



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 10:30 AM EDT

PDB ID : 1FRV / pdb_00001frv
Title : CRYSTAL STRUCTURE OF THE OXIDIZED FORM OF NI-FE HYDROGENASE
Authors : Volbeda, A.; Frey, M.; Fontecilla-Camps, J.C.
Deposited on : 1996-03-28
Resolution : 2.85 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

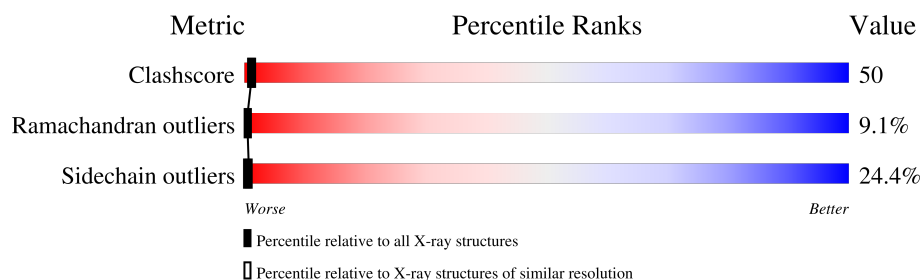
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	264	
1	C	264	
2	B	536	
2	D	536	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SF4	C	265	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12268 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.

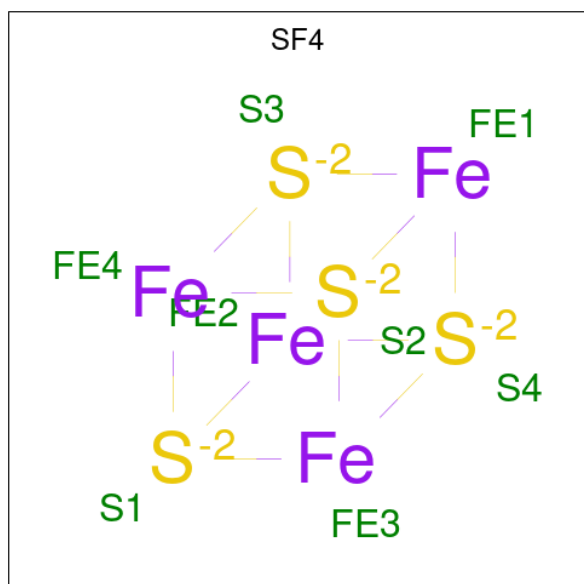
- Molecule 1 is a protein called HYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1961	1247	328	367	19			
1	C	262	Total	C	N	O	S	0	0	0
			1961	1247	328	367	19			

- Molecule 2 is a protein called HYDROGENASE.

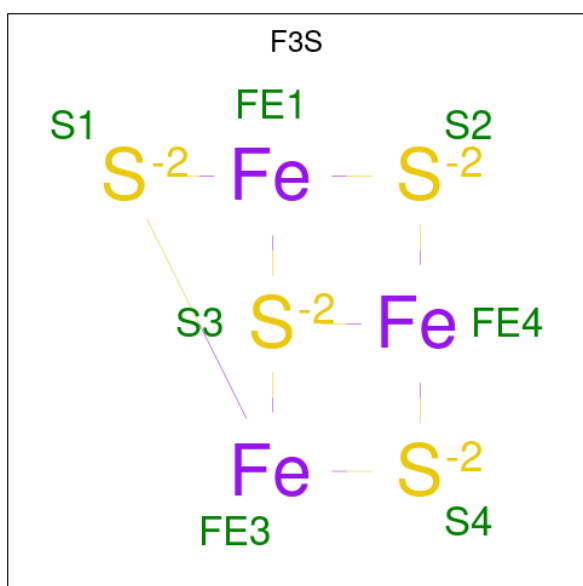
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			
2	D	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			

- Molecule 3 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	A	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		
3	C	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 4 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	C	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ni	0	0
			1	1		
5	D	1	Total	Ni	0	0
			1	1		

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Fe 1	0	0
6	D	1	Total 1	Fe 1	0	0

- Molecule 7 is water.

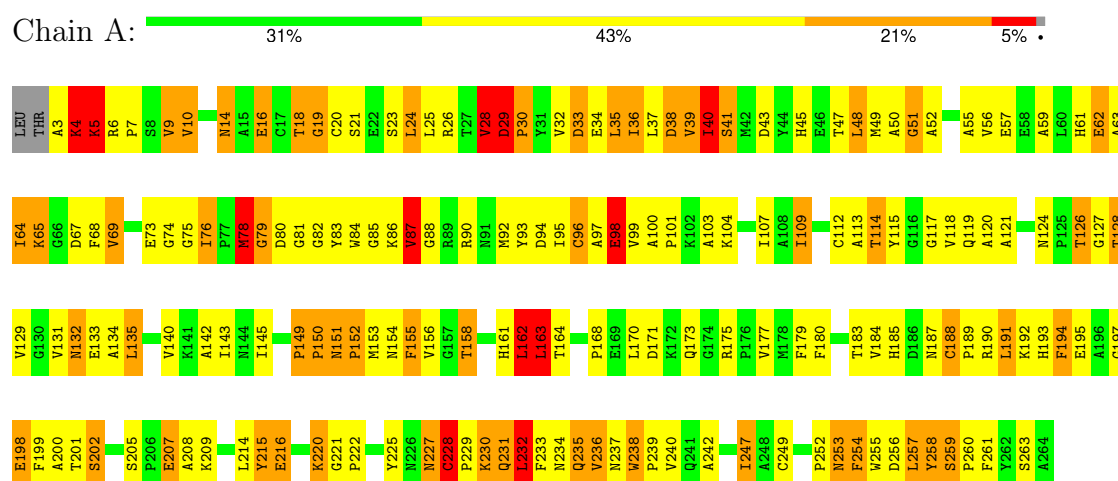
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total 3	O 3	0	0
7	D	3	Total 3	O 3	0	0

3 Residue-property plots

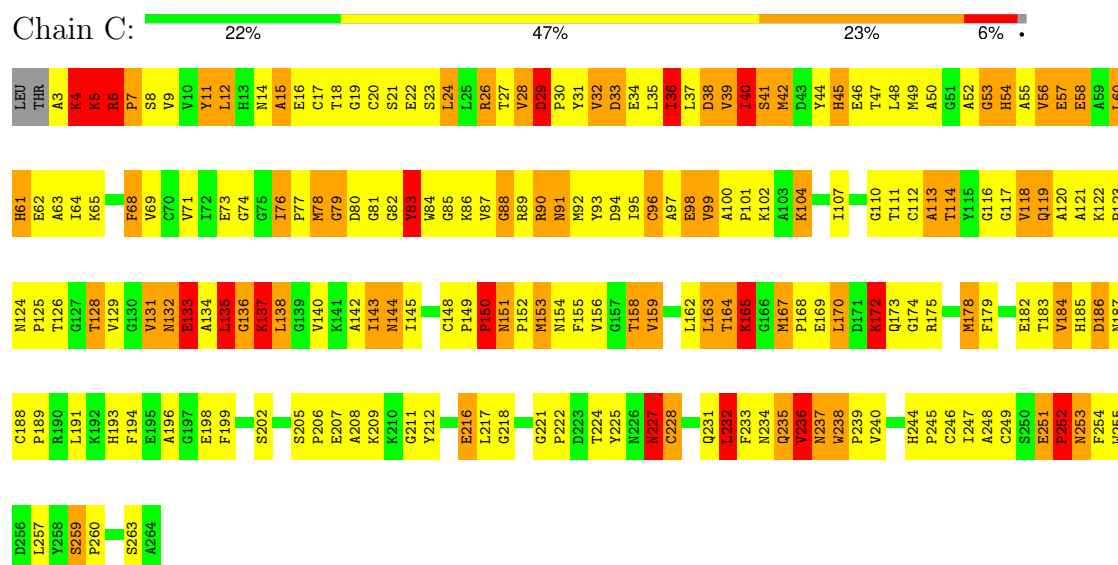
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: HYDROGENASE

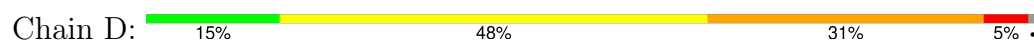


• Molecule 1: HYDROGENASE



• Molecule 2: HYDROGENASE





R497	R498	L499	S500	A501	S502	E503	S504	A505	L506	E507	S508	P509	P510	E511	A512	D513	P514	K515	R516	P517	S518	E519	I520	L521	R522	T523	V524	H525	S526	V527	D528	P529	C530	I531	A532	C533	G534	V535	H536																					
V436	A437	A438		D441	D442	L443	Y444	T445	D446	Y447	Q448	Y449	P450	T451	E452	S453	Q454	G455	V456	G457	F458	V459	M460	A461	P462	R463	G464	V465	L466	S467	H468	V469	L470	V471	Q472	R473	G474	G475	L476	L477	S478	N479	F480	Q481	H482	V483	V484	P485	S486	T487	H488	N489	L490	G491	P492	R493	C494	A495	F496	
V375	L376	V377	A378	S379	A380	K381	K382	H383	E384	P385	T386	V387	K388	A389	V390	D391	L392	V393	L394	K395	T396	L397	G398	V399	G400	P401	E402	A403	L404	F405	S406	T407	L408	G409	R410	T411	A412	A413	R414	G415	T416	Q417	C418	L419	T420	A421			E424	V425	E426	V427	N428	L429	D430	K431	L432	E433	A434	N435

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.60Å 93.90Å 69.20Å 89.80° 102.90° 90.80°	Depositor
Resolution (Å)	8.00 – 2.85	Depositor
% Data completeness (in resolution range)	85.3 (8.00-2.85)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12268	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: F3S, SF4, FE, NI

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	1.05	1/2014 (0.0%)	2.02	62/2738 (2.3%)
1	C	1.05	2/2014 (0.1%)	1.94	68/2738 (2.5%)
2	B	1.01	3/4251 (0.1%)	1.89	99/5782 (1.7%)
2	D	1.01	2/4251 (0.0%)	1.90	111/5782 (1.9%)
All	All	1.02	8/12530 (0.1%)	1.92	340/17040 (2.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	40	THR	CA-CB	7.32	1.60	1.53
2	D	491	GLY	N-CA	6.24	1.53	1.44
1	A	76	ILE	CA-CB	5.91	1.61	1.54
2	B	470	ILE	CA-CB	5.70	1.61	1.54
2	B	220	THR	CA-CB	5.41	1.61	1.53
1	C	76	ILE	CA-CB	5.37	1.61	1.54
1	C	164	THR	CA-CB	5.25	1.61	1.53
2	B	229	THR	CA-CB	5.18	1.61	1.54

All (340) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	348	PHE	CA-CB-CG	14.91	128.71	113.80
1	A	76	ILE	N-CA-C	13.23	123.66	108.05
1	A	185	HIS	CA-CB-CG	12.21	126.00	113.80
2	D	366	ALA	N-CA-C	12.08	125.60	111.71
1	A	99	VAL	N-CA-C	11.35	121.83	110.82
1	A	254	PHE	CA-CB-CG	11.34	125.14	113.80
2	B	40	THR	N-CA-C	11.15	127.22	113.17
2	B	67	VAL	N-CA-C	-10.96	100.12	110.42
2	D	365	GLU	CA-C-N	10.93	136.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	365	GLU	C-N-CA	10.93	136.02	120.28
2	B	312	ASP	CA-CB-CG	10.88	123.48	112.60
1	A	74	GLY	N-CA-C	10.87	138.94	113.18
2	D	34	ASN	CA-CB-CG	-10.81	101.79	112.60
2	B	64	ALA	N-CA-C	-10.63	99.70	111.07
2	D	382	LYS	N-CA-C	10.41	126.09	111.52
2	B	348	PHE	CA-CB-CG	9.53	123.33	113.80
2	B	225	VAL	N-CA-C	-9.51	97.41	109.30
1	A	179	PHE	CA-CB-CG	9.45	123.25	113.80
2	D	40	THR	N-CA-C	9.16	124.03	109.83
1	C	116	GLY	N-CA-C	-9.11	101.46	112.48
1	C	218	GLY	N-CA-C	9.06	128.21	115.43
1	C	164	THR	N-CA-C	9.02	120.80	110.97
1	C	199	PHE	CA-CB-CG	9.02	122.82	113.80
1	C	116	GLY	CA-C-O	-8.91	114.48	122.24
2	D	490	LEU	CA-C-O	-8.90	110.38	121.50
2	D	226	GLY	N-CA-C	-8.89	103.39	113.79
2	B	470	ILE	N-CA-C	8.85	121.01	108.36
2	B	77	VAL	N-CA-C	-8.69	101.87	110.30
1	A	215	TYR	CA-C-N	8.57	132.70	120.79
1	A	215	TYR	C-N-CA	8.57	132.70	120.79
2	D	312	ASP	CA-CB-CG	8.33	120.93	112.60
2	B	317	ASP	CA-CB-CG	8.19	120.79	112.60
1	A	171	ASP	CA-CB-CG	8.18	120.78	112.60
2	B	313	ASP	CA-CB-CG	8.09	120.69	112.60
2	B	114	HIS	N-CA-C	8.00	122.47	112.87
2	D	494	CYS	N-CA-C	-7.99	100.58	110.41
2	B	8	LYS	N-CA-C	7.91	122.59	109.46
2	B	63	ARG	CD-NE-CZ	7.91	135.47	124.40
1	C	81	GLY	N-CA-C	-7.78	105.10	115.21
1	C	82	GLY	N-CA-C	7.78	125.53	114.64
1	A	39	VAL	N-CA-C	7.77	117.76	111.62
2	D	207	ALA	CA-C-N	7.76	130.68	120.28
2	D	207	ALA	C-N-CA	7.76	130.68	120.28
2	D	165	GLY	N-CA-C	-7.75	102.39	114.10
2	D	67	VAL	N-CA-C	-7.73	105.16	111.81
2	D	379	TYR	N-CA-C	-7.62	102.57	111.03
1	A	30	PRO	N-CA-C	-7.61	98.11	110.74
2	B	214	GLY	N-CA-C	7.57	123.68	113.99
1	A	28	VAL	CA-C-O	-7.55	114.16	121.63
2	D	227	GLY	N-CA-C	7.55	131.07	113.18
1	A	150	PRO	N-CA-C	7.46	123.21	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	40	THR	N-CA-CB	-7.43	100.26	111.19
1	C	228	CYS	N-CA-C	7.40	123.67	113.16
2	B	365	GLU	CA-C-N	7.39	131.91	120.82
2	B	365	GLU	C-N-CA	7.39	131.91	120.82
2	D	100	MET	N-CA-C	-7.37	102.88	112.68
2	B	358	LYS	N-CA-C	-7.33	101.07	110.53
2	B	226	GLY	N-CA-C	-7.33	104.38	114.64
2	B	349	HIS	CA-CB-CG	-7.33	106.47	113.80
2	B	114	HIS	CA-CB-CG	-7.29	106.51	113.80
2	B	213	PHE	CA-C-N	7.26	133.23	120.74
2	B	213	PHE	C-N-CA	7.26	133.23	120.74
2	D	487	THR	N-CA-CB	7.21	121.13	110.53
1	C	89	ARG	N-CA-C	-7.21	102.56	113.51
2	D	59	HIS	CA-CB-CG	-7.18	106.62	113.80
1	A	230	LYS	N-CA-C	7.17	122.32	113.50
2	B	516	ARG	O-C-N	7.17	126.42	121.19
2	B	73	ALA	N-CA-C	-7.13	103.11	111.03
2	B	443	LEU	N-CA-C	-7.13	97.34	109.24
1	C	7	PRO	N-CA-C	7.10	121.52	110.80
2	D	67	VAL	CB-CA-C	7.10	119.72	111.55
2	D	467	SER	CA-CB-OG	7.07	125.24	111.10
1	C	165	LYS	N-CA-C	7.07	122.77	113.30
1	A	259	SER	O-C-N	-7.02	115.38	121.35
1	C	29	ASP	N-CA-C	-7.00	94.34	109.81
2	B	200	LEU	N-CA-C	-6.98	104.57	113.23
1	A	149	PRO	CA-C-N	6.93	127.08	119.87
1	A	149	PRO	C-N-CA	6.93	127.08	119.87
2	B	219	HIS	CA-C-N	6.91	131.30	121.42
2	B	219	HIS	C-N-CA	6.91	131.30	121.42
2	D	509	THR	O-C-N	6.88	127.42	121.30
2	B	225	VAL	CA-C-O	-6.85	113.23	121.04
1	A	238	TRP	CA-CB-CG	6.84	126.60	113.60
2	D	137	LEU	CB-CA-C	6.82	123.17	110.70
1	C	99	VAL	N-CA-C	6.80	116.93	110.53
2	D	209	ALA	N-CA-C	-6.78	103.89	111.28
1	C	259	SER	O-C-N	-6.75	116.28	121.55
2	D	332	ASP	CA-CB-CG	6.75	119.35	112.60
2	B	464	GLY	N-CA-C	6.73	120.34	111.52
2	D	166	GLN	N-CA-C	-6.73	105.07	113.55
1	C	5	LYS	N-CA-C	6.69	121.80	111.56
1	A	194	PHE	CA-CB-CG	-6.68	107.12	113.80
2	B	345	TRP	N-CA-CB	6.66	121.74	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	417	GLN	O-C-N	6.65	129.17	122.12
1	C	252	PRO	N-CA-C	6.63	126.12	112.47
2	D	101	GLY	N-CA-C	-6.59	104.66	112.64
2	D	256	VAL	N-CA-C	6.57	122.94	113.16
2	D	479	ASN	CA-CB-CG	6.55	119.15	112.60
2	B	119	ASP	CA-CB-CG	6.54	119.14	112.60
2	B	464	GLY	CA-C-O	6.51	128.32	122.01
2	B	248	GLU	CA-CB-CG	6.50	127.10	114.10
1	A	231	GLN	N-CA-C	-6.49	104.05	112.68
2	D	241	GLU	CA-CB-CG	6.49	127.07	114.10
1	A	38	ASP	CA-CB-CG	6.47	119.07	112.60
1	C	144	ASN	N-CA-C	6.45	119.07	109.59
2	D	24	GLU	CB-CG-CD	6.44	123.55	112.60
2	D	298	THR	N-CA-CB	6.40	119.48	110.07
2	D	108	HIS	N-CA-C	6.38	119.23	111.82
1	C	246	CYS	N-CA-C	-6.38	101.51	110.50
2	B	298	THR	CB-CA-C	6.37	117.11	109.85
2	D	492	PRO	N-CA-C	6.37	125.59	112.47
1	C	136	GLY	N-CA-C	-6.36	104.94	112.64
1	C	56	VAL	N-CA-C	-6.33	104.58	110.53
2	D	29	GLY	N-CA-C	6.33	125.91	114.46
1	A	98	GLU	CA-C-N	6.28	129.72	120.74
1	A	98	GLU	C-N-CA	6.28	129.72	120.74
2	B	289	ASP	N-CA-C	-6.25	97.62	108.69
2	D	471	VAL	N-CA-CB	6.24	120.30	111.82
2	B	72	HIS	CA-CB-CG	6.23	120.03	113.80
1	C	169	GLU	N-CA-CB	6.23	120.33	110.23
1	C	11	TYR	CA-CB-CG	6.22	125.09	113.90
2	D	513	ASP	N-CA-CB	6.20	121.40	110.37
2	B	366	ALA	N-CA-C	6.17	121.55	111.37
1	A	51	GLY	CA-C-O	-6.17	116.11	122.28
2	D	347	GLU	N-CA-C	6.15	123.90	110.80
1	A	78	MET	N-CA-C	-6.12	105.30	112.89
2	D	39	SER	CA-C-O	-6.12	114.01	121.36
2	B	236	PRO	N-CA-C	-6.12	105.55	113.57
1	C	36	ILE	N-CA-C	6.11	118.72	111.09
1	C	40	ILE	N-CA-C	6.10	122.03	109.34
1	A	228	CYS	O-C-N	6.09	126.17	120.51
1	C	186	ASP	CA-CB-CG	-6.08	106.52	112.60
2	B	226	GLY	CA-C-N	6.07	133.31	121.41
2	B	226	GLY	C-N-CA	6.07	133.31	121.41
2	D	220	THR	N-CA-CB	-6.07	101.20	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	29	ASP	N-CA-CB	6.07	121.17	110.37
2	D	130	ASP	CA-CB-CG	6.06	118.66	112.60
2	D	127	LEU	N-CA-C	-6.05	104.61	111.14
2	B	49	LEU	N-CA-C	6.03	118.64	111.71
2	B	365	GLU	N-CA-C	6.03	120.08	109.96
2	D	367	PHE	N-CA-C	6.02	123.62	110.80
1	C	54	HIS	N-CA-C	6.01	119.88	112.54
2	D	417	GLN	O-C-N	6.01	130.58	122.59
1	A	131	VAL	N-CA-C	6.00	116.47	110.23
1	A	132	ASN	CB-CA-C	6.00	120.36	111.06
2	B	39	SER	N-CA-C	-5.99	100.08	109.25
1	C	133	GLU	N-CA-C	-5.97	98.09	110.80
2	B	191	ILE	N-CA-C	-5.96	105.04	110.82
1	C	38	ASP	CA-C-O	-5.96	115.11	121.78
1	C	46	GLU	CB-CG-CD	5.95	122.72	112.60
2	D	281	LEU	N-CA-CB	-5.95	100.36	111.13
1	A	29	ASP	N-CA-C	-5.94	96.68	109.81
2	B	23	ILE	N-CA-CB	5.94	119.36	111.64
1	A	88	GLY	N-CA-C	-5.92	105.79	114.61
2	B	122	ASN	CA-CB-CG	5.92	118.52	112.60
1	C	7	PRO	CA-C-O	5.91	127.76	121.03
2	D	81	ASP	O-C-N	5.91	128.15	122.07
2	B	372	LEU	N-CA-C	-5.89	103.83	111.02
2	D	40	THR	CA-C-O	5.89	127.15	121.67
2	B	520	ILE	CA-C-N	5.89	130.55	120.72
2	B	520	ILE	C-N-CA	5.89	130.55	120.72
2	B	172	ASN	CA-C-N	5.88	129.11	120.82
2	B	172	ASN	C-N-CA	5.88	129.11	120.82
2	B	256	VAL	N-CA-C	5.87	121.54	109.34
1	C	238	TRP	CA-CB-CG	5.86	124.73	113.60
2	B	184	LEU	N-CA-C	5.85	118.76	109.64
2	D	274	ILE	CB-CA-C	5.84	119.32	110.62
2	D	39	SER	N-CA-C	-5.84	101.04	110.32
2	B	7	ASN	CA-CB-CG	-5.83	106.78	112.60
1	C	163	LEU	CA-C-N	5.82	128.33	120.65
1	C	163	LEU	C-N-CA	5.82	128.33	120.65
1	A	4	LYS	CA-C-N	5.82	132.65	121.54
1	A	4	LYS	C-N-CA	5.82	132.65	121.54
2	B	39	SER	CB-CA-C	5.82	119.83	110.29
2	B	436	VAL	N-CA-C	-5.82	104.84	110.42
1	A	109	ILE	N-CA-C	5.82	116.67	108.36
1	C	119	GLN	N-CA-C	-5.80	104.86	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	116	HIS	N-CA-C	5.80	118.72	111.24
1	A	220	LYS	CA-C-N	5.79	125.36	121.13
1	A	220	LYS	C-N-CA	5.79	125.36	121.13
2	D	64	ALA	N-CA-C	-5.79	104.57	111.69
2	D	365	GLU	N-CA-C	5.79	119.52	110.32
2	D	114	HIS	N-CA-C	5.78	118.36	111.71
1	C	78	MET	CA-C-N	5.78	132.74	121.41
1	C	78	MET	C-N-CA	5.78	132.74	121.41
2	D	114	HIS	CA-CB-CG	-5.78	108.03	113.80
2	D	443	LEU	N-CA-C	-5.77	100.98	109.81
1	C	184	VAL	N-CA-C	-5.76	104.89	110.42
2	B	511	ILE	CA-C-N	5.76	129.06	120.31
2	B	511	ILE	C-N-CA	5.76	129.06	120.31
1	A	40	ILE	N-CA-C	5.75	121.29	109.34
1	A	216	GLU	CB-CA-C	-5.74	101.80	110.92
1	A	216	GLU	N-CA-C	5.72	118.00	111.02
2	B	487	THR	N-CA-C	-5.72	105.18	111.82
2	B	67	VAL	O-C-N	5.71	128.05	121.94
2	D	242	PHE	N-CA-C	-5.71	104.67	111.69
1	A	232	LEU	CA-C-N	5.68	128.78	120.71
1	A	232	LEU	C-N-CA	5.68	128.78	120.71
1	A	30	PRO	N-CA-CB	5.68	106.10	102.92
2	B	171	THR	CA-CB-OG1	-5.67	101.09	109.60
2	B	449	TYR	O-C-N	5.67	126.13	121.31
1	A	61	HIS	CA-CB-CG	-5.66	108.14	113.80
2	D	483	VAL	CB-CA-C	5.66	118.16	111.32
2	B	335	HIS	N-CA-C	-5.65	102.28	110.08
2	B	80	VAL	N-CA-C	-5.64	105.35	110.82
2	D	356	TRP	N-CA-C	-5.64	106.56	113.50
2	D	402	GLU	N-CA-C	-5.63	106.41	113.28
1	A	200	ALA	N-CA-C	-5.62	101.38	110.32
1	C	196	ALA	N-CA-C	-5.62	104.66	112.30
1	C	68	PHE	CA-C-O	5.61	126.65	120.31
2	D	198	GLU	N-CA-C	-5.58	105.28	111.36
2	D	516	ARG	O-C-N	5.57	125.25	121.19
1	C	99	VAL	CA-C-N	5.57	127.05	120.09
1	C	99	VAL	C-N-CA	5.57	127.05	120.09
1	C	6	ARG	CA-C-N	5.56	125.74	119.90
1	C	6	ARG	C-N-CA	5.56	125.74	119.90
2	D	312	ASP	N-CA-C	-5.56	102.29	110.52
1	A	155	PHE	CA-CB-CG	5.55	119.35	113.80
1	C	170	LEU	N-CA-C	5.54	118.26	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	236	VAL	N-CA-CB	-5.54	102.10	111.23
2	D	443	LEU	CA-C-O	-5.54	115.15	121.68
1	A	43	ASP	CB-CA-C	5.53	120.25	110.85
2	B	490	LEU	CA-C-O	-5.53	114.87	121.89
2	B	48	ILE	CA-C-N	5.52	128.23	120.28
2	B	48	ILE	C-N-CA	5.52	128.23	120.28
2	D	32	ILE	N-CA-C	5.52	116.25	108.36
1	A	87	VAL	CB-CA-C	5.51	120.25	110.71
2	B	63	ARG	CB-CA-C	5.51	120.19	110.37
2	B	64	ALA	O-C-N	5.51	127.75	122.07
1	C	83	TYR	N-CA-C	5.50	122.52	110.80
1	A	51	GLY	N-CA-C	-5.49	104.17	112.41
1	A	82	GLY	N-CA-C	-5.48	107.02	116.01
2	D	504	GLN	OE1-CD-NE2	5.48	128.08	122.60
2	D	190	LEU	CB-CA-C	5.47	119.98	110.79
2	D	323	VAL	N-CA-CB	5.47	120.25	111.23
2	B	98	LEU	N-CA-C	-5.46	104.97	111.03
2	D	187	GLU	CA-C-N	5.46	128.54	120.74
2	D	187	GLU	C-N-CA	5.46	128.54	120.74
2	D	406	SER	N-CA-C	5.46	117.55	109.69
2	D	39	SER	CA-C-N	-5.45	113.76	121.83
2	D	39	SER	C-N-CA	-5.45	113.76	121.83
2	D	350	GLY	N-CA-C	-5.45	100.25	113.18
1	A	94	ASP	CA-CB-CG	5.45	118.05	112.60
1	C	263	SER	CA-C-N	5.45	131.51	121.70
1	C	263	SER	C-N-CA	5.45	131.51	121.70
2	D	255	GLN	CA-C-N	5.45	129.25	121.02
2	D	255	GLN	C-N-CA	5.45	129.25	121.02
2	D	267	PHE	CA-CB-CG	-5.45	108.35	113.80
1	A	188	CYS	CB-CA-C	5.43	116.53	108.87
1	A	97	ALA	CA-C-N	5.42	127.80	120.65
1	A	97	ALA	C-N-CA	5.42	127.80	120.65
2	D	497	ARG	N-CA-C	5.42	122.34	110.80
2	D	312	ASP	CB-CA-C	5.41	119.30	109.83
1	A	104	LYS	N-CA-C	-5.41	105.39	111.28
2	B	491	GLY	O-C-N	5.41	127.18	121.77
2	B	220	THR	N-CA-C	5.40	118.72	110.20
2	B	459	VAL	O-C-N	5.39	129.00	123.18
2	D	91	ASN	N-CA-C	-5.39	105.44	112.23
1	C	137	LYS	N-CA-C	5.37	117.13	111.28
2	D	245	LEU	CA-C-N	5.36	127.47	120.28
2	D	245	LEU	C-N-CA	5.36	127.47	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	376	LEU	N-CA-C	-5.35	104.87	111.40
2	B	355	SER	N-CA-C	5.34	117.51	109.23
2	D	20	HIS	CA-CB-CG	-5.34	108.46	113.80
2	B	528	ASP	CA-CB-CG	5.33	117.93	112.60
1	C	208	ALA	N-CA-C	-5.33	105.13	111.69
2	D	490	LEU	N-CA-C	-5.33	101.60	109.86
1	A	247	ILE	N-CA-C	5.32	117.22	112.17
1	C	251	GLU	CA-C-N	5.31	126.48	119.84
1	C	251	GLU	C-N-CA	5.31	126.48	119.84
2	B	288	THR	CB-CA-C	5.31	117.98	109.07
2	B	34	ASN	N-CA-C	5.30	122.08	110.80
1	A	191	LEU	N-CA-C	-5.29	105.41	111.07
2	B	90	GLU	CB-CG-CD	5.29	121.59	112.60
1	C	49	MET	N-CA-C	5.29	117.69	110.24
1	C	48	LEU	CA-C-N	5.28	128.34	120.90
1	C	48	LEU	C-N-CA	5.28	128.34	120.90
2	B	300	GLN	CA-C-O	-5.28	114.67	120.69
2	D	112	PHE	N-CA-CB	5.28	117.84	109.82
2	D	298	THR	CA-C-N	5.27	125.28	119.90
2	D	298	THR	C-N-CA	5.27	125.28	119.90
2	D	242	PHE	N-CA-CB	5.27	118.05	110.20
2	D	78	ARG	O-C-N	5.27	127.50	122.07
2	D	91	ASN	CA-CB-CG	5.26	117.86	112.60
2	D	165	GLY	O-C-N	5.26	127.56	122.41
2	D	471	VAL	O-C-N	5.26	128.65	123.18
1	C	150	PRO	N-CA-C	5.24	123.27	112.47
2	B	405	PHE	CA-CB-CG	-5.24	108.56	113.80
2	D	502	VAL	N-CA-CB	5.23	116.32	110.51
1	C	15	ALA	N-CA-C	-5.22	101.26	109.25
1	A	40	ILE	N-CA-CB	-5.22	102.61	111.23
2	D	68	CYS	N-CA-C	-5.22	107.43	112.97
1	A	76	ILE	CB-CA-C	-5.22	105.00	110.53
2	B	429	LEU	N-CA-C	-5.22	105.49	111.07
2	D	478	GLU	N-CA-C	-5.22	104.51	111.24
2	D	509	THR	N-CA-C	-5.20	101.99	109.48
2	B	98	LEU	CA-C-N	5.20	127.20	120.44
2	B	98	LEU	C-N-CA	5.20	127.20	120.44
2	B	372	LEU	O-C-N	5.20	127.64	122.08
2	D	220	THR	CA-CB-CG2	5.20	119.33	110.50
2	D	314	PHE	CA-CB-CG	5.19	118.99	113.80
2	D	78	ARG	CD-NE-CZ	-5.19	117.13	124.40
1	A	201	THR	N-CA-C	-5.19	106.98	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	104	LYS	N-CA-C	-5.19	106.79	113.01
1	C	114	THR	CA-CB-CG2	5.18	119.30	110.50
2	B	284	GLY	N-CA-C	-5.17	106.16	112.68
2	D	450	PRO	N-CA-C	-5.17	101.81	112.47
2	D	266	GLY	CA-C-N	5.15	127.90	120.38
2	D	266	GLY	C-N-CA	5.15	127.90	120.38
2	B	65	CYS	CB-CA-C	5.15	121.26	111.17
2	B	78	ARG	N-CA-C	5.14	118.32	111.75
2	D	295	SER	N-CA-C	-5.13	105.86	112.68
1	A	30	PRO	O-C-N	5.13	126.37	122.73
2	B	343	PRO	N-CA-C	5.12	119.53	111.38
2	B	521	LEU	N-CA-C	5.12	118.78	112.54
2	B	444	TYR	CA-CB-CG	-5.12	104.69	113.90
2	D	298	THR	CB-CA-C	5.12	115.23	110.17
2	B	226	GLY	CA-C-O	5.11	124.86	119.03
2	B	53	ASP	O-C-N	5.10	126.83	121.42
1	C	169	GLU	CB-CG-CD	5.10	121.28	112.60
2	D	391	ASP	CA-CB-CG	5.10	117.70	112.60
2	B	224	VAL	CA-C-O	-5.09	116.36	121.45
1	A	19	GLY	CA-C-N	5.09	127.10	120.28
1	A	19	GLY	C-N-CA	5.09	127.10	120.28
2	D	43	ARG	CD-NE-CZ	5.09	131.52	124.40
2	D	12	ASP	O-C-N	-5.08	115.49	121.23
1	C	178	MET	O-C-N	5.07	127.49	122.12
2	B	40	THR	N-CA-CB	-5.07	102.99	110.49
1	C	113	ALA	CA-C-N	5.05	127.00	120.44
1	C	113	ALA	C-N-CA	5.05	127.00	120.44
1	C	227	ASN	CA-CB-CG	5.04	117.64	112.60
1	C	29	ASP	O-C-N	5.04	127.11	121.32
1	C	88	GLY	N-CA-C	-5.04	108.37	115.32
1	A	29	ASP	CB-CA-C	5.03	120.08	110.17
2	B	288	THR	CA-C-O	5.03	124.35	118.97
2	B	460	ASN	O-C-N	5.03	127.97	122.64
2	D	281	LEU	N-CA-C	5.03	117.34	108.75
2	D	262	LEU	CB-CA-C	5.02	119.12	110.79
1	C	96	CYS	N-CA-C	-5.01	105.89	111.36
2	D	154	VAL	O-C-N	5.00	126.79	121.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1961	0	1879	162	0
1	C	1961	0	1879	207	0
2	B	4145	0	4073	382	1
2	D	4145	0	4073	513	1
3	A	16	0	0	2	0
3	C	16	0	0	3	0
4	A	7	0	0	0	0
4	C	7	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	3	0	0	0	0
7	D	3	0	0	0	0
All	All	12268	0	11904	1205	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 50.

All (1205) 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:308:LEU:HD21	2:B:405:PHE:HZ	1.15	1.07
2:D:14:ILE:HG13	2:D:21:LEU:HD13	1.30	1.07
1:C:29:ASP:HB3	1:C:30:PRO:HD3	1.30	1.06
2:D:27:VAL:HG22	2:D:32:ILE:HA	1.38	1.02
1:A:29:ASP:HB3	1:A:30:PRO:HD3	1.41	1.01
2:D:208:ARG:HG2	2:D:245:LEU:HD21	1.38	1.00
1:C:137:LYS:HG2	1:C:138:LEU:HD13	1.46	0.97
1:C:231:GLN:O	1:C:232:LEU:HB2	1.61	0.97
2:D:32:ILE:HD12	2:D:509:THR:HB	1.49	0.94
2:B:14:ILE:HD11	2:B:23:ILE:HG12	1.49	0.94
2:B:173:ALA:HB3	2:B:176:LEU:HG	1.48	0.94
2:B:141:LEU:HD21	2:B:263:ALA:HB2	1.49	0.93
1:C:149:PRO:HG3	2:D:218:PRO:HG2	1.51	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:VAL:HG11	2:D:381:LYS:HD2	1.52	0.92
1:C:29:ASP:HB3	1:C:30:PRO:CD	1.99	0.91
2:D:466:LEU:HD13	2:D:484:VAL:HG13	1.50	0.91
2:D:108:HIS:ND1	2:D:418:CYS:HB2	1.87	0.89
2:D:109:LEU:HD21	2:D:253:ILE:HG12	1.54	0.89
2:B:308:LEU:HD21	2:B:405:PHE:CZ	2.08	0.89
1:A:29:ASP:HB3	1:A:30:PRO:CD	2.02	0.88
1:A:100:ALA:HB3	1:A:101:PRO:HD3	1.54	0.88
2:B:89:PRO:HD3	2:B:445:THR:OG1	1.74	0.88
2:B:472:GLN:HE22	2:B:475:GLY:H	1.18	0.88
1:C:9:VAL:HG22	1:C:69:VAL:HB	1.56	0.88
2:D:321:GLU:HG2	2:D:360:PRO:HB3	1.55	0.87
2:D:50:LYS:HE2	2:D:478:GLU:O	1.74	0.87
1:A:28:VAL:O	1:A:30:PRO:HD2	1.75	0.87
2:B:261:LEU:HD11	2:B:412:ALA:HA	1.57	0.87
1:C:36:ILE:HD11	1:C:42:MET:HB2	1.57	0.86
1:C:77:PRO:HA	1:C:128:THR:HA	1.57	0.86
2:D:527:TYR:C	2:D:529:PRO:HD3	2.01	0.86
2:B:96:ARG:HH21	2:B:227:GLY:HA2	1.41	0.85
2:D:14:ILE:HG13	2:D:21:LEU:CD1	2.05	0.85
2:D:323:VAL:HG11	2:D:328:TYR:HB2	1.59	0.85
2:B:127:LEU:HD23	2:B:158:VAL:HG12	1.60	0.84
2:D:410:ARG:HG2	2:D:410:ARG:HH11	1.40	0.84
2:D:358:LYS:O	2:D:360:PRO:HD3	1.76	0.84
1:C:28:VAL:O	1:C:30:PRO:HD2	1.77	0.84
2:D:528:ASP:N	2:D:529:PRO:HD3	1.93	0.83
1:A:145:ILE:HD11	1:A:158:THR:HG21	1.60	0.82
2:D:78:ARG:HH11	2:D:459:VAL:HG22	1.43	0.82
1:A:29:ASP:CB	1:A:30:PRO:HD3	2.09	0.82
1:C:135:LEU:HB3	1:C:140:VAL:HG21	1.60	0.82
1:A:193:HIS:HB3	1:A:198:GLU:O	1.80	0.82
2:B:510:PRO:O	2:B:519:GLU:HG3	1.79	0.82
1:A:35:LEU:HA	1:A:39:VAL:HB	1.62	0.81
2:D:21:LEU:HD22	2:D:22:ARG:H	1.46	0.81
2:B:108:HIS:HE1	2:B:417:GLN:HE21	1.27	0.81
2:D:143:PRO:HD2	2:D:255:GLN:HG3	1.59	0.80
1:C:29:ASP:CB	1:C:30:PRO:HD3	2.11	0.80
2:D:388:LYS:C	2:D:388:LYS:HD3	2.07	0.80
2:B:390:VAL:HG23	2:B:394:LEU:HD13	1.63	0.79
2:B:108:HIS:HE1	2:B:417:GLN:NE2	1.80	0.79
1:A:132:ASN:HD22	1:A:142:ALA:N	1.79	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:ALA:HB3	2:B:440:LYS:CG	2.13	0.79
2:B:467:SER:OG	2:B:469:TRP:NE1	2.16	0.78
2:B:77:VAL:HG11	2:B:223:THR:HB	1.65	0.78
1:C:40:ILE:O	1:C:41:SER:HB3	1.81	0.78
2:D:10:VAL:HG13	2:D:24:GLU:HG2	1.64	0.78
1:A:220:LYS:C	1:A:222:PRO:HD2	2.08	0.78
1:A:239:PRO:HB3	2:B:221:GLN:NE2	1.99	0.78
2:D:112:PHE:HB2	2:D:257:TYR:HE1	1.47	0.78
2:B:467:SER:HG	2:B:469:TRP:NE1	1.81	0.77
2:D:393:VAL:O	2:D:397:LEU:HB2	1.84	0.77
2:D:472:GLN:HE22	2:D:475:GLY:H	1.28	0.77
1:A:153:MET:HE1	1:A:231:GLN:HG3	1.65	0.77
1:A:3:ALA:O	1:A:4:LYS:HB2	1.85	0.77
1:C:6:ARG:HB2	1:C:6:ARG:NH1	2.00	0.77
1:A:253:ASN:HB3	1:A:257:LEU:HD13	1.67	0.77
2:B:345:TRP:CZ2	2:B:347:GLU:HA	2.20	0.77
2:B:108:HIS:CE1	2:B:417:GLN:HE21	2.02	0.77
2:D:528:ASP:N	2:D:529:PRO:CD	2.48	0.77
2:B:30:GLY:O	2:B:510:PRO:HA	1.84	0.76
1:C:9:VAL:HB	1:C:40:ILE:HD11	1.65	0.76
2:D:323:VAL:O	2:D:324:LYS:HB3	1.83	0.76
1:C:134:ALA:C	1:C:136:GLY:H	1.91	0.76
2:B:360:PRO:HD3	2:B:487:THR:HG22	1.68	0.76
2:B:139:ASN:HD21	2:B:145:LYS:HG3	1.51	0.76
1:C:235:GLN:HE21	2:D:208:ARG:HH21	1.30	0.76
1:A:214:LEU:HD12	1:A:240:VAL:HG13	1.68	0.76
1:A:85:GLY:HA3	1:A:92:MET:SD	2.24	0.76
3:C:267:SF4:S2	2:D:63:ARG:HG2	2.26	0.76
1:A:78:MET:HE1	1:A:134:ALA:HB1	1.68	0.76
2:D:387:VAL:HA	2:D:390:VAL:HG12	1.66	0.75
2:D:39:SER:OG	2:D:357:MET:HG3	1.86	0.75
2:D:139:ASN:HD21	2:D:145:LYS:HG3	1.49	0.75
2:B:94:LEU:O	2:B:98:LEU:HB2	1.87	0.75
2:D:270:ASN:H	2:D:270:ASN:ND2	1.85	0.75
2:D:322:HIS:HB2	2:D:359:ALA:HB3	1.69	0.74
1:A:249:CYS:HA	1:A:254:PHE:CE2	2.23	0.74
2:B:253:ILE:HD13	2:B:418:CYS:SG	2.27	0.74
2:D:26:GLU:O	2:D:33:LYS:HB3	1.87	0.74
2:B:302:VAL:O	2:B:311:VAL:HA	1.87	0.74
2:D:351:GLU:HG3	2:D:353:ARG:HE	1.53	0.74
2:B:243:ARG:HB2	2:B:429:LEU:HD21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:LYS:HE3	1:C:91:ASN:OD1	1.88	0.73
2:D:485:PRO:C	2:D:487:THR:H	1.95	0.73
2:D:111:HIS:HA	2:D:115:LEU:HB2	1.68	0.73
2:D:88:ILE:HG21	2:D:96:ARG:HH12	1.54	0.73
1:A:150:PRO:O	1:A:151:ASN:CB	2.37	0.73
1:A:197:GLY:HA3	2:D:235:ARG:NH1	2.04	0.73
2:B:357:MET:HE2	2:B:534:GLY:HA3	1.70	0.73
2:D:78:ARG:NH1	2:D:459:VAL:HG22	2.04	0.73
2:D:68:CYS:O	2:D:71:VAL:HG22	1.89	0.73
1:A:221:GLY:N	1:A:222:PRO:CD	2.50	0.73
2:B:139:ASN:ND2	2:B:145:LYS:HG3	2.03	0.73
1:C:153:MET:HE3	1:C:179:PHE:HE1	1.53	0.72
1:C:17:CYS:HB2	2:D:65:CYS:HA	1.71	0.72
2:D:15:THR:HG23	2:D:16:ARG:H	1.55	0.72
2:D:471:VAL:HG23	2:D:478:GLU:HB3	1.72	0.72
1:A:197:GLY:HA3	2:D:235:ARG:HH12	1.53	0.72
2:B:337:TYR:OH	2:B:456:VAL:HG12	1.88	0.72
2:D:144:ARG:HG2	2:D:255:GLN:HG2	1.71	0.72
1:A:45:HIS:HD2	1:A:47:THR:H	1.38	0.72
2:B:347:GLU:O	2:B:348:PHE:HB2	1.88	0.72
1:A:150:PRO:O	1:A:151:ASN:HB3	1.89	0.72
1:C:44:TYR:CE2	1:C:60:LEU:HB2	2.24	0.71
1:C:119:GLN:CG	2:D:43:ARG:HG2	2.21	0.71
2:D:32:ILE:HG22	2:D:507:ILE:HA	1.73	0.71
2:D:253:ILE:O	2:D:257:TYR:HB3	1.90	0.71
1:A:55:ALA:HB1	2:B:172:ASN:HB3	1.72	0.71
1:A:205:SER:OG	1:A:207:GLU:HG2	1.90	0.71
2:D:315:ASN:ND2	2:D:318:LEU:HG	2.05	0.71
2:B:382:LYS:O	2:B:383:HIS:C	2.33	0.71
1:C:80:ASP:H	1:C:84:TRP:HE1	1.39	0.71
2:D:129:ALA:O	2:D:131:PRO:HD3	1.90	0.71
2:B:355:SER:HB3	2:B:492:PRO:HD3	1.72	0.70
1:A:183:THR:HA	1:A:225:TYR:HA	1.72	0.70
2:D:34:ASN:O	2:D:35:ALA:HB3	1.89	0.70
2:D:324:LYS:HB2	2:D:331:ALA:HB1	1.73	0.70
2:B:319:ILE:HD12	2:B:319:ILE:C	2.16	0.70
2:B:383:HIS:NE2	2:B:385:PRO:HG2	2.06	0.70
2:B:472:GLN:NE2	2:B:475:GLY:H	1.89	0.70
2:D:340:VAL:HG23	2:D:342:LYS:HG3	1.73	0.70
2:D:372:LEU:HD22	2:D:410:ARG:HD3	1.73	0.70
2:D:484:VAL:HG11	2:D:533:CYS:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:511:ILE:HA	2:D:519:GLU:HG3	1.72	0.70
1:C:6:ARG:HB2	1:C:6:ARG:HH11	1.56	0.70
2:D:356:TRP:HB3	2:D:535:VAL:CG1	2.22	0.70
2:B:340:VAL:O	2:B:358:LYS:NZ	2.25	0.69
1:C:234:ASN:OD1	2:D:211:ALA:HB2	1.92	0.69
1:A:120:ALA:HA	1:A:124:ASN:ND2	2.08	0.69
1:C:153:MET:HE3	1:C:179:PHE:CE1	2.27	0.69
2:D:88:ILE:HD12	2:D:92:ALA:HB3	1.75	0.69
1:A:24:LEU:HD11	1:A:155:PHE:CE1	2.28	0.69
2:B:15:THR:HG23	2:B:16:ARG:H	1.57	0.69
1:C:9:VAL:CB	1:C:40:ILE:HD11	2.22	0.69
1:C:119:GLN:HG3	2:D:43:ARG:HG2	1.73	0.69
1:C:143:ILE:HD13	1:C:170:LEU:HD11	1.74	0.69
1:C:55:ALA:HB1	2:D:172:ASN:HB2	1.73	0.69
2:D:53:ASP:O	2:D:56:ASP:HB2	1.92	0.69
1:A:5:LYS:HB3	1:A:6:ARG:HD3	1.74	0.69
2:B:329:GLU:HG3	2:B:342:LYS:HG3	1.74	0.69
2:B:70:TYR:OH	2:B:74:LEU:HG	1.92	0.68
2:D:14:ILE:O	2:D:14:ILE:HG22	1.93	0.68
1:A:132:ASN:HD22	1:A:142:ALA:H	1.39	0.68
2:B:283:CYS:O	2:B:300:GLN:HB2	1.94	0.68
2:D:142:SER:HB2	2:D:143:PRO:CD	2.23	0.68
1:A:227:ASN:HD22	1:A:227:ASN:H	1.41	0.68
2:B:379:TYR:CD1	2:B:387:VAL:HG12	2.29	0.68
2:D:270:ASN:H	2:D:270:ASN:HD22	1.40	0.68
2:D:287:PRO:HB3	2:D:296:ARG:HG2	1.76	0.67
1:C:235:GLN:HE21	2:D:208:ARG:NH2	1.93	0.67
2:D:388:LYS:HD3	2:D:388:LYS:O	1.94	0.67
1:C:202:SER:O	1:C:205:SER:OG	2.13	0.67
1:C:94:ASP:O	1:C:97:ALA:HB3	1.95	0.67
2:D:424:GLU:OE1	2:D:424:GLU:HA	1.95	0.67
1:A:78:MET:HE1	1:A:134:ALA:CB	2.24	0.67
2:B:75:ALA:HB2	2:B:459:VAL:HG23	1.75	0.67
2:D:21:LEU:HD22	2:D:22:ARG:N	2.09	0.67
2:B:241:GLU:O	2:B:245:LEU:HD22	1.94	0.67
1:C:118:VAL:O	2:D:48:ILE:HD13	1.94	0.67
2:B:425:VAL:HA	2:B:428:TRP:CE3	2.30	0.66
2:B:514:PRO:O	2:B:517:PRO:HD3	1.95	0.66
2:D:25:VAL:HG12	2:D:35:ALA:CB	2.25	0.66
1:C:158:THR:O	1:C:162:LEU:HD22	1.95	0.66
2:D:485:PRO:C	2:D:487:THR:N	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:ARG:NH2	2:B:227:GLY:HA2	2.10	0.66
1:C:24:LEU:HD21	1:C:155:PHE:CE2	2.31	0.66
2:D:22:ARG:NH1	2:D:24:GLU:OE2	2.29	0.66
2:D:86:VAL:HG23	2:D:447:TRP:HB3	1.78	0.66
2:D:120:TRP:O	2:D:184:LEU:HD22	1.95	0.66
2:B:395:LYS:O	2:B:396:THR:C	2.38	0.66
1:C:134:ALA:O	1:C:136:GLY:N	2.29	0.66
2:B:91:ASN:HB2	2:B:442:ASP:O	1.96	0.66
2:D:340:VAL:HG21	2:D:342:LYS:HE3	1.77	0.66
1:A:249:CYS:HA	1:A:254:PHE:CD2	2.31	0.66
1:C:20:CYS:O	1:C:23:SER:HB3	1.94	0.66
2:D:49:LEU:HD11	2:D:57:ALA:HA	1.78	0.66
2:D:27:VAL:CG2	2:D:32:ILE:HA	2.23	0.66
1:C:137:LYS:HD3	1:C:138:LEU:HD22	1.78	0.65
2:B:109:LEU:HD21	2:B:252:PHE:CE2	2.31	0.65
1:C:90:ARG:HB2	1:C:95:ILE:HD11	1.77	0.65
2:D:158:VAL:O	2:D:162:VAL:HG23	1.97	0.65
2:D:356:TRP:HB3	2:D:535:VAL:HG11	1.77	0.65
2:D:185:PRO:HG2	2:D:188:VAL:HB	1.76	0.65
2:B:344:LYS:HE2	2:B:344:LYS:HA	1.78	0.65
2:D:31:LYS:HA	2:D:510:PRO:HA	1.77	0.65
2:D:324:LYS:HB2	2:D:331:ALA:CB	2.27	0.65
2:B:226:GLY:O	2:B:444:TYR:HA	1.97	0.65
1:C:55:ALA:HB1	2:D:172:ASN:CB	2.26	0.65
2:D:49:LEU:HG	2:D:477:ILE:HD13	1.77	0.65
2:D:348:PHE:O	2:D:349:HIS:HB2	1.96	0.65
1:A:189:PRO:C	1:A:191:LEU:H	2.04	0.65
2:B:278:SER:O	2:B:279:ASN:HB2	1.96	0.65
2:B:382:LYS:O	2:B:384:GLU:N	2.29	0.64
2:B:390:VAL:CG2	2:B:394:LEU:HD13	2.27	0.64
2:B:127:LEU:HD11	2:B:159:LYS:HG3	1.79	0.64
2:B:280:PHE:HB3	2:B:373:ALA:CB	2.28	0.64
2:B:380:ALA:O	2:B:381:LYS:HG3	1.96	0.64
2:D:112:PHE:CB	2:D:257:TYR:HE1	2.10	0.64
1:A:109:ILE:HG13	1:A:150:PRO:HG2	1.78	0.64
2:D:14:ILE:CG1	2:D:21:LEU:HD13	2.18	0.64
2:B:277:THR:HG22	2:B:504:GLN:HE21	1.61	0.64
2:D:161:LEU:HA	2:D:164:SER:OG	1.97	0.64
2:B:33:LYS:HG2	2:B:33:LYS:O	1.98	0.64
1:C:14:ASN:HA	1:C:92:MET:SD	2.38	0.64
1:C:159:VAL:HA	1:C:162:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:TRP:CD1	2:D:493:ARG:HH21	2.16	0.64
2:D:531:ILE:O	2:D:535:VAL:HG23	1.97	0.64
1:A:168:PRO:O	1:A:170:LEU:HD13	1.99	0.63
1:C:117:GLY:O	1:C:120:ALA:N	2.30	0.63
1:C:36:ILE:HD11	1:C:42:MET:HE3	1.80	0.63
1:C:98:GLU:HG3	1:C:99:VAL:N	2.12	0.63
2:D:82:ASN:HD22	2:D:456:VAL:H	1.44	0.63
2:B:74:LEU:HD12	2:B:100:MET:HE2	1.81	0.63
2:D:139:ASN:OD1	2:D:146:THR:N	2.24	0.63
2:D:173:ALA:HB3	2:D:176:LEU:HG	1.78	0.63
1:A:14:ASN:HD22	1:A:92:MET:HB3	1.62	0.63
2:B:466:LEU:HD13	2:B:484:VAL:HG13	1.81	0.63
1:C:170:LEU:HA	1:C:175:ARG:O	1.97	0.63
2:D:245:LEU:O	2:D:249:VAL:HG23	1.96	0.63
1:C:236:VAL:O	1:C:237:ASN:HB2	1.97	0.63
2:D:86:VAL:HG22	2:D:445:THR:HG22	1.80	0.63
2:B:95:MET:HE2	2:B:233:SER:OG	1.99	0.63
2:B:198:GLU:C	2:B:200:LEU:H	2.07	0.63
1:A:24:LEU:HD11	1:A:155:PHE:CD1	2.34	0.63
2:D:25:VAL:HG12	2:D:35:ALA:HB2	1.81	0.63
2:D:69:THR:O	2:D:70:TYR:HB3	1.98	0.63
1:A:193:HIS:HA	1:A:198:GLU:HG3	1.80	0.63
2:B:311:VAL:HG21	2:B:380:ALA:HB1	1.80	0.63
2:D:515:LYS:O	2:D:516:ARG:HG3	1.98	0.63
2:D:377:VAL:O	2:D:381:LYS:HB2	1.99	0.62
2:D:502:VAL:HG23	2:D:527:TYR:CD2	2.34	0.62
1:C:24:LEU:C	1:C:26:ARG:H	2.06	0.62
2:D:132:ALA:HA	2:D:148:THR:OG1	1.99	0.62
2:B:473:ARG:HB3	2:B:478:GLU:OE2	1.99	0.62
2:B:14:ILE:HG22	2:B:14:ILE:O	1.98	0.62
2:B:336:PRO:O	2:B:338:LYS:N	2.32	0.62
1:A:161:HIS:ND1	1:A:168:PRO:HG3	2.14	0.62
2:D:131:PRO:HG3	2:D:155:GLN:OE1	1.98	0.62
2:D:83:CYS:HB2	2:D:454:GLN:C	2.25	0.62
1:A:197:GLY:CA	2:D:235:ARG:HH12	2.13	0.62
1:C:259:SER:HA	1:C:260:PRO:C	2.25	0.62
2:D:357:MET:HE2	2:D:534:GLY:HA3	1.82	0.62
2:D:361:ARG:HD3	2:D:366:ALA:HA	1.82	0.62
1:A:4:LYS:HD2	1:A:5:LYS:H	1.65	0.62
1:C:7:PRO:HD2	1:C:40:ILE:HA	1.82	0.62
2:B:335:HIS:CD2	2:B:336:PRO:HD2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:ASN:HD21	2:D:317:ASP:HB2	1.65	0.61
1:C:56:VAL:C	1:C:58:GLU:H	2.08	0.61
2:B:277:THR:HG21	2:B:527:TYR:OH	1.99	0.61
2:B:383:HIS:CD2	2:B:385:PRO:HG2	2.35	0.61
1:C:144:ASN:HB2	1:C:174:GLY:O	1.99	0.61
2:D:41:LEU:O	2:D:535:VAL:HG11	2.00	0.61
1:A:253:ASN:O	1:A:257:LEU:HB2	2.01	0.61
1:C:91:ASN:O	1:C:95:ILE:HD12	2.00	0.61
1:C:134:ALA:C	1:C:136:GLY:N	2.51	0.61
2:D:166:GLN:O	2:D:168:GLY:N	2.32	0.61
2:D:531:ILE:N	2:D:531:ILE:HD12	2.16	0.61
1:C:260:PRO:HA	2:D:56:ASP:OD2	2.01	0.61
2:D:179:HIS:HE2	2:D:516:ARG:HB2	1.66	0.61
2:D:410:ARG:HG2	2:D:410:ARG:NH1	2.09	0.61
2:B:108:HIS:CE1	2:B:417:GLN:NE2	2.63	0.61
2:D:241:GLU:O	2:D:245:LEU:HB2	2.01	0.61
2:D:351:GLU:HG3	2:D:353:ARG:NE	2.16	0.61
2:B:38:MET:HG2	2:B:354:TYR:HB2	1.82	0.60
2:B:67:VAL:HG23	2:B:68:CYS:H	1.66	0.60
2:B:378:ALA:HB3	2:B:386:THR:HG21	1.81	0.60
1:C:224:THR:CG2	1:C:248:ALA:HA	2.30	0.60
2:D:32:ILE:HG13	2:D:509:THR:O	2.00	0.60
1:C:53:GLY:O	1:C:56:VAL:HG22	2.01	0.60
2:D:349:HIS:O	2:D:352:ASP:N	2.34	0.60
2:D:503:GLU:O	2:D:506:LEU:HB2	2.00	0.60
2:B:274:ILE:HD11	2:B:509:THR:HG23	1.83	0.60
2:B:502:VAL:HG23	2:B:527:TYR:CD2	2.36	0.60
1:C:255:TRP:HB3	2:D:60:PHE:CZ	2.35	0.60
2:D:122:ASN:ND2	2:D:175:PHE:HB2	2.16	0.60
2:D:235:ARG:HB3	2:D:237:GLU:OE2	2.01	0.60
2:D:247:LYS:HD2	2:D:248:GLU:N	2.16	0.60
2:B:109:LEU:HD21	2:B:252:PHE:HE2	1.65	0.60
2:D:274:ILE:CD1	2:D:510:PRO:HD3	2.32	0.60
1:C:145:ILE:HG22	1:C:150:PRO:HB3	1.83	0.60
2:D:11:VAL:HG22	2:D:14:ILE:HD13	1.84	0.60
2:D:185:PRO:O	2:D:188:VAL:HB	2.01	0.60
2:D:251:GLU:O	2:D:255:GLN:HB2	2.02	0.60
2:B:198:GLU:O	2:B:201:ARG:N	2.27	0.60
1:C:40:ILE:HG23	1:C:41:SER:H	1.67	0.60
2:D:271:TRP:CE3	2:D:274:ILE:HG23	2.36	0.60
2:D:274:ILE:HD12	2:D:510:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:C	1:A:235:GLN:NE2	2.60	0.60
1:C:3:ALA:N	2:D:165:GLY:O	2.35	0.60
1:C:9:VAL:HA	1:C:69:VAL:O	2.01	0.60
1:C:54:HIS:HA	1:C:57:GLU:CB	2.32	0.60
2:D:62:GLN:HG2	2:D:62:GLN:O	1.99	0.60
2:D:269:LYS:HE3	2:D:399:VAL:HG13	1.82	0.60
1:A:20:CYS:SG	1:A:150:PRO:HD3	2.41	0.59
2:B:170:PHE:O	2:B:173:ALA:HB2	2.01	0.59
2:D:179:HIS:ND1	2:D:181:ALA:HB3	2.16	0.59
2:B:395:LYS:HG2	2:B:396:THR:N	2.14	0.59
2:B:454:GLN:HG3	2:B:471:VAL:HG22	1.84	0.59
2:B:345:TRP:CE2	2:B:347:GLU:HA	2.36	0.59
1:C:64:ILE:HD12	1:C:102:LYS:HE3	1.84	0.59
2:B:362:TYR:CG	2:B:363:LYS:N	2.70	0.59
2:B:384:GLU:HB3	2:B:385:PRO:HD3	1.84	0.59
2:D:271:TRP:CZ3	2:D:274:ILE:HG12	2.37	0.59
2:D:472:GLN:HE22	2:D:475:GLY:N	2.00	0.59
2:D:122:ASN:OD1	2:D:124:ALA:HB3	2.01	0.59
2:B:84:VAL:HG12	2:B:86:VAL:HG22	1.83	0.59
1:C:135:LEU:O	1:C:140:VAL:HG23	2.01	0.59
2:D:310:LYS:C	2:D:311:VAL:HG23	2.28	0.59
2:D:516:ARG:N	2:D:517:PRO:HD3	2.17	0.59
1:A:234:ASN:ND2	2:B:217:ASN:HB3	2.17	0.59
1:C:54:HIS:HA	1:C:57:GLU:HB2	1.85	0.59
2:D:27:VAL:CG2	2:D:32:ILE:HG12	2.33	0.59
2:D:500:SER:HB2	2:D:503:GLU:HG3	1.84	0.59
2:D:88:ILE:HG13	2:D:88:ILE:O	2.02	0.59
2:B:183:VAL:HG12	2:B:183:VAL:O	2.03	0.59
2:D:347:GLU:O	2:D:348:PHE:HB2	2.03	0.59
2:D:484:VAL:HG12	2:D:485:PRO:HD2	1.84	0.59
1:A:232:LEU:HD13	1:A:237:ASN:N	2.18	0.58
2:D:62:GLN:OE1	2:D:219:HIS:HA	2.03	0.58
1:C:111:THR:HA	1:C:114:THR:OG1	2.04	0.58
2:B:113:TYR:HE2	2:B:195:HIS:HB2	1.67	0.58
2:B:280:PHE:HB3	2:B:373:ALA:HB2	1.85	0.58
1:C:191:LEU:O	1:C:194:PHE:HB3	2.03	0.58
2:D:372:LEU:HA	2:D:375:VAL:CG2	2.34	0.58
2:B:224:VAL:O	2:B:227:GLY:HA2	2.02	0.58
2:B:302:VAL:HG13	2:B:312:ASP:O	2.02	0.58
2:D:199:ALA:C	2:D:201:ARG:H	2.10	0.58
2:D:372:LEU:O	2:D:375:VAL:HG23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HD13	1:A:163:LEU:H	1.67	0.58
2:B:355:SER:CB	2:B:492:PRO:HD3	2.32	0.58
2:B:435:ASN:O	2:B:438:ALA:HB3	2.04	0.58
2:D:324:LYS:HD3	2:D:495:ALA:CB	2.33	0.58
1:A:220:LYS:C	1:A:222:PRO:CD	2.77	0.58
2:D:80:VAL:O	2:D:84:VAL:HB	2.03	0.58
2:B:70:TYR:HD1	2:B:220:THR:HG21	1.68	0.58
2:B:122:ASN:O	2:B:123:VAL:C	2.47	0.58
1:C:173:GLN:HA	1:C:173:GLN:NE2	2.19	0.58
2:D:113:TYR:O	2:D:117:ALA:HB3	2.03	0.58
2:D:185:PRO:HG2	2:D:188:VAL:CG2	2.33	0.58
1:A:40:ILE:HG23	1:A:41:SER:H	1.69	0.57
1:A:62:GLU:O	1:A:65:LYS:HB2	2.03	0.57
2:B:156:ALA:HA	2:B:159:LYS:HB2	1.86	0.57
2:D:199:ALA:C	2:D:201:ARG:N	2.60	0.57
2:D:265:ALA:O	2:D:266:GLY:C	2.47	0.57
2:D:387:VAL:HA	2:D:390:VAL:CG1	2.34	0.57
2:D:449:TYR:C	2:D:450:PRO:O	2.45	0.57
2:B:11:VAL:O	2:B:11:VAL:HG22	2.04	0.57
2:B:64:ALA:HB3	2:B:72:HIS:CD2	2.39	0.57
2:B:127:LEU:HD11	2:B:159:LYS:CG	2.32	0.57
1:C:35:LEU:O	1:C:40:ILE:HG22	2.04	0.57
2:B:404:LEU:O	2:B:409:GLY:HA3	2.05	0.57
2:B:496:GLU:HB3	2:B:498:LYS:NZ	2.19	0.57
2:D:470:ILE:HG13	2:D:480:PHE:CD2	2.40	0.57
1:A:239:PRO:HB3	2:B:221:GLN:HE21	1.69	0.57
1:C:56:VAL:C	1:C:58:GLU:N	2.62	0.57
1:A:68:PHE:CE1	1:A:103:ALA:HB2	2.40	0.57
2:D:355:SER:CB	2:D:492:PRO:HD3	2.34	0.57
1:C:122:LYS:O	2:D:48:ILE:HG23	2.04	0.57
2:B:22:ARG:HG2	2:B:38:MET:HB2	1.87	0.57
2:B:82:ASN:HD22	2:B:455:GLY:HA2	1.69	0.57
2:D:286:PHE:HB3	2:D:428:TRP:CZ2	2.40	0.57
2:D:463:ARG:O	2:D:485:PRO:HB2	2.05	0.57
1:C:34:GLU:O	1:C:39:VAL:HG23	2.04	0.57
2:B:96:ARG:NH2	2:B:227:GLY:CA	2.68	0.57
2:D:17:ILE:HD12	2:D:531:ILE:CD1	2.34	0.57
1:A:28:VAL:O	1:A:30:PRO:CD	2.51	0.56
2:B:34:ASN:O	2:B:35:ALA:O	2.23	0.56
2:B:234:LEU:HD12	2:B:436:VAL:HG21	1.85	0.56
2:D:232:ASP:OD1	2:D:235:ARG:NE	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:315:ASN:HD22	2:D:318:LEU:HG	1.70	0.56
2:D:363:LYS:C	2:D:365:GLU:H	2.13	0.56
1:A:86:LYS:HE3	2:B:345:TRP:CH2	2.41	0.56
2:B:182:TYR:CE1	2:B:518:VAL:HG21	2.40	0.56
2:B:272:ALA:O	2:B:406:SER:HB3	2.06	0.56
2:B:392:LEU:HD23	2:B:393:VAL:N	2.20	0.56
1:C:27:THR:OG1	1:C:156:VAL:HG21	2.05	0.56
2:D:72:HIS:O	2:D:73:ALA:C	2.48	0.56
2:D:86:VAL:HG22	2:D:445:THR:CG2	2.36	0.56
2:D:340:VAL:CG2	2:D:342:LYS:HG3	2.35	0.56
2:B:113:TYR:CE2	2:B:195:HIS:HB2	2.40	0.56
2:B:471:VAL:O	2:B:478:GLU:HB2	2.05	0.56
2:D:509:THR:CG2	2:D:519:GLU:HB2	2.36	0.56
2:B:89:PRO:HD3	2:B:445:THR:HG1	1.68	0.56
1:C:74:GLY:O	1:C:112:CYS:HB3	2.05	0.56
2:D:329:GLU:HB2	2:D:344:LYS:HZ2	1.70	0.56
2:D:311:VAL:HG21	2:D:380:ALA:O	2.06	0.56
2:D:327:TRP:HZ2	2:D:348:PHE:HA	1.71	0.56
2:D:397:LEU:HB3	2:D:399:VAL:HG22	1.88	0.56
2:B:43:ARG:NH2	2:B:532:ALA:O	2.39	0.56
2:D:208:ARG:HG2	2:D:245:LEU:CD2	2.25	0.56
2:D:315:ASN:HD21	2:D:317:ASP:CB	2.18	0.56
2:B:89:PRO:O	2:B:92:ALA:N	2.38	0.56
2:B:323:VAL:O	2:B:325:TYR:N	2.36	0.56
1:C:85:GLY:C	1:C:92:MET:HE3	2.30	0.56
2:B:499:LEU:HD23	2:B:503:GLU:HB3	1.87	0.56
1:C:50:ALA:HB2	2:D:118:LEU:HD23	1.88	0.56
2:B:134:ALA:O	2:B:191:ILE:HD11	2.06	0.56
2:B:401:PRO:O	2:B:404:LEU:HB2	2.06	0.56
2:D:234:LEU:HD21	2:D:443:LEU:HD21	1.87	0.56
2:D:234:LEU:CD2	2:D:443:LEU:HD21	2.36	0.55
2:D:394:LEU:HD12	2:D:399:VAL:HG23	1.87	0.55
1:A:126:THR:HG21	2:B:42:PHE:O	2.06	0.55
1:A:188:CYS:O	1:A:191:LEU:HB2	2.06	0.55
1:C:167:MET:HG3	1:C:168:PRO:CD	2.36	0.55
1:C:135:LEU:HB3	1:C:140:VAL:CG2	2.36	0.55
2:D:433:GLU:O	2:D:437:LYS:CG	2.54	0.55
1:A:56:VAL:O	1:A:59:ALA:HB3	2.07	0.55
2:B:311:VAL:HG21	2:B:380:ALA:CB	2.36	0.55
2:B:323:VAL:HG23	2:B:331:ALA:HA	1.88	0.55
1:C:24:LEU:C	1:C:26:ARG:N	2.63	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:101:GLY:O	2:D:105:MET:HG3	2.05	0.55
1:C:29:ASP:O	1:C:31:TYR:HD1	1.89	0.55
2:B:23:ILE:HD12	2:B:524:VAL:HG21	1.88	0.55
2:D:17:ILE:HD12	2:D:531:ILE:HD13	1.87	0.55
2:D:493:ARG:HH12	2:D:499:LEU:HD23	1.69	0.55
2:B:438:ALA:CB	2:B:440:LYS:CG	2.85	0.55
1:C:100:ALA:C	1:C:102:LYS:H	2.15	0.55
2:D:12:ASP:HB2	2:D:22:ARG:HG3	1.89	0.55
2:D:389:ALA:O	2:D:393:VAL:HG12	2.07	0.55
2:D:457:GLY:O	2:D:467:SER:HA	2.07	0.55
2:B:259:THR:O	2:B:262:LEU:HB2	2.06	0.55
2:B:239:ILE:HG23	2:B:429:LEU:HD11	1.89	0.55
2:B:399:VAL:HG23	2:B:400:GLY:N	2.21	0.55
2:D:408:LEU:O	2:D:412:ALA:N	2.40	0.55
1:A:40:ILE:O	1:A:41:SER:CB	2.55	0.55
1:A:221:GLY:HA3	3:A:265:SF4:S3	2.47	0.55
2:B:347:GLU:O	2:B:348:PHE:CB	2.54	0.55
2:B:387:VAL:O	2:B:389:ALA:N	2.40	0.55
2:B:387:VAL:C	2:B:389:ALA:N	2.65	0.55
1:A:84:TRP:O	2:B:41:LEU:HA	2.06	0.54
2:B:345:TRP:HZ2	2:B:347:GLU:OE2	1.89	0.54
2:D:485:PRO:O	2:D:488:TRP:N	2.35	0.54
2:B:198:GLU:C	2:B:200:LEU:N	2.64	0.54
2:D:58:GLN:HG3	2:D:59:HIS:N	2.21	0.54
2:D:196:TYR:HD1	2:D:197:LEU:HD23	1.72	0.54
2:D:320:GLU:HG3	2:D:333:ALA:HB1	1.89	0.54
2:D:323:VAL:CG1	2:D:328:TYR:HB2	2.35	0.54
1:A:26:ARG:NH1	2:B:203:GLN:OE1	2.41	0.54
1:A:112:CYS:SG	1:A:117:GLY:HA3	2.47	0.54
2:B:14:ILE:HD11	2:B:23:ILE:CG1	2.31	0.54
1:C:35:LEU:O	1:C:39:VAL:HB	2.07	0.54
2:D:487:THR:OG1	2:D:534:GLY:HA2	2.07	0.54
1:A:90:ARG:NH1	1:A:98:GLU:OE1	2.35	0.54
1:A:234:ASN:O	1:A:235:GLN:HG2	2.07	0.54
2:B:118:LEU:HD12	2:B:118:LEU:H	1.71	0.54
2:B:214:GLY:O	2:B:215:ALA:HB3	2.08	0.54
2:D:302:VAL:O	2:D:311:VAL:HA	2.07	0.54
2:B:244:LYS:O	2:B:247:LYS:HG3	2.07	0.54
1:C:117:GLY:C	1:C:119:GLN:N	2.64	0.54
1:C:145:ILE:HD12	1:C:154:ASN:O	2.07	0.54
2:D:162:VAL:C	2:D:164:SER:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:ARG:CG	2:D:245:LEU:HD21	2.26	0.54
2:D:278:SER:O	2:D:279:ASN:HB2	2.08	0.54
2:D:285:GLU:HB2	2:D:460:ASN:HB3	1.88	0.54
2:D:484:VAL:HG12	2:D:485:PRO:CD	2.38	0.54
2:B:348:PHE:C	2:B:350:GLY:H	2.14	0.54
1:A:221:GLY:N	1:A:222:PRO:HD2	2.17	0.54
2:B:350:GLY:C	2:B:352:ASP:N	2.63	0.54
2:B:387:VAL:O	2:B:388:LYS:C	2.51	0.54
2:B:524:VAL:O	2:B:529:PRO:HD3	2.08	0.54
2:D:11:VAL:HG13	2:D:23:ILE:HG13	1.90	0.54
1:A:3:ALA:N	2:B:165:GLY:HA3	2.23	0.54
2:B:281:LEU:CD2	2:B:369:VAL:HG12	2.38	0.54
2:B:304:TRP:HH2	2:B:363:LYS:HB2	1.72	0.54
2:B:484:VAL:HG12	2:B:485:PRO:HD2	1.90	0.54
2:B:500:SER:O	2:B:501:ALA:C	2.51	0.54
2:D:164:SER:HB3	2:D:166:GLN:HG3	1.88	0.54
2:D:509:THR:HG23	2:D:519:GLU:HB2	1.89	0.54
2:B:222:PHE:CE1	2:B:223:THR:HG23	2.43	0.54
2:B:242:PHE:CD1	2:B:243:ARG:N	2.76	0.54
2:B:484:VAL:CG1	2:B:485:PRO:HD2	2.38	0.54
1:C:123:PRO:HD3	2:D:48:ILE:HA	1.90	0.54
2:D:10:VAL:HG11	2:D:22:ARG:NH2	2.23	0.54
2:B:11:VAL:O	2:B:14:ILE:HD13	2.09	0.53
2:B:67:VAL:HG23	2:B:68:CYS:N	2.23	0.53
2:D:243:ARG:O	2:D:244:LYS:C	2.51	0.53
2:B:103:GLN:O	2:B:107:ASP:HB2	2.08	0.53
2:D:81:ASP:HB3	2:D:86:VAL:HG12	1.90	0.53
2:D:199:ALA:O	2:D:201:ARG:N	2.41	0.53
2:D:328:TYR:CE2	2:D:358:LYS:HG3	2.43	0.53
2:B:89:PRO:HB2	2:B:442:ASP:O	2.09	0.53
1:C:100:ALA:N	1:C:101:PRO:CD	2.71	0.53
2:D:123:VAL:O	2:D:124:ALA:C	2.51	0.53
2:D:362:TYR:O	2:D:364:GLY:N	2.42	0.53
1:A:214:LEU:O	1:A:215:TYR:C	2.51	0.53
2:B:243:ARG:HA	2:B:246:TYR:HB3	1.91	0.53
1:C:173:GLN:OE1	1:C:252:PRO:HG2	2.08	0.53
2:D:39:SER:CB	2:D:357:MET:HG3	2.38	0.53
2:B:70:TYR:O	2:B:73:ALA:N	2.36	0.53
2:B:137:LEU:O	2:B:140:ASP:HB2	2.09	0.53
1:C:185:HIS:HB3	1:C:222:PRO:HA	1.91	0.53
1:A:175:ARG:HD2	1:A:180:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LEU:HA	2:B:77:VAL:HG22	1.91	0.53
1:C:114:THR:HG22	1:C:144:ASN:HB3	1.90	0.53
1:C:237:ASN:CG	1:C:238:TRP:H	2.17	0.53
2:D:302:VAL:HG23	2:D:367:PHE:CE2	2.44	0.53
1:A:4:LYS:CD	1:A:5:LYS:H	2.22	0.53
1:A:33:ASP:O	1:A:37:LEU:HB2	2.09	0.53
1:A:93:TYR:O	1:A:96:CYS:HB2	2.09	0.53
2:B:494:CYS:SG	2:B:498:LYS:NZ	2.82	0.53
1:C:60:LEU:O	1:C:63:ALA:N	2.42	0.53
1:C:238:TRP:HB2	1:C:239:PRO:CD	2.39	0.53
2:D:138:ALA:HB2	2:D:191:ILE:HD13	1.91	0.53
1:A:194:PHE:HD2	1:A:195:GLU:OE2	1.92	0.53
1:A:214:LEU:CD1	1:A:240:VAL:HG13	2.37	0.53
2:D:10:VAL:HG13	2:D:24:GLU:CG	2.35	0.53
2:D:14:ILE:HG22	2:D:17:ILE:HG23	1.89	0.53
2:D:300:GLN:O	2:D:381:LYS:HE2	2.09	0.53
1:C:77:PRO:HB2	1:C:84:TRP:HB2	1.90	0.52
1:C:84:TRP:CG	1:C:126:THR:HB	2.44	0.52
2:D:32:ILE:N	2:D:509:THR:O	2.42	0.52
2:D:198:GLU:O	2:D:202:VAL:HG23	2.09	0.52
2:D:283:CYS:HB3	2:D:465:MET:CG	2.38	0.52
2:B:242:PHE:HD1	2:B:243:ARG:N	2.08	0.52
2:B:336:PRO:C	2:B:338:LYS:H	2.17	0.52
2:B:490:LEU:HD11	2:B:529:PRO:HA	1.91	0.52
2:D:51:GLY:HA2	2:D:477:ILE:O	2.09	0.52
2:D:327:TRP:CZ2	2:D:348:PHE:HD1	2.27	0.52
2:D:435:ASN:HA	2:D:438:ALA:HB3	1.92	0.52
1:A:86:LYS:O	2:B:40:THR:HG23	2.10	0.52
1:C:88:GLY:C	1:C:90:ARG:H	2.15	0.52
2:D:34:ASN:O	2:D:35:ALA:CB	2.56	0.52
2:D:234:LEU:HG	2:D:436:VAL:CG2	2.39	0.52
2:D:323:VAL:HG23	2:D:331:ALA:HA	1.90	0.52
2:B:142:SER:O	2:B:144:ARG:N	2.39	0.52
2:B:184:LEU:HD13	2:B:268:TYR:CE2	2.44	0.52
1:C:91:ASN:O	1:C:94:ASP:HB2	2.09	0.52
2:D:300:GLN:HG2	2:D:301:GLY:N	2.25	0.52
1:C:119:GLN:HG2	2:D:43:ARG:HG2	1.89	0.52
2:D:271:TRP:HE1	2:D:522:ARG:NH1	2.07	0.52
2:D:496:GLU:O	2:D:498:LYS:HD2	2.10	0.52
2:D:384:GLU:N	2:D:385:PRO:HD2	2.24	0.52
1:A:10:VAL:HG12	1:A:10:VAL:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:VAL:O	1:C:30:PRO:CD	2.53	0.52
1:A:135:LEU:O	1:A:140:VAL:HB	2.10	0.52
2:B:371:PRO:HA	2:B:374:SER:HB2	1.90	0.52
1:C:123:PRO:CD	2:D:48:ILE:HA	2.39	0.52
1:C:167:MET:HG3	1:C:168:PRO:HD2	1.92	0.52
2:D:400:GLY:O	2:D:403:ALA:HB3	2.10	0.52
1:A:234:ASN:HD21	2:B:217:ASN:HB3	1.75	0.52
2:D:122:ASN:CG	2:D:175:PHE:HB2	2.35	0.52
2:D:134:ALA:O	2:D:135:ALA:C	2.53	0.52
1:A:119:GLN:HG2	2:B:43:ARG:HG2	1.91	0.52
1:A:187:ASN:ND2	1:A:230:LYS:HE3	2.25	0.52
2:D:71:VAL:HG11	2:D:462:PRO:HD3	1.92	0.52
2:D:88:ILE:HG21	2:D:96:ARG:NH1	2.22	0.52
2:D:285:GLU:O	2:D:286:PHE:HB2	2.09	0.52
2:D:341:THR:OG1	2:D:481:GLN:NE2	2.39	0.52
1:A:220:LYS:HG2	1:A:258:TYR:CD1	2.45	0.51
2:B:62:GLN:HG3	2:B:73:ALA:HB2	1.92	0.51
2:B:354:TYR:OH	2:B:493:ARG:HG3	2.10	0.51
2:B:278:SER:O	2:B:279:ASN:CB	2.57	0.51
2:B:321:GLU:HA	2:B:360:PRO:HA	1.92	0.51
2:D:185:PRO:HG2	2:D:188:VAL:CB	2.40	0.51
2:B:20:HIS:CB	2:B:40:THR:HG22	2.40	0.51
2:B:274:ILE:HD12	2:B:510:PRO:HD2	1.92	0.51
1:C:151:ASN:HB2	1:C:233:PHE:CE1	2.44	0.51
2:D:280:PHE:HB3	2:D:373:ALA:HA	1.91	0.51
1:A:90:ARG:HG3	1:A:95:ILE:HG12	1.92	0.51
2:B:95:MET:HE1	2:B:230:ASN:O	2.10	0.51
1:C:125:PRO:HB3	2:D:47:MET:HE2	1.92	0.51
1:C:183:THR:HG22	1:C:225:TYR:CZ	2.45	0.51
2:D:499:LEU:H	2:D:499:LEU:HD12	1.75	0.51
1:A:28:VAL:O	1:A:29:ASP:HB3	2.10	0.51
2:B:95:MET:CE	2:B:233:SER:OG	2.59	0.51
2:B:222:PHE:O	2:B:228:CYS:HA	2.11	0.51
1:C:151:ASN:HB2	1:C:233:PHE:HE1	1.75	0.51
2:B:8:LYS:HA	2:B:25:VAL:O	2.11	0.51
2:B:81:ASP:OD1	2:B:225:VAL:HG13	2.11	0.51
2:B:473:ARG:O	2:B:476:LYS:HG2	2.09	0.51
2:B:480:PHE:HD1	2:B:480:PHE:O	1.94	0.51
2:D:17:ILE:CD1	2:D:21:LEU:HB3	2.40	0.51
2:D:62:GLN:HA	2:D:72:HIS:HB2	1.92	0.51
2:D:202:VAL:HG21	2:D:252:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:VAL:HG21	2:D:252:PHE:CE2	2.45	0.51
2:D:268:TYR:O	2:D:271:TRP:HB2	2.11	0.51
2:D:321:GLU:OE1	2:D:358:LYS:HD2	2.11	0.51
2:D:349:HIS:N	2:D:353:ARG:O	2.36	0.51
2:B:28:GLU:HG3	2:B:33:LYS:HD2	1.92	0.51
2:B:89:PRO:C	2:B:91:ASN:N	2.68	0.51
2:D:71:VAL:HG23	2:D:72:HIS:HD2	1.75	0.51
2:D:110:VAL:HA	2:D:114:HIS:ND1	2.26	0.51
2:D:357:MET:SD	2:D:486:SER:O	2.69	0.51
2:D:372:LEU:O	2:D:376:LEU:HG	2.11	0.51
2:B:379:TYR:C	2:B:381:LYS:H	2.19	0.51
2:D:308:LEU:N	2:D:308:LEU:HD23	2.25	0.51
2:B:281:LEU:HB3	2:B:367:PHE:CD2	2.46	0.51
1:C:118:VAL:HG12	1:C:255:TRP:CE2	2.46	0.51
2:D:239:ILE:HG23	2:D:429:LEU:HD11	1.92	0.51
2:B:75:ALA:HB2	2:B:459:VAL:CG2	2.40	0.50
2:B:215:ALA:HB2	2:B:221:GLN:O	2.11	0.50
1:C:77:PRO:C	1:C:79:GLY:H	2.18	0.50
1:C:113:ALA:O	1:C:131:VAL:HG23	2.11	0.50
2:D:271:TRP:HA	2:D:274:ILE:CG2	2.41	0.50
2:D:384:GLU:HB3	2:D:385:PRO:CD	2.41	0.50
1:A:52:ALA:HB2	2:B:521:LEU:HD21	1.92	0.50
1:A:118:VAL:HG12	1:A:255:TRP:CZ2	2.46	0.50
2:B:25:VAL:HG21	2:B:520:ILE:HD11	1.93	0.50
2:B:142:SER:OG	2:B:144:ARG:HB2	2.10	0.50
2:B:416:ILE:O	2:B:420:THR:HG23	2.10	0.50
2:B:421:ALA:O	2:B:425:VAL:HG23	2.11	0.50
2:D:48:ILE:O	2:D:52:ARG:NH1	2.39	0.50
2:D:383:HIS:O	2:D:386:THR:N	2.42	0.50
2:B:344:LYS:HA	2:B:344:LYS:CE	2.39	0.50
1:C:143:ILE:O	1:C:143:ILE:HG13	2.10	0.50
2:D:54:PRO:C	2:D:56:ASP:H	2.18	0.50
2:D:400:GLY:HA3	2:D:402:GLU:OE2	2.10	0.50
2:D:472:GLN:NE2	2:D:475:GLY:H	2.03	0.50
2:D:513:ASP:OD1	2:D:513:ASP:C	2.52	0.50
1:A:124:ASN:HD21	1:A:128:THR:H	1.59	0.50
2:B:20:HIS:HB3	2:B:40:THR:HG22	1.94	0.50
2:B:94:LEU:HD23	2:B:432:LEU:CA	2.42	0.50
2:B:230:ASN:ND2	2:B:233:SER:HB3	2.26	0.50
2:D:271:TRP:HA	2:D:274:ILE:HG23	1.93	0.50
1:C:29:ASP:O	1:C:31:TYR:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:18:GLU:CD	2:D:18:GLU:C	2.79	0.50
2:D:394:LEU:HD21	2:D:401:PRO:HA	1.94	0.50
2:D:515:LYS:C	2:D:516:ARG:HG3	2.36	0.50
2:B:195:HIS:O	2:B:196:TYR:C	2.53	0.50
2:B:389:ALA:HB1	2:B:416:ILE:HG12	1.93	0.50
2:D:106:HIS:CE1	2:D:203:GLN:HB2	2.46	0.50
2:D:142:SER:HB2	2:D:143:PRO:HD2	1.94	0.50
2:D:258:ILE:HG23	2:D:262:LEU:HD12	1.94	0.50
1:A:234:ASN:C	1:A:235:GLN:HE21	2.19	0.50
2:B:470:ILE:HG13	2:B:471:VAL:N	2.25	0.50
1:C:9:VAL:CG1	1:C:40:ILE:HD11	2.42	0.50
1:A:4:LYS:CG	1:A:5:LYS:H	2.25	0.50
1:A:19:GLY:HA3	3:A:267:SF4:S4	2.52	0.50
2:B:160:ALA:HA	2:B:163:GLU:HG3	1.94	0.50
2:B:386:THR:O	2:B:389:ALA:HB3	2.12	0.50
2:B:387:VAL:HA	2:B:390:VAL:CG1	2.42	0.50
2:B:395:LYS:O	2:B:398:GLY:N	2.44	0.50
2:D:14:ILE:O	2:D:14:ILE:CG2	2.60	0.50
2:D:107:ASP:OD2	2:D:462:PRO:HG2	2.12	0.50
1:C:20:CYS:HB2	1:C:73:GLU:OE2	2.11	0.49
2:D:283:CYS:HB3	2:D:465:MET:HG2	1.93	0.49
2:B:362:TYR:O	2:B:363:LYS:C	2.55	0.49
2:D:88:ILE:HD12	2:D:92:ALA:CB	2.40	0.49
1:A:18:THR:OG1	2:B:18:GLU:HG2	2.13	0.49
1:C:83:TYR:CD1	1:C:83:TYR:C	2.89	0.49
1:C:233:PHE:C	1:C:235:GLN:H	2.20	0.49
2:D:146:THR:O	2:D:147:THR:HG23	2.13	0.49
2:D:346:THR:HG21	2:D:353:ARG:HD2	1.95	0.49
1:A:126:THR:O	1:A:127:GLY:C	2.56	0.49
1:A:259:SER:HA	1:A:260:PRO:C	2.37	0.49
2:B:424:GLU:HG3	2:B:428:TRP:CZ2	2.47	0.49
2:D:36:TRP:HB3	2:D:354:TYR:CE2	2.47	0.49
2:D:484:VAL:CG1	2:D:533:CYS:HB3	2.41	0.49
2:B:304:TRP:HH2	2:B:363:LYS:CB	2.25	0.49
2:B:393:VAL:O	2:B:395:LYS:N	2.45	0.49
2:B:464:GLY:C	2:B:485:PRO:HG3	2.37	0.49
1:C:76:ILE:CG2	1:C:93:TYR:HB2	2.41	0.49
2:B:70:TYR:CD1	2:B:220:THR:HG21	2.47	0.49
2:B:127:LEU:HD21	2:B:159:LYS:HG3	1.93	0.49
1:C:15:ALA:HA	2:D:41:LEU:CD2	2.43	0.49
1:C:26:ARG:HA	2:D:204:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:107:ASP:CG	2:D:463:ARG:HH12	2.20	0.49
2:D:306:ASN:HB3	2:D:405:PHE:CE1	2.47	0.49
1:A:16:GLU:HB3	1:A:73:GLU:HG2	1.95	0.49
2:B:14:ILE:HG12	2:B:21:LEU:O	2.13	0.49
1:C:15:ALA:HA	2:D:41:LEU:HD21	1.94	0.49
1:C:36:ILE:CD1	1:C:42:MET:HB2	2.36	0.49
2:D:37:SER:H	2:D:354:TYR:HE2	1.61	0.49
2:D:369:VAL:O	2:D:489:ASN:ND2	2.40	0.49
1:C:191:LEU:O	1:C:191:LEU:HD12	2.12	0.49
1:A:194:PHE:HE1	1:A:215:TYR:CD1	2.31	0.49
2:B:527:TYR:O	2:B:528:ASP:C	2.55	0.49
1:C:86:LYS:O	2:D:40:THR:HG23	2.13	0.49
2:D:183:VAL:HG23	2:D:183:VAL:O	2.12	0.49
2:D:261:LEU:HD11	2:D:411:THR:HG22	1.94	0.48
1:A:256:ASP:OD1	2:B:52:ARG:NH2	2.45	0.48
2:B:22:ARG:HD3	2:B:38:MET:SD	2.53	0.48
2:B:118:LEU:HD12	2:B:118:LEU:N	2.28	0.48
2:B:513:ASP:OD2	2:B:516:ARG:HD3	2.13	0.48
1:C:80:ASP:H	1:C:84:TRP:NE1	2.07	0.48
2:D:82:ASN:ND2	2:D:455:GLY:HA2	2.27	0.48
2:D:409:GLY:O	2:D:412:ALA:HB3	2.13	0.48
1:A:50:ALA:HB2	2:B:118:LEU:HD23	1.94	0.48
2:B:11:VAL:O	2:B:14:ILE:CD1	2.61	0.48
2:B:53:ASP:OD2	2:B:55:ARG:HB2	2.13	0.48
2:B:54:PRO:HB3	2:B:470:ILE:HD13	1.94	0.48
1:C:6:ARG:HE	1:C:38:ASP:HA	1.79	0.48
2:D:126:ALA:HB1	2:D:190:LEU:HB2	1.95	0.48
2:D:134:ALA:HB1	2:D:151:LEU:HD13	1.95	0.48
2:D:209:ALA:HB1	2:D:242:PHE:CE2	2.48	0.48
2:D:531:ILE:CD1	2:D:531:ILE:H	2.27	0.48
2:B:112:PHE:HD2	2:B:113:TYR:CD1	2.32	0.48
2:B:195:HIS:ND1	2:B:260:ASP:OD2	2.36	0.48
1:A:188:CYS:SG	1:A:189:PRO:HD2	2.54	0.48
2:B:496:GLU:O	2:B:498:LYS:N	2.47	0.48
2:B:502:VAL:HG23	2:B:527:TYR:CE2	2.47	0.48
1:C:110:GLY:H	1:C:150:PRO:HG2	1.77	0.48
1:C:118:VAL:HG12	1:C:255:TRP:CZ2	2.49	0.48
2:D:344:LYS:HG3	2:D:345:TRP:N	2.28	0.48
2:B:94:LEU:HD23	2:B:432:LEU:HA	1.95	0.48
2:B:231:TYR:O	2:B:234:LEU:HB2	2.12	0.48
1:C:151:ASN:HD22	1:C:227:ASN:HD21	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:PHE:C	1:C:235:GLN:N	2.72	0.48
2:D:42:PHE:HE1	2:D:328:TYR:HH	1.58	0.48
2:D:250:ARG:HG2	2:D:250:ARG:HH11	1.78	0.48
1:A:189:PRO:C	1:A:191:LEU:N	2.71	0.48
2:B:25:VAL:HG11	2:B:32:ILE:HD12	1.95	0.48
2:B:70:TYR:CZ	2:B:74:LEU:HG	2.47	0.48
2:D:490:LEU:HD11	2:D:529:PRO:HG3	1.96	0.48
1:A:3:ALA:O	1:A:4:LYS:CB	2.59	0.48
2:B:110:VAL:O	2:B:110:VAL:CG1	2.61	0.48
2:D:70:TYR:O	2:D:71:VAL:C	2.56	0.48
2:D:222:PHE:O	2:D:228:CYS:HA	2.13	0.48
1:A:51:GLY:O	2:B:15:THR:HG21	2.14	0.48
2:B:348:PHE:C	2:B:350:GLY:N	2.72	0.48
1:C:184:VAL:N	1:C:224:THR:O	2.43	0.48
2:D:383:HIS:C	2:D:385:PRO:HD2	2.38	0.48
1:A:33:ASP:O	1:A:34:GLU:C	2.57	0.48
1:A:63:ALA:C	1:A:65:LYS:H	2.22	0.48
1:C:193:HIS:CE1	1:C:212:TYR:CE1	3.01	0.48
2:D:130:ASP:HB3	2:D:133:LYS:HB2	1.96	0.48
2:B:375:VAL:HG21	2:B:416:ILE:HG22	1.95	0.47
2:D:82:ASN:ND2	2:D:456:VAL:H	2.11	0.47
2:D:460:ASN:ND2	2:D:464:GLY:O	2.44	0.47
1:A:202:SER:O	1:A:208:ALA:HB2	2.14	0.47
2:B:26:GLU:HG2	2:B:33:LYS:HD3	1.95	0.47
2:B:247:LYS:HD2	2:B:248:GLU:N	2.29	0.47
2:D:95:MET:HG2	2:D:222:PHE:HE2	1.77	0.47
1:A:100:ALA:CB	1:A:101:PRO:HD3	2.33	0.47
2:B:153:ALA:O	2:B:154:VAL:C	2.57	0.47
2:D:111:HIS:O	2:D:112:PHE:C	2.56	0.47
2:D:289:ASP:HB3	2:D:292:ASP:HB3	1.95	0.47
1:A:84:TRP:CG	1:A:126:THR:HG22	2.49	0.47
2:B:17:ILE:HG21	2:B:529:PRO:HG2	1.97	0.47
2:B:105:MET:O	2:B:109:LEU:HB2	2.15	0.47
2:B:272:ALA:HB2	2:B:408:LEU:HD12	1.96	0.47
1:C:216:GLU:HA	1:C:216:GLU:OE1	2.15	0.47
2:D:293:LEU:C	2:D:295:SER:H	2.22	0.47
2:D:387:VAL:CA	2:D:390:VAL:HG12	2.42	0.47
2:D:395:LYS:HE2	2:D:396:THR:OG1	2.14	0.47
1:A:247:ILE:HB	1:A:261:PHE:CE1	2.49	0.47
2:B:311:VAL:HG12	2:B:381:LYS:HE3	1.96	0.47
2:B:515:LYS:C	2:B:516:ARG:HG3	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:GLN:NE2	2:D:190:LEU:HD22	2.29	0.47
2:B:271:TRP:CZ3	2:B:274:ILE:HD13	2.50	0.47
2:B:456:VAL:HG21	2:B:458:PHE:CZ	2.49	0.47
1:C:17:CYS:O	1:C:18:THR:HB	2.14	0.47
1:C:173:GLN:HA	1:C:173:GLN:HE21	1.79	0.47
2:D:100:MET:O	2:D:101:GLY:C	2.58	0.47
2:D:275:GLY:O	2:D:406:SER:HA	2.15	0.47
2:D:470:ILE:HG13	2:D:480:PHE:HD2	1.78	0.47
2:D:531:ILE:N	2:D:531:ILE:CD1	2.77	0.47
1:A:40:ILE:O	1:A:41:SER:HB2	2.14	0.47
1:A:48:LEU:O	2:B:169:ILE:HG23	2.14	0.47
1:A:173:GLN:HA	1:A:173:GLN:HE21	1.79	0.47
1:A:192:LYS:HA	1:A:192:LYS:HD3	1.68	0.47
1:A:209:LYS:HG2	2:B:231:TYR:CE1	2.50	0.47
1:A:234:ASN:HA	1:A:235:GLN:NE2	2.29	0.47
2:B:490:LEU:CD2	2:B:529:PRO:HB3	2.44	0.47
1:C:172:LYS:HA	1:C:172:LYS:HD3	1.47	0.47
2:D:144:ARG:HD3	2:D:255:GLN:HG2	1.97	0.47
2:D:154:VAL:O	2:D:158:VAL:HG23	2.15	0.47
2:D:168:GLY:O	2:D:169:ILE:C	2.57	0.47
2:D:315:ASN:HD22	2:D:318:LEU:H	1.62	0.47
2:D:349:HIS:O	2:D:350:GLY:C	2.57	0.47
2:D:517:PRO:O	2:D:519:GLU:N	2.48	0.47
1:A:153:MET:HE2	1:A:153:MET:HB3	1.75	0.47
1:A:238:TRP:CZ3	1:A:240:VAL:HG23	2.50	0.47
2:D:347:GLU:O	2:D:348:PHE:CB	2.62	0.47
2:D:361:ARG:HH21	2:D:494:CYS:N	2.12	0.47
1:A:118:VAL:HG12	1:A:255:TRP:CE2	2.50	0.47
2:B:323:VAL:HG11	2:B:328:TYR:HB2	1.96	0.47
1:C:92:MET:HE2	2:D:20:HIS:CD2	2.50	0.47
2:D:88:ILE:HD13	2:D:96:ARG:HH11	1.80	0.47
1:A:232:LEU:HB2	1:A:237:ASN:O	2.15	0.47
2:B:34:ASN:HB3	2:B:36:TRP:CH2	2.50	0.47
2:B:118:LEU:H	2:B:118:LEU:CD1	2.28	0.47
2:B:490:LEU:CD1	2:B:529:PRO:HB3	2.45	0.47
1:C:24:LEU:HD21	1:C:155:PHE:CD2	2.50	0.47
1:C:162:LEU:HD22	1:C:162:LEU:H	1.80	0.47
2:D:32:ILE:CG2	2:D:507:ILE:HA	2.42	0.47
1:A:149:PRO:HG3	2:B:218:PRO:HG2	1.96	0.46
1:C:22:GLU:OE1	1:C:26:ARG:NH2	2.46	0.46
1:C:121:ALA:HB3	2:D:48:ILE:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:PRO:O	1:C:151:ASN:HB3	2.16	0.46
1:C:238:TRP:HB2	1:C:239:PRO:HD2	1.96	0.46
2:D:361:ARG:HH21	2:D:494:CYS:H	1.63	0.46
1:A:191:LEU:O	1:A:194:PHE:N	2.43	0.46
2:B:432:LEU:O	2:B:436:VAL:HG23	2.15	0.46
2:B:484:VAL:HG23	2:B:536:HIS:CE1	2.50	0.46
1:C:44:TYR:O	1:C:45:HIS:HB2	2.14	0.46
1:C:76:ILE:HG21	1:C:93:TYR:HB2	1.96	0.46
1:C:119:GLN:HB3	1:C:128:THR:HG21	1.97	0.46
1:C:185:HIS:HB2	1:C:221:GLY:C	2.40	0.46
2:D:137:LEU:O	2:D:141:LEU:HD22	2.15	0.46
2:D:271:TRP:NE1	2:D:522:ARG:NH1	2.63	0.46
2:D:452:GLU:HB3	2:D:473:ARG:HA	1.96	0.46
2:B:119:ASP:HB3	2:B:522:ARG:HG3	1.97	0.46
2:B:360:PRO:CD	2:B:487:THR:HG22	2.41	0.46
2:D:357:MET:CE	2:D:534:GLY:HA3	2.44	0.46
1:A:6:ARG:HB3	1:A:7:PRO:CD	2.45	0.46
1:C:185:HIS:HA	3:C:265:SF4:S3	2.56	0.46
2:D:485:PRO:O	2:D:487:THR:N	2.47	0.46
1:A:100:ALA:HB3	1:A:101:PRO:CD	2.38	0.46
1:A:162:LEU:C	1:A:164:THR:H	2.23	0.46
2:B:480:PHE:CD1	2:B:480:PHE:C	2.93	0.46
2:D:471:VAL:CG2	2:D:479:ASN:HB3	2.46	0.46
1:A:180:PHE:O	1:A:225:TYR:HB3	2.15	0.46
2:B:387:VAL:HA	2:B:390:VAL:HG13	1.97	0.46
1:C:191:LEU:HA	3:C:265:SF4:S1	2.56	0.46
1:C:234:ASN:O	1:C:235:GLN:HG2	2.16	0.46
2:D:34:ASN:HD21	2:D:493:ARG:HH22	1.63	0.46
2:D:393:VAL:HG11	2:D:416:ILE:HD11	1.97	0.46
2:D:472:GLN:NE2	2:D:475:GLY:N	2.61	0.46
1:A:162:LEU:O	1:A:164:THR:N	2.49	0.46
2:B:15:THR:HG23	2:B:16:ARG:N	2.28	0.46
1:C:224:THR:HG21	1:C:248:ALA:HA	1.98	0.46
1:A:7:PRO:O	1:A:40:ILE:O	2.33	0.46
1:A:79:GLY:C	1:A:81:GLY:H	2.24	0.46
1:A:114:THR:OG1	1:A:115:TYR:N	2.47	0.46
2:B:390:VAL:O	2:B:391:ASP:C	2.59	0.46
2:D:285:GLU:HA	2:D:296:ARG:HD3	1.98	0.46
2:D:346:THR:CG2	2:D:353:ARG:HD2	2.45	0.46
2:D:357:MET:SD	2:D:487:THR:HA	2.56	0.46
2:D:441:ASP:OD1	2:D:441:ASP:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:LEU:HG	2:B:42:PHE:N	2.25	0.46
2:D:464:GLY:HA3	2:D:485:PRO:HB3	1.97	0.46
2:B:34:ASN:HB3	2:B:36:TRP:CZ3	2.51	0.46
2:B:384:GLU:HB3	2:B:385:PRO:CD	2.45	0.46
1:C:117:GLY:O	1:C:119:GLN:N	2.48	0.46
2:D:371:PRO:O	2:D:375:VAL:HG22	2.16	0.46
2:D:482:HIS:HB2	2:D:536:HIS:NE2	2.31	0.46
2:D:502:VAL:O	2:D:506:LEU:HD23	2.15	0.46
2:B:11:VAL:HG22	2:B:14:ILE:HD13	1.98	0.45
2:B:52:ARG:O	2:B:477:ILE:HG13	2.15	0.45
2:B:134:ALA:O	2:B:137:LEU:HB3	2.15	0.45
2:B:300:GLN:HE21	2:B:300:GLN:HB3	1.49	0.45
1:C:77:PRO:HA	1:C:128:THR:CA	2.39	0.45
2:D:21:LEU:HB2	2:D:531:ILE:HG12	1.98	0.45
2:D:234:LEU:HD12	2:D:234:LEU:HA	1.76	0.45
2:D:384:GLU:HB3	2:D:385:PRO:HD3	1.98	0.45
2:D:494:CYS:SG	2:D:496:GLU:HB3	2.56	0.45
1:C:12:LEU:N	1:C:12:LEU:HD23	2.31	0.45
1:C:224:THR:HG23	1:C:248:ALA:HA	1.98	0.45
2:D:465:MET:HE3	2:D:465:MET:HB3	1.88	0.45
2:D:497:ARG:O	2:D:498:LYS:C	2.58	0.45
1:A:21:SER:O	1:A:25:LEU:HD13	2.16	0.45
2:B:279:ASN:OD1	2:B:305:GLY:N	2.34	0.45
2:B:386:THR:O	2:B:390:VAL:HG12	2.17	0.45
2:B:495:ALA:C	2:B:497:ARG:H	2.22	0.45
1:C:60:LEU:O	1:C:61:HIS:C	2.60	0.45
2:D:21:LEU:HB2	2:D:531:ILE:HD11	1.98	0.45
2:D:350:GLY:C	2:D:351:GLU:HG2	2.41	0.45
1:C:99:VAL:O	1:C:102:LYS:HB2	2.16	0.45
1:C:117:GLY:O	1:C:118:VAL:C	2.60	0.45
2:D:18:GLU:HG3	2:D:67:VAL:HG13	1.99	0.45
2:D:84:VAL:CG2	2:D:449:TYR:HD1	2.29	0.45
2:D:315:ASN:HA	2:D:316:PRO:HD2	1.84	0.45
1:A:35:LEU:HA	1:A:39:VAL:CB	2.42	0.45
2:B:119:ASP:O	2:B:522:ARG:NE	2.40	0.45
2:D:43:ARG:NH2	2:D:64:ALA:O	2.46	0.45
2:D:278:SER:O	2:D:279:ASN:CB	2.64	0.45
2:D:302:VAL:HG13	2:D:312:ASP:O	2.17	0.45
2:D:527:TYR:CA	2:D:529:PRO:HD3	2.46	0.45
1:A:14:ASN:O	1:A:16:GLU:HG3	2.17	0.45
2:B:80:VAL:O	2:B:83:CYS:N	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ILE:O	1:C:41:SER:CB	2.60	0.45
1:C:52:ALA:O	1:C:53:GLY:C	2.59	0.45
2:D:244:LYS:O	2:D:247:LYS:HG3	2.17	0.45
2:D:393:VAL:HG22	2:D:394:LEU:N	2.32	0.45
2:D:520:ILE:HG22	2:D:521:LEU:N	2.31	0.45
1:A:247:ILE:HB	1:A:261:PHE:CD1	2.52	0.45
2:B:344:LYS:HB3	2:B:345:TRP:H	1.58	0.45
1:C:8:SER:O	1:C:68:PHE:HA	2.17	0.45
2:D:54:PRO:C	2:D:56:ASP:N	2.73	0.45
2:D:74:LEU:HD22	2:D:74:LEU:O	2.16	0.45
2:D:86:VAL:HG13	2:D:87:LYS:N	2.31	0.45
2:D:217:ASN:C	2:D:217:ASN:HD22	2.25	0.45
2:D:315:ASN:ND2	2:D:317:ASP:N	2.64	0.45
2:D:523:THR:O	2:D:524:VAL:C	2.60	0.45
1:C:42:MET:HB2	1:C:42:MET:HE3	1.89	0.45
2:D:26:GLU:HG3	2:D:33:LYS:HB3	1.97	0.45
2:D:49:LEU:HG	2:D:477:ILE:CD1	2.45	0.45
2:D:79:ALA:O	2:D:82:ASN:HB3	2.17	0.45
2:D:230:ASN:ND2	2:D:233:SER:HB3	2.32	0.45
1:A:228:CYS:HB3	1:A:233:PHE:CE2	2.52	0.45
2:B:111:HIS:CD2	2:B:111:HIS:C	2.95	0.45
2:B:170:PHE:O	2:B:171:THR:C	2.59	0.45
2:B:363:LYS:C	2:B:363:LYS:HD3	2.42	0.45
1:C:182:GLU:OE1	1:C:187:ASN:OD1	2.35	0.45
1:A:242:ALA:HA	2:B:230:ASN:OD1	2.17	0.45
2:B:74:LEU:C	2:B:76:SER:N	2.75	0.45
2:B:76:SER:HG	2:B:480:PHE:HZ	1.65	0.45
2:B:316:PRO:HB2	2:B:469:TRP:HH2	1.82	0.45
2:B:350:GLY:C	2:B:352:ASP:H	2.25	0.45
2:D:30:GLY:C	2:D:31:LYS:O	2.59	0.45
2:D:254:GLU:O	2:D:255:GLN:C	2.60	0.45
1:A:80:ASP:O	1:A:83:TYR:HE2	2.01	0.44
2:B:369:VAL:HG23	2:B:370:GLY:N	2.32	0.44
2:B:394:LEU:HD11	2:B:404:LEU:HG	1.98	0.44
1:C:4:LYS:HB3	1:C:5:LYS:H	1.40	0.44
2:D:36:TRP:HB3	2:D:354:TYR:CD2	2.52	0.44
1:C:54:HIS:HA	1:C:57:GLU:HB3	1.99	0.44
2:D:232:ASP:C	2:D:234:LEU:H	2.25	0.44
2:D:277:THR:HG21	2:D:527:TYR:OH	2.16	0.44
2:D:366:ALA:O	2:D:367:PHE:O	2.36	0.44
2:B:450:PRO:O	2:B:451:THR:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:LEU:O	2:D:97:ASN:HB2	2.18	0.44
2:D:296:ARG:O	2:D:297:TYR:C	2.60	0.44
2:D:324:LYS:HD3	2:D:495:ALA:HA	1.99	0.44
2:D:345:TRP:CZ2	2:D:347:GLU:HA	2.51	0.44
1:A:90:ARG:HH22	1:A:98:GLU:HG3	1.82	0.44
2:B:25:VAL:CG2	2:B:520:ILE:HD11	2.47	0.44
2:B:61:THR:C	2:B:63:ARG:N	2.72	0.44
2:B:147:THR:O	2:B:150:SER:N	2.47	0.44
2:B:387:VAL:CG2	2:B:388:LYS:N	2.81	0.44
2:B:393:VAL:C	2:B:395:LYS:N	2.74	0.44
1:C:132:ASN:ND2	1:C:142:ALA:H	2.16	0.44
2:D:12:ASP:C	2:D:12:ASP:OD1	2.61	0.44
2:D:278:SER:HA	2:D:306:ASN:HD21	1.82	0.44
2:D:310:LYS:HD2	2:D:310:LYS:HA	1.75	0.44
2:D:315:ASN:ND2	2:D:315:ASN:C	2.75	0.44
2:B:280:PHE:CD2	2:B:376:LEU:HD12	2.52	0.44
2:B:336:PRO:C	2:B:338:LYS:N	2.73	0.44
1:C:52:ALA:HB2	2:D:521:LEU:HD11	1.99	0.44
2:D:227:GLY:O	2:D:444:TYR:N	2.49	0.44
2:D:344:LYS:O	2:D:345:TRP:HB3	2.17	0.44
2:B:343:PRO:HB3	2:B:356:TRP:HZ3	1.82	0.44
1:C:167:MET:HA	1:C:168:PRO:HD3	1.81	0.44
2:D:184:LEU:HB3	2:D:189:ASP:OD1	2.18	0.44
2:D:355:SER:HB3	2:D:492:PRO:HD3	2.00	0.44
1:C:91:ASN:HB2	1:C:94:ASP:OD1	2.18	0.44
1:C:238:TRP:CH2	1:C:240:VAL:HB	2.53	0.44
2:D:255:GLN:O	2:D:259:THR:CG2	2.65	0.44
2:D:296:ARG:O	2:D:298:THR:N	2.51	0.44
2:D:491:GLY:O	2:D:500:SER:CB	2.65	0.44
1:A:121:ALA:HB3	2:B:48:ILE:HG12	2.00	0.44
2:B:36:TRP:CD1	2:B:349:HIS:HE1	2.36	0.44
2:B:211:ALA:O	2:B:215:ALA:N	2.48	0.44
2:B:281:LEU:HD23	2:B:369:VAL:HG12	2.00	0.44
2:B:379:TYR:CD1	2:B:390:VAL:HG11	2.53	0.44
2:B:384:GLU:O	2:B:387:VAL:HG22	2.18	0.44
2:D:326:SER:C	2:D:328:TYR:H	2.25	0.44
2:D:370:GLY:O	2:D:374:SER:OG	2.28	0.44
2:D:456:VAL:HG21	2:D:469:TRP:CH2	2.53	0.44
2:B:308:LEU:N	2:B:308:LEU:HD23	2.32	0.44
2:B:387:VAL:HG23	2:B:388:LYS:N	2.32	0.44
1:C:124:ASN:HD22	1:C:124:ASN:HA	1.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:THR:OG1	1:C:165:LYS:N	2.50	0.44
2:D:74:LEU:O	2:D:77:VAL:HG22	2.17	0.44
1:A:4:LYS:CG	1:A:5:LYS:N	2.80	0.43
2:B:9:ILE:N	2:B:25:VAL:O	2.47	0.43
2:B:94:LEU:HD23	2:B:432:LEU:HB2	1.99	0.43
2:B:387:VAL:O	2:B:390:VAL:N	2.51	0.43
1:A:228:CYS:N	1:A:229:PRO:CD	2.81	0.43
2:B:74:LEU:O	2:B:76:SER:N	2.51	0.43
1:C:132:ASN:ND2	1:C:142:ALA:N	2.66	0.43
2:D:123:VAL:HG13	2:D:193:THR:CG2	2.48	0.43
2:D:147:THR:O	2:D:150:SER:N	2.49	0.43
2:D:336:PRO:HB2	2:D:469:TRP:CG	2.53	0.43
2:D:452:GLU:HA	2:D:472:GLN:O	2.18	0.43
2:B:264:VAL:C	2:B:266:GLY:N	2.75	0.43
1:C:188:CYS:HA	1:C:189:PRO:HD3	1.80	0.43
2:D:435:ASN:O	2:D:438:ALA:HB3	2.18	0.43
2:D:517:PRO:O	2:D:518:VAL:C	2.61	0.43
2:B:46:GLU:HG2	2:B:482:HIS:CD2	2.54	0.43
2:B:431:LYS:O	2:B:434:ALA:HB3	2.19	0.43
2:B:478:GLU:O	2:B:479:ASN:HB2	2.18	0.43
2:D:137:LEU:HA	2:D:140:ASP:HB2	2.01	0.43
2:D:472:GLN:HA	2:D:478:GLU:HB2	2.01	0.43
2:B:389:ALA:O	2:B:393:VAL:HG23	2.19	0.43
2:B:511:ILE:CG2	2:B:519:GLU:HG2	2.47	0.43
1:C:182:GLU:C	1:C:225:TYR:CD1	2.97	0.43
2:D:325:TYR:HD2	2:D:493:ARG:O	2.01	0.43
1:A:9:VAL:CB	1:A:40:ILE:HD11	2.49	0.43
1:A:18:THR:HG22	1:A:21:SER:HB2	2.01	0.43
2:B:23:ILE:CD1	2:B:524:VAL:HG21	2.48	0.43
2:B:452:GLU:HB3	2:B:473:ARG:HD2	2.01	0.43
1:C:255:TRP:HB3	2:D:60:PHE:HZ	1.82	0.43
2:D:23:ILE:HD11	2:D:520:ILE:HD13	2.01	0.43
2:D:147:THR:O	2:D:148:THR:C	2.62	0.43
2:D:409:GLY:HA2	2:D:412:ALA:HB3	2.01	0.43
1:A:23:SER:O	1:A:152:PRO:HG3	2.17	0.43
2:B:100:MET:HE3	2:B:459:VAL:HG13	2.00	0.43
2:B:384:GLU:N	2:B:385:PRO:HD2	2.33	0.43
1:C:4:LYS:HB2	2:D:164:SER:O	2.18	0.43
2:D:12:ASP:HB2	2:D:22:ARG:CG	2.48	0.43
2:D:153:ALA:O	2:D:156:ALA:HB3	2.18	0.43
2:D:262:LEU:HD23	2:D:262:LEU:HA	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:372:LEU:HA	2:D:375:VAL:HG22	1.99	0.43
2:D:390:VAL:CG2	2:D:404:LEU:HD11	2.49	0.43
2:B:14:ILE:O	2:B:14:ILE:CG2	2.66	0.43
2:B:80:VAL:C	2:B:82:ASN:N	2.73	0.43
2:B:142:SER:C	2:B:144:ARG:N	2.77	0.43
1:C:17:CYS:C	1:C:19:GLY:H	2.26	0.43
2:D:112:PHE:O	2:D:117:ALA:N	2.44	0.43
2:D:390:VAL:O	2:D:393:VAL:HG13	2.18	0.43
2:B:49:LEU:HA	2:B:52:ARG:HD2	2.01	0.43
2:B:76:SER:O	2:B:77:VAL:C	2.60	0.43
2:B:486:SER:HB3	2:B:490:LEU:HD12	2.01	0.43
1:C:150:PRO:O	1:C:151:ASN:O	2.37	0.43
2:D:9:ILE:HD11	2:D:511:ILE:HD12	2.01	0.43
2:D:34:ASN:ND2	2:D:36:TRP:CZ2	2.87	0.43
2:D:355:SER:HB3	2:D:492:PRO:CD	2.48	0.43
2:D:506:LEU:HD22	2:D:506:LEU:HA	1.87	0.43
2:D:527:TYR:C	2:D:529:PRO:CD	2.81	0.43
2:B:80:VAL:HA	2:B:83:CYS:SG	2.59	0.43
2:B:179:HIS:HB3	2:B:182:TYR:HD1	1.84	0.43
2:B:484:VAL:HG11	2:B:533:CYS:HB3	2.00	0.43
2:D:376:LEU:O	2:D:379:TYR:N	2.51	0.43
2:D:458:PHE:CD1	2:D:467:SER:HB3	2.54	0.43
2:D:502:VAL:CG1	2:D:503:GLU:N	2.82	0.43
1:C:145:ILE:HD11	1:C:158:THR:HG21	2.00	0.42
1:C:255:TRP:HE3	2:D:60:PHE:CE1	2.36	0.42
2:D:524:VAL:C	2:D:526:SER:N	2.77	0.42
1:A:239:PRO:CB	2:B:221:GLN:NE2	2.79	0.42
2:B:11:VAL:HG22	2:B:14:ILE:CD1	2.48	0.42
2:B:71:VAL:HG23	2:B:466:LEU:CD2	2.49	0.42
2:B:198:GLU:O	2:B:200:LEU:N	2.52	0.42
2:B:498:LYS:NZ	2:B:498:LYS:HB2	2.33	0.42
2:D:63:ARG:HG3	2:D:219:HIS:NE2	2.35	0.42
2:D:293:LEU:O	2:D:296:ARG:HG3	2.19	0.42
2:D:307:ASP:C	2:D:309:SER:H	2.27	0.42
2:D:467:SER:OG	2:D:483:VAL:CG2	2.68	0.42
2:D:509:THR:HA	2:D:510:PRO:HD3	1.84	0.42
1:A:14:ASN:ND2	1:A:92:MET:HB3	2.32	0.42
1:A:75:GLY:N	1:A:113:ALA:HA	2.35	0.42
2:B:135:ALA:HB2	2:B:151:LEU:HD12	2.01	0.42
2:B:419:LEU:HD12	2:B:419:LEU:HA	1.87	0.42
1:C:52:ALA:HB3	2:D:174:TYR:OH	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:VAL:O	1:C:58:GLU:N	2.52	0.42
2:D:238:ARG:HD2	2:D:238:ARG:HA	1.82	0.42
2:D:311:VAL:CG1	2:D:381:LYS:HD2	2.37	0.42
2:D:387:VAL:CG2	2:D:388:LYS:N	2.82	0.42
1:A:220:LYS:HG2	1:A:258:TYR:HD1	1.84	0.42
2:B:375:VAL:HG11	2:B:416:ILE:HG21	2.02	0.42
2:B:388:LYS:HB3	2:B:388:LYS:HE2	1.78	0.42
2:D:92:ALA:HA	2:D:228:CYS:SG	2.60	0.42
2:D:123:VAL:HG13	2:D:193:THR:HG21	2.00	0.42
2:D:129:ALA:HA	2:D:187:GLU:OE1	2.20	0.42
2:D:216:LYS:HG2	2:D:219:HIS:O	2.20	0.42
2:D:298:THR:HA	2:D:299:PRO:HD2	1.78	0.42
2:B:67:VAL:CG2	2:B:68:CYS:H	2.32	0.42
2:B:184:LEU:HA	2:B:185:PRO:HD3	1.85	0.42
2:B:244:LYS:O	2:B:248:GLU:HG2	2.19	0.42
1:A:145:ILE:HG22	1:A:150:PRO:HB3	2.01	0.42
2:B:213:PHE:O	2:B:230:ASN:ND2	2.50	0.42
2:B:234:LEU:O	2:B:235:ARG:C	2.61	0.42
2:B:362:TYR:CD2	2:B:363:LYS:N	2.71	0.42
2:D:112:PHE:HB2	2:D:257:TYR:CE1	2.38	0.42
2:D:316:PRO:O	2:D:319:ILE:HG23	2.19	0.42
1:A:227:ASN:HD22	1:A:227:ASN:N	2.10	0.42
2:B:260:ASP:O	2:B:261:LEU:C	2.63	0.42
2:D:10:VAL:HG11	2:D:22:ARG:CZ	2.49	0.42
2:D:34:ASN:HD21	2:D:493:ARG:NH2	2.18	0.42
2:D:179:HIS:HA	2:D:180:PRO:HD2	1.73	0.42
2:D:278:SER:HB3	2:D:306:ASN:OD1	2.20	0.42
2:D:434:ALA:O	2:D:435:ASN:C	2.63	0.42
1:A:9:VAL:HG22	1:A:69:VAL:HG12	2.00	0.42
2:B:119:ASP:HB3	2:B:522:ARG:CG	2.50	0.42
2:B:292:ASP:HB3	2:B:295:SER:HB3	2.02	0.42
2:B:323:VAL:CG1	2:B:328:TYR:HB2	2.50	0.42
2:B:371:PRO:O	2:B:372:LEU:C	2.62	0.42
2:B:395:LYS:O	2:B:397:LEU:N	2.53	0.42
1:C:17:CYS:HB2	2:D:65:CYS:CA	2.45	0.42
2:D:214:GLY:O	2:D:215:ALA:HB3	2.20	0.42
2:D:280:PHE:HE2	2:D:306:ASN:ND2	2.17	0.42
2:D:284:GLY:HA2	2:D:298:THR:O	2.19	0.42
2:D:484:VAL:HG21	2:D:533:CYS:O	2.20	0.42
2:B:44:GLY:O	2:B:48:ILE:HD12	2.20	0.42
1:C:148:CYS:HB3	1:C:249:CYS:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:TRP:HB3	2:D:535:VAL:HG13	2.00	0.42
2:B:34:ASN:O	2:B:35:ALA:C	2.63	0.42
2:B:272:ALA:HA	2:B:406:SER:OG	2.20	0.42
1:C:244:HIS:CG	1:C:245:PRO:HD2	2.55	0.42
2:D:83:CYS:HB3	2:D:455:GLY:HA3	2.01	0.42
2:D:258:ILE:O	2:D:259:THR:C	2.61	0.42
2:D:417:GLN:C	2:D:419:LEU:H	2.28	0.42
1:A:238:TRP:CZ3	1:A:240:VAL:CG2	3.03	0.41
2:B:336:PRO:HG2	2:B:469:TRP:CE2	2.54	0.41
2:B:454:GLN:CG	2:B:471:VAL:HG22	2.48	0.41
1:C:14:ASN:CA	1:C:92:MET:SD	3.07	0.41
1:C:14:ASN:ND2	1:C:96:CYS:SG	2.80	0.41
1:C:62:GLU:O	1:C:65:LYS:HB2	2.20	0.41
2:D:276:LYS:HA	2:D:405:PHE:O	2.19	0.41
2:D:316:PRO:C	2:D:318:LEU:N	2.76	0.41
1:A:35:LEU:C	1:A:37:LEU:H	2.28	0.41
1:C:97:ALA:O	1:C:101:PRO:HG3	2.20	0.41
1:C:117:GLY:C	1:C:119:GLN:H	2.27	0.41
2:D:179:HIS:HB3	2:D:182:TYR:HD1	1.85	0.41
2:D:414:ARG:HB2	2:D:414:ARG:NH1	2.34	0.41
2:B:133:LYS:HB3	2:B:187:GLU:OE1	2.20	0.41
1:C:11:TYR:CE2	1:C:71:VAL:HG11	2.56	0.41
1:C:93:TYR:HE1	1:C:135:LEU:HD13	1.84	0.41
1:C:96:CYS:O	1:C:101:PRO:HD3	2.21	0.41
1:C:221:GLY:N	1:C:222:PRO:CD	2.83	0.41
2:D:139:ASN:OD1	2:D:145:LYS:HA	2.20	0.41
2:D:147:THR:O	2:D:150:SER:OG	2.25	0.41
2:D:308:LEU:HD21	2:D:405:PHE:HZ	1.85	0.41
2:B:195:HIS:O	2:B:198:GLU:N	2.48	0.41
2:D:244:LYS:O	2:D:247:LYS:HE2	2.21	0.41
2:D:302:VAL:HG23	2:D:367:PHE:HE2	1.84	0.41
2:B:83:CYS:HA	2:B:454:GLN:O	2.20	0.41
2:B:84:VAL:CG1	2:B:86:VAL:HG22	2.51	0.41
1:C:20:CYS:HB2	1:C:73:GLU:CD	2.46	0.41
1:C:135:LEU:O	1:C:136:GLY:C	2.63	0.41
1:C:209:LYS:C	1:C:211:GLY:N	2.76	0.41
2:D:95:MET:HG2	2:D:95:MET:O	2.20	0.41
2:D:397:LEU:HB3	2:D:399:VAL:CG2	2.50	0.41
1:A:87:VAL:HG22	1:A:95:ILE:CD1	2.49	0.41
1:A:151:ASN:O	1:A:152:PRO:C	2.64	0.41
2:B:214:GLY:O	2:B:215:ALA:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:SER:HB3	2:B:306:ASN:OD1	2.21	0.41
1:C:28:VAL:HG21	1:C:235:GLN:NE2	2.36	0.41
1:C:236:VAL:CG1	2:D:212:ILE:HD13	2.49	0.41
2:D:142:SER:HB3	2:D:259:THR:HG21	2.03	0.41
1:A:29:ASP:CG	1:A:30:PRO:HD3	2.45	0.41
1:A:162:LEU:C	1:A:164:THR:N	2.79	0.41
2:B:424:GLU:O	2:B:425:VAL:C	2.62	0.41
1:C:61:HIS:O	1:C:65:LYS:HG3	2.20	0.41
1:A:199:PHE:HB2	1:A:216:GLU:HG3	2.03	0.41
2:B:271:TRP:HH2	2:B:519:GLU:HB3	1.86	0.41
2:B:480:PHE:HD1	2:B:480:PHE:C	2.28	0.41
1:C:14:ASN:OD1	1:C:14:ASN:N	2.53	0.41
1:C:205:SER:HA	1:C:206:PRO:HD3	1.90	0.41
2:D:250:ARG:HG2	2:D:250:ARG:NH1	2.33	0.41
2:D:413:ALA:O	2:D:416:ILE:N	2.53	0.41
2:D:524:VAL:HG13	2:D:529:PRO:HG2	2.01	0.41
2:D:531:ILE:HD12	2:D:531:ILE:H	1.81	0.41
2:B:70:TYR:CE2	2:B:99:THR:HG22	2.55	0.41
2:B:322:HIS:NE2	2:B:361:ARG:HB2	2.36	0.41
2:B:409:GLY:O	2:B:410:ARG:C	2.64	0.41
2:B:473:ARG:HB3	2:B:478:GLU:CG	2.51	0.41
1:C:60:LEU:O	1:C:62:GLU:N	2.54	0.41
2:D:11:VAL:HG11	2:D:520:ILE:HG21	2.03	0.41
2:D:21:LEU:HB2	2:D:531:ILE:CG1	2.50	0.41
2:D:28:GLU:OE2	2:D:33:LYS:NZ	2.50	0.41
2:D:69:THR:O	2:D:70:TYR:CB	2.66	0.41
2:D:69:THR:OG1	2:D:219:HIS:N	2.51	0.41
2:D:71:VAL:HG12	2:D:100:MET:HE1	2.03	0.41
2:D:74:LEU:HD23	2:D:74:LEU:HA	1.86	0.41
2:D:104:TYR:HD1	2:D:462:PRO:HG3	1.86	0.41
2:D:179:HIS:C	2:D:181:ALA:N	2.76	0.41
2:D:340:VAL:HG23	2:D:341:THR:N	2.35	0.41
2:D:387:VAL:C	2:D:389:ALA:N	2.78	0.41
2:D:494:CYS:O	2:D:495:ALA:C	2.64	0.41
1:A:154:ASN:O	1:A:158:THR:HB	2.21	0.41
2:B:242:PHE:CE1	2:B:429:LEU:HD22	2.56	0.41
2:B:350:GLY:O	2:B:351:GLU:C	2.63	0.41
2:B:533:CYS:O	2:B:536:HIS:ND1	2.53	0.41
1:C:18:THR:O	1:C:21:SER:N	2.54	0.41
2:D:49:LEU:HA	2:D:52:ARG:HD2	2.02	0.41
2:D:517:PRO:C	2:D:519:GLU:N	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:VAL:HG23	1:A:119:GLN:N	2.36	0.40
2:B:88:ILE:HA	2:B:89:PRO:HD3	1.98	0.40
1:C:9:VAL:HG11	1:C:40:ILE:HD11	2.04	0.40
2:D:14:ILE:HG22	2:D:17:ILE:CG2	2.50	0.40
2:D:95:MET:CE	2:D:234:LEU:HD13	2.51	0.40
2:D:279:ASN:C	2:D:280:PHE:CG	2.99	0.40
2:D:417:GLN:C	2:D:419:LEU:N	2.77	0.40
2:D:513:ASP:HA	2:D:514:PRO:HD2	1.85	0.40
1:A:231:GLN:O	1:A:232:LEU:HG	2.22	0.40
2:B:126:ALA:C	2:B:128:ASN:N	2.79	0.40
2:B:182:TYR:CZ	2:B:518:VAL:HG21	2.55	0.40
2:B:300:GLN:CD	2:B:300:GLN:C	2.89	0.40
2:B:395:LYS:C	2:B:397:LEU:N	2.77	0.40
2:B:408:LEU:HD23	2:B:408:LEU:HA	1.79	0.40
2:D:19:GLY:HA3	2:D:531:ILE:HB	2.04	0.40
2:D:125:ASN:OD1	2:D:186:ALA:HB2	2.21	0.40
2:D:127:LEU:HD11	2:D:162:VAL:HG21	2.02	0.40
2:D:493:ARG:HB3	2:D:497:ARG:O	2.21	0.40
2:D:524:VAL:CG1	2:D:529:PRO:HG2	2.51	0.40
1:A:30:PRO:HG2	1:A:156:VAL:HG11	2.03	0.40
2:B:335:HIS:CG	2:B:336:PRO:HD2	2.56	0.40
2:B:414:ARG:O	2:B:414:ARG:HG3	2.21	0.40
1:C:251:GLU:HA	1:C:252:PRO:HD3	1.84	0.40
2:D:152:LYS:HE2	2:D:152:LYS:HB3	1.84	0.40
2:D:186:ALA:C	2:D:188:VAL:N	2.78	0.40
2:D:280:PHE:HA	2:D:368:GLU:O	2.21	0.40
2:D:472:GLN:HE21	2:D:472:GLN:HB2	1.72	0.40
1:A:228:CYS:O	1:A:232:LEU:HB3	2.21	0.40
2:B:25:VAL:HB	2:B:32:ILE:HG23	2.03	0.40
2:B:74:LEU:HA	2:B:74:LEU:HD23	1.87	0.40
2:B:350:GLY:O	2:B:353:ARG:N	2.47	0.40
1:C:32:VAL:O	1:C:33:ASP:C	2.64	0.40
2:D:104:TYR:HD2	2:D:421:ALA:CB	2.34	0.40
2:D:268:TYR:HB3	2:D:271:TRP:HD1	1.84	0.40
2:D:281:LEU:HD13	2:D:302:VAL:HB	2.03	0.40
1:A:33:ASP:OD2	2:B:201:ARG:NH2	2.55	0.40
1:A:84:TRP:CD2	1:A:126:THR:HG22	2.57	0.40
2:B:68:CYS:O	2:B:68:CYS:SG	2.79	0.40
2:B:500:SER:O	2:B:503:GLU:N	2.55	0.40
1:C:24:LEU:O	1:C:26:ARG:N	2.55	0.40
1:C:42:MET:HA	1:C:42:MET:HE2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:MET:H	2:D:38:MET:HG3	1.64	0.40
2:D:205:LYS:HB2	2:D:205:LYS:HE3	1.57	0.40
2:D:373:ALA:O	2:D:377:VAL:HG23	2.22	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:430:ASP:OD2	2:D:31:LYS:NZ[1_565]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/264 (98%)	198 (76%)	42 (16%)	20 (8%)	1	1
1	C	260/264 (98%)	192 (74%)	43 (16%)	25 (10%)	0	0
2	B	528/536 (98%)	387 (73%)	94 (18%)	47 (9%)	0	0
2	D	528/536 (98%)	379 (72%)	97 (18%)	52 (10%)	0	0
All	All	1576/1600 (98%)	1156 (73%)	276 (18%)	144 (9%)	0	0

All (144) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	29	ASP
1	A	41	SER
1	A	79	GLY
2	B	35	ALA
2	B	129	ALA
2	B	171	THR

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Mol	Chain	Res	Type
2	B	337	TYR
2	B	348	PHE
2	B	367	PHE
2	B	492	PRO
2	B	497	ARG
1	C	4	LYS
1	C	29	ASP
1	C	41	SER
1	C	53	GLY
1	C	79	GLY
1	C	131	VAL
1	C	133	GLU
1	C	150	PRO
2	D	15	THR
2	D	70	TYR
2	D	167	LEU
2	D	219	HIS
2	D	279	ASN
2	D	348	PHE
2	D	367	PHE
2	D	381	LYS
1	A	35	LEU
1	A	38	ASP
1	A	162	LEU
1	A	163	LEU
1	A	252	PRO
2	B	16	ARG
2	B	113	TYR
2	B	118	LEU
2	B	168	GLY
2	B	178	GLY
2	B	215	ALA
2	B	227	GLY
2	B	279	ASN
2	B	362	TYR
2	B	394	LEU
2	B	421	ALA
1	C	45	HIS
1	C	252	PRO
2	D	31	LYS
2	D	228	CYS
2	D	254	GLU

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Mol	Chain	Res	Type
2	D	255	GLN
2	D	266	GLY
2	D	296	ARG
2	D	297	TYR
2	D	324	LYS
2	D	327	TRP
2	D	345	TRP
2	D	363	LYS
2	D	364	GLY
2	D	444	TYR
2	D	496	GLU
2	D	498	LYS
1	A	114	THR
1	A	232	LEU
2	B	74	LEU
2	B	75	ALA
2	B	219	HIS
2	B	324	LYS
2	B	383	HIS
2	B	388	LYS
2	B	479	ASN
2	B	501	ALA
1	C	39	VAL
1	C	61	HIS
1	C	135	LEU
1	C	151	ASN
1	C	153	MET
1	C	163	LEU
1	C	172	LYS
1	C	253	ASN
2	D	71	VAL
2	D	117	ALA
2	D	169	ILE
2	D	200	LEU
2	D	329	GLU
2	D	349	HIS
2	D	395	LYS
2	D	492	PRO
2	D	525	HIS
1	A	5	LYS
1	A	64	ILE
1	A	151	ASN

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Mol	Chain	Res	Type
1	A	190	ARG
1	A	258	TYR
2	B	128	ASN
2	B	199	ALA
2	B	323	VAL
2	B	380	ALA
2	B	382	LYS
1	C	60	LEU
1	C	83	TYR
1	C	232	LEU
1	C	254	PHE
2	D	35	ALA
2	D	113	TYR
2	D	331	ALA
2	D	359	ALA
2	D	376	LEU
2	D	418	CYS
1	A	14	ASN
1	A	152	PRO
1	A	236	VAL
2	B	34	ASN
2	B	123	VAL
2	B	150	SER
2	B	222	PHE
2	B	228	CYS
2	B	311	VAL
2	B	465	MET
1	C	47	THR
1	C	237	ASN
2	D	275	GLY
2	D	294	ASN
2	D	486	SER
2	B	71	VAL
2	B	336	PRO
2	B	444	TYR
2	D	48	ILE
2	D	311	VAL
2	D	360	PRO
2	D	377	VAL
2	D	384	GLU
2	D	518	VAL
2	D	529	PRO

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Mol	Chain	Res	Type
2	B	364	GLY
2	B	485	PRO
2	B	17	ILE
2	B	131	PRO
2	D	524	VAL
1	C	152	PRO
2	D	86	VAL
1	A	36	ILE
2	D	286	PHE
2	D	514	PRO
2	B	393	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	205/211 (97%)	158 (77%)	47 (23%)	1	0
1	C	205/211 (97%)	154 (75%)	51 (25%)	0	0
2	B	431/441 (98%)	335 (78%)	96 (22%)	1	0
2	D	431/441 (98%)	315 (73%)	116 (27%)	0	0
All	All	1272/1304 (98%)	962 (76%)	310 (24%)	1	0

All (310) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	LYS
1	A	9	VAL
1	A	10	VAL
1	A	16	GLU
1	A	18	THR
1	A	24	LEU
1	A	28	VAL
1	A	32	VAL
1	A	33	ASP

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Mol	Chain	Res	Type
1	A	36	ILE
1	A	40	ILE
1	A	48	LEU
1	A	49	MET
1	A	57	GLU
1	A	62	GLU
1	A	64	ILE
1	A	65	LYS
1	A	67	ASP
1	A	69	VAL
1	A	76	ILE
1	A	78	MET
1	A	87	VAL
1	A	96	CYS
1	A	98	GLU
1	A	107	ILE
1	A	126	THR
1	A	128	THR
1	A	129	VAL
1	A	133	GLU
1	A	135	LEU
1	A	143	ILE
1	A	158	THR
1	A	162	LEU
1	A	163	LEU
1	A	177	VAL
1	A	184	VAL
1	A	198	GLU
1	A	202	SER
1	A	207	GLU
1	A	227	ASN
1	A	228	CYS
1	A	235	GLN
1	A	236	VAL
1	A	253	ASN
1	A	257	LEU
1	A	263	SER
2	B	11	VAL
2	B	21	LEU
2	B	23	ILE
2	B	34	ASN
2	B	40	THR

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Mol	Chain	Res	Type
2	B	41	LEU
2	B	48	ILE
2	B	49	LEU
2	B	50	LYS
2	B	53	ASP
2	B	58	GLN
2	B	63	ARG
2	B	65	CYS
2	B	71	VAL
2	B	74	LEU
2	B	76	SER
2	B	80	VAL
2	B	86	VAL
2	B	93	THR
2	B	98	LEU
2	B	99	THR
2	B	103	GLN
2	B	109	LEU
2	B	110	VAL
2	B	127	LEU
2	B	144	ARG
2	B	147	THR
2	B	148	THR
2	B	152	LYS
2	B	158	VAL
2	B	166	GLN
2	B	172	ASN
2	B	184	LEU
2	B	220	THR
2	B	222	PHE
2	B	229	THR
2	B	232	ASP
2	B	234	LEU
2	B	244	LYS
2	B	245	LEU
2	B	253	ILE
2	B	255	GLN
2	B	261	LEU
2	B	270	ASN
2	B	274	ILE
2	B	278	SER
2	B	281	LEU

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Mol	Chain	Res	Type
2	B	288	THR
2	B	289	ASP
2	B	300	GLN
2	B	302	VAL
2	B	308	LEU
2	B	318	LEU
2	B	319	ILE
2	B	338	LYS
2	B	342	LYS
2	B	344	LYS
2	B	348	PHE
2	B	363	LYS
2	B	365	GLU
2	B	369	VAL
2	B	388	LYS
2	B	390	VAL
2	B	392	LEU
2	B	394	LEU
2	B	395	LYS
2	B	396	THR
2	B	399	VAL
2	B	402	GLU
2	B	407	THR
2	B	408	LEU
2	B	410	ARG
2	B	414	ARG
2	B	416	ILE
2	B	435	ASN
2	B	451	THR
2	B	452	GLU
2	B	454	GLN
2	B	456	VAL
2	B	467	SER
2	B	470	ILE
2	B	472	GLN
2	B	481	GLN
2	B	482	HIS
2	B	483	VAL
2	B	484	VAL
2	B	490	LEU
2	B	496	GLU
2	B	498	LYS

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Mol	Chain	Res	Type
2	B	502	VAL
2	B	511	ILE
2	B	516	ARG
2	B	518	VAL
2	B	519	GLU
2	B	520	ILE
2	B	536	HIS
1	C	4	LYS
1	C	5	LYS
1	C	6	ARG
1	C	12	LEU
1	C	16	GLU
1	C	24	LEU
1	C	26	ARG
1	C	28	VAL
1	C	32	VAL
1	C	33	ASP
1	C	36	ILE
1	C	37	LEU
1	C	40	ILE
1	C	42	MET
1	C	57	GLU
1	C	58	GLU
1	C	78	MET
1	C	87	VAL
1	C	90	ARG
1	C	91	ASN
1	C	98	GLU
1	C	104	LYS
1	C	107	ILE
1	C	118	VAL
1	C	128	THR
1	C	129	VAL
1	C	132	ASN
1	C	133	GLU
1	C	135	LEU
1	C	137	LYS
1	C	138	LEU
1	C	143	ILE
1	C	158	THR
1	C	159	VAL
1	C	165	LYS

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Mol	Chain	Res	Type
1	C	167	MET
1	C	172	LYS
1	C	178	MET
1	C	186	ASP
1	C	198	GLU
1	C	207	GLU
1	C	216	GLU
1	C	217	LEU
1	C	227	ASN
1	C	228	CYS
1	C	232	LEU
1	C	235	GLN
1	C	236	VAL
1	C	247	ILE
1	C	253	ASN
1	C	257	LEU
2	D	9	ILE
2	D	11	VAL
2	D	16	ARG
2	D	21	LEU
2	D	22	ARG
2	D	23	ILE
2	D	26	GLU
2	D	27	VAL
2	D	38	MET
2	D	40	THR
2	D	63	ARG
2	D	67	VAL
2	D	74	LEU
2	D	80	VAL
2	D	83	CYS
2	D	84	VAL
2	D	86	VAL
2	D	88	ILE
2	D	90	GLU
2	D	94	LEU
2	D	98	LEU
2	D	99	THR
2	D	116	HIS
2	D	120	TRP
2	D	133	LYS
2	D	136	ARG

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Mol	Chain	Res	Type
2	D	137	LEU
2	D	140	ASP
2	D	141	LEU
2	D	144	ARG
2	D	150	SER
2	D	161	LEU
2	D	164	SER
2	D	166	GLN
2	D	169	ILE
2	D	170	PHE
2	D	171	THR
2	D	184	LEU
2	D	188	VAL
2	D	190	LEU
2	D	196	TYR
2	D	198	GLU
2	D	204	VAL
2	D	210	MET
2	D	217	ASN
2	D	221	GLN
2	D	234	LEU
2	D	237	GLU
2	D	241	GLU
2	D	244	LYS
2	D	247	LYS
2	D	249	VAL
2	D	250	ARG
2	D	255	GLN
2	D	258	ILE
2	D	269	LYS
2	D	270	ASN
2	D	274	ILE
2	D	276	LYS
2	D	278	SER
2	D	287	PRO
2	D	300	GLN
2	D	302	VAL
2	D	303	ILE
2	D	308	LEU
2	D	310	LYS
2	D	311	VAL
2	D	319	ILE

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Mol	Chain	Res	Type
2	D	320	GLU
2	D	326	SER
2	D	332	ASP
2	D	338	LYS
2	D	340	VAL
2	D	344	LYS
2	D	348	PHE
2	D	351	GLU
2	D	365	GLU
2	D	375	VAL
2	D	381	LYS
2	D	387	VAL
2	D	393	VAL
2	D	394	LEU
2	D	397	LEU
2	D	410	ARG
2	D	416	ILE
2	D	426	GLU
2	D	430	ASP
2	D	432	LEU
2	D	436	VAL
2	D	442	ASP
2	D	443	LEU
2	D	445	THR
2	D	446	ASP
2	D	448	GLN
2	D	451	THR
2	D	452	GLU
2	D	470	ILE
2	D	472	GLN
2	D	478	GLU
2	D	481	GLN
2	D	482	HIS
2	D	484	VAL
2	D	487	THR
2	D	498	LYS
2	D	499	LEU
2	D	500	SER
2	D	502	VAL
2	D	506	LEU
2	D	507	ILE
2	D	515	LYS

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Mol	Chain	Res	Type
2	D	518	VAL
2	D	519	GLU
2	D	526	SER
2	D	529	PRO
2	D	531	ILE
2	D	535	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	45	HIS
1	A	124	ASN
1	A	132	ASN
1	A	173	GLN
1	A	187	ASN
1	A	193	HIS
1	A	227	ASN
1	A	231	GLN
1	A	235	GLN
1	A	241	GLN
2	B	20	HIS
2	B	34	ASN
2	B	82	ASN
2	B	108	HIS
2	B	125	ASN
2	B	128	ASN
2	B	172	ASN
2	B	270	ASN
2	B	335	HIS
2	B	383	HIS
2	B	417	GLN
2	B	460	ASN
2	B	472	GLN
2	B	479	ASN
2	B	481	GLN
2	B	482	HIS
2	B	504	GLN
1	C	13	HIS
1	C	124	ASN
1	C	193	HIS
1	C	227	ASN

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Mol	Chain	Res	Type
1	C	235	GLN
1	C	241	GLN
2	D	7	ASN
2	D	34	ASN
2	D	72	HIS
2	D	82	ASN
2	D	106	HIS
2	D	172	ASN
2	D	217	ASN
2	D	270	ASN
2	D	306	ASN
2	D	315	ASN
2	D	417	GLN
2	D	460	ASN
2	D	472	GLN
2	D	479	ASN
2	D	481	GLN
2	D	504	GLN
2	D	525	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z > 2$
4	F3S	C	266	1	0,9,9	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		
3	SF4	A	267	1	0,12,12	-	-	-		
3	SF4	A	265	1	0,12,12	-	-	-		
3	SF4	C	267	1	0,12,12	-	-	-		
3	SF4	C	265	1	0,12,12	-	-	-		

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
4	F3S	C	266	1	-	-	0/3/3/3
4	F3S	A	266	1	-	-	0/3/3/3
3	SF4	A	267	1	-	-	0/6/5/5
3	SF4	A	265	1	-	-	0/6/5/5
3	SF4	C	267	1	-	-	0/6/5/5
3	SF4	C	265	1	-	-	0/6/5/5

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	267	SF4	1	0
3	A	265	SF4	1	0
3	C	267	SF4	1	0
3	C	265	SF4	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.