



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:02 AM UTC

PDB ID : 1N0V / pdb_00001n0v
Title : Crystal structure of elongation factor 2
Authors : Joergensen, R.; Ortiz, P.A.; Carr-Schmid, A.; Nissen, P.; Kinzy, T.G.; Andersen, G.R.
Deposited on : 2002-10-15
Resolution : 2.85 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

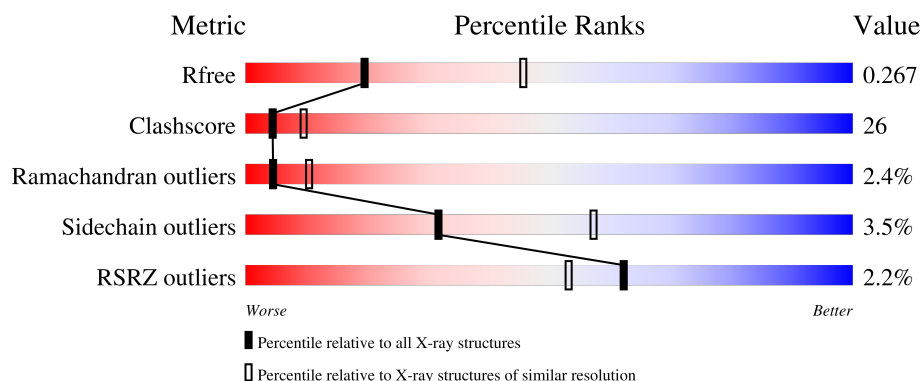
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	C	842	
1	D	842	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12838 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.

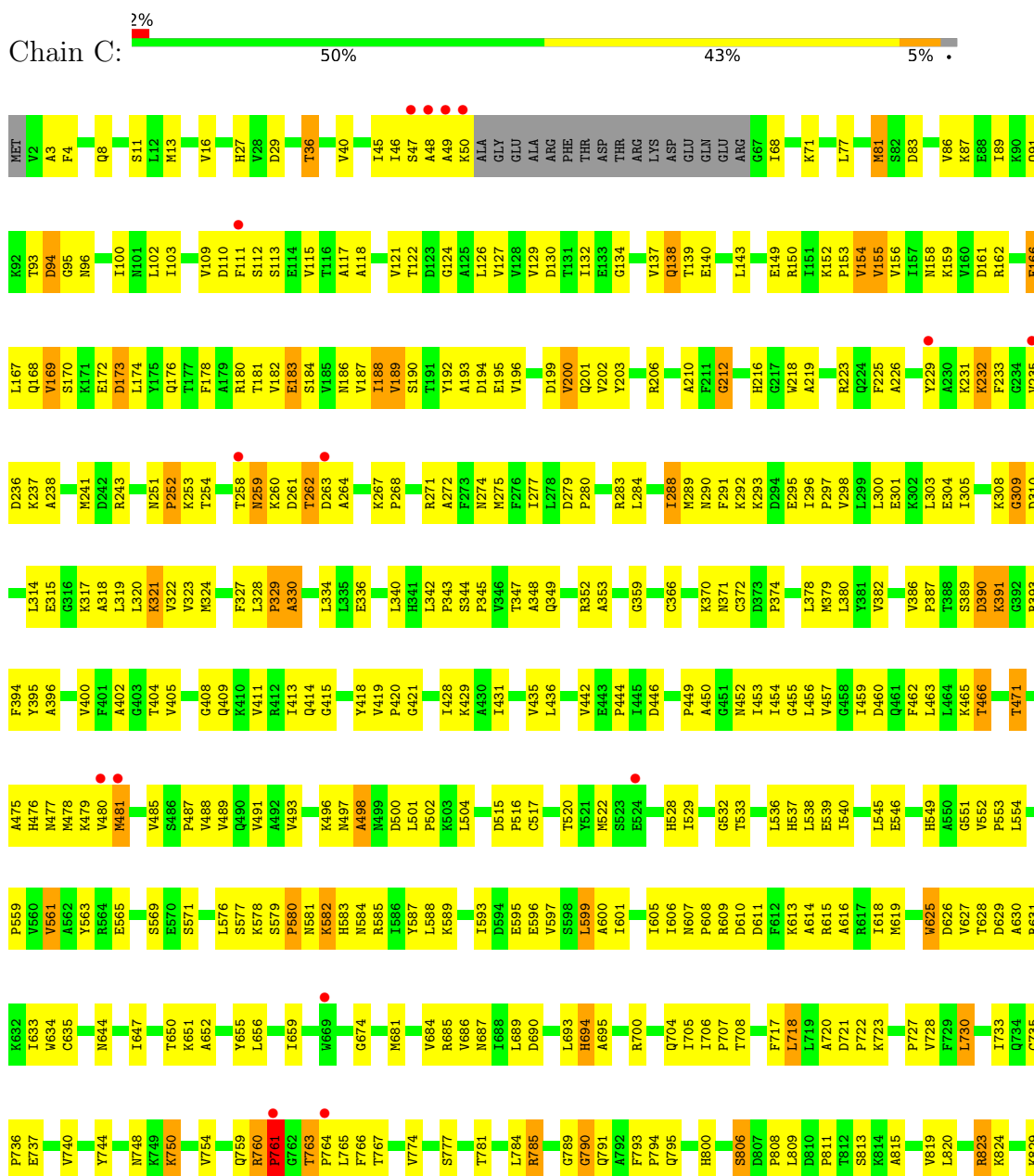
- Molecule 1 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	825	Total	C	N	O	S	0	0	0
			6419	4084	1096	1209	30			
1	D	825	Total	C	N	O	S	0	0	0
			6419	4084	1096	1209	30			

3 Residue-property plots [i](#)

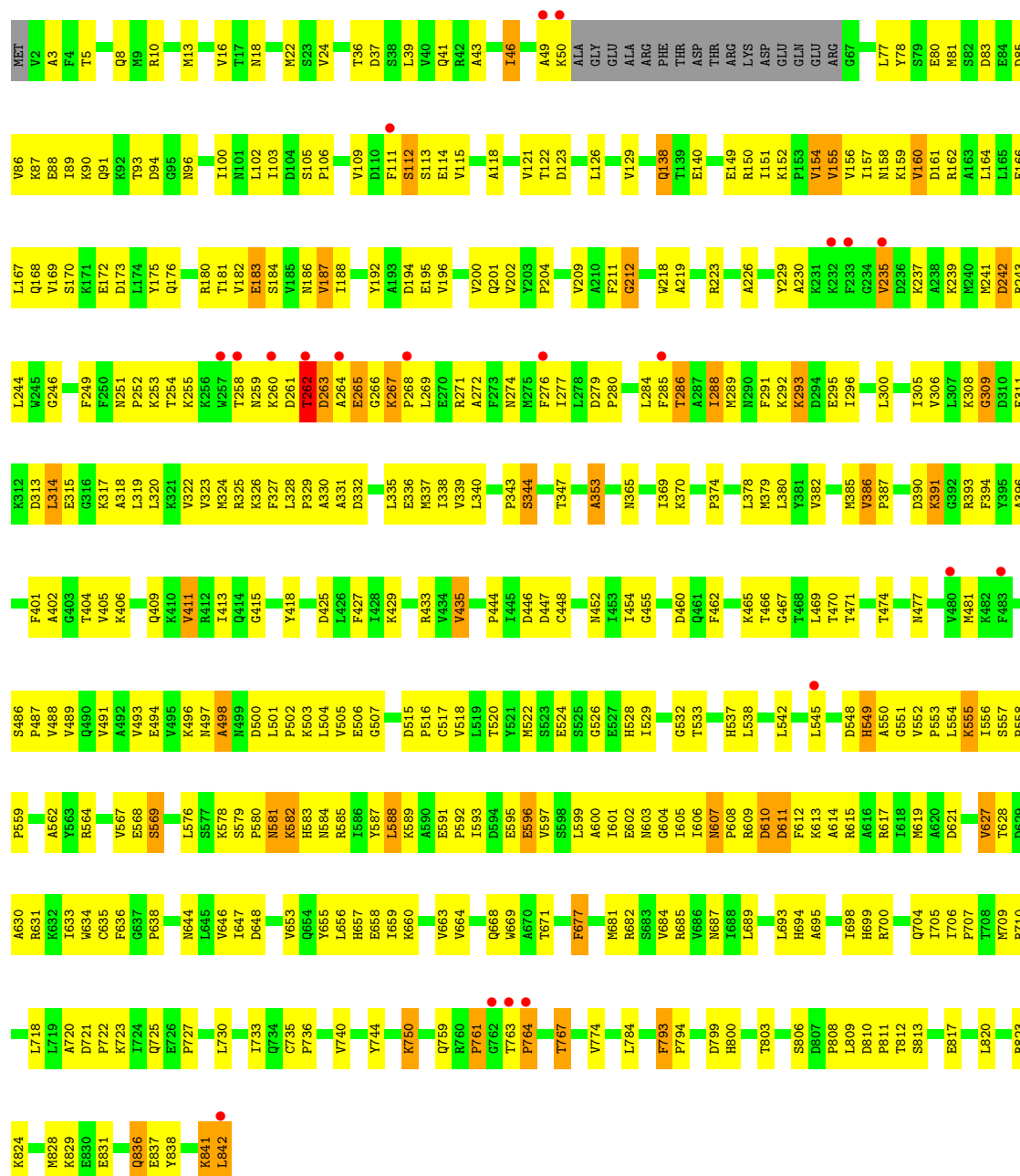
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Elongation factor 2





● Molecule 1: Elongation factor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.83Å 114.55Å 177.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.85 30.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.85) 96.2 (30.00-2.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.84Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.273 0.228 , 0.267	Depositor DCC
R_{free} test set	1101 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12838	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% 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	C	0.53	0/6543	1.03	40/8859 (0.5%)
1	D	0.56	0/6543	1.06	44/8859 (0.5%)
All	All	0.55	0/13086	1.04	84/17718 (0.5%)

There are no bond length outliers.

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	ASP	N-CA-C	16.45	129.29	111.03
1	C	760	ARG	CA-C-N	12.69	135.70	119.84
1	C	760	ARG	C-N-CA	12.69	135.70	119.84
1	D	264	ALA	N-CA-C	9.59	121.50	111.14
1	C	763	THR	N-CA-C	8.32	121.77	110.29
1	C	192	TYR	N-CA-C	7.53	121.36	112.93
1	D	764	PRO	N-CA-C	-7.43	106.08	114.92
1	D	268	PRO	N-CA-C	7.34	122.78	111.11
1	C	288	ILE	N-CA-C	7.26	117.39	110.42
1	D	340	LEU	N-CA-C	6.95	121.21	112.87
1	D	267	LYS	CA-C-N	6.87	126.89	119.89
1	D	267	LYS	C-N-CA	6.87	126.89	119.89
1	D	607	ASN	CA-C-N	6.84	126.80	119.28
1	D	607	ASN	C-N-CA	6.84	126.80	119.28
1	D	149	GLU	N-CA-C	-6.63	104.32	112.88
1	D	591	GLU	CA-C-N	6.48	126.24	119.76
1	D	591	GLU	C-N-CA	6.48	126.24	119.76
1	D	411	VAL	N-CA-C	6.46	118.08	108.46
1	D	155	VAL	N-CA-C	6.43	119.17	109.20
1	D	793	PHE	CA-C-N	6.42	126.37	120.21
1	D	793	PHE	C-N-CA	6.42	126.37	120.21
1	C	415	GLY	CA-C-N	6.38	125.61	118.97
1	C	415	GLY	C-N-CA	6.38	125.61	118.97
1	C	838	TYR	N-CA-C	-6.36	104.97	114.64
1	C	359	GLY	CA-C-N	6.29	127.70	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	359	GLY	C-N-CA	6.29	127.70	119.84
1	D	446	ASP	N-CA-C	6.25	117.76	111.07
1	C	137	VAL	N-CA-C	6.21	116.39	110.42
1	D	580	PRO	N-CA-C	-6.21	105.26	113.65
1	C	155	VAL	N-CA-C	6.18	118.78	109.20
1	D	154	VAL	N-CA-C	-6.18	99.80	108.27
1	D	266	GLY	N-CA-C	-6.18	98.54	113.18
1	C	580	PRO	N-CA-C	-6.16	105.51	113.57
1	C	763	THR	CA-C-N	6.15	127.53	119.84
1	C	763	THR	C-N-CA	6.15	127.53	119.84
1	D	115	VAL	N-CA-C	-6.15	104.51	110.72
1	C	721	ASP	CA-C-N	6.13	125.89	119.76
1	C	721	ASP	C-N-CA	6.13	125.89	119.76
1	D	569	SER	N-CA-C	6.12	115.93	107.73
1	C	793	PHE	CA-C-N	6.09	127.49	120.98
1	C	793	PHE	C-N-CA	6.09	127.49	120.98
1	C	733	ILE	N-CA-C	6.08	116.63	107.75
1	D	242	ASP	N-CA-C	-6.05	104.01	111.40
1	C	348	ALA	N-CA-C	6.02	118.37	111.02
1	C	561	VAL	N-CA-C	6.00	116.75	107.99
1	D	636	PHE	N-CA-C	-5.98	101.36	110.14
1	C	694	HIS	N-CA-C	-5.97	102.65	110.53
1	D	705	ILE	N-CA-C	5.97	116.14	110.53
1	C	353	ALA	N-CA-C	5.96	117.47	110.97
1	D	593	ILE	N-CA-C	-5.89	99.93	108.36
1	D	195	GLU	N-CA-C	-5.84	105.31	113.37
1	D	730	LEU	N-CA-C	-5.84	99.01	108.52
1	D	160	VAL	N-CA-C	-5.83	104.83	110.72
1	D	435	VAL	N-CA-C	5.78	116.69	108.42
1	D	750	LYS	N-CA-C	5.76	119.50	111.56
1	C	475	ALA	N-CA-C	5.74	118.80	110.42
1	C	275	MET	N-CA-C	5.74	117.61	111.36
1	C	761	PRO	N-CA-C	5.73	124.28	112.47
1	C	446	ASP	N-CA-C	5.70	117.17	111.07
1	D	212	GLY	N-CA-C	5.70	118.55	110.74
1	D	262	THR	N-CA-C	-5.70	104.04	111.74
1	C	154	VAL	N-CA-C	-5.67	97.54	109.34
1	C	777	SER	N-CA-C	5.67	119.82	113.01
1	D	353	ALA	N-CA-C	5.67	117.94	111.02
1	C	750	LYS	N-CA-C	5.58	117.59	110.61
1	C	593	ILE	N-CA-C	-5.50	100.47	108.17
1	D	288	ILE	N-CA-C	5.46	117.88	111.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	ASP	CB-CA-C	-5.43	102.54	110.95
1	C	202	VAL	N-CA-C	5.42	117.12	108.87
1	D	581	ASN	N-CA-C	-5.31	105.18	110.97
1	C	173	ASP	N-CA-C	-5.30	105.19	110.97
1	C	94	ASP	CB-CA-C	-5.28	103.73	111.23
1	D	187	VAL	N-CA-C	-5.27	105.36	110.42
1	C	187	VAL	N-CA-C	-5.21	105.46	110.72
1	D	841	LYS	N-CA-C	5.18	116.62	111.07
1	D	344	SER	N-CA-C	-5.17	103.43	110.36
1	D	695	ALA	N-CA-C	5.17	116.91	111.28
1	C	115	VAL	N-CA-C	-5.09	105.75	110.53
1	C	95	GLY	N-CA-C	-5.09	106.59	112.29
1	C	195	GLU	N-CA-C	-5.08	107.15	113.19
1	D	611	ASP	N-CA-C	-5.07	102.14	109.59
1	C	212	GLY	N-CA-C	5.03	117.38	110.69
1	D	721	ASP	CA-C-N	5.03	124.94	119.76
1	D	721	ASP	C-N-CA	5.03	124.94	119.76

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	C	6419	0	6492	344	0
1	D	6419	0	6492	338	0
All	All	12838	0	12984	682	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 26.

All (682) 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:D:289:MET:HE1	1:D:317:LYS:HG2	1.31	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:644:ASN:HD22	1:D:684:VAL:H	1.15	0.95
1:C:418:TYR:HB3	1:C:477:ASN:HD21	1.27	0.95
1:D:391:LYS:HA	1:D:391:LYS:HE2	1.50	0.94
1:C:644:ASN:HD22	1:C:684:VAL:HB	1.33	0.93
1:D:841:LYS:O	1:D:842:LEU:HB3	1.69	0.93
1:C:659:ILE:HD13	1:C:693:LEU:HD21	1.50	0.93
1:D:533:THR:H	1:D:537:HIS:HD2	1.03	0.93
1:D:258:THR:HG22	1:D:260:LYS:H	1.34	0.92
1:D:91:GLN:HE22	1:D:344:SER:H	1.07	0.92
1:C:685:ARG:HE	1:C:687:ASN:HD21	1.10	0.92
1:C:258:THR:HG22	1:C:260:LYS:H	1.34	0.92
1:D:685:ARG:HE	1:D:687:ASN:HD21	1.09	0.91
1:C:607:ASN:HD21	1:C:609:ARG:HH21	1.16	0.91
1:D:494:GLU:HB2	1:D:555:LYS:HD3	1.52	0.91
1:C:156:VAL:HG22	1:C:210:ALA:HB3	1.52	0.89
1:D:607:ASN:HD21	1:D:609:ARG:NH2	1.69	0.89
1:D:126:LEU:HD11	1:D:156:VAL:HG23	1.54	0.89
1:D:488:VAL:HG23	1:D:489:VAL:HG23	1.56	0.88
1:D:619:MET:HE1	1:D:633:ILE:HD11	1.55	0.88
1:D:265:GLU:HG2	1:D:267:LYS:NZ	1.89	0.88
1:C:619:MET:HE1	1:C:633:ILE:HD11	1.56	0.87
1:D:91:GLN:NE2	1:D:344:SER:H	1.73	0.86
1:D:288:ILE:HG23	1:D:319:LEU:HD23	1.59	0.85
1:C:759:GLN:HB2	1:C:766:PHE:CE1	2.11	0.85
1:D:251:ASN:HB3	1:D:254:THR:OG1	1.77	0.84
1:C:501:LEU:HB3	1:C:502:PRO:HD3	1.60	0.84
1:D:694:HIS:O	1:D:700:ARG:HD3	1.79	0.83
1:D:140:GLU:HG3	1:D:188:ILE:HD13	1.62	0.82
1:D:262:THR:HA	1:D:267:LYS:O	1.79	0.82
1:C:223:ARG:HG3	1:C:241:MET:HE1	1.60	0.81
1:C:391:LYS:HE2	1:C:391:LYS:HA	1.62	0.81
1:D:324:MET:HA	1:D:324:MET:HE2	1.63	0.81
1:D:533:THR:H	1:D:537:HIS:CD2	1.95	0.80
1:C:744:TYR:CE1	1:C:754:VAL:HG21	2.18	0.79
1:C:615:ARG:HG2	1:C:619:MET:HE2	1.64	0.78
1:D:186:ASN:HB3	1:D:201:GLN:HE21	1.48	0.78
1:C:744:TYR:HE1	1:C:754:VAL:HG21	1.47	0.78
1:D:784:LEU:HD23	1:D:794:PRO:HG3	1.64	0.78
1:C:607:ASN:HD21	1:C:609:ARG:NH2	1.81	0.77
1:D:3:ALA:HA	1:D:46:ILE:O	1.84	0.77
1:C:305:ILE:HG21	1:C:323:VAL:HG13	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:619:MET:HE3	1:D:630:ALA:HB1	1.65	0.76
1:D:126:LEU:HD11	1:D:156:VAL:CG2	2.15	0.76
1:C:36:THR:HG22	1:C:102:LEU:HD21	1.65	0.76
1:D:487:PRO:HA	1:D:532:GLY:O	1.86	0.76
1:D:94:ASP:C	1:D:94:ASP:OD1	2.28	0.75
1:C:291:PHE:HE1	1:C:315:GLU:HB3	1.52	0.75
1:D:533:THR:N	1:D:537:HIS:HD2	1.83	0.75
1:D:265:GLU:HB3	1:D:267:LYS:HD2	1.69	0.75
1:C:169:VAL:HG22	1:C:170:SER:H	1.52	0.74
1:C:324:MET:HE2	1:C:324:MET:HA	1.69	0.74
1:D:150:ARG:NH1	1:D:196:VAL:HG11	2.03	0.74
1:D:619:MET:HE1	1:D:633:ILE:CD1	2.17	0.73
1:C:91:GLN:HE21	1:C:347:THR:CB	2.01	0.73
1:C:140:GLU:HG3	1:C:188:ILE:HD13	1.68	0.72
1:D:106:PRO:HG2	1:D:114:GLU:HG3	1.70	0.72
1:C:809:LEU:O	1:C:811:PRO:HD3	1.90	0.72
1:C:500:ASP:HB3	1:C:552:VAL:HG11	1.71	0.72
1:C:94:ASP:OD1	1:C:94:ASP:C	2.31	0.71
1:D:226:ALA:O	1:D:230:ALA:HB2	1.90	0.71
1:D:644:ASN:ND2	1:D:684:VAL:H	1.87	0.71
1:D:491:VAL:HG21	1:D:542:LEU:HD11	1.71	0.71
1:D:569:SER:O	1:D:720:ALA:HB1	1.91	0.71
1:D:91:GLN:HE22	1:D:344:SER:N	1.85	0.71
1:C:153:PRO:HD2	1:C:200:VAL:HG22	1.73	0.70
1:C:784:LEU:HD23	1:C:794:PRO:HG3	1.73	0.70
1:D:615:ARG:HG2	1:D:619:MET:HE2	1.74	0.70
1:D:155:VAL:HG23	1:D:202:VAL:HG11	1.72	0.70
1:D:152:LYS:HG3	1:D:200:VAL:CG2	2.21	0.70
1:C:533:THR:H	1:C:537:HIS:HD2	1.40	0.70
1:C:49:ALA:O	1:C:50:LYS:CB	2.40	0.69
1:D:808:PRO:HG2	1:D:809:LEU:HD12	1.72	0.69
1:C:49:ALA:O	1:C:50:LYS:HB2	1.92	0.69
1:C:279:ASP:HB3	1:C:280:PRO:HD3	1.74	0.69
1:D:784:LEU:CD2	1:D:794:PRO:HG3	2.23	0.69
1:D:260:LYS:HB2	1:D:263:ASP:HB2	1.75	0.68
1:D:693:LEU:HB3	1:D:700:ARG:HD2	1.75	0.68
1:D:162:ARG:O	1:D:166:GLU:HB2	1.93	0.68
1:D:279:ASP:HB3	1:D:280:PRO:HD3	1.74	0.68
1:D:406:LYS:HB3	1:D:447:ASP:HB3	1.75	0.68
1:D:500:ASP:CB	1:D:552:VAL:HG11	2.24	0.68
1:D:305:ILE:HG21	1:D:323:VAL:HG13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLN:HE22	1:C:343:PRO:HA	1.58	0.68
1:D:265:GLU:HG2	1:D:267:LYS:HZ2	1.58	0.68
1:D:669:TRP:HD1	1:D:710:ARG:NH1	1.90	0.68
1:C:581:ASN:ND2	1:C:704:GLN:HG3	2.08	0.68
1:C:289:MET:HE1	1:C:317:LYS:HG2	1.75	0.67
1:D:507:GLY:HA3	1:D:550:ALA:HB2	1.75	0.67
1:D:186:ASN:HB3	1:D:201:GLN:NE2	2.09	0.67
1:D:806:SER:HB2	1:D:813:SER:HB2	1.76	0.67
1:D:172:GLU:HA	1:D:274:ASN:HD21	1.60	0.66
1:C:626:ASP:OD2	1:C:628:THR:HB	1.96	0.66
1:D:194:ASP:C	1:D:196:VAL:H	2.04	0.66
1:D:260:LYS:HD2	1:D:263:ASP:OD1	1.96	0.66
1:D:433:ARG:HE	1:D:444:PRO:HB3	1.59	0.66
1:D:588:LEU:C	1:D:588:LEU:HD12	2.21	0.66
1:D:659:ILE:HD13	1:D:693:LEU:HD21	1.78	0.65
1:C:68:ILE:HD13	1:C:390:ASP:HB2	1.79	0.65
1:C:533:THR:H	1:C:537:HIS:CD2	2.14	0.65
1:C:644:ASN:ND2	1:C:684:VAL:HB	2.10	0.65
1:C:607:ASN:ND2	1:C:609:ARG:HH21	1.93	0.65
1:C:91:GLN:HE22	1:C:344:SER:H	1.45	0.65
1:C:169:VAL:HG22	1:C:173:ASP:HB2	1.78	0.65
1:D:496:LYS:HD2	1:D:553:PRO:HB3	1.79	0.65
1:C:706:ILE:HB	1:C:707:PRO:HD3	1.79	0.65
1:D:394:PHE:CZ	1:D:516:PRO:HG3	2.32	0.65
1:C:454:ILE:HG13	1:C:455:GLY:H	1.62	0.65
1:D:579:SER:HB2	1:D:704:GLN:OE1	1.96	0.65
1:D:581:ASN:O	1:D:582:LYS:HB2	1.96	0.64
1:D:613:LYS:HE3	1:D:631:ARG:HH12	1.63	0.64
1:C:117:ALA:HB2	1:C:481:MET:CE	2.28	0.64
1:C:611:ASP:OD2	1:C:613:LYS:HB2	1.97	0.64
1:D:219:ALA:HB3	1:D:330:ALA:HA	1.79	0.64
1:D:235:VAL:HG11	1:D:239:LYS:CG	2.27	0.64
1:D:91:GLN:HE21	1:D:347:THR:CB	2.10	0.64
1:D:595:GLU:O	1:D:599:LEU:HD22	1.96	0.64
1:D:374:PRO:O	1:D:404:THR:HG23	1.97	0.64
1:C:153:PRO:HD2	1:C:200:VAL:CG2	2.27	0.64
1:D:600:ALA:HB1	1:D:606:ILE:HG12	1.80	0.64
1:D:647:ILE:N	1:D:647:ILE:HD12	2.13	0.64
1:C:391:LYS:HE2	1:C:391:LYS:CA	2.27	0.63
1:D:435:VAL:HG12	1:D:444:PRO:HA	1.80	0.63
1:D:581:ASN:HD21	1:D:699:HIS:HB3	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASP:O	1:C:87:LYS:HG3	1.99	0.63
1:C:91:GLN:NE2	1:C:344:SER:H	1.96	0.63
1:D:265:GLU:HG2	1:D:267:LYS:CD	2.27	0.63
1:C:619:MET:HE1	1:C:633:ILE:CD1	2.26	0.63
1:D:394:PHE:N	1:D:460:ASP:OD2	2.24	0.63
1:C:413:ILE:HD11	1:C:459:ILE:HD12	1.82	0.62
1:C:382:VAL:O	1:C:466:THR:HG22	1.99	0.62
1:D:109:VAL:HG21	1:D:138:GLN:HG3	1.82	0.62
1:C:140:GLU:HG3	1:C:188:ILE:CD1	2.30	0.62
1:C:500:ASP:CB	1:C:552:VAL:HG11	2.29	0.62
1:C:488:VAL:HG23	1:C:489:VAL:HG23	1.82	0.62
1:D:111:PHE:O	1:D:113:SER:N	2.33	0.62
1:C:86:VAL:HG21	1:C:96:ASN:OD1	2.00	0.62
1:C:630:ALA:O	1:C:633:ILE:HG13	1.98	0.61
1:D:235:VAL:HG11	1:D:239:LYS:HG2	1.82	0.61
1:D:194:ASP:HB3	1:D:196:VAL:HG23	1.82	0.61
1:C:578:LYS:HB3	1:C:585:ARG:HG2	1.82	0.61
1:C:600:ALA:HB1	1:C:606:ILE:HG12	1.82	0.61
1:C:823:ARG:HH11	1:C:823:ARG:HB3	1.63	0.61
1:C:581:ASN:HB3	1:C:583:HIS:H	1.64	0.61
1:C:435:VAL:HG12	1:C:444:PRO:HA	1.83	0.61
1:C:578:LYS:HA	1:C:584:ASN:O	2.01	0.61
1:D:379:MET:HB2	1:D:402:ALA:HB3	1.81	0.61
1:C:580:PRO:HD2	1:C:704:GLN:OE1	2.00	0.60
1:D:258:THR:HG22	1:D:259:ASN:N	2.15	0.60
1:D:454:ILE:HG13	1:D:455:GLY:H	1.66	0.60
1:D:155:VAL:O	1:D:337:MET:HE1	2.00	0.60
1:C:588:LEU:C	1:C:588:LEU:HD12	2.27	0.60
1:D:653:VAL:HG11	1:D:656:LEU:HD13	1.83	0.60
1:D:251:ASN:ND2	1:D:269:LEU:HD21	2.16	0.60
1:D:583:HIS:HB3	1:D:694:HIS:HB2	1.84	0.60
1:D:685:ARG:HE	1:D:687:ASN:ND2	1.92	0.60
1:C:569:SER:O	1:C:720:ALA:HB1	2.02	0.60
1:D:129:VAL:HG11	1:D:181:THR:HG21	1.84	0.60
1:D:251:ASN:HD22	1:D:269:LEU:HD21	1.64	0.60
1:C:429:LYS:HE2	1:C:462:PHE:CZ	2.36	0.60
1:C:496:LYS:HD2	1:C:553:PRO:HB3	1.82	0.60
1:C:497:ASN:HB2	1:C:500:ASP:OD2	2.00	0.60
1:D:258:THR:HG22	1:D:260:LYS:N	2.12	0.60
1:D:327:PHE:O	1:D:328:LEU:HD23	2.02	0.59
1:D:842:LEU:HD23	1:D:842:LEU:OXT	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:LYS:HE3	1:D:462:PHE:CE1	2.38	0.59
1:D:106:PRO:CG	1:D:114:GLU:HG3	2.31	0.59
1:C:303:LEU:O	1:C:304:GLU:HB2	2.02	0.59
1:C:13:MET:HG2	1:C:452:ASN:ND2	2.18	0.59
1:C:296:ILE:O	1:C:300:LEU:HD13	2.03	0.59
1:C:465:LYS:NZ	1:C:517:CYS:SG	2.71	0.58
1:C:685:ARG:HE	1:C:687:ASN:ND2	1.91	0.58
1:C:4:PHE:O	1:C:47:SER:HA	2.03	0.58
1:D:391:LYS:HE2	1:D:391:LYS:CA	2.29	0.58
1:D:555:LYS:O	1:D:555:LYS:HG2	2.02	0.58
1:D:411:VAL:HG11	1:D:469:LEU:HG	1.84	0.58
1:C:717:PHE:HD2	1:C:718:LEU:CD1	2.16	0.58
1:C:155:VAL:HG12	1:C:156:VAL:N	2.19	0.58
1:C:186:ASN:HB3	1:C:201:GLN:NE2	2.19	0.58
1:D:465:LYS:HE3	1:D:517:CYS:SG	2.43	0.58
1:D:605:ILE:HD12	1:D:605:ILE:H	1.69	0.58
1:C:629:ASP:HB3	1:C:647:ILE:HG21	1.84	0.57
1:D:353:ALA:HB3	1:D:370:LYS:HG2	1.86	0.57
1:C:226:ALA:HB3	1:C:241:MET:HE2	1.85	0.57
1:C:463:LEU:HD22	1:C:466:THR:O	2.04	0.57
1:D:454:ILE:HG13	1:D:455:GLY:N	2.20	0.57
1:C:576:LEU:HD11	1:C:585:ARG:HD3	1.87	0.57
1:C:823:ARG:HE	1:C:832:VAL:HG22	1.69	0.57
1:D:581:ASN:HB2	1:D:704:GLN:OE1	2.04	0.57
1:D:627:VAL:HG13	1:D:628:THR:N	2.20	0.57
1:C:89:ILE:HG22	1:C:91:GLN:HB3	1.87	0.57
1:D:49:ALA:O	1:D:50:LYS:HB2	2.04	0.57
1:C:291:PHE:CE1	1:C:315:GLU:HB3	2.37	0.56
1:D:5:THR:OG1	1:D:8:GLN:HG3	2.05	0.56
1:D:36:THR:HG22	1:D:102:LEU:HD21	1.86	0.56
1:D:235:VAL:CG1	1:D:239:LYS:HB3	2.35	0.56
1:D:249:PHE:CZ	1:D:261:ASP:HB3	2.40	0.56
1:C:232:LYS:O	1:C:232:LYS:HG2	2.05	0.56
1:C:327:PHE:O	1:C:328:LEU:HD23	2.04	0.56
1:C:722:PRO:O	1:C:723:LYS:HG3	2.05	0.56
1:D:24:VAL:HG23	1:D:102:LEU:HD11	1.87	0.56
1:D:155:VAL:HG12	1:D:156:VAL:N	2.20	0.56
1:D:578:LYS:HD3	1:D:585:ARG:NH2	2.20	0.56
1:C:71:LYS:HB3	1:C:386:VAL:HG23	1.86	0.56
1:C:251:ASN:HB3	1:C:254:THR:OG1	2.04	0.56
1:D:318:ALA:O	1:D:322:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:ILE:HB	1:D:427:PHE:HB2	1.87	0.56
1:C:295:GLU:C	1:C:297:PRO:HD2	2.30	0.56
1:C:336:GLU:HG2	1:C:340:LEU:HD12	1.88	0.56
1:C:4:PHE:HB3	1:C:8:GLN:HB2	1.86	0.56
1:C:150:ARG:NH1	1:C:196:VAL:HG21	2.21	0.56
1:D:89:ILE:HG21	1:D:93:THR:HG21	1.86	0.56
1:C:379:MET:HB2	1:C:402:ALA:HB3	1.88	0.56
1:C:737:GLU:HB2	1:C:766:PHE:CD2	2.40	0.56
1:D:584:ASN:HD21	1:D:700:ARG:HG2	1.71	0.56
1:C:190:SER:HB3	1:C:201:GLN:NE2	2.21	0.55
1:D:285:PHE:CE1	1:D:320:LEU:HD21	2.41	0.55
1:D:300:LEU:HG	1:D:305:ILE:HB	1.87	0.55
1:D:589:LYS:HE2	1:D:689:LEU:HD11	1.88	0.55
1:D:820:LEU:HG	1:D:824:LYS:HE2	1.87	0.55
1:C:235:VAL:HG12	1:C:236:ASP:N	2.21	0.55
1:D:103:ILE:HD13	1:D:121:VAL:CG2	2.36	0.55
1:D:277:ILE:O	1:D:280:PRO:HD2	2.07	0.55
1:D:596:GLU:HA	1:D:596:GLU:OE1	2.07	0.55
1:C:405:VAL:HA	1:C:409:GLN:OE1	2.07	0.55
1:C:485:VAL:O	1:C:485:VAL:HG22	2.06	0.55
1:D:429:LYS:HG3	1:D:462:PHE:CZ	2.42	0.55
1:D:607:ASN:HD21	1:D:609:ARG:CZ	2.19	0.55
1:C:396:ALA:HB3	1:C:456:LEU:HB2	1.88	0.55
1:D:289:MET:HE1	1:D:317:LYS:CG	2.21	0.55
1:D:489:VAL:HG12	1:D:538:LEU:HD22	1.88	0.55
1:C:522:MET:HE1	1:C:528:HIS:CE1	2.40	0.55
1:C:587:TYR:O	1:C:689:LEU:N	2.35	0.55
1:D:603:ASN:O	1:D:605:ILE:HD12	2.07	0.55
1:C:387:PRO:HG3	1:C:394:PHE:HE1	1.71	0.55
1:C:552:VAL:HG13	1:C:553:PRO:HD2	1.89	0.55
1:C:27:HIS:CE1	1:C:29:ASP:HB2	2.42	0.54
1:C:219:ALA:HB3	1:C:330:ALA:HA	1.90	0.54
1:C:199:ASP:C	1:C:201:GLN:H	2.15	0.54
1:D:646:VAL:C	1:D:647:ILE:HD12	2.32	0.54
1:D:664:VAL:O	1:D:668:GLN:HG2	2.07	0.54
1:C:218:TRP:C	1:C:330:ALA:HB2	2.33	0.54
1:C:366:CYS:O	1:C:370:LYS:HG3	2.08	0.54
1:C:46:ILE:O	1:C:47:SER:C	2.50	0.54
1:C:619:MET:O	1:C:625:TRP:HB2	2.08	0.54
1:C:374:PRO:O	1:C:404:THR:HG23	2.08	0.54
1:D:13:MET:HB3	1:D:452:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:545:LEU:O	1:D:550:ALA:HB3	2.08	0.54
1:C:585:ARG:HG3	1:C:585:ARG:HH11	1.72	0.54
1:C:806:SER:HB3	1:C:813:SER:HB2	1.90	0.54
1:C:152:LYS:HG3	1:C:200:VAL:CG2	2.38	0.53
1:D:86:VAL:HG21	1:D:96:ASN:OD1	2.08	0.53
1:D:192:TYR:HA	1:D:763:THR:HG22	1.88	0.53
1:D:474:THR:O	1:D:474:THR:HG22	2.08	0.53
1:C:647:ILE:HD12	1:C:647:ILE:N	2.23	0.53
1:C:579:SER:OG	1:C:581:ASN:HB2	2.08	0.53
1:D:260:LYS:O	1:D:263:ASP:HB2	2.09	0.53
1:D:581:ASN:ND2	1:D:699:HIS:HB3	2.24	0.53
1:C:493:VAL:O	1:C:528:HIS:HB2	2.09	0.53
1:D:226:ALA:HB2	1:D:241:MET:HB3	1.89	0.53
1:C:150:ARG:HH12	1:C:196:VAL:HG21	1.73	0.53
1:C:319:LEU:O	1:C:323:VAL:HG23	2.09	0.53
1:D:515:ASP:HB3	1:D:518:VAL:CG1	2.38	0.53
1:C:162:ARG:HG3	1:C:166:GLU:OE2	2.09	0.53
1:C:320:LEU:C	1:C:322:VAL:H	2.17	0.53
1:C:150:ARG:NH1	1:C:196:VAL:HG11	2.24	0.53
1:D:194:ASP:C	1:D:196:VAL:N	2.65	0.53
1:D:265:GLU:HG2	1:D:267:LYS:HZ3	1.70	0.53
1:C:705:ILE:O	1:C:708:THR:N	2.42	0.53
1:C:89:ILE:HD13	1:C:93:THR:HG21	1.90	0.53
1:C:178:PHE:O	1:C:182:VAL:HG23	2.09	0.53
1:D:169:VAL:HG22	1:D:170:SER:N	2.23	0.53
1:C:597:VAL:O	1:C:601:ILE:HG13	2.09	0.52
1:D:172:GLU:HA	1:D:172:GLU:OE1	2.09	0.52
1:C:155:VAL:CG1	1:C:156:VAL:N	2.71	0.52
1:C:501:LEU:HB3	1:C:502:PRO:CD	2.37	0.52
1:C:842:LEU:HD23	1:C:842:LEU:OXT	2.09	0.52
1:D:533:THR:O	1:D:533:THR:HG22	2.09	0.52
1:C:466:THR:HG21	1:C:481:MET:SD	2.48	0.52
1:C:576:LEU:HD13	1:C:587:TYR:CE1	2.44	0.52
1:D:169:VAL:CG2	1:D:173:ASP:HB2	2.39	0.52
1:D:284:LEU:HD13	1:D:324:MET:HE1	1.92	0.52
1:D:597:VAL:O	1:D:601:ILE:HG13	2.09	0.52
1:D:515:ASP:HB3	1:D:518:VAL:HG12	1.91	0.52
1:D:308:LYS:O	1:D:309:GLY:C	2.51	0.52
1:D:331:ALA:O	1:D:332:ASP:C	2.53	0.52
1:D:501:LEU:HB3	1:D:502:PRO:HD3	1.91	0.52
1:C:129:VAL:HG11	1:C:181:THR:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:TYR:O	1:C:233:PHE:HB2	2.09	0.52
1:C:378:LEU:H	1:C:471:THR:HB	1.74	0.52
1:C:581:ASN:O	1:C:582:LYS:CB	2.57	0.52
1:D:94:ASP:OD1	1:D:94:ASP:O	2.26	0.52
1:D:235:VAL:HG12	1:D:239:LYS:HB3	1.91	0.52
1:C:532:GLY:HA3	1:C:538:LEU:HD13	1.92	0.52
1:D:567:VAL:HG23	1:D:592:PRO:HG3	1.90	0.52
1:C:194:ASP:C	1:C:196:VAL:H	2.18	0.51
1:C:413:ILE:HD13	1:C:459:ILE:HG23	1.90	0.51
1:C:418:TYR:HB3	1:C:477:ASN:ND2	2.11	0.51
1:D:390:ASP:O	1:D:391:LYS:HB2	2.10	0.51
1:D:634:TRP:O	1:D:635:CYS:HB3	2.09	0.51
1:D:813:SER:O	1:D:817:GLU:HB2	2.10	0.51
1:C:763:THR:C	1:C:765:LEU:H	2.17	0.51
1:D:103:ILE:HD13	1:D:121:VAL:HG23	1.91	0.51
1:C:809:LEU:HD12	1:C:809:LEU:H	1.76	0.51
1:D:89:ILE:HG21	1:D:93:THR:CG2	2.41	0.51
1:D:466:THR:HG22	1:D:467:GLY:N	2.25	0.51
1:C:203:TYR:HB2	1:C:206:ARG:HG2	1.92	0.51
1:D:548:ASP:O	1:D:549:HIS:C	2.54	0.51
1:D:727:PRO:HG2	1:D:774:VAL:HB	1.92	0.51
1:D:603:ASN:HB2	1:D:605:ILE:HD13	1.92	0.51
1:C:111:PHE:CZ	1:C:540:ILE:HD12	2.45	0.51
1:C:152:LYS:HG3	1:C:200:VAL:HG23	1.92	0.51
1:C:226:ALA:CB	1:C:241:MET:HE2	2.40	0.51
1:D:226:ALA:CB	1:D:241:MET:HB3	2.40	0.51
1:D:595:GLU:O	1:D:599:LEU:CD2	2.58	0.51
1:D:313:ASP:O	1:D:315:GLU:HG3	2.11	0.51
1:D:313:ASP:OD1	1:D:314:LEU:N	2.44	0.51
1:D:382:VAL:O	1:D:466:THR:HG23	2.11	0.51
1:C:169:VAL:HG22	1:C:173:ASP:CB	2.41	0.51
1:C:308:LYS:O	1:C:309:GLY:C	2.53	0.51
1:D:313:ASP:O	1:D:314:LEU:C	2.54	0.51
1:C:124:GLY:HA3	1:C:342:LEU:HD22	1.93	0.51
1:C:212:GLY:HA2	1:C:218:TRP:CZ3	2.46	0.51
1:C:290:ASN:HB3	1:C:292:LYS:HE2	1.93	0.50
1:D:183:GLU:OE1	1:D:183:GLU:HA	2.11	0.50
1:D:496:LYS:HE3	1:D:554:LEU:O	2.11	0.50
1:C:284:LEU:HD12	1:C:324:MET:HE1	1.91	0.50
1:D:22:MET:HE3	1:D:338:ILE:HD11	1.93	0.50
1:D:466:THR:OG1	1:D:481:MET:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:828:MET:O	1:D:829:LYS:C	2.53	0.50
1:C:785:ARG:HB2	1:C:790:GLY:HA2	1.93	0.50
1:D:551:GLY:O	1:D:552:VAL:HG23	2.11	0.50
1:C:110:ASP:OD1	1:C:781:THR:HG21	2.11	0.50
1:D:229:TYR:CE2	1:D:276:PHE:HB3	2.46	0.50
1:C:841:LYS:O	1:C:842:LEU:HB3	2.11	0.50
1:D:501:LEU:C	1:D:501:LEU:HD23	2.37	0.50
1:C:520:THR:HA	1:C:529:ILE:O	2.11	0.50
1:D:37:ASP:O	1:D:41:GLN:HG2	2.11	0.50
1:C:428:ILE:C	1:C:429:LYS:HD2	2.36	0.50
1:D:501:LEU:O	1:D:505:VAL:HG23	2.12	0.50
1:D:43:ALA:HB1	1:D:78:TYR:O	2.11	0.49
1:D:162:ARG:HG3	1:D:166:GLU:OE2	2.11	0.49
1:C:289:MET:HE1	1:C:317:LYS:CG	2.41	0.49
1:D:237:LYS:O	1:D:241:MET:HG2	2.12	0.49
1:D:562:ALA:O	1:D:727:PRO:HD3	2.12	0.49
1:C:111:PHE:O	1:C:113:SER:N	2.45	0.49
1:C:225:PHE:CE2	1:C:277:ILE:HG23	2.48	0.49
1:C:288:ILE:HA	1:C:296:ILE:HD11	1.95	0.49
1:C:823:ARG:NH1	1:C:829:LYS:O	2.45	0.49
1:C:45:ILE:C	1:C:46:ILE:HG13	2.38	0.49
1:C:36:THR:O	1:C:40:VAL:HG23	2.12	0.49
1:C:138:GLN:HG3	1:C:139:THR:N	2.27	0.49
1:C:737:GLU:CD	1:C:766:PHE:HE2	2.20	0.49
1:C:831:GLU:OE1	1:C:831:GLU:N	2.42	0.49
1:D:77:LEU:HB2	1:D:100:ILE:HB	1.94	0.49
1:D:291:PHE:O	1:D:293:LYS:N	2.45	0.49
1:D:500:ASP:HB3	1:D:552:VAL:HG11	1.93	0.49
1:C:27:HIS:ND1	1:C:29:ASP:HB2	2.26	0.49
1:C:420:PRO:HG2	1:C:476:HIS:CD2	2.48	0.49
1:D:378:LEU:O	1:D:470:THR:HA	2.12	0.49
1:D:660:LYS:O	1:D:664:VAL:HG23	2.13	0.49
1:C:581:ASN:O	1:C:582:LYS:HB2	2.13	0.49
1:C:3:ALA:HA	1:C:46:ILE:O	2.12	0.49
1:C:455:GLY:O	1:C:456:LEU:HD23	2.13	0.49
1:C:504:LEU:HD13	1:C:554:LEU:HD21	1.95	0.49
1:D:600:ALA:CB	1:D:606:ILE:HG12	2.42	0.49
1:C:390:ASP:O	1:C:391:LYS:HB2	2.12	0.48
1:C:394:PHE:N	1:C:460:ASP:OD2	2.43	0.48
1:C:453:ILE:O	1:C:453:ILE:HG22	2.13	0.48
1:C:728:VAL:HB	1:C:800:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:ILE:HD12	1:D:211:PHE:CE1	2.48	0.48
1:C:634:TRP:O	1:C:635:CYS:HB3	2.12	0.48
1:C:501:LEU:C	1:C:501:LEU:HD23	2.38	0.48
1:D:568:GLU:HB2	1:D:723:LYS:HD3	1.94	0.48
1:C:118:ALA:O	1:C:121:VAL:HG22	2.13	0.48
1:C:203:TYR:HB2	1:C:206:ARG:CG	2.44	0.48
1:C:717:PHE:HD2	1:C:718:LEU:HD13	1.78	0.48
1:D:265:GLU:CB	1:D:267:LYS:HD2	2.42	0.48
1:D:548:ASP:O	1:D:550:ALA:N	2.47	0.48
1:D:733:ILE:O	1:D:767:THR:HA	2.12	0.48
1:C:478:MET:O	1:C:480:VAL:HG13	2.13	0.48
1:D:369:ILE:HD12	1:D:401:PHE:HB3	1.93	0.48
1:C:156:VAL:HG21	1:C:334:LEU:CD2	2.43	0.48
1:C:193:ALA:O	1:C:194:ASP:C	2.56	0.48
1:C:454:ILE:HG13	1:C:455:GLY:N	2.26	0.48
1:C:613:LYS:HG2	1:C:631:ARG:NH1	2.27	0.48
1:C:727:PRO:O	1:C:774:VAL:HG23	2.13	0.48
1:C:650:THR:HG22	1:C:690:ASP:HA	1.94	0.48
1:C:315:GLU:O	1:C:318:ALA:HB3	2.14	0.48
1:D:448:CYS:SG	1:D:452:ASN:HB2	2.54	0.48
1:D:164:LEU:HD12	1:D:285:PHE:CE1	2.48	0.48
1:C:16:VAL:O	1:C:345:PRO:HD2	2.14	0.47
1:C:127:VAL:HG21	1:C:143:LEU:HD13	1.97	0.47
1:C:318:ALA:O	1:C:322:VAL:HG23	2.15	0.47
1:C:345:PRO:O	1:C:349:GLN:HG3	2.13	0.47
1:C:789:GLY:O	1:C:791:GLN:N	2.47	0.47
1:D:671:THR:HA	1:D:681:MET:HG3	1.96	0.47
1:D:10:ARG:O	1:D:10:ARG:NH1	2.47	0.47
1:C:126:LEU:HD21	1:C:334:LEU:HD22	1.96	0.47
1:D:706:ILE:HB	1:D:707:PRO:HD3	1.96	0.47
1:C:515:ASP:OD2	1:C:537:HIS:HE1	1.97	0.47
1:D:36:THR:HA	1:D:39:LEU:HD12	1.97	0.47
1:D:503:LYS:O	1:D:506:GLU:HB3	2.15	0.47
1:D:607:ASN:ND2	1:D:609:ARG:NH2	2.52	0.47
1:C:71:LYS:HB3	1:C:386:VAL:CG2	2.43	0.47
1:C:587:TYR:HD2	1:C:690:ASP:O	1.98	0.47
1:D:253:LYS:O	1:D:255:LYS:HG2	2.15	0.47
1:D:261:ASP:C	1:D:262:THR:HG23	2.39	0.47
1:D:325:ARG:O	1:D:329:PRO:HG3	2.14	0.47
1:D:677:PHE:N	1:D:677:PHE:CD2	2.83	0.47
1:C:129:VAL:HG11	1:C:181:THR:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:371:ASN:O	1:C:372:CYS:C	2.58	0.47
1:C:174:LEU:HD11	1:C:178:PHE:CZ	2.50	0.47
1:C:694:HIS:O	1:C:700:ARG:HD3	2.15	0.47
1:C:45:ILE:HG22	1:C:46:ILE:N	2.30	0.46
1:D:80:GLU:O	1:D:81:MET:HE2	2.14	0.46
1:C:820:LEU:HG	1:C:824:LYS:HE3	1.98	0.46
1:D:112:SER:HA	1:D:793:PHE:CZ	2.51	0.46
1:D:491:VAL:HG13	1:D:538:LEU:HD21	1.97	0.46
1:D:604:GLY:O	1:D:607:ASN:HB2	2.15	0.46
1:D:722:PRO:O	1:D:723:LYS:HD2	2.15	0.46
1:C:158:ASN:O	1:C:159:LYS:HB2	2.16	0.46
1:C:626:ASP:O	1:C:628:THR:N	2.48	0.46
1:D:172:GLU:HA	1:D:274:ASN:ND2	2.30	0.46
1:D:285:PHE:CD1	1:D:320:LEU:HD21	2.50	0.46
1:D:647:ILE:N	1:D:647:ILE:CD1	2.77	0.46
1:C:237:LYS:O	1:C:238:ALA:C	2.59	0.46
1:D:167:LEU:O	1:D:168:GLN:C	2.57	0.46
1:D:169:VAL:HG22	1:D:170:SER:O	2.16	0.46
1:D:391:LYS:HA	1:D:391:LYS:CE	2.34	0.46
1:C:259:ASN:OD1	1:C:259:ASN:N	2.43	0.46
1:C:479:LYS:HZ2	1:C:760:ARG:HH12	1.64	0.46
1:D:155:VAL:CG1	1:D:156:VAL:N	2.79	0.46
1:C:231:LYS:C	1:C:233:PHE:H	2.24	0.46
1:C:740:VAL:HG12	1:C:744:TYR:CE2	2.51	0.46
1:D:524:GLU:C	1:D:526:GLY:H	2.22	0.46
1:C:129:VAL:HG13	1:C:134:GLY:C	2.41	0.46
1:C:194:ASP:C	1:C:196:VAL:N	2.73	0.46
1:C:429:LYS:HG3	1:C:462:PHE:CE2	2.50	0.46
1:C:487:PRO:HA	1:C:532:GLY:O	2.15	0.46
1:C:565:GLU:OE1	1:C:674:GLY:HA3	2.16	0.46
1:C:585:ARG:HG3	1:C:585:ARG:NH1	2.30	0.46
1:D:160:VAL:HG23	1:D:212:GLY:O	2.16	0.46
1:D:578:LYS:HE3	1:D:582:LYS:HZ3	1.81	0.46
1:C:216:HIS:HA	1:C:321:LYS:HG2	1.97	0.46
1:D:166:GLU:HB3	1:D:167:LEU:HD12	1.98	0.46
1:D:609:ARG:O	1:D:610:ASP:O	2.33	0.46
1:C:117:ALA:HB2	1:C:481:MET:HE3	1.97	0.46
1:C:393:ARG:NH1	1:C:460:ASP:HB2	2.31	0.46
1:C:400:VAL:HG12	1:C:450:ALA:HA	1.98	0.46
1:C:577:SER:O	1:C:585:ARG:HA	2.16	0.46
1:C:615:ARG:HG2	1:C:619:MET:CE	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ILE:HD12	1:D:122:THR:HG22	1.97	0.46
1:D:170:SER:OG	1:D:173:ASP:OD2	2.33	0.46
1:D:258:THR:HG22	1:D:259:ASN:H	1.79	0.46
1:D:271:ARG:O	1:D:272:ALA:C	2.58	0.46
1:D:655:TYR:O	1:D:656:LEU:C	2.58	0.46
1:C:16:VAL:O	1:C:16:VAL:HG12	2.15	0.45
1:C:263:ASP:O	1:C:264:ALA:HB3	2.16	0.45
1:C:380:LEU:HD12	1:C:400:VAL:HG22	1.98	0.45
1:C:496:LYS:HD2	1:C:553:PRO:CB	2.45	0.45
1:C:408:GLY:N	1:C:431:ILE:O	2.48	0.45
1:C:283:ARG:HG2	1:C:283:ARG:HH11	1.80	0.45
1:C:647:ILE:HD13	1:C:685:ARG:HG3	1.99	0.45
1:D:335:LEU:O	1:D:336:GLU:C	2.58	0.45
1:D:617:ARG:HG2	1:D:621:ASP:OD2	2.16	0.45
1:D:644:ASN:HD21	1:D:682:ARG:CA	2.29	0.45
1:C:169:VAL:HG22	1:C:170:SER:N	2.28	0.45
1:C:309:GLY:O	1:C:310:ASP:C	2.60	0.45
1:C:314:LEU:HD13	1:C:322:VAL:HG21	1.97	0.45
1:C:730:LEU:HD12	1:C:730:LEU:C	2.42	0.45
1:C:188:ILE:O	1:C:189:VAL:C	2.59	0.45
1:C:237:LYS:O	1:C:241:MET:HG2	2.17	0.45
1:C:393:ARG:HH11	1:C:460:ASP:HB2	1.82	0.45
1:C:395:TYR:CE1	1:C:457:VAL:HG13	2.52	0.45
1:C:497:ASN:O	1:C:498:ALA:C	2.59	0.45
1:C:613:LYS:HG2	1:C:631:ARG:HH12	1.82	0.45
1:D:22:MET:HE3	1:D:338:ILE:CD1	2.45	0.45
1:D:386:VAL:HA	1:D:387:PRO:HD3	1.82	0.45
1:D:740:VAL:HG12	1:D:744:TYR:CE2	2.52	0.45
1:C:189:VAL:CG1	1:C:200:VAL:HG13	2.47	0.45
1:D:161:ASP:CG	1:D:162:ARG:N	2.74	0.45
1:C:109:VAL:HG21	1:C:138:GLN:HB2	1.97	0.45
1:C:138:GLN:CG	1:C:139:THR:N	2.80	0.45
1:C:189:VAL:HG13	1:C:200:VAL:HG13	1.99	0.45
1:C:428:ILE:O	1:C:429:LYS:HD2	2.17	0.45
1:C:808:PRO:HG2	1:C:809:LEU:HD12	1.99	0.45
1:D:581:ASN:O	1:D:582:LYS:CB	2.63	0.45
1:C:459:ILE:O	1:C:459:ILE:HG22	2.16	0.45
1:D:380:LEU:HD23	1:D:380:LEU:C	2.42	0.45
1:C:77:LEU:HB2	1:C:100:ILE:HB	1.99	0.45
1:C:117:ALA:HB2	1:C:481:MET:HE1	1.98	0.45
1:C:404:THR:HG22	1:C:449:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:799:ASP:OD1	1:D:800:HIS:HD2	2.00	0.45
1:C:183:GLU:OE1	1:C:183:GLU:HA	2.17	0.45
1:D:605:ILE:HD12	1:D:605:ILE:N	2.30	0.45
1:C:478:MET:O	1:C:479:LYS:C	2.60	0.44
1:C:479:LYS:NZ	1:C:760:ARG:NH1	2.65	0.44
1:D:390:ASP:O	1:D:393:ARG:HG2	2.17	0.44
1:D:576:LEU:HD13	1:D:587:TYR:CE1	2.53	0.44
1:C:296:ILE:N	1:C:297:PRO:HD2	2.32	0.44
1:D:16:VAL:C	1:D:18:ASN:N	2.74	0.44
1:D:49:ALA:O	1:D:50:LYS:CB	2.66	0.44
1:D:111:PHE:N	1:D:111:PHE:CD2	2.84	0.44
1:C:320:LEU:C	1:C:322:VAL:N	2.76	0.44
1:D:291:PHE:CE1	1:D:315:GLU:HB3	2.52	0.44
1:D:200:VAL:O	1:D:200:VAL:HG13	2.17	0.44
1:C:36:THR:CG2	1:C:102:LEU:HD21	2.42	0.44
1:C:103:ILE:HD11	1:C:453:ILE:HG12	1.99	0.44
1:D:520:THR:HA	1:D:529:ILE:O	2.18	0.44
1:C:111:PHE:HE1	1:C:540:ILE:HG13	1.83	0.44
1:C:183:GLU:O	1:C:184:SER:C	2.59	0.44
1:D:613:LYS:HE3	1:D:631:ARG:HH22	1.82	0.44
1:D:112:SER:CB	1:D:794:PRO:O	2.65	0.44
1:D:249:PHE:CD2	1:D:249:PHE:N	2.86	0.44
1:D:493:VAL:O	1:D:528:HIS:HB2	2.18	0.44
1:C:3:ALA:HB1	1:C:48:ALA:HB2	2.00	0.44
1:C:819:VAL:O	1:C:823:ARG:HG3	2.18	0.44
1:D:123:ASP:O	1:D:151:ILE:HG23	2.18	0.44
1:D:823:ARG:NH1	1:D:829:LYS:O	2.51	0.44
1:C:111:PHE:CE1	1:C:540:ILE:HG13	2.54	0.43
1:C:389:SER:O	1:C:391:LYS:N	2.48	0.43
1:C:515:ASP:HA	1:C:516:PRO:HD3	1.83	0.43
1:D:81:MET:HB3	1:D:85:ASP:HB2	1.99	0.43
1:D:183:GLU:O	1:D:187:VAL:HG23	2.18	0.43
1:D:204:PRO:HA	1:D:209:VAL:HB	1.98	0.43
1:D:235:VAL:HG21	1:D:243:ARG:NH1	2.33	0.43
1:C:500:ASP:O	1:C:501:LEU:C	2.61	0.43
1:C:705:ILE:O	1:C:706:ILE:C	2.61	0.43
1:D:181:THR:O	1:D:182:VAL:C	2.61	0.43
1:D:265:GLU:HB3	1:D:267:LYS:CD	2.45	0.43
1:C:8:GLN:O	1:C:11:SER:HB3	2.18	0.43
1:C:607:ASN:HA	1:C:608:PRO:HD3	1.78	0.43
1:C:681:MET:HE2	1:C:717:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ILE:HD12	1:C:162:ARG:CD	2.49	0.43
1:C:329:PRO:O	1:C:330:ALA:C	2.60	0.43
1:C:686:VAL:C	1:C:687:ASN:HD22	2.27	0.43
1:D:85:ASP:OD1	1:D:223:ARG:NH2	2.45	0.43
1:D:311:GLU:OE1	1:D:326:LYS:HE3	2.19	0.43
1:D:405:VAL:HA	1:D:409:GLN:OE1	2.19	0.43
1:D:607:ASN:HA	1:D:608:PRO:HD3	1.77	0.43
1:D:677:PHE:N	1:D:677:PHE:HD2	2.15	0.43
1:C:429:LYS:HG3	1:C:462:PHE:CZ	2.53	0.43
1:D:91:GLN:HE22	1:D:343:PRO:HA	1.82	0.43
1:D:223:ARG:HG2	1:D:223:ARG:HH11	1.84	0.43
1:C:103:ILE:HD13	1:C:121:VAL:HG23	2.01	0.43
1:C:261:ASP:OD1	1:C:261:ASP:C	2.61	0.43
1:C:605:ILE:HD12	1:C:605:ILE:N	2.34	0.43
1:C:186:ASN:OD1	1:C:201:GLN:HB3	2.18	0.43
1:C:261:ASP:OD1	1:C:262:THR:N	2.52	0.43
1:D:382:VAL:HG13	1:D:396:ALA:HB1	2.00	0.43
1:D:415:GLY:HA3	1:D:425:ASP:OD1	2.19	0.43
1:D:658:GLU:OE1	1:D:700:ARG:NH2	2.50	0.43
1:D:588:LEU:C	1:D:588:LEU:CD1	2.92	0.43
1:C:546:GLU:HB2	1:C:554:LEU:HD12	2.00	0.43
1:D:365:ASN:O	1:D:369:ILE:HG12	2.18	0.43
1:D:558:PRO:HA	1:D:559:PRO:HD3	1.91	0.43
1:D:725:GLN:HE21	1:D:803:THR:HG1	1.61	0.43
1:D:836:GLN:C	1:D:838:TYR:H	2.27	0.43
1:C:130:ASP:OD1	1:C:159:LYS:HD3	2.19	0.43
1:C:251:ASN:HB3	1:C:254:THR:HG1	1.83	0.43
1:C:298:VAL:O	1:C:301:GLU:HB3	2.19	0.43
1:C:614:ALA:O	1:C:618:ILE:HG13	2.19	0.43
1:C:243:ARG:O	1:C:272:ALA:HB3	2.19	0.42
1:C:616:ALA:HA	1:C:630:ALA:HB1	2.00	0.42
1:D:235:VAL:CG1	1:D:239:LYS:HG2	2.49	0.42
1:D:251:ASN:CG	1:D:254:THR:HG23	2.43	0.42
1:D:295:GLU:O	1:D:296:ILE:C	2.61	0.42
1:D:524:GLU:C	1:D:526:GLY:N	2.77	0.42
1:C:81:MET:O	1:C:96:ASN:HB3	2.18	0.42
1:D:176:GLN:HB3	1:D:180:ARG:HH12	1.84	0.42
1:D:306:VAL:O	1:D:306:VAL:HG23	2.18	0.42
1:D:504:LEU:O	1:D:505:VAL:C	2.62	0.42
1:C:122:THR:O	1:C:352:ARG:NH2	2.52	0.42
1:C:161:ASP:OD2	1:C:161:ASP:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:GLN:O	1:C:168:GLN:HG3	2.18	0.42
1:C:252:PRO:O	1:C:253:LYS:C	2.61	0.42
1:D:277:ILE:C	1:D:280:PRO:HD2	2.44	0.42
1:C:150:ARG:HH12	1:C:196:VAL:HG11	1.84	0.42
1:C:267:LYS:HA	1:C:268:PRO:HD3	1.89	0.42
1:D:292:LYS:HD3	1:D:295:GLU:OE2	2.19	0.42
1:D:552:VAL:HG13	1:D:553:PRO:HD2	2.00	0.42
1:D:584:ASN:HD22	1:D:693:LEU:HA	1.84	0.42
1:C:103:ILE:HD12	1:C:122:THR:HG22	2.02	0.42
1:C:763:THR:HA	1:C:764:PRO:HD3	1.75	0.42
1:C:824:LYS:HE2	1:C:830:GLU:CD	2.45	0.42
1:D:123:ASP:C	1:D:151:ILE:HG23	2.44	0.42
1:D:611:ASP:OD2	1:D:613:LYS:HB2	2.19	0.42
1:C:314:LEU:O	1:C:315:GLU:HG3	2.20	0.42
1:C:489:VAL:HG12	1:C:538:LEU:HD22	2.01	0.42
1:C:545:LEU:HA	1:C:549:HIS:HB2	1.99	0.42
1:D:810:ASP:O	1:D:812:THR:N	2.52	0.42
1:D:258:THR:CG2	1:D:259:ASN:N	2.82	0.42
1:D:829:LYS:HE2	1:D:831:GLU:OE1	2.19	0.42
1:D:320:LEU:C	1:D:322:VAL:N	2.77	0.42
1:D:411:VAL:CG1	1:D:469:LEU:HG	2.48	0.42
1:C:4:PHE:CD1	1:C:8:GLN:NE2	2.87	0.42
1:C:176:GLN:O	1:C:180:ARG:HG3	2.20	0.42
1:D:265:GLU:HG2	1:D:267:LYS:CE	2.49	0.42
1:D:556:ILE:HG22	1:D:557:SER:N	2.35	0.42
1:D:638:PRO:HG3	1:D:671:THR:C	2.45	0.42
1:C:328:LEU:O	1:C:330:ALA:N	2.53	0.42
1:D:103:ILE:HD13	1:D:121:VAL:HG21	2.02	0.42
1:D:129:VAL:HG11	1:D:181:THR:CG2	2.48	0.42
1:D:169:VAL:CG2	1:D:170:SER:N	2.83	0.42
1:D:305:ILE:HD11	1:D:327:PHE:CD1	2.55	0.42
1:C:581:ASN:O	1:C:582:LYS:CG	2.68	0.41
1:D:118:ALA:O	1:D:122:THR:HG23	2.20	0.41
1:D:279:ASP:O	1:D:280:PRO:C	2.62	0.41
1:D:504:LEU:O	1:D:507:GLY:N	2.53	0.41
1:D:648:ASP:OD1	1:D:648:ASP:C	2.63	0.41
1:C:91:GLN:HE22	1:C:344:SER:N	2.13	0.41
1:C:414:GLN:HB2	1:C:477:ASN:OD1	2.20	0.41
1:C:748:ASN:C	1:C:750:LYS:H	2.27	0.41
1:D:83:ASP:O	1:D:87:LYS:HG3	2.20	0.41
1:C:149:GLU:O	1:C:150:ARG:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:VAL:HG12	1:C:236:ASP:H	1.84	0.41
1:C:479:LYS:NZ	1:C:760:ARG:HH12	2.18	0.41
1:C:561:VAL:O	1:C:563:TYR:CD2	2.73	0.41
1:C:579:SER:HB2	1:C:704:GLN:OE1	2.20	0.41
1:D:152:LYS:HG3	1:D:200:VAL:HG21	1.99	0.41
1:D:379:MET:SD	1:D:470:THR:HG22	2.60	0.41
1:C:16:VAL:O	1:C:16:VAL:CG1	2.68	0.41
1:C:595:GLU:O	1:C:599:LEU:HD22	2.20	0.41
1:C:737:GLU:OE2	1:C:766:PHE:HE2	2.03	0.41
1:D:112:SER:HB2	1:D:794:PRO:O	2.21	0.41
1:D:385:MET:HE3	1:D:394:PHE:HB3	2.02	0.41
1:D:599:LEU:O	1:D:602:GLU:N	2.53	0.41
1:C:695:ALA:O	1:C:700:ARG:NH1	2.53	0.41
1:D:192:TYR:CE1	1:D:764:PRO:HD2	2.55	0.41
1:D:612:PHE:CE1	1:D:613:LYS:HG2	2.55	0.41
1:C:533:THR:N	1:C:537:HIS:HD2	2.14	0.41
1:D:183:GLU:O	1:D:184:SER:C	2.62	0.41
1:D:320:LEU:C	1:D:322:VAL:H	2.27	0.41
1:C:295:GLU:O	1:C:296:ILE:C	2.63	0.41
1:C:419:VAL:HG12	1:C:421:GLY:H	1.85	0.41
1:C:735:CYS:SG	1:C:736:PRO:HD2	2.60	0.41
1:D:474:THR:O	1:D:474:THR:CG2	2.69	0.41
1:D:497:ASN:O	1:D:498:ALA:C	2.64	0.41
1:D:655:TYR:O	1:D:658:GLU:HB2	2.21	0.41
1:C:533:THR:O	1:C:533:THR:HG22	2.20	0.41
1:C:718:LEU:HD13	1:C:718:LEU:N	2.36	0.41
1:D:158:ASN:CG	1:D:159:LYS:N	2.78	0.41
1:D:285:PHE:O	1:D:286:THR:C	2.63	0.41
1:D:486:SER:HA	1:D:487:PRO:HD3	1.87	0.41
1:D:614:ALA:O	1:D:615:ARG:C	2.63	0.41
1:C:94:ASP:OD1	1:C:94:ASP:O	2.38	0.41
1:C:189:VAL:O	1:C:193:ALA:HB2	2.20	0.41
1:C:271:ARG:HG3	1:C:271:ARG:HH11	1.86	0.41
1:C:300:LEU:HG	1:C:305:ILE:HB	2.02	0.41
1:C:522:MET:HE1	1:C:528:HIS:ND1	2.36	0.41
1:D:181:THR:O	1:D:184:SER:N	2.54	0.41
1:D:218:TRP:HB3	1:D:324:MET:HB3	2.02	0.41
1:D:500:ASP:O	1:D:501:LEU:C	2.64	0.41
1:D:515:ASP:HA	1:D:516:PRO:HD3	1.93	0.41
1:D:522:MET:HE2	1:D:522:MET:HA	2.02	0.41
1:D:613:LYS:CE	1:D:631:ARG:HH22	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:O	1:C:168:GLN:C	2.64	0.41
1:C:314:LEU:HD22	1:C:318:ALA:HB1	2.03	0.41
1:C:685:ARG:NE	1:C:687:ASN:HD21	1.94	0.41
1:D:88:GLU:O	1:D:90:LYS:HD2	2.21	0.41
1:C:172:GLU:HA	1:C:274:ASN:HD21	1.86	0.40
1:C:491:VAL:HG12	1:C:559:PRO:HA	2.02	0.40
1:C:551:GLY:O	1:C:552:VAL:HG23	2.22	0.40
1:D:111:PHE:HB3	1:D:114:GLU:HG2	2.03	0.40
1:D:836:GLN:HE21	1:D:836:GLN:HB2	1.62	0.40
1:C:109:VAL:O	1:C:109:VAL:HG12	2.21	0.40
1:C:571:SER:HB2	1:C:589:LYS:HG2	2.02	0.40
1:C:836:GLN:HE21	1:C:836:GLN:HB2	1.69	0.40
1:D:418:TYR:HB3	1:D:477:ASN:HD21	1.87	0.40
1:D:465:LYS:CE	1:D:517:CYS:SG	3.09	0.40
1:C:436:LEU:O	1:C:442:VAL:HA	2.21	0.40
1:C:655:TYR:O	1:C:656:LEU:C	2.63	0.40
1:C:651:LYS:O	1:C:652:ALA:C	2.64	0.40
1:C:785:ARG:O	1:C:789:GLY:N	2.54	0.40
1:D:175:TYR:OH	1:D:246:GLY:HA2	2.21	0.40
1:D:252:PRO:O	1:D:255:LYS:HG2	2.21	0.40
1:D:735:CYS:HA	1:D:736:PRO:HD3	1.97	0.40
1:C:91:GLN:NE2	1:C:347:THR:CB	2.78	0.40
1:C:760:ARG:HA	1:C:761:PRO:HD3	1.78	0.40
1:C:806:SER:HB2	1:C:815:ALA:CB	2.52	0.40
1:D:663:VAL:HG13	1:D:709:MET:HG2	2.03	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	C	821/842 (98%)	713 (87%)	85 (10%)	23 (3%)	4 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	821/842 (98%)	735 (90%)	70 (8%)	16 (2%)	6	14
All	All	1642/1684 (98%)	1448 (88%)	155 (9%)	39 (2%)	4	10

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	112	SER
1	D	112	SER
1	D	309	GLY
1	D	549	HIS
1	D	610	ASP
1	C	309	GLY
1	C	610	ASP
1	C	627	VAL
1	C	790	GLY
1	C	795	GLN
1	D	293	LYS
1	D	314	LEU
1	D	582	LYS
1	C	329	PRO
1	C	498	ALA
1	C	582	LYS
1	D	286	THR
1	D	391	LYS
1	D	498	ALA
1	D	657	HIS
1	C	232	LYS
1	C	293	LYS
1	C	330	ALA
1	C	536	LEU
1	D	811	PRO
1	C	166	GLU
1	C	200	VAL
1	C	321	LYS
1	C	761	PRO
1	C	188	ILE
1	C	189	VAL
1	C	252	PRO
1	C	390	ASP
1	C	391	LYS
1	D	244	LEU
1	D	627	VAL

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Mol	Chain	Res	Type
1	D	761	PRO
1	C	169	VAL
1	D	339	VAL

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	C	701/715 (98%)	677 (97%)	24 (3%)	32	58
1	D	701/715 (98%)	676 (96%)	25 (4%)	31	56
All	All	1402/1430 (98%)	1353 (96%)	49 (4%)	32	57

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	36	THR
1	C	81	MET
1	C	138	GLN
1	C	154	VAL
1	C	183	GLU
1	C	259	ASN
1	C	262	THR
1	C	411	VAL
1	C	466	THR
1	C	471	THR
1	C	481	MET
1	C	539	GLU
1	C	596	GLU
1	C	599	LEU
1	C	625	TRP
1	C	718	LEU
1	C	730	LEU
1	C	761	PRO
1	C	767	THR
1	C	785	ARG

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Mol	Chain	Res	Type
1	C	806	SER
1	C	823	ARG
1	C	836	GLN
1	C	842	LEU
1	D	46	ILE
1	D	105	SER
1	D	138	GLN
1	D	154	VAL
1	D	183	GLU
1	D	235	VAL
1	D	242	ASP
1	D	262	THR
1	D	265	GLU
1	D	386	VAL
1	D	471	THR
1	D	555	LYS
1	D	564	ARG
1	D	588	LEU
1	D	596	GLU
1	D	677	PHE
1	D	698	ILE
1	D	718	LEU
1	D	750	LYS
1	D	759	GLN
1	D	761	PRO
1	D	767	THR
1	D	836	GLN
1	D	837	GLU
1	D	842	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	91	GLN
1	C	101	ASN
1	C	108	HIS
1	C	138	GLN
1	C	201	GLN
1	C	452	ASN
1	C	477	ASN
1	C	490	GLN
1	C	537	HIS

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Mol	Chain	Res	Type
1	C	641	ASN
1	C	644	ASN
1	C	654	GLN
1	C	687	ASN
1	C	748	ASN
1	C	753	GLN
1	C	800	HIS
1	C	836	GLN
1	D	30	HIS
1	D	91	GLN
1	D	138	GLN
1	D	176	GLN
1	D	201	GLN
1	D	274	ASN
1	D	341	HIS
1	D	414	GLN
1	D	452	ASN
1	D	537	HIS
1	D	584	ASN
1	D	644	ASN
1	D	687	ASN
1	D	753	GLN
1	D	759	GLN
1	D	800	HIS
1	D	826	HIS
1	D	836	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	C	825/842 (97%)	0.05	16 (1%) 66 59	32, 55, 95, 123	0
1	D	825/842 (97%)	0.03	21 (2%) 58 49	29, 51, 99, 127	0
All	All	1650/1684 (97%)	0.04	37 (2%) 62 53	29, 54, 97, 127	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	48	ALA	4.6
1	D	264	ALA	4.1
1	D	232	LYS	3.7
1	C	481	MET	3.3
1	C	49	ALA	3.2
1	D	258	THR	3.2
1	D	50	LYS	3.1
1	C	263	ASP	3.1
1	D	763	THR	3.0
1	D	480	VAL	3.0
1	C	480	VAL	2.9
1	D	262	THR	2.9
1	C	229	TYR	2.9
1	D	49	ALA	2.8
1	D	285	PHE	2.7
1	D	764	PRO	2.6
1	C	235	VAL	2.6
1	C	764	PRO	2.5
1	D	233	PHE	2.4
1	D	762	GLY	2.4
1	D	483	PHE	2.4
1	D	111	PHE	2.4
1	D	268	PRO	2.4
1	D	257	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	842	LEU	2.4
1	C	50	LYS	2.3
1	C	47	SER	2.3
1	C	111	PHE	2.3
1	D	260	LYS	2.1
1	C	669	TRP	2.1
1	C	842	LEU	2.1
1	C	258	THR	2.1
1	D	276	PHE	2.1
1	C	761	PRO	2.1
1	D	545	LEU	2.1
1	D	235	VAL	2.0
1	C	524	GLU	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.