



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:18 AM UTC

PDB ID : 2VDT / pdb_00002vdt
Title : Crystallographic structure of Levansucrase from Bacillus subtilis mutant S164A
Authors : Ortiz-Soto, M.E.; Rivera, M.; Rudino-Pinera, E.; Olvera, C.; Lopez-Munguia, A.
Deposited on : 2007-10-11
Resolution : 3.20 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

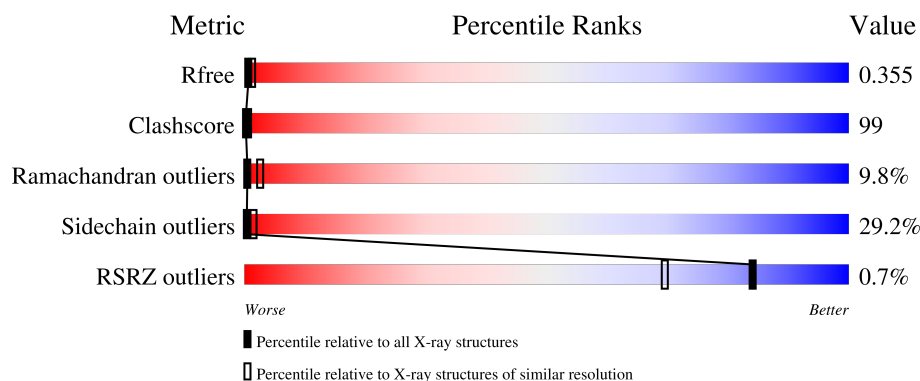
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	439	12% 42% 37% 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3485 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 LEVANSUCRASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3484	2196	579	700	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	ALA	SER	engineered mutation	UNP P05655

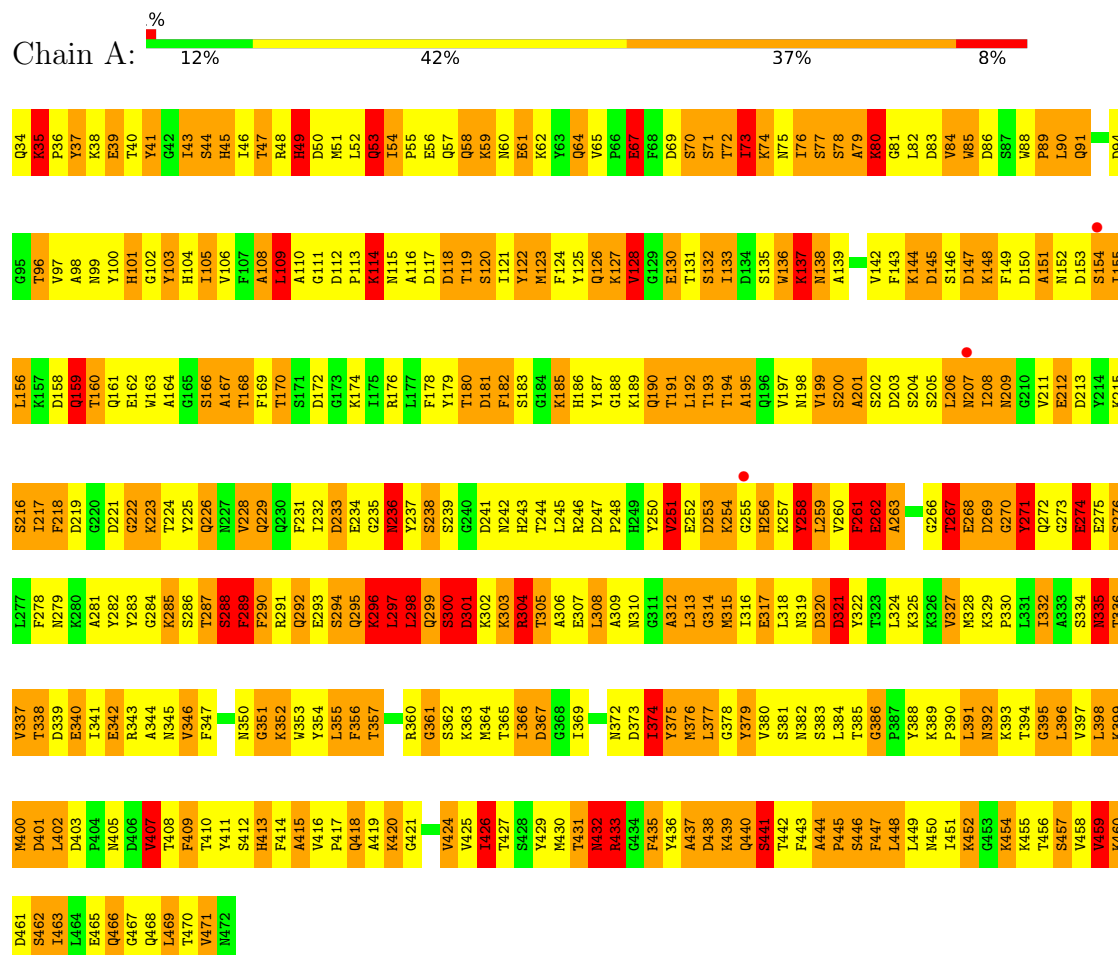
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

3 Residue-property plots

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

• Molecule 1: LEVANSUCRASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.88Å 55.80Å 124.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.41 – 3.20 39.41 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.7 (39.41-3.20) 89.6 (39.41-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.03 (at 3.18Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.265 , 0.297 0.260 , 0.355	Depositor DCC
R_{free} test set	248 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	65.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	3485	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
CA

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	0.98	10/3560 (0.3%)	1.83	124/4811 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CG-CD	-7.10	1.34	1.52
1	A	374	ILE	CA-CB	-6.85	1.48	1.55
1	A	298	LEU	CA-C	-6.50	1.43	1.52
1	A	128	VAL	N-CA	-6.22	1.40	1.46
1	A	61	GLU	CA-CB	-5.91	1.42	1.53
1	A	61	GLU	CB-CG	-5.61	1.35	1.52
1	A	297	LEU	CA-C	-5.59	1.45	1.52
1	A	297	LEU	C-O	-5.39	1.17	1.24
1	A	365	THR	CA-CB	-5.28	1.46	1.53
1	A	459	VAL	CA-CB	5.22	1.60	1.54

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	LEU	N-CA-C	-14.49	92.59	110.41
1	A	301	ASP	N-CA-C	-13.66	92.31	113.89
1	A	147	ASP	N-CA-C	13.00	124.98	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLU	N-CA-C	-12.42	96.25	111.40
1	A	136	TRP	N-CA-C	12.25	128.91	112.25
1	A	114	LYS	CD-CE-NZ	11.80	149.67	111.90
1	A	271	TYR	N-CA-C	11.44	127.92	109.85
1	A	164	ALA	N-CA-C	11.27	127.16	110.48
1	A	261	PHE	N-CA-C	10.60	124.22	109.18
1	A	421	GLY	N-CA-C	-10.28	100.96	111.85
1	A	327	VAL	N-CA-C	-10.20	93.52	108.71
1	A	432	ASN	N-CA-C	10.02	125.12	110.28
1	A	53	GLN	N-CA-C	-10.01	101.20	113.41
1	A	127	LYS	CA-C-N	-9.88	105.83	121.34
1	A	127	LYS	C-N-CA	-9.88	105.83	121.34
1	A	35	LYS	CA-C-N	9.81	129.87	119.76
1	A	35	LYS	C-N-CA	9.81	129.87	119.76
1	A	304	ARG	N-CA-C	9.70	121.79	111.03
1	A	61	GLU	N-CA-C	9.53	124.44	113.01
1	A	356	PHE	N-CA-C	9.42	121.06	108.07
1	A	256	HIS	N-CA-C	-9.32	94.59	109.59
1	A	396	LEU	N-CA-C	-9.27	95.57	110.32
1	A	128	VAL	N-CA-C	9.18	124.45	112.98
1	A	269	ASP	N-CA-C	-9.07	96.01	109.62
1	A	94	ASP	N-CA-C	8.93	123.97	112.89
1	A	76	ILE	N-CA-C	8.89	120.69	107.80
1	A	391	LEU	N-CA-C	-8.86	97.35	110.46
1	A	103	TYR	N-CA-C	8.80	123.63	108.76
1	A	376	MET	N-CA-C	-8.79	94.11	109.06
1	A	64	GLN	N-CA-C	8.76	123.62	108.02
1	A	130	GLU	N-CA-C	8.48	123.07	110.52
1	A	271	TYR	N-CA-CB	-8.46	97.50	111.20
1	A	375	TYR	N-CA-C	8.37	121.43	108.96
1	A	90	LEU	N-CA-C	-8.31	97.38	109.59
1	A	297	LEU	CA-C-N	8.27	135.62	121.14
1	A	297	LEU	C-N-CA	8.27	135.62	121.14
1	A	108	ALA	N-CA-C	8.18	123.09	110.42
1	A	409	PHE	N-CA-C	-8.17	99.73	110.43
1	A	132	SER	N-CA-C	8.12	122.28	110.42
1	A	444	ALA	N-CA-C	-8.09	99.88	110.39
1	A	258	TYR	N-CA-C	8.05	122.58	109.94
1	A	267	THR	N-CA-C	8.04	123.66	112.72
1	A	435	PHE	N-CA-C	7.91	121.45	111.24
1	A	170	THR	N-CA-C	7.76	121.44	110.50
1	A	312	ALA	N-CA-C	7.73	120.62	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	303	LYS	CA-C-N	7.64	131.02	120.63
1	A	303	LYS	C-N-CA	7.64	131.02	120.63
1	A	342	GLU	N-CA-C	7.64	121.57	109.50
1	A	300	SER	CA-CB-OG	-7.62	95.87	111.10
1	A	372	ASN	N-CA-C	-7.59	104.16	113.50
1	A	74	LYS	N-CA-C	-7.52	98.51	109.18
1	A	253	ASP	N-CA-C	-7.50	94.83	110.80
1	A	67	GLU	N-CA-C	-7.42	99.04	110.10
1	A	460	LYS	N-CA-C	7.37	121.35	110.30
1	A	313	LEU	N-CA-C	-7.36	96.74	108.73
1	A	298	LEU	CA-CB-CG	7.29	141.81	116.30
1	A	305	THR	N-CA-C	-7.28	103.50	112.38
1	A	61	GLU	CB-CG-CD	-7.21	100.35	112.60
1	A	156	LEU	N-CA-C	7.20	121.89	113.18
1	A	366	ILE	N-CA-C	7.17	117.78	106.88
1	A	201	ALA	N-CA-C	7.17	121.13	109.59
1	A	297	LEU	N-CA-C	7.15	126.03	110.80
1	A	298	LEU	N-CA-C	-7.13	104.05	112.89
1	A	298	LEU	CB-CA-C	7.03	124.67	109.99
1	A	446	SER	N-CA-C	-7.01	98.88	109.60
1	A	458	VAL	N-CA-C	-6.94	99.64	109.63
1	A	218	PHE	N-CA-C	6.85	120.68	109.24
1	A	263	ALA	N-CA-C	6.81	117.63	108.23
1	A	469	LEU	N-CA-C	-6.76	104.93	113.72
1	A	62	LYS	N-CA-C	-6.67	104.04	111.71
1	A	437	ALA	N-CA-C	6.57	120.94	112.26
1	A	289	PHE	N-CA-C	-6.55	96.85	110.80
1	A	79	ALA	N-CA-C	6.53	118.06	111.07
1	A	298	LEU	N-CA-CB	-6.52	99.78	110.40
1	A	314	GLY	N-CA-C	6.50	123.92	112.10
1	A	217	ILE	CB-CA-C	-6.46	103.42	111.94
1	A	41	TYR	N-CA-C	6.43	120.45	112.47
1	A	36	PRO	N-CA-C	6.43	121.17	111.14
1	A	208	ILE	N-CA-C	6.40	122.65	109.34
1	A	353	TRP	N-CA-C	6.35	118.63	108.41
1	A	167	ALA	CA-C-N	-6.32	109.47	121.54
1	A	167	ALA	C-N-CA	-6.32	109.47	121.54
1	A	361	GLY	N-CA-C	-6.18	105.30	112.83
1	A	303	LYS	N-CA-C	-6.11	104.69	111.36
1	A	101	HIS	N-CA-C	6.01	123.60	110.80
1	A	335	ASN	N-CA-C	5.97	123.52	110.80
1	A	217	ILE	N-CA-C	5.95	116.16	110.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	VAL	N-CA-C	5.88	116.28	107.51
1	A	226	GLN	N-CA-C	5.87	118.29	108.73
1	A	294	SER	N-CA-C	-5.85	104.90	111.28
1	A	143	PHE	N-CA-C	5.83	119.56	110.17
1	A	300	SER	CB-CA-C	-5.80	98.88	110.42
1	A	98	ALA	CA-C-N	-5.79	114.19	122.77
1	A	98	ALA	C-N-CA	-5.79	114.19	122.77
1	A	321	ASP	N-CA-C	-5.79	105.88	113.17
1	A	407	VAL	N-CA-C	-5.78	105.21	113.07
1	A	299	GLN	O-C-N	5.74	129.72	122.37
1	A	426	ILE	N-CA-C	5.62	116.46	107.98
1	A	151	ALA	N-CA-C	5.56	117.78	111.11
1	A	299	GLN	CA-C-N	5.54	132.13	121.54
1	A	299	GLN	C-N-CA	5.54	132.13	121.54
1	A	424	VAL	N-CA-C	-5.52	99.83	108.95
1	A	351	GLY	N-CA-C	5.47	122.32	115.21
1	A	223	LYS	N-CA-C	-5.45	106.76	113.41
1	A	122	TYR	N-CA-C	-5.43	102.85	110.35
1	A	98	ALA	N-CA-C	5.40	117.89	109.52
1	A	262	GLU	N-CA-C	-5.39	100.91	109.96
1	A	297	LEU	CA-C-O	5.38	128.21	120.51
1	A	315	MET	N-CA-C	5.29	117.86	109.50
1	A	395	GLY	N-CA-C	-5.29	106.75	114.90
1	A	231	PHE	N-CA-C	-5.26	106.37	112.89
1	A	222	GLY	N-CA-C	5.25	125.62	113.18
1	A	193	THR	N-CA-C	5.25	118.29	109.95
1	A	84	VAL	N-CA-CB	-5.22	105.55	112.34
1	A	84	VAL	N-CA-C	5.20	116.18	107.18
1	A	337	VAL	CB-CA-C	-5.13	105.14	112.22
1	A	418	GLN	CA-C-N	5.12	127.90	120.79
1	A	418	GLN	C-N-CA	5.12	127.90	120.79
1	A	49	HIS	N-CA-C	-5.12	99.91	110.80
1	A	145	ASP	N-CA-C	-5.11	105.15	111.33
1	A	159	GLN	N-CA-C	-5.04	103.13	110.24
1	A	415	ALA	N-CA-C	5.01	117.45	108.17
1	A	296	LYS	O-C-N	5.01	129.26	122.59
1	A	451	ILE	CB-CA-C	-5.01	102.05	110.71

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	271	TYR	Sidechain
1	A	296	LYS	Mainchain
1	A	379	TYR	Sidechain
1	A	386	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3484	0	3346	677	3
2	A	1	0	0	0	0
All	All	3485	0	3346	677	3

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 99.

All (677) 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:A:355:LEU:HD23	1:A:388:TYR:CD2	1.40	1.56
1:A:355:LEU:CD2	1:A:388:TYR:CD2	2.07	1.36
1:A:355:LEU:HD23	1:A:388:TYR:CE2	1.65	1.29
1:A:355:LEU:CD2	1:A:388:TYR:CE2	2.17	1.25
1:A:297:LEU:O	1:A:300:SER:HB3	1.31	1.24
1:A:430:MET:HB2	1:A:444:ALA:HB2	1.21	1.19
1:A:56:GLU:O	1:A:59:LYS:HG3	1.42	1.15
1:A:198:ASN:ND2	1:A:212:GLU:HG2	1.62	1.14
1:A:300:SER:HB2	1:A:302:LYS:N	1.65	1.11
1:A:85:TRP:CD2	1:A:433:ARG:HD2	1.86	1.10
1:A:163:TRP:HB2	1:A:180:THR:HB	1.33	1.09
1:A:41:TYR:CE2	1:A:270:GLY:HA3	1.87	1.09
1:A:123:MET:HE2	1:A:208:ILE:HD11	1.30	1.08
1:A:271:TYR:CE1	1:A:272:GLN:HG2	1.88	1.08
1:A:198:ASN:HD21	1:A:212:GLU:HG2	1.16	1.07
1:A:127:LYS:HD2	1:A:130:GLU:OE2	1.54	1.07
1:A:37:TYR:O	1:A:279:ASN:HA	1.56	1.05
1:A:297:LEU:O	1:A:300:SER:CB	2.07	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLN:NE2	1:A:179:TYR:OH	1.94	1.00
1:A:355:LEU:HD22	1:A:388:TYR:CE2	1.94	0.99
1:A:300:SER:HB2	1:A:302:LYS:H	0.84	0.99
1:A:316:ILE:HD12	1:A:324:LEU:HD13	1.45	0.99
1:A:99:ASN:HD21	1:A:102:GLY:H	1.03	0.97
1:A:420:LYS:NZ	1:A:420:LYS:HB3	1.80	0.97
1:A:209:ASN:H	1:A:209:ASN:HD22	1.09	0.96
1:A:74:LYS:H	1:A:466:GLN:HE22	1.08	0.96
1:A:430:MET:HB2	1:A:444:ALA:CB	1.96	0.95
1:A:55:PRO:HA	1:A:58:GLN:NE2	1.81	0.95
1:A:55:PRO:HA	1:A:58:GLN:HE22	1.31	0.94
1:A:125:TYR:OH	1:A:137:LYS:HE2	1.66	0.94
1:A:420:LYS:HB3	1:A:420:LYS:HZ3	1.27	0.94
1:A:57:GLN:NE2	1:A:394:THR:HG21	1.82	0.92
1:A:315:MET:HE1	1:A:385:THR:HG22	1.48	0.92
1:A:419:ALA:O	1:A:420:LYS:HG2	1.69	0.92
1:A:209:ASN:HD22	1:A:209:ASN:N	1.67	0.92
1:A:241:ASP:HB2	1:A:308:LEU:HD22	1.49	0.91
1:A:246:ARG:HG2	1:A:262:GLU:HG2	1.52	0.91
1:A:198:ASN:HD21	1:A:212:GLU:CG	1.81	0.91
1:A:99:ASN:ND2	1:A:102:GLY:H	1.68	0.91
1:A:309:ALA:HA	1:A:339:ASP:HB2	1.53	0.91
1:A:85:TRP:CE3	1:A:433:ARG:HD2	2.07	0.90
1:A:153:ASP:OD1	1:A:216:SER:OG	1.90	0.90
1:A:65:VAL:HG23	1:A:398:LEU:CD2	2.01	0.89
1:A:78:SER:HB3	1:A:138:ASN:N	1.88	0.89
1:A:252:GLU:HG2	1:A:257:LYS:CA	2.03	0.88
1:A:300:SER:CB	1:A:302:LYS:H	1.80	0.88
1:A:430:MET:CB	1:A:444:ALA:HB2	2.04	0.88
1:A:124:PHE:CE1	1:A:138:ASN:HB2	2.08	0.88
1:A:376:MET:C	1:A:377:LEU:HD23	1.99	0.88
1:A:119:THR:OG1	1:A:161:GLN:OE1	1.89	0.88
1:A:246:ARG:CG	1:A:262:GLU:HG2	2.06	0.86
1:A:53:GLN:C	1:A:55:PRO:HD2	2.01	0.86
1:A:209:ASN:H	1:A:209:ASN:ND2	1.72	0.86
1:A:294:SER:HA	1:A:297:LEU:HD23	1.58	0.86
1:A:313:LEU:HG	1:A:341:ILE:HD12	1.57	0.86
1:A:252:GLU:HG2	1:A:257:LYS:HB3	1.58	0.85
1:A:179:TYR:CE2	1:A:193:THR:HG21	2.11	0.85
1:A:222:GLY:O	1:A:267:THR:HG23	1.75	0.85
1:A:411:TYR:HB3	1:A:429:TYR:CE2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLU:HG2	1:A:257:LYS:HA	1.58	0.84
1:A:49:HIS:O	1:A:53:GLN:NE2	2.11	0.84
1:A:48:ARG:HG3	1:A:282:TYR:O	1.77	0.84
1:A:267:THR:O	1:A:268:GLU:HG3	1.77	0.84
1:A:43:ILE:HG22	1:A:329:LYS:CD	2.09	0.83
1:A:334:SER:OG	1:A:338:THR:O	1.96	0.82
1:A:316:ILE:HD12	1:A:324:LEU:CD1	2.08	0.82
1:A:381:SER:OG	1:A:386:GLY:O	1.95	0.82
1:A:166:SER:OG	1:A:248:PRO:O	1.98	0.82
1:A:208:ILE:HG22	1:A:208:ILE:O	1.79	0.82
1:A:244:THR:HG22	1:A:246:ARG:NH1	1.95	0.82
1:A:77:SER:O	1:A:80:LYS:HD3	1.80	0.81
1:A:252:GLU:HG2	1:A:257:LYS:CB	2.11	0.81
1:A:253:ASP:O	1:A:255:GLY:N	2.14	0.81
1:A:172:ASP:OD1	1:A:174:LYS:HG2	1.80	0.80
1:A:315:MET:SD	1:A:328:MET:HE2	2.21	0.80
1:A:43:ILE:HG22	1:A:329:LYS:HD3	1.63	0.80
1:A:57:GLN:HE22	1:A:394:THR:CG2	1.95	0.80
1:A:294:SER:O	1:A:298:LEU:HD13	1.81	0.80
1:A:75:ASN:ND2	1:A:440:GLN:HB2	1.96	0.80
1:A:99:ASN:HD21	1:A:102:GLY:N	1.78	0.80
1:A:315:MET:CE	1:A:385:THR:HG22	2.10	0.80
1:A:90:LEU:HD12	1:A:168:THR:O	1.82	0.80
1:A:202:SER:O	1:A:204:SER:N	2.15	0.80
1:A:267:THR:HG22	1:A:271:TYR:CE2	2.17	0.79
1:A:355:LEU:HD23	1:A:388:TYR:HD2	1.44	0.79
1:A:449:LEU:HD12	1:A:450:ASN:N	1.98	0.79
1:A:303:LYS:O	1:A:306:ALA:HB3	1.83	0.79
1:A:198:ASN:ND2	1:A:212:GLU:CG	2.41	0.79
1:A:123:MET:HE2	1:A:208:ILE:CD1	2.11	0.79
1:A:74:LYS:H	1:A:466:GLN:NE2	1.79	0.79
1:A:61:GLU:O	1:A:61:GLU:HG2	1.82	0.79
1:A:273:GLY:O	1:A:276:SER:OG	2.01	0.78
1:A:251:VAL:HG13	1:A:252:GLU:N	1.95	0.78
1:A:271:TYR:HD1	1:A:272:GLN:H	1.32	0.78
1:A:271:TYR:HE1	1:A:272:GLN:HG2	1.42	0.78
1:A:413:HIS:HA	1:A:427:THR:O	1.84	0.78
1:A:361:GLY:HA2	1:A:364:MET:SD	2.24	0.77
1:A:449:LEU:HD12	1:A:457:SER:O	1.84	0.77
1:A:407:VAL:HG22	1:A:439:LYS:NZ	2.00	0.77
1:A:65:VAL:CG2	1:A:398:LEU:HD21	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:PHE:N	1:A:261:PHE:CD2	2.53	0.77
1:A:407:VAL:HG22	1:A:439:LYS:HZ1	1.49	0.76
1:A:37:TYR:CE2	1:A:278:PHE:C	2.64	0.76
1:A:37:TYR:CE2	1:A:279:ASN:N	2.54	0.76
1:A:207:ASN:H	1:A:207:ASN:HD22	1.31	0.76
1:A:355:LEU:HD22	1:A:388:TYR:CZ	2.19	0.76
1:A:416:VAL:HG12	1:A:418:GLN:NE2	2.00	0.76
1:A:452:LYS:HD2	1:A:452:LYS:O	1.86	0.76
1:A:41:TYR:CE2	1:A:270:GLY:CA	2.67	0.76
1:A:198:ASN:O	1:A:199:VAL:HG23	1.86	0.76
1:A:312:ALA:HA	1:A:341:ILE:HD11	1.68	0.76
1:A:271:TYR:HD1	1:A:272:GLN:N	1.83	0.75
1:A:285:LYS:HB3	1:A:289:PHE:CD2	2.20	0.75
1:A:293:GLU:O	1:A:297:LEU:HB2	1.86	0.75
1:A:37:TYR:HE2	1:A:278:PHE:C	1.94	0.75
1:A:236:ASN:CG	1:A:237:TYR:H	1.93	0.75
1:A:89:PRO:O	1:A:91:GLN:HG3	1.87	0.75
1:A:449:LEU:HD11	1:A:457:SER:H	1.51	0.75
1:A:57:GLN:NE2	1:A:394:THR:CG2	2.49	0.74
1:A:163:TRP:HB2	1:A:180:THR:CB	2.16	0.74
1:A:44:SER:C	1:A:45:HIS:CD2	2.65	0.74
1:A:153:ASP:HB3	1:A:156:LEU:HB2	1.70	0.74
1:A:85:TRP:CE3	1:A:85:TRP:N	2.56	0.74
1:A:252:GLU:CG	1:A:257:LYS:HB3	2.16	0.74
1:A:65:VAL:CG2	1:A:398:LEU:CD2	2.65	0.74
1:A:179:TYR:CE2	1:A:193:THR:CG2	2.70	0.74
1:A:310:ASN:CG	1:A:310:ASN:O	2.28	0.74
1:A:379:TYR:HB3	1:A:388:TYR:HB3	1.67	0.74
1:A:407:VAL:O	1:A:431:THR:OG1	2.06	0.74
1:A:229:GLN:NE2	1:A:233:ASP:OD1	2.21	0.73
1:A:73:ILE:HG13	1:A:430:MET:SD	2.28	0.73
1:A:78:SER:HB3	1:A:138:ASN:H	1.51	0.73
1:A:343:ARG:CD	1:A:412:SER:OG	2.36	0.73
1:A:51:MET:O	1:A:366:ILE:HG21	1.88	0.73
1:A:315:MET:SD	1:A:385:THR:HG22	2.28	0.73
1:A:236:ASN:OD1	1:A:237:TYR:HD2	1.72	0.73
1:A:271:TYR:CD1	1:A:272:GLN:N	2.57	0.72
1:A:319:ASN:HB3	1:A:321:ASP:OD1	1.89	0.72
1:A:54:ILE:O	1:A:58:GLN:HB3	1.90	0.72
1:A:144:LYS:HB3	1:A:146:SER:OG	1.89	0.72
1:A:236:ASN:O	1:A:239:SER:OG	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:VAL:CG2	1:A:439:LYS:HZ1	2.02	0.72
1:A:241:ASP:OD1	1:A:242:ASN:N	2.22	0.71
1:A:318:LEU:O	1:A:325:LYS:HE3	1.89	0.71
1:A:236:ASN:ND2	1:A:237:TYR:N	2.38	0.71
1:A:271:TYR:CD1	1:A:272:GLN:HG2	2.24	0.71
1:A:207:ASN:N	1:A:207:ASN:ND2	2.38	0.71
1:A:43:ILE:HD12	1:A:330:PRO:HG2	1.72	0.71
1:A:90:LEU:HD11	1:A:169:PHE:HB2	1.72	0.71
1:A:115:ASN:HB3	1:A:118:ASP:HB3	1.73	0.71
1:A:287:THR:O	1:A:289:PHE:N	2.24	0.71
1:A:297:LEU:HB3	1:A:298:LEU:HB3	1.72	0.71
1:A:194:THR:CG2	1:A:217:ILE:HD11	2.21	0.71
1:A:181:ASP:HB3	1:A:191:THR:HG22	1.72	0.70
1:A:168:THR:HG23	1:A:169:PHE:N	2.05	0.70
1:A:355:LEU:CD2	1:A:388:TYR:CG	2.74	0.70
1:A:319:ASN:CB	1:A:321:ASP:OD1	2.40	0.70
1:A:180:THR:HG21	1:A:246:ARG:HB3	1.72	0.70
1:A:49:HIS:O	1:A:52:LEU:N	2.21	0.70
1:A:350:ASN:OD1	1:A:420:LYS:CE	2.39	0.70
1:A:225:TYR:OH	1:A:328:MET:O	2.06	0.70
1:A:301:ASP:O	1:A:302:LYS:HG3	1.91	0.70
1:A:400:MET:SD	1:A:400:MET:C	2.75	0.69
1:A:83:ASP:C	1:A:85:TRP:HZ3	2.00	0.69
1:A:298:LEU:C	1:A:300:SER:H	1.99	0.69
1:A:390:PRO:HB3	1:A:395:GLY:N	2.07	0.69
1:A:301:ASP:C	1:A:302:LYS:HG3	2.16	0.69
1:A:439:LYS:NZ	1:A:439:LYS:HB3	2.07	0.69
1:A:192:LEU:HB2	1:A:218:PHE:H	1.58	0.69
1:A:392:ASN:ND2	1:A:396:LEU:O	2.18	0.69
1:A:361:GLY:O	1:A:364:MET:HG2	1.92	0.68
1:A:151:ALA:O	1:A:152:ASN:HB2	1.93	0.68
1:A:65:VAL:HG22	1:A:398:LEU:HD21	1.76	0.68
1:A:69:ASP:O	1:A:72:THR:OG1	2.08	0.68
1:A:199:VAL:HG22	1:A:208:ILE:HA	1.74	0.68
1:A:260:VAL:HA	1:A:314:GLY:O	1.92	0.68
1:A:161:GLN:HB2	1:A:182:PHE:CE2	2.29	0.68
1:A:360:ARG:C	1:A:364:MET:HE3	2.19	0.68
1:A:407:VAL:CG2	1:A:439:LYS:NZ	2.56	0.68
1:A:343:ARG:HD2	1:A:412:SER:OG	1.93	0.67
1:A:126:GLN:HB2	1:A:135:SER:O	1.94	0.67
1:A:224:THR:O	1:A:269:ASP:OD2	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:O	1:A:161:GLN:HG2	1.95	0.67
1:A:366:ILE:CG2	1:A:369:ILE:HD12	2.24	0.67
1:A:248:PRO:HB2	1:A:259:LEU:HD13	1.76	0.67
1:A:355:LEU:HD21	1:A:388:TYR:CD2	2.27	0.67
1:A:241:ASP:HB2	1:A:308:LEU:CD2	2.25	0.67
1:A:310:ASN:OD1	1:A:339:ASP:OD1	2.13	0.66
1:A:312:ALA:CA	1:A:341:ILE:HD11	2.24	0.66
1:A:448:LEU:HB2	1:A:462:SER:CB	2.25	0.66
1:A:258:TYR:CD1	1:A:258:TYR:N	2.64	0.66
1:A:34:GLN:HG3	1:A:35:LYS:N	2.11	0.66
1:A:376:MET:O	1:A:377:LEU:HD23	1.95	0.66
1:A:297:LEU:O	1:A:300:SER:CA	2.43	0.66
1:A:48:ARG:O	1:A:52:LEU:HG	1.95	0.66
1:A:226:GLN:O	1:A:243:HIS:HE1	1.78	0.66
1:A:85:TRP:NE1	1:A:109:LEU:HD12	2.10	0.66
1:A:241:ASP:CB	1:A:308:LEU:HD22	2.26	0.66
1:A:448:LEU:N	1:A:462:SER:OG	2.28	0.66
1:A:317:GLU:C	1:A:318:LEU:HD23	2.21	0.65
1:A:346:VAL:HG23	1:A:355:LEU:HB2	1.79	0.65
1:A:185:LYS:O	1:A:185:LYS:HD3	1.96	0.65
1:A:439:LYS:HB3	1:A:439:LYS:HZ3	1.61	0.65
1:A:350:ASN:OD1	1:A:420:LYS:HE2	1.95	0.65
1:A:52:LEU:HD23	1:A:366:ILE:HG23	1.78	0.65
1:A:57:GLN:HE21	1:A:394:THR:HG21	1.60	0.65
1:A:61:GLU:O	1:A:61:GLU:CG	2.44	0.65
1:A:78:SER:HB2	1:A:124:PHE:CE1	2.32	0.65
1:A:246:ARG:HH21	1:A:342:GLU:CG	2.10	0.65
1:A:272:GLN:HB3	1:A:310:ASN:HB3	1.79	0.65
1:A:104:HIS:N	1:A:128:VAL:HG23	2.11	0.65
1:A:128:VAL:HG13	1:A:128:VAL:O	1.97	0.65
1:A:236:ASN:CG	1:A:237:TYR:N	2.51	0.65
1:A:312:ALA:C	1:A:341:ILE:HD11	2.21	0.65
1:A:189:LYS:HG3	1:A:228:VAL:HB	1.79	0.64
1:A:411:TYR:O	1:A:412:SER:HB3	1.97	0.64
1:A:90:LEU:HB3	1:A:105:ILE:HG22	1.79	0.64
1:A:343:ARG:HD3	1:A:412:SER:OG	1.97	0.64
1:A:47:THR:OG1	1:A:50:ASP:OD1	2.15	0.64
1:A:273:GLY:O	1:A:307:GLU:HB3	1.97	0.64
1:A:274:GLU:HG3	1:A:307:GLU:OE2	1.98	0.64
1:A:124:PHE:CD1	1:A:138:ASN:HB2	2.32	0.64
1:A:194:THR:HG22	1:A:217:ILE:CD1	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:CD1	1:A:168:THR:O	2.46	0.64
1:A:161:GLN:HB2	1:A:182:PHE:CD2	2.33	0.64
1:A:179:TYR:HE2	1:A:193:THR:HG21	1.59	0.64
1:A:52:LEU:CD2	1:A:366:ILE:HG23	2.28	0.64
1:A:118:ASP:OD1	1:A:118:ASP:C	2.41	0.64
1:A:73:ILE:CG1	1:A:430:MET:SD	2.86	0.63
1:A:75:ASN:HD21	1:A:440:GLN:HB2	1.60	0.63
1:A:163:TRP:CB	1:A:180:THR:HB	2.19	0.63
1:A:226:GLN:OE1	1:A:243:HIS:ND1	2.29	0.63
1:A:261:PHE:O	1:A:313:LEU:HA	1.98	0.63
1:A:181:ASP:HB2	1:A:193:THR:OG1	1.99	0.63
1:A:37:TYR:HE2	1:A:279:ASN:N	1.95	0.62
1:A:43:ILE:HG22	1:A:329:LYS:HD2	1.81	0.62
1:A:43:ILE:HG13	1:A:44:SER:O	1.99	0.62
1:A:410:THR:O	1:A:413:HIS:CE1	2.52	0.62
1:A:448:LEU:HB2	1:A:462:SER:OG	1.99	0.62
1:A:85:TRP:CZ2	1:A:433:ARG:NE	2.68	0.62
1:A:468:GLN:HG2	1:A:470:THR:O	2.00	0.62
1:A:410:THR:O	1:A:413:HIS:HE1	1.82	0.62
1:A:236:ASN:OD1	1:A:237:TYR:CD2	2.53	0.62
1:A:315:MET:HE1	1:A:385:THR:CG2	2.27	0.62
1:A:54:ILE:N	1:A:55:PRO:HD2	2.15	0.62
1:A:84:VAL:H	1:A:441:SER:CB	2.12	0.62
1:A:89:PRO:HB3	1:A:469:LEU:HD22	1.82	0.62
1:A:366:ILE:HB	1:A:369:ILE:HD12	1.80	0.62
1:A:125:TYR:CZ	1:A:137:LYS:HB2	2.33	0.62
1:A:207:ASN:HD22	1:A:207:ASN:N	1.98	0.62
1:A:144:LYS:O	1:A:147:ASP:HB2	2.00	0.62
1:A:449:LEU:HD12	1:A:450:ASN:H	1.62	0.62
1:A:454:LYS:HD3	1:A:454:LYS:C	2.25	0.62
1:A:285:LYS:HB3	1:A:289:PHE:HD2	1.65	0.61
1:A:340:GLU:CG	1:A:340:GLU:O	2.48	0.61
1:A:190:GLN:OE1	1:A:244:THR:HA	1.99	0.61
1:A:225:TYR:HE2	1:A:327:VAL:CG1	2.14	0.61
1:A:304:ARG:C	1:A:306:ALA:N	2.55	0.61
1:A:412:SER:O	1:A:413:HIS:C	2.43	0.61
1:A:465:GLU:O	1:A:467:GLY:N	2.33	0.61
1:A:192:LEU:O	1:A:217:ILE:N	2.33	0.61
1:A:379:TYR:N	1:A:379:TYR:CD2	2.67	0.61
1:A:246:ARG:HH21	1:A:342:GLU:HG3	1.64	0.61
1:A:337:VAL:O	1:A:338:THR:HB	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:PRO:CA	1:A:58:GLN:NE2	2.60	0.61
1:A:85:TRP:CE2	1:A:433:ARG:HD2	2.36	0.61
1:A:452:LYS:HD2	1:A:452:LYS:C	2.24	0.61
1:A:83:ASP:C	1:A:85:TRP:CZ3	2.79	0.61
1:A:355:LEU:HB3	1:A:388:TYR:CE2	2.37	0.60
1:A:338:THR:OG1	1:A:363:LYS:O	2.08	0.60
1:A:123:MET:CE	1:A:208:ILE:HD11	2.20	0.60
1:A:85:TRP:HE1	1:A:109:LEU:HD12	1.66	0.60
1:A:262:GLU:HB2	1:A:341:ILE:O	2.01	0.60
1:A:127:LYS:CD	1:A:130:GLU:OE2	2.40	0.60
1:A:294:SER:HA	1:A:297:LEU:CD2	2.30	0.60
1:A:84:VAL:H	1:A:441:SER:HB3	1.64	0.59
1:A:145:ASP:O	1:A:148:LYS:NZ	2.32	0.59
1:A:319:ASN:O	1:A:322:TYR:N	2.27	0.59
1:A:321:ASP:OD1	1:A:321:ASP:N	2.35	0.59
1:A:115:ASN:HD22	1:A:118:ASP:HB2	1.67	0.59
1:A:361:GLY:HA2	1:A:364:MET:HE3	1.85	0.59
1:A:456:THR:O	1:A:457:SER:HB3	2.02	0.59
1:A:190:GLN:HB3	1:A:245:LEU:O	2.03	0.59
1:A:194:THR:HG21	1:A:217:ILE:HD11	1.84	0.59
1:A:213:ASP:OD1	1:A:215:LYS:HE2	2.02	0.59
1:A:234:GLU:HB3	1:A:239:SER:HB2	1.84	0.59
1:A:38:LYS:HA	1:A:279:ASN:OD1	2.03	0.59
1:A:112:ASP:OD1	1:A:114:LYS:HG2	2.03	0.59
1:A:46:ILE:O	1:A:46:ILE:HG22	2.01	0.58
1:A:128:VAL:O	1:A:128:VAL:CG1	2.50	0.58
1:A:286:SER:O	1:A:289:PHE:HB3	2.03	0.58
1:A:401:ASP:OD1	1:A:401:ASP:N	2.31	0.58
1:A:78:SER:CB	1:A:138:ASN:HB3	2.33	0.58
1:A:202:SER:C	1:A:204:SER:H	2.11	0.58
1:A:378:GLY:C	1:A:379:TYR:CD2	2.81	0.58
1:A:381:SER:OG	1:A:382:ASN:N	2.36	0.58
1:A:84:VAL:N	1:A:441:SER:HB3	2.18	0.58
1:A:460:LYS:O	1:A:461:ASP:HB2	2.03	0.58
1:A:54:ILE:O	1:A:54:ILE:HG22	2.04	0.58
1:A:193:THR:CG2	1:A:194:THR:N	2.67	0.58
1:A:207:ASN:H	1:A:207:ASN:ND2	1.95	0.58
1:A:53:GLN:C	1:A:55:PRO:CD	2.75	0.58
1:A:246:ARG:HG3	1:A:262:GLU:HG2	1.82	0.58
1:A:262:GLU:CD	1:A:341:ILE:O	2.47	0.58
1:A:391:LEU:C	1:A:393:LYS:H	2.12	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:GLU:HG2	1:A:41:TYR:CE1	2.39	0.57
1:A:41:TYR:CZ	1:A:270:GLY:CA	2.86	0.57
1:A:110:ALA:HB3	1:A:122:TYR:CD1	2.39	0.57
1:A:361:GLY:HA2	1:A:364:MET:CG	2.34	0.57
1:A:449:LEU:CD1	1:A:457:SER:O	2.51	0.57
1:A:160:THR:HG23	1:A:183:SER:HA	1.87	0.57
1:A:158:ASP:O	1:A:183:SER:HB2	2.04	0.57
1:A:153:ASP:CG	1:A:216:SER:OG	2.48	0.57
1:A:334:SER:OG	1:A:334:SER:O	2.23	0.57
1:A:346:VAL:HG23	1:A:355:LEU:CB	2.34	0.57
1:A:319:ASN:OD1	1:A:325:LYS:HB2	2.05	0.56
1:A:408:THR:HG22	1:A:430:MET:HE2	1.86	0.56
1:A:213:ASP:OD1	1:A:215:LYS:NZ	2.39	0.56
1:A:56:GLU:O	1:A:59:LYS:CG	2.34	0.56
1:A:90:LEU:CD1	1:A:169:PHE:HB2	2.34	0.56
1:A:127:LYS:CB	1:A:130:GLU:OE2	2.54	0.56
1:A:304:ARG:C	1:A:306:ALA:H	2.12	0.56
1:A:199:VAL:HG13	1:A:207:ASN:O	2.06	0.56
1:A:228:VAL:O	1:A:232:ILE:HG13	2.05	0.56
1:A:338:THR:HB	1:A:364:MET:HB3	1.88	0.56
1:A:40:THR:HG22	1:A:281:ALA:HB1	1.87	0.55
1:A:47:THR:OG1	1:A:50:ASP:CG	2.49	0.55
1:A:39:GLU:O	1:A:279:ASN:ND2	2.33	0.55
1:A:83:ASP:O	1:A:85:TRP:CZ3	2.59	0.55
1:A:121:ILE:O	1:A:142:VAL:HG23	2.07	0.55
1:A:433:ARG:HG3	1:A:441:SER:OG	2.06	0.55
1:A:78:SER:HB2	1:A:138:ASN:HB3	1.87	0.55
1:A:70:SER:C	1:A:72:THR:H	2.14	0.55
1:A:248:PRO:CB	1:A:259:LEU:HD13	2.36	0.55
1:A:283:TYR:CD2	1:A:290:PHE:HD1	2.24	0.55
1:A:309:ALA:HA	1:A:339:ASP:CB	2.32	0.55
1:A:391:LEU:HD12	1:A:397:VAL:CG2	2.37	0.55
1:A:34:GLN:HG3	1:A:35:LYS:H	1.72	0.55
1:A:313:LEU:HD22	1:A:344:ALA:HB2	1.88	0.55
1:A:317:GLU:O	1:A:318:LEU:HD23	2.05	0.55
1:A:43:ILE:O	1:A:45:HIS:NE2	2.40	0.55
1:A:85:TRP:CD2	1:A:85:TRP:N	2.73	0.55
1:A:198:ASN:HD22	1:A:212:GLU:HG2	1.66	0.55
1:A:274:GLU:CG	1:A:307:GLU:OE2	2.54	0.55
1:A:274:GLU:O	1:A:275:GLU:C	2.50	0.54
1:A:131:THR:OG1	1:A:132:SER:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:ASN:OD1	1:A:346:VAL:N	2.37	0.54
1:A:381:SER:CB	1:A:386:GLY:O	2.55	0.54
1:A:399:LYS:C	1:A:399:LYS:HD3	2.33	0.54
1:A:50:ASP:C	1:A:53:GLN:HE21	2.14	0.54
1:A:181:ASP:OD1	1:A:181:ASP:C	2.50	0.54
1:A:361:GLY:CA	1:A:364:MET:HE3	2.37	0.54
1:A:400:MET:SD	1:A:401:ASP:N	2.81	0.54
1:A:267:THR:C	1:A:268:GLU:HG3	2.33	0.54
1:A:53:GLN:NE2	1:A:53:GLN:N	2.56	0.54
1:A:126:GLN:NE2	1:A:135:SER:OG	2.40	0.54
1:A:136:TRP:O	1:A:137:LYS:C	2.49	0.54
1:A:319:ASN:HB2	1:A:321:ASP:OD1	2.08	0.54
1:A:70:SER:C	1:A:72:THR:N	2.63	0.54
1:A:315:MET:SD	1:A:328:MET:CE	2.95	0.54
1:A:454:LYS:HD3	1:A:454:LYS:O	2.08	0.54
1:A:470:THR:O	1:A:471:VAL:HG23	2.07	0.54
1:A:37:TYR:H	1:A:37:TYR:HD2	1.56	0.54
1:A:64:GLN:O	1:A:65:VAL:C	2.50	0.54
1:A:79:ALA:HB2	1:A:124:PHE:CZ	2.43	0.54
1:A:439:LYS:NZ	1:A:439:LYS:CB	2.69	0.53
1:A:391:LEU:O	1:A:393:LYS:N	2.41	0.53
1:A:399:LYS:C	1:A:399:LYS:CD	2.81	0.53
1:A:39:GLU:HG2	1:A:41:TYR:CZ	2.44	0.53
1:A:49:HIS:CG	1:A:285:LYS:HB2	2.43	0.53
1:A:105:ILE:C	1:A:106:VAL:HG23	2.32	0.53
1:A:266:GLY:O	1:A:271:TYR:HB2	2.07	0.53
1:A:361:GLY:HA2	1:A:364:MET:CE	2.38	0.53
1:A:127:LYS:HB2	1:A:130:GLU:CD	2.34	0.53
1:A:269:ASP:O	1:A:270:GLY:O	2.27	0.53
1:A:181:ASP:CB	1:A:193:THR:OG1	2.56	0.53
1:A:185:LYS:C	1:A:185:LYS:CD	2.82	0.53
1:A:194:THR:OG1	1:A:195:ALA:N	2.41	0.53
1:A:380:VAL:HG22	1:A:381:SER:N	2.23	0.53
1:A:286:SER:O	1:A:287:THR:O	2.27	0.53
1:A:347:PHE:CD1	1:A:347:PHE:C	2.87	0.53
1:A:199:VAL:HG22	1:A:208:ILE:HG12	1.92	0.52
1:A:89:PRO:O	1:A:91:GLN:CG	2.56	0.52
1:A:320:ASP:OD2	1:A:320:ASP:N	2.37	0.52
1:A:436:TYR:HB2	1:A:439:LYS:HB2	1.91	0.52
1:A:420:LYS:NZ	1:A:420:LYS:CB	2.65	0.52
1:A:435:PHE:N	1:A:435:PHE:CD1	2.76	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:THR:O	1:A:195:ALA:HB2	2.10	0.52
1:A:287:THR:O	1:A:290:PHE:HB3	2.09	0.52
1:A:124:PHE:HA	1:A:138:ASN:HA	1.92	0.52
1:A:65:VAL:HG23	1:A:398:LEU:HD22	1.87	0.52
1:A:78:SER:HB2	1:A:124:PHE:HE1	1.75	0.52
1:A:238:SER:O	1:A:239:SER:C	2.53	0.52
1:A:401:ASP:O	1:A:402:LEU:C	2.53	0.52
1:A:79:ALA:HB2	1:A:124:PHE:HZ	1.75	0.51
1:A:361:GLY:N	1:A:364:MET:HE3	2.24	0.51
1:A:383:SER:O	1:A:384:LEU:C	2.52	0.51
1:A:45:HIS:CD2	1:A:45:HIS:N	2.78	0.51
1:A:105:ILE:HG13	1:A:125:TYR:HB2	1.92	0.51
1:A:133:ILE:HB	1:A:466:GLN:HB2	1.92	0.51
1:A:366:ILE:CB	1:A:369:ILE:HD12	2.41	0.51
1:A:391:LEU:C	1:A:393:LYS:N	2.65	0.51
1:A:132:SER:O	1:A:135:SER:HB3	2.10	0.51
1:A:254:LYS:O	1:A:256:HIS:CD2	2.64	0.51
1:A:293:GLU:HA	1:A:293:GLU:OE1	2.10	0.51
1:A:419:ALA:O	1:A:420:LYS:CG	2.50	0.51
1:A:470:THR:C	1:A:471:VAL:HG23	2.36	0.51
1:A:104:HIS:HB2	1:A:126:GLN:HG2	1.92	0.51
1:A:435:PHE:N	1:A:435:PHE:HD1	2.08	0.51
1:A:46:ILE:O	1:A:47:THR:C	2.53	0.51
1:A:347:PHE:CD2	1:A:417:PRO:HG3	2.45	0.51
1:A:189:LYS:NZ	1:A:219:ASP:HB2	2.26	0.50
1:A:356:PHE:O	1:A:357:THR:HB	2.10	0.50
1:A:335:ASN:O	1:A:336:THR:HG23	2.11	0.50
1:A:409:PHE:CD2	1:A:432:ASN:OD1	2.65	0.50
1:A:213:ASP:OD1	1:A:215:LYS:CE	2.60	0.50
1:A:361:GLY:HA2	1:A:364:MET:HG2	1.92	0.50
1:A:382:ASN:OD1	1:A:383:SER:N	2.45	0.50
1:A:192:LEU:HB2	1:A:218:PHE:N	2.25	0.50
1:A:224:THR:HG22	1:A:225:TYR:CE2	2.47	0.50
1:A:301:ASP:O	1:A:301:ASP:CG	2.54	0.50
1:A:253:ASP:O	1:A:254:LYS:C	2.54	0.50
1:A:263:ALA:N	1:A:312:ALA:O	2.45	0.50
1:A:272:GLN:HB3	1:A:310:ASN:CB	2.40	0.50
1:A:48:ARG:O	1:A:49:HIS:C	2.55	0.50
1:A:194:THR:HG22	1:A:217:ILE:HD12	1.92	0.50
1:A:430:MET:HB2	1:A:444:ALA:CA	2.40	0.50
1:A:437:ALA:O	1:A:438:ASP:CG	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:LYS:HB3	1:A:268:GLU:CD	2.36	0.50
1:A:294:SER:O	1:A:298:LEU:CD1	2.57	0.50
1:A:117:ASP:HA	1:A:161:GLN:HE22	1.77	0.50
1:A:138:ASN:OD1	1:A:138:ASN:C	2.55	0.50
1:A:212:GLU:O	1:A:213:ASP:C	2.54	0.49
1:A:100:TYR:O	1:A:101:HIS:HB2	2.12	0.49
1:A:149:PHE:C	1:A:151:ALA:N	2.69	0.49
1:A:403:ASP:OD2	1:A:405:ASN:HB2	2.11	0.49
1:A:414:PHE:HB3	1:A:427:THR:OG1	2.13	0.49
1:A:84:VAL:N	1:A:441:SER:CB	2.74	0.49
1:A:236:ASN:ND2	1:A:236:ASN:C	2.69	0.49
1:A:459:VAL:HG12	1:A:462:SER:HB3	1.95	0.49
1:A:53:GLN:N	1:A:53:GLN:CD	2.70	0.49
1:A:182:PHE:CD2	1:A:182:PHE:C	2.90	0.49
1:A:445:PRO:C	1:A:446:SER:O	2.51	0.49
1:A:374:ILE:C	1:A:375:TYR:CD2	2.90	0.49
1:A:41:TYR:HE2	1:A:270:GLY:HA3	1.69	0.49
1:A:49:HIS:HB2	1:A:289:PHE:CE2	2.48	0.49
1:A:103:TYR:C	1:A:128:VAL:HG23	2.37	0.49
1:A:295:GLN:O	1:A:296:LYS:C	2.56	0.49
1:A:49:HIS:O	1:A:50:ASP:C	2.56	0.49
1:A:91:GLN:HB3	1:A:96:THR:O	2.13	0.49
1:A:54:ILE:N	1:A:55:PRO:CD	2.75	0.49
1:A:37:TYR:CD2	1:A:278:PHE:C	2.90	0.48
1:A:193:THR:HG22	1:A:194:THR:N	2.28	0.48
1:A:223:LYS:HB3	1:A:268:GLU:OE1	2.13	0.48
1:A:450:ASN:HB3	1:A:457:SER:HG	1.79	0.48
1:A:54:ILE:O	1:A:54:ILE:CG2	2.61	0.48
1:A:90:LEU:CB	1:A:105:ILE:HG22	2.41	0.48
1:A:89:PRO:HG2	1:A:91:GLN:HG2	1.95	0.48
1:A:145:ASP:C	1:A:148:LYS:HZ3	2.19	0.48
1:A:208:ILE:O	1:A:208:ILE:CG2	2.52	0.48
1:A:233:ASP:OD1	1:A:233:ASP:N	2.45	0.48
1:A:186:HIS:O	1:A:187:TYR:HB2	2.13	0.48
1:A:160:THR:O	1:A:161:GLN:CG	2.61	0.48
1:A:201:ALA:HB2	1:A:206:LEU:HD21	1.96	0.48
1:A:54:ILE:O	1:A:58:GLN:CD	2.57	0.48
1:A:78:SER:HB2	1:A:138:ASN:CB	2.44	0.48
1:A:202:SER:C	1:A:204:SER:N	2.71	0.48
1:A:246:ARG:HG2	1:A:262:GLU:CG	2.35	0.48
1:A:252:GLU:HA	1:A:256:HIS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:VAL:HG12	1:A:418:GLN:HE22	1.74	0.48
1:A:256:HIS:HB2	1:A:258:TYR:OH	2.13	0.48
1:A:345:ASN:ND2	1:A:414:PHE:CZ	2.82	0.48
1:A:430:MET:O	1:A:431:THR:O	2.32	0.48
1:A:272:GLN:HB3	1:A:310:ASN:CG	2.39	0.47
1:A:405:ASN:O	1:A:436:TYR:OH	2.29	0.47
1:A:224:THR:HG22	1:A:225:TYR:CD2	2.49	0.47
1:A:163:TRP:CB	1:A:180:THR:CB	2.86	0.47
1:A:248:PRO:HB2	1:A:259:LEU:CD1	2.44	0.47
1:A:292:GLN:HE21	1:A:292:GLN:HB3	1.45	0.47
1:A:450:ASN:HB3	1:A:457:SER:OG	2.13	0.47
1:A:54:ILE:HA	1:A:57:GLN:HG2	1.97	0.47
1:A:189:LYS:HG3	1:A:228:VAL:CG1	2.43	0.47
1:A:126:GLN:CG	1:A:127:LYS:N	2.78	0.47
1:A:449:LEU:CD1	1:A:457:SER:C	2.87	0.47
1:A:402:LEU:O	1:A:403:ASP:C	2.58	0.47
1:A:55:PRO:O	1:A:58:GLN:NE2	2.48	0.47
1:A:252:GLU:CD	1:A:257:LYS:HB3	2.40	0.47
1:A:342:GLU:O	1:A:343:ARG:HB2	2.14	0.47
1:A:361:GLY:C	1:A:364:MET:HG2	2.39	0.47
1:A:373:ASP:HB3	1:A:375:TYR:CE2	2.49	0.47
1:A:414:PHE:HB3	1:A:427:THR:HG1	1.80	0.47
1:A:448:LEU:CB	1:A:462:SER:OG	2.62	0.47
1:A:462:SER:O	1:A:463:ILE:C	2.58	0.47
1:A:85:TRP:CH2	1:A:111:GLY:N	2.82	0.47
1:A:200:SER:OG	1:A:209:ASN:ND2	2.48	0.47
1:A:83:ASP:O	1:A:85:TRP:HZ3	1.95	0.47
1:A:269:ASP:O	1:A:270:GLY:C	2.58	0.47
1:A:416:VAL:O	1:A:424:VAL:HB	2.15	0.47
1:A:37:TYR:CD2	1:A:37:TYR:N	2.83	0.46
1:A:84:VAL:C	1:A:441:SER:HB3	2.41	0.46
1:A:125:TYR:CE2	1:A:137:LYS:HB2	2.50	0.46
1:A:287:THR:C	1:A:289:PHE:N	2.73	0.46
1:A:189:LYS:HG3	1:A:228:VAL:CB	2.44	0.46
1:A:225:TYR:HE2	1:A:327:VAL:HG13	1.79	0.46
1:A:346:VAL:HA	1:A:355:LEU:HA	1.97	0.46
1:A:347:PHE:CD1	1:A:347:PHE:O	2.68	0.46
1:A:355:LEU:HB3	1:A:388:TYR:HE2	1.80	0.46
1:A:41:TYR:CZ	1:A:270:GLY:HA3	2.41	0.46
1:A:131:THR:HB	1:A:465:GLU:HG3	1.97	0.46
1:A:182:PHE:HA	1:A:189:LYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:GLY:O	1:A:286:SER:N	2.47	0.46
1:A:37:TYR:CD2	1:A:279:ASN:HA	2.50	0.46
1:A:131:THR:CB	1:A:465:GLU:HG3	2.45	0.46
1:A:337:VAL:O	1:A:364:MET:HA	2.14	0.46
1:A:78:SER:CB	1:A:138:ASN:N	2.72	0.46
1:A:108:ALA:C	1:A:109:LEU:O	2.50	0.46
1:A:258:TYR:CE2	1:A:317:GLU:HG3	2.50	0.46
1:A:407:VAL:O	1:A:407:VAL:HG13	2.15	0.46
1:A:407:VAL:HG12	1:A:408:THR:HG23	1.98	0.46
1:A:248:PRO:HB2	1:A:259:LEU:HD22	1.98	0.46
1:A:48:ARG:O	1:A:49:HIS:O	2.33	0.46
1:A:304:ARG:NH2	1:A:308:LEU:HD21	2.30	0.46
1:A:179:TYR:CE2	1:A:193:THR:HG22	2.51	0.46
1:A:347:PHE:CE2	1:A:417:PRO:HG3	2.51	0.46
1:A:375:TYR:CB	1:A:377:LEU:HD21	2.46	0.46
1:A:162:GLU:HG2	1:A:179:TYR:CE1	2.51	0.46
1:A:102:GLY:O	1:A:128:VAL:N	2.49	0.45
1:A:137:LYS:HB3	1:A:137:LYS:HE3	1.72	0.45
1:A:208:ILE:O	1:A:209:ASN:C	2.58	0.45
1:A:340:GLU:O	1:A:340:GLU:HG3	2.15	0.45
1:A:450:ASN:HB2	1:A:459:VAL:HG23	1.98	0.45
1:A:119:THR:C	1:A:120:SER:OG	2.59	0.45
1:A:90:LEU:HD21	1:A:100:TYR:HB2	1.98	0.45
1:A:127:LYS:HB2	1:A:130:GLU:OE2	2.17	0.45
1:A:415:ALA:HA	1:A:426:ILE:HD13	1.98	0.45
1:A:83:ASP:HB3	1:A:441:SER:HB2	1.98	0.45
1:A:125:TYR:HA	1:A:136:TRP:HZ3	1.81	0.45
1:A:426:ILE:HG22	1:A:447:PHE:CE2	2.52	0.45
1:A:192:LEU:N	1:A:218:PHE:O	2.37	0.45
1:A:338:THR:O	1:A:338:THR:HG23	2.16	0.45
1:A:355:LEU:HD21	1:A:388:TYR:CG	2.48	0.45
1:A:52:LEU:HD23	1:A:366:ILE:CG2	2.47	0.45
1:A:392:ASN:O	1:A:393:LYS:HB2	2.16	0.45
1:A:232:ILE:O	1:A:232:ILE:HG22	2.16	0.45
1:A:416:VAL:HG12	1:A:418:GLN:HE21	1.78	0.45
1:A:131:THR:OG1	1:A:465:GLU:HG3	2.17	0.45
1:A:153:ASP:OD1	1:A:156:LEU:HG	2.17	0.45
1:A:37:TYR:HD2	1:A:37:TYR:N	2.14	0.45
1:A:44:SER:HB2	1:A:332:ILE:HD12	1.99	0.45
1:A:153:ASP:O	1:A:154:SER:C	2.60	0.45
1:A:335:ASN:O	1:A:336:THR:OG1	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:GLN:HE21	1:A:35:LYS:H	1.65	0.44
1:A:90:LEU:HA	1:A:167:ALA:HB3	1.98	0.44
1:A:49:HIS:NE2	1:A:285:LYS:HD3	2.33	0.44
1:A:85:TRP:CE2	1:A:433:ARG:CD	2.99	0.44
1:A:217:ILE:HG22	1:A:218:PHE:HB2	1.99	0.44
1:A:352:LYS:HG3	1:A:354:TYR:CE2	2.52	0.44
1:A:83:ASP:OD1	1:A:440:GLN:CG	2.65	0.44
1:A:85:TRP:CD1	1:A:109:LEU:HD12	2.52	0.44
1:A:352:LYS:HD2	1:A:354:TYR:OH	2.17	0.44
1:A:399:LYS:NZ	1:A:401:ASP:OD2	2.44	0.44
1:A:37:TYR:HD2	1:A:278:PHE:O	2.01	0.44
1:A:74:LYS:N	1:A:466:GLN:HE22	1.93	0.44
1:A:315:MET:O	1:A:316:ILE:CG2	2.66	0.44
1:A:361:GLY:O	1:A:362:SER:C	2.60	0.44
1:A:123:MET:O	1:A:139:ALA:HB3	2.17	0.44
1:A:180:THR:HG23	1:A:246:ARG:HA	2.00	0.44
1:A:197:VAL:O	1:A:197:VAL:HG12	2.17	0.44
1:A:78:SER:HB2	1:A:124:PHE:CD1	2.52	0.44
1:A:292:GLN:O	1:A:295:GLN:HB2	2.18	0.44
1:A:123:MET:O	1:A:123:MET:CG	2.65	0.43
1:A:329:LYS:HG3	1:A:330:PRO:O	2.18	0.43
1:A:345:ASN:HB3	1:A:356:PHE:HB2	1.99	0.43
1:A:390:PRO:HB3	1:A:395:GLY:CA	2.48	0.43
1:A:415:ALA:HA	1:A:426:ILE:CD1	2.47	0.43
1:A:43:ILE:O	1:A:45:HIS:CD2	2.71	0.43
1:A:85:TRP:CE2	1:A:433:ARG:NE	2.86	0.43
1:A:360:ARG:NE	1:A:411:TYR:OH	2.51	0.43
1:A:82:LEU:HD11	1:A:122:TYR:CZ	2.53	0.43
1:A:126:GLN:HG3	1:A:127:LYS:N	2.32	0.43
1:A:180:THR:CG2	1:A:246:ARG:HB3	2.44	0.43
1:A:229:GLN:O	1:A:233:ASP:OD1	2.35	0.43
1:A:319:ASN:C	1:A:321:ASP:H	2.26	0.43
1:A:115:ASN:ND2	1:A:118:ASP:HB2	2.33	0.43
1:A:169:PHE:HD1	1:A:174:LYS:O	2.01	0.43
1:A:413:HIS:ND1	1:A:413:HIS:N	2.64	0.43
1:A:443:PHE:O	1:A:466:GLN:OE1	2.36	0.43
1:A:176:ARG:HG3	1:A:178:PHE:CE1	2.53	0.43
1:A:179:TYR:HE2	1:A:193:THR:CG2	2.19	0.43
1:A:378:GLY:C	1:A:391:LEU:HG	2.44	0.43
1:A:420:LYS:HZ3	1:A:420:LYS:CB	2.14	0.43
1:A:79:ALA:O	1:A:80:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:HIS:CG	1:A:128:VAL:HG22	2.54	0.43
1:A:185:LYS:HD3	1:A:185:LYS:C	2.44	0.43
1:A:273:GLY:C	1:A:276:SER:OG	2.61	0.43
1:A:374:ILE:HG22	1:A:400:MET:HB3	2.01	0.43
1:A:40:THR:HG22	1:A:281:ALA:CB	2.47	0.43
1:A:50:ASP:O	1:A:53:GLN:HG2	2.19	0.43
1:A:55:PRO:C	1:A:58:GLN:NE2	2.76	0.43
1:A:287:THR:HB	1:A:288:SER:H	1.15	0.43
1:A:126:GLN:NE2	1:A:136:TRP:CE2	2.86	0.43
1:A:127:LYS:CB	1:A:130:GLU:CD	2.92	0.43
1:A:145:ASP:HA	1:A:148:LYS:HZ1	1.83	0.43
1:A:266:GLY:O	1:A:269:ASP:OD1	2.36	0.43
1:A:132:SER:O	1:A:135:SER:N	2.45	0.43
1:A:149:PHE:O	1:A:150:ASP:C	2.62	0.43
1:A:52:LEU:C	1:A:55:PRO:HD2	2.44	0.42
1:A:290:PHE:CD2	1:A:291:ARG:N	2.87	0.42
1:A:399:LYS:HD3	1:A:400:MET:N	2.34	0.42
1:A:168:THR:HB	1:A:250:TYR:CD2	2.54	0.42
1:A:213:ASP:CG	1:A:215:LYS:NZ	2.77	0.42
1:A:345:ASN:ND2	1:A:414:PHE:CE1	2.87	0.42
1:A:50:ASP:C	1:A:52:LEU:H	2.27	0.42
1:A:201:ALA:HA	1:A:206:LEU:HD23	2.00	0.42
1:A:241:ASP:OD1	1:A:241:ASP:C	2.59	0.42
1:A:380:VAL:CG2	1:A:381:SER:N	2.82	0.42
1:A:440:GLN:O	1:A:441:SER:C	2.62	0.42
1:A:442:THR:OG1	1:A:443:PHE:N	2.52	0.42
1:A:53:GLN:O	1:A:55:PRO:N	2.52	0.42
1:A:85:TRP:CE3	1:A:433:ARG:CD	2.93	0.42
1:A:117:ASP:HA	1:A:161:GLN:NE2	2.34	0.42
1:A:125:TYR:HA	1:A:136:TRP:CZ3	2.55	0.42
1:A:161:GLN:HB2	1:A:182:PHE:HE2	1.77	0.42
1:A:197:VAL:HG12	1:A:199:VAL:CG2	2.50	0.42
1:A:413:HIS:H	1:A:413:HIS:HD1	1.66	0.42
1:A:86:ASP:HB2	1:A:109:LEU:HG	2.02	0.42
1:A:124:PHE:CE1	1:A:138:ASN:CB	2.94	0.42
1:A:287:THR:O	1:A:290:PHE:N	2.53	0.42
1:A:366:ILE:O	1:A:367:ASP:C	2.62	0.42
1:A:399:LYS:HZ1	1:A:401:ASP:CG	2.27	0.42
1:A:178:PHE:CD2	1:A:259:LEU:HD11	2.55	0.42
1:A:236:ASN:C	1:A:236:ASN:HD22	2.28	0.42
1:A:49:HIS:C	1:A:53:GLN:NE2	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ASN:CG	1:A:237:TYR:HD2	2.27	0.42
1:A:313:LEU:HD13	1:A:356:PHE:O	2.19	0.42
1:A:78:SER:C	1:A:138:ASN:HB3	2.45	0.42
1:A:83:ASP:C	1:A:84:VAL:HG23	2.45	0.42
1:A:224:THR:C	1:A:266:GLY:HA3	2.44	0.42
1:A:37:TYR:HE2	1:A:278:PHE:CA	2.33	0.41
1:A:57:GLN:C	1:A:59:LYS:H	2.28	0.41
1:A:65:VAL:CG2	1:A:398:LEU:HD22	2.48	0.41
1:A:235:GLY:O	1:A:236:ASN:ND2	2.53	0.41
1:A:88:TRP:CD1	1:A:167:ALA:HB2	2.55	0.41
1:A:247:ASP:OD1	1:A:247:ASP:N	2.52	0.41
1:A:37:TYR:O	1:A:279:ASN:CA	2.46	0.41
1:A:69:ASP:OD1	1:A:71:SER:OG	2.37	0.41
1:A:155:ILE:H	1:A:155:ILE:HG12	1.31	0.41
1:A:191:THR:HG23	1:A:192:LEU:N	2.34	0.41
1:A:399:LYS:NZ	1:A:401:ASP:HB3	2.35	0.41
1:A:465:GLU:HB2	1:A:468:GLN:OE1	2.20	0.41
1:A:114:LYS:HG2	1:A:114:LYS:H	1.22	0.41
1:A:57:GLN:HG3	1:A:58:GLN:N	2.32	0.41
1:A:85:TRP:N	1:A:85:TRP:HE3	2.16	0.41
1:A:197:VAL:O	1:A:198:ASN:C	2.61	0.41
1:A:335:ASN:O	1:A:336:THR:CB	2.69	0.41
1:A:357:THR:O	1:A:376:MET:HA	2.20	0.41
1:A:361:GLY:CA	1:A:364:MET:HG2	2.51	0.41
1:A:116:ALA:C	1:A:117:ASP:OD1	2.64	0.41
1:A:377:LEU:HD23	1:A:377:LEU:N	2.34	0.41
1:A:250:TYR:HA	1:A:259:LEU:HD23	2.02	0.41
1:A:266:GLY:N	1:A:269:ASP:OD1	2.54	0.41
1:A:298:LEU:C	1:A:300:SER:N	2.73	0.40
1:A:319:ASN:O	1:A:321:ASP:N	2.54	0.40
1:A:81:GLY:HA2	1:A:440:GLN:OE1	2.21	0.40
1:A:287:THR:C	1:A:289:PHE:H	2.29	0.40
1:A:315:MET:SD	1:A:385:THR:CG2	3.06	0.40
1:A:391:LEU:HD12	1:A:397:VAL:HG22	2.02	0.40
1:A:60:ASN:OD1	1:A:61:GLU:N	2.55	0.40
1:A:242:ASN:O	1:A:339:ASP:OD2	2.39	0.40
1:A:440:GLN:O	1:A:442:THR:N	2.54	0.40
1:A:85:TRP:HH2	1:A:111:GLY:N	2.19	0.40
1:A:163:TRP:O	1:A:179:TYR:HD1	2.04	0.40
1:A:163:TRP:O	1:A:179:TYR:HB2	2.20	0.40
1:A:201:ALA:HB2	1:A:206:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:HG22	1:A:314:GLY:O	2.21	0.40
1:A:182:PHE:CE1	1:A:188:GLY:HA2	2.56	0.40
1:A:197:VAL:HG12	1:A:199:VAL:HG23	2.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLU:OE2	1:A:454:LYS:NZ[3_545]	1.97	0.23
1:A:59:LYS:NZ	1:A:351:GLY:O[3_545]	2.03	0.17
1:A:99:ASN:CG	1:A:319:ASN:ND2[4_455]	2.04	0.16

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	437/439 (100%)	313 (72%)	81 (18%)	43 (10%)	0 2

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASP
1	A	236	ASN
1	A	254	LYS
1	A	270	GLY
1	A	276	SER
1	A	287	THR
1	A	288	SER
1	A	296	LYS
1	A	297	LEU
1	A	300	SER
1	A	466	GLN

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Mol	Chain	Res	Type
1	A	49	HIS
1	A	285	LYS
1	A	335	ASN
1	A	336	THR
1	A	431	THR
1	A	441	SER
1	A	457	SER
1	A	47	THR
1	A	80	LYS
1	A	137	LYS
1	A	289	PHE
1	A	290	PHE
1	A	357	THR
1	A	392	ASN
1	A	402	LEU
1	A	413	HIS
1	A	54	ILE
1	A	96	THR
1	A	113	PRO
1	A	268	GLU
1	A	338	THR
1	A	367	ASP
1	A	438	ASP
1	A	195	ALA
1	A	433	ARG
1	A	471	VAL
1	A	73	ILE
1	A	346	VAL
1	A	463	ILE
1	A	89	PRO
1	A	228	VAL
1	A	251	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	A	383/383 (100%)	271 (71%)	112 (29%)	0 1

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	37	TYR
1	A	39	GLU
1	A	43	ILE
1	A	44	SER
1	A	45	HIS
1	A	53	GLN
1	A	58	GLN
1	A	59	LYS
1	A	67	GLU
1	A	70	SER
1	A	71	SER
1	A	72	THR
1	A	73	ILE
1	A	76	ILE
1	A	77	SER
1	A	78	SER
1	A	80	LYS
1	A	85	TRP
1	A	91	GLN
1	A	97	VAL
1	A	105	ILE
1	A	109	LEU
1	A	114	LYS
1	A	118	ASP
1	A	119	THR
1	A	120	SER
1	A	123	MET
1	A	126	GLN
1	A	128	VAL
1	A	133	ILE
1	A	137	LYS
1	A	138	ASN
1	A	144	LYS
1	A	148	LYS
1	A	154	SER
1	A	155	ILE
1	A	159	GLN

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Mol	Chain	Res	Type
1	A	160	THR
1	A	166	SER
1	A	168	THR
1	A	170	THR
1	A	180	THR
1	A	181	ASP
1	A	182	PHE
1	A	185	LYS
1	A	190	GLN
1	A	191	THR
1	A	192	LEU
1	A	194	THR
1	A	199	VAL
1	A	200	SER
1	A	205	SER
1	A	206	LEU
1	A	207	ASN
1	A	209	ASN
1	A	211	VAL
1	A	212	GLU
1	A	216	SER
1	A	221	ASP
1	A	229	GLN
1	A	233	ASP
1	A	236	ASN
1	A	238	SER
1	A	251	VAL
1	A	258	TYR
1	A	259	LEU
1	A	261	PHE
1	A	262	GLU
1	A	267	THR
1	A	274	GLU
1	A	288	SER
1	A	289	PHE
1	A	292	GLN
1	A	295	GLN
1	A	297	LEU
1	A	298	LEU
1	A	299	GLN
1	A	301	ASP
1	A	304	ARG

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Mol	Chain	Res	Type
1	A	305	THR
1	A	308	LEU
1	A	317	GLU
1	A	320	ASP
1	A	321	ASP
1	A	332	ILE
1	A	340	GLU
1	A	352	LYS
1	A	355	LEU
1	A	374	ILE
1	A	377	LEU
1	A	389	LYS
1	A	398	LEU
1	A	399	LYS
1	A	400	MET
1	A	401	ASP
1	A	407	VAL
1	A	420	LYS
1	A	426	ILE
1	A	432	ASN
1	A	433	ARG
1	A	439	LYS
1	A	440	GLN
1	A	441	SER
1	A	445	PRO
1	A	447	PHE
1	A	448	LEU
1	A	452	LYS
1	A	454	LYS
1	A	455	LYS
1	A	459	VAL
1	A	462	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	53	GLN
1	A	57	GLN
1	A	58	GLN
1	A	99	ASN
1	A	126	GLN

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Mol	Chain	Res	Type
1	A	159	GLN
1	A	186	HIS
1	A	196	GLN
1	A	198	ASN
1	A	207	ASN
1	A	209	ASN
1	A	227	ASN
1	A	229	GLN
1	A	230	GLN
1	A	256	HIS
1	A	292	GLN
1	A	418	GLN
1	A	432	ASN
1	A	450	ASN
1	A	466	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	439/439 (100%)	-0.07	3 (0%) 84 69	31, 52, 67, 79	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	GLY	2.4
1	A	207	ASN	2.3
1	A	154	SER	2.2

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	1473	1/1	0.97	0.06	75,75,75,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.