



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2024 – 04:15 PM EDT

PDB ID : 1FRV
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.

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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

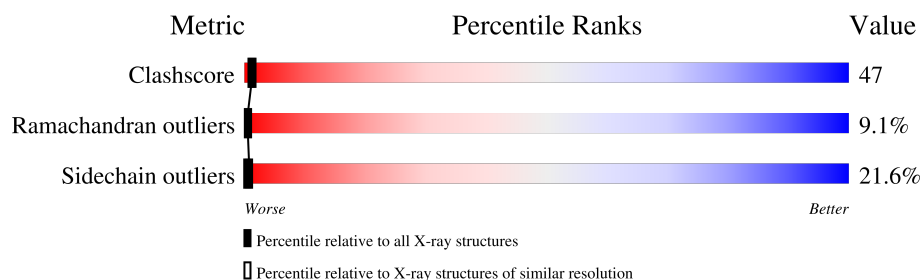
1 Overall quality at a glance

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	180529	1351 (2.88-2.84)
Ramachandran outliers	177936	1318 (2.88-2.84)
Sidechain outliers	177891	1319 (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 6 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.

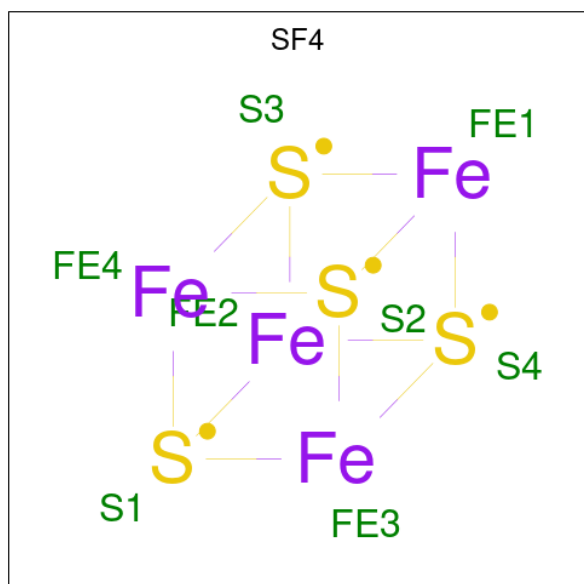
- Molecule 1 is a protein called HYDROGENASE.

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.

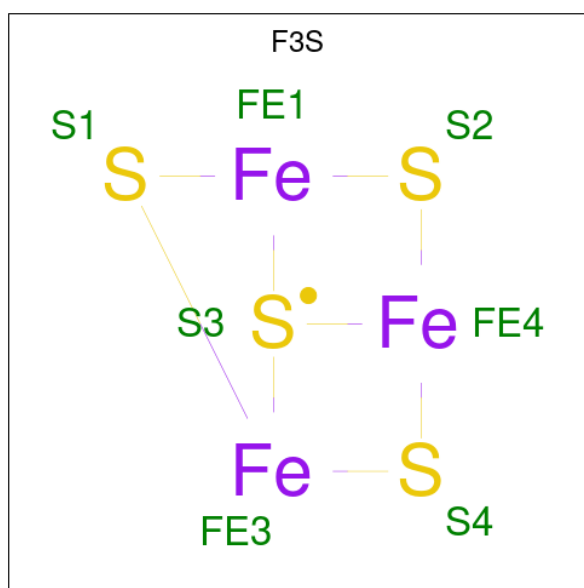
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			
2	D	530	Total	C	N	O	S	0	0	0
			4145	2645	725	758	17			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: 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 (three-letter code: F3S) (formula: Fe_3S_4).

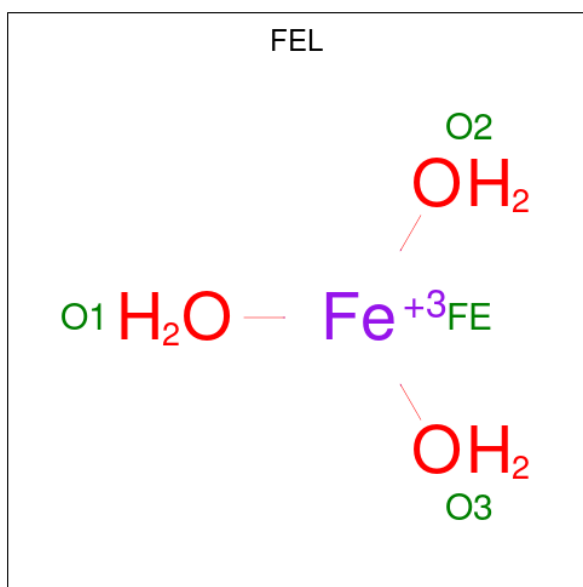


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			7	3	4		
4	C	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 5 is NICKEL (II) ION (three-letter code: 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 HYDRATED FE (three-letter code: FEL) (formula: FeH_6O_3).



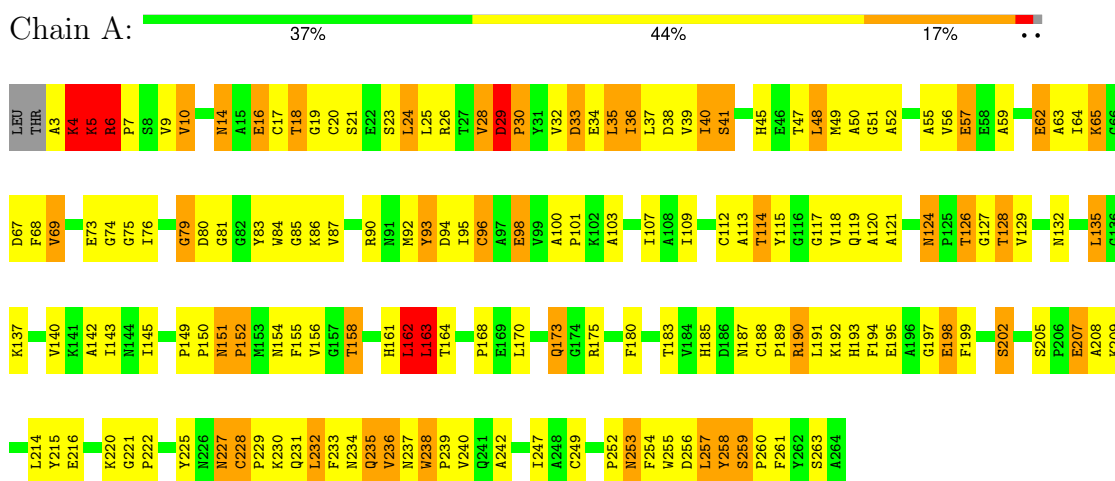
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	Fe	O	0	0
			4	1	3		
6	D	1	Total	Fe	O	0	0
			4	1	3		

3 Residue-property plots

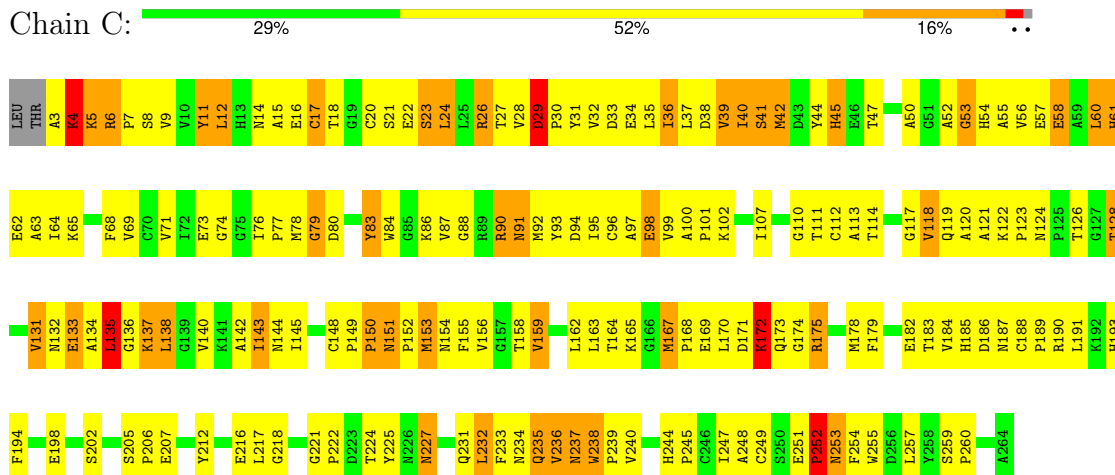
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

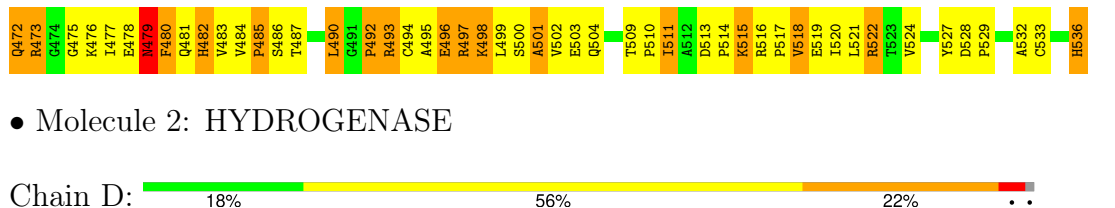


• Molecule 1: HYDROGENASE



• Molecule 2: HYDROGENASE





Chain D: 18% 56% 22% ..

E503	E504	E505	E506	E507	E508	E509	E510	E511	E512	E513	E514	E515	E516	E517	E518	E519	E520	E521	E522	E523	E524	E525	E526	E527	E528	E529	E530	E531	E532	E533	E534	E535	E536	E537	E538	E539	E540	E541	E542	E543	E544	E545	E546	E547	E548	E549	E550	E551	E552
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

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 ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.84	0/2014	1.43	12/2738 (0.4%)
1	C	0.84	0/2014	1.44	11/2738 (0.4%)
2	B	0.81	0/4251	1.45	37/5782 (0.6%)
2	D	0.81	0/4251	1.45	36/5782 (0.6%)
All	All	0.82	0/12530	1.45	96/17040 (0.6%)

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	63	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	C	190	ARG	NE-CZ-NH1	11.18	125.89	120.30
2	B	414	ARG	NE-CZ-NH1	11.16	125.88	120.30
2	D	16	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	A	74	GLY	N-CA-C	10.34	138.94	113.10
2	B	414	ARG	NE-CZ-NH2	-9.89	115.36	120.30
2	B	522	ARG	NE-CZ-NH2	-9.37	115.62	120.30
2	B	63	ARG	NE-CZ-NH2	-9.21	115.70	120.30
2	B	78	ARG	NE-CZ-NH1	9.15	124.88	120.30
2	B	63	ARG	CD-NE-CZ	8.48	135.47	123.60
2	B	493	ARG	NE-CZ-NH1	7.87	124.24	120.30
2	B	136	ARG	NE-CZ-NH1	7.74	124.17	120.30
2	D	43	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	C	11	TYR	CB-CG-CD1	7.63	125.58	121.00
2	D	96	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	B	144	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	185	HIS	CA-CB-CG	7.30	126.00	113.60
2	D	43	ARG	NE-CZ-NH2	-7.24	116.68	120.30
2	D	463	ARG	NE-CZ-NH2	-7.21	116.70	120.30
2	D	227	GLY	N-CA-C	7.19	131.07	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	16	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	190	ARG	NE-CZ-NH1	6.89	123.75	120.30
2	B	43	ARG	NE-CZ-NH2	-6.85	116.88	120.30
2	B	522	ARG	NE-CZ-NH1	6.83	123.72	120.30
2	D	137	LEU	CB-CA-C	6.83	123.17	110.20
1	C	11	TYR	CB-CG-CD2	-6.79	116.92	121.00
1	A	238	TRP	CA-CB-CG	6.79	126.60	113.70
2	D	493	ARG	NE-CZ-NH1	6.58	123.59	120.30
2	D	243	ARG	NE-CZ-NH2	-6.57	117.02	120.30
2	B	473	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	B	442	ASP	CB-CG-OD2	-6.37	112.57	118.30
2	B	248	GLU	CA-CB-CG	6.23	127.10	113.40
2	D	241	GLU	CA-CB-CG	6.21	127.07	113.40
2	B	353	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	B	345	TRP	N-CA-CB	6.19	121.74	110.60
2	D	348	PHE	CA-CB-CG	6.17	128.71	113.90
1	C	29	ASP	N-CA-C	-6.17	94.34	111.00
2	B	312	ASP	CB-CG-OD1	6.15	123.84	118.30
1	C	11	TYR	CA-CB-CG	6.15	125.09	113.40
2	B	81	ASP	CB-CG-OD1	-6.07	112.83	118.30
1	C	218	GLY	N-CA-C	6.04	128.21	113.10
2	B	40	THR	N-CA-C	6.01	127.22	111.00
2	D	513	ASP	N-CA-CB	6.00	121.40	110.60
1	A	190	ARG	NE-CZ-NH2	-5.95	117.32	120.30
1	C	29	ASP	N-CA-CB	5.87	121.17	110.60
2	D	137	LEU	CA-CB-CG	5.86	128.78	115.30
2	D	463	ARG	NE-CZ-NH1	5.84	123.22	120.30
2	B	78	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	238	TRP	CA-CB-CG	5.81	124.73	113.70
2	D	56	ASP	CB-CG-OD2	-5.75	113.13	118.30
2	D	365	GLU	C-N-CA	5.73	136.02	121.70
2	B	90	GLU	CG-CD-OE1	5.71	129.73	118.30
2	D	487	THR	N-CA-CB	5.70	121.13	110.30
1	A	57	GLU	CG-CD-OE2	-5.67	106.96	118.30
2	D	43	ARG	CD-NE-CZ	5.66	131.52	123.60
1	A	94	ASP	CB-CG-OD1	5.63	123.37	118.30
2	D	382	LYS	N-CA-C	5.59	126.09	111.00
1	A	93	TYR	CB-CG-CD1	5.59	124.35	121.00
1	A	6	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	B	200	LEU	CA-CB-CG	5.56	128.08	115.30
2	D	353	ARG	NE-CZ-NH1	5.53	123.07	120.30
2	D	167	LEU	CA-CB-CG	5.52	128.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	238	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	B	65	CYS	CB-CA-C	5.43	121.26	110.40
2	D	366	ALA	N-CA-C	5.41	125.60	111.00
1	C	169	GLU	N-CA-CB	5.40	120.33	110.60
1	C	252	PRO	N-CA-C	5.39	126.12	112.10
1	A	30	PRO	N-CA-C	-5.38	98.11	112.10
2	D	295	SER	N-CA-CB	5.38	118.57	110.50
2	D	467	SER	N-CA-CB	5.37	118.56	110.50
2	B	522	ARG	CD-NE-CZ	5.33	131.06	123.60
1	A	29	ASP	N-CA-C	-5.30	96.68	111.00
2	B	260	ASP	CB-CG-OD1	-5.29	113.54	118.30
2	D	40	THR	N-CA-CB	-5.28	100.26	110.30
2	D	34	ASN	CA-CB-CG	-5.28	101.79	113.40
2	B	260	ASP	CB-CG-OD2	5.28	123.05	118.30
2	B	226	GLY	C-N-CA	5.24	133.31	122.30
1	C	175	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	B	213	PHE	C-N-CA	5.20	133.23	122.30
2	D	467	SER	CA-CB-OG	5.20	125.24	111.20
2	D	492	PRO	N-CA-C	5.19	125.59	112.10
2	B	473	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	D	190	LEU	CB-CA-C	5.15	119.98	110.20
2	D	350	GLY	N-CA-C	-5.14	100.25	113.10
2	D	29	GLY	N-CA-C	5.12	125.91	113.10
2	B	39	SER	CB-CA-C	5.12	119.83	110.10
2	B	115	LEU	CA-CB-CG	5.12	127.07	115.30
2	B	90	GLU	OE1-CD-OE2	-5.11	117.17	123.30
2	B	443	LEU	N-CA-C	-5.06	97.34	111.00
2	D	250	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	D	21	LEU	CA-CB-CG	5.04	126.89	115.30
2	B	225	VAL	N-CA-C	-5.03	97.41	111.00
2	D	281	LEU	N-CA-CB	-5.02	100.36	110.40
2	B	493	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	48	LEU	CA-CB-CG	5.00	126.81	115.30
2	B	463	ARG	NE-CZ-NH2	-5.00	117.80	120.30

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	155	0
1	C	1961	0	1879	195	0
2	B	4145	0	4073	362	1
2	D	4145	0	4073	487	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	4	0	0	0	0
6	D	4	0	0	0	0
All	All	12268	0	11904	1142	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 47.

All (1142) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:527:TYR:C	2:D:529:PRO:HD3	2.01	0.79
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
2:B:438:ALA:HB3	2:B:440:LYS:CG	2.13	0.79
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: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:D:393:VAL:O	2:D:397:LEU:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:467:SER:OG	2:B:469:TRP:NE1	2.16	0.77
2:D:472:GLN:HE22	2:D:475:GLY:H	1.28	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
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
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:D:388:LYS:C	2:D:388:LYS:HD3	2.07	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
1:C:86:LYS:HE3	1:C:91:ASN:OD1	1.88	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
1:A:220:LYS:C	1:A:222:PRO:HD2	2.08	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:150:PRO:O	1:A:151:ASN:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:CYS:HB2	2:D:65:CYS:HA	1.71	0.72
1:C:134:ALA:C	1:C:136:GLY:H	1.91	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: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
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: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
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
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
2:D:485:PRO:C	2:D:487:THR:H	1.95	0.69
1:C:55:ALA:HB1	2:D:172:ASN:HB2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:388:LYS:HD3	2:D:388:LYS:O	1.94	0.67
1:C:235:GLN:HE21	2:D:208:ARG:NH2	1.93	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
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: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:B:382:LYS:O	2:B:383:HIS:C	2.33	0.66
2:D:120:TRP:O	2:D:184:LEU:HD22	1.95	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:D:348:PHE:O	2:D:349:HIS:HB2	1.96	0.65
2:B:109:LEU:HD21	2:B:252:PHE:CE2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:ARG:HB2	1:C:95:ILE:HD11	1.77	0.65
2:B:319:ILE:HD12	2:B:319:ILE:C	2.16	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: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
1:C:98:GLU:HG3	1:C:99:VAL:N	2.12	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
1:C:134:ALA:C	1:C:136:GLY:N	2.51	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
2:D:82:ASN:HD22	2:D:456:VAL:H	1.44	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:197:GLY:CA	2:D:235:ARG:HH12	2.13	0.62
1:C:36:ILE:HD11	1:C:42:MET:HE3	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
2:D:315:ASN:HD21	2:D:317:ASP:HB2	1.65	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
2:D:485:PRO:C	2:D:487:THR:N	2.53	0.61
2:B:395:LYS:HG2	2:B:396:THR:N	2.14	0.61
2:B:395:LYS:O	2:B:396:THR:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:189:PRO:C	1:A:191:LEU:H	2.04	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:372:LEU:O	2:D:375:VAL:HG23	2.03	0.58
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
1:C:24:LEU:C	1:C:26:ARG:H	2.06	0.58
2:D:324:LYS:HD3	2:D:495:ALA:CB	2.33	0.58
2:B:198:GLU:C	2:B:200:LEU:H	2.07	0.58
1:C:56:VAL:C	1:C:58:GLU:H	2.08	0.58
2:D:80:VAL:O	2:D:84:VAL:HB	2.03	0.58
2:B:11:VAL:O	2:B:11:VAL:HG22	2.04	0.58
2:B:70:TYR:HD1	2:B:220:THR:HG21	1.68	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:387:VAL:HA	2:D:390:VAL:CG1	2.34	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:A:68:PHE:CE1	1:A:103:ALA:HB2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:SER:HA	1:C:260:PRO:C	2.25	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:B:95:MET:HE1	2:B:233:SER:OG	2.05	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:D:83:CYS:HB2	2:D:454:GLN:C	2.25	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
2:D:315:ASN:HD22	2:D:318:LEU:HG	1.70	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: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
1:C:74:GLY:O	1:C:112:CYS:HB3	2.05	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:89:PRO:HD3	2:B:445:THR:HG1	1.69	0.55
1:C:167:MET:HG3	1:C:168:PRO:CD	2.36	0.55
2:B:399:VAL:HG23	2:B:400:GLY:N	2.21	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
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
1:C:153:MET:HE2	1:C:231:GLN:HG3	1.89	0.55
1:A:234:ASN:C	1:A:235:GLN:NE2	2.60	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
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: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
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: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:310:LYS:C	2:D:311:VAL:HG23	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:ILE:HD12	1:C:154:ASN:O	2.07	0.54
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:D:199:ALA:C	2:D:201:ARG:H	2.10	0.54
1:A:221:GLY:N	1:A:222:PRO:HD2	2.17	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: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:449:TYR:C	2:D:450:PRO:O	2.45	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:362:TYR:O	2:D:364:GLY:N	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:TYR:O	2:B:73:ALA:N	2.36	0.53
2:B:122:ASN:O	2:B:123:VAL:C	2.47	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
2:B:74:LEU:HA	2:B:77:VAL:HG22	1.91	0.53
2:D:199:ALA:C	2:D:201:ARG:N	2.60	0.53
1:C:114:THR:HG22	1:C:144:ASN:HB3	1.90	0.53
2:D:265:ALA:O	2:D:266:GLY:C	2.47	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
1:C:56:VAL:C	1:C:58:GLU:N	2.62	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: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
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

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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	0.52
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
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:363:LYS:C	2:D:365:GLU:H	2.13	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
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:72:HIS:O	2:D:73:ALA:C	2.48	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:350:GLY:C	2:B:352:ASP:N	2.63	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
1:C:24:LEU:C	1:C:26:ARG:N	2.63	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:C:117:GLY:C	1:C:119:GLN:N	2.64	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: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: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: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
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:198:GLU:C	2:B:200:LEU:N	2.64	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:230:ASN:ND2	2:B:233:SER:HB3	2.26	0.50
1:C:100:ALA:C	1:C:102:LYS:H	2.15	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
2:D:394:LEU:HD21	2:D:401:PRO:HA	1.94	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
2:B:387:VAL:C	2:B:389:ALA:N	2.65	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: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
2:B:348:PHE:C	2:B:350:GLY:H	2.14	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
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:162:VAL:C	2:D:164:SER:H	2.15	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:VAL:O	2:B:388:LYS:C	2.51	0.49
2:B:500:SER:O	2:B:501:ALA:C	2.51	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
1:C:86:LYS:O	2:D:40:THR:HG23	2.13	0.49
2:D:243:ARG:O	2:D:244:LYS:C	2.51	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
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
1:A:214:LEU:O	1:A:215:TYR:C	2.51	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:123:VAL:O	2:D:124:ALA:C	2.51	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
2:D:42:PHE:HE1	2:D:328:TYR:HH	1.58	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:250:ARG:HG2	2:D:250:ARG:HH11	1.78	0.48
2:D:513:ASP:OD1	2:D:513:ASP:C	2.52	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
1:C:237:ASN:CG	1:C:238:TRP:H	2.17	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:CG1	2:B:110:VAL:O	2.61	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
1:C:88:GLY:C	1:C:90:ARG:H	2.15	0.48
1:C:184:VAL:N	1:C:224:THR:O	2.43	0.48
2:B:336:PRO:C	2:B:338:LYS:H	2.17	0.48
1:C:17:CYS:O	1:C:18:THR:HB	2.14	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:D:357:MET:CE	2:D:534:GLY:HA3	2.44	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:89:PRO:C	2:B:91:ASN:N	2.68	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:D:276:LYS:HZ3	2:D:276:LYS:N	2.11	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: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: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:173:GLN:HA	1:C:173:GLN:HE21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:205:SER:HG	1:A:207:GLU:HG2	1.77	0.47
1:A:209:LYS:HG2	2:B:231:TYR:CE1	2.50	0.47
1:A:220:LYS:C	1:A:222:PRO:CD	2.77	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:122:ASN:CG	2:D:175:PHE:HB2	2.35	0.47
2:D:134:ALA:O	2:D:135:ALA:C	2.53	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:315:ASN:HD22	2:D:318:LEU:H	1.62	0.47
2:D:517:PRO:O	2:D:519:GLU:N	2.48	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:76:SER:HG	2:B:480:PHE:HZ	1.64	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
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
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:379:TYR:C	2:B:381:LYS:H	2.19	0.46
2:B:387:VAL:HA	2:B:390:VAL:HG13	1.97	0.46
1:C:77:PRO:C	1:C:79:GLY:H	2.18	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:114:THR:OG1	1:A:115:TYR:N	2.47	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:464:GLY:HA3	2:D:485:PRO:HB3	1.97	0.46
2:D:515:LYS:C	2:D:516:ARG:HG3	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:21:SER:O	1:A:25:LEU:HD13	2.16	0.45
2:B:195:HIS:O	2:B:196:TYR:C	2.53	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:D:21:LEU:HB2	2:D:531:ILE:HD11	1.98	0.45
2:B:498:LYS:HZ2	2:B:498:LYS:HB2	1.81	0.45
1:C:99:VAL:O	1:C:102:LYS:HB2	2.16	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
1:A:234:ASN:C	1:A:235:GLN:HE21	2.19	0.45
2:B:80:VAL:O	2:B:83:CYS:N	2.48	0.45
1:C:40:ILE:O	1:C:41:SER:CB	2.60	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: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:315:ASN:ND2	2:D:317:ASP:N	2.64	0.45
1:C:42:MET:HE2	1:C:42:MET:HA	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:362:TYR:O	2:B:363:LYS:C	2.55	0.45
1:C:182:GLU:OE1	1:C:187:ASN:OD1	2.35	0.45
2:D:54:PRO:C	2:D:56:ASP:H	2.18	0.45
1:A:126:THR:O	1:A:127:GLY:C	2.56	0.45
1:A:242:ALA:HA	2:B:230:ASN:OD1	2.17	0.45
1:A:259:SER:HA	1:A:260:PRO:C	2.37	0.45
2:B:316:PRO:HB2	2:B:469:TRP:HH2	1.82	0.45
1:C:83:TYR:CD1	1:C:83:TYR:C	2.89	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
2:B:464:GLY:C	2:B:485:PRO:HG3	2.37	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:107:ASP:CG	2:D:463:ARG:HH12	2.20	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:D:94:LEU:O	2:D:97:ASN:HB2	2.18	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: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
1:C:132:ASN:ND2	1:C:142:ALA:H	2.16	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:B:280:PHE:CD2	2:B:376:LEU:HD12	2.52	0.44
2:B:527:TYR:O	2:B:528:ASP:C	2.55	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
1:C:233:PHE:C	1:C:235:GLN:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:LEU:HD12	2:B:100:MET:HE2	1.99	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: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
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
2:D:383:HIS:C	2:D:385:PRO:HD2	2.38	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
1:A:189:PRO:C	1:A:191:LEU:N	2.71	0.43
1:C:188:CYS:HA	1:C:189:PRO:HD3	1.80	0.43
1:C:233:PHE:C	1:C:235:GLN:N	2.72	0.43
2:D:435:ASN:O	2:D:438:ALA:HB3	2.18	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:348:PHE:C	2:B:350:GLY:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:70:TYR:O	2:D:71:VAL:C	2.56	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: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
1:A:33:ASP:O	1:A:34:GLU:C	2.57	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
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
1:A:63:ALA:C	1:A:65:LYS:H	2.22	0.43
2:B:14:ILE:O	2:B:14:ILE:CG2	2.66	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: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:B:80:VAL:HA	2:B:83:CYS:SG	2.59	0.43
2:B:153:ALA:O	2:B:154:VAL:C	2.57	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:111:HIS:O	2:D:112:PHE:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:293:LEU:C	2:D:295:SER:H	2.22	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:496:GLU:HB3	2:B:498:LYS:HZ1	1.84	0.42
2:B:498:LYS:NZ	2:B:498:LYS:HB2	2.33	0.42
2:B:515:LYS:C	2:B:516:ARG:HG3	2.39	0.42
2:D:54:PRO:C	2:D:56:ASP:N	2.73	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:387:VAL:CG2	2:D:388:LYS:N	2.82	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
1:C:56:VAL:O	1:C:58:GLU:N	2.52	0.42
2:D:100:MET:O	2:D:101:GLY:C	2.58	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:491:GLY:O	2:D:500:SER:OG	2.35	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:D:349:HIS:O	2:D:350:GLY:C	2.57	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
2:D:168:GLY:O	2:D:169:ILE:C	2.57	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:153:MET:HE3	1:C:179:PHE:CE1	2.54	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:95:MET:HG2	2:D:95:MET:O	2.20	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
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:395:LYS:O	2:B:397:LEU:N	2.53	0.42
2:B:495:ALA:C	2:B:497:ARG:H	2.22	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
2:D:356:TRP:HB3	2:D:535:VAL:HG13	2.00	0.42
2:B:80:VAL:C	2:B:82:ASN:N	2.73	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
1:A:238:TRP:CZ3	1:A:240:VAL:CG2	3.03	0.41
2:B:61:THR:C	2:B:63:ARG:N	2.72	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:OD1	1:C:14:ASN:N	2.53	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
1:C:97:ALA:O	1:C:101:PRO:HG3	2.20	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
1:A:162:LEU:C	1:A:164:THR:H	2.23	0.41
2:B:133:LYS:HB3	2:B:187:GLU:OE1	2.20	0.41
2:B:480:PHE:CD1	2:B:480:PHE:C	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:185:HIS:HB2	1:C:221:GLY:C	2.40	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
1:A:79:GLY:C	1:A:81:GLY:H	2.24	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
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
2:B:214:GLY:O	2:B:215:ALA:CB	2.68	0.41
2:B:278:SER:HB3	2:B:306:ASN:OD1	2.21	0.41
2:B:390:VAL:O	2:B:391:ASP:C	2.59	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
2:D:441:ASP:C	2:D:441:ASP:OD1	2.59	0.41
2:B:336:PRO:C	2:B:338:LYS:N	2.73	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
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:276:LYS:HZ3	2:D:276:LYS:H	1.68	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:170:PHE:O	2:B:171:THR:C	2.59	0.41
2:B:264:VAL:C	2:B:266:GLY:N	2.75	0.41
2:B:322:HIS:NE2	2:B:361:ARG:HB2	2.36	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:18:GLU:CD	2:D:18:GLU:C	2.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:LEU:HB2	2:D:531:ILE:CG1	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: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:340:VAL:HG23	2:D:341:THR:N	2.35	0.41
2:D:497:ARG:O	2:D:498:LYS:C	2.58	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: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
1:C:60:LEU:O	1:C:61:HIS:C	2.60	0.41
2:D:49:LEU:HA	2:D:52:ARG:HD2	2.02	0.41
2:D:350:GLY:C	2:D:351:GLU:HG2	2.41	0.41
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
1:C:117:GLY:O	1:C:118:VAL:C	2.60	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: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:182:TYR:CZ	2:B:518:VAL:HG21	2.55	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:74:LEU:C	2:B:76:SER:N	2.75	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:52:ALA:O	1:C:53:GLY:C	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:350:GLY:O	2:B:353:ARG:N	2.47	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
2:D:315:ASN:ND2	2:D:315:ASN:C	2.75	0.40
2:D:523:THR:O	2:D:524:VAL:C	2.60	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
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:217:ASN:C	2:D:217:ASN:HD22	2.25	0.40
2:D:254:GLU:O	2:D:255:GLN:C	2.60	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	160 (78%)	45 (22%)	1	0
1	C	205/211 (97%)	161 (78%)	44 (22%)	1	0
2	B	431/441 (98%)	346 (80%)	85 (20%)	1	1
2	D	431/441 (98%)	330 (77%)	101 (23%)	0	0
All	All	1272/1304 (98%)	997 (78%)	275 (22%)	1	0

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	LYS
1	A	6	ARG
1	A	10	VAL
1	A	16	GLU
1	A	17	CYS
1	A	18	THR
1	A	24	LEU
1	A	28	VAL
1	A	32	VAL
1	A	33	ASP
1	A	36	ILE
1	A	40	ILE
1	A	49	MET
1	A	57	GLU
1	A	62	GLU
1	A	65	LYS
1	A	67	ASP
1	A	69	VAL
1	A	76	ILE
1	A	96	CYS
1	A	98	GLU
1	A	107	ILE
1	A	124	ASN
1	A	126	THR
1	A	128	THR
1	A	129	VAL
1	A	135	LEU
1	A	137	LYS
1	A	143	ILE
1	A	158	THR
1	A	162	LEU
1	A	163	LEU
1	A	173	GLN
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

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Mol	Chain	Res	Type
1	A	259	SER
1	A	263	SER
2	B	11	VAL
2	B	21	LEU
2	B	23	ILE
2	B	34	ASN
2	B	40	THR
2	B	41	LEU
2	B	48	ILE
2	B	49	LEU
2	B	50	LYS
2	B	52	ARG
2	B	53	ASP
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	93	THR
2	B	99	THR
2	B	103	GLN
2	B	109	LEU
2	B	127	LEU
2	B	133	LYS
2	B	144	ARG
2	B	147	THR
2	B	148	THR
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	242	PHE
2	B	244	LYS
2	B	245	LEU
2	B	247	LYS
2	B	255	GLN

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Mol	Chain	Res	Type
2	B	257	TYR
2	B	261	LEU
2	B	270	ASN
2	B	278	SER
2	B	281	LEU
2	B	288	THR
2	B	289	ASP
2	B	293	LEU
2	B	300	GLN
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	388	LYS
2	B	390	VAL
2	B	392	LEU
2	B	394	LEU
2	B	395	LYS
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	456	VAL
2	B	467	SER
2	B	470	ILE
2	B	472	GLN
2	B	479	ASN
2	B	480	PHE
2	B	481	GLN
2	B	482	HIS
2	B	483	VAL
2	B	490	LEU
2	B	496	GLU
2	B	498	LYS
2	B	511	ILE

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Mol	Chain	Res	Type
2	B	515	LYS
2	B	518	VAL
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	17	CYS
1	C	23	SER
1	C	24	LEU
1	C	26	ARG
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	58	GLU
1	C	78	MET
1	C	87	VAL
1	C	90	ARG
1	C	91	ASN
1	C	98	GLU
1	C	107	ILE
1	C	118	VAL
1	C	128	THR
1	C	133	GLU
1	C	135	LEU
1	C	137	LYS
1	C	138	LEU
1	C	143	ILE
1	C	159	VAL
1	C	167	MET
1	C	171	ASP
1	C	172	LYS
1	C	178	MET
1	C	186	ASP
1	C	198	GLU
1	C	207	GLU
1	C	217	LEU
1	C	227	ASN

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Mol	Chain	Res	Type
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	21	LEU
2	D	22	ARG
2	D	26	GLU
2	D	38	MET
2	D	40	THR
2	D	63	ARG
2	D	74	LEU
2	D	83	CYS
2	D	86	VAL
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
2	D	137	LEU
2	D	140	ASP
2	D	141	LEU
2	D	144	ARG
2	D	150	SER
2	D	155	GLN
2	D	159	LYS
2	D	161	LEU
2	D	164	SER
2	D	166	GLN
2	D	169	ILE
2	D	170	PHE
2	D	184	LEU
2	D	196	TYR
2	D	210	MET
2	D	217	ASN
2	D	221	GLN
2	D	222	PHE
2	D	234	LEU

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Mol	Chain	Res	Type
2	D	237	GLU
2	D	241	GLU
2	D	244	LYS
2	D	246	TYR
2	D	247	LYS
2	D	250	ARG
2	D	255	GLN
2	D	258	ILE
2	D	260	ASP
2	D	270	ASN
2	D	274	ILE
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	315	ASN
2	D	319	ILE
2	D	320	GLU
2	D	326	SER
2	D	332	ASP
2	D	344	LYS
2	D	348	PHE
2	D	351	GLU
2	D	354	TYR
2	D	356	TRP
2	D	365	GLU
2	D	375	VAL
2	D	379	TYR
2	D	381	LYS
2	D	383	HIS
2	D	392	LEU
2	D	393	VAL
2	D	394	LEU
2	D	397	LEU
2	D	410	ARG
2	D	426	GLU
2	D	430	ASP
2	D	432	LEU
2	D	442	ASP
2	D	443	LEU

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Mol	Chain	Res	Type
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	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
2	D	518	VAL
2	D	526	SER
2	D	529	PRO
2	D	535	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
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	227	ASN
1	A	231	GLN
1	A	235	GLN
1	A	241	GLN
1	A	253	ASN
2	B	34	ASN
2	B	82	ASN
2	B	108	HIS
2	B	125	ASN

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Mol	Chain	Res	Type
2	B	128	ASN
2	B	172	ASN
2	B	221	GLN
2	B	270	ASN
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
1	C	235	GLN
1	C	241	GLN
2	D	34	ASN
2	D	72	HIS
2	D	82	ASN
2	D	172	ASN
2	D	217	ASN
2	D	255	GLN
2	D	270	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	482	HIS
2	D	525	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
3	SF4	A	267	1	0,12,12	-	-	-		
4	F3S	C	266	1	0,9,9	-	-	-		
4	F3S	A	266	1	0,9,9	-	-	-		
6	FEL	B	537	2	0,3,3	-	-	-		
3	SF4	A	265	1	0,12,12	-	-	-		
3	SF4	C	267	1	0,12,12	-	-	-		
6	FEL	D	537	2	0,3,3	-	-	-		
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
3	SF4	A	267	1	-	-	0/6/5/5
4	F3S	C	266	1	-	-	0/3/3/3
4	F3S	A	266	1	-	-	0/3/3/3
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 [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

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.