THR	3.3
1	B	532	GLY	3.2
1	A	423	GLU	3.2
1	B	281	PHE	3.2
1	C	723	ASP	3.2
1	A	429	GLU	3.2
1	A	877	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	672	VAL	3.1
1	C	811	TYR	3.1
1	C	355	MET	3.1
1	B	529	ASP	3.1
1	B	611	ALA	3.0
1	B	612	ASN	3.0
1	B	694	LYS	3.0
1	C	82	SER	2.9
1	C	87	THR	2.9
1	B	609	VAL	2.9
1	C	824	SER	2.9
1	A	628	PHE	2.9
1	A	674	LEU	2.9
1	C	7	ASP	2.8
1	C	513	PHE	2.8
1	B	575	MET	2.8
1	B	672	VAL	2.8
1	C	54	ALA	2.8
1	C	128	SER	2.8
1	C	89	GLN	2.8
1	B	366	LEU	2.7
1	A	676	THR	2.7
1	A	826	GLU	2.7
1	C	696	THR	2.7
1	A	985	GLY	2.6
1	C	691	GLY	2.6
1	A	69	MET	2.6
1	B	643	LYS	2.6
1	B	984	LEU	2.6
1	C	55	LYS	2.6
1	C	705	GLU	2.6
1	A	37	THR	2.6
1	C	453	PHE	2.6
1	B	144	ASN	2.6
1	A	868	LEU	2.6
1	C	351	VAL	2.6
1	C	872	GLN	2.5
1	B	286	ALA	2.5
1	C	496	MET	2.5
1	A	467	TYR	2.5
1	A	113	LEU	2.5
1	B	176	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	57	TRP	2.5
1	B	124	GLN	2.5
1	A	615	PHE	2.5
1	B	563	PHE	2.5
1	C	119	PRO	2.5
1	A	1040	ILE	2.4
1	C	6	ILE	2.4
1	C	121	GLU	2.4
1	C	226	LYS	2.4
1	C	494	ALA	2.4
1	A	662	MET	2.4
1	C	86	GLY	2.4
1	A	148	THR	2.3
1	C	495	THR	2.3
1	B	645	GLU	2.3
1	A	112	GLN	2.3
1	C	224	PRO	2.2
1	A	981	ALA	2.2
1	A	668	LEU	2.2
1	B	1026	PHE	2.2
1	C	964	THR	2.2
1	C	834	GLY	2.2
2	D	115	THR	2.2
1	C	284	GLN	2.2
1	C	264	ASP	2.2
1	A	971	ARG	2.2
1	A	38	ILE	2.2
1	C	118	LEU	2.2
1	C	702	LEU	2.2
1	B	813	SER	2.2
1	B	719	ASN	2.2
1	C	83	ASP	2.2
1	A	620	ARG	2.1
1	B	282	ASN	2.1
2	E	145	PHE	2.1
1	C	408	ASP	2.1
1	C	497	LEU	2.1
1	A	244	GLU	2.1
1	A	543	VAL	2.1
1	B	525	HIS	2.1
1	B	392	THR	2.1
1	C	357	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	402	ILE	2.1
1	A	774	MET	2.1
1	C	401	ALA	2.1
1	C	726	GLN	2.1
1	B	720	GLY	2.1
2	D	74	ASN	2.1
1	B	786	ILE	2.1
2	E	139	VAL	2.0
1	B	608	SER	2.0
1	A	804	PHE	2.0
1	B	130	GLU	2.0
1	C	743	ILE	2.0
1	C	470	PHE	2.0
1	A	972	LEU	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 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.