



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:12 PM UTC

PDB ID : 4W1Y / pdb_00004w1y
Title : Crystal structure of Escherichia coli Tryptophanase in 'semi-holo' form
Authors : Goldgur, Y.
Deposited on : 2014-08-13
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
Mogul : 2022.3.0, CSD as543be (2022)
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

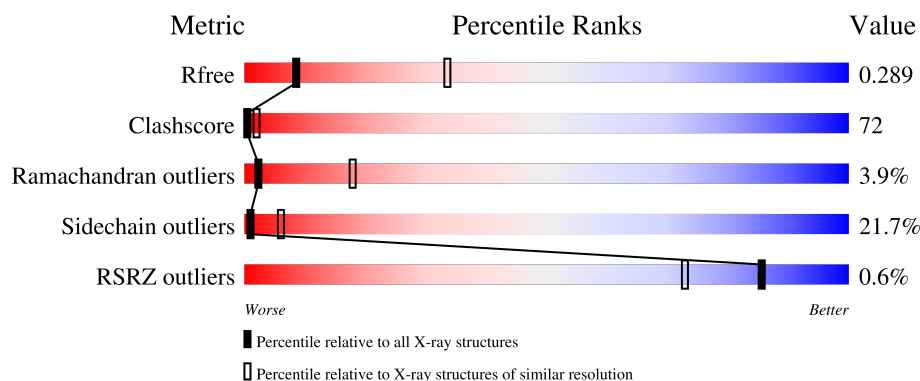
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

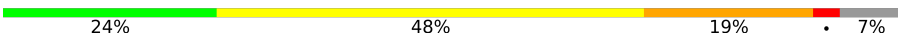
The reported resolution of this entry is 3.20 Å.

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	467	
2	B	467	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6957 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 Tryptophanase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	P	S	0	0	0
			3428	2181	575	650	1	21			

- Molecule 2 is a protein called Tryptophanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	433	Total	C	N	O	S	0	0	0
			3412	2175	575	641	21			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

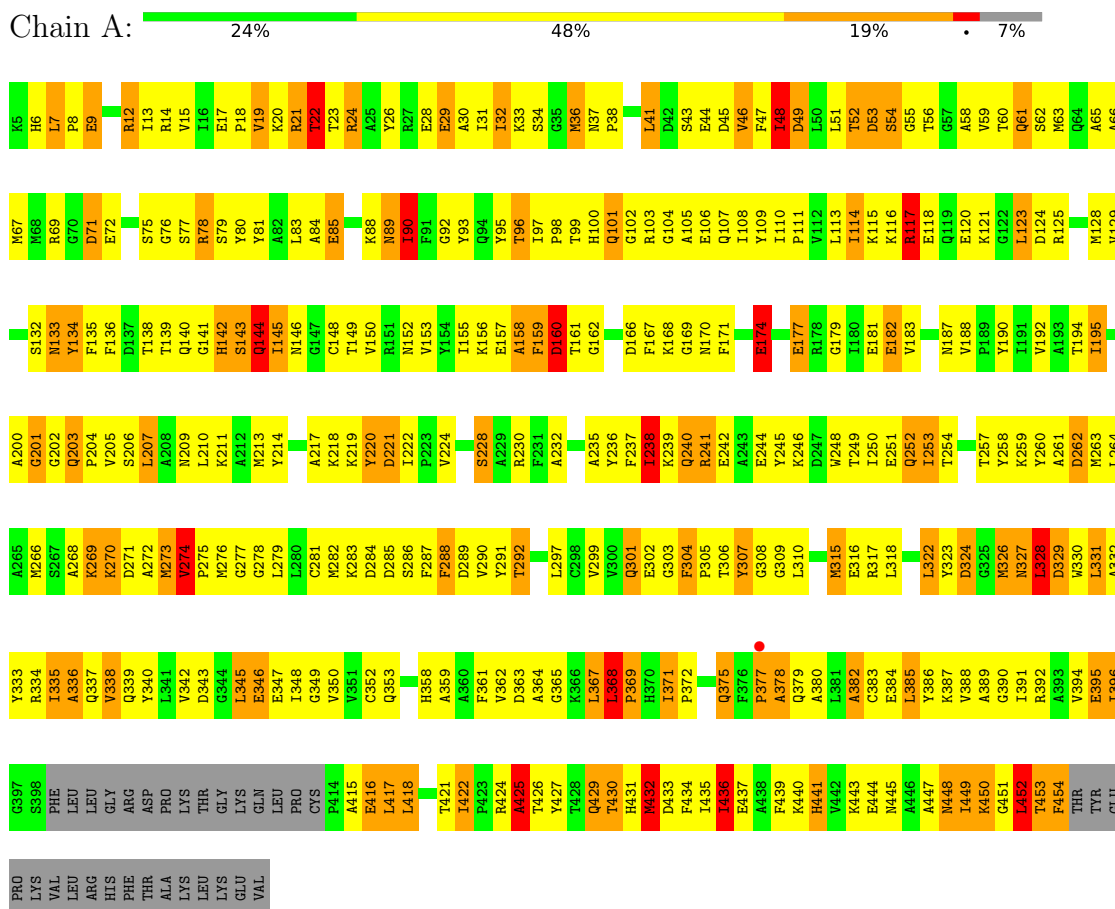
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total 42	O 42	0	0
4	B	65	Total 65	O 65	0	0

3 Residue-property plots

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

• Molecule 1: Tryptophanase



• Molecule 2: Tryptophanase



T455	E395	A319	Y258	S197	Y134
Y456	I396	V320	K259	M198	PHE
E457	G397	Y323	Y260	S199	PHE
P458	S398		A261	A200	ASP
K459	PHE		D262	G201	THR
V460	LEU	M326	M263	G202	THR
L461	LEU	M327	L264	Q203	GLN
R462	GLY	L328	A265	P204	GLY
H463	ARG	D329	M266	V205	HIS
F464	ASP	W330	S267	S206	SER
T465	PRO	L331	A268	L207	GLN
A466	LYS	A332	K269	A208	ILE
K467	THR	Y333	K270	N209	ASN
L468	GLY	R334	D271	L210	GLY
K469	LYS	I335	A272	K211	
E470	GLN	A336	M273	A212	
V471	LEU	Q337	V274	M213	
	PRO	V338	P275	M214	
	C413	Q339	M276	S215	V153
	P414	Y340	G277	I216	Y154
	A415	L341	G278	A217	I155
	E416		L279	K218	K156
	L417	Q353	L280	K219	E157
	L418	Q354	C281	Y220	F159
	B419	A355	M282	D221	D160
	L420	G356	K283	I222	T161
	T421	G357	D284	P223	G162
	I422	H358	D285	V224	V163
	P423	A359	S286	V225	R164
	R424	A360	F287	M226	Y165
	A425	F361	F288	D227	D166
	T426	V362	D289	S228	F167
	Y427	D363	V290	A229	K168
	T428	A364	Y291	R230	G169
	Q429		T292	F231	N170
	T430	L367	E293	A232	F171
	H431	L368	C294	E233	D172
	M432		R295	M234	L173
	D433	I371	T296	A235	E174
	F434	P372	L297	Y236	G175
	I435		C298		L176
	L436	Q375	V299	K239	E177
	B437	F376	V300	Q240	R178
	M438	P377	Q301	R241	G179
	F439	A378	E302	E242	I180
	K440	Q379	GLY	A243	E181
	H441	A380	PHE	E244	E182
	V442	L381	PRO	Y245	V183
	K443	A382	THR	K246	G184
	E444	C383	TYR	D247	
	M445	E384	GLY	W248	M187
	A446	L385	G309	T249	V188
	A447	Y386	L310	I250	P189
	N448	K387	E311	E251	Y190
	T449	V388		Q252	I191
	K450	A389	A314	I253	V192
	G451		M315	T254	A193
	L452	R392	E316	R255	T194
	T453	A393	R317	E256	I195
	F454	V394	L318	T257	T196

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	109.97Å 109.97Å 238.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20 15.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	94.7 (15.00-3.20) 94.0 (15.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.214 , 0.290 0.212 , 0.289	Depositor DCC
R_{free} test set	1207 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	86.8	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 74.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6957	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: SO4, LLP

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	1.27	16/3473 (0.5%)	1.53	57/4692 (1.2%)
2	B	1.35	13/3478 (0.4%)	1.62	66/4694 (1.4%)
All	All	1.31	29/6951 (0.4%)	1.58	123/9386 (1.3%)

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	1
2	B	0	2
All	All	0	3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	422	ILE	CA-CB	-12.26	1.43	1.54
1	A	396	ILE	CA-CB	7.06	1.64	1.54
1	A	417	LEU	CA-C	6.52	1.61	1.52
2	B	423	PRO	N-CA	-6.37	1.39	1.47
2	B	108	ILE	CA-C	6.18	1.60	1.52
2	B	71	ASP	CA-C	-6.04	1.45	1.52
2	B	255	ARG	CA-C	5.78	1.60	1.52
1	A	101	GLN	CA-C	5.75	1.59	1.52
1	A	71	ASP	CA-C	-5.73	1.45	1.52
1	A	59	VAL	C-O	5.71	1.29	1.23
2	B	83	LEU	CA-C	-5.69	1.45	1.52
1	A	416	GLU	CA-C	5.47	1.60	1.52
2	B	310	LEU	N-CA	5.43	1.52	1.46
2	B	467	LYS	CA-C	5.41	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	389	ALA	N-CA	5.38	1.52	1.45
1	A	49	ASP	N-CA	-5.34	1.39	1.46
2	B	249	THR	CA-CB	-5.32	1.45	1.53
1	A	451	GLY	N-CA	5.31	1.50	1.45
2	B	421	THR	CA-CB	-5.30	1.44	1.53
1	A	415	ALA	N-CA	5.29	1.53	1.46
2	B	83	LEU	C-O	-5.28	1.18	1.24
1	A	250	ILE	CA-CB	-5.18	1.47	1.54
2	B	74	TYR	N-CA	-5.14	1.40	1.46
1	A	32	ILE	CA-CB	5.11	1.60	1.54
1	A	338	VAL	CA-CB	-5.10	1.48	1.54
1	A	46	VAL	CA-CB	-5.07	1.48	1.54
2	B	234	ASN	N-CA	-5.05	1.40	1.46
1	A	97	ILE	CA-CB	-5.02	1.48	1.54
1	A	278	GLY	N-CA	5.01	1.50	1.45

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	183	VAL	N-CA-C	12.73	122.21	111.90
1	A	22	THR	N-CA-C	10.26	125.10	108.99
2	B	108	ILE	N-CA-C	10.25	121.07	110.72
2	B	74	TYR	N-CA-C	-10.02	100.37	112.59
2	B	17	GLU	CA-C-N	9.85	129.95	119.90
2	B	17	GLU	C-N-CA	9.85	129.95	119.90
2	B	422	ILE	CA-C-N	9.59	131.10	119.98
2	B	422	ILE	C-N-CA	9.59	131.10	119.98
2	B	222	ILE	CA-C-N	-9.05	110.54	120.14
2	B	222	ILE	C-N-CA	-9.05	110.54	120.14
1	A	228	SER	N-CA-C	8.38	122.82	112.59
2	B	375	GLN	N-CA-C	-8.32	98.17	110.48
1	A	415	ALA	N-CA-C	8.23	122.28	108.20
2	B	338	VAL	N-CA-C	-8.05	102.22	111.00
1	A	452	LEU	N-CA-C	7.97	121.19	109.07
2	B	419	ARG	N-CA-C	7.94	122.37	109.59
2	B	310	LEU	N-CA-C	7.90	122.26	108.75
2	B	266	MET	CB-CG-SD	-7.88	89.05	112.70
2	B	184	GLY	CA-C-N	7.83	128.55	119.47
2	B	184	GLY	C-N-CA	7.83	128.55	119.47
2	B	320	VAL	N-CA-C	-7.78	105.60	111.90
1	A	274	VAL	CA-C-N	7.77	128.48	119.47
1	A	274	VAL	C-N-CA	7.77	128.48	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	VAL	CB-CA-C	-7.74	100.14	111.68
1	A	97	ILE	CB-CA-C	-7.66	102.05	110.85
1	A	417	LEU	N-CA-C	7.66	119.65	108.86
1	A	436	ILE	N-CA-C	-7.53	102.39	110.23
2	B	71	ASP	N-CA-C	-7.51	96.17	108.41
1	A	449	ILE	N-CA-C	7.47	119.59	108.46
1	A	273	MET	N-CA-C	7.16	121.59	112.86
1	A	432	MET	N-CA-C	-7.09	103.16	111.03
2	B	256	GLU	N-CA-C	-6.94	103.65	111.07
1	A	106	GLU	N-CA-C	6.90	118.46	111.07
1	A	71	ASP	N-CA-C	-6.89	97.97	109.07
1	A	201	GLY	N-CA-C	-6.85	105.78	115.30
1	A	75	SER	N-CA-C	6.71	119.35	108.34
1	A	418	LEU	N-CA-C	6.49	119.51	109.07
1	A	19	VAL	N-CA-C	6.47	117.43	108.12
2	B	203	GLN	CA-C-N	6.47	127.92	119.84
2	B	203	GLN	C-N-CA	6.47	127.92	119.84
2	B	368	LEU	CA-C-N	6.46	126.39	119.28
2	B	368	LEU	C-N-CA	6.46	126.39	119.28
2	B	422	ILE	N-CA-C	6.46	117.91	107.71
1	A	17	GLU	CA-C-N	6.43	126.40	119.78
1	A	17	GLU	C-N-CA	6.43	126.40	119.78
2	B	435	ILE	CB-CA-C	-6.36	103.56	111.70
1	A	203	GLN	CA-C-N	6.34	127.77	119.84
1	A	203	GLN	C-N-CA	6.34	127.77	119.84
1	A	301	GLN	N-CA-C	6.33	120.86	111.04
2	B	188	VAL	CA-C-N	6.33	127.75	119.84
2	B	188	VAL	C-N-CA	6.33	127.75	119.84
1	A	65	ALA	N-CA-C	-6.32	104.32	111.14
1	A	48	ILE	N-CA-C	-6.30	96.23	109.34
2	B	388	VAL	N-CA-C	6.28	116.43	110.53
1	A	241	ARG	N-CA-C	6.25	120.50	112.12
2	B	56	THR	N-CA-C	-6.24	103.73	113.02
1	A	304	PHE	N-CA-C	6.19	118.50	109.71
2	B	220	TYR	N-CA-C	-6.16	105.63	113.02
1	A	378	ALA	N-CA-C	-6.09	97.82	110.80
2	B	278	GLY	N-CA-C	-6.02	99.40	110.97
1	A	90	ILE	N-CA-C	-6.00	105.00	110.82
2	B	83	LEU	N-CA-C	-5.98	104.68	111.14
2	B	274	VAL	CA-C-N	5.95	125.49	119.19
2	B	274	VAL	C-N-CA	5.95	125.49	119.19
1	A	30	ALA	N-CA-C	5.93	118.23	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	LEU	CA-C-N	5.91	125.87	119.78
2	B	7	LEU	C-N-CA	5.91	125.87	119.78
2	B	114	ILE	CB-CA-C	-5.86	104.46	111.97
1	A	299	VAL	CB-CA-C	-5.78	101.82	111.29
2	B	421	THR	CA-C-N	-5.77	115.15	123.28
2	B	421	THR	C-N-CA	-5.77	115.15	123.28
2	B	252	GLN	N-CA-C	-5.74	104.02	111.02
2	B	183	VAL	CA-C-O	-5.73	114.92	120.30
1	A	144	GLN	N-CA-C	-5.71	105.20	111.82
2	B	53	ASP	CB-CA-C	-5.69	102.30	111.28
1	A	53	ASP	N-CA-C	-5.66	106.37	113.28
2	B	468	LEU	N-CA-C	5.66	118.46	110.14
1	A	220	TYR	N-CA-C	-5.65	106.36	113.20
2	B	241	ARG	N-CA-C	5.64	122.81	110.80
2	B	286	SER	N-CA-C	-5.63	106.11	112.87
1	A	207	LEU	N-CA-C	-5.63	105.05	111.07
2	B	416	GLU	N-CA-C	5.60	117.81	107.73
1	A	7	LEU	N-CA-C	-5.58	102.60	110.29
2	B	428	THR	N-CA-C	5.58	118.59	110.17
2	B	13	ILE	CB-CA-C	-5.57	102.79	111.26
2	B	217	ALA	N-CA-C	-5.53	106.46	113.43
2	B	386	TYR	CA-CB-CG	-5.51	103.97	113.90
2	B	251	GLU	N-CA-C	-5.48	104.83	112.45
1	A	363	ASP	N-CA-CB	5.45	118.54	109.60
2	B	21	ARG	N-CA-C	5.43	118.91	110.17
2	B	44	GLU	N-CA-C	-5.41	99.28	110.80
2	B	132	SER	CA-C-N	-5.39	113.26	120.54
2	B	132	SER	C-N-CA	-5.39	113.26	120.54
1	A	368	LEU	CA-C-N	5.37	126.55	119.84
1	A	368	LEU	C-N-CA	5.37	126.55	119.84
1	A	97	ILE	CA-C-N	-5.35	114.09	120.13
1	A	97	ILE	C-N-CA	-5.35	114.09	120.13
1	A	89	ASN	N-CA-C	5.34	117.10	111.28
1	A	29	GLU	CA-C-N	5.33	127.74	120.54
1	A	29	GLU	C-N-CA	5.33	127.74	120.54
2	B	359	ALA	N-CA-C	5.33	115.32	108.34
2	B	61	GLN	CA-C-N	-5.29	112.78	120.29
2	B	61	GLN	C-N-CA	-5.29	112.78	120.29
1	A	61	GLN	N-CA-C	-5.28	104.77	111.11
1	A	367	LEU	N-CA-C	-5.26	105.54	111.28
2	B	442	VAL	CB-CA-C	-5.26	105.23	111.81
1	A	174	GLU	N-CA-C	5.24	116.79	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	GLU	CB-CA-C	-5.22	105.01	110.33
2	B	183	VAL	CA-C-N	5.22	131.09	121.70
2	B	183	VAL	C-N-CA	5.22	131.09	121.70
2	B	114	ILE	N-CA-CB	5.17	116.60	110.55
1	A	375	GLN	N-CA-C	-5.13	102.68	110.28
1	A	425	ALA	CA-C-N	-5.13	113.65	122.79
1	A	425	ALA	C-N-CA	-5.13	113.65	122.79
1	A	160	ASP	CB-CA-C	5.12	119.08	110.88
1	A	67	MET	N-CA-C	-5.11	106.55	112.89
2	B	188	VAL	N-CA-C	-5.05	102.20	107.60
2	B	430	THR	N-CA-C	-5.04	105.23	111.33
2	B	165	TYR	N-CA-C	-5.03	101.49	109.59
1	A	348	ILE	N-CA-C	-5.03	107.01	112.80
1	A	54	SER	N-CA-C	5.03	116.98	109.59
1	A	117	ARG	N-CA-C	5.01	117.64	111.82
2	B	427	TYR	N-CA-C	5.01	117.93	110.52

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	453	THR	Peptide
2	B	162	GLY	Peptide
2	B	309	GLY	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3428	0	3371	446	0
2	B	3412	0	3395	546	1
3	B	10	0	0	1	0
4	A	42	0	0	29	0
4	B	65	0	0	41	0
All	All	6957	0	6766	975	1

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 72.

All (975) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:THR:CG2	2:B:27:ARG:HH11	1.02	1.58
2:B:22:THR:CG2	2:B:27:ARG:HG3	1.39	1.52
2:B:450:LYS:HB2	2:B:470:GLU:CD	1.31	1.51
2:B:375:GLN:HE21	2:B:471:VAL:CG1	1.26	1.46
1:A:170:ASN:CB	1:A:209:ASN:ND2	1.79	1.45
2:B:22:THR:HG21	2:B:27:ARG:CG	1.57	1.35
2:B:375:GLN:HG2	2:B:471:VAL:CG2	1.55	1.34
2:B:451:GLY:O	2:B:470:GLU:HA	1.19	1.34
2:B:455:THR:HG23	4:B:645:HOH:O	1.17	1.32
2:B:375:GLN:NE2	2:B:471:VAL:CG1	1.93	1.29
1:A:200:ALA:CB	1:A:203:GLN:HG2	1.63	1.26
2:B:450:LYS:HB2	2:B:470:GLU:OE1	1.26	1.26
1:A:170:ASN:HB3	1:A:209:ASN:ND2	0.93	1.25
2:B:353:GLN:OE1	2:B:417:LEU:HD21	1.24	1.25
2:B:161:THR:CG2	2:B:354:GLN:OE1	1.85	1.24
1:A:60:THR:OG1	1:A:63:MET:HG3	1.33	1.23
2:B:377:PRO:HD2	2:B:416:GLU:OE2	1.39	1.22
2:B:22:THR:HG22	2:B:27:ARG:NH1	0.89	1.21
2:B:170:ASN:HB3	2:B:209:ASN:OD1	1.39	1.20
2:B:31:ILE:CD1	2:B:383:CYS:HB3	1.72	1.19
1:A:450:LYS:HD3	1:A:450:LYS:N	1.46	1.19
1:A:445:ASN:O	1:A:449:ILE:HG13	1.42	1.18
2:B:198:ASN:HB3	4:B:627:HOH:O	1.42	1.18
1:A:262:ASP:HB3	1:A:287:PHE:CE2	1.78	1.18
1:A:200:ALA:HB1	1:A:203:GLN:CG	1.73	1.17
2:B:22:THR:CG2	2:B:27:ARG:NH1	1.74	1.17
2:B:450:LYS:CB	2:B:470:GLU:CD	2.17	1.16
2:B:353:GLN:O	2:B:354:GLN:HG2	1.46	1.15
2:B:389:ALA:HB1	2:B:434:PHE:CE2	1.84	1.12
1:A:170:ASN:CB	1:A:209:ASN:HD22	1.47	1.12
1:A:36:MET:HA	1:A:36:MET:HE2	1.18	1.11
2:B:451:GLY:O	2:B:470:GLU:CA	1.98	1.10
2:B:389:ALA:HB1	2:B:434:PHE:HE2	0.95	1.10
2:B:251:GLU:HG3	2:B:326:MET:CE	1.81	1.10
2:B:245:TYR:O	2:B:247:ASP:N	1.86	1.09
2:B:372:PRO:HD2	2:B:375:GLN:HB2	1.33	1.09
2:B:134:TYR:CD1	2:B:199:SER:HB3	1.88	1.08
2:B:375:GLN:HG2	2:B:471:VAL:HG21	1.29	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:SER:O	2:B:44:GLU:CB	1.96	1.07
1:A:170:ASN:CG	1:A:209:ASN:HD22	1.63	1.07
2:B:381:LEU:HG	4:B:620:HOH:O	1.55	1.07
2:B:9:GLU:HG3	2:B:333:TYR:CE1	1.90	1.06
2:B:327:ASN:ND2	2:B:330:TRP:H	1.51	1.06
2:B:375:GLN:CD	2:B:471:VAL:HB	1.79	1.06
1:A:432:MET:HE2	1:A:432:MET:HA	1.32	1.06
2:B:39:PHE:CE2	2:B:51:LEU:HD21	1.91	1.05
2:B:363:ASP:OD1	4:B:628:HOH:O	1.74	1.05
2:B:9:GLU:HG3	2:B:333:TYR:CZ	1.90	1.04
1:A:204:PRO:HG3	1:A:237:PHE:CD2	1.91	1.04
2:B:38:PRO:O	2:B:41:LEU:HB2	1.60	1.01
2:B:199:SER:O	4:B:623:HOH:O	1.77	1.01
2:B:379:GLN:HG2	2:B:395:GLU:OE1	1.61	1.00
2:B:375:GLN:HE21	2:B:471:VAL:HG11	0.85	1.00
2:B:251:GLU:HG3	2:B:326:MET:HE1	1.40	1.00
1:A:38:PRO:O	1:A:41:LEU:HB2	1.60	0.99
2:B:31:ILE:HD11	2:B:383:CYS:HB3	1.44	0.99
2:B:251:GLU:CG	2:B:326:MET:HE1	1.92	0.99
2:B:375:GLN:NE2	2:B:471:VAL:CB	2.25	0.99
2:B:450:LYS:HB2	2:B:470:GLU:OE2	1.63	0.99
1:A:159:PHE:O	1:A:353:GLN:NE2	1.95	0.99
2:B:361:PHE:HB2	4:B:624:HOH:O	1.61	0.98
2:B:164:ARG:HG3	4:B:657:HOH:O	1.61	0.98
2:B:450:LYS:CB	2:B:470:GLU:OE2	2.10	0.98
1:A:117:ARG:HG3	1:A:117:ARG:HH11	1.29	0.98
1:A:202:GLY:HA3	4:A:536:HOH:O	1.62	0.98
2:B:353:GLN:OE1	2:B:417:LEU:CD2	2.12	0.97
1:A:450:LYS:HD3	1:A:450:LYS:H	1.23	0.97
2:B:452:LEU:HA	2:B:469:LYS:O	1.65	0.97
2:B:198:ASN:N	2:B:198:ASN:OD1	1.95	0.97
1:A:32:ILE:HD11	4:A:524:HOH:O	1.64	0.97
2:B:133:ASN:N	2:B:133:ASN:HD22	1.61	0.97
2:B:43:SER:O	2:B:44:GLU:HB3	1.15	0.97
2:B:450:LYS:CD	2:B:470:GLU:OE2	2.13	0.96
1:A:36:MET:HA	1:A:36:MET:CE	1.94	0.96
2:B:296:THR:O	2:B:299:VAL:HG22	1.66	0.95
1:A:307:TYR:HD1	1:A:309:GLY:H	1.14	0.94
2:B:22:THR:HG22	2:B:27:ARG:CZ	1.98	0.94
1:A:133:ASN:HD22	1:A:133:ASN:H	1.11	0.94
2:B:375:GLN:CG	2:B:471:VAL:HG21	1.97	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ASP:CB	1:A:287:PHE:CE2	2.50	0.94
2:B:40:LEU:HD11	2:B:465:THR:HA	1.48	0.94
2:B:22:THR:O	2:B:27:ARG:NH1	2.01	0.94
1:A:141:GLY:O	1:A:145:ILE:HB	1.67	0.94
2:B:467:LYS:HB2	4:B:647:HOH:O	1.68	0.94
1:A:36:MET:HE2	1:A:36:MET:CA	1.98	0.93
1:A:429:GLN:O	1:A:432:MET:HB2	1.66	0.93
2:B:375:GLN:CG	2:B:471:VAL:CG2	2.47	0.93
1:A:200:ALA:HB1	1:A:203:GLN:HG2	0.94	0.93
2:B:375:GLN:NE2	2:B:471:VAL:HB	1.82	0.93
1:A:32:ILE:HA	1:A:36:MET:CE	2.00	0.92
2:B:22:THR:HG23	2:B:27:ARG:HG3	1.51	0.92
2:B:240:GLN:HB2	4:B:632:HOH:O	1.69	0.92
1:A:166:ASP:HB2	4:A:528:HOH:O	1.68	0.92
2:B:389:ALA:CB	2:B:434:PHE:HE2	1.81	0.92
1:A:365:GLY:O	1:A:368:LEU:C	2.12	0.92
2:B:117:ARG:HH21	2:B:222:ILE:HD13	1.35	0.92
1:A:450:LYS:N	1:A:450:LYS:CD	2.29	0.92
2:B:375:GLN:HG2	2:B:471:VAL:CB	1.99	0.91
1:A:391:ILE:HD13	1:A:435:ILE:HG23	1.53	0.91
1:A:432:MET:HE2	1:A:432:MET:CA	2.01	0.91
1:A:60:THR:HG1	1:A:63:MET:HG3	1.26	0.91
1:A:135:PHE:CE2	1:A:150:VAL:HB	2.07	0.90
2:B:154:TYR:HD2	2:B:154:TYR:H	0.92	0.90
2:B:6:HIS:CD2	2:B:429:GLN:HB2	2.07	0.90
2:B:375:GLN:NE2	2:B:471:VAL:HG11	1.70	0.89
2:B:22:THR:HG21	2:B:27:ARG:HG3	0.90	0.89
2:B:171:PHE:HB2	2:B:209:ASN:HD21	1.37	0.89
2:B:368:LEU:HB3	2:B:371:ILE:CD1	2.02	0.89
2:B:22:THR:HG22	2:B:27:ARG:HH12	1.32	0.89
2:B:375:GLN:NE2	2:B:471:VAL:HG12	1.84	0.88
2:B:451:GLY:O	2:B:470:GLU:HG2	1.73	0.88
1:A:32:ILE:HA	1:A:36:MET:HE1	1.54	0.88
1:A:143:SER:O	1:A:148:CYS:O	1.92	0.87
1:A:249:THR:O	1:A:253:ILE:HD12	1.73	0.87
2:B:378:ALA:CB	2:B:395:GLU:HG3	2.05	0.87
1:A:432:MET:HA	1:A:432:MET:CE	2.05	0.87
2:B:22:THR:HG21	2:B:27:ARG:CD	2.05	0.87
2:B:202:GLY:CA	2:B:358:HIS:CD2	2.58	0.87
2:B:22:THR:CG2	2:B:27:ARG:CG	2.30	0.86
2:B:450:LYS:HD2	2:B:470:GLU:OE2	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:ASP:HA	1:A:436:ILE:HD12	1.56	0.86
1:A:170:ASN:CB	1:A:209:ASN:HD21	1.66	0.86
2:B:331:LEU:O	2:B:335:ILE:HG13	1.75	0.86
2:B:271:ASP:OD1	2:B:424:ARG:NH2	2.08	0.86
1:A:15:VAL:HB	2:B:15:VAL:HB	1.57	0.85
1:A:331:LEU:O	1:A:335:ILE:HG12	1.75	0.85
2:B:22:THR:HG21	2:B:27:ARG:HH11	1.33	0.85
2:B:327:ASN:HD21	2:B:330:TRP:H	1.22	0.85
2:B:230:ARG:HH11	2:B:230:ARG:CG	1.89	0.85
2:B:395:GLU:HB3	4:B:637:HOH:O	1.76	0.85
1:A:372:PRO:O	1:A:375:GLN:O	1.94	0.84
2:B:161:THR:HG23	2:B:354:GLN:OE1	1.77	0.84
2:B:22:THR:CB	2:B:27:ARG:HH11	1.89	0.84
2:B:450:LYS:CB	2:B:470:GLU:OE1	2.18	0.84
2:B:31:ILE:HD11	2:B:383:CYS:CB	2.07	0.84
1:A:60:THR:OG1	1:A:63:MET:CG	2.21	0.84
1:A:327:ASN:ND2	1:A:330:TRP:H	1.75	0.84
2:B:353:GLN:O	2:B:354:GLN:CG	2.26	0.83
2:B:209:ASN:C	2:B:209:ASN:HD22	1.85	0.83
2:B:202:GLY:HA2	2:B:358:HIS:CD2	2.13	0.83
2:B:368:LEU:O	2:B:371:ILE:HD12	1.79	0.82
2:B:161:THR:HG22	2:B:354:GLN:OE1	1.77	0.82
1:A:9:GLU:OE2	1:A:333:TYR:CE1	2.33	0.82
1:A:449:ILE:C	1:A:450:LYS:HD3	2.05	0.82
1:A:251:GLU:HG2	1:A:326:MET:HE1	1.61	0.82
1:A:19:VAL:HG12	2:B:11:PHE:HA	1.62	0.82
1:A:54:SER:HB2	1:A:270:LLP:HE3	1.60	0.82
2:B:354:GLN:NE2	4:B:653:HOH:O	2.12	0.82
1:A:289:ASP:HB3	4:A:537:HOH:O	1.80	0.81
1:A:114:ILE:HG21	1:A:125:ARG:HH12	1.44	0.81
1:A:345:LEU:HD23	1:A:436:ILE:HG23	1.62	0.81
2:B:196:THR:CG2	2:B:203:GLN:O	2.29	0.81
2:B:161:THR:HG21	2:B:354:GLN:OE1	1.81	0.81
2:B:453:THR:N	2:B:469:LYS:O	2.14	0.81
2:B:170:ASN:CB	2:B:209:ASN:OD1	2.26	0.81
1:A:422:ILE:O	1:A:422:ILE:HG22	1.77	0.80
1:A:161:THR:HG22	1:A:353:GLN:CD	2.05	0.80
2:B:117:ARG:HG2	2:B:117:ARG:HH11	1.46	0.80
2:B:251:GLU:CG	2:B:326:MET:CE	2.54	0.79
2:B:381:LEU:CG	4:B:620:HOH:O	2.20	0.79
2:B:31:ILE:HG13	4:B:659:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:THR:HG23	2:B:203:GLN:O	1.82	0.79
2:B:375:GLN:CG	2:B:471:VAL:HB	2.11	0.79
1:A:200:ALA:O	1:A:203:GLN:NE2	2.16	0.78
2:B:361:PHE:CD1	2:B:419:ARG:HB2	2.18	0.78
2:B:368:LEU:HB3	2:B:371:ILE:HD13	1.62	0.78
1:A:54:SER:O	1:A:56:THR:HG23	1.84	0.78
2:B:31:ILE:CD1	2:B:383:CYS:CB	2.58	0.78
2:B:21:ARG:NH2	2:B:47:PHE:CZ	2.51	0.78
1:A:268:ALA:O	1:A:274:VAL:HG23	1.84	0.78
1:A:431:HIS:O	1:A:435:ILE:HG13	1.82	0.77
2:B:456:TYR:HB3	4:B:647:HOH:O	1.84	0.77
2:B:236:TYR:CD2	2:B:335:ILE:HD12	2.18	0.77
2:B:154:TYR:HD2	2:B:154:TYR:N	1.76	0.77
2:B:161:THR:CG2	2:B:354:GLN:CD	2.58	0.77
2:B:40:LEU:CD1	2:B:465:THR:HA	2.15	0.77
1:A:365:GLY:O	1:A:368:LEU:O	2.03	0.77
2:B:167:PHE:HB3	2:B:170:ASN:HD21	1.49	0.76
1:A:169:GLY:O	1:A:205:VAL:HG22	1.84	0.76
2:B:31:ILE:HD11	2:B:383:CYS:SG	2.24	0.76
1:A:161:THR:HG23	1:A:353:GLN:NE2	2.01	0.76
2:B:196:THR:CG2	2:B:203:GLN:C	2.59	0.76
1:A:200:ALA:CB	1:A:203:GLN:CG	2.49	0.76
1:A:350:VAL:HG22	1:A:367:LEU:HD13	1.67	0.75
1:A:117:ARG:HH11	1:A:117:ARG:CG	1.98	0.75
2:B:375:GLN:CG	2:B:471:VAL:CB	2.64	0.75
1:A:251:GLU:CG	1:A:326:MET:HE1	2.16	0.75
2:B:50:LEU:HD12	2:B:420:LEU:HD23	1.69	0.75
2:B:180:ILE:O	2:B:184:GLY:HA2	1.86	0.75
2:B:224:VAL:CG1	2:B:261:ALA:HA	2.16	0.75
1:A:135:PHE:CZ	1:A:150:VAL:CG1	2.69	0.75
1:A:161:THR:HG22	1:A:353:GLN:HA	1.67	0.75
2:B:63:MET:HE1	2:B:273:MET:HB2	1.67	0.75
1:A:454:PHE:CE2	4:A:529:HOH:O	2.39	0.75
2:B:133:ASN:HD22	2:B:133:ASN:H	1.31	0.75
2:B:154:TYR:N	2:B:154:TYR:CD2	2.46	0.75
1:A:454:PHE:HE2	4:A:529:HOH:O	1.69	0.75
2:B:375:GLN:HE21	2:B:471:VAL:CB	1.96	0.75
1:A:433:ASP:HA	1:A:436:ILE:CD1	2.16	0.75
2:B:354:GLN:CD	4:B:653:HOH:O	2.30	0.74
2:B:31:ILE:HD12	2:B:383:CYS:HB3	1.69	0.74
1:A:9:GLU:OE1	2:B:428:THR:HG21	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:GLU:C	2:B:183:VAL:H	1.94	0.74
2:B:389:ALA:CB	2:B:434:PHE:CE2	2.64	0.74
1:A:133:ASN:H	1:A:133:ASN:ND2	1.83	0.74
2:B:337:GLN:O	2:B:337:GLN:HG2	1.86	0.74
2:B:381:LEU:CD1	4:B:620:HOH:O	2.35	0.74
2:B:451:GLY:O	2:B:470:GLU:CB	2.35	0.74
2:B:368:LEU:HD13	4:B:630:HOH:O	1.87	0.74
1:A:28:GLU:O	1:A:32:ILE:HG12	1.88	0.73
2:B:117:ARG:HH11	2:B:117:ARG:CG	2.00	0.73
2:B:375:GLN:HG2	2:B:471:VAL:HG23	1.63	0.73
1:A:6:HIS:ND1	1:A:429:GLN:HB2	2.03	0.73
1:A:449:ILE:HA	1:A:450:LYS:HD3	1.69	0.73
1:A:238:ILE:HG23	1:A:242:GLU:HB3	1.71	0.73
2:B:108:ILE:HD11	2:B:298:CYS:SG	2.28	0.73
2:B:460:VAL:O	4:B:601:HOH:O	2.06	0.73
2:B:22:THR:C	2:B:27:ARG:HH12	1.95	0.72
1:A:161:THR:CG2	1:A:353:GLN:CD	2.62	0.72
1:A:327:ASN:ND2	1:A:327:ASN:C	2.47	0.72
2:B:419:ARG:HG2	2:B:420:LEU:N	2.04	0.72
2:B:451:GLY:O	2:B:470:GLU:CG	2.37	0.72
2:B:28:GLU:O	2:B:29:GLU:C	2.33	0.72
1:A:6:HIS:CE1	1:A:337:GLN:HG3	2.25	0.72
1:A:41:LEU:HD21	1:A:386:TYR:CD2	2.25	0.71
2:B:99:THR:OG1	2:B:278:GLY:HA3	1.90	0.71
1:A:20:LYS:HD3	4:A:532:HOH:O	1.89	0.71
1:A:55:GLY:N	1:A:269:LYS:HB3	2.04	0.71
2:B:133:ASN:N	2:B:133:ASN:ND2	2.37	0.71
2:B:422:ILE:HG23	2:B:423:PRO:HD2	1.72	0.71
2:B:214:TYR:HB2	2:B:260:TYR:HB3	1.72	0.71
2:B:445:ASN:C	2:B:447:ALA:H	1.98	0.71
1:A:249:THR:OG1	1:A:252:GLN:HB2	1.91	0.71
1:A:238:ILE:O	1:A:239:LYS:C	2.31	0.71
2:B:251:GLU:HG3	2:B:326:MET:HE3	1.73	0.71
2:B:372:PRO:O	2:B:375:GLN:O	2.09	0.71
1:A:204:PRO:HG3	1:A:237:PHE:HD2	1.56	0.71
2:B:9:GLU:HG3	2:B:333:TYR:OH	1.91	0.71
2:B:181:GLU:C	2:B:183:VAL:N	2.44	0.71
2:B:189:PRO:HB2	2:B:190:TYR:CD1	2.26	0.71
1:A:72:GLU:HA	4:A:538:HOH:O	1.90	0.70
1:A:98:PRO:O	1:A:308:GLY:HA3	1.91	0.70
2:B:251:GLU:HG2	2:B:326:MET:HE1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:THR:CB	2:B:27:ARG:NH1	2.52	0.70
1:A:133:ASN:HD21	1:A:194:THR:H	1.39	0.70
2:B:6:HIS:CE1	2:B:337:GLN:HG3	2.26	0.69
2:B:445:ASN:O	2:B:447:ALA:N	2.25	0.69
1:A:450:LYS:H	1:A:450:LYS:CD	1.97	0.69
2:B:43:SER:C	2:B:45:ASP:H	1.99	0.69
2:B:262:ASP:HB3	2:B:287:PHE:CE2	2.28	0.69
2:B:361:PHE:CE1	2:B:419:ARG:HD3	2.27	0.69
1:A:55:GLY:H	1:A:269:LYS:HB3	1.58	0.69
2:B:50:LEU:HD13	2:B:421:THR:H	1.57	0.69
2:B:378:ALA:HB3	2:B:395:GLU:HG3	1.73	0.69
1:A:327:ASN:C	1:A:327:ASN:HD22	2.01	0.69
1:A:124:ASP:HB3	1:A:187:ASN:HD21	1.56	0.69
2:B:327:ASN:ND2	2:B:330:TRP:N	2.36	0.69
1:A:135:PHE:CZ	1:A:150:VAL:HG12	2.29	0.68
1:A:171:PHE:N	1:A:209:ASN:HD21	1.90	0.68
1:A:371:ILE:CG2	1:A:377:PRO:HB3	2.22	0.68
1:A:214:TYR:HB2	1:A:260:TYR:HB3	1.76	0.68
1:A:9:GLU:OE2	1:A:333:TYR:HE1	1.74	0.68
1:A:32:ILE:CA	1:A:36:MET:HE1	2.23	0.68
2:B:110:ILE:O	2:B:114:ILE:HG13	1.94	0.68
1:A:254:THR:HA	4:A:527:HOH:O	1.93	0.68
2:B:245:TYR:O	2:B:246:LYS:C	2.37	0.68
2:B:452:LEU:CA	2:B:469:LYS:O	2.41	0.68
2:B:6:HIS:HB2	2:B:340:TYR:CD1	2.28	0.68
2:B:375:GLN:HG2	2:B:471:VAL:HB	1.71	0.68
1:A:8:PRO:HG2	2:B:21:ARG:NH2	2.09	0.68
1:A:449:ILE:CA	1:A:450:LYS:HD3	2.23	0.67
2:B:245:TYR:C	2:B:247:ASP:N	2.52	0.67
1:A:288:PHE:CD1	1:A:288:PHE:C	2.73	0.67
1:A:171:PHE:H	1:A:209:ASN:HD21	1.43	0.67
2:B:202:GLY:HA3	2:B:358:HIS:CD2	2.28	0.67
1:A:93:TYR:CE2	1:A:283:LYS:HB2	2.30	0.67
2:B:240:GLN:HG2	2:B:241:ARG:HG3	1.74	0.67
1:A:9:GLU:CG	2:B:431:HIS:CE1	2.78	0.66
1:A:384:GLU:O	1:A:388:VAL:HG12	1.95	0.66
2:B:195:ILE:HG23	2:B:234:ASN:CG	2.20	0.66
1:A:248:TRP:CD1	4:A:517:HOH:O	2.47	0.66
2:B:21:ARG:HH21	2:B:47:PHE:HZ	1.42	0.66
1:A:385:LEU:HD11	1:A:439:PHE:CE1	2.30	0.66
1:A:327:ASN:HD21	1:A:330:TRP:H	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:O	1:A:116:LYS:C	2.34	0.66
1:A:274:VAL:HG12	1:A:317:ARG:HE	1.61	0.66
1:A:445:ASN:HD22	1:A:449:ILE:CG1	2.09	0.66
1:A:214:TYR:HD2	1:A:260:TYR:HD1	1.43	0.66
2:B:110:ILE:HB	2:B:111:PRO:HD3	1.77	0.66
2:B:117:ARG:NH2	2:B:222:ILE:HD13	2.08	0.66
2:B:179:GLY:HA2	2:B:182:GLU:OE2	1.96	0.66
1:A:449:ILE:HA	1:A:450:LYS:CD	2.26	0.65
1:A:251:GLU:CG	1:A:326:MET:CE	2.74	0.65
1:A:336:ALA:O	1:A:339:GLN:HB3	1.95	0.65
1:A:20:LYS:HB2	4:A:512:HOH:O	1.95	0.65
2:B:378:ALA:HB3	2:B:395:GLU:CG	2.25	0.65
1:A:103:ARG:O	1:A:107:GLN:HG3	1.96	0.65
2:B:196:THR:HG23	2:B:203:GLN:C	2.20	0.65
2:B:6:HIS:HE1	2:B:337:GLN:HG3	1.61	0.65
1:A:24:ARG:CZ	4:A:511:HOH:O	2.44	0.65
2:B:230:ARG:HH11	2:B:230:ARG:HG2	1.61	0.65
2:B:239:LYS:HB2	2:B:253:ILE:CD1	2.27	0.65
1:A:333:TYR:C	1:A:333:TYR:CD2	2.75	0.65
2:B:245:TYR:C	2:B:247:ASP:H	2.05	0.65
1:A:135:PHE:CE2	1:A:150:VAL:CB	2.81	0.64
1:A:135:PHE:CE2	1:A:150:VAL:CG1	2.80	0.64
2:B:230:ARG:HH11	2:B:230:ARG:HG3	1.62	0.64
2:B:379:GLN:HB2	2:B:452:LEU:HD12	1.79	0.64
2:B:39:PHE:CD2	2:B:51:LEU:HD21	2.33	0.64
1:A:88:LYS:O	1:A:92:GLY:HA2	1.97	0.64
2:B:224:VAL:HG12	2:B:261:ALA:HA	1.79	0.64
1:A:90:ILE:HD11	1:A:323:TYR:CE2	2.33	0.64
1:A:170:ASN:HB3	1:A:209:ASN:HD21	0.82	0.64
1:A:83:LEU:HD23	1:A:315:MET:HG2	1.78	0.64
2:B:21:ARG:NE	2:B:47:PHE:CE1	2.66	0.64
2:B:428:THR:O	2:B:432:MET:HG2	1.98	0.64
2:B:216:ILE:HG22	2:B:216:ILE:O	1.97	0.63
2:B:330:TRP:HH2	2:B:424:ARG:HB3	1.64	0.63
1:A:262:ASP:HB3	1:A:287:PHE:CD2	2.29	0.63
2:B:37:ASN:ND2	2:B:463:HIS:O	2.29	0.63
2:B:86:SER:HB2	2:B:323:TYR:CE1	2.33	0.63
2:B:443:LYS:HG2	2:B:443:LYS:O	1.98	0.63
2:B:201:GLY:O	2:B:356:GLY:HA3	1.97	0.63
2:B:327:ASN:HD22	2:B:330:TRP:H	1.41	0.63
2:B:375:GLN:HA	2:B:452:LEU:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LEU:CD2	1:A:436:ILE:HG23	2.29	0.63
1:A:352:CYS:CB	1:A:361:PHE:O	2.47	0.63
2:B:384:GLU:O	2:B:388:VAL:HG23	1.99	0.62
1:A:289:ASP:O	1:A:292:THR:HB	1.98	0.62
2:B:93:TYR:HB3	2:B:282:MET:O	1.98	0.62
1:A:380:ALA:N	1:A:452:LEU:HD11	2.14	0.62
2:B:80:TYR:N	2:B:315:MET:HE3	2.14	0.62
2:B:327:ASN:HD21	2:B:330:TRP:N	1.95	0.62
2:B:372:PRO:CD	2:B:375:GLN:OE1	2.47	0.62
2:B:384:GLU:OE1	2:B:387:LYS:HE2	1.99	0.62
2:B:224:VAL:HG12	2:B:261:ALA:CB	2.29	0.62
1:A:251:GLU:HG2	1:A:326:MET:CE	2.30	0.62
1:A:41:LEU:HD21	1:A:386:TYR:CE2	2.35	0.62
1:A:437:GLU:OE1	1:A:437:GLU:HA	2.00	0.62
1:A:46:VAL:HG12	1:A:47:PHE:N	2.11	0.62
2:B:17:GLU:O	2:B:17:GLU:HG2	1.98	0.62
1:A:28:GLU:OE2	1:A:387:LYS:HD3	2.00	0.62
2:B:167:PHE:O	2:B:170:ASN:ND2	2.33	0.61
2:B:372:PRO:HD2	2:B:375:GLN:CB	2.22	0.61
1:A:228:SER:HB2	1:A:266:MET:HB2	1.82	0.61
2:B:161:THR:HG21	2:B:354:GLN:CD	2.24	0.61
2:B:48:ILE:HD11	2:B:431:HIS:HD2	1.65	0.61
2:B:354:GLN:O	4:B:624:HOH:O	2.16	0.61
2:B:124:ASP:OD1	2:B:124:ASP:C	2.42	0.61
2:B:230:ARG:HG3	2:B:358:HIS:CE1	2.36	0.61
2:B:207:LEU:HD13	2:B:245:TYR:CZ	2.35	0.61
1:A:287:PHE:HA	4:A:537:HOH:O	2.00	0.61
2:B:103:ARG:O	2:B:107:GLN:HG3	2.01	0.61
2:B:32:ILE:O	2:B:35:GLY:N	2.34	0.61
2:B:80:TYR:C	2:B:80:TYR:CD2	2.78	0.61
1:A:132:SER:HB3	1:A:135:PHE:CE2	2.37	0.60
1:A:285:ASP:C	1:A:287:PHE:H	2.08	0.60
2:B:88:LYS:O	2:B:92:GLY:HA2	2.01	0.60
2:B:327:ASN:HD22	2:B:330:TRP:HB3	1.66	0.60
2:B:291:TYR:CZ	2:B:295:ARG:HD2	2.36	0.60
2:B:378:ALA:HB3	2:B:395:GLU:CD	2.27	0.60
2:B:441:HIS:N	2:B:441:HIS:ND1	2.49	0.60
1:A:99:THR:HG21	1:A:105:ALA:N	2.17	0.60
1:A:29:GLU:OE2	1:A:29:GLU:HA	2.01	0.60
1:A:76:GLY:N	1:A:306:THR:HG21	2.16	0.60
1:A:220:TYR:N	1:A:220:TYR:CD1	2.68	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:SER:OG	1:A:190:TYR:OH	2.18	0.60
2:B:355:ALA:N	4:B:619:HOH:O	2.34	0.60
1:A:102:GLY:N	1:A:270:LLP:OP2	2.34	0.60
1:A:379:GLN:OE1	1:A:395:GLU:HG2	2.02	0.60
2:B:361:PHE:CE1	2:B:419:ARG:HB2	2.35	0.60
1:A:251:GLU:HG3	1:A:326:MET:HE3	1.84	0.60
1:A:269:LYS:HD3	1:A:276:MET:HA	1.82	0.60
2:B:51:LEU:HD23	2:B:392:ARG:HD3	1.84	0.60
2:B:445:ASN:C	2:B:447:ALA:N	2.59	0.60
1:A:303:GLY:HA3	1:A:307:TYR:HE1	1.66	0.59
2:B:254:THR:O	2:B:258:TYR:HD2	1.85	0.59
1:A:200:ALA:HB3	1:A:203:GLN:HG2	1.76	0.59
2:B:378:ALA:CB	2:B:395:GLU:CG	2.80	0.59
1:A:268:ALA:HB1	1:A:274:VAL:HG21	1.84	0.59
2:B:340:TYR:C	2:B:340:TYR:CD2	2.80	0.59
1:A:135:PHE:CZ	1:A:150:VAL:HG11	2.36	0.59
2:B:40:LEU:CD1	2:B:464:PHE:O	2.50	0.59
2:B:217:ALA:O	2:B:221:ASP:N	2.36	0.59
2:B:232:ALA:HB1	2:B:331:LEU:HD21	1.84	0.59
2:B:211:LYS:HD3	2:B:260:TYR:OH	2.03	0.59
1:A:21:ARG:NH1	1:A:47:PHE:CE1	2.71	0.59
1:A:132:SER:OG	1:A:134:TYR:O	2.10	0.59
1:A:445:ASN:HD22	1:A:449:ILE:HG13	1.68	0.59
1:A:46:VAL:CG1	1:A:47:PHE:N	2.62	0.59
2:B:239:LYS:HD2	2:B:248:TRP:O	2.03	0.59
2:B:171:PHE:CD1	2:B:213:MET:HG3	2.37	0.59
2:B:214:TYR:HD1	2:B:224:VAL:HG21	1.67	0.59
1:A:161:THR:CG2	1:A:353:GLN:NE2	2.66	0.58
1:A:170:ASN:CA	1:A:209:ASN:ND2	2.62	0.58
2:B:51:LEU:HD23	2:B:392:ARG:CD	2.33	0.58
2:B:189:PRO:HB2	2:B:190:TYR:HD1	1.66	0.58
2:B:339:GLN:O	2:B:340:TYR:C	2.44	0.58
1:A:114:ILE:HG21	1:A:125:ARG:NH1	2.18	0.58
1:A:195:ILE:O	1:A:195:ILE:HG12	2.02	0.58
2:B:195:ILE:CD1	2:B:226:MET:SD	2.91	0.58
1:A:352:CYS:HB3	1:A:361:PHE:O	2.04	0.58
2:B:110:ILE:HB	2:B:111:PRO:CD	2.32	0.58
2:B:450:LYS:CG	2:B:470:GLU:OE2	2.51	0.58
2:B:327:ASN:ND2	2:B:327:ASN:C	2.61	0.58
2:B:161:THR:HG23	2:B:354:GLN:CD	2.26	0.57
2:B:209:ASN:C	2:B:209:ASN:ND2	2.59	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:LEU:HD12	2:B:318:LEU:O	2.04	0.57
1:A:24:ARG:HD3	4:A:511:HOH:O	2.04	0.57
2:B:166:ASP:HB3	2:B:241:ARG:HD3	1.86	0.57
2:B:116:LYS:HE2	2:B:120:GLU:OE2	2.04	0.57
2:B:43:SER:C	2:B:45:ASP:N	2.61	0.57
2:B:268:ALA:O	2:B:272:ALA:HB3	2.05	0.57
2:B:449:ILE:HG22	4:B:630:HOH:O	2.04	0.57
2:B:220:TYR:N	2:B:220:TYR:CD1	2.72	0.57
1:A:107:GLN:HG2	1:A:142:HIS:CE1	2.39	0.57
1:A:230:ARG:HA	1:A:271:ASP:CG	2.30	0.57
1:A:90:ILE:HD11	1:A:323:TYR:CD2	2.40	0.57
1:A:96:THR:O	1:A:96:THR:HG22	2.04	0.56
1:A:159:PHE:C	1:A:353:GLN:NE2	2.63	0.56
2:B:39:PHE:HE2	2:B:51:LEU:HD21	1.60	0.56
2:B:171:PHE:N	2:B:209:ASN:OD1	2.37	0.56
2:B:181:GLU:O	2:B:183:VAL:N	2.38	0.56
2:B:194:THR:HG21	2:B:198:ASN:ND2	2.20	0.56
2:B:170:ASN:N	2:B:170:ASN:HD22	2.03	0.56
2:B:182:GLU:O	2:B:182:GLU:HG2	2.04	0.56
1:A:183:VAL:HG12	1:A:183:VAL:O	2.04	0.56
1:A:445:ASN:O	1:A:445:ASN:ND2	2.38	0.56
2:B:189:PRO:O	2:B:223:PRO:HD2	2.05	0.56
2:B:334:ARG:C	2:B:334:ARG:CD	2.77	0.56
1:A:34:SER:HB3	1:A:41:LEU:HD12	1.86	0.56
1:A:80:TYR:CD2	1:A:80:TYR:C	2.82	0.56
1:A:429:GLN:O	1:A:432:MET:CB	2.49	0.56
2:B:118:GLU:CD	2:B:125:ARG:HH21	2.12	0.56
1:A:37:ASN:OD1	1:A:37:ASN:C	2.48	0.56
1:A:58:ALA:HB3	1:A:425:ALA:HB3	1.87	0.56
1:A:251:GLU:HG3	1:A:326:MET:CE	2.35	0.56
2:B:165:TYR:HB3	2:B:168:LYS:HD3	1.87	0.56
1:A:168:LYS:HB3	1:A:203:GLN:HG3	1.88	0.56
1:A:343:ASP:O	1:A:347:GLU:HG3	2.06	0.56
1:A:269:LYS:C	1:A:270:LLP:HD3	2.31	0.56
1:A:380:ALA:H	1:A:452:LEU:HD11	1.70	0.56
2:B:9:GLU:CG	2:B:333:TYR:OH	2.53	0.56
2:B:86:SER:HA	4:B:664:HOH:O	2.05	0.56
2:B:228:SER:HB3	2:B:231:PHE:HB3	1.88	0.56
2:B:451:GLY:C	2:B:470:GLU:HA	2.21	0.56
2:B:467:LYS:HB3	4:B:643:HOH:O	2.06	0.56
2:B:9:GLU:HA	2:B:333:TYR:CE1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:GLU:HG2	2:B:431:HIS:CE1	2.40	0.55
1:A:110:ILE:HB	1:A:111:PRO:HD3	1.87	0.55
2:B:195:ILE:HD11	2:B:226:MET:SD	2.45	0.55
2:B:316:GLU:O	2:B:319:ALA:HB3	2.06	0.55
2:B:438:ALA:O	2:B:442:VAL:HG23	2.06	0.55
2:B:445:ASN:N	4:B:629:HOH:O	2.38	0.55
1:A:8:PRO:HG2	2:B:21:ARG:HH22	1.70	0.55
1:A:327:ASN:HD21	1:A:329:ASP:HB2	1.71	0.55
2:B:182:GLU:O	2:B:182:GLU:CG	2.54	0.55
2:B:330:TRP:CH2	2:B:424:ARG:HB3	2.41	0.55
2:B:220:TYR:O	2:B:221:ASP:C	2.48	0.55
2:B:90:ILE:HG22	2:B:91:PHE:CD2	2.42	0.55
2:B:230:ARG:CG	2:B:230:ARG:NH1	2.61	0.55
1:A:128:MET:SD	1:A:148:CYS:HB2	2.47	0.55
1:A:183:VAL:O	1:A:183:VAL:CG1	2.54	0.55
1:A:79:SER:OG	1:A:316:GLU:HG2	2.07	0.55
1:A:358:HIS:ND1	4:A:536:HOH:O	2.33	0.55
2:B:383:CYS:O	2:B:387:LYS:CG	2.55	0.55
1:A:188:VAL:HG11	1:A:222:ILE:HD13	1.87	0.55
1:A:331:LEU:O	1:A:335:ILE:CG1	2.50	0.55
2:B:117:ARG:C	2:B:119:GLN:N	2.65	0.55
2:B:202:GLY:CA	2:B:358:HIS:HD2	2.13	0.55
1:A:76:GLY:H	1:A:306:THR:HG21	1.72	0.55
2:B:95:TYR:O	2:B:281:CYS:HA	2.07	0.55
1:A:371:ILE:HG22	1:A:377:PRO:HB3	1.89	0.54
1:A:104:GLY:O	1:A:105:ALA:C	2.50	0.54
1:A:307:TYR:HD1	1:A:308:GLY:N	2.05	0.54
1:A:432:MET:CA	1:A:432:MET:CE	2.75	0.54
2:B:81:TYR:O	2:B:85:GLU:HB2	2.07	0.54
2:B:463:HIS:HB2	4:B:665:HOH:O	2.08	0.54
1:A:7:LEU:HD12	1:A:336:ALA:HB2	1.90	0.54
1:A:93:TYR:HD1	1:A:93:TYR:N	2.05	0.54
1:A:365:GLY:O	1:A:369:PRO:N	2.41	0.54
2:B:242:GLU:CD	2:B:245:TYR:HE1	2.15	0.54
2:B:251:GLU:OE2	2:B:251:GLU:N	2.41	0.54
1:A:124:ASP:HB3	1:A:187:ASN:ND2	2.23	0.54
1:A:364:ALA:HB1	1:A:377:PRO:O	2.08	0.54
2:B:117:ARG:O	2:B:118:GLU:C	2.50	0.54
2:B:194:THR:HG21	2:B:198:ASN:CG	2.32	0.54
2:B:290:VAL:HG23	4:B:650:HOH:O	2.08	0.54
2:B:353:GLN:C	2:B:354:GLN:HG2	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:ILE:CD1	2:B:298:CYS:SG	2.94	0.54
1:A:270:LLP:HD3	1:A:270:LLP:N	2.23	0.54
2:B:132:SER:O	2:B:133:ASN:C	2.49	0.54
2:B:334:ARG:O	2:B:334:ARG:HD3	2.08	0.54
1:A:32:ILE:HD13	1:A:36:MET:HE1	1.89	0.53
1:A:217:ALA:O	1:A:221:ASP:HA	2.08	0.53
2:B:161:THR:HG23	2:B:354:GLN:NE2	2.24	0.53
1:A:107:GLN:HG2	1:A:142:HIS:NE2	2.23	0.53
1:A:204:PRO:CG	1:A:237:PHE:CD2	2.81	0.53
1:A:262:ASP:HB3	1:A:287:PHE:HE2	1.59	0.53
1:A:340:TYR:C	1:A:340:TYR:CD2	2.85	0.53
1:A:93:TYR:HB3	1:A:282:MET:O	2.08	0.53
1:A:307:TYR:HD1	1:A:309:GLY:N	1.94	0.53
2:B:6:HIS:NE2	2:B:429:GLN:HB2	2.23	0.53
2:B:230:ARG:NH1	4:B:616:HOH:O	2.39	0.53
2:B:376:PHE:HZ	2:B:454:PHE:CE1	2.26	0.53
1:A:224:VAL:HG12	1:A:261:ALA:CB	2.39	0.53
2:B:201:GLY:O	2:B:356:GLY:CA	2.57	0.53
2:B:17:GLU:O	2:B:17:GLU:CG	2.56	0.53
1:A:109:TYR:CD1	1:A:109:TYR:C	2.87	0.53
1:A:220:TYR:HD1	1:A:220:TYR:H	1.56	0.53
1:A:333:TYR:O	1:A:334:ARG:C	2.48	0.53
2:B:117:ARG:O	2:B:119:GLN:N	2.42	0.53
2:B:422:ILE:CG2	2:B:423:PRO:HD2	2.39	0.53
1:A:335:ILE:O	1:A:336:ALA:C	2.50	0.53
2:B:134:TYR:CE1	2:B:199:SER:HB3	2.41	0.53
2:B:372:PRO:HD3	2:B:375:GLN:OE1	2.07	0.53
2:B:383:CYS:O	2:B:387:LYS:HG2	2.08	0.53
1:A:9:GLU:HG3	2:B:431:HIS:CE1	2.44	0.53
1:A:394:VAL:HG22	1:A:395:GLU:H	1.74	0.53
2:B:106:GLU:O	2:B:107:GLN:C	2.50	0.53
2:B:230:ARG:NH1	2:B:358:HIS:ND1	2.57	0.53
1:A:93:TYR:N	1:A:93:TYR:CD1	2.77	0.53
1:A:88:LYS:O	1:A:92:GLY:N	2.40	0.52
1:A:166:ASP:O	1:A:241:ARG:NH1	2.41	0.52
1:A:361:PHE:N	1:A:361:PHE:CD2	2.77	0.52
2:B:384:GLU:HA	2:B:387:LYS:HG3	1.90	0.52
1:A:135:PHE:CE1	1:A:150:VAL:HG11	2.44	0.52
2:B:102:GLY:HA3	2:B:267:SER:HB2	1.91	0.52
2:B:460:VAL:HG22	2:B:461:LEU:HG	1.91	0.52
1:A:9:GLU:CG	2:B:431:HIS:HE1	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:LEU:O	2:B:371:ILE:CD1	2.56	0.52
2:B:117:ARG:CG	2:B:117:ARG:NH1	2.69	0.52
2:B:195:ILE:CG2	2:B:234:ASN:CB	2.88	0.52
2:B:288:PHE:CD1	2:B:288:PHE:C	2.87	0.52
2:B:42:ASP:O	2:B:45:ASP:HB2	2.09	0.52
2:B:84:ALA:CB	2:B:96:THR:HB	2.39	0.52
2:B:133:ASN:H	2:B:133:ASN:ND2	2.05	0.52
1:A:93:TYR:CG	1:A:283:LYS:HA	2.45	0.52
1:A:270:LLP:N	1:A:270:LLP:CD	2.72	0.52
1:A:282:MET:SD	1:A:282:MET:N	2.83	0.52
1:A:371:ILE:HG21	1:A:377:PRO:HB3	1.91	0.52
2:B:64:GLN:O	2:B:65:ALA:C	2.53	0.52
1:A:32:ILE:HA	1:A:36:MET:HE3	1.90	0.52
1:A:21:ARG:NH1	1:A:47:PHE:CD1	2.78	0.52
1:A:268:ALA:HB1	1:A:274:VAL:CG2	2.39	0.52
2:B:196:THR:HG22	2:B:197:SER:N	2.25	0.52
1:A:93:TYR:CD2	1:A:283:LYS:CA	2.93	0.52
1:A:327:ASN:ND2	1:A:330:TRP:HB3	2.25	0.52
1:A:375:GLN:O	1:A:377:PRO:HD3	2.10	0.52
1:A:391:ILE:CD1	1:A:435:ILE:HG23	2.34	0.52
1:A:76:GLY:H	1:A:306:THR:CG2	2.23	0.51
2:B:452:LEU:HA	2:B:470:GLU:HA	1.91	0.51
1:A:93:TYR:OH	1:A:258:TYR:O	2.17	0.51
1:A:100:HIS:ND1	1:A:302:GLU:OE1	2.34	0.51
2:B:432:MET:HA	2:B:435:ILE:HD13	1.92	0.51
1:A:138:THR:O	1:A:142:HIS:HB2	2.11	0.51
2:B:230:ARG:HA	2:B:271:ASP:CG	2.36	0.51
1:A:340:TYR:CZ	1:A:429:GLN:NE2	2.79	0.51
2:B:263:MET:HB2	2:B:282:MET:HG3	1.91	0.51
2:B:361:PHE:CE1	2:B:419:ARG:CD	2.94	0.51
2:B:431:HIS:O	2:B:435:ILE:HD12	2.11	0.51
1:A:340:TYR:OH	1:A:433:ASP:OD1	2.22	0.51
2:B:123:LEU:HD23	2:B:123:LEU:C	2.35	0.51
2:B:168:LYS:HB3	2:B:203:GLN:HB3	1.92	0.51
1:A:24:ARG:NE	4:A:520:HOH:O	1.91	0.51
1:A:117:ARG:CG	1:A:117:ARG:NH1	2.67	0.51
2:B:47:PHE:CD2	2:B:48:ILE:HG13	2.46	0.51
2:B:86:SER:HB2	2:B:323:TYR:HE1	1.72	0.51
2:B:311:GLU:O	2:B:314:ALA:HB3	2.11	0.51
1:A:214:TYR:CD2	1:A:260:TYR:HA	2.46	0.51
1:A:254:THR:HG23	4:A:527:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:ASP:OD2	2:B:163:VAL:CG2	2.59	0.51
1:A:88:LYS:O	1:A:92:GLY:CA	2.58	0.51
2:B:22:THR:C	2:B:27:ARG:NH1	2.62	0.51
2:B:264:LEU:C	2:B:264:LEU:HD12	2.36	0.51
1:A:248:TRP:CD1	1:A:248:TRP:H	2.29	0.50
1:A:285:ASP:C	1:A:287:PHE:N	2.69	0.50
1:A:170:ASN:CA	1:A:209:ASN:HD21	2.22	0.50
2:B:93:TYR:CE1	2:B:283:LYS:HG3	2.45	0.50
2:B:134:TYR:CG	2:B:199:SER:HB3	2.44	0.50
2:B:195:ILE:HD12	2:B:226:MET:SD	2.51	0.50
2:B:394:VAL:HG22	2:B:396:ILE:HD13	1.93	0.50
1:A:14:ARG:HE	1:A:14:ARG:HA	1.75	0.50
1:A:179:GLY:HA2	1:A:182:GLU:OE2	2.11	0.50
1:A:217:ALA:O	1:A:221:ASP:CA	2.59	0.50
2:B:196:THR:H	2:B:230:ARG:HB2	1.76	0.50
1:A:307:TYR:O	1:A:308:GLY:C	2.54	0.50
2:B:450:LYS:HD3	2:B:470:GLU:OE2	2.05	0.50
2:B:9:GLU:HA	2:B:333:TYR:CD1	2.47	0.50
1:A:425:ALA:O	2:B:13:ILE:HB	2.11	0.50
2:B:22:THR:HG21	2:B:27:ARG:HD3	1.90	0.50
2:B:367:LEU:HD11	2:B:443:LYS:HB2	1.94	0.50
1:A:77:SER:H	1:A:306:THR:CG2	2.25	0.50
2:B:230:ARG:HG3	2:B:358:HIS:HE1	1.76	0.50
1:A:8:PRO:CG	2:B:21:ARG:HH22	2.25	0.50
1:A:38:PRO:HG2	1:A:382:ALA:HB1	1.93	0.50
1:A:214:TYR:CB	1:A:260:TYR:HB3	2.42	0.50
2:B:51:LEU:HB2	2:B:392:ARG:HD2	1.92	0.50
1:A:34:SER:HB3	1:A:41:LEU:CD1	2.42	0.49
2:B:97:ILE:O	2:B:97:ILE:HG22	2.11	0.49
1:A:83:LEU:CD2	1:A:315:MET:HG2	2.42	0.49
1:A:93:TYR:CD2	1:A:283:LYS:HA	2.47	0.49
2:B:361:PHE:CE1	2:B:419:ARG:CB	2.95	0.49
1:A:359:ALA:HB3	1:A:361:PHE:HE2	1.76	0.49
1:A:434:PHE:O	1:A:437:GLU:HB3	2.13	0.49
2:B:161:THR:HG23	2:B:354:GLN:HE22	1.77	0.49
2:B:220:TYR:N	2:B:220:TYR:HD1	2.09	0.49
1:A:9:GLU:HA	1:A:333:TYR:CD1	2.46	0.49
1:A:153:VAL:HG23	1:A:153:VAL:O	2.12	0.49
1:A:346:GLU:O	1:A:349:GLY:N	2.43	0.49
2:B:269:LYS:HA	2:B:274:VAL:O	2.12	0.49
2:B:328:LEU:O	2:B:329:ASP:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:440:LYS:O	2:B:441:HIS:C	2.55	0.49
1:A:110:ILE:N	1:A:111:PRO:HD2	2.27	0.49
1:A:242:GLU:HG2	1:A:245:TYR:CD2	2.48	0.49
1:A:395:GLU:O	1:A:396:ILE:C	2.55	0.49
1:A:251:GLU:O	1:A:254:THR:HB	2.12	0.49
2:B:126:SER:OG	2:B:127:LYS:HE2	2.13	0.49
2:B:191:ILE:HD12	2:B:222:ILE:HG21	1.93	0.49
1:A:365:GLY:O	1:A:369:PRO:CA	2.61	0.49
2:B:110:ILE:HD12	4:B:658:HOH:O	2.12	0.49
2:B:327:ASN:ND2	2:B:330:TRP:HB3	2.27	0.49
1:A:31:ILE:HG23	1:A:32:ILE:N	2.27	0.49
1:A:47:PHE:CD2	1:A:48:ILE:HG13	2.47	0.49
1:A:432:MET:HE2	1:A:432:MET:N	2.26	0.49
2:B:361:PHE:HA	4:B:633:HOH:O	2.12	0.49
1:A:114:ILE:CG2	1:A:125:ARG:HH12	2.20	0.49
1:A:210:LEU:O	1:A:213:MET:HE3	2.13	0.49
1:A:219:LYS:C	1:A:221:ASP:H	2.19	0.49
1:A:284:ASP:OD1	1:A:286:SER:OG	2.21	0.49
2:B:95:TYR:HB2	2:B:282:MET:HB2	1.95	0.49
2:B:358:HIS:CE1	4:B:616:HOH:O	2.65	0.49
2:B:432:MET:HE2	2:B:435:ILE:CD1	2.42	0.49
1:A:52:THR:OG1	1:A:53:ASP:N	2.44	0.49
1:A:118:GLU:HA	1:A:123:LEU:H	1.78	0.49
1:A:368:LEU:HB2	1:A:371:ILE:HD13	1.94	0.49
2:B:168:LYS:HB3	2:B:203:GLN:HG3	1.94	0.49
2:B:375:GLN:CD	2:B:471:VAL:CB	2.59	0.49
1:A:134:TYR:HA	1:A:152:ASN:OD1	2.12	0.48
2:B:216:ILE:O	2:B:216:ILE:CG2	2.60	0.48
2:B:378:ALA:HB1	2:B:395:GLU:HG3	1.88	0.48
2:B:453:THR:HG22	2:B:469:LYS:HG3	1.94	0.48
1:A:288:PHE:O	1:A:289:ASP:C	2.56	0.48
2:B:358:HIS:O	2:B:421:THR:HG22	2.13	0.48
2:B:26:TYR:C	2:B:28:GLU:H	2.22	0.48
1:A:95:TYR:O	1:A:281:CYS:HA	2.14	0.48
1:A:263:MET:HB2	1:A:281:CYS:O	2.14	0.48
1:A:340:TYR:OH	1:A:429:GLN:NE2	2.39	0.48
1:A:424:ARG:O	1:A:426:THR:N	2.46	0.48
2:B:468:LEU:HD12	2:B:468:LEU:N	2.28	0.48
1:A:13:ILE:HD13	2:B:13:ILE:HD13	1.96	0.48
2:B:83:LEU:HD11	2:B:318:LEU:HG	1.96	0.48
2:B:107:GLN:HA	4:B:658:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:GLY:O	1:A:369:PRO:HA	2.14	0.48
1:A:18:PRO:HA	2:B:11:PHE:HB3	1.96	0.48
1:A:307:TYR:HB2	1:A:310:LEU:O	2.13	0.48
2:B:80:TYR:N	2:B:315:MET:CE	2.77	0.48
2:B:360:ALA:HB3	2:B:420:LEU:HB2	1.95	0.48
1:A:55:GLY:H	1:A:269:LYS:CB	2.26	0.48
1:A:90:ILE:CG1	1:A:323:TYR:CE2	2.97	0.48
1:A:291:TYR:O	1:A:292:THR:C	2.56	0.48
1:A:369:PRO:HA	4:A:515:HOH:O	2.13	0.48
2:B:285:ASP:C	2:B:287:PHE:N	2.65	0.48
1:A:240:GLN:HG3	1:A:241:ARG:HG3	1.95	0.48
1:A:315:MET:O	1:A:316:GLU:C	2.57	0.48
1:A:327:ASN:HD22	1:A:330:TRP:HB3	1.78	0.48
2:B:439:PHE:HA	2:B:442:VAL:CG2	2.44	0.48
1:A:369:PRO:HD2	4:A:526:HOH:O	2.14	0.47
2:B:181:GLU:O	2:B:182:GLU:C	2.53	0.47
1:A:26:TYR:CD1	1:A:26:TYR:C	2.88	0.47
2:B:230:ARG:CG	4:B:616:HOH:O	2.62	0.47
2:B:396:ILE:HG22	2:B:396:ILE:O	2.14	0.47
2:B:233:GLU:O	2:B:234:ASN:C	2.57	0.47
1:A:24:ARG:H	1:A:24:ARG:HG2	1.37	0.47
1:A:77:SER:O	1:A:80:TYR:HB3	2.15	0.47
2:B:28:GLU:HA	2:B:31:ILE:HG22	1.96	0.47
2:B:224:VAL:HG12	2:B:261:ALA:CA	2.42	0.47
2:B:239:LYS:CD	2:B:248:TRP:O	2.61	0.47
1:A:9:GLU:OE2	1:A:333:TYR:CZ	2.68	0.47
2:B:285:ASP:C	2:B:287:PHE:H	2.22	0.47
1:A:159:PHE:C	1:A:353:GLN:HE22	2.23	0.47
1:A:84:ALA:HA	1:A:96:THR:HG21	1.97	0.47
1:A:149:THR:HG22	1:A:150:VAL:N	2.30	0.47
1:A:167:PHE:O	1:A:170:ASN:ND2	2.48	0.47
1:A:248:TRP:CD1	1:A:248:TRP:N	2.83	0.47
1:A:449:ILE:HG22	1:A:450:LYS:N	2.29	0.47
2:B:32:ILE:HG22	2:B:33:LYS:N	2.30	0.47
2:B:242:GLU:O	2:B:243:ALA:C	2.58	0.47
2:B:427:TYR:HB3	2:B:431:HIS:CB	2.44	0.47
1:A:424:ARG:O	1:A:425:ALA:C	2.55	0.47
2:B:79:SER:O	2:B:80:TYR:C	2.58	0.47
2:B:174:GLU:O	2:B:177:GLU:HB2	2.14	0.47
2:B:439:PHE:HA	2:B:442:VAL:HG23	1.97	0.47
1:A:237:PHE:O	1:A:238:ILE:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ALA:CB	1:A:274:VAL:HG21	2.44	0.47
2:B:432:MET:HA	2:B:435:ILE:CD1	2.44	0.47
1:A:60:THR:O	1:A:61:GLN:C	2.58	0.46
1:A:90:ILE:HG13	1:A:323:TYR:CE2	2.50	0.46
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.54	0.46
1:A:144:GLN:OE1	1:A:149:THR:HG23	2.15	0.46
1:A:290:VAL:HG12	1:A:291:TYR:N	2.30	0.46
1:A:328:LEU:O	1:A:329:ASP:C	2.58	0.46
2:B:90:ILE:HD11	2:B:323:TYR:CD2	2.50	0.46
2:B:432:MET:HE2	2:B:435:ILE:HD13	1.97	0.46
1:A:24:ARG:NE	4:A:511:HOH:O	2.46	0.46
1:A:338:VAL:HB	4:A:514:HOH:O	2.16	0.46
2:B:80:TYR:H	2:B:315:MET:CE	2.28	0.46
2:B:201:GLY:O	2:B:356:GLY:C	2.58	0.46
2:B:262:ASP:CB	2:B:287:PHE:CE2	2.97	0.46
2:B:361:PHE:CE1	2:B:419:ARG:CG	2.98	0.46
2:B:63:MET:HE1	2:B:273:MET:CB	2.41	0.46
1:A:32:ILE:CA	1:A:36:MET:CE	2.84	0.46
2:B:6:HIS:HB2	2:B:340:TYR:CE1	2.51	0.46
2:B:230:ARG:HA	2:B:271:ASP:OD2	2.15	0.46
1:A:24:ARG:NH1	4:A:511:HOH:O	2.47	0.46
1:A:114:ILE:CG2	1:A:125:ARG:NH1	2.76	0.46
1:A:117:ARG:HG3	1:A:117:ARG:NH1	2.09	0.46
1:A:135:PHE:CE2	1:A:150:VAL:HG11	2.50	0.46
1:A:171:PHE:H	1:A:209:ASN:ND2	2.09	0.46
2:B:249:THR:HG23	2:B:252:GLN:OE1	2.16	0.46
2:B:251:GLU:CG	2:B:326:MET:HE3	2.38	0.46
2:B:330:TRP:O	2:B:333:TYR:HB3	2.14	0.46
1:A:248:TRP:HB2	1:A:253:ILE:HD11	1.98	0.46
1:A:440:LYS:O	1:A:441:HIS:C	2.58	0.46
2:B:242:GLU:HB3	2:B:245:TYR:HD1	1.81	0.46
2:B:341:LEU:HD13	2:B:432:MET:SD	2.56	0.46
2:B:418:LEU:C	2:B:418:LEU:HD13	2.41	0.46
2:B:429:GLN:O	2:B:430:THR:C	2.57	0.46
2:B:54:SER:O	2:B:56:THR:HG23	2.16	0.46
2:B:93:TYR:N	2:B:93:TYR:CD1	2.83	0.46
2:B:381:LEU:HD23	2:B:418:LEU:HG	1.98	0.46
1:A:361:PHE:N	1:A:361:PHE:HD2	2.12	0.46
2:B:50:LEU:HD12	2:B:420:LEU:CD2	2.44	0.46
2:B:65:ALA:O	2:B:66:ALA:C	2.55	0.46
2:B:93:TYR:N	2:B:93:TYR:HD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:SER:C	2:B:217:ALA:H	2.24	0.46
2:B:436:ILE:O	2:B:439:PHE:HB2	2.15	0.46
1:A:24:ARG:CD	4:A:511:HOH:O	2.61	0.45
1:A:26:TYR:OH	1:A:45:ASP:OD1	2.23	0.45
1:A:38:PRO:HD3	1:A:379:GLN:HE22	1.81	0.45
1:A:253:ILE:O	1:A:257:THR:OG1	2.29	0.45
1:A:384:GLU:O	1:A:385:LEU:C	2.58	0.45
1:A:429:GLN:O	1:A:432:MET:N	2.49	0.45
2:B:28:GLU:C	2:B:30:ALA:N	2.66	0.45
2:B:123:LEU:HD23	2:B:124:ASP:N	2.31	0.45
2:B:427:TYR:HB3	2:B:431:HIS:HB2	1.98	0.45
1:A:89:ASN:OD1	1:A:89:ASN:N	2.45	0.45
1:A:200:ALA:C	1:A:203:GLN:HE21	2.18	0.45
1:A:369:PRO:C	1:A:371:ILE:H	2.24	0.45
2:B:376:PHE:HA	2:B:377:PRO:HD3	1.83	0.45
1:A:143:SER:C	1:A:148:CYS:O	2.59	0.45
1:A:155:ILE:O	1:A:156:LYS:C	2.59	0.45
2:B:367:LEU:O	2:B:368:LEU:HD23	2.16	0.45
1:A:224:VAL:O	1:A:261:ALA:HB1	2.17	0.45
2:B:172:ASP:O	2:B:173:LEU:C	2.58	0.45
1:A:31:ILE:O	1:A:36:MET:HE2	2.16	0.45
1:A:101:GLN:OE1	1:A:103:ARG:HD2	2.17	0.45
1:A:149:THR:HG22	1:A:150:VAL:H	1.81	0.45
1:A:322:LEU:HD23	1:A:322:LEU:HA	1.74	0.45
1:A:371:ILE:HG22	1:A:377:PRO:CG	2.47	0.45
2:B:239:LYS:HB2	2:B:253:ILE:HD11	1.98	0.45
1:A:159:PHE:N	1:A:159:PHE:CD1	2.85	0.45
2:B:40:LEU:HD12	2:B:464:PHE:O	2.16	0.45
2:B:157:GLU:O	2:B:158:ALA:C	2.60	0.45
2:B:196:THR:CG2	2:B:197:SER:N	2.79	0.45
2:B:196:THR:HG21	2:B:203:GLN:C	2.41	0.45
1:A:427:TYR:HB3	1:A:431:HIS:ND1	2.32	0.45
2:B:234:ASN:O	2:B:235:ALA:C	2.57	0.45
1:A:19:VAL:HG12	2:B:11:PHE:CA	2.41	0.45
1:A:72:GLU:CA	4:A:538:HOH:O	2.59	0.45
1:A:246:LYS:O	1:A:246:LYS:HG2	2.17	0.45
1:A:448:ASN:ND2	1:A:448:ASN:H	2.15	0.45
2:B:22:THR:CG2	2:B:27:ARG:CZ	2.77	0.45
2:B:160:ASP:OD2	2:B:163:VAL:HG23	2.17	0.45
2:B:169:GLY:C	4:B:656:HOH:O	2.59	0.45
2:B:214:TYR:CD1	2:B:224:VAL:HG21	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:226:MET:HG2	2:B:258:TYR:CE1	2.52	0.45
1:A:55:GLY:CA	1:A:269:LYS:HB3	2.47	0.45
1:A:69:ARG:O	1:A:316:GLU:HG3	2.17	0.45
1:A:95:TYR:HB2	1:A:282:MET:HB2	1.99	0.45
1:A:271:ASP:O	1:A:273:MET:HG2	2.16	0.45
2:B:383:CYS:O	2:B:387:LYS:HG3	2.16	0.45
2:B:450:LYS:HB3	2:B:470:GLU:OE2	2.10	0.45
2:B:118:GLU:OE2	2:B:125:ARG:NH2	2.49	0.44
2:B:207:LEU:HD13	2:B:245:TYR:CE2	2.52	0.44
2:B:256:GLU:HA	2:B:259:LYS:HE3	1.99	0.44
1:A:21:ARG:HG3	4:A:534:HOH:O	2.17	0.44
1:A:136:PHE:HD2	1:A:138:THR:OG1	1.99	0.44
1:A:323:TYR:O	1:A:324:ASP:C	2.60	0.44
2:B:327:ASN:HD22	2:B:327:ASN:C	2.25	0.44
2:B:413:CYS:SG	2:B:413:CYS:O	2.75	0.44
1:A:155:ILE:O	1:A:158:ALA:HB2	2.18	0.44
1:A:326:MET:O	1:A:327:ASN:C	2.55	0.44
1:A:394:VAL:O	1:A:418:LEU:HD12	2.17	0.44
2:B:102:GLY:O	2:B:103:ARG:C	2.60	0.44
2:B:230:ARG:HD3	2:B:424:ARG:HH22	1.82	0.44
2:B:333:TYR:CD2	2:B:333:TYR:C	2.94	0.44
1:A:248:TRP:HB2	1:A:253:ILE:CD1	2.48	0.44
2:B:445:ASN:OD1	2:B:448:ASN:CG	2.60	0.44
2:B:452:LEU:HB3	2:B:468:LEU:HB3	1.98	0.44
2:B:7:LEU:HD12	2:B:336:ALA:HB2	1.98	0.44
2:B:93:TYR:CG	2:B:283:LYS:HA	2.53	0.44
2:B:317:ARG:O	2:B:320:VAL:N	2.37	0.44
2:B:452:LEU:C	2:B:469:LYS:O	2.61	0.44
1:A:307:TYR:HD1	1:A:307:TYR:C	2.25	0.44
2:B:83:LEU:CD1	2:B:318:LEU:HG	2.47	0.44
2:B:210:LEU:HD23	2:B:210:LEU:HA	1.59	0.44
2:B:230:ARG:HG3	4:B:616:HOH:O	2.17	0.44
1:A:200:ALA:CB	1:A:203:GLN:CB	2.96	0.44
1:A:307:TYR:C	1:A:307:TYR:CD1	2.96	0.44
1:A:436:ILE:H	1:A:436:ILE:HG13	1.72	0.44
2:B:6:HIS:HE1	2:B:337:GLN:CG	2.30	0.44
2:B:133:ASN:ND2	2:B:134:TYR:H	2.16	0.44
2:B:368:LEU:HB3	2:B:371:ILE:HD11	1.93	0.44
1:A:33:LYS:HB2	1:A:33:LYS:HE3	1.74	0.44
2:B:117:ARG:NE	2:B:188:VAL:O	2.51	0.44
2:B:169:GLY:O	2:B:205:VAL:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:PHE:CG	2:B:213:MET:HG3	2.53	0.44
2:B:211:LYS:HD3	2:B:260:TYR:CZ	2.53	0.44
2:B:227:ASP:C	2:B:227:ASP:OD1	2.61	0.44
1:A:6:HIS:CE1	1:A:429:GLN:HA	2.53	0.44
1:A:188:VAL:CG1	1:A:222:ILE:HD13	2.48	0.44
1:A:232:ALA:HB1	1:A:331:LEU:HD21	2.00	0.44
2:B:116:LYS:O	2:B:120:GLU:HG3	2.18	0.44
1:A:167:PHE:HE2	1:A:238:ILE:HG12	1.82	0.43
2:B:26:TYR:C	2:B:28:GLU:N	2.76	0.43
2:B:33:LYS:C	2:B:35:GLY:H	2.25	0.43
2:B:211:LYS:O	2:B:212:ALA:C	2.59	0.43
2:B:274:VAL:HA	2:B:275:PRO:HD3	1.73	0.43
2:B:339:GLN:O	2:B:341:LEU:N	2.51	0.43
2:B:379:GLN:O	2:B:382:ALA:HB3	2.18	0.43
2:B:384:GLU:OE1	2:B:387:LYS:CE	2.64	0.43
2:B:445:ASN:OD1	2:B:448:ASN:OD1	2.36	0.43
1:A:13:ILE:HG23	2:B:13:ILE:HG23	2.00	0.43
1:A:124:ASP:CB	1:A:187:ASN:HD21	2.28	0.43
1:A:194:THR:C	1:A:195:ILE:CG2	2.91	0.43
1:A:329:ASP:O	1:A:332:ALA:HB3	2.17	0.43
1:A:340:TYR:CD2	1:A:340:TYR:O	2.71	0.43
2:B:50:LEU:CD1	2:B:421:THR:H	2.28	0.43
2:B:359:ALA:CB	2:B:419:ARG:HD2	2.48	0.43
1:A:129:VAL:O	1:A:188:VAL:HA	2.19	0.43
1:A:430:THR:O	1:A:431:HIS:C	2.60	0.43
2:B:440:LYS:O	2:B:443:LYS:N	2.51	0.43
1:A:46:VAL:HG11	1:A:49:ASP:HB2	1.99	0.43
1:A:371:ILE:HG22	1:A:377:PRO:CB	2.49	0.43
2:B:334:ARG:C	2:B:334:ARG:HD3	2.42	0.43
1:A:251:GLU:HB2	4:A:533:HOH:O	2.18	0.43
1:A:264:LEU:C	1:A:264:LEU:HD12	2.43	0.43
1:A:307:TYR:CD1	1:A:308:GLY:N	2.86	0.43
1:A:437:GLU:OE1	1:A:437:GLU:CA	2.56	0.43
1:A:181:GLU:O	1:A:183:VAL:N	2.51	0.43
2:B:199:SER:C	4:B:623:HOH:O	2.46	0.43
2:B:123:LEU:HD23	2:B:124:ASP:C	2.44	0.43
2:B:196:THR:HG22	2:B:203:GLN:O	2.17	0.43
2:B:225:VAL:HA	2:B:263:MET:O	2.19	0.43
2:B:287:PHE:HA	4:B:650:HOH:O	2.17	0.43
2:B:297:LEU:HD12	2:B:297:LEU:HA	1.55	0.43
2:B:334:ARG:O	2:B:338:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:THR:HB	2:B:471:VAL:HG22	2.00	0.43
1:A:7:LEU:HD12	1:A:336:ALA:CB	2.48	0.43
1:A:352:CYS:HB2	1:A:361:PHE:O	2.16	0.43
1:A:382:ALA:O	1:A:383:CYS:C	2.62	0.43
2:B:437:GLU:HA	2:B:437:GLU:OE1	2.18	0.43
1:A:77:SER:O	1:A:78:ARG:C	2.61	0.43
1:A:161:THR:HG23	1:A:353:GLN:CD	2.37	0.43
1:A:251:GLU:HG3	4:A:533:HOH:O	2.17	0.43
2:B:102:GLY:CA	2:B:267:SER:HB2	2.49	0.43
2:B:174:GLU:O	2:B:175:GLY:C	2.61	0.43
2:B:199:SER:O	2:B:200:ALA:C	2.61	0.43
2:B:279:LEU:HD23	2:B:279:LEU:HA	1.76	0.43
2:B:397:GLY:O	2:B:398:SER:C	2.62	0.43
2:B:450:LYS:HD2	2:B:470:GLU:CD	2.44	0.43
1:A:71:ASP:HB2	1:A:78:ARG:HD3	2.00	0.42
1:A:133:ASN:ND2	1:A:133:ASN:N	2.52	0.42
1:A:245:TYR:HD1	1:A:248:TRP:CE2	2.37	0.42
2:B:372:PRO:CD	2:B:375:GLN:HB2	2.23	0.42
1:A:346:GLU:HA	1:A:346:GLU:OE1	2.19	0.42
2:B:16:ILE:O	2:B:16:ILE:HG13	2.19	0.42
2:B:72:GLU:HG3	4:B:611:HOH:O	2.19	0.42
1:A:36:MET:CE	1:A:36:MET:CA	2.73	0.42
1:A:160:ASP:C	1:A:162:GLY:H	2.27	0.42
1:A:371:ILE:HG22	1:A:377:PRO:HG3	2.02	0.42
2:B:177:GLU:HA	2:B:177:GLU:OE1	2.19	0.42
2:B:361:PHE:CZ	2:B:419:ARG:HD3	2.53	0.42
1:A:13:ILE:CD1	2:B:13:ILE:HD13	2.50	0.42
1:A:110:ILE:HB	1:A:111:PRO:CD	2.50	0.42
1:A:334:ARG:C	1:A:334:ARG:CD	2.93	0.42
2:B:67:MET:HE2	2:B:317:ARG:NH1	2.33	0.42
2:B:327:ASN:HD21	2:B:329:ASP:HB2	1.85	0.42
1:A:32:ILE:N	1:A:36:MET:HE1	2.33	0.42
1:A:38:PRO:O	1:A:41:LEU:N	2.49	0.42
2:B:48:ILE:HD11	2:B:431:HIS:CD2	2.49	0.42
2:B:198:ASN:CB	4:B:627:HOH:O	2.25	0.42
2:B:197:SER:O	2:B:202:GLY:HA2	2.20	0.42
1:A:98:PRO:HD2	1:A:305:PRO:O	2.19	0.42
2:B:418:LEU:C	2:B:418:LEU:CD1	2.93	0.42
1:A:77:SER:H	1:A:306:THR:HG23	1.84	0.42
1:A:90:ILE:CD1	1:A:323:TYR:CE2	3.01	0.42
1:A:100:HIS:O	1:A:277:GLY:CA	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PHE:O	1:A:140:GLN:HG2	2.18	0.42
1:A:339:GLN:O	1:A:342:VAL:N	2.52	0.42
2:B:110:ILE:N	2:B:111:PRO:HD2	2.34	0.42
2:B:354:GLN:HB3	4:B:619:HOH:O	2.19	0.42
1:A:28:GLU:O	1:A:29:GLU:C	2.63	0.42
1:A:290:VAL:O	1:A:291:TYR:C	2.63	0.42
2:B:165:TYR:HD1	2:B:166:ASP:H	1.68	0.42
1:A:235:ALA:O	1:A:236:TYR:C	2.62	0.42
2:B:436:ILE:O	2:B:439:PHE:N	2.53	0.42
1:A:72:GLU:C	4:A:538:HOH:O	2.63	0.41
1:A:93:TYR:CD2	1:A:283:LYS:N	2.88	0.41
1:A:12:ARG:NH1	2:B:49:ASP:HB2	2.35	0.41
1:A:219:LYS:C	1:A:221:ASP:N	2.78	0.41
1:A:368:LEU:HA	1:A:369:PRO:HD3	1.54	0.41
2:B:195:ILE:HG23	2:B:234:ASN:CB	2.50	0.41
2:B:260:TYR:CD2	2:B:260:TYR:N	2.87	0.41
1:A:61:GLN:O	1:A:62:SER:C	2.63	0.41
1:A:214:TYR:CD2	1:A:260:TYR:HD1	2.30	0.41
1:A:268:ALA:O	1:A:274:VAL:CG2	2.63	0.41
2:B:99:THR:OG1	2:B:278:GLY:CA	2.64	0.41
2:B:372:PRO:HD2	2:B:375:GLN:OE1	2.19	0.41
1:A:26:TYR:CD1	1:A:26:TYR:O	2.73	0.41
1:A:123:LEU:HD23	1:A:123:LEU:C	2.46	0.41
2:B:375:GLN:HG3	2:B:471:VAL:HG21	1.92	0.41
2:B:445:ASN:O	2:B:446:ALA:C	2.64	0.41
2:B:168:LYS:HB3	2:B:203:GLN:CB	2.50	0.41
2:B:429:GLN:O	2:B:432:MET:N	2.54	0.41
1:A:107:GLN:HB2	1:A:301:GLN:OE1	2.20	0.41
1:A:279:LEU:HA	1:A:279:LEU:HD23	1.43	0.41
1:A:284:ASP:C	1:A:286:SER:N	2.78	0.41
1:A:328:LEU:HB3	1:A:329:ASP:H	1.59	0.41
1:A:453:THR:HB	4:A:508:HOH:O	2.20	0.41
1:A:272:ALA:C	1:A:273:MET:HG2	2.45	0.41
2:B:188:VAL:HA	2:B:189:PRO:HD3	1.76	0.41
2:B:230:ARG:C	2:B:271:ASP:OD2	2.63	0.41
1:A:12:ARG:NH2	2:B:46:VAL:O	2.54	0.41
1:A:128:MET:HG3	1:A:148:CYS:HB2	2.02	0.41
1:A:201:GLY:HA2	1:A:361:PHE:CE2	2.56	0.41
1:A:386:TYR:HA	1:A:391:ILE:O	2.21	0.41
2:B:21:ARG:HD3	2:B:21:ARG:HA	1.97	0.41
2:B:50:LEU:HD22	2:B:50:LEU:HA	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:501:SO4:O1	4:B:602:HOH:O	2.22	0.41
1:A:81:TYR:O	1:A:85:GLU:HB2	2.21	0.41
1:A:318:LEU:HD12	1:A:322:LEU:HG	2.02	0.41
2:B:77:SER:O	2:B:78:ARG:C	2.61	0.41
2:B:109:TYR:CD1	2:B:109:TYR:C	2.99	0.41
2:B:128:MET:HA	2:B:187:ASN:HB3	2.03	0.41
2:B:364:ALA:O	2:B:368:LEU:N	2.54	0.41
1:A:21:ARG:O	1:A:22:THR:HG23	2.21	0.40
1:A:174:GLU:HA	1:A:177:GLU:HB2	2.03	0.40
1:A:181:GLU:O	1:A:182:GLU:C	2.63	0.40
1:A:337:GLN:O	1:A:338:VAL:C	2.63	0.40
2:B:81:TYR:O	2:B:82:ALA:C	2.64	0.40
2:B:97:ILE:HG21	2:B:97:ILE:HD13	1.56	0.40
2:B:112:VAL:HG11	2:B:290:VAL:HG13	2.03	0.40
2:B:168:LYS:HB3	2:B:203:GLN:CG	2.51	0.40
2:B:359:ALA:HB1	2:B:419:ARG:HD2	2.03	0.40
1:A:47:PHE:HB3	1:A:390:GLY:O	2.22	0.40
1:A:254:THR:O	1:A:257:THR:HB	2.21	0.40
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.65	0.40
2:B:395:GLU:CB	4:B:637:HOH:O	2.50	0.40
2:B:457:GLU:HA	2:B:458:PRO:HD3	1.97	0.40
1:A:38:PRO:O	1:A:41:LEU:CB	2.50	0.40
1:A:71:ASP:OD1	1:A:78:ARG:N	2.54	0.40
2:B:51:LEU:HD23	2:B:392:ARG:HD2	2.01	0.40
2:B:330:TRP:O	2:B:331:LEU:C	2.64	0.40
1:A:63:MET:O	1:A:66:ALA:HB3	2.21	0.40
1:A:304:PHE:HA	1:A:305:PRO:HD3	1.82	0.40
2:B:26:TYR:O	2:B:28:GLU:N	2.55	0.40
2:B:33:LYS:C	2:B:35:GLY:N	2.80	0.40
2:B:52:THR:OG1	2:B:53:ASP:N	2.53	0.40
2:B:120:GLU:HG3	2:B:120:GLU:H	1.52	0.40
2:B:364:ALA:O	2:B:368:LEU:HB2	2.22	0.40
1:A:269:LYS:HD2	1:A:275:PRO:O	2.22	0.40
2:B:115:LYS:O	2:B:116:LYS:C	2.64	0.40
2:B:458:PRO:HD2	2:B:462:ARG:HA	2.04	0.40

All (1) 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)
2:B:103:ARG:NH1	2:B:301:GLN:O[8_665]	2.16	0.04

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	430/467 (92%)	331 (77%)	81 (19%)	18 (4%)	2	16
2	B	425/467 (91%)	327 (77%)	83 (20%)	15 (4%)	3	20
All	All	855/934 (92%)	658 (77%)	164 (19%)	33 (4%)	2	18

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	LEU
2	B	246	LYS
1	A	157	GLU
1	A	238	ILE
2	B	243	ALA
2	B	425	ALA
2	B	446	ALA
1	A	158	ALA
1	A	182	GLU
1	A	329	ASP
1	A	378	ALA
1	A	425	ALA
1	A	443	LYS
2	B	340	TYR
1	A	324	ASP
1	A	336	ALA
1	A	447	ALA
2	B	27	ARG
2	B	30	ALA
1	A	221	ASP
1	A	322	LEU
1	A	369	PRO
1	A	382	ALA
1	A	441	HIS
2	B	25	ALA

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Mol	Chain	Res	Type
2	B	75	SER
2	B	103	ARG
2	B	118	GLU
2	B	244	GLU
2	B	414	PRO
2	B	216	ILE
1	A	377	PRO
2	B	204	PRO

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	356/385 (92%)	275 (77%)	81 (23%)	1	5
2	B	358/386 (93%)	284 (79%)	74 (21%)	1	7
All	All	714/771 (93%)	559 (78%)	155 (22%)	1	6

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	12	ARG
1	A	21	ARG
1	A	22	THR
1	A	23	THR
1	A	24	ARG
1	A	36	MET
1	A	41	LEU
1	A	43	SER
1	A	44	GLU
1	A	48	ILE
1	A	51	LEU
1	A	52	THR
1	A	78	ARG
1	A	85	GLU

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Mol	Chain	Res	Type
1	A	90	ILE
1	A	96	THR
1	A	108	ILE
1	A	114	ILE
1	A	117	ARG
1	A	120	GLU
1	A	121	LYS
1	A	123	LEU
1	A	133	ASN
1	A	134	TYR
1	A	139	THR
1	A	142	HIS
1	A	143	SER
1	A	144	GLN
1	A	145	ILE
1	A	146	ASN
1	A	159	PHE
1	A	160	ASP
1	A	174	GLU
1	A	177	GLU
1	A	192	VAL
1	A	195	ILE
1	A	206	SER
1	A	207	LEU
1	A	211	LYS
1	A	218	LYS
1	A	238	ILE
1	A	240	GLN
1	A	244	GLU
1	A	252	GLN
1	A	253	ILE
1	A	259	LYS
1	A	262	ASP
1	A	269	LYS
1	A	274	VAL
1	A	288	PHE
1	A	292	THR
1	A	297	LEU
1	A	307	TYR
1	A	315	MET
1	A	326	MET
1	A	327	ASN

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Mol	Chain	Res	Type
1	A	328	LEU
1	A	331	LEU
1	A	335	ILE
1	A	345	LEU
1	A	346	GLU
1	A	362	VAL
1	A	368	LEU
1	A	371	ILE
1	A	385	LEU
1	A	392	ARG
1	A	395	GLU
1	A	416	GLU
1	A	417	LEU
1	A	421	THR
1	A	422	ILE
1	A	429	GLN
1	A	430	THR
1	A	432	MET
1	A	436	ILE
1	A	444	GLU
1	A	448	ASN
1	A	450	LYS
1	A	452	LEU
1	A	454	PHE
2	B	13	ILE
2	B	18	PRO
2	B	28	GLU
2	B	32	ILE
2	B	33	LYS
2	B	34	SER
2	B	41	LEU
2	B	44	GLU
2	B	50	LEU
2	B	51	LEU
2	B	52	THR
2	B	54	SER
2	B	62	SER
2	B	64	GLN
2	B	68	MET
2	B	71	ASP
2	B	100	HIS
2	B	112	VAL

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Mol	Chain	Res	Type
2	B	117	ARG
2	B	120	GLU
2	B	123	LEU
2	B	127	LYS
2	B	129	VAL
2	B	133	ASN
2	B	153	VAL
2	B	154	TYR
2	B	155	ILE
2	B	168	LYS
2	B	183	VAL
2	B	191	ILE
2	B	192	VAL
2	B	194	THR
2	B	198	ASN
2	B	207	LEU
2	B	209	ASN
2	B	211	LYS
2	B	215	SER
2	B	218	LYS
2	B	220	TYR
2	B	222	ILE
2	B	228	SER
2	B	230	ARG
2	B	239	LYS
2	B	240	GLN
2	B	246	LYS
2	B	252	GLN
2	B	263	MET
2	B	264	LEU
2	B	267	SER
2	B	269	LYS
2	B	273	MET
2	B	276	MET
2	B	283	LYS
2	B	288	PHE
2	B	292	THR
2	B	293	GLU
2	B	300	VAL
2	B	301	GLN
2	B	302	GLU
2	B	327	ASN

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Mol	Chain	Res	Type
2	B	328	LEU
2	B	335	ILE
2	B	371	ILE
2	B	394	VAL
2	B	398	SER
2	B	417	LEU
2	B	418	LEU
2	B	421	THR
2	B	440	LYS
2	B	441	HIS
2	B	442	VAL
2	B	443	LYS
2	B	448	ASN
2	B	459	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	119	GLN
1	A	133	ASN
1	A	144	GLN
1	A	146	ASN
1	A	187	ASN
1	A	198	ASN
1	A	209	ASN
1	A	234	ASN
1	A	327	ASN
1	A	358	HIS
1	A	445	ASN
1	A	448	ASN
2	B	6	HIS
2	B	64	GLN
2	B	94	GLN
2	B	101	GLN
2	B	133	ASN
2	B	152	ASN
2	B	170	ASN
2	B	327	ASN
2	B	375	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	LLP	A	270	1	23,24,25	2.18	6 (26%)	25,32,34	2.52	7 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	270	1	-	4/16/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	LLP	O3-C3	-6.65	1.21	1.36
1	A	270	LLP	C4-C4'	3.31	1.53	1.46
1	A	270	LLP	C2-N1	3.17	1.39	1.33
1	A	270	LLP	C6-N1	2.91	1.40	1.34
1	A	270	LLP	C4'-NZ	2.67	1.36	1.27
1	A	270	LLP	CE-NZ	2.24	1.51	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	LLP	OP4-C5'-C5	7.27	122.98	109.36
1	A	270	LLP	C4-C3-C2	7.13	124.16	120.14
1	A	270	LLP	CE-NZ-C4'	-3.47	107.62	118.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	LLP	OP3-P-OP1	3.04	122.68	110.83
1	A	270	LLP	C3-C2-N1	-2.65	117.62	120.96
1	A	270	LLP	OP3-P-OP4	-2.10	101.19	106.67
1	A	270	LLP	CD-CG-CB	2.04	121.33	113.62

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	270	LLP	C4-C5-C5'-OP4
1	A	270	LLP	C6-C5-C5'-OP4
1	A	270	LLP	C4-C4'-NZ-CE
1	A	270	LLP	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	270	LLP	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	500	-	4,4,4	0.24	0	6,6,6	0.58	0
3	SO4	B	501	-	4,4,4	0.28	0	6,6,6	0.22	0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	SO4	1	0

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	434/467 (92%)	-0.55	1 (0%) 91 85	50, 82, 120, 126	0
2	B	433/467 (92%)	-0.39	4 (0%) 81 64	48, 82, 129, 170	0
All	All	867/934 (92%)	-0.47	5 (0%) 85 73	48, 82, 121, 170	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	302	GLU	3.3
1	A	377	PRO	2.4
2	B	468	LEU	2.2
2	B	471	VAL	2.1
2	B	395	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	270	24/25	0.96	0.08	63,73,78,80	0

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($\text{\AA}^2$)	Q<0.9
3	SO4	B	501	5/5	0.85	0.13	184,184,184,185	0
3	SO4	B	500	5/5	0.93	0.11	110,110,111,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.