



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:23 AM UTC

PDB ID : 1Z01 / pdb_00001z01
Title : 2-Oxoquinoline 8-Monooxygenase Component: Active site Modulation by
Rieske-[2Fe-2S] Center Oxidation/Reduction
Authors : Martins, B.M.; Svetlitchnaia, T.; Dobbek, H.
Deposited on : 2005-03-01
Resolution : 1.80 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

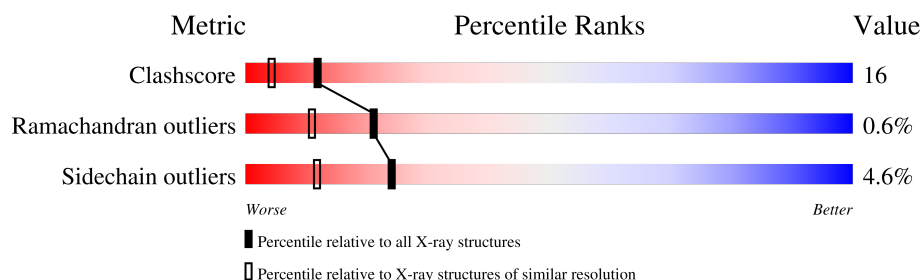
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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	446	
1	B	446	
1	C	446	
1	D	446	
1	E	446	
1	F	446	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 24517 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 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3454	2211	592	635	16			
1	B	427	Total	C	N	O	S	0	0	0
			3454	2211	592	635	16			
1	C	427	Total	C	N	O	S	0	0	0
			3454	2211	592	635	16			
1	D	427	Total	C	N	O	S	0	0	0
			3454	2211	592	635	16			
1	E	427	Total	C	N	O	S	0	0	0
			3454	2211	592	635	16			
1	F	427	Total	C	N	O	S	0	0	0
			3454	2211	592	635	16			

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		
2	B	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	E	1	Total	Fe	0	0
			1	1		
2	F	1	Total	Fe	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		
3	E	1	Total	Fe	S	0	0
			4	2	2		
3	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is water.

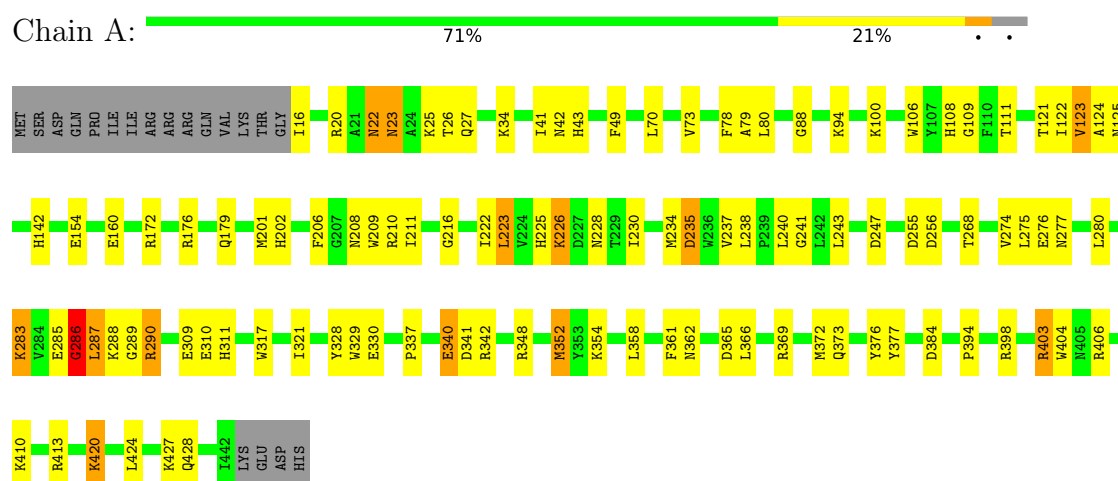
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	668	Total	O	0	0
			668	668		
4	B	620	Total	O	0	0
			620	620		
4	C	603	Total	O	0	0
			603	603		
4	D	663	Total	O	0	0
			663	663		
4	E	590	Total	O	0	0
			590	590		
4	F	619	Total	O	0	0
			619	619		

3 Residue-property plots

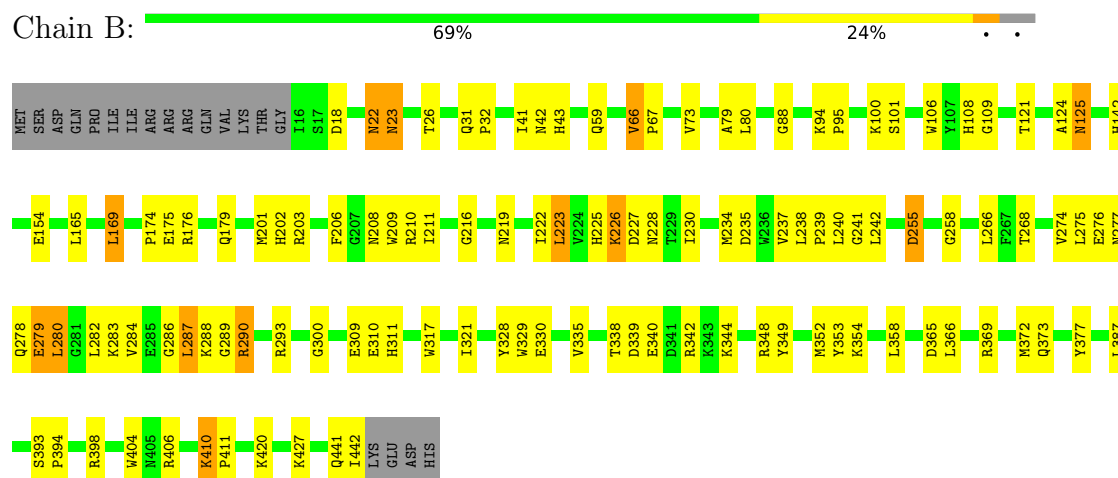
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

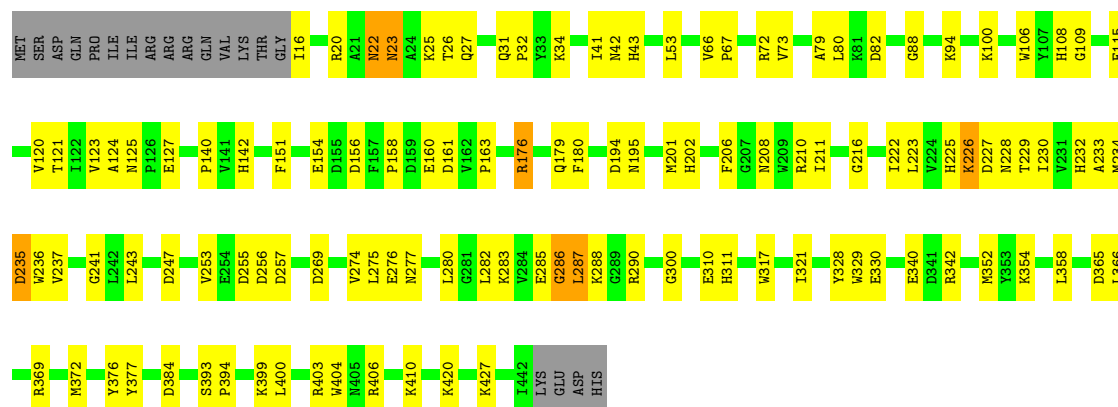


- Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component



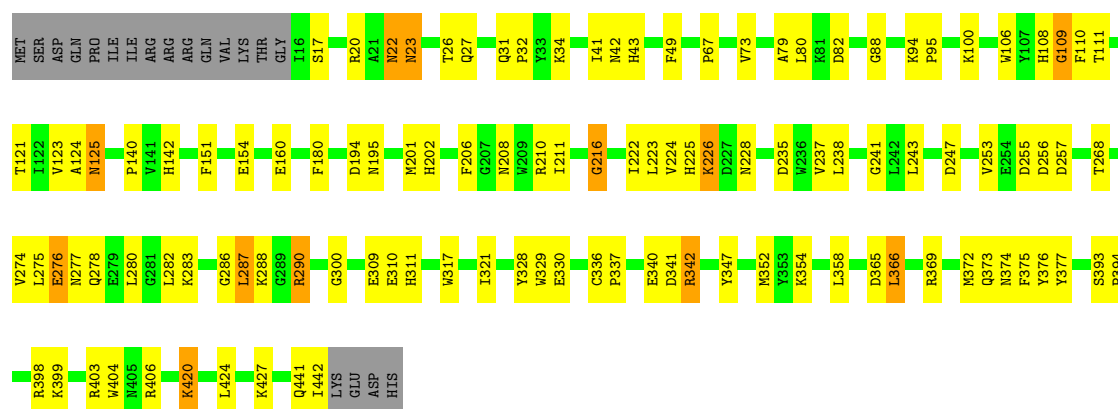
- Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component





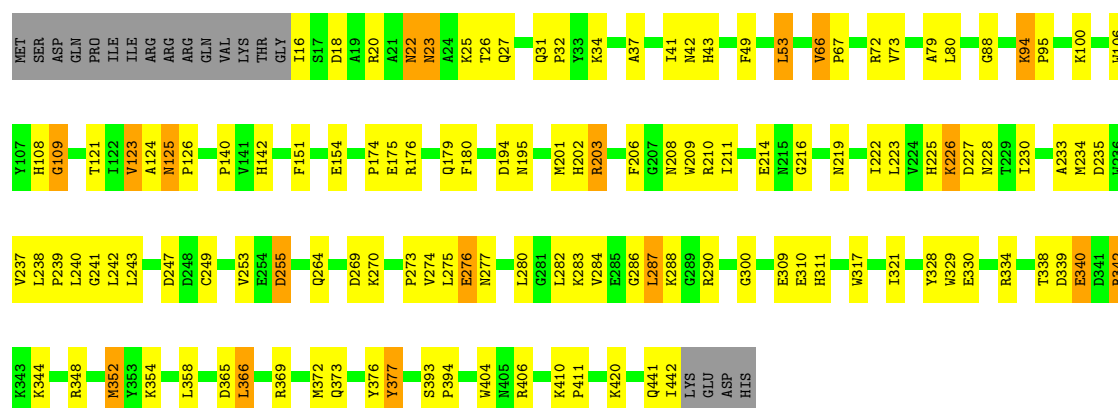
- Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain D: 70% 23%



- Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain E: 67% 25%



- Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain F: 68% 25%

L358	D365	L366	R369	K372	Q373	Y377	D384	L387	S393	P394	R398	W404	N405	R406	K410	P411	G412	R413	K420	K427	Q428	I442	LYS	GLU	ASP	HIS	L242	L243	D247	D248	C249	V253	E254	D255	D256	D257	G258	F259	K260	Q264	W265	L266	D269	K270	V274	L275	E276	N277	L280	K283	G286	L287	K288	G289	R290	R293	G300	E310	H311	W317	I321	Y328	W329	E330	E340	D341	R342	M352	Y353	K354																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.46Å 166.96Å 173.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	98.7 (20.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	24517	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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: FES, FE

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	0.43	0/3560	0.95	17/4853 (0.4%)
1	B	0.41	0/3560	0.94	15/4853 (0.3%)
1	C	0.40	0/3560	0.92	10/4853 (0.2%)
1	D	0.40	0/3560	0.93	17/4853 (0.4%)
1	E	0.40	0/3560	0.93	14/4853 (0.3%)
1	F	0.40	0/3560	0.92	14/4853 (0.3%)
All	All	0.41	0/21360	0.93	87/29118 (0.3%)

There are no bond length outliers.

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	321	ILE	N-CA-C	-8.69	103.32	111.48
1	F	321	ILE	N-CA-C	-8.15	103.93	111.67
1	B	88	GLY	N-CA-C	8.11	126.70	114.61
1	A	88	GLY	N-CA-C	8.09	126.31	114.10
1	E	321	ILE	N-CA-C	-8.05	103.91	111.48
1	D	321	ILE	N-CA-C	-7.77	104.18	111.48
1	C	88	GLY	N-CA-C	7.65	126.00	114.61
1	A	321	ILE	N-CA-C	-7.57	104.37	111.48
1	D	88	GLY	N-CA-C	7.43	126.35	114.90
1	E	88	GLY	N-CA-C	7.42	126.33	114.90
1	F	88	GLY	N-CA-C	7.38	126.27	114.90
1	A	268	THR	N-CA-C	-7.21	98.69	108.86
1	B	321	ILE	N-CA-C	-7.20	104.71	111.48
1	A	377	TYR	N-CA-C	6.57	119.28	111.33
1	B	268	THR	N-CA-C	-6.57	99.17	108.96
1	A	125	ASN	CA-C-N	6.56	126.25	119.56
1	A	125	ASN	C-N-CA	6.56	126.25	119.56
1	D	268	THR	N-CA-C	-6.55	99.62	108.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	GLY	CA-C-N	6.48	126.46	119.78
1	B	258	GLY	C-N-CA	6.48	126.46	119.78
1	C	276	GLU	N-CA-C	6.44	118.96	109.24
1	F	404	TRP	N-CA-C	6.35	121.81	113.30
1	B	276	GLU	N-CA-C	6.35	118.82	109.24
1	D	125	ASN	CA-C-N	6.32	126.01	119.82
1	D	125	ASN	C-N-CA	6.32	126.01	119.82
1	E	404	TRP	N-CA-C	6.30	121.74	113.30
1	F	276	GLU	N-CA-C	6.23	118.65	109.24
1	C	404	TRP	N-CA-C	6.23	121.65	113.30
1	A	376	TYR	N-CA-C	6.21	120.98	113.41
1	A	276	GLU	N-CA-C	6.17	118.56	109.24
1	D	377	TYR	N-CA-C	6.16	118.50	111.11
1	E	125	ASN	CA-C-N	6.15	125.85	119.82
1	E	125	ASN	C-N-CA	6.15	125.85	119.82
1	E	276	GLU	N-CA-C	6.13	118.49	109.24
1	B	125	ASN	CA-C-N	6.12	125.82	119.82
1	B	125	ASN	C-N-CA	6.12	125.82	119.82
1	E	49	PHE	N-CA-C	-6.10	101.45	110.48
1	A	404	TRP	N-CA-C	6.04	120.67	112.88
1	F	125	ASN	CA-C-N	6.03	125.73	119.82
1	F	125	ASN	C-N-CA	6.03	125.73	119.82
1	F	109	GLY	N-CA-C	6.00	123.63	115.30
1	B	216	GLY	N-CA-C	5.99	120.14	112.83
1	C	109	GLY	N-CA-C	5.93	123.55	115.30
1	D	216	GLY	N-CA-C	5.93	120.07	112.83
1	A	373	GLN	N-CA-C	5.89	117.70	111.28
1	D	109	GLY	N-CA-C	5.86	123.15	115.36
1	B	404	TRP	N-CA-C	5.83	121.11	113.30
1	E	376	TYR	N-CA-C	5.78	120.46	113.41
1	D	376	TYR	N-CA-C	5.77	120.45	113.41
1	E	216	GLY	N-CA-C	5.77	119.87	112.83
1	D	404	TRP	N-CA-C	5.73	120.98	113.30
1	B	377	TYR	N-CA-C	5.71	117.97	111.11
1	F	216	GLY	N-CA-C	5.66	119.74	112.83
1	B	373	GLN	N-CA-C	5.64	117.43	111.28
1	A	49	PHE	N-CA-C	-5.64	101.36	110.32
1	F	377	TYR	N-CA-C	5.63	117.86	111.11
1	E	377	TYR	N-CA-C	5.61	117.84	111.11
1	E	373	GLN	N-CA-C	5.58	118.08	111.33
1	D	276	GLU	N-CA-C	5.56	117.64	109.24
1	E	109	GLY	N-CA-C	5.50	122.95	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	GLY	N-CA-C	5.48	119.51	112.83
1	E	66	VAL	N-CA-C	5.46	113.27	107.76
1	A	420	LYS	N-CA-C	5.39	119.58	112.89
1	C	66	VAL	N-CA-C	5.39	113.20	107.76
1	D	373	GLN	N-CA-C	5.38	117.15	111.28
1	C	377	TYR	N-CA-C	5.37	117.55	111.11
1	F	49	PHE	N-CA-C	-5.26	102.69	110.48
1	B	420	LYS	N-CA-C	5.25	119.75	113.23
1	B	109	GLY	N-CA-C	5.20	122.53	115.30
1	B	66	VAL	N-CA-C	5.19	113.00	107.76
1	C	376	TYR	N-CA-C	5.18	119.73	113.41
1	F	373	GLN	N-CA-C	5.17	117.31	111.11
1	D	49	PHE	N-CA-C	-5.16	102.12	110.32
1	A	403	ARG	N-CA-C	5.15	118.03	111.69
1	A	286	GLY	N-CA-C	-5.14	101.00	113.18
1	F	258	GLY	CA-C-N	5.08	124.98	119.85
1	F	258	GLY	C-N-CA	5.08	124.98	119.85
1	D	336	CYS	CA-C-N	5.07	124.24	118.97
1	D	336	CYS	C-N-CA	5.07	124.24	118.97
1	D	420	LYS	N-CA-C	5.07	119.51	113.23
1	A	384	ASP	N-CA-C	5.06	119.46	113.28
1	C	233	ALA	N-CA-C	-5.06	105.85	112.23
1	E	233	ALA	N-CA-C	-5.06	105.86	112.23
1	A	109	GLY	N-CA-C	5.05	122.32	115.30
1	D	238	LEU	N-CA-C	5.04	117.32	110.01
1	F	384	ASP	N-CA-C	5.04	119.42	113.28
1	C	384	ASP	N-CA-C	5.01	119.39	113.28

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	3454	0	3307	102	0
1	B	3454	0	3307	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3454	0	3307	99	0
1	D	3454	0	3307	101	0
1	E	3454	0	3307	133	0
1	F	3454	0	3307	109	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	4	0	0	1	0
3	B	4	0	0	1	0
3	C	4	0	0	1	0
3	D	4	0	0	1	0
3	E	4	0	0	1	0
3	F	4	0	0	1	0
4	A	668	0	0	25	0
4	B	620	0	0	39	0
4	C	603	0	0	19	0
4	D	663	0	0	18	0
4	E	590	0	0	35	0
4	F	619	0	0	19	0
All	All	24517	0	19842	642	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 16.

All (642) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PRO:HB3	1:F:127:GLU:OE2	1.51	1.10
1:A:287:LEU:H	1:A:287:LEU:HD23	0.96	1.09
1:E:222:ILE:HG21	4:E:980:HOH:O	1.61	0.98
1:A:287:LEU:HD23	1:A:287:LEU:N	1.80	0.96
1:C:287:LEU:H	1:C:287:LEU:HD23	1.31	0.95
1:A:287:LEU:H	1:A:287:LEU:CD2	1.81	0.94
1:C:22:ASN:HD22	1:C:22:ASN:H	1.14	0.92
1:B:287:LEU:HD23	1:B:287:LEU:H	1.33	0.91
1:E:22:ASN:HD22	1:E:22:ASN:H	1.15	0.91
1:F:22:ASN:HD22	1:F:22:ASN:H	1.16	0.91
1:E:225:HIS:HD1	1:E:228:ASN:HD21	1.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ASN:H	1:D:22:ASN:HD22	1.19	0.90
1:E:287:LEU:H	1:E:287:LEU:HD23	1.35	0.90
1:A:225:HIS:HD1	1:A:228:ASN:HD21	1.14	0.90
1:D:287:LEU:HD23	1:D:287:LEU:H	1.35	0.90
1:B:225:HIS:HD1	1:B:228:ASN:HD21	1.19	0.90
1:D:225:HIS:HD1	1:D:228:ASN:HD21	1.20	0.89
1:B:222:ILE:HG21	4:B:1071:HOH:O	1.71	0.89
1:C:225:HIS:HD1	1:C:228:ASN:HD21	1.20	0.89
1:F:225:HIS:HD1	1:F:228:ASN:HD21	1.18	0.89
1:B:22:ASN:H	1:B:22:ASN:HD22	1.15	0.88
1:A:22:ASN:HD22	1:A:22:ASN:H	1.18	0.86
1:A:208:ASN:HD21	1:A:210:ARG:HE	1.22	0.85
1:B:335:VAL:HB	1:D:278:GLN:HE22	1.39	0.85
1:F:208:ASN:HD21	1:F:210:ARG:HE	1.26	0.84
1:E:282:LEU:HG	4:E:737:HOH:O	1.78	0.84
1:B:284:VAL:HB	4:B:689:HOH:O	1.78	0.83
1:C:280:LEU:HB3	4:C:1076:HOH:O	1.77	0.83
1:B:208:ASN:HD21	1:B:210:ARG:HE	1.25	0.83
1:B:165:LEU:HG	1:B:169:LEU:CD1	2.10	0.81
1:C:232:HIS:HB2	4:C:1096:HOH:O	1.79	0.81
1:B:43:HIS:HE1	1:B:406:ARG:H	1.26	0.80
1:D:282:LEU:HG	4:D:645:HOH:O	1.80	0.80
1:E:290:ARG:HG3	4:E:725:HOH:O	1.81	0.80
1:A:201:MET:HE1	1:A:354:LYS:HE3	1.65	0.79
1:A:256:ASP:HB3	4:A:836:HOH:O	1.82	0.79
1:B:288:LYS:HE3	4:B:1024:HOH:O	1.82	0.79
1:D:208:ASN:HD21	1:D:210:ARG:HE	1.28	0.79
1:E:290:ARG:HH21	1:E:309:GLU:HA	1.47	0.78
1:F:287:LEU:HD23	1:F:287:LEU:H	1.48	0.78
1:F:208:ASN:ND2	1:F:210:ARG:HE	1.81	0.78
1:B:335:VAL:HB	1:D:278:GLN:NE2	1.98	0.77
1:B:121:THR:HG21	1:C:280:LEU:HD13	1.66	0.77
1:D:121:THR:HG21	1:E:280:LEU:HD13	1.66	0.77
1:A:208:ASN:ND2	1:A:210:ARG:HE	1.82	0.77
1:F:237:VAL:CG1	1:F:286:GLY:O	2.33	0.77
1:E:43:HIS:HE1	1:E:406:ARG:H	1.31	0.77
1:A:121:THR:HG21	1:B:280:LEU:HD13	1.64	0.77
1:C:208:ASN:ND2	1:C:210:ARG:HE	1.83	0.77
1:C:283:LYS:HE2	4:C:1068:HOH:O	1.86	0.76
1:E:288:LYS:HE3	4:E:1006:HOH:O	1.86	0.75
1:B:208:ASN:ND2	1:B:210:ARG:HE	1.84	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:ASN:HD21	1:C:210:ARG:HE	1.30	0.75
1:D:275:LEU:HG	4:D:950:HOH:O	1.87	0.75
1:E:43:HIS:CE1	1:E:406:ARG:H	2.05	0.75
1:C:43:HIS:HE1	1:C:406:ARG:H	1.32	0.74
1:D:43:HIS:HE1	1:D:406:ARG:H	1.35	0.74
1:F:23:ASN:ND2	1:F:26:THR:H	1.84	0.74
1:B:43:HIS:CE1	1:B:406:ARG:H	2.05	0.74
1:D:208:ASN:ND2	1:D:210:ARG:HE	1.85	0.73
1:B:275:LEU:HA	4:B:689:HOH:O	1.89	0.73
1:C:201:MET:HE1	1:C:354:LYS:HE3	1.69	0.73
1:D:201:MET:HE1	1:D:354:LYS:HE3	1.70	0.73
1:A:225:HIS:HD1	1:A:228:ASN:ND2	1.86	0.72
1:E:348:ARG:O	1:E:352:MET:HB3	1.89	0.72
1:C:23:ASN:ND2	1:C:26:THR:H	1.88	0.72
1:A:43:HIS:HE1	1:A:406:ARG:H	1.36	0.72
1:B:222:ILE:HG22	4:B:614:HOH:O	1.90	0.71
1:C:16:ILE:N	4:C:1086:HOH:O	2.23	0.71
1:B:287:LEU:HD12	4:B:994:HOH:O	1.89	0.71
1:F:201:MET:HE1	1:F:354:LYS:HE3	1.73	0.71
1:E:201:MET:HE1	1:E:354:LYS:HE3	1.72	0.71
1:E:342:ARG:HH11	1:E:342:ARG:HG3	1.55	0.71
1:C:43:HIS:CE1	1:C:406:ARG:H	2.09	0.70
1:B:238:LEU:HD23	4:B:729:HOH:O	1.91	0.70
1:C:330:GLU:HG2	1:C:358:LEU:HD22	1.72	0.70
1:D:43:HIS:CE1	1:D:406:ARG:H	2.10	0.70
1:E:211:ILE:HG23	1:E:372:MET:HE3	1.74	0.70
1:E:339:ASP:HA	1:E:342:ARG:NH1	2.07	0.70
4:B:522:HOH:O	1:D:283:LYS:HG3	1.92	0.69
1:E:273:PRO:HB3	4:E:987:HOH:O	1.92	0.69
1:C:285:GLU:O	1:C:285:GLU:HG3	1.91	0.69
1:E:208:ASN:ND2	1:E:210:ARG:HB2	2.07	0.69
1:A:43:HIS:CE1	1:A:406:ARG:H	2.11	0.69
1:C:108:HIS:HB2	3:C:500:FES:S1	2.33	0.68
1:F:256:ASP:HB3	4:F:960:HOH:O	1.94	0.68
1:A:211:ILE:HG23	1:A:372:MET:HE3	1.76	0.68
1:F:42:ASN:HD21	1:F:154:GLU:H	1.42	0.68
1:F:237:VAL:HG11	1:F:286:GLY:HA3	1.76	0.68
1:A:277:ASN:HD22	1:A:280:LEU:H	1.42	0.67
1:E:37:ALA:HA	1:E:210:ARG:NH2	2.09	0.67
1:F:43:HIS:HE1	1:F:406:ARG:H	1.39	0.67
1:E:53:LEU:HD23	1:E:72:ARG:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ASN:ND2	1:E:26:THR:H	1.93	0.67
1:B:22:ASN:HD22	1:B:22:ASN:N	1.91	0.67
1:A:330:GLU:HG2	1:A:358:LEU:HD22	1.77	0.66
1:B:226:LYS:HD3	1:B:227:ASP:OD2	1.95	0.66
1:E:282:LEU:HD23	4:E:808:HOH:O	1.94	0.66
1:D:277:ASN:HD22	1:D:280:LEU:H	1.44	0.66
1:E:22:ASN:HD22	1:E:22:ASN:N	1.90	0.66
1:F:43:HIS:CE1	1:F:406:ARG:H	2.13	0.66
1:A:238:LEU:HA	4:A:840:HOH:O	1.95	0.66
1:B:239:PRO:O	4:B:1071:HOH:O	2.12	0.66
1:D:330:GLU:OE1	1:D:358:LEU:HA	1.96	0.66
1:B:203:ARG:HD3	4:B:794:HOH:O	1.93	0.66
1:C:256:ASP:HB3	4:C:1077:HOH:O	1.96	0.66
1:F:287:LEU:HD23	1:F:287:LEU:N	2.10	0.66
1:A:108:HIS:HB2	3:A:500:FES:S1	2.36	0.65
1:E:42:ASN:HD21	1:E:154:GLU:H	1.44	0.65
1:F:277:ASN:HD22	1:F:280:LEU:H	1.44	0.65
1:B:226:LYS:HB2	1:B:226:LYS:NZ	2.11	0.65
1:B:344:LYS:HE3	4:D:1150:HOH:O	1.95	0.65
1:E:121:THR:HG21	1:F:280:LEU:HD13	1.77	0.65
1:A:285:GLU:HG3	1:A:285:GLU:O	1.95	0.65
1:F:211:ILE:HG23	1:F:372:MET:HE3	1.77	0.65
1:B:283:LYS:HE3	4:B:912:HOH:O	1.96	0.65
1:E:287:LEU:HD12	4:E:902:HOH:O	1.97	0.65
1:D:124:ALA:O	1:E:274:VAL:HG21	1.97	0.64
1:B:201:MET:HE1	1:B:354:LYS:HE3	1.80	0.64
1:C:53:LEU:CD2	1:C:72:ARG:HB2	2.27	0.64
1:B:342:ARG:HG3	1:B:342:ARG:HH11	1.62	0.64
1:B:222:ILE:HD12	1:B:241:GLY:HA2	1.79	0.64
1:B:339:ASP:HA	1:B:342:ARG:NH1	2.12	0.64
1:B:290:ARG:NH2	1:B:309:GLU:HA	2.13	0.64
1:D:22:ASN:HD22	1:D:22:ASN:N	1.92	0.63
1:A:23:ASN:ND2	1:A:26:THR:H	1.96	0.63
1:A:275:LEU:HG	4:A:926:HOH:O	1.97	0.63
1:C:237:VAL:HB	1:C:286:GLY:O	1.97	0.63
1:C:277:ASN:HD22	1:C:280:LEU:H	1.45	0.63
1:D:23:ASN:ND2	1:D:26:THR:H	1.97	0.63
1:E:239:PRO:HG2	4:E:980:HOH:O	1.98	0.63
1:E:222:ILE:HG22	4:E:699:HOH:O	1.98	0.63
1:A:311:HIS:HD2	4:A:975:HOH:O	1.81	0.63
1:A:124:ALA:O	1:B:274:VAL:HG21	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ASN:ND2	1:B:26:THR:H	1.97	0.63
1:F:225:HIS:HD1	1:F:228:ASN:ND2	1.94	0.63
1:A:222:ILE:HD12	1:A:241:GLY:HA2	1.80	0.62
1:E:225:HIS:HD1	1:E:228:ASN:ND2	1.93	0.62
1:F:226:LYS:HB2	1:F:226:LYS:NZ	2.14	0.62
1:B:142:HIS:HD2	4:B:625:HOH:O	1.82	0.62
1:C:222:ILE:HD12	1:C:241:GLY:HA2	1.80	0.62
1:C:277:ASN:ND2	1:C:280:LEU:H	1.96	0.62
1:A:176:ARG:HD3	1:A:179:GLN:NE2	2.13	0.62
1:A:223:LEU:HD12	4:A:1053:HOH:O	1.99	0.62
1:F:260:LYS:HD3	4:F:880:HOH:O	2.00	0.62
1:F:277:ASN:ND2	1:F:280:LEU:H	1.97	0.62
1:D:256:ASP:HB3	4:D:960:HOH:O	2.00	0.62
1:D:206:PHE:CD1	1:F:427:LYS:HD2	2.35	0.62
1:E:203:ARG:HG2	4:E:845:HOH:O	1.99	0.62
1:F:142:HIS:HD2	4:F:527:HOH:O	1.82	0.61
1:D:211:ILE:HG23	1:D:372:MET:HE3	1.81	0.61
1:F:16:ILE:N	4:F:891:HOH:O	2.33	0.61
1:C:282:LEU:HG	4:C:1076:HOH:O	2.00	0.61
1:B:225:HIS:HD1	1:B:228:ASN:ND2	1.95	0.61
1:F:79:ALA:C	1:F:80:LEU:HD12	2.25	0.61
1:A:238:LEU:HD23	4:A:840:HOH:O	1.99	0.61
1:B:211:ILE:HG23	1:B:372:MET:HE3	1.82	0.61
1:C:42:ASN:HD21	1:C:154:GLU:H	1.49	0.61
1:E:277:ASN:HD22	1:E:280:LEU:H	1.47	0.61
1:C:79:ALA:C	1:C:80:LEU:HD12	2.25	0.61
1:B:239:PRO:HG2	4:B:1071:HOH:O	2.01	0.61
1:E:240:LEU:HD23	4:E:1089:HOH:O	2.00	0.61
1:B:108:HIS:HB2	3:B:500:FES:S1	2.40	0.61
1:B:310:GLU:HG3	4:B:1011:HOH:O	2.01	0.61
1:C:287:LEU:H	1:C:287:LEU:CD2	2.08	0.61
1:C:23:ASN:HD22	1:C:26:THR:H	1.49	0.61
1:E:22:ASN:H	1:E:22:ASN:ND2	1.95	0.61
1:E:79:ALA:C	1:E:80:LEU:HD12	2.26	0.61
1:B:282:LEU:HG	4:B:665:HOH:O	2.00	0.60
1:C:22:ASN:HD22	1:C:22:ASN:N	1.90	0.60
1:E:53:LEU:CD2	1:E:72:ARG:HB2	2.31	0.60
1:E:95:PRO:HG2	1:E:441:GLN:OE1	2.00	0.60
1:D:342:ARG:HG2	4:D:1146:HOH:O	2.00	0.60
1:E:311:HIS:HD2	4:E:834:HOH:O	1.84	0.60
1:B:22:ASN:H	1:B:22:ASN:ND2	1.95	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LEU:HB2	4:B:893:HOH:O	2.01	0.60
1:C:222:ILE:HG22	4:C:1011:HOH:O	2.02	0.60
1:D:108:HIS:HB2	3:D:500:FES:S1	2.41	0.60
1:D:226:LYS:HB2	1:D:226:LYS:NZ	2.16	0.60
1:A:226:LYS:HB2	1:A:226:LYS:NZ	2.16	0.59
1:E:344:LYS:HE3	4:E:1075:HOH:O	2.01	0.59
1:D:222:ILE:HD12	1:D:241:GLY:HA2	1.85	0.59
1:F:237:VAL:HG12	1:F:286:GLY:O	2.03	0.59
1:B:42:ASN:HD21	1:B:154:GLU:H	1.49	0.59
1:C:176:ARG:HD2	1:C:179:GLN:NE2	2.18	0.59
1:E:284:VAL:HB	4:E:795:HOH:O	2.02	0.59
1:F:226:LYS:HD3	1:F:227:ASP:OD2	2.01	0.59
1:A:79:ALA:C	1:A:80:LEU:HD12	2.27	0.59
1:B:226:LYS:HB2	1:B:226:LYS:HZ2	1.67	0.59
1:F:22:ASN:HD22	1:F:22:ASN:N	1.95	0.59
1:A:23:ASN:C	1:A:23:ASN:HD22	2.11	0.59
1:A:237:VAL:HB	1:A:286:GLY:O	2.02	0.59
1:A:16:ILE:N	4:A:870:HOH:O	2.34	0.59
1:A:42:ASN:HD21	1:A:154:GLU:H	1.51	0.59
1:D:42:ASN:HD21	1:D:154:GLU:H	1.51	0.59
1:D:427:LYS:HD2	1:E:206:PHE:CD1	2.38	0.59
1:C:226:LYS:HB2	1:C:226:LYS:NZ	2.17	0.58
1:D:225:HIS:HD1	1:D:228:ASN:ND2	1.96	0.58
1:D:95:PRO:HG2	1:D:441:GLN:OE1	2.03	0.58
1:D:277:ASN:ND2	1:D:280:LEU:H	2.00	0.58
1:E:342:ARG:HG3	1:E:342:ARG:NH1	2.16	0.58
1:C:330:GLU:OE1	1:C:358:LEU:HA	2.03	0.58
1:E:27:GLN:HE21	1:E:34:LYS:HZ1	1.51	0.58
1:C:156:ASP:HB3	4:C:719:HOH:O	2.03	0.58
1:F:237:VAL:CG1	1:F:237:VAL:O	2.51	0.58
1:B:101:SER:HA	4:B:1115:HOH:O	2.03	0.57
1:B:330:GLU:HG2	1:B:358:LEU:HD22	1.86	0.57
1:F:20:ARG:HD2	1:F:22:ASN:HD21	1.69	0.57
1:F:287:LEU:HA	4:F:725:HOH:O	2.04	0.57
1:A:201:MET:CE	1:A:354:LYS:HE3	2.34	0.57
1:E:108:HIS:HB2	3:E:500:FES:S1	2.44	0.57
1:A:111:THR:HG21	1:B:280:LEU:HD11	1.86	0.57
1:C:310:GLU:O	1:C:311:HIS:HB2	2.04	0.57
1:F:310:GLU:O	1:F:311:HIS:HB2	2.05	0.57
1:B:165:LEU:HG	1:B:169:LEU:HD11	1.86	0.57
1:C:27:GLN:HE21	1:C:34:LYS:HZ1	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:PHE:CD1	1:C:427:LYS:HD2	2.40	0.57
1:B:95:PRO:HG2	1:B:441:GLN:OE1	2.04	0.57
1:E:222:ILE:HD12	1:E:241:GLY:HA2	1.86	0.57
1:E:37:ALA:CA	1:E:210:ARG:NH2	2.67	0.57
1:C:243:LEU:HD11	1:C:274:VAL:HG22	1.87	0.57
1:B:348:ARG:HD2	4:B:1062:HOH:O	2.05	0.56
1:D:142:HIS:HD2	4:D:536:HOH:O	1.88	0.56
1:F:203:ARG:HD3	4:F:893:HOH:O	2.05	0.56
1:F:211:ILE:CG2	1:F:372:MET:HE3	2.35	0.56
1:E:201:MET:CE	1:E:354:LYS:HE3	2.36	0.56
1:E:237:VAL:HB	1:E:286:GLY:O	2.05	0.56
1:A:290:ARG:HD3	4:A:673:HOH:O	2.05	0.56
1:A:413:ARG:HG3	4:B:830:HOH:O	2.05	0.56
1:E:142:HIS:HD2	4:E:654:HOH:O	1.89	0.56
1:C:342:ARG:HG3	1:C:342:ARG:HH11	1.69	0.56
1:A:277:ASN:ND2	1:A:280:LEU:H	2.02	0.56
1:F:59:GLN:NE2	4:F:736:HOH:O	2.39	0.56
1:B:23:ASN:C	1:B:23:ASN:HD22	2.14	0.55
1:D:23:ASN:HD22	1:D:23:ASN:C	2.15	0.55
1:B:79:ALA:C	1:B:80:LEU:HD12	2.31	0.55
1:D:287:LEU:H	1:D:287:LEU:CD2	2.15	0.55
1:B:165:LEU:HG	1:B:169:LEU:HD13	1.89	0.55
1:B:278:GLN:O	1:B:279:GLU:O	2.24	0.55
1:B:311:HIS:HD2	4:B:504:HOH:O	1.88	0.55
1:E:330:GLU:OE1	1:E:358:LEU:HA	2.07	0.55
1:F:41:ILE:O	1:F:42:ASN:HB2	2.07	0.55
1:C:399:LYS:O	1:C:403:ARG:HG3	2.06	0.55
1:D:317:TRP:HB2	1:D:329:TRP:HB2	1.88	0.55
1:D:20:ARG:HD2	1:D:22:ASN:HD21	1.72	0.55
1:A:23:ASN:HD22	1:A:26:THR:H	1.55	0.55
1:E:23:ASN:C	1:E:23:ASN:HD22	2.15	0.55
1:A:226:LYS:HD3	4:A:1136:HOH:O	2.06	0.54
1:D:23:ASN:HD22	1:D:26:THR:H	1.54	0.54
1:E:275:LEU:HA	4:E:795:HOH:O	2.06	0.54
1:B:124:ALA:O	1:C:274:VAL:HG21	2.05	0.54
1:B:237:VAL:HB	1:B:286:GLY:O	2.07	0.54
1:A:27:GLN:HE21	1:A:34:LYS:HZ1	1.55	0.54
1:E:176:ARG:HD3	1:E:179:GLN:NE2	2.23	0.54
1:F:23:ASN:HD22	1:F:26:THR:H	1.53	0.54
1:B:73:VAL:HG13	1:B:100:LYS:HD2	1.90	0.54
1:D:365:ASP:O	1:D:369:ARG:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:ASN:HD22	1:E:26:THR:H	1.56	0.54
1:E:282:LEU:HD22	4:E:969:HOH:O	2.06	0.54
1:E:287:LEU:HB2	4:E:902:HOH:O	2.08	0.54
1:C:211:ILE:HG23	1:C:372:MET:HE3	1.90	0.54
1:D:125:ASN:HA	1:E:243:LEU:HD21	1.89	0.54
1:B:223:LEU:O	1:B:226:LYS:HG2	2.08	0.54
1:A:20:ARG:HD2	1:A:22:ASN:HD21	1.73	0.54
1:A:362:ASN:HB3	4:A:1126:HOH:O	2.08	0.54
1:D:201:MET:CE	1:D:354:LYS:HE3	2.37	0.54
1:E:125:ASN:HA	1:F:243:LEU:HD21	1.90	0.54
1:F:330:GLU:HG2	1:F:358:LEU:HD22	1.89	0.53
1:A:243:LEU:HD21	1:C:125:ASN:HA	1.90	0.53
1:A:274:VAL:HG21	1:C:124:ALA:O	2.08	0.53
1:B:41:ILE:O	1:B:42:ASN:HB2	2.09	0.53
1:F:237:VAL:HG11	1:F:286:GLY:CA	2.38	0.53
1:A:427:LYS:HD2	1:B:206:PHE:CD1	2.43	0.53
1:B:365:ASP:O	1:B:369:ARG:HG3	2.08	0.53
1:B:342:ARG:HG3	1:B:342:ARG:NH1	2.21	0.53
1:C:23:ASN:HD22	1:C:23:ASN:C	2.16	0.53
1:E:243:LEU:HD11	1:E:274:VAL:HG22	1.91	0.53
1:D:366:LEU:HD21	4:D:533:HOH:O	2.08	0.53
1:B:280:LEU:CD1	1:B:280:LEU:H	2.21	0.53
1:F:23:ASN:HD22	1:F:23:ASN:C	2.17	0.53
1:F:340:GLU:HG2	4:F:916:HOH:O	2.08	0.53
1:E:226:LYS:HB2	1:E:226:LYS:NZ	2.22	0.53
1:E:284:VAL:HG22	4:E:993:HOH:O	2.09	0.53
1:B:202:HIS:HA	1:B:328:TYR:O	2.09	0.53
1:A:208:ASN:HD21	1:A:210:ARG:NE	2.00	0.53
1:C:142:HIS:HD2	4:C:739:HOH:O	1.91	0.53
1:C:280:LEU:HD23	4:C:1076:HOH:O	2.08	0.53
1:E:41:ILE:O	1:E:42:ASN:HB2	2.09	0.53
1:A:121:THR:HG21	1:B:277:ASN:HD21	1.73	0.52
1:C:225:HIS:HD1	1:C:228:ASN:ND2	1.98	0.52
1:E:239:PRO:O	4:E:980:HOH:O	2.19	0.52
1:B:283:LYS:HE2	4:B:914:HOH:O	2.09	0.52
1:D:202:HIS:HA	1:D:328:TYR:O	2.09	0.52
1:F:275:LEU:O	1:F:283:LYS:HA	2.09	0.52
1:F:365:ASP:O	1:F:369:ARG:HG3	2.09	0.52
1:A:424:LEU:HG	4:B:708:HOH:O	2.08	0.52
1:C:53:LEU:HD23	1:C:72:ARG:HB2	1.91	0.52
1:D:41:ILE:O	1:D:42:ASN:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:GLU:HG2	1:E:358:LEU:HD22	1.92	0.52
1:E:243:LEU:CD1	1:E:274:VAL:HG22	2.39	0.52
1:D:311:HIS:HD2	4:D:977:HOH:O	1.93	0.52
1:A:330:GLU:OE1	1:A:358:LEU:HA	2.10	0.52
1:A:121:THR:CG2	1:B:280:LEU:HD13	2.36	0.52
1:B:23:ASN:HD22	1:B:26:THR:H	1.57	0.52
1:B:176:ARG:HD3	1:B:179:GLN:NE2	2.25	0.52
1:C:41:ILE:O	1:C:42:ASN:HB2	2.10	0.52
1:E:27:GLN:HE21	1:E:34:LYS:NZ	2.08	0.52
1:E:339:ASP:N	1:E:342:ARG:HH12	2.08	0.52
1:F:412:GLY:O	1:F:413:ARG:HD3	2.10	0.52
1:A:420:LYS:HE2	4:A:901:HOH:O	2.10	0.52
1:B:201:MET:CE	1:B:354:LYS:HE3	2.40	0.52
4:D:971:HOH:O	1:F:442:ILE:HG21	2.10	0.52
1:F:20:ARG:HD2	1:F:22:ASN:ND2	2.25	0.52
1:F:201:MET:CE	1:F:354:LYS:HE3	2.40	0.52
1:B:330:GLU:OE1	1:B:358:LEU:HA	2.09	0.51
1:B:125:ASN:HA	1:C:243:LEU:HD21	1.92	0.51
1:E:277:ASN:ND2	1:E:280:LEU:H	2.09	0.51
1:E:280:LEU:HB3	4:E:737:HOH:O	2.10	0.51
1:E:420:LYS:NZ	4:E:865:HOH:O	2.27	0.51
1:A:365:ASP:O	1:A:369:ARG:HG3	2.10	0.51
1:B:18:ASP:HB3	4:B:978:HOH:O	2.09	0.51
1:C:342:ARG:HG3	1:C:342:ARG:NH1	2.23	0.51
1:F:243:LEU:HD11	1:F:274:VAL:HG22	1.92	0.51
1:A:27:GLN:HE21	1:A:34:LYS:NZ	2.08	0.51
1:A:283:LYS:O	1:A:283:LYS:HG2	2.05	0.51
1:F:108:HIS:HB2	3:F:500:FES:S1	2.51	0.51
1:A:202:HIS:HA	1:A:328:TYR:O	2.11	0.51
1:B:240:LEU:HD11	4:B:893:HOH:O	2.10	0.51
1:C:403:ARG:HD3	4:C:1058:HOH:O	2.10	0.51
1:D:394:PRO:O	1:D:398:ARG:HG3	2.11	0.51
1:A:289:GLY:HA3	4:A:1155:HOH:O	2.11	0.51
1:E:124:ALA:O	1:F:274:VAL:HG21	2.10	0.51
1:D:121:THR:HG21	1:E:277:ASN:HD21	1.76	0.51
1:F:243:LEU:CD1	1:F:274:VAL:HG22	2.41	0.51
1:B:284:VAL:HG22	4:B:1030:HOH:O	2.09	0.51
1:D:79:ALA:C	1:D:80:LEU:HD12	2.36	0.50
1:D:399:LYS:O	1:D:403:ARG:HG3	2.12	0.50
1:A:41:ILE:O	1:A:42:ASN:HB2	2.10	0.50
1:F:226:LYS:HB2	1:F:226:LYS:HZ2	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HB3	4:B:665:HOH:O	2.09	0.50
1:B:290:ARG:HH21	1:B:309:GLU:HA	1.76	0.50
1:E:140:PRO:HD2	1:E:151:PHE:HB3	1.94	0.50
1:F:176:ARG:HD3	1:F:179:GLN:NE2	2.26	0.50
1:C:243:LEU:CD1	1:C:274:VAL:HG22	2.41	0.50
1:C:275:LEU:O	1:C:283:LYS:HA	2.12	0.50
1:B:310:GLU:O	1:B:311:HIS:HB2	2.12	0.50
1:A:22:ASN:H	1:A:22:ASN:ND2	1.98	0.50
1:A:142:HIS:HD2	4:A:527:HOH:O	1.93	0.50
1:D:290:ARG:NH2	1:D:309:GLU:HA	2.27	0.50
1:F:317:TRP:HB2	1:F:329:TRP:HB2	1.93	0.50
1:C:115:GLU:HG2	4:C:1097:HOH:O	2.12	0.50
1:C:230:ILE:HD11	4:C:1022:HOH:O	2.10	0.50
1:D:22:ASN:H	1:D:22:ASN:ND2	1.98	0.50
1:E:377:TYR:HB3	4:E:875:HOH:O	2.11	0.50
1:B:410:LYS:NZ	4:B:899:HOH:O	2.44	0.50
1:A:340:GLU:HG2	4:A:1006:HOH:O	2.11	0.49
1:D:237:VAL:HB	1:D:286:GLY:O	2.12	0.49
1:D:243:LEU:HD21	1:F:125:ASN:HA	1.93	0.49
1:E:211:ILE:CG2	1:E:372:MET:HE3	2.42	0.49
1:F:208:ASN:HD21	1:F:210:ARG:NE	2.03	0.49
1:F:216:GLY:HA3	4:F:684:HOH:O	2.12	0.49
1:C:20:ARG:HD2	1:C:22:ASN:HD21	1.77	0.49
1:E:365:ASP:O	1:E:369:ARG:HG3	2.11	0.49
1:F:67:PRO:HB2	1:F:82:ASP:HB3	1.94	0.49
1:F:208:ASN:ND2	1:F:210:ARG:HB2	2.27	0.49
1:D:288:LYS:HG3	4:D:965:HOH:O	2.12	0.49
1:E:339:ASP:CA	1:E:342:ARG:NH1	2.75	0.49
1:A:310:GLU:O	1:A:311:HIS:HB2	2.12	0.49
1:D:111:THR:HG21	1:E:280:LEU:HD11	1.94	0.49
1:D:424:LEU:HG	4:E:871:HOH:O	2.12	0.49
1:E:338:THR:C	1:E:342:ARG:HH12	2.20	0.49
1:A:428:GLN:NE2	4:A:1046:HOH:O	2.44	0.49
1:C:365:ASP:O	1:C:369:ARG:HG3	2.12	0.49
1:D:121:THR:CG2	1:E:280:LEU:HD13	2.38	0.49
1:B:211:ILE:CG2	1:B:372:MET:HE3	2.42	0.49
1:E:18:ASP:HB2	4:E:965:HOH:O	2.11	0.49
1:E:42:ASN:ND2	1:E:154:GLU:H	2.08	0.49
1:C:226:LYS:HB2	1:C:226:LYS:HZ2	1.76	0.49
1:B:278:GLN:HG3	4:B:1114:HOH:O	2.12	0.49
1:B:287:LEU:H	1:B:287:LEU:CD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:PRO:HD3	4:E:767:HOH:O	2.12	0.49
1:A:290:ARG:NH2	1:A:309:GLU:HA	2.28	0.49
1:B:73:VAL:HG11	1:B:100:LYS:O	2.12	0.49
1:E:255:ASP:O	4:E:715:HOH:O	2.20	0.49
1:A:211:ILE:CG2	1:A:372:MET:HE3	2.42	0.48
1:F:223:LEU:O	1:F:226:LYS:HG2	2.13	0.48
1:D:280:LEU:HD13	1:F:121:THR:HG21	1.94	0.48
1:F:42:ASN:ND2	1:F:154:GLU:H	2.07	0.48
1:B:59:GLN:NE2	4:B:905:HOH:O	2.46	0.48
1:C:202:HIS:HA	1:C:328:TYR:O	2.13	0.48
1:C:234:MET:O	1:C:236:TRP:CD1	2.66	0.48
1:D:17:SER:HB3	1:F:130:LEU:HD11	1.95	0.48
1:D:330:GLU:CG	1:D:358:LEU:HD22	2.44	0.48
1:F:234:MET:HE3	4:F:871:HOH:O	2.14	0.48
1:D:208:ASN:ND2	1:D:210:ARG:H	2.11	0.48
1:E:338:THR:C	1:E:342:ARG:NH1	2.72	0.48
1:F:27:GLN:NE2	1:F:34:LYS:HZ1	2.12	0.48
1:F:275:LEU:HG	4:F:737:HOH:O	2.12	0.48
1:B:230:ILE:O	1:B:234:MET:HG2	2.14	0.48
1:C:127:GLU:OE1	4:C:777:HOH:O	2.20	0.48
1:C:208:ASN:HD21	1:C:210:ARG:NE	2.04	0.48
1:E:344:LYS:HG3	4:E:789:HOH:O	2.13	0.48
1:F:266:LEU:HD12	1:F:293:ARG:HA	1.96	0.48
1:E:275:LEU:O	1:E:283:LYS:HA	2.14	0.48
1:B:266:LEU:HD12	1:B:293:ARG:HA	1.95	0.48
1:B:275:LEU:O	1:B:283:LYS:HA	2.14	0.48
1:E:290:ARG:NE	4:E:725:HOH:O	2.47	0.48
1:E:339:ASP:HA	1:E:342:ARG:HH11	1.78	0.48
1:A:342:ARG:HG3	1:A:342:ARG:HH11	1.79	0.48
1:C:256:ASP:CG	1:C:257:ASP:H	2.22	0.47
1:D:280:LEU:HB3	4:D:645:HOH:O	2.14	0.47
1:D:347:TYR:HA	4:D:764:HOH:O	2.13	0.47
1:C:67:PRO:HB2	1:C:82:ASP:HB3	1.96	0.47
1:C:211:ILE:CG2	1:C:372:MET:HE3	2.44	0.47
1:C:234:MET:HE3	4:C:879:HOH:O	2.13	0.47
1:D:256:ASP:HA	4:D:872:HOH:O	2.13	0.47
1:F:237:VAL:O	1:F:237:VAL:HG13	2.14	0.47
1:C:226:LYS:HG3	1:C:227:ASP:OD2	2.14	0.47
1:F:22:ASN:H	1:F:22:ASN:ND2	1.96	0.47
1:A:235:ASP:HA	4:A:830:HOH:O	2.15	0.47
1:A:275:LEU:O	1:A:283:LYS:HA	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:TRP:HB2	1:B:329:TRP:HB2	1.95	0.47
1:B:287:LEU:HB2	4:B:994:HOH:O	2.15	0.47
1:D:106:TRP:H	1:D:106:TRP:CD1	2.33	0.47
1:E:210:ARG:O	1:E:214:GLU:HG3	2.14	0.47
1:E:287:LEU:H	1:E:287:LEU:CD2	2.15	0.47
1:F:27:GLN:HE21	1:F:34:LYS:NZ	2.12	0.47
1:A:310:GLU:HG3	4:A:1084:HOH:O	2.14	0.47
1:C:420:LYS:NZ	4:C:1093:HOH:O	2.39	0.47
1:D:27:GLN:HE21	1:D:34:LYS:NZ	2.12	0.47
1:E:240:LEU:HD12	1:E:274:VAL:HG12	1.96	0.47
1:E:310:GLU:O	1:E:311:HIS:HB2	2.15	0.47
1:A:42:ASN:ND2	1:A:154:GLU:H	2.13	0.47
1:B:106:TRP:CD1	1:B:106:TRP:H	2.32	0.47
1:A:394:PRO:O	1:A:398:ARG:HG3	2.15	0.46
1:F:202:HIS:HA	1:F:328:TYR:O	2.14	0.46
1:F:222:ILE:HD12	1:F:241:GLY:HA2	1.97	0.46
1:A:172:ARG:HB3	4:A:620:HOH:O	2.15	0.46
1:A:337:PRO:HD2	1:A:341:ASP:OD1	2.15	0.46
1:D:275:LEU:O	1:D:283:LYS:HA	2.15	0.46
1:F:288:LYS:HB3	1:F:288:LYS:HE2	1.73	0.46
1:F:342:ARG:HG3	1:F:342:ARG:HH11	1.79	0.46
1:B:338:THR:C	1:B:342:ARG:NH1	2.74	0.46
1:C:288:LYS:HE2	1:C:288:LYS:HB3	1.68	0.46
4:D:529:HOH:O	1:E:420:LYS:HD3	2.16	0.46
1:E:317:TRP:HB2	1:E:329:TRP:HB2	1.97	0.46
1:A:234:MET:HE1	4:A:677:HOH:O	2.13	0.46
1:A:348:ARG:O	1:A:352:MET:HB3	2.15	0.46
1:B:339:ASP:HA	1:B:342:ARG:HH11	1.79	0.46
1:B:287:LEU:HD23	1:B:287:LEU:N	2.14	0.46
1:B:311:HIS:HE1	4:B:964:HOH:O	1.98	0.46
1:B:441:GLN:O	1:B:442:ILE:HB	2.16	0.46
1:C:393:SER:HB2	1:C:394:PRO:CD	2.46	0.46
1:D:290:ARG:NH2	4:D:726:HOH:O	2.49	0.46
1:F:237:VAL:CG1	1:F:286:GLY:C	2.88	0.46
1:F:238:LEU:HD23	4:F:935:HOH:O	2.15	0.46
1:A:22:ASN:HD22	1:A:22:ASN:N	1.94	0.46
1:E:109:GLY:O	1:E:123:VAL:HG23	2.15	0.46
1:E:264:GLN:NE2	1:E:393:SER:OG	2.45	0.46
1:F:208:ASN:ND2	1:F:210:ARG:H	2.13	0.46
1:B:279:GLU:O	1:B:280:LEU:C	2.58	0.46
1:D:27:GLN:HE21	1:D:34:LYS:HZ1	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:GLU:O	1:D:311:HIS:HB2	2.15	0.46
1:D:288:LYS:HE2	1:D:288:LYS:HB3	1.82	0.45
1:D:337:PRO:HG3	4:D:1045:HOH:O	2.16	0.45
1:E:37:ALA:N	1:E:210:ARG:NH2	2.65	0.45
1:E:208:ASN:ND2	1:E:210:ARG:H	2.15	0.45
1:F:330:GLU:OE1	1:F:358:LEU:HA	2.16	0.45
1:B:165:LEU:O	1:B:169:LEU:HD12	2.16	0.45
1:B:338:THR:C	1:B:342:ARG:HH12	2.24	0.45
1:B:121:THR:CG2	1:C:280:LEU:HD13	2.44	0.45
1:E:202:HIS:HA	1:E:328:TYR:O	2.16	0.45
1:B:31:GLN:HB3	1:B:32:PRO:HD3	1.98	0.45
1:B:335:VAL:HB	1:D:278:GLN:CD	2.41	0.45
1:C:282:LEU:HD22	4:C:877:HOH:O	2.16	0.45
1:E:20:ARG:HD2	1:E:22:ASN:HD21	1.82	0.45
1:C:275:LEU:N	1:C:275:LEU:HD12	2.32	0.45
1:D:287:LEU:HD23	1:D:287:LEU:N	2.17	0.45
1:D:337:PRO:HD2	1:D:341:ASP:OD1	2.17	0.45
1:A:100:LYS:HE3	4:A:865:HOH:O	2.16	0.45
1:A:106:TRP:CD1	1:A:106:TRP:H	2.35	0.45
1:C:42:ASN:ND2	1:C:154:GLU:H	2.13	0.45
1:D:226:LYS:HB2	1:D:226:LYS:HZ2	1.80	0.45
1:D:330:GLU:HG2	1:D:358:LEU:HD22	1.97	0.45
1:E:106:TRP:CD1	1:E:106:TRP:H	2.34	0.45
1:F:230:ILE:O	1:F:234:MET:HG2	2.16	0.45
1:A:73:VAL:HG13	1:A:100:LYS:HD2	1.98	0.45
1:A:317:TRP:HB2	1:A:329:TRP:HB2	1.99	0.45
1:B:209:TRP:CE2	1:B:210:ARG:HG3	2.51	0.45
1:E:194:ASP:O	1:E:195:ASN:HB2	2.16	0.45
1:B:73:VAL:CG1	1:B:100:LYS:HD2	2.46	0.45
1:B:280:LEU:N	1:B:280:LEU:HD12	2.31	0.45
1:C:73:VAL:HG11	1:C:100:LYS:O	2.16	0.45
1:A:226:LYS:HB2	1:A:226:LYS:HZ2	1.81	0.45
1:A:342:ARG:HG3	1:A:342:ARG:NH1	2.32	0.45
1:B:277:ASN:N	4:B:893:HOH:O	2.49	0.45
1:E:275:LEU:O	1:E:284:VAL:N	2.45	0.45
1:C:201:MET:CE	1:C:354:LYS:HE3	2.42	0.44
1:E:31:GLN:HB3	1:E:32:PRO:HD3	1.98	0.44
1:C:140:PRO:HD2	1:C:151:PHE:HB3	1.99	0.44
1:E:230:ILE:O	1:E:234:MET:HG2	2.18	0.44
1:C:194:ASP:O	1:C:195:ASN:HB2	2.16	0.44
1:F:393:SER:HB2	1:F:394:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:ARG:HG3	1:F:342:ARG:NH1	2.31	0.44
1:B:275:LEU:HG	4:B:1053:HOH:O	2.16	0.44
1:D:211:ILE:CG2	1:D:372:MET:HE3	2.44	0.44
1:E:208:ASN:HD21	1:E:210:ARG:HB2	1.80	0.44
1:E:393:SER:HB2	1:E:394:PRO:CD	2.47	0.44
1:A:287:LEU:N	1:A:287:LEU:CD2	2.55	0.44
1:D:20:ARG:HD2	1:D:22:ASN:ND2	2.33	0.44
1:C:73:VAL:HG13	1:C:100:LYS:HD2	2.00	0.44
1:E:287:LEU:HD23	1:E:287:LEU:N	2.16	0.44
1:A:223:LEU:CD1	4:A:1053:HOH:O	2.61	0.44
1:A:228:ASN:ND2	1:A:361:PHE:HA	2.33	0.44
1:D:375:PHE:CG	1:F:88:GLY:HA3	2.52	0.44
1:F:428:GLN:NE2	4:F:748:HOH:O	2.50	0.44
1:A:70:LEU:HA	1:A:78:PHE:O	2.18	0.44
1:B:282:LEU:CB	4:B:893:HOH:O	2.61	0.44
1:B:394:PRO:O	1:B:398:ARG:HG3	2.18	0.44
1:D:216:GLY:HA3	4:D:584:HOH:O	2.18	0.44
1:F:180:PHE:HZ	1:F:253:VAL:HG21	1.83	0.44
1:A:122:ILE:O	1:A:123:VAL:C	2.61	0.43
1:C:27:GLN:HE21	1:C:34:LYS:NZ	2.16	0.43
1:E:208:ASN:HD22	1:E:210:ARG:HB2	1.81	0.43
1:E:209:TRP:CE2	1:E:210:ARG:HG3	2.52	0.43
1:F:287:LEU:N	1:F:287:LEU:CD2	2.81	0.43
1:B:219:ASN:HB3	1:B:242:LEU:HB2	2.01	0.43
1:F:100:LYS:HE3	4:F:1071:HOH:O	2.18	0.43
1:F:264:GLN:NE2	1:F:393:SER:OG	2.51	0.43
1:D:208:ASN:HD21	1:D:210:ARG:NE	2.07	0.43
1:C:20:ARG:HD2	1:C:22:ASN:ND2	2.33	0.43
1:D:275:LEU:HD12	1:D:275:LEU:N	2.33	0.43
1:A:275:LEU:N	1:A:275:LEU:HD12	2.34	0.43
1:A:16:ILE:N	4:A:896:HOH:O	2.51	0.43
1:A:73:VAL:CG1	1:A:100:LYS:HD2	2.49	0.43
1:E:334:ARG:NH1	4:E:1055:HOH:O	2.46	0.43
1:B:339:ASP:N	1:B:342:ARG:HH12	2.17	0.43
1:D:224:VAL:HA	4:F:875:HOH:O	2.19	0.43
1:E:174:PRO:O	1:E:175:GLU:C	2.60	0.43
1:F:442:ILE:HB	4:F:686:HOH:O	2.19	0.43
1:A:209:TRP:CE2	1:A:210:ARG:HG3	2.54	0.43
1:D:274:VAL:HG21	1:F:124:ALA:O	2.19	0.42
1:D:393:SER:HB2	1:D:394:PRO:CD	2.49	0.42
1:E:94:LYS:NZ	4:E:995:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:LEU:N	1:E:275:LEU:HD12	2.34	0.42
1:F:442:ILE:HG22	4:F:741:HOH:O	2.19	0.42
1:B:42:ASN:ND2	1:B:154:GLU:H	2.14	0.42
1:F:420:LYS:NZ	4:F:709:HOH:O	2.48	0.42
1:A:230:ILE:O	1:A:234:MET:HG2	2.19	0.42
1:B:255:ASP:HB2	4:B:902:HOH:O	2.19	0.42
1:C:73:VAL:CG1	1:C:100:LYS:HD2	2.49	0.42
1:C:158:PRO:HG2	1:C:161:ASP:OD1	2.19	0.42
1:E:66:VAL:HA	1:E:67:PRO:HD3	1.88	0.42
1:F:106:TRP:CD1	1:F:106:TRP:H	2.37	0.42
1:B:208:ASN:ND2	1:B:210:ARG:HB2	2.35	0.42
1:E:95:PRO:CG	1:E:441:GLN:OE1	2.68	0.42
1:F:22:ASN:ND2	1:F:387:LEU:H	2.18	0.42
1:F:31:GLN:HB3	1:F:32:PRO:HD3	2.01	0.42
1:F:73:VAL:HG13	1:F:100:LYS:HD2	2.02	0.42
1:F:410:LYS:HB2	1:F:410:LYS:NZ	2.33	0.42
1:A:20:ARG:HD2	1:A:22:ASN:ND2	2.35	0.42
1:B:165:LEU:CG	1:B:169:LEU:HD11	2.47	0.42
1:F:194:ASP:O	1:F:195:ASN:HB2	2.19	0.42
1:F:249:CYS:HA	1:F:270:LYS:HB3	2.02	0.42
1:B:280:LEU:CD1	1:B:280:LEU:N	2.81	0.42
1:C:163:PRO:HG3	1:C:406:ARG:CZ	2.50	0.42
1:D:31:GLN:N	1:D:32:PRO:CD	2.83	0.42
1:E:73:VAL:HG11	1:E:100:LYS:O	2.18	0.42
1:F:73:VAL:HG11	1:F:100:LYS:O	2.20	0.42
1:F:394:PRO:O	1:F:398:ARG:HG3	2.20	0.42
1:A:403:ARG:HG3	4:A:648:HOH:O	2.19	0.42
1:C:106:TRP:CD1	1:C:106:TRP:H	2.36	0.42
1:B:280:LEU:C	4:B:665:HOH:O	2.63	0.42
1:D:290:ARG:HH21	1:D:309:GLU:HA	1.85	0.42
1:F:125:ASN:N	1:F:126:PRO:CD	2.82	0.42
1:B:240:LEU:HD12	1:B:274:VAL:HG12	2.02	0.42
1:C:31:GLN:HB3	1:C:32:PRO:HD3	2.01	0.42
1:B:427:LYS:HD2	1:C:206:PHE:CD1	2.55	0.42
1:A:240:LEU:HD12	1:A:274:VAL:HG12	2.01	0.41
1:C:274:VAL:C	1:C:275:LEU:HD12	2.45	0.41
1:C:400:LEU:HD12	1:C:400:LEU:C	2.45	0.41
1:D:180:PHE:HZ	1:D:253:VAL:HG21	1.85	0.41
1:D:194:ASP:O	1:D:195:ASN:HB2	2.19	0.41
1:E:73:VAL:HG13	1:E:100:LYS:HD2	2.02	0.41
1:E:340:GLU:O	1:E:340:GLU:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:219:ASN:HB3	1:E:242:LEU:HB2	2.02	0.41
1:E:238:LEU:HD23	4:E:671:HOH:O	2.20	0.41
1:F:140:PRO:HD2	1:F:151:PHE:HB3	2.02	0.41
1:F:275:LEU:N	1:F:275:LEU:HD12	2.35	0.41
1:B:349:TYR:HA	1:B:353:TYR:HB2	2.02	0.41
1:B:22:ASN:HB3	1:B:387:LEU:HD12	2.02	0.41
1:E:16:ILE:N	4:E:959:HOH:O	2.53	0.41
1:E:239:PRO:HA	4:E:795:HOH:O	2.21	0.41
1:E:441:GLN:O	1:E:442:ILE:HB	2.20	0.41
1:B:165:LEU:CD1	1:B:169:LEU:HD11	2.51	0.41
1:C:216:GLY:HA3	4:C:717:HOH:O	2.20	0.41
1:C:317:TRP:HB2	1:C:329:TRP:HB2	2.02	0.41
1:D:67:PRO:HB2	1:D:82:ASP:HB3	2.02	0.41
1:A:27:GLN:NE2	1:A:34:LYS:NZ	2.69	0.41
1:A:283:LYS:O	1:A:283:LYS:CG	2.65	0.41
1:B:66:VAL:HA	1:B:67:PRO:HD3	1.93	0.41
1:D:73:VAL:CG1	1:D:100:LYS:HD2	2.50	0.41
1:C:120:VAL:O	1:C:121:THR:HB	2.21	0.41
1:B:411:PRO:HD3	4:B:847:HOH:O	2.20	0.41
1:C:140:PRO:HA	4:C:636:HOH:O	2.21	0.41
1:C:180:PHE:HZ	1:C:253:VAL:HG21	1.85	0.41
1:E:226:LYS:HG3	1:E:227:ASP:OD2	2.20	0.41
1:F:209:TRP:CE2	1:F:210:ARG:HG3	2.56	0.41
1:A:70:LEU:N	1:A:70:LEU:HD12	2.36	0.41
1:B:311:HIS:CE1	1:D:276:GLU:OE1	2.73	0.41
1:B:393:SER:HB2	1:B:394:PRO:CD	2.50	0.41
1:E:31:GLN:N	1:E:32:PRO:CD	2.84	0.41
1:F:186:PRO:HB3	4:F:921:HOH:O	2.20	0.41
1:A:288:LYS:HG3	4:A:1067:HOH:O	2.21	0.41
1:D:256:ASP:CG	1:D:257:ASP:H	2.28	0.41
1:E:366:LEU:HD22	4:E:522:HOH:O	2.20	0.41
1:A:176:ARG:NH1	4:A:1134:HOH:O	2.45	0.40
1:B:203:ARG:NH1	4:B:1060:HOH:O	2.54	0.40
1:B:289:GLY:HA3	4:B:613:HOH:O	2.20	0.40
1:C:79:ALA:O	1:C:80:LEU:HD12	2.21	0.40
1:C:208:ASN:ND2	1:C:210:ARG:HB2	2.36	0.40
1:D:109:GLY:O	1:D:110:PHE:C	2.63	0.40
1:D:274:VAL:C	1:D:275:LEU:HD12	2.46	0.40
1:E:125:ASN:N	1:E:126:PRO:CD	2.84	0.40
1:E:180:PHE:HZ	1:E:253:VAL:HG21	1.86	0.40
1:A:243:LEU:CD1	1:A:274:VAL:HG22	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:PRO:O	1:B:175:GLU:C	2.64	0.40
1:B:275:LEU:N	1:B:275:LEU:HD12	2.36	0.40
1:D:420:LYS:HE2	4:D:1032:HOH:O	2.21	0.40
1:B:208:ASN:ND2	1:B:210:ARG:H	2.19	0.40
1:C:234:MET:O	1:C:236:TRP:N	2.54	0.40
1:D:95:PRO:CG	1:D:441:GLN:OE1	2.69	0.40
1:D:374:ASN:HD22	1:D:374:ASN:HA	1.66	0.40
1:B:339:ASP:CA	1:B:342:ARG:NH1	2.81	0.40
1:D:27:GLN:NE2	1:D:34:LYS:NZ	2.70	0.40
1:D:140:PRO:HD2	1:D:151:PHE:HB3	2.04	0.40
1:E:276:GLU:HB3	1:E:283:LYS:HB2	2.04	0.40
1:F:42:ASN:HD22	1:F:153:ARG:HA	1.87	0.40
1:F:219:ASN:HB3	1:F:242:LEU:HB2	2.02	0.40
1:D:441:GLN:O	1:D:442:ILE:HB	2.22	0.40
1:E:27:GLN:NE2	1:E:34:LYS:NZ	2.70	0.40
1:E:249:CYS:HA	1:E:270:LYS:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	425/446 (95%)	398 (94%)	25 (6%)	2 (0%)	24	14
1	B	425/446 (95%)	399 (94%)	23 (5%)	3 (1%)	18	8
1	C	425/446 (95%)	395 (93%)	26 (6%)	4 (1%)	14	5
1	D	425/446 (95%)	401 (94%)	22 (5%)	2 (0%)	24	14
1	E	425/446 (95%)	400 (94%)	23 (5%)	2 (0%)	24	14
1	F	425/446 (95%)	400 (94%)	23 (5%)	2 (0%)	24	14
All	All	2550/2676 (95%)	2393 (94%)	142 (6%)	15 (1%)	21	11

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	279	GLU
1	C	235	ASP
1	A	123	VAL
1	C	123	VAL
1	D	123	VAL
1	B	280	LEU
1	F	123	VAL
1	E	123	VAL
1	A	286	GLY
1	C	300	GLY
1	B	300	GLY
1	C	286	GLY
1	F	300	GLY
1	D	300	GLY
1	E	300	GLY

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	373/392 (95%)	356 (95%)	17 (5%)	24	12
1	B	373/392 (95%)	359 (96%)	14 (4%)	29	17
1	C	373/392 (95%)	354 (95%)	19 (5%)	21	9
1	D	373/392 (95%)	358 (96%)	15 (4%)	28	15
1	E	373/392 (95%)	355 (95%)	18 (5%)	23	11
1	F	373/392 (95%)	353 (95%)	20 (5%)	20	8
All	All	2238/2352 (95%)	2135 (95%)	103 (5%)	24	12

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	23	ASN

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Mol	Chain	Res	Type
1	A	25	LYS
1	A	94	LYS
1	A	160	GLU
1	A	223	LEU
1	A	226	LYS
1	A	235	ASP
1	A	247	ASP
1	A	255	ASP
1	A	283	LYS
1	A	287	LEU
1	A	290	ARG
1	A	340	GLU
1	A	352	MET
1	A	366	LEU
1	A	410	LYS
1	B	22	ASN
1	B	23	ASN
1	B	94	LYS
1	B	169	LEU
1	B	223	LEU
1	B	226	LYS
1	B	235	ASP
1	B	255	ASP
1	B	287	LEU
1	B	290	ARG
1	B	340	GLU
1	B	352	MET
1	B	366	LEU
1	B	410	LYS
1	C	22	ASN
1	C	23	ASN
1	C	25	LYS
1	C	94	LYS
1	C	160	GLU
1	C	176	ARG
1	C	223	LEU
1	C	226	LYS
1	C	229	THR
1	C	235	ASP
1	C	247	ASP
1	C	255	ASP
1	C	269	ASP

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Mol	Chain	Res	Type
1	C	287	LEU
1	C	290	ARG
1	C	340	GLU
1	C	352	MET
1	C	366	LEU
1	C	410	LYS
1	D	22	ASN
1	D	23	ASN
1	D	94	LYS
1	D	160	GLU
1	D	223	LEU
1	D	226	LYS
1	D	235	ASP
1	D	247	ASP
1	D	255	ASP
1	D	287	LEU
1	D	290	ARG
1	D	340	GLU
1	D	342	ARG
1	D	352	MET
1	D	366	LEU
1	E	22	ASN
1	E	23	ASN
1	E	25	LYS
1	E	53	LEU
1	E	94	LYS
1	E	203	ARG
1	E	223	LEU
1	E	226	LYS
1	E	235	ASP
1	E	247	ASP
1	E	255	ASP
1	E	269	ASP
1	E	287	LEU
1	E	340	GLU
1	E	342	ARG
1	E	352	MET
1	E	366	LEU
1	E	410	LYS
1	F	22	ASN
1	F	23	ASN
1	F	25	LYS

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Mol	Chain	Res	Type
1	F	94	LYS
1	F	160	GLU
1	F	203	ARG
1	F	223	LEU
1	F	226	LYS
1	F	229	THR
1	F	235	ASP
1	F	237	VAL
1	F	247	ASP
1	F	255	ASP
1	F	269	ASP
1	F	287	LEU
1	F	290	ARG
1	F	340	GLU
1	F	352	MET
1	F	366	LEU
1	F	410	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (114) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	23	ASN
1	A	27	GLN
1	A	42	ASN
1	A	43	HIS
1	A	62	GLN
1	A	142	HIS
1	A	179	GLN
1	A	195	ASN
1	A	199	HIS
1	A	208	ASN
1	A	228	ASN
1	A	232	HIS
1	A	264	GLN
1	A	277	ASN
1	A	311	HIS
1	A	346	GLN
1	A	374	ASN
1	A	428	GLN
1	A	441	GLN
1	B	22	ASN

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Mol	Chain	Res	Type
1	B	23	ASN
1	B	27	GLN
1	B	42	ASN
1	B	43	HIS
1	B	62	GLN
1	B	142	HIS
1	B	167	HIS
1	B	179	GLN
1	B	195	ASN
1	B	208	ASN
1	B	228	ASN
1	B	232	HIS
1	B	264	GLN
1	B	277	ASN
1	B	311	HIS
1	B	346	GLN
1	B	374	ASN
1	C	22	ASN
1	C	23	ASN
1	C	27	GLN
1	C	42	ASN
1	C	43	HIS
1	C	62	GLN
1	C	142	HIS
1	C	179	GLN
1	C	195	ASN
1	C	208	ASN
1	C	228	ASN
1	C	232	HIS
1	C	264	GLN
1	C	277	ASN
1	C	311	HIS
1	C	346	GLN
1	C	351	HIS
1	C	374	ASN
1	C	428	GLN
1	C	441	GLN
1	D	22	ASN
1	D	23	ASN
1	D	27	GLN
1	D	42	ASN
1	D	43	HIS

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Mol	Chain	Res	Type
1	D	62	GLN
1	D	142	HIS
1	D	179	GLN
1	D	195	ASN
1	D	208	ASN
1	D	228	ASN
1	D	232	HIS
1	D	264	GLN
1	D	277	ASN
1	D	311	HIS
1	D	346	GLN
1	D	374	ASN
1	D	428	GLN
1	E	22	ASN
1	E	23	ASN
1	E	27	GLN
1	E	42	ASN
1	E	43	HIS
1	E	62	GLN
1	E	142	HIS
1	E	179	GLN
1	E	195	ASN
1	E	208	ASN
1	E	228	ASN
1	E	232	HIS
1	E	264	GLN
1	E	277	ASN
1	E	311	HIS
1	E	346	GLN
1	E	374	ASN
1	E	428	GLN
1	F	22	ASN
1	F	23	ASN
1	F	27	GLN
1	F	42	ASN
1	F	43	HIS
1	F	62	GLN
1	F	142	HIS
1	F	167	HIS
1	F	179	GLN
1	F	195	ASN
1	F	208	ASN

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Mol	Chain	Res	Type
1	F	228	ASN
1	F	232	HIS
1	F	264	GLN
1	F	277	ASN
1	F	346	GLN
1	F	351	HIS
1	F	374	ASN
1	F	428	GLN
1	F	441	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FES	D	500	1	0,4,4	-	-	-		
3	FES	B	500	1	0,4,4	-	-	-		
3	FES	F	500	1	0,4,4	-	-	-		
3	FES	C	500	1	0,4,4	-	-	-		
3	FES	A	500	1	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FES	E	500	1	0,4,4	-	-	-		

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	FES	D	500	1	-	-	0/1/1/1
3	FES	B	500	1	-	-	0/1/1/1
3	FES	F	500	1	-	-	0/1/1/1
3	FES	C	500	1	-	-	0/1/1/1
3	FES	A	500	1	-	-	0/1/1/1
3	FES	E	500	1	-	-	0/1/1/1

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.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	500	FES	1	0
3	B	500	FES	1	0
3	F	500	FES	1	0
3	C	500	FES	1	0
3	A	500	FES	1	0
3	E	500	FES	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.