



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:35 AM UTC

PDB ID : 1G20 / pdb_00001g20
Title : MGATP-BOUND AND NUCLEOTIDE-FREE STRUCTURES OF A NITROGENASE PROTEIN COMPLEX BETWEEN LEU127DEL-FE PROTEIN AND THE MOFE PROTEIN
Authors : Chiu, H.-J.; Peters, J.W.; Lanzilotta, W.N.; Ryle, M.J.; Seefeldt, L.C.; Howard, J.B.; Rees, D.C.
Deposited on : 2000-10-16
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	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)	:	2.49

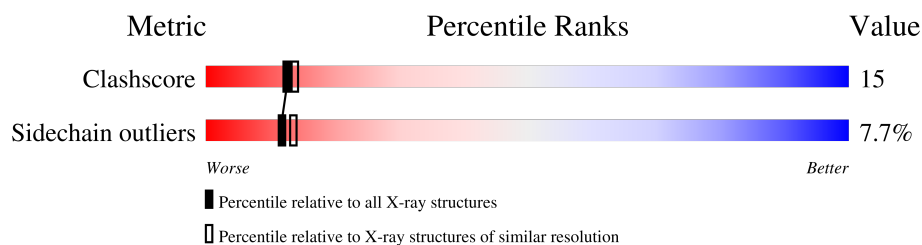
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6851 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	492	68% 24% 5% .
1	C	492	65% 28% . .
2	B	523	75% 21% .
2	D	523	72% 24% .
3	E	289	55% 29% 5% 10%
3	F	289	46% 40% . 10%
3	G	289	49% 35% 5% 11%
3	H	289	49% 36% 5% 9%

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
5	CFM	A	1496	-	-	X	-
5	CFM	C	3496	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24903 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 NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			
1	C	476	Total	C	N	O	S	0	0	0
			3776	2402	642	708	24			

- Molecule 2 is a protein called NITROGENASE MOLYBDENUM-IRON PROTEIN BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			
2	D	522	Total	C	N	O	S	0	0	0
			4174	2666	705	775	28			

- Molecule 3 is a protein called NITROGENASE IRON PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	259	Total	C	N	O	S	3	0	0
			1953	1227	330	376	20			
3	F	260	Total	C	N	O	S	0	0	0
			1952	1226	327	379	20			
3	G	257	Total	C	N	O	S	5	0	0
			1938	1219	327	372	20			
3	H	262	Total	C	N	O	S	3	0	0
			1984	1244	337	383	20			

There are 4 discrepancies between the modelled and reference sequences:

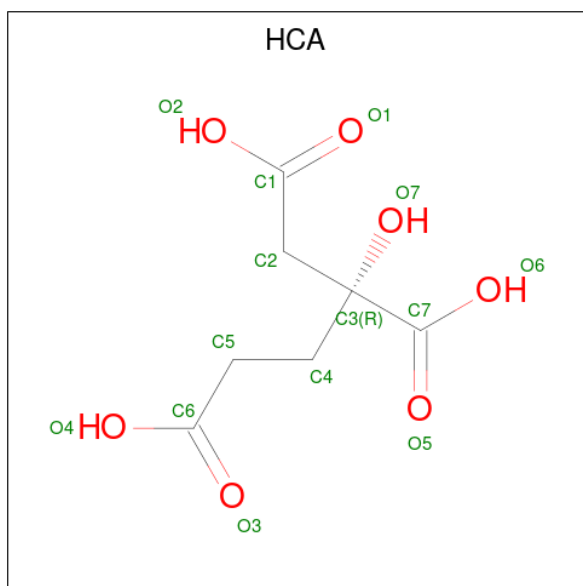
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	deletion	UNP P00459
F	?	-	LEU	deletion	UNP P00459
G	?	-	LEU	deletion	UNP P00459

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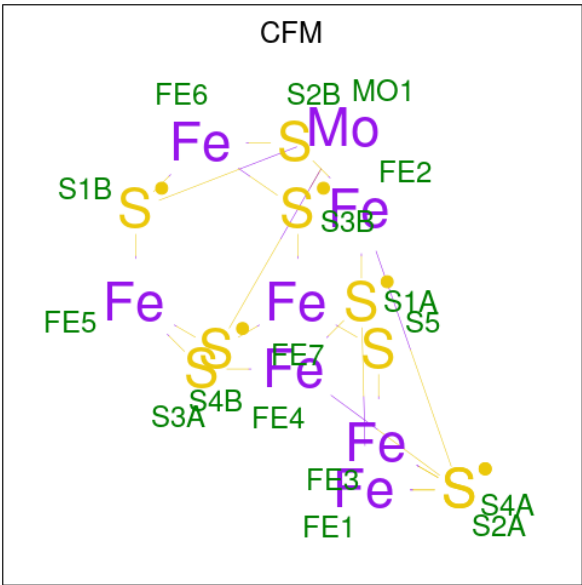
Chain	Residue	Modelled	Actual	Comment	Reference
H	?	-	LEU	deletion	UNP P00459

- Molecule 4 is 3-HYDROXY-3-CARBOXY-ADIPIC ACID (CCD ID: HCA) (formula: $C_7H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			14	7	7		
4	C	1	Total	C	O	0	0
			14	7	7		

- Molecule 5 is FE-MO-S CLUSTER (CCD ID: CFM) (formula: Fe_7MoS_9).

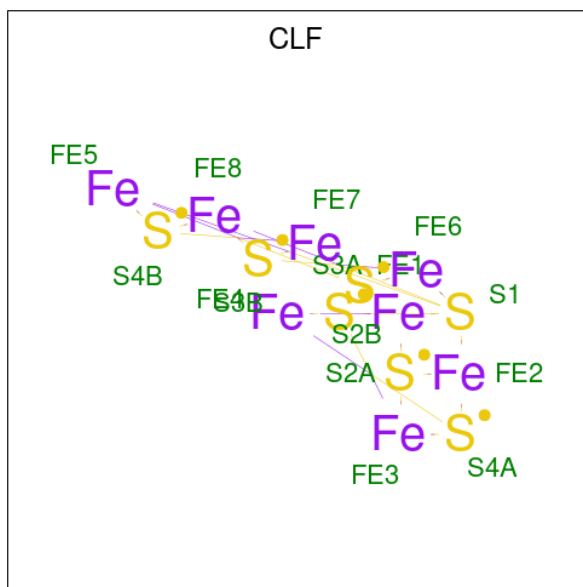


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Fe	Mo	S	0	0
			17	7	1	9		
5	C	1	Total	Fe	Mo	S	0	0
			17	7	1	9		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

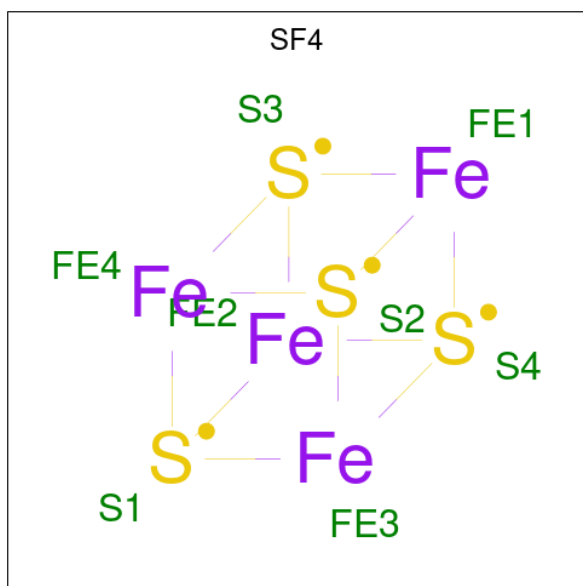
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	D	1	Total	Ca	0	0
			1	1		

- Molecule 7 is FE(8)-S(7) CLUSTER (CCD ID: CLF) (formula: Fe₈S₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			15	8	7		
7	D	1	Total	Fe	S	0	0
			15	8	7		

- Molecule 8 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	E	1	Total	Fe	S	0	0
			8	4	4		
8	G	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 9 is water.

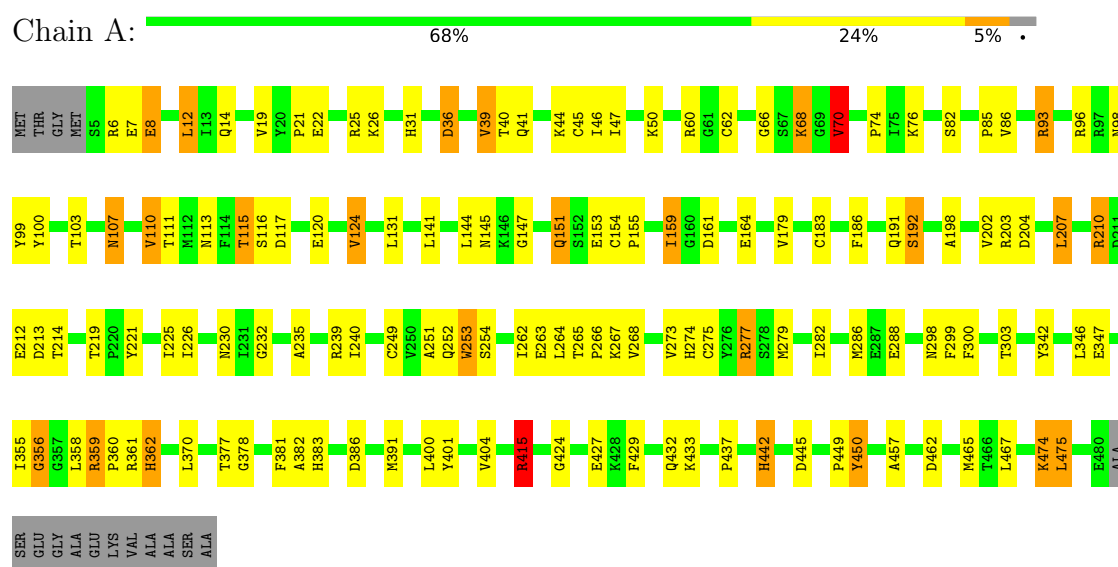
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	211	Total 211	O 211	0	0
9	B	309	Total 309	O 309	0	0
9	C	104	Total 104	O 104	0	0
9	D	235	Total 235	O 235	0	0
9	E	56	Total 56	O 56	0	0
9	F	62	Total 62	O 62	0	0
9	G	37	Total 37	O 37	0	0
9	H	52	Total 52	O 52	0	0

3 Residue-property plots

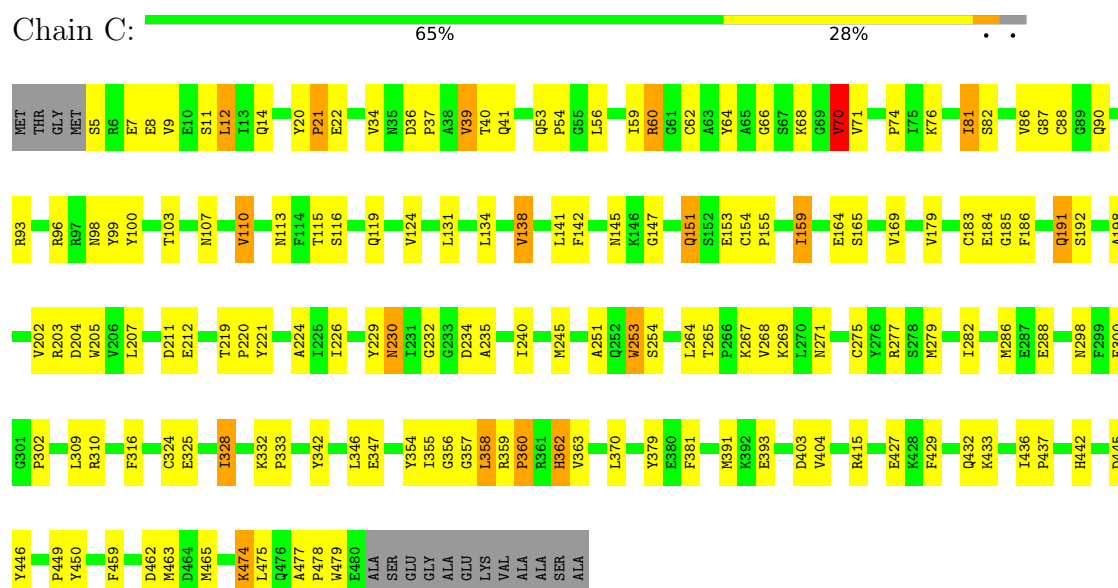
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

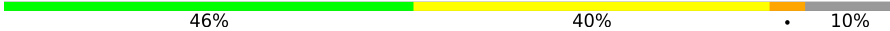
Note EDS was not executed.

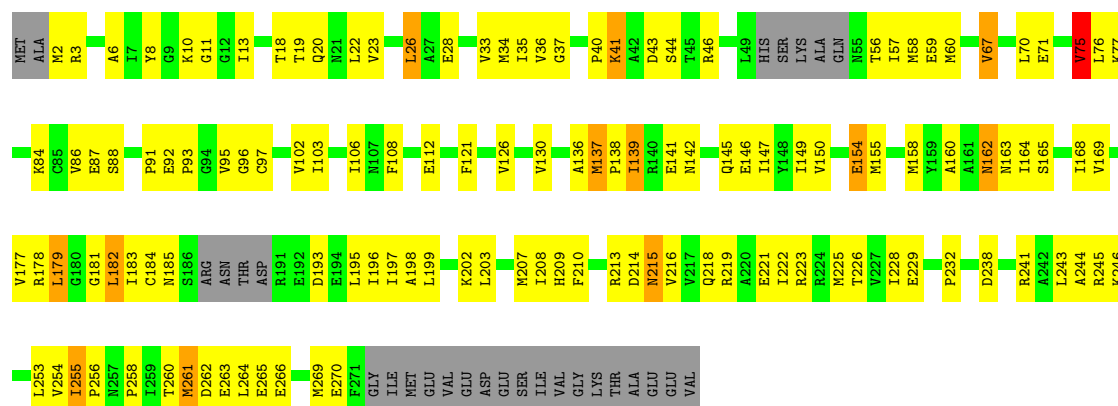
• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN



• Molecule 1: NITROGENASE MOLYBDENUM-IRON PROTEIN ALPHA CHAIN

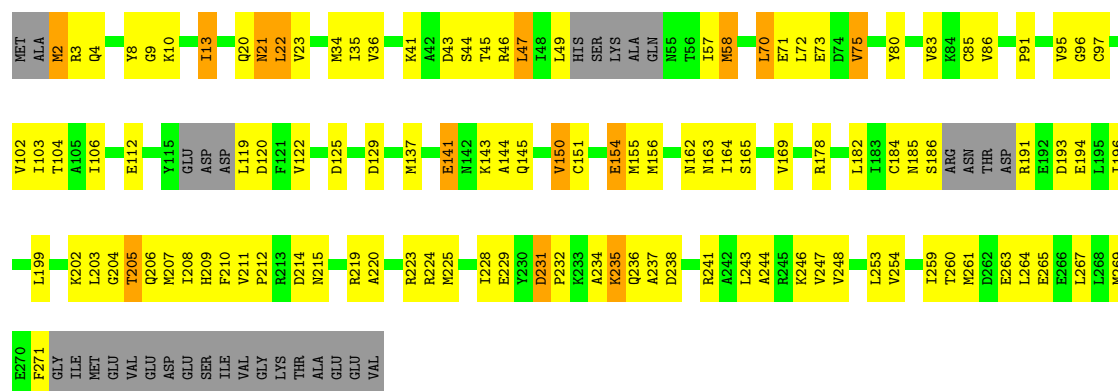


Chain F: 



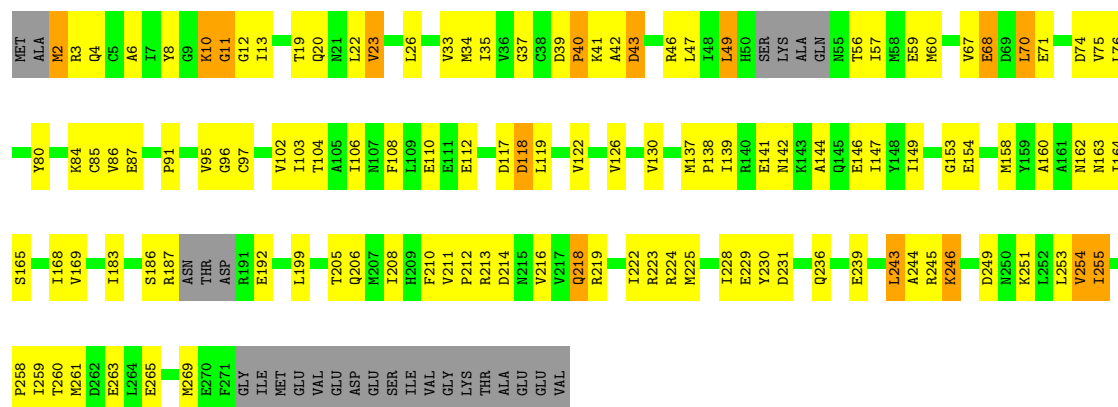
• Molecule 3: NITROGENASE IRON PROTEIN

Chain G: 



• Molecule 3: NITROGENASE IRON PROTEIN

Chain H: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	264.24Å 111.46Å 121.59Å 90.00° 97.40° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20	Depositor
% Data completeness (in resolution range)	89.1 (20.00-2.20)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24903	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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, HCA, CLF, CFM, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.58	0/3864	1.25	42/5212 (0.8%)
1	C	0.58	0/3864	1.27	43/5212 (0.8%)
2	B	0.58	0/4280	1.19	35/5786 (0.6%)
2	D	0.53	0/4280	1.16	32/5786 (0.6%)
3	E	0.35	0/1973	0.99	9/2654 (0.3%)
3	F	0.34	0/1973	0.97	10/2655 (0.4%)
3	G	0.38	0/1958	0.98	5/2633 (0.2%)
3	H	0.39	0/2006	1.01	11/2699 (0.4%)
All	All	0.51	0/24198	1.15	187/32637 (0.6%)

There are no bond length outliers.

All (187) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	VAL	N-CA-C	12.33	122.42	111.81
1	C	76	LYS	N-CA-C	11.45	123.76	111.28
2	D	213	MET	N-CA-C	11.40	124.82	111.71
1	A	70	VAL	N-CA-C	11.12	120.90	111.90
1	A	76	LYS	N-CA-C	11.02	123.29	111.28
3	H	118	ASP	N-CA-C	10.10	124.80	108.63
1	C	20	TYR	N-CA-C	9.46	123.13	110.08
1	C	362	HIS	N-CA-C	9.01	122.27	111.82
2	B	12	TYR	N-CA-C	-8.59	96.23	109.64
1	C	211	ASP	N-CA-C	-8.19	98.36	110.48
1	C	110	VAL	N-CA-C	8.18	118.27	110.42
2	D	12	TYR	N-CA-C	-8.00	97.16	109.64
2	B	498	VAL	CB-CA-C	-7.96	101.23	112.22
1	A	110	VAL	N-CA-C	7.84	117.94	110.42
2	D	49	THR	N-CA-C	7.79	119.99	110.41
2	D	149	VAL	N-CA-C	7.65	119.93	108.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	260	VAL	CB-CA-C	-7.56	101.79	112.22
1	A	22	GLU	N-CA-C	7.51	120.42	111.33
1	A	381	PHE	N-CA-C	7.45	122.43	112.30
2	D	391	VAL	N-CA-C	7.37	117.50	110.42
1	C	99	TYR	N-CA-C	7.37	120.37	110.35
2	B	237	PHE	N-CA-C	-7.37	103.18	111.14
3	G	231	ASP	CA-C-N	-7.33	110.68	119.84
3	G	231	ASP	C-N-CA	-7.33	110.68	119.84
1	A	347	GLU	N-CA-C	7.30	120.53	110.24
1	C	347	GLU	N-CA-C	7.28	120.51	110.24
2	B	368	ALA	N-CA-C	-7.25	97.92	109.59
1	A	60	ARG	N-CA-C	7.24	119.66	110.24
2	D	214	ASP	N-CA-C	7.23	120.20	111.82
3	F	255	ILE	N-CA-C	-7.22	99.69	107.77
2	D	237	PHE	N-CA-C	-7.17	103.55	111.36
2	D	358	SER	N-CA-C	7.17	122.20	113.17
3	H	255	ILE	N-CA-C	-7.16	100.53	107.76
3	G	207	MET	N-CA-C	-7.16	96.89	108.41
3	H	211	VAL	CA-C-N	6.99	127.40	119.92
3	H	211	VAL	C-N-CA	6.99	127.40	119.92
3	E	92	GLU	N-CA-C	-6.93	100.11	110.24
1	A	86	VAL	N-CA-C	6.92	121.85	111.89
1	C	39	VAL	CB-CA-C	-6.84	100.07	111.29
2	B	478	HIS	N-CA-C	6.83	120.98	112.24
1	C	192	SER	N-CA-C	6.81	118.70	111.28
2	D	212	SER	N-CA-C	6.78	121.40	113.20
2	B	213	MET	N-CA-C	6.77	120.64	112.38
2	D	368	ALA	N-CA-C	-6.75	98.19	109.07
2	B	18	GLN	N-CA-C	6.72	119.46	111.33
2	D	520	ASP	N-CA-C	6.70	119.95	110.50
1	A	99	TYR	N-CA-C	6.69	119.45	110.35
2	B	93	GLN	N-CA-C	6.67	119.56	111.82
1	C	22	GLU	N-CA-C	6.63	119.35	111.33
2	B	228	PRO	N-CA-C	6.61	122.25	113.40
2	B	212	SER	N-CA-C	6.58	120.98	113.15
2	D	5	VAL	N-CA-C	6.51	120.16	111.17
1	C	342	TYR	N-CA-C	6.44	121.22	113.23
2	B	214	ASP	N-CA-C	6.43	119.11	111.71
2	B	5	VAL	N-CA-C	6.41	120.01	111.17
3	G	224	ARG	N-CA-C	6.41	120.25	111.54
2	B	49	THR	N-CA-C	6.40	118.59	110.33
2	B	358	SER	N-CA-C	6.37	121.20	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	381	PHE	N-CA-C	6.37	122.51	113.02
2	D	325	THR	N-CA-C	-6.37	103.86	111.69
2	B	149	VAL	N-CA-C	6.33	117.92	108.23
2	D	175	ILE	N-CA-C	-6.32	104.01	109.19
1	C	279	MET	N-CA-C	6.32	120.28	111.56
1	A	207	LEU	N-CA-C	6.31	118.97	111.33
2	B	428	TRP	N-CA-C	-6.31	104.63	112.90
1	C	39	VAL	N-CA-C	6.30	122.45	109.34
3	F	92	GLU	N-CA-C	-6.27	102.92	110.13
1	A	442	HIS	N-CA-C	-6.24	101.53	111.02
1	C	185	GLY	N-CA-C	6.24	121.57	113.27
1	C	393	GLU	N-CA-C	6.18	117.68	111.07
1	A	342	TYR	N-CA-C	6.10	120.89	112.90
1	C	21	PRO	N-CA-C	-6.09	101.69	111.38
2	B	145	ASP	N-CA-C	-6.09	105.67	113.23
1	C	86	VAL	N-CA-C	6.06	118.63	111.05
1	C	253	TRP	N-CA-C	6.04	118.14	108.41
1	A	44	LYS	N-CA-C	-6.03	105.10	112.88
1	A	210	ARG	CB-CG-CD	6.03	125.16	111.30
1	A	253	TRP	N-CA-C	6.03	118.59	108.23
1	C	116	SER	N-CA-C	-6.02	105.97	113.38
1	A	212	GLU	CA-C-N	6.01	129.92	121.02
1	A	212	GLU	C-N-CA	6.01	129.92	121.02
1	C	60	ARG	N-CA-C	6.00	118.29	110.43
2	D	145	ASP	N-CA-C	-5.97	106.00	113.28
1	A	277	ARG	N-CA-C	5.93	117.41	111.07
1	C	71	VAL	N-CA-C	5.90	116.11	110.74
2	D	468	ARG	N-CA-C	5.90	119.08	108.17
3	F	226	THR	N-CA-C	-5.89	101.28	110.42
1	A	251	ALA	N-CA-C	5.89	118.36	109.23
3	E	187	ARG	N-CA-C	-5.88	106.08	113.72
1	A	362	HIS	N-CA-C	5.88	118.64	111.82
1	A	45	CYS	CA-C-N	-5.87	113.03	122.25
1	A	45	CYS	C-N-CA	-5.87	113.03	122.25
1	A	432	GLN	N-CA-C	-5.86	104.97	111.36
2	D	475	ASP	N-CA-C	5.86	120.05	113.02
1	A	21	PRO	N-CA-C	-5.79	102.73	111.41
1	A	450	TYR	N-CA-C	-5.79	106.08	114.12
1	C	251	ALA	N-CA-C	5.78	118.19	109.23
1	C	436	ILE	N-CA-C	5.78	114.24	107.77
2	D	498	VAL	CB-CA-C	-5.77	104.26	112.22
2	D	428	TRP	N-CA-C	-5.75	104.99	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	87	PRO	N-CA-C	-5.73	102.14	110.80
2	B	341	PRO	N-CA-C	5.73	120.22	111.34
1	A	124	VAL	N-CA-C	5.72	116.50	110.72
1	C	12	LEU	N-CA-C	-5.70	104.99	111.14
1	C	37	PRO	N-CA-C	5.66	121.28	113.98
1	C	179	VAL	N-CA-C	5.66	114.18	107.73
1	C	11	SER	N-CA-C	-5.63	105.91	112.89
1	C	119	GLN	N-CA-C	-5.62	101.59	109.69
2	B	367	PHE	N-CA-C	5.62	118.62	109.24
3	E	126	VAL	N-CA-C	5.62	117.68	108.97
1	C	450	TYR	N-CA-C	-5.60	106.33	114.12
1	A	153	GLU	N-CA-C	-5.59	101.92	110.14
1	A	39	VAL	N-CA-C	5.58	120.94	109.34
1	C	56	LEU	N-CA-C	5.55	119.75	112.92
2	D	228	PRO	N-CA-C	5.51	120.79	113.40
3	F	261	MET	N-CA-C	-5.48	105.46	111.82
3	H	254	VAL	N-CA-C	5.48	118.00	108.90
3	F	126	VAL	N-CA-C	5.47	117.77	109.12
3	H	43	ASP	N-CA-C	-5.46	99.83	108.73
1	C	234	ASP	N-CA-C	5.46	117.66	111.11
3	G	205	THR	CB-CA-C	-5.46	108.57	116.54
1	A	424	GLY	N-CA-C	5.44	120.02	112.57
1	A	279	MET	N-CA-C	5.43	119.68	112.30
2	B	520	ASP	N-CA-C	5.42	118.30	110.28
2	D	359	HIS	N-CA-C	5.42	117.94	111.71
1	C	7	GLU	N-CA-C	-5.41	107.05	113.97
1	C	474	LYS	N-CA-C	5.40	119.43	112.41
3	E	231	ASP	CA-C-N	5.39	124.57	118.97
3	E	231	ASP	C-N-CA	5.39	124.57	118.97
1	A	474	LYS	N-CA-C	5.38	119.16	112.59
2	B	467	ILE	N-CA-C	-5.37	99.42	107.37
2	D	256	ASP	N-CA-CB	-5.36	103.64	111.20
3	F	139	ILE	N-CA-C	5.36	116.68	111.91
1	A	192	SER	N-CA-C	5.34	117.53	111.11
1	A	213	ASP	N-CA-C	5.34	117.92	109.96
3	H	42	ALA	CA-C-N	-5.33	115.68	122.77
3	H	42	ALA	C-N-CA	-5.33	115.68	122.77
2	D	363	HIS	N-CA-C	5.32	118.02	110.10
2	D	284	ALA	N-CA-C	5.31	121.54	109.81
1	C	432	GLN	N-CA-C	-5.30	105.67	111.82
2	B	363	HIS	N-CA-C	5.30	117.86	109.96
1	C	142	PHE	CA-C-N	5.29	125.61	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	142	PHE	C-N-CA	5.29	125.61	119.47
3	E	226	THR	N-CA-C	-5.29	103.06	110.35
1	C	191	GLN	N-CA-C	-5.28	106.34	112.89
2	B	373	PRO	N-CA-C	5.28	121.62	113.75
2	B	517	TYR	N-CA-C	-5.27	106.11	112.54
2	D	478	HIS	N-CA-C	5.26	119.28	112.86
3	E	255	ILE	N-CA-C	-5.26	102.34	107.55
1	A	361	ARG	N-CA-C	-5.24	107.54	114.04
2	D	123	ALA	N-CA-C	-5.24	105.75	111.82
2	D	379	LEU	N-CA-C	-5.23	105.66	111.36
2	B	299	GLU	N-CA-C	5.23	117.06	111.36
1	A	240	ILE	N-CA-C	-5.22	105.44	110.72
1	A	179	VAL	N-CA-C	5.22	113.62	107.77
2	D	467	ILE	N-CA-C	-5.22	99.65	107.37
1	C	81	ILE	N-CA-C	5.21	115.59	107.99
2	B	322	LEU	N-CA-C	5.20	116.81	111.03
1	C	205	TRP	N-CA-C	5.20	120.62	113.97
2	B	418	ASN	N-CA-C	-5.17	106.21	112.88
2	B	451	ILE	N-CA-C	-5.16	105.50	110.72
3	H	39	ASP	CA-C-N	5.15	125.44	119.47
3	H	39	ASP	C-N-CA	5.15	125.44	119.47
3	F	136	ALA	N-CA-C	-5.15	106.40	113.30
1	A	116	SER	N-CA-C	-5.15	106.69	113.17
2	B	500	SER	N-CA-C	-5.13	105.38	111.69
2	B	210	LEU	N-CA-C	5.13	117.27	111.11
1	A	273	VAL	N-CA-C	5.13	115.73	107.73
3	E	132	CYS	N-CA-C	5.13	115.11	107.88
2	B	446	SER	N-CA-C	5.12	118.63	112.38
2	B	503	GLU	N-CA-C	-5.12	105.61	111.14
3	H	11	GLY	N-CA-C	5.12	125.31	113.18
2	D	351	LEU	N-CA-C	-5.10	105.80	111.36
1	A	36	ASP	N-CA-C	-5.07	97.58	108.64
1	A	356	GLY	N-CA-C	5.06	125.17	113.18
1	A	415	ARG	CA-C-N	5.06	127.39	120.46
1	A	415	ARG	C-N-CA	5.06	127.39	120.46
2	D	238	ARG	N-CA-C	5.05	116.79	111.28
3	F	44	SER	N-CA-C	5.05	119.44	113.28
2	B	222	LYS	N-CA-C	5.04	118.55	111.74
1	C	240	ILE	N-CA-C	-5.04	104.79	111.09
2	D	210	LEU	N-CA-C	5.04	117.43	111.33
3	E	175	GLY	N-CA-C	5.04	118.78	110.77
3	F	75	VAL	N-CA-C	5.04	116.14	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	207	LEU	N-CA-C	5.03	118.19	111.75
2	D	31	PHE	N-CA-C	5.01	121.13	113.61
3	F	93	PRO	N-CA-C	5.01	118.95	111.14

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	3776	0	3708	89	0
1	C	3776	0	3708	101	0
2	B	4174	0	4087	61	0
2	D	4174	0	4087	80	0
3	E	1953	0	1971	77	0
3	F	1952	0	1958	106	0
3	G	1938	0	1958	121	0
3	H	1984	0	1993	141	0
4	A	14	0	6	3	0
4	C	14	0	6	2	0
5	A	17	0	0	5	0
5	C	17	0	0	6	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	B	15	0	0	1	0
7	D	15	0	0	1	0
8	E	8	0	0	0	0
8	G	8	0	0	0	0
9	A	211	0	0	6	0
9	B	309	0	0	6	0
9	C	104	0	0	1	0
9	D	235	0	0	6	0
9	E	56	0	0	2	0
9	F	62	0	0	0	0
9	G	37	0	0	0	0
9	H	52	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	24903	0	23482	722	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (722) 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)
3:G:231:ASP:OD2	3:G:234:ALA:HB2	1.31	1.25
3:G:129:ASP:CG	3:H:41:LYS:HZ3	1.48	1.21
1:C:253:TRP:CZ3	1:C:282:ILE:HD13	1.78	1.16
1:A:275:CYS:HA	1:A:358:LEU:HD22	1.28	1.14
3:F:23:VAL:HG21	3:F:35:ILE:HD11	1.32	1.04
3:G:23:VAL:HG21	3:G:35:ILE:HD11	1.40	1.01
1:A:210:ARG:HD3	1:A:263:GLU:CB	1.90	1.01
3:G:215:ASN:O	3:G:219:ARG:HG3	1.62	0.99
1:A:210:ARG:HD3	1:A:263:GLU:HB3	1.01	0.99
3:G:129:ASP:CG	3:H:41:LYS:NZ	2.21	0.98
3:G:219:ARG:O	3:G:223:ARG:HD3	1.66	0.95
3:E:162:ASN:HD21	3:E:259:ILE:H	1.09	0.94
1:C:39:VAL:HG23	1:C:391:MET:HG3	1.49	0.94
1:C:325:GLU:HA	1:C:328:ILE:CG2	1.99	0.93
1:C:253:TRP:HZ3	1:C:282:ILE:HD13	1.14	0.93
1:C:324:CYS:O	1:C:328:ILE:HG22	1.68	0.92
1:A:8:GLU:HA	1:A:8:GLU:OE1	1.70	0.90
1:A:39:VAL:HG21	1:A:391:MET:HE3	1.54	0.90
1:A:359:ARG:HG3	5:A:1496:CFM:S3A	2.13	0.89
3:G:205:THR:HG23	3:G:206:GLN:H	1.38	0.88
3:H:118:ASP:C	3:H:119:LEU:HD12	1.99	0.88
1:A:210:ARG:CD	1:A:263:GLU:HB3	1.97	0.87
1:A:68:LYS:HB2	1:A:151:GLN:HG2	1.54	0.87
3:E:228:ILE:H	3:E:228:ILE:HD12	1.41	0.86
1:A:36:ASP:O	1:A:39:VAL:HG22	1.77	0.85
3:E:225:MET:HE2	3:E:229:GLU:HG2	1.59	0.84
3:H:46:ARG:NH2	3:H:224:ARG:HE	1.75	0.84
1:A:39:VAL:CG2	1:A:391:MET:HE3	2.07	0.84
3:E:57:ILE:HG12	3:E:75:VAL:HG21	1.59	0.83
3:H:154:GLU:HB2	3:H:187:ARG:NH1	1.93	0.83
1:A:210:ARG:HD2	1:A:263:GLU:OE2	1.79	0.83
3:E:23:VAL:HG21	3:E:35:ILE:HD11	1.59	0.82
3:F:34:MET:HE2	3:F:76:LEU:HD21	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:231:ASP:OD2	3:G:234:ALA:CB	2.23	0.81
3:G:129:ASP:CB	3:H:41:LYS:HE2	2.12	0.80
3:G:58:MET:HE1	3:G:104:THR:HG21	1.63	0.79
3:G:205:THR:HG23	3:G:206:GLN:N	1.96	0.79
1:C:39:VAL:O	1:C:41:GLN:N	2.16	0.79
3:H:106:ILE:HB	3:H:137:MET:HE3	1.65	0.78
3:F:103:ILE:HA	3:F:137:MET:HG3	1.64	0.78
3:G:72:LEU:HB2	3:G:112:GLU:HG2	1.64	0.78
2:D:413:SER:O	2:D:417:LYS:HE3	1.83	0.77
3:H:76:LEU:HD23	3:H:86:VAL:HG22	1.65	0.77
3:G:228:ILE:H	3:G:228:ILE:HD12	1.48	0.77
2:D:118:MET:HE2	2:D:154:MET:SD	2.25	0.76
3:F:260:THR:HG22	3:F:262:ASP:H	1.51	0.76
1:C:221:TYR:HA	1:C:316:PHE:CE2	2.21	0.76
3:F:225:MET:HE2	3:F:229:GLU:HG2	1.67	0.75
3:G:244:ALA:O	3:G:248:VAL:HG23	1.86	0.75
1:A:68:LYS:HD2	1:A:68:LYS:C	2.12	0.75
3:G:129:ASP:HB3	3:H:41:LYS:HE2	1.69	0.75
1:A:442:HIS:ND1	4:A:1494:HCA:H52	2.02	0.74
3:F:182:LEU:HD21	3:F:199:LEU:HD12	1.68	0.74
3:G:231:ASP:CG	3:G:231:ASP:O	2.30	0.73
3:H:219:ARG:O	3:H:222:ILE:HG12	1.88	0.73
1:A:275:CYS:HA	1:A:358:LEU:CD2	2.15	0.73
3:H:6:ALA:HB3	3:H:147:ILE:CD1	2.18	0.73
3:F:162:ASN:HD21	3:F:258:PRO:HA	1.51	0.73
1:C:81:ILE:HD13	1:C:134:LEU:HD21	1.69	0.72
3:G:8:TYR:HB3	3:G:164:ILE:HD13	1.71	0.72
2:B:216:LYS:HG2	2:B:285:PRO:HB2	1.70	0.72
2:D:304:PHE:O	2:D:308:THR:HB	1.90	0.72
3:H:265:GLU:O	3:H:269:MET:HG2	1.90	0.72
3:H:139:ILE:HG22	3:H:147:ILE:HD11	1.72	0.71
1:C:39:VAL:HG21	1:C:391:MET:CE	2.20	0.71
3:H:8:TYR:HB3	3:H:164:ILE:HD13	1.70	0.71
1:A:7:GLU:OE1	1:A:7:GLU:N	2.23	0.71
3:G:129:ASP:OD2	3:H:41:LYS:HD3	1.91	0.70
1:C:253:TRP:CH2	1:C:282:ILE:HD13	2.27	0.70
2:D:96:VAL:HG21	2:D:115:SER:HB2	1.73	0.70
3:E:162:ASN:HD21	3:E:259:ILE:N	1.89	0.70
3:H:154:GLU:HB2	3:H:187:ARG:HH12	1.55	0.69
1:A:31:HIS:O	1:A:46:ILE:HD11	1.92	0.69
2:D:362:LEU:HD13	2:D:386:LEU:HG	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:44:SER:HB3	3:G:125:ASP:OD2	1.93	0.69
3:E:228:ILE:HD12	3:E:228:ILE:N	2.08	0.68
1:C:298:ASN:HD21	1:C:300:PHE:HB2	1.58	0.68
2:B:96:VAL:HG21	2:B:115:SER:HB2	1.77	0.67
1:C:310:ARG:NH1	1:C:328:ILE:HD13	2.09	0.67
3:F:266:GLU:O	3:F:270:GLU:HG3	1.95	0.67
3:G:155:MET:HE3	3:G:155:MET:O	1.95	0.67
3:G:208:ILE:O	3:G:246:LYS:HD3	1.94	0.67
3:H:10:LYS:HE2	3:H:10:LYS:HA	1.77	0.67
1:A:415:ARG:HA	1:A:415:ARG:NE	2.09	0.67
3:G:237:ALA:O	3:G:241:ARG:HG3	1.94	0.67
2:B:473:ILE:HD12	2:B:479:LEU:HD23	1.77	0.67
1:A:232:GLY:O	1:A:449:PRO:HD3	1.95	0.67
3:G:22:LEU:HG	3:G:243:LEU:HD22	1.76	0.67
3:E:217:VAL:HB	3:E:218:GLN:OE1	1.94	0.67
1:A:230:ASN:HD22	1:A:235:ALA:H	1.42	0.66
3:F:146:GLU:HG2	3:F:253:LEU:HD11	1.76	0.66
1:C:39:VAL:CG2	1:C:391:MET:HG3	2.23	0.66
2:D:118:MET:HB3	2:D:154:MET:HE1	1.76	0.66
3:G:49:LEU:HD11	3:G:85:CYS:SG	2.35	0.66
3:G:243:LEU:O	3:G:247:VAL:HG23	1.95	0.66
3:E:155:MET:HG2	3:F:221:GLU:OE2	1.96	0.66
1:A:103:THR:H	1:A:107:ASN:HD21	1.43	0.65
3:F:13:ILE:HG22	3:F:185:ASN:HD22	1.60	0.65
1:C:229:TYR:CE1	5:C:3496:CFM:S2A	2.89	0.65
3:G:162:ASN:HD21	3:G:259:ILE:H	1.45	0.65
3:H:2:MET:HE3	3:H:122:VAL:HG23	1.79	0.65
3:G:129:ASP:OD2	3:H:41:LYS:CE	2.45	0.65
1:C:39:VAL:HG21	1:C:391:MET:HE3	1.77	0.65
2:B:348:ARG:HG3	2:B:487:TYR:CE2	2.32	0.65
2:B:414:PRO:HA	2:B:417:LYS:HD2	1.78	0.65
1:A:219:THR:HG22	1:A:221:TYR:H	1.62	0.64
3:F:76:LEU:HD23	3:F:86:VAL:HG13	1.80	0.64
3:G:129:ASP:CB	3:H:41:LYS:CE	2.75	0.64
1:C:220:PRO:O	1:C:316:PHE:HE2	1.81	0.64
3:E:12:GLY:H	3:F:10:LYS:HZ2	1.45	0.64
1:A:442:HIS:CG	4:A:1494:HCA:H52	2.33	0.64
3:G:106:ILE:HB	3:G:137:MET:HE3	1.78	0.64
3:E:228:ILE:H	3:E:228:ILE:CD1	2.10	0.64
1:C:232:GLY:O	1:C:449:PRO:HD3	1.98	0.64
1:C:159:ILE:HG13	3:H:97:CYS:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:95:VAL:HG22	3:H:96:GLY:H	1.63	0.63
3:H:254:VAL:HG22	3:H:255:ILE:N	2.12	0.63
1:C:265:THR:HG22	1:C:286:MET:HE1	1.79	0.63
3:H:2:MET:HE2	3:H:3:ARG:N	2.13	0.63
3:E:18:THR:HG21	3:E:185:ASN:OD1	1.99	0.63
3:F:214:ASP:OD2	3:F:216:VAL:HG23	1.98	0.63
1:C:40:THR:HG22	1:C:40:THR:O	1.99	0.63
3:H:10:LYS:HE2	3:H:11:GLY:H	1.62	0.63
3:F:254:VAL:HG12	3:F:255:ILE:N	2.12	0.63
3:G:129:ASP:CB	3:H:41:LYS:NZ	2.61	0.63
2:D:85:THR:HG21	2:D:146:MET:HE2	1.81	0.62
3:G:2:MET:CE	3:G:122:VAL:HG23	2.28	0.62
3:H:261:MET:O	3:H:265:GLU:HG3	1.99	0.62
3:H:10:LYS:HG2	3:H:160:ALA:CB	2.30	0.62
3:G:155:MET:HE1	3:G:264:LEU:HD23	1.81	0.62
1:C:154:CYS:HB2	1:C:155:PRO:HD3	1.81	0.62
3:G:36:VAL:HA	3:G:86:VAL:HG23	1.80	0.62
1:C:36:ASP:O	1:C:39:VAL:HG13	1.99	0.62
2:D:360:THR:HB	9:D:3531:HOH:O	1.98	0.62
3:F:262:ASP:O	3:F:266:GLU:HG3	2.00	0.62
1:A:145:ASN:HD22	1:A:147:GLY:H	1.47	0.62
1:C:68:LYS:HB2	1:C:151:GLN:HG2	1.81	0.62
2:D:86:MET:HG2	2:D:138:CYS:SG	2.40	0.62
3:E:57:ILE:CG1	3:E:75:VAL:HG21	2.29	0.62
3:H:56:THR:HG23	3:H:59:GLU:OE2	1.99	0.62
3:E:15:LYS:HG2	3:E:150:VAL:HG11	1.80	0.62
3:F:20:GLN:HA	3:F:23:VAL:HG22	1.82	0.62
2:D:394:LEU:HD13	2:D:430:LEU:HB2	1.82	0.61
3:H:210:PHE:O	3:H:212:PRO:HD3	2.00	0.61
1:A:415:ARG:NE	1:A:415:ARG:CA	2.61	0.61
3:H:43:ASP:OD2	3:H:46:ARG:HB2	2.00	0.61
3:F:198:ALA:O	3:F:202:LYS:HG2	2.00	0.61
3:G:260:THR:HG23	3:G:263:GLU:H	1.64	0.61
3:G:129:ASP:CG	3:H:41:LYS:CE	2.74	0.61
2:D:299:GLU:O	2:D:303:LYS:HG3	2.01	0.61
3:H:223:ARG:O	3:H:225:MET:HG2	2.00	0.61
1:C:103:THR:H	1:C:107:ASN:HD21	1.47	0.61
3:H:10:LYS:HG2	3:H:160:ALA:HB2	1.83	0.61
3:H:95:VAL:HG22	3:H:96:GLY:N	2.16	0.61
3:H:102:VAL:O	3:H:106:ILE:HG12	2.01	0.61
2:B:67:ALA:H	2:B:396:HIS:HD2	1.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:HIS:CG	4:C:3494:HCA:H52	2.35	0.61
3:E:103:ILE:HG12	3:E:137:MET:HG3	1.83	0.61
1:A:66:GLY:O	1:A:70:VAL:HG22	2.01	0.60
1:A:68:LYS:HD2	1:A:68:LYS:O	2.01	0.60
1:A:442:HIS:HB2	9:A:1509:HOH:O	1.99	0.60
3:E:214:ASP:CG	3:E:216:VAL:HG22	2.27	0.60
3:H:22:LEU:HD23	3:H:26:LEU:HD13	1.83	0.60
3:F:179:LEU:HD22	3:F:181:GLY:H	1.65	0.60
1:A:207:LEU:HD22	1:A:282:ILE:HD11	1.83	0.60
1:C:221:TYR:HA	1:C:316:PHE:HE2	1.65	0.60
1:C:359:ARG:NH1	5:C:3496:CFM:S4B	2.74	0.60
3:F:40:PRO:HG2	3:F:41:LYS:HD3	1.82	0.60
3:F:260:THR:HB	3:F:263:GLU:HG3	1.82	0.60
3:E:162:ASN:ND2	3:E:259:ILE:H	1.91	0.60
1:C:275:CYS:HA	1:C:358:LEU:HG	1.84	0.60
2:D:243:MET:HE3	9:D:3722:HOH:O	2.01	0.59
1:C:64:TYR:CE2	1:C:88:CYS:HB3	2.37	0.59
1:C:230:ASN:HD22	1:C:235:ALA:H	1.48	0.59
2:D:216:LYS:HG2	2:D:285:PRO:HB2	1.84	0.59
3:E:15:LYS:HG2	3:E:150:VAL:CG1	2.32	0.59
3:G:260:THR:CG2	3:G:263:GLU:HG3	2.31	0.59
3:F:158:MET:HE1	3:F:195:LEU:HD11	1.84	0.59
3:G:228:ILE:HD12	3:G:228:ILE:N	2.15	0.59
3:F:28:GLU:OE1	3:F:241:ARG:HD3	2.03	0.59
3:G:102:VAL:O	3:G:106:ILE:HG12	2.02	0.59
1:C:124:VAL:O	3:H:91:PRO:HB3	2.02	0.59
3:G:231:ASP:O	3:G:231:ASP:OD1	2.21	0.59
3:G:202:LYS:HG3	3:G:267:LEU:HD11	1.85	0.59
3:H:57:ILE:HD11	3:H:86:VAL:HG11	1.85	0.59
1:C:325:GLU:O	1:C:328:ILE:HG23	2.02	0.58
3:G:2:MET:HE1	3:G:122:VAL:HG23	1.84	0.58
3:G:2:MET:HE2	3:G:3:ARG:N	2.18	0.58
3:G:215:ASN:C	3:G:219:ARG:HG3	2.29	0.58
1:C:442:HIS:HB2	9:C:3565:HOH:O	2.03	0.58
3:H:119:LEU:HD12	3:H:119:LEU:N	2.17	0.58
3:E:219:ARG:O	3:E:223:ARG:HD3	2.02	0.58
2:D:304:PHE:CZ	2:D:308:THR:HG21	2.38	0.58
3:E:76:LEU:HD23	3:E:86:VAL:HG13	1.85	0.58
3:G:10:LYS:NZ	3:G:156:MET:HB3	2.18	0.58
3:G:228:ILE:H	3:G:228:ILE:CD1	2.16	0.58
3:F:6:ALA:HB3	3:F:147:ILE:CD1	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:71:GLU:HG3	3:G:73:GLU:OE1	2.04	0.58
1:A:415:ARG:HA	1:A:415:ARG:CZ	2.34	0.58
2:D:304:PHE:CE1	2:D:308:THR:HG21	2.39	0.58
3:G:129:ASP:OD2	3:H:41:LYS:NZ	2.33	0.57
2:B:468:ARG:HB3	2:B:473:ILE:HD13	1.86	0.57
1:C:96:ARG:HD2	5:C:3496:CFM:S3B	2.44	0.57
1:C:141:LEU:HD21	2:D:56:ASN:HA	1.86	0.57
3:G:21:ASN:N	3:G:21:ASN:HD22	1.99	0.57
1:C:298:ASN:HD22	1:C:300:PHE:H	1.52	0.57
3:F:102:VAL:O	3:F:106:ILE:HG12	2.04	0.57
3:F:225:MET:HE2	3:F:229:GLU:CG	2.33	0.57
3:G:235:LYS:HE2	3:G:235:LYS:HA	1.87	0.57
3:H:23:VAL:HG21	3:H:35:ILE:HD11	1.87	0.57
3:H:146:GLU:HG2	3:H:253:LEU:HD21	1.86	0.57
1:C:253:TRP:CZ3	1:C:282:ILE:CD1	2.71	0.57
3:F:179:LEU:HD12	3:F:256:PRO:HB3	1.86	0.57
2:D:372:ASP:O	2:D:376:VAL:HG12	2.05	0.57
3:E:179:LEU:HD22	3:E:181:GLY:H	1.70	0.57
2:B:85:THR:HG21	2:B:146:MET:HE2	1.87	0.56
3:H:228:ILE:HD12	3:H:228:ILE:H	1.70	0.56
1:C:325:GLU:HA	1:C:328:ILE:HG21	1.81	0.56
3:G:2:MET:HE2	3:G:3:ARG:H	1.70	0.56
3:H:23:VAL:HG11	3:H:35:ILE:HD11	1.86	0.56
3:H:162:ASN:HD21	3:H:259:ILE:H	1.51	0.56
3:H:26:LEU:HD12	3:H:244:ALA:HB1	1.88	0.56
3:H:6:ALA:HB3	3:H:147:ILE:HD12	1.87	0.56
3:G:129:ASP:OD2	3:H:41:LYS:CD	2.54	0.56
1:A:93:ARG:HD2	1:A:111:THR:O	2.06	0.56
3:F:76:LEU:HD22	3:F:84:LYS:HB3	1.87	0.56
3:H:218:GLN:O	3:H:222:ILE:HG23	2.05	0.56
3:H:117:ASP:O	3:H:119:LEU:HD13	2.06	0.56
3:H:103:ILE:HA	3:H:137:MET:HE2	1.88	0.56
3:H:46:ARG:NH2	3:H:224:ARG:NE	2.50	0.56
2:D:95:CYS:HB3	2:D:99:PHE:CZ	2.40	0.55
2:D:414:PRO:O	2:D:417:LYS:HG2	2.06	0.55
3:E:106:ILE:HD11	3:E:138:PRO:HG3	1.87	0.55
1:A:186:PHE:HB3	2:B:154:MET:HE3	1.89	0.55
2:D:198:ASP:HB2	2:D:297:HIS:O	2.05	0.55
2:D:417:LYS:N	2:D:417:LYS:HE2	2.21	0.55
3:E:225:MET:HE2	3:E:229:GLU:CG	2.34	0.55
3:F:228:ILE:HD12	3:F:228:ILE:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:34:MET:HE2	3:G:119:LEU:HD21	1.87	0.55
2:B:236:ASN:HB3	2:B:485:LEU:HD22	1.87	0.55
2:D:358:SER:HB3	2:D:498:VAL:HG11	1.88	0.55
3:H:57:ILE:CG1	3:H:75:VAL:HG21	2.37	0.55
1:A:265:THR:HG22	1:A:286:MET:HE1	1.88	0.55
2:D:124:VAL:HG11	3:G:58:MET:HG2	1.89	0.55
3:G:165:SER:O	3:G:169:VAL:HG23	2.06	0.55
1:A:39:VAL:HG23	1:A:391:MET:HE3	1.88	0.55
3:F:77:LYS:NZ	3:F:77:LYS:HB3	2.22	0.55
3:H:214:ASP:OD2	3:H:216:VAL:HG23	2.05	0.55
3:H:117:ASP:OD1	3:H:119:LEU:HD11	2.07	0.55
3:H:228:ILE:HD12	3:H:228:ILE:N	2.22	0.55
1:C:298:ASN:ND2	1:C:300:PHE:H	2.05	0.55
3:F:36:VAL:HA	3:F:86:VAL:HG23	1.88	0.55
1:C:325:GLU:CA	1:C:328:ILE:CG2	2.82	0.54
3:F:178:ARG:HB2	3:F:253:LEU:HB3	1.89	0.54
3:H:146:GLU:HG2	3:H:253:LEU:CD2	2.37	0.54
1:C:354:TYR:CZ	1:C:404:VAL:HG12	2.43	0.54
2:D:151:THR:HG23	2:D:162:LEU:HD11	1.89	0.54
3:G:46:ARG:HG3	3:G:46:ARG:HH11	1.71	0.54
1:C:219:THR:HG22	1:C:221:TYR:H	1.72	0.54
3:E:231:ASP:OD2	3:E:234:ALA:HB2	2.07	0.54
3:G:261:MET:HG2	3:H:46:ARG:NH2	2.22	0.54
2:B:315:LYS:C	2:B:315:LYS:HD2	2.31	0.54
2:B:383:LEU:HD23	2:B:390:PRO:HB3	1.90	0.54
3:F:23:VAL:HG21	3:F:35:ILE:CD1	2.22	0.54
3:F:160:ALA:O	3:F:164:ILE:HG13	2.08	0.54
3:F:199:LEU:O	3:F:203:LEU:HD13	2.07	0.54
3:F:95:VAL:HG22	3:F:96:GLY:H	1.72	0.54
1:C:442:HIS:CE1	5:C:3496:CFM:S1B	3.02	0.53
3:E:182:LEU:O	3:E:208:ILE:HG22	2.08	0.53
1:A:25:ARG:NH1	1:A:26:LYS:HG2	2.24	0.53
2:B:43:VAL:O	2:B:47:THR:HG23	2.09	0.53
3:E:72:LEU:HB2	3:E:112:GLU:HG2	1.89	0.53
3:G:184:CYS:SG	3:G:196:ILE:HG13	2.48	0.53
3:G:45:THR:O	3:G:49:LEU:HD13	2.09	0.53
3:H:23:VAL:HB	3:H:33:VAL:HG11	1.91	0.53
3:E:26:LEU:HD12	3:E:244:ALA:HB1	1.91	0.53
3:G:129:ASP:HB2	3:H:41:LYS:NZ	2.24	0.53
1:A:214:THR:HA	9:A:1659:HOH:O	2.08	0.53
3:F:178:ARG:CB	3:F:253:LEU:HB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ARG:HD2	1:C:403:ASP:OD2	2.08	0.53
3:G:204:GLY:O	3:G:254:VAL:HG21	2.09	0.53
2:D:118:MET:CE	2:D:154:MET:SD	2.96	0.52
3:E:170:LYS:HB2	3:E:170:LYS:NZ	2.24	0.52
2:D:119:THR:HG22	2:D:120:GLU:N	2.24	0.52
3:F:254:VAL:CG1	3:F:255:ILE:N	2.72	0.52
3:G:260:THR:HG22	3:G:263:GLU:HG3	1.92	0.52
3:H:103:ILE:HG12	3:H:137:MET:HG3	1.90	0.52
1:A:230:ASN:HD22	1:A:235:ALA:N	2.07	0.52
1:C:226:ILE:HA	1:C:253:TRP:HB2	1.91	0.52
1:C:245:MET:SD	1:C:309:LEU:HD22	2.49	0.52
3:G:154:GLU:OE1	3:G:155:MET:N	2.32	0.52
3:G:205:THR:CG2	3:G:206:GLN:H	2.07	0.52
3:H:40:PRO:HD3	9:H:320:HOH:O	2.10	0.52
1:C:62:CYS:O	1:C:191:GLN:HA	2.10	0.52
3:E:269:MET:HG3	3:F:222:ILE:HG21	1.90	0.52
3:H:60:MET:CE	3:H:74:ASP:HB3	2.39	0.52
1:C:74:PRO:HB2	1:C:254:SER:HB3	1.91	0.52
1:A:154:CYS:HB2	1:A:155:PRO:HD3	1.91	0.52
1:C:265:THR:O	1:C:268:VAL:HG22	2.09	0.52
1:A:265:THR:O	1:A:268:VAL:HG22	2.10	0.52
1:A:275:CYS:CA	1:A:358:LEU:HD22	2.20	0.52
3:E:131:VAL:CG1	3:F:41:LYS:HD2	2.39	0.52
3:F:154:GLU:OE1	3:F:155:MET:N	2.42	0.52
3:G:260:THR:HG22	3:G:263:GLU:OE2	2.10	0.52
3:H:2:MET:CE	3:H:122:VAL:HG23	2.39	0.52
1:C:141:LEU:HD11	2:D:55:LEU:HB3	1.90	0.52
3:F:57:ILE:HG12	3:F:75:VAL:HG21	1.91	0.52
3:H:245:ARG:HG3	3:H:245:ARG:HH11	1.75	0.52
3:H:106:ILE:O	3:H:110:GLU:HG2	2.11	0.51
3:H:117:ASP:OD1	3:H:119:LEU:CD1	2.58	0.51
1:A:12:LEU:HG	1:A:415:ARG:HG2	1.91	0.51
3:E:244:ALA:O	3:E:248:VAL:HG23	2.10	0.51
1:C:253:TRP:CH2	1:C:282:ILE:CD1	2.92	0.51
3:E:33:VAL:HG13	3:E:121:PHE:HB2	1.91	0.51
3:F:106:ILE:HB	3:F:137:MET:HE3	1.92	0.51
3:G:41:LYS:HZ3	3:H:41:LYS:HZ1	1.57	0.51
3:G:231:ASP:O	3:G:232:PRO:C	2.51	0.51
3:H:205:THR:HG23	3:H:206:GLN:N	2.25	0.51
3:H:260:THR:OG1	3:H:263:GLU:HG3	2.10	0.51
3:E:235:LYS:HE2	3:E:235:LYS:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:4:GLN:HB2	3:G:144:ALA:HA	1.91	0.51
2:B:74:GLY:HA3	2:B:193:HIS:O	2.10	0.51
2:B:151:THR:HG23	2:B:162:LEU:HD11	1.92	0.51
1:A:429:PHE:O	1:A:433:LYS:HD3	2.11	0.51
1:C:151:GLN:HG3	1:C:183:CYS:SG	2.50	0.51
3:H:46:ARG:HG3	3:H:46:ARG:HH11	1.76	0.51
3:F:182:LEU:CD2	3:F:199:LEU:HD12	2.41	0.51
3:F:183:ILE:HG12	3:F:208:ILE:CG2	2.41	0.51
2:B:100:ARG:HD2	2:B:111:VAL:O	2.09	0.51
1:C:90:GLN:HG3	2:D:68:LYS:O	2.11	0.51
1:A:355:ILE:HG22	1:A:356:GLY:H	1.75	0.51
2:B:86:MET:HG2	2:B:138:CYS:SG	2.51	0.51
1:C:357:GLY:HA2	1:C:379:TYR:HD2	1.76	0.51
2:D:68:LYS:HE2	2:D:396:HIS:CE1	2.45	0.50
3:H:68:GLU:H	3:H:68:GLU:CD	2.18	0.50
3:E:145:GLN:HE21	3:E:145:GLN:N	2.08	0.50
3:H:154:GLU:O	3:H:158:MET:HG3	2.11	0.50
3:H:187:ARG:HA	3:H:213:ARG:CZ	2.42	0.50
3:H:249:ASP:O	3:H:251:LYS:HD2	2.11	0.50
3:H:60:MET:HB3	3:H:70:LEU:HD21	1.93	0.50
2:B:163:ASN:HD22	2:B:183:PHE:HE2	1.58	0.50
2:B:376:VAL:O	2:B:380:VAL:HG23	2.12	0.50
2:D:45:GLN:O	2:D:48:THR:HB	2.12	0.50
3:H:164:ILE:O	3:H:168:ILE:HG13	2.12	0.50
2:B:3:GLN:NE2	2:B:9:LYS:H	2.10	0.50
2:D:228:PRO:HA	2:D:293:LEU:HD12	1.93	0.50
3:E:22:LEU:O	3:E:22:LEU:HD22	2.11	0.50
1:A:198:ALA:O	1:A:202:VAL:HG23	2.12	0.50
2:D:233:TYR:HB2	2:D:236:ASN:ND2	2.27	0.50
3:F:76:LEU:CD2	3:F:86:VAL:HG13	2.41	0.50
3:H:23:VAL:CG2	3:H:35:ILE:HD11	2.42	0.50
1:C:220:PRO:HA	1:C:269:LYS:HE2	1.93	0.50
1:C:359:ARG:O	1:C:363:VAL:HG22	2.12	0.50
3:E:154:GLU:OE1	3:E:155:MET:N	2.45	0.49
3:E:183:ILE:HG12	3:E:208:ILE:CG2	2.42	0.49
3:G:95:VAL:HG22	3:G:96:GLY:H	1.77	0.49
3:H:37:GLY:HA3	3:H:87:GLU:OE2	2.12	0.49
1:A:159:ILE:HG13	3:F:97:CYS:HB2	1.94	0.49
2:D:257:PRO:HB2	2:D:261:LEU:HD22	1.94	0.49
3:H:57:ILE:HG12	3:H:75:VAL:HG21	1.92	0.49
3:H:141:GLU:O	3:H:142:ASN:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:TYR:CE2	1:A:110:VAL:HB	2.47	0.49
1:A:226:ILE:HA	1:A:253:TRP:HB2	1.93	0.49
2:B:85:THR:HG22	2:B:146:MET:HB3	1.94	0.49
3:E:28:GLU:OE1	3:E:241:ARG:NH1	2.39	0.49
3:F:215:ASN:O	3:F:219:ARG:HG3	2.12	0.49
3:H:23:VAL:CG1	3:H:35:ILE:HD11	2.42	0.49
2:B:211:LYS:HG3	9:B:1631:HOH:O	2.11	0.49
1:C:90:GLN:OE1	1:C:90:GLN:HA	2.10	0.49
1:C:459:PHE:O	1:C:463:MET:HG2	2.12	0.49
1:A:96:ARG:HD2	5:A:1496:CFM:S3B	2.52	0.49
1:C:87:GLY:HA3	7:D:3498:CLF:S2B	2.53	0.49
3:F:260:THR:HG22	3:F:261:MET:N	2.28	0.49
3:H:254:VAL:CG2	3:H:255:ILE:N	2.74	0.49
3:F:6:ALA:HB3	3:F:147:ILE:HD12	1.93	0.49
3:G:49:LEU:HD12	3:G:49:LEU:N	2.28	0.49
1:A:85:PRO:HB2	7:B:1498:CLF:S2B	2.53	0.49
1:A:239:ARG:HG3	2:B:23:MET:SD	2.53	0.49
3:G:225:MET:SD	3:G:229:GLU:OE2	2.71	0.49
2:B:45:GLN:O	2:B:48:THR:HB	2.13	0.49
2:B:431:ARG:HD2	2:B:454:ASP:OD1	2.13	0.49
1:C:230:ASN:HD22	1:C:235:ALA:N	2.10	0.48
2:D:100:ARG:HD2	2:D:111:VAL:O	2.13	0.48
3:F:26:LEU:CD1	3:F:244:ALA:HB1	2.43	0.48
2:B:522:VAL:HG23	1:C:446:TYR:CE2	2.48	0.48
2:D:324:TRP:CE2	2:D:381:LYS:HD2	2.48	0.48
2:D:400:LYS:O	2:D:404:LYS:HG2	2.13	0.48
1:A:277:ARG:O	1:A:277:ARG:HD3	2.13	0.48
2:D:85:THR:HG22	2:D:146:MET:HB3	1.95	0.48
3:E:8:TYR:HB3	3:E:164:ILE:HD13	1.94	0.48
3:H:103:ILE:HA	3:H:137:MET:HG3	1.95	0.48
1:C:184:GLU:HG3	1:C:186:PHE:CZ	2.49	0.48
3:E:12:GLY:N	3:F:10:LYS:HE3	2.29	0.48
3:E:106:ILE:CG2	3:E:143:LYS:HZ1	2.27	0.48
3:G:103:ILE:HG12	3:G:137:MET:HG3	1.95	0.48
1:C:253:TRP:HZ3	1:C:282:ILE:CD1	2.05	0.48
3:G:58:MET:HE3	3:G:58:MET:HA	1.95	0.48
3:H:60:MET:HE3	3:H:74:ASP:HB3	1.96	0.48
3:H:108:PHE:CZ	3:H:112:GLU:HG3	2.49	0.48
3:H:126:VAL:HG22	3:H:138:PRO:HG2	1.95	0.48
3:H:22:LEU:O	3:H:26:LEU:HD13	2.14	0.48
2:B:234:LEU:HD22	2:B:480:HIS:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:184:CYS:SG	3:F:196:ILE:HG13	2.54	0.48
1:C:81:ILE:HD13	1:C:134:LEU:CD2	2.42	0.47
3:F:228:ILE:O	3:F:232:PRO:HG3	2.14	0.47
3:G:41:LYS:NZ	3:G:129:ASP:OD1	2.47	0.47
1:A:253:TRP:CZ2	1:A:262:ILE:HG23	2.49	0.47
3:E:220:ALA:HB1	3:E:225:MET:O	2.14	0.47
3:G:10:LYS:HZ2	3:G:156:MET:HB3	1.79	0.47
1:A:265:THR:N	1:A:266:PRO:HD2	2.29	0.47
1:A:303:THR:HG22	9:A:1547:HOH:O	2.14	0.47
3:H:68:GLU:N	3:H:68:GLU:OE1	2.46	0.47
1:A:210:ARG:CD	1:A:263:GLU:OE2	2.59	0.47
3:E:20:GLN:O	3:E:23:VAL:HG22	2.14	0.47
3:E:218:GLN:OE1	3:E:218:GLN:N	2.47	0.47
3:F:130:VAL:O	3:F:130:VAL:HG23	2.13	0.47
3:E:166:LYS:HG2	3:E:258:PRO:HG3	1.97	0.47
3:F:58:MET:HG2	3:F:88:SER:O	2.14	0.47
1:A:442:HIS:CE1	5:A:1496:CFM:S1B	3.07	0.47
2:B:225:ASN:HB3	2:B:254:LEU:HD11	1.96	0.47
2:D:416:GLY:C	2:D:417:LYS:HE2	2.40	0.47
2:B:247:MET:HG2	2:B:341:PRO:HD3	1.97	0.47
1:C:203:ARG:HG3	1:C:204:ASP:N	2.30	0.47
1:C:462:ASP:HA	1:C:465:MET:HG2	1.97	0.47
1:A:47:ILE:HD12	1:A:50:LYS:HG3	1.97	0.47
2:D:67:ALA:H	2:D:396:HIS:HD2	1.63	0.47
2:D:74:GLY:HA3	2:D:193:HIS:O	2.15	0.47
2:D:96:VAL:CG2	2:D:115:SER:HB2	2.43	0.47
2:D:373:PRO:O	2:D:377:MET:HB2	2.15	0.47
3:F:103:ILE:HG12	3:F:137:MET:HG2	1.95	0.47
3:F:183:ILE:HG12	3:F:208:ILE:HG22	1.97	0.47
9:A:1624:HOH:O	2:B:119:THR:HG23	2.15	0.47
2:D:158:ILE:HG22	3:G:97:CYS:HB2	1.97	0.47
3:H:231:ASP:CG	3:H:231:ASP:O	2.59	0.47
2:B:236:ASN:HD21	2:B:484:THR:HB	1.79	0.46
1:C:429:PHE:O	1:C:433:LYS:HD3	2.14	0.46
2:D:9:LYS:HB3	2:D:13:PRO:HD2	1.96	0.46
3:G:41:LYS:NZ	3:H:41:LYS:HZ1	2.12	0.46
1:C:355:ILE:HB	1:C:360:PRO:HD3	1.97	0.46
3:G:73:GLU:H	3:G:73:GLU:CD	2.24	0.46
3:H:10:LYS:CE	3:H:11:GLY:H	2.29	0.46
3:H:130:VAL:HG23	3:H:130:VAL:O	2.15	0.46
3:H:225:MET:HE2	3:H:229:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD13	2:B:43:VAL:HG21	1.97	0.46
1:C:198:ALA:O	1:C:202:VAL:HG23	2.15	0.46
3:H:119:LEU:N	3:H:119:LEU:CD1	2.78	0.46
1:A:298:ASN:HD21	1:A:300:PHE:HB2	1.80	0.46
1:C:66:GLY:O	1:C:70:VAL:HG22	2.14	0.46
3:F:207:MET:HE1	3:F:210:PHE:HB2	1.97	0.46
3:G:261:MET:HG2	3:H:46:ARG:CZ	2.45	0.46
1:A:274:HIS:HE1	1:A:299:PHE:H	1.62	0.46
1:A:382:ALA:HB1	1:A:386:ASP:HB2	1.97	0.46
2:B:93:GLN:HG2	9:B:1547:HOH:O	2.15	0.46
2:D:411:ALA:HA	2:D:417:LYS:NZ	2.30	0.46
3:F:26:LEU:HD13	3:F:244:ALA:HB1	1.98	0.46
3:F:33:VAL:HG12	3:F:34:MET:N	2.29	0.46
3:F:207:MET:HE3	3:F:209:HIS:C	2.41	0.46
3:H:126:VAL:CG2	3:H:138:PRO:HG2	2.45	0.46
1:A:113:ASN:ND2	9:A:1527:HOH:O	2.43	0.46
1:A:151:GLN:HG3	1:A:183:CYS:SG	2.56	0.46
1:A:225:ILE:HD12	1:A:252:GLN:HG2	1.97	0.46
1:C:165:SER:O	1:C:169:VAL:HG22	2.15	0.46
3:H:245:ARG:HD2	9:H:321:HOH:O	2.13	0.46
3:G:10:LYS:HE2	3:H:11:GLY:C	2.40	0.46
1:A:103:THR:H	1:A:107:ASN:ND2	2.11	0.46
1:A:355:ILE:HB	1:A:360:PRO:HD3	1.97	0.46
1:A:449:PRO:O	1:A:450:TYR:HD2	1.99	0.46
2:D:103:PHE:HB3	2:D:111:VAL:HG11	1.98	0.46
3:E:205:THR:HG23	3:E:206:GLN:N	2.31	0.46
3:E:261:MET:HG2	3:F:46:ARG:CZ	2.46	0.46
3:G:41:LYS:NZ	3:H:41:LYS:NZ	2.63	0.46
1:A:62:CYS:O	1:A:191:GLN:HA	2.16	0.46
2:B:324:TRP:CZ3	2:B:378:GLY:HA2	2.51	0.46
2:D:43:VAL:O	2:D:47:THR:HG23	2.16	0.46
9:B:1500:HOH:O	1:C:433:LYS:HE2	2.16	0.46
1:C:359:ARG:HH11	1:C:442:HIS:HA	1.81	0.46
3:F:67:VAL:HG12	3:F:108:PHE:CD1	2.51	0.46
3:F:137:MET:N	3:F:138:PRO:CD	2.79	0.46
1:A:120:GLU:HG3	2:B:190:VAL:HG22	1.97	0.45
3:E:145:GLN:HE21	3:E:145:GLN:CA	2.29	0.45
3:G:238:ASP:HA	3:G:241:ARG:HD2	1.98	0.45
3:H:67:VAL:HG21	3:H:104:THR:CG2	2.46	0.45
2:B:457:HIS:CD2	2:D:512:MET:HB3	2.50	0.45
4:C:3494:HCA:H22	5:C:3496:CFM:S3B	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:119:THR:HG22	2:D:120:GLU:H	1.81	0.45
3:E:70:LEU:HB3	3:E:108:PHE:CE1	2.51	0.45
3:G:70:LEU:HD23	3:G:71:GLU:N	2.31	0.45
3:G:80:TYR:O	3:G:83:VAL:HG23	2.17	0.45
3:E:11:GLY:C	3:E:13:ILE:H	2.24	0.45
3:F:225:MET:HE2	3:F:229:GLU:CD	2.41	0.45
3:H:68:GLU:CD	3:H:68:GLU:N	2.75	0.45
3:H:19:THR:O	3:H:23:VAL:HG13	2.16	0.45
3:G:46:ARG:HG3	3:G:46:ARG:NH1	2.28	0.45
3:G:214:ASP:HB3	3:G:236:GLN:NE2	2.31	0.45
3:F:37:GLY:HA3	3:F:87:GLU:OE2	2.16	0.45
3:G:267:LEU:O	3:G:271:PHE:HD1	2.00	0.45
3:H:71:GLU:OE1	3:H:71:GLU:HA	2.16	0.45
3:H:208:ILE:HG13	3:H:246:LYS:HB3	1.99	0.45
3:E:126:VAL:HG12	3:E:128:GLY:N	2.32	0.45
3:F:165:SER:O	3:F:169:VAL:HG23	2.16	0.45
3:G:178:ARG:CB	3:G:253:LEU:HB3	2.47	0.45
3:G:185:ASN:O	3:G:186:SER:C	2.59	0.45
1:A:6:ARG:CB	1:A:7:GLU:OE1	2.65	0.45
2:B:71:GLN:O	2:B:196:GLY:HA3	2.17	0.45
3:F:147:ILE:O	3:F:179:LEU:HD23	2.16	0.45
3:G:129:ASP:HB2	3:H:41:LYS:HZ1	1.81	0.45
3:G:199:LEU:O	3:G:203:LEU:HD13	2.16	0.45
3:H:33:VAL:HG12	3:H:34:MET:N	2.32	0.45
1:A:74:PRO:HB2	1:A:254:SER:HB3	1.98	0.45
3:H:57:ILE:HD11	3:H:86:VAL:CG1	2.46	0.45
2:B:103:PHE:HB3	2:B:111:VAL:HG11	1.99	0.45
2:B:406:VAL:HA	2:B:409:ILE:HD12	1.98	0.45
3:E:20:GLN:HA	3:E:23:VAL:HG22	1.99	0.45
3:E:150:VAL:HA	3:E:183:ILE:O	2.17	0.44
3:F:18:THR:HG21	3:F:185:ASN:OD1	2.17	0.44
3:F:139:ILE:HG22	3:F:147:ILE:HD11	1.98	0.44
3:H:80:TYR:CD1	3:H:80:TYR:C	2.94	0.44
1:A:225:ILE:HG13	1:A:249:CYS:SG	2.57	0.44
4:A:1494:HCA:H22	5:A:1496:CFM:S3B	2.57	0.44
2:D:119:THR:CG2	2:D:120:GLU:H	2.30	0.44
3:G:9:GLY:HA3	3:G:150:VAL:HG22	1.99	0.44
3:G:41:LYS:NZ	3:G:129:ASP:H	2.15	0.44
3:G:72:LEU:O	3:G:75:VAL:HG12	2.18	0.44
3:H:70:LEU:HB3	3:H:108:PHE:CE1	2.53	0.44
3:H:84:LYS:NZ	3:H:117:ASP:OD2	2.45	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:260:VAL:HG22	9:D:3516:HOH:O	2.17	0.44
2:D:381:LYS:O	2:D:385:GLU:HG3	2.17	0.44
3:F:256:PRO:O	3:F:258:PRO:HD3	2.17	0.44
3:H:103:ILE:HG12	3:H:137:MET:CG	2.48	0.44
1:C:100:TYR:CE2	1:C:110:VAL:HB	2.53	0.44
1:C:298:ASN:HD22	1:C:298:ASN:C	2.25	0.44
1:C:325:GLU:HA	1:C:328:ILE:HG23	1.94	0.44
3:F:238:ASP:CG	3:F:241:ARG:HH21	2.26	0.44
3:F:253:LEU:N	3:F:253:LEU:HD22	2.32	0.44
3:E:144:ALA:O	3:E:177:VAL:HG23	2.17	0.44
3:F:261:MET:SD	3:F:264:LEU:HD23	2.58	0.44
3:G:209:HIS:CG	3:G:210:PHE:N	2.86	0.44
3:G:212:PRO:HG2	3:G:236:GLN:OE1	2.17	0.44
3:H:23:VAL:HG21	3:H:35:ILE:CD1	2.48	0.44
1:C:138:VAL:HG12	2:D:62:LEU:HD22	1.98	0.44
3:E:88:SER:HB2	3:E:105:ALA:CB	2.48	0.44
3:F:146:GLU:HG2	3:F:253:LEU:CD1	2.47	0.44
3:H:75:VAL:HG22	9:H:293:HOH:O	2.17	0.44
1:A:378:GLY:HA3	1:A:401:TYR:CD2	2.53	0.44
3:F:8:TYR:O	3:F:149:ILE:HA	2.17	0.44
3:F:154:GLU:O	3:F:158:MET:HG3	2.18	0.44
2:D:234:LEU:HD23	2:D:480:HIS:HD2	1.83	0.44
3:E:29:MET:HE3	3:E:245:ARG:CZ	2.48	0.44
3:E:145:GLN:HG2	9:E:5326:HOH:O	2.18	0.44
3:F:164:ILE:O	3:F:168:ILE:HG13	2.18	0.44
3:H:10:LYS:HA	3:H:10:LYS:CE	2.46	0.44
1:C:68:LYS:CB	1:C:151:GLN:HG2	2.47	0.43
2:D:376:VAL:HG13	2:D:402:TRP:HZ2	1.83	0.43
3:E:88:SER:HB2	3:E:105:ALA:HB2	2.00	0.43
3:G:141:GLU:O	3:G:143:LYS:HG2	2.17	0.43
3:H:8:TYR:O	3:H:149:ILE:HA	2.17	0.43
2:B:369:LEU:HD13	2:B:379:LEU:HD12	2.00	0.43
2:B:502:LEU:HD11	2:D:477:HIS:CD2	2.53	0.43
2:D:151:THR:CG2	2:D:162:LEU:HD21	2.48	0.43
3:G:265:GLU:O	3:G:269:MET:HG3	2.18	0.43
2:B:118:MET:HB3	2:B:154:MET:HE1	2.01	0.43
1:C:39:VAL:HG21	1:C:391:MET:HE2	1.94	0.43
2:D:100:ARG:HA	2:D:111:VAL:HG21	1.99	0.43
3:H:186:SER:HA	3:H:192:GLU:OE1	2.18	0.43
1:A:192:SER:OG	1:A:383:HIS:HE1	2.01	0.43
2:B:96:VAL:CG2	2:B:115:SER:HB2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:HIS:HE1	5:C:3496:CFM:S1B	2.41	0.43
3:G:70:LEU:HD23	3:G:71:GLU:H	1.82	0.43
1:C:355:ILE:HG22	1:C:356:GLY:H	1.84	0.43
2:D:124:VAL:O	3:G:91:PRO:HB3	2.17	0.43
3:F:77:LYS:HB3	3:F:77:LYS:HZ3	1.83	0.43
3:F:245:ARG:HG2	3:F:245:ARG:HH11	1.83	0.43
3:G:182:LEU:O	3:G:208:ILE:HG22	2.18	0.43
3:H:147:ILE:HG21	3:H:168:ILE:HD11	2.01	0.43
3:E:137:MET:N	3:E:138:PRO:CD	2.82	0.43
3:F:177:VAL:O	3:F:177:VAL:HG13	2.18	0.43
3:H:4:GLN:HB2	3:H:144:ALA:HA	2.00	0.43
1:A:82:SER:HB2	1:A:115:THR:HG22	1.99	0.43
2:B:473:ILE:CD1	2:B:479:LEU:HD23	2.48	0.43
3:E:261:MET:O	3:E:265:GLU:HG3	2.18	0.43
1:A:39:VAL:O	1:A:41:GLN:N	2.51	0.43
1:A:475:LEU:HD22	2:D:352:VAL:HG11	2.00	0.43
2:D:28:ARG:HA	2:D:32:GLU:HB2	2.00	0.43
2:D:96:VAL:HA	2:D:99:PHE:CD2	2.53	0.43
3:G:163:ASN:HD22	3:G:163:ASN:HA	1.64	0.43
3:H:183:ILE:HD13	3:H:243:LEU:HD11	2.00	0.43
1:C:477:ALA:HA	1:C:478:PRO:HD2	1.89	0.43
3:F:179:LEU:CD2	3:F:181:GLY:H	2.29	0.43
3:G:4:GLN:CB	3:G:144:ALA:HA	2.48	0.43
1:A:124:VAL:O	3:F:91:PRO:HB3	2.19	0.43
1:A:462:ASP:HA	1:A:465:MET:HG2	2.01	0.43
2:B:96:VAL:O	2:B:100:ARG:HG3	2.19	0.43
2:B:310:LYS:HE2	9:B:1755:HOH:O	2.19	0.43
2:B:376:VAL:HG13	2:B:402:TRP:HZ2	1.84	0.43
3:E:34:MET:HE2	3:E:76:LEU:HD21	2.01	0.43
3:F:179:LEU:HD22	3:F:181:GLY:N	2.33	0.43
3:G:2:MET:HE2	3:G:120:ASP:O	2.18	0.43
2:D:509:THR:O	2:D:516:ASP:HA	2.19	0.42
3:E:182:LEU:HD22	3:E:200:ALA:HB2	2.00	0.42
3:E:189:THR:HG22	3:F:213:ARG:HH22	1.84	0.42
3:E:228:ILE:O	3:E:232:PRO:HG3	2.19	0.42
3:G:259:ILE:HD11	3:G:264:LEU:HD13	2.01	0.42
1:C:82:SER:HB3	1:C:153:GLU:OE1	2.19	0.42
1:C:224:ALA:HB3	1:C:271:ASN:HD22	1.84	0.42
3:F:43:ASP:CG	3:F:46:ARG:HB2	2.44	0.42
1:A:274:HIS:HD2	9:A:1639:HOH:O	2.02	0.42
2:B:206:ARG:HA	2:B:304:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:ASN:C	1:C:113:ASN:ND2	2.77	0.42
2:D:523:ARG:HD2	9:D:3587:HOH:O	2.18	0.42
3:E:162:ASN:ND2	3:E:259:ILE:HG12	2.35	0.42
3:E:188:ASN:C	3:E:188:ASN:HD22	2.25	0.42
3:H:49:LEU:HD13	3:H:85:CYS:SG	2.59	0.42
3:H:162:ASN:HD21	3:H:258:PRO:HA	1.83	0.42
1:A:203:ARG:HG3	1:A:204:ASP:N	2.35	0.42
2:B:198:ASP:HB2	2:B:297:HIS:O	2.20	0.42
2:D:119:THR:CG2	2:D:120:GLU:N	2.82	0.42
3:G:43:ASP:OD1	3:G:46:ARG:HB2	2.20	0.42
3:H:10:LYS:O	3:H:13:ILE:HG12	2.20	0.42
3:H:46:ARG:HG3	3:H:46:ARG:NH1	2.33	0.42
2:D:479:LEU:HB2	9:D:3510:HOH:O	2.18	0.42
3:F:3:ARG:O	3:F:121:PHE:HA	2.19	0.42
3:F:41:LYS:HD3	3:F:41:LYS:N	2.35	0.42
2:B:348:ARG:HD3	1:C:479:TRP:CH2	2.54	0.42
2:D:320:MET:HE3	2:D:484:THR:HG23	2.02	0.42
3:G:10:LYS:HZ1	3:G:156:MET:HB3	1.85	0.42
2:B:146:MET:HG3	2:B:180:PRO:HB2	2.01	0.42
3:F:56:THR:HG23	3:F:59:GLU:OE2	2.20	0.42
3:G:20:GLN:HA	3:G:23:VAL:HG22	2.00	0.42
3:G:21:ASN:N	3:G:21:ASN:ND2	2.67	0.42
3:H:165:SER:O	3:H:169:VAL:HG23	2.19	0.42
3:H:183:ILE:HG12	3:H:208:ILE:CG2	2.50	0.42
1:A:115:THR:HB	1:A:117:ASP:H	1.84	0.42
1:C:36:ASP:O	1:C:39:VAL:CG1	2.67	0.42
2:B:509:THR:HG21	2:B:518:ASN:HD22	1.83	0.42
3:E:152:SER:O	3:E:196:ILE:HD11	2.19	0.42
3:F:46:ARG:HG3	3:F:46:ARG:HH11	1.85	0.42
3:F:208:ILE:O	3:F:246:LYS:HD3	2.20	0.42
3:G:43:ASP:CG	3:G:46:ARG:HB2	2.44	0.42
3:G:205:THR:CG2	3:G:206:GLN:N	2.65	0.42
3:H:236:GLN:O	3:H:239:GLU:HB2	2.19	0.42
2:B:479:LEU:HB2	9:B:1507:HOH:O	2.20	0.42
1:C:282:ILE:O	1:C:286:MET:HG3	2.19	0.42
1:C:325:GLU:C	1:C:328:ILE:HG23	2.45	0.42
2:D:192:SER:OG	2:D:194:VAL:HG22	2.20	0.42
3:E:110:GLU:HG3	3:E:143:LYS:HZ3	1.85	0.42
2:B:104:ASN:OD1	2:B:111:VAL:HG22	2.21	0.41
2:B:322:LEU:HD23	1:C:474:LYS:HD3	2.02	0.41
2:B:348:ARG:O	2:B:352:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:VAL:HG22	9:B:1630:HOH:O	2.20	0.41
1:C:145:ASN:HD22	1:C:147:GLY:H	1.67	0.41
3:E:222:ILE:HG22	3:F:269:MET:HE3	2.02	0.41
3:E:269:MET:HE3	3:F:223:ARG:CZ	2.50	0.41
3:H:8:TYR:CB	3:H:164:ILE:HD13	2.46	0.41
1:C:59:ILE:HD12	1:C:354:TYR:CE2	2.55	0.41
2:D:369:LEU:HD12	2:D:376:VAL:HG23	2.01	0.41
3:H:205:THR:OG1	3:H:206:GLN:N	2.50	0.41
1:A:68:LYS:CB	1:A:151:GLN:HG2	2.37	0.41
1:C:62:CYS:SG	1:C:64:TYR:HB3	2.61	0.41
3:E:219:ARG:HD2	9:E:5334:HOH:O	2.19	0.41
3:G:20:GLN:OE1	3:G:47:LEU:HB2	2.20	0.41
1:A:96:ARG:NH2	5:A:1496:CFM:S5	2.93	0.41
2:B:247:MET:HG2	2:B:341:PRO:CD	2.50	0.41
1:C:159:ILE:CG1	3:H:97:CYS:HB2	2.49	0.41
2:D:376:VAL:HG13	2:D:402:TRP:CZ2	2.55	0.41
3:F:11:GLY:C	3:F:13:ILE:H	2.27	0.41
3:H:76:LEU:HD23	3:H:86:VAL:CG2	2.44	0.41
2:D:10:ALA:O	2:D:14:LEU:HB2	2.20	0.41
2:D:39:LYS:HD2	2:D:39:LYS:HA	1.84	0.41
1:C:357:GLY:HA2	1:C:379:TYR:CD2	2.54	0.41
3:H:153:GLY:HA3	3:H:192:GLU:HG3	2.03	0.41
1:A:159:ILE:HD11	3:F:97:CYS:CB	2.49	0.41
3:F:141:GLU:O	3:F:142:ASN:HB2	2.21	0.41
1:C:5:SER:HA	1:C:8:GLU:HB3	2.03	0.41
1:C:53:GLN:HA	1:C:54:PRO:HD2	1.91	0.41
1:C:220:PRO:O	1:C:316:PHE:CE2	2.67	0.41
1:C:328:ILE:O	1:C:328:ILE:HG13	2.13	0.41
3:F:56:THR:OG1	3:F:59:GLU:HG2	2.21	0.41
3:G:10:LYS:NZ	3:H:12:GLY:HA2	2.36	0.41
3:G:191:ARG:C	3:G:193:ASP:N	2.76	0.41
3:G:220:ALA:HB1	3:G:225:MET:O	2.21	0.41
3:H:208:ILE:CG1	3:H:246:LYS:HB3	2.51	0.41
1:A:39:VAL:O	1:A:40:THR:C	2.64	0.41
1:A:298:ASN:ND2	1:A:300:PHE:H	2.19	0.41
2:B:402:TRP:CZ2	2:B:406:VAL:HG21	2.56	0.41
1:C:9:VAL:HG23	1:C:34:VAL:HG11	2.03	0.41
3:E:23:VAL:HG23	3:E:24:ALA:N	2.36	0.41
3:E:222:ILE:CG2	3:F:269:MET:HE3	2.51	0.41
3:F:8:TYR:HB3	3:F:164:ILE:HD13	2.02	0.41
3:F:19:THR:O	3:F:23:VAL:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:23:VAL:CG2	3:F:35:ILE:HD11	2.24	0.41
3:F:60:MET:HB3	3:F:70:LEU:HD21	2.03	0.41
3:F:162:ASN:HD21	3:F:258:PRO:CA	2.26	0.41
3:G:211:VAL:HA	3:G:212:PRO:HD2	1.94	0.41
3:G:228:ILE:O	3:G:232:PRO:HG3	2.20	0.41
3:H:10:LYS:HE2	3:H:11:GLY:N	2.32	0.41
3:H:103:ILE:HA	3:H:137:MET:CE	2.49	0.41
1:A:355:ILE:CD1	1:A:359:ARG:HB2	2.51	0.41
2:D:277:THR:HG1	2:D:280:GLU:HG3	1.86	0.41
2:D:377:MET:HG3	2:D:406:VAL:HG22	2.02	0.41
3:E:26:LEU:CD1	3:E:244:ALA:HB1	2.50	0.41
3:G:13:ILE:CD1	3:G:151:CYS:HA	2.51	0.41
1:C:332:LYS:N	1:C:333:PRO:HD2	2.36	0.40
2:D:46:TRP:C	2:D:48:THR:H	2.29	0.40
2:D:449:LYS:HB2	2:D:449:LYS:HE3	1.95	0.40
3:E:208:ILE:HD11	3:E:246:LYS:HB3	2.02	0.40
3:H:10:LYS:HE2	3:H:10:LYS:CA	2.49	0.40
3:H:20:GLN:OE1	3:H:47:LEU:HB2	2.21	0.40
2:B:497:LEU:O	2:B:501:ILE:HG13	2.22	0.40
3:G:194:GLU:HB3	3:G:271:PHE:HE2	1.86	0.40
1:A:457:ALA:CB	2:B:3:GLN:HG2	2.51	0.40
2:D:445:ASN:HB2	2:D:472:PRO:O	2.21	0.40
3:E:23:VAL:O	3:E:26:LEU:HB2	2.22	0.40
3:F:261:MET:O	3:F:265:GLU:HG3	2.21	0.40
3:G:57:ILE:HG23	3:G:70:LEU:CD1	2.51	0.40
3:G:261:MET:CG	3:H:46:ARG:NH2	2.84	0.40
3:H:229:GLU:O	3:H:230:TYR:C	2.64	0.40
1:A:474:LYS:O	2:D:348:ARG:NH1	2.55	0.40
3:E:187:ARG:O	3:E:188:ASN:HB3	2.20	0.40
2:D:331:LYS:HD2	2:D:331:LYS:HA	1.93	0.40
2:D:373:PRO:HG2	9:D:3554:HOH:O	2.21	0.40
3:F:193:ASP:O	3:F:197:ILE:HG13	2.22	0.40
3:G:72:LEU:HB2	3:G:112:GLU:CG	2.44	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	405/415 (98%)	373 (92%)	32 (8%)	11	13
1	C	405/415 (98%)	375 (93%)	30 (7%)	13	14
2	B	454/455 (100%)	419 (92%)	35 (8%)	12	13
2	D	454/455 (100%)	421 (93%)	33 (7%)	13	15
3	E	206/233 (88%)	185 (90%)	21 (10%)	7	7
3	F	205/233 (88%)	186 (91%)	19 (9%)	8	9
3	G	204/233 (88%)	191 (94%)	13 (6%)	16	19
3	H	209/233 (90%)	197 (94%)	12 (6%)	18	23
All	All	2542/2672 (95%)	2347 (92%)	195 (8%)	12	13

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	12	LEU
1	A	14	GLN
1	A	19	VAL
1	A	68	LYS
1	A	70	VAL
1	A	93	ARG
1	A	98	ASN
1	A	107	ASN
1	A	115	THR
1	A	131	LEU
1	A	141	LEU
1	A	151	GLN
1	A	159	ILE
1	A	161	ASP
1	A	164	GLU
1	A	264	LEU
1	A	267	LYS
1	A	288	GLU

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Mol	Chain	Res	Type
1	A	346	LEU
1	A	359	ARG
1	A	362	HIS
1	A	370	LEU
1	A	377	THR
1	A	400	LEU
1	A	404	VAL
1	A	415	ARG
1	A	427	GLU
1	A	437	PRO
1	A	445	ASP
1	A	467	LEU
1	A	475	LEU
2	B	13	PRO
2	B	14	LEU
2	B	24	LEU
2	B	28	ARG
2	B	38	ASP
2	B	48	THR
2	B	55	LEU
2	B	150	SER
2	B	154	MET
2	B	172	GLU
2	B	177	ASP
2	B	210	LEU
2	B	234	LEU
2	B	258	GLU
2	B	260	VAL
2	B	261	LEU
2	B	281	MET
2	B	315	LYS
2	B	316	LEU
2	B	369	LEU
2	B	379	LEU
2	B	381	LYS
2	B	383	LEU
2	B	384	LEU
2	B	386	LEU
2	B	453	ARG
2	B	461	GLU
2	B	468	ARG
2	B	473	ILE

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Mol	Chain	Res	Type
2	B	479	LEU
2	B	484	THR
2	B	485	LEU
2	B	498	VAL
2	B	522	VAL
2	B	523	ARG
1	C	12	LEU
1	C	14	GLN
1	C	21	PRO
1	C	70	VAL
1	C	93	ARG
1	C	98	ASN
1	C	115	THR
1	C	131	LEU
1	C	138	VAL
1	C	151	GLN
1	C	159	ILE
1	C	164	GLU
1	C	212	GLU
1	C	230	ASN
1	C	264	LEU
1	C	267	LYS
1	C	277	ARG
1	C	288	GLU
1	C	302	PRO
1	C	328	ILE
1	C	346	LEU
1	C	358	LEU
1	C	360	PRO
1	C	362	HIS
1	C	370	LEU
1	C	415	ARG
1	C	427	GLU
1	C	437	PRO
1	C	445	ASP
1	C	475	LEU
2	D	3	GLN
2	D	11	SER
2	D	13	PRO
2	D	14	LEU
2	D	24	LEU
2	D	38	ASP

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Mol	Chain	Res	Type
2	D	48	THR
2	D	55	LEU
2	D	87	PRO
2	D	153	CYS
2	D	154	MET
2	D	172	GLU
2	D	210	LEU
2	D	211	LYS
2	D	214	ASP
2	D	258	GLU
2	D	260	VAL
2	D	261	LEU
2	D	281	MET
2	D	316	LEU
2	D	360	THR
2	D	379	LEU
2	D	383	LEU
2	D	384	LEU
2	D	386	LEU
2	D	456	LEU
2	D	461	GLU
2	D	468	ARG
2	D	473	ILE
2	D	479	LEU
2	D	484	THR
2	D	498	VAL
2	D	523	ARG
3	E	22	LEU
3	E	26	LEU
3	E	33	VAL
3	E	67	VAL
3	E	70	LEU
3	E	71	GLU
3	E	145	GLN
3	E	150	VAL
3	E	154	GLU
3	E	156	MET
3	E	163	ASN
3	E	170	LYS
3	E	179	LEU
3	E	199	LEU
3	E	203	LEU

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Mol	Chain	Res	Type
3	E	215	ASN
3	E	218	GLN
3	E	228	ILE
3	E	235	LYS
3	E	243	LEU
3	E	253	LEU
3	F	2	MET
3	F	22	LEU
3	F	26	LEU
3	F	41	LYS
3	F	67	VAL
3	F	71	GLU
3	F	75	VAL
3	F	112	GLU
3	F	137	MET
3	F	145	GLN
3	F	150	VAL
3	F	154	GLU
3	F	162	ASN
3	F	163	ASN
3	F	179	LEU
3	F	182	LEU
3	F	215	ASN
3	F	218	GLN
3	F	243	LEU
3	G	2	MET
3	G	13	ILE
3	G	21	ASN
3	G	22	LEU
3	G	47	LEU
3	G	58	MET
3	G	70	LEU
3	G	75	VAL
3	G	141	GLU
3	G	145	GLN
3	G	150	VAL
3	G	154	GLU
3	G	235	LYS
3	H	2	MET
3	H	10	LYS
3	H	23	VAL
3	H	40	PRO

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Mol	Chain	Res	Type
3	H	49	LEU
3	H	68	GLU
3	H	70	LEU
3	H	163	ASN
3	H	199	LEU
3	H	218	GLN
3	H	243	LEU
3	H	246	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	107	ASN
1	A	113	ASN
1	A	145	ASN
1	A	151	GLN
1	A	230	ASN
1	A	271	ASN
1	A	274	HIS
1	A	298	ASN
1	A	321	GLN
1	A	383	HIS
2	B	3	GLN
2	B	37	GLN
2	B	130	ASN
2	B	163	ASN
2	B	168	ASN
2	B	185	HIS
2	B	294	GLN
2	B	396	HIS
2	B	457	HIS
2	B	518	ASN
2	B	519	HIS
1	C	14	GLN
1	C	107	ASN
1	C	113	ASN
1	C	119	GLN
1	C	145	ASN
1	C	230	ASN
1	C	252	GLN
1	C	271	ASN

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Mol	Chain	Res	Type
1	C	298	ASN
1	C	383	HIS
2	D	3	GLN
2	D	53	GLN
2	D	168	ASN
2	D	185	HIS
2	D	396	HIS
2	D	457	HIS
2	D	513	GLN
2	D	519	HIS
3	E	142	ASN
3	E	145	GLN
3	E	162	ASN
3	E	163	ASN
3	E	188	ASN
3	E	201	ASN
3	E	215	ASN
3	F	4	GLN
3	F	142	ASN
3	F	145	GLN
3	F	162	ASN
3	F	163	ASN
3	F	185	ASN
3	F	201	ASN
3	F	206	GLN
3	F	215	ASN
3	F	250	ASN
3	F	257	ASN
3	G	4	GLN
3	G	21	ASN
3	G	142	ASN
3	G	162	ASN
3	G	163	ASN
3	G	201	ASN
3	H	4	GLN
3	H	162	ASN
3	H	163	ASN
3	H	206	GLN
3	H	257	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 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$
5	CFM	C	3496	1	0,24,24	-	-	-		
8	SF4	G	7290	3	0,12,12	-	-	-		
7	CLF	B	1498	1,2	0,24,24	-	-	-		
4	HCA	A	1494	-	13,13,13	2.63	4 (30%)	15,18,18	3.60	7 (46%)
5	CFM	A	1496	1	0,24,24	-	-	-		
4	HCA	C	3494	-	13,13,13	2.99	5 (38%)	15,18,18	4.24	9 (60%)
8	SF4	E	5290	3	0,12,12	-	-	-		
7	CLF	D	3498	1,2	0,24,24	-	-	-		

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
8	SF4	G	7290	3	-	-	0/6/5/5
7	CLF	B	1498	1,2	-	-	0/12/10/10

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HCA	A	1494	-	-	4/17/17/17	-
4	HCA	C	3494	-	-	5/17/17/17	-
8	SF4	E	5290	3	-	-	0/6/5/5
7	CLF	D	3498	1,2	-	-	0/12/10/10

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3494	HCA	O5-C7	8.80	1.49	1.22
4	A	1494	HCA	O5-C7	7.30	1.45	1.22
4	C	3494	HCA	C3-C7	3.50	1.57	1.53
4	C	3494	HCA	O1-C1	3.37	1.33	1.22
4	A	1494	HCA	O6-C7	-3.35	1.18	1.30
4	A	1494	HCA	O1-C1	2.95	1.31	1.22
4	A	1494	HCA	C3-C7	2.66	1.56	1.53
4	C	3494	HCA	O6-C7	-2.62	1.21	1.30
4	C	3494	HCA	O3-C6	2.19	1.29	1.22

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3494	HCA	O7-C3-C4	-10.40	92.25	108.88
4	C	3494	HCA	O7-C3-C2	-8.49	90.01	109.38
4	A	1494	HCA	O7-C3-C2	-8.19	90.70	109.38
4	A	1494	HCA	O7-C3-C4	-7.49	96.90	108.88
4	A	1494	HCA	C3-C2-C1	6.10	130.60	113.92
4	C	3494	HCA	C3-C2-C1	6.04	130.45	113.92
4	C	3494	HCA	O5-C7-C3	-3.76	114.80	122.09
4	C	3494	HCA	O7-C3-C7	3.45	113.85	108.96
4	A	1494	HCA	O6-C7-C3	2.94	118.79	113.14
4	C	3494	HCA	O2-C1-O1	-2.74	116.30	123.33
4	A	1494	HCA	O2-C1-O1	-2.56	116.75	123.33
4	C	3494	HCA	O3-C6-C5	-2.51	115.14	123.09
4	A	1494	HCA	O3-C6-C5	-2.39	115.50	123.09
4	C	3494	HCA	O1-C1-C2	2.35	129.60	122.95
4	C	3494	HCA	O6-C7-C3	2.25	117.46	113.14
4	A	1494	HCA	O1-C1-C2	2.20	129.17	122.95

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3494	HCA	C1-C2-C3-C4
4	C	3494	HCA	O7-C3-C4-C5
4	A	1494	HCA	C1-C2-C3-C4
4	A	1494	HCA	C7-C3-C4-C5
4	C	3494	HCA	C7-C3-C4-C5
4	A	1494	HCA	C4-C3-C7-O5
4	C	3494	HCA	C4-C3-C7-O5
4	A	1494	HCA	C4-C5-C6-O3
4	C	3494	HCA	C4-C5-C6-O3

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	3496	CFM	6	0
7	B	1498	CLF	1	0
4	A	1494	HCA	3	0
5	A	1496	CFM	5	0
4	C	3494	HCA	2	0
7	D	3498	CLF	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.