



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:45 PM UTC

PDB ID : 1Z02 / pdb_00001z02
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

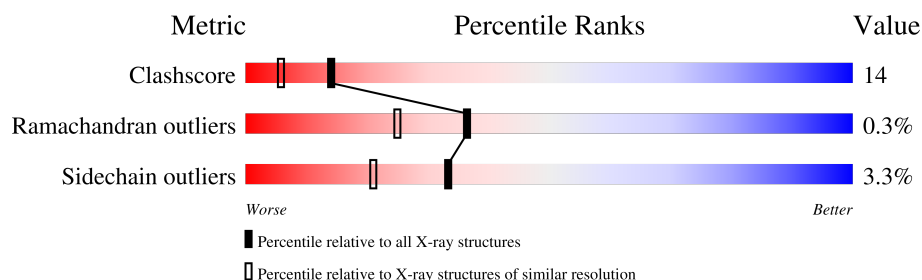
1 Overall quality at a glance

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	71% 22% . .
1	B	446	74% 19% . .
1	C	446	70% 23% . .
1	D	446	73% 21% . .
1	E	446	72% 21% . .
1	F	446	74% 20% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25843 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.

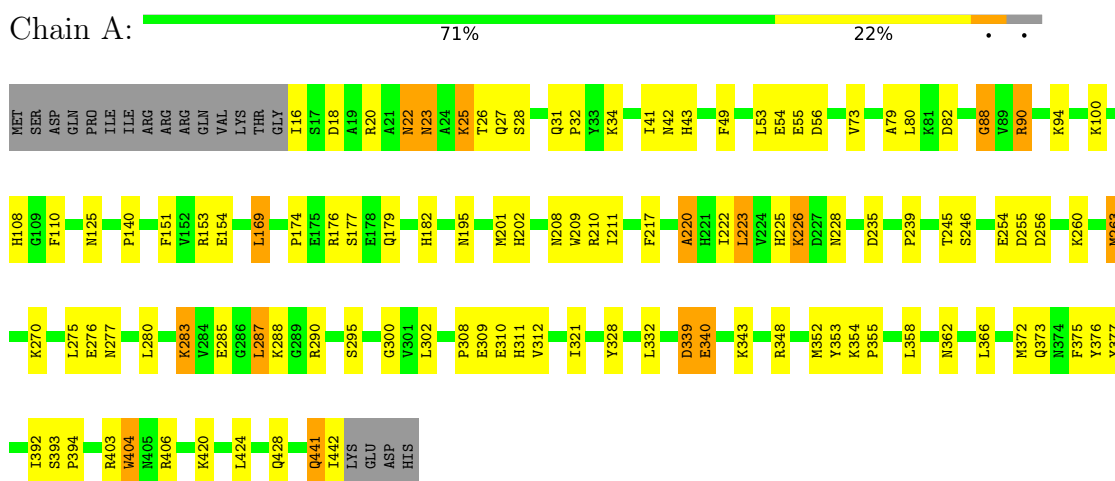
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	795	Total	O	0	0
			795	795		
4	B	890	Total	O	0	0
			890	890		
4	C	841	Total	O	0	0
			841	841		
4	D	817	Total	O	0	0
			817	817		
4	E	874	Total	O	0	0
			874	874		
4	F	872	Total	O	0	0
			872	872		

3 Residue-property plots

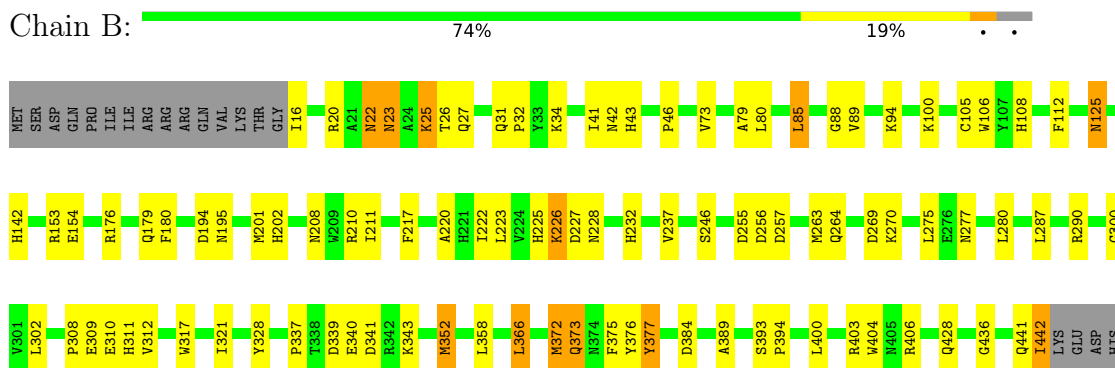
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

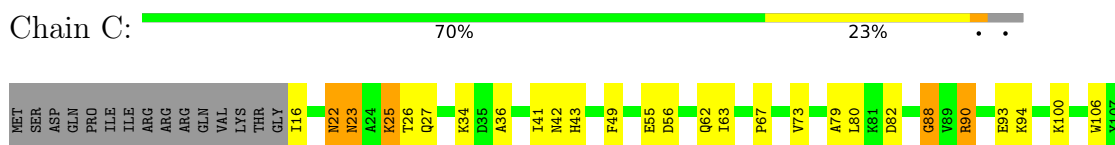
- Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

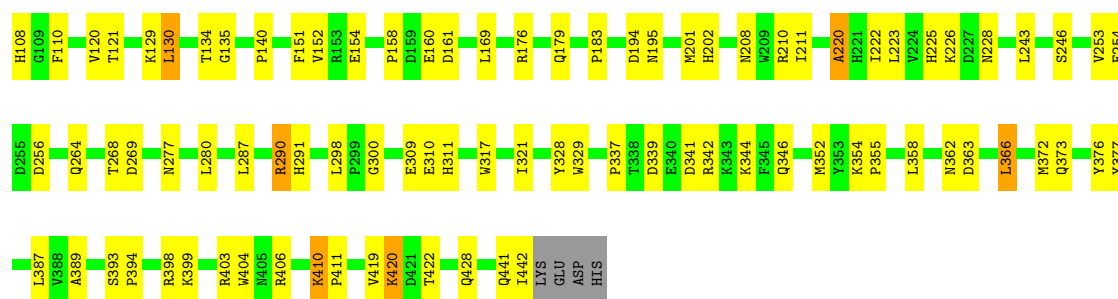


- Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component



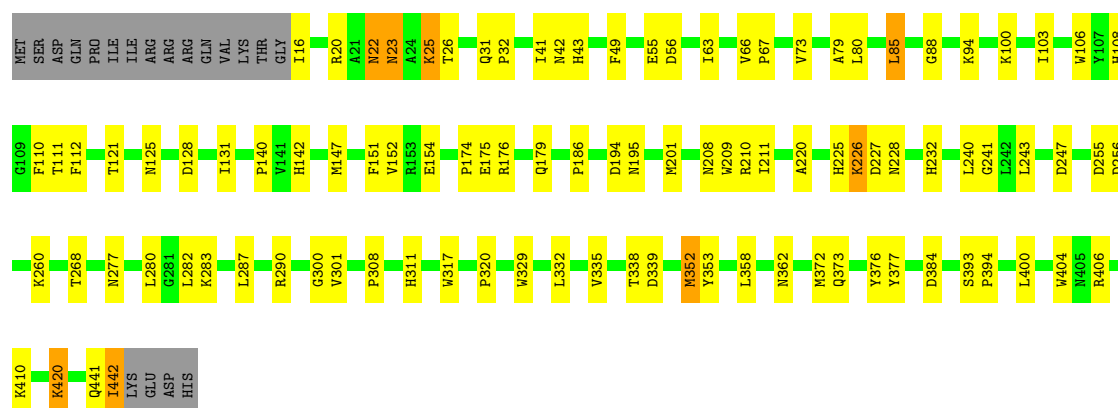
- Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component





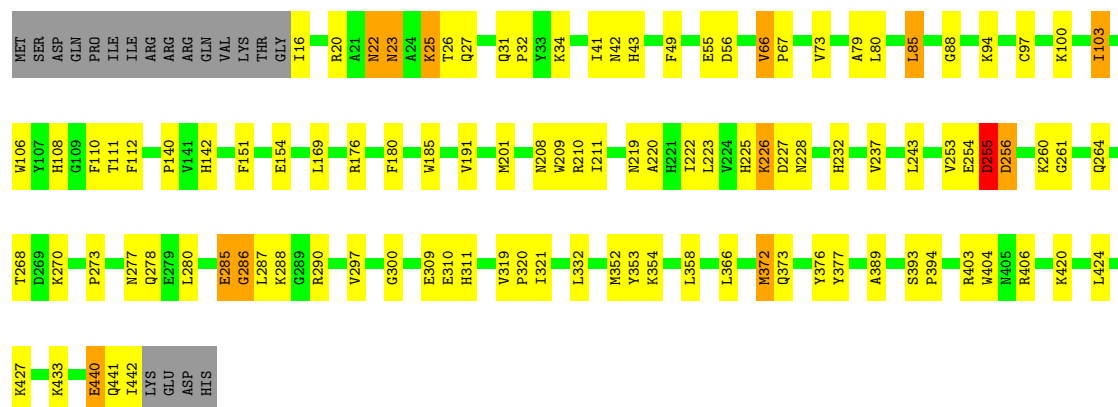
- Molecule 1: 2-oxo-1,2-dihydroquinoline 8-monooxygenase, oxygenase component

Chain D: 73% 21%



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

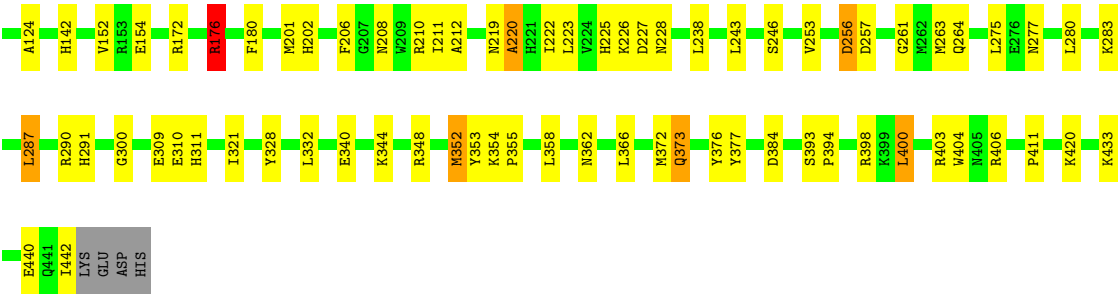
Chain E: 72% 21%



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

Chain F: 74% 20%





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	102.03Å 169.97Å 175.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80	Depositor
% Data completeness (in resolution range)	98.2 (20.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	25843	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	0.50	3/3560 (0.1%)	0.92	14/4853 (0.3%)
1	B	0.46	1/3560 (0.0%)	0.96	12/4853 (0.2%)
1	C	0.46	0/3560	0.93	13/4853 (0.3%)
1	D	0.46	0/3560	0.91	13/4853 (0.3%)
1	E	0.45	1/3560 (0.0%)	0.94	12/4853 (0.2%)
1	F	0.47	1/3560 (0.0%)	0.92	9/4853 (0.2%)
All	All	0.47	6/21360 (0.0%)	0.93	73/29118 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	MET	SD-CE	-9.00	1.57	1.79
1	F	176	ARG	CD-NE	6.83	1.55	1.46
1	A	287	LEU	CG-CD2	-6.44	1.31	1.52
1	A	223	LEU	CG-CD1	-5.56	1.34	1.52
1	B	372	MET	SD-CE	-5.41	1.66	1.79
1	E	372	MET	SD-CE	-5.28	1.66	1.79

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	ILE	N-CA-C	-8.79	104.00	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	321	ILE	N-CA-C	-8.55	103.44	111.48
1	B	256	ASP	N-CA-C	8.25	119.96	110.97
1	F	321	ILE	N-CA-C	-8.18	103.79	111.48
1	C	321	ILE	N-CA-C	-7.73	104.22	111.48
1	E	377	TYR	N-CA-C	7.45	119.04	111.07
1	B	88	GLY	N-CA-C	7.35	125.56	114.61
1	D	256	ASP	N-CA-C	7.32	119.95	111.02
1	E	373	GLN	N-CA-C	7.29	119.86	111.11
1	B	373	GLN	N-CA-C	7.07	119.59	111.11
1	B	376	TYR	N-CA-C	6.90	121.83	113.41
1	F	373	GLN	N-CA-C	6.72	119.47	111.33
1	F	377	TYR	N-CA-C	6.72	118.26	111.07
1	A	373	GLN	N-CA-C	6.67	119.40	111.33
1	A	321	ILE	N-CA-C	-6.60	105.28	111.48
1	E	404	TRP	N-CA-C	6.49	122.00	113.30
1	D	377	TYR	N-CA-C	6.49	118.90	111.11
1	E	220	ALA	N-CA-C	6.45	119.14	108.49
1	C	373	GLN	N-CA-C	6.42	119.10	111.33
1	C	404	TRP	N-CA-C	6.37	121.83	113.30
1	B	404	TRP	N-CA-C	6.25	121.68	113.30
1	A	376	TYR	N-CA-C	6.22	121.00	113.41
1	D	376	TYR	N-CA-C	6.22	120.99	113.41
1	F	220	ALA	N-CA-C	6.20	118.72	108.49
1	A	404	TRP	N-CA-C	6.13	121.51	113.30
1	C	376	TYR	N-CA-C	6.09	120.84	113.41
1	E	88	GLY	N-CA-C	6.07	123.65	114.61
1	C	420	LYS	N-CA-C	6.04	120.65	113.28
1	A	377	TYR	N-CA-C	5.98	117.47	111.07
1	A	209	TRP	N-CA-C	5.96	117.78	111.28
1	A	340	GLU	N-CA-C	-5.94	104.38	111.69
1	B	220	ALA	N-CA-C	5.94	118.99	107.71
1	C	268	THR	N-CA-C	-5.88	100.63	108.34
1	A	362	ASN	N-CA-C	5.87	119.71	112.54
1	C	377	TYR	N-CA-C	5.84	118.12	111.11
1	B	377	TYR	N-CA-C	5.84	118.11	111.11
1	A	88	GLY	N-CA-C	5.70	123.68	114.90
1	D	404	TRP	N-CA-C	5.66	120.88	113.30
1	B	436	GLY	N-CA-C	5.65	119.06	111.20
1	F	404	TRP	N-CA-C	5.65	120.87	113.30
1	F	384	ASP	N-CA-C	5.57	120.08	113.28
1	A	110	PHE	N-CA-C	-5.56	101.81	110.10
1	B	125	ASN	CA-C-N	5.53	125.20	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	ASN	C-N-CA	5.53	125.20	119.56
1	E	268	THR	N-CA-C	-5.52	101.08	108.86
1	F	376	TYR	N-CA-C	5.51	120.14	113.41
1	E	376	TYR	N-CA-C	5.47	120.23	113.50
1	D	420	LYS	N-CA-C	5.45	119.65	112.89
1	E	49	PHE	N-CA-C	-5.45	102.42	110.48
1	C	110	PHE	N-CA-C	-5.43	102.00	110.10
1	F	88	GLY	N-CA-C	5.42	123.11	115.30
1	D	268	THR	N-CA-C	-5.42	101.06	109.14
1	C	220	ALA	N-CA-C	5.41	118.56	107.37
1	A	256	ASP	CB-CA-C	-5.39	102.65	110.96
1	C	88	GLY	N-CA-C	5.36	123.02	115.30
1	B	384	ASP	N-CA-C	5.33	119.76	113.16
1	A	441	GLN	N-CA-C	5.31	118.65	110.42
1	D	384	ASP	N-CA-C	5.30	119.75	113.28
1	D	373	GLN	N-CA-C	5.30	120.11	111.37
1	C	36	ALA	N-CA-C	5.30	118.81	111.55
1	D	362	ASN	N-CA-C	5.30	119.00	112.54
1	C	49	PHE	N-CA-C	-5.28	103.42	110.55
1	E	185	TRP	N-CA-C	5.27	112.96	108.22
1	D	110	PHE	N-CA-C	-5.26	102.27	110.10
1	D	49	PHE	N-CA-C	-5.23	102.74	110.48
1	E	66	VAL	N-CA-C	5.21	113.02	107.76
1	C	362	ASN	N-CA-C	5.18	119.31	112.89
1	A	220	ALA	N-CA-C	5.17	117.52	107.71
1	D	88	GLY	N-CA-C	5.08	122.73	114.90
1	A	49	PHE	N-CA-C	-5.05	103.01	110.48
1	D	220	ALA	N-CA-C	5.02	118.17	107.67
1	E	110	PHE	N-CA-C	-5.02	102.62	110.10
1	F	362	ASN	N-CA-C	5.00	118.64	112.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	176	ARG	Sidechain

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	85	0
1	C	3454	0	3307	96	0
1	D	3454	0	3307	98	0
1	E	3454	0	3307	104	0
1	F	3454	0	3307	107	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	795	0	0	34	0
4	B	890	0	0	25	0
4	C	841	0	0	30	0
4	D	817	0	0	30	0
4	E	874	0	0	25	0
4	F	872	0	0	36	0
All	All	25843	0	19842	579	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 14.

All (579) 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:A:239:PRO:HA	4:A:836:HOH:O	1.55	1.07
1:C:442:ILE:HG22	1:C:442:ILE:O	1.57	1.02
1:E:211:ILE:HG23	1:E:372:MET:HE2	1.41	1.00
1:C:220:ALA:HB3	4:C:1156:HOH:O	1.63	0.98
1:D:22:ASN:H	1:D:22:ASN:HD22	1.12	0.98
1:F:211:ILE:HG23	1:F:372:MET:HE2	1.47	0.97
4:A:1170:HOH:O	1:C:130:LEU:HG	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:22:ASN:HD22	1:F:22:ASN:H	1.15	0.95
1:F:442:ILE:HG22	1:F:442:ILE:O	1.65	0.94
1:A:263:MET:HE3	1:A:295:SER:HB3	1.48	0.93
1:C:22:ASN:HD22	1:C:22:ASN:H	1.15	0.93
1:B:211:ILE:HG23	1:B:372:MET:HE2	1.51	0.90
1:D:140:PRO:HG2	1:D:151:PHE:HB3	1.54	0.89
1:B:22:ASN:H	1:B:22:ASN:HD22	1.15	0.89
1:A:22:ASN:HD22	1:A:22:ASN:H	1.21	0.89
1:E:22:ASN:HD22	1:E:22:ASN:H	1.15	0.88
1:A:287:LEU:HD22	4:A:1105:HOH:O	1.73	0.87
1:A:287:LEU:CD2	4:A:1105:HOH:O	2.22	0.87
1:C:344:LYS:HD2	4:C:1250:HOH:O	1.76	0.85
1:C:208:ASN:HD21	1:C:210:ARG:HE	1.22	0.85
1:E:191:VAL:HB	4:E:1331:HOH:O	1.77	0.84
1:F:226:LYS:HD3	4:F:1240:HOH:O	1.77	0.83
1:E:140:PRO:HG2	1:E:151:PHE:HB3	1.60	0.82
1:F:124:ALA:HB3	4:F:1344:HOH:O	1.80	0.82
1:D:208:ASN:HD21	1:D:210:ARG:HE	1.28	0.82
1:D:225:HIS:HD1	1:D:228:ASN:HD21	1.27	0.82
1:A:404:TRP:HH2	4:A:1253:HOH:O	1.63	0.81
1:C:208:ASN:ND2	1:C:210:ARG:HE	1.80	0.80
1:D:290:ARG:HD3	4:D:864:HOH:O	1.81	0.79
1:C:225:HIS:HD1	1:C:228:ASN:HD21	1.30	0.79
1:E:225:HIS:HD1	1:E:228:ASN:HD21	1.27	0.79
1:A:208:ASN:HD21	1:A:210:ARG:HE	1.32	0.78
1:B:225:HIS:HD1	1:B:228:ASN:HD21	1.29	0.78
1:F:23:ASN:ND2	1:F:26:THR:H	1.80	0.78
1:A:442:ILE:HD12	4:B:1254:HOH:O	1.85	0.77
1:F:225:HIS:HD1	1:F:228:ASN:HD21	1.31	0.76
1:C:287:LEU:H	1:C:287:LEU:HD23	1.51	0.76
1:D:352:MET:HG2	4:D:1238:HOH:O	1.85	0.76
1:D:226:LYS:HD3	4:F:1162:HOH:O	1.84	0.76
1:E:208:ASN:HD21	1:E:210:ARG:HE	1.32	0.76
1:B:287:LEU:HD23	1:B:287:LEU:H	1.50	0.76
1:F:256:ASP:HB3	4:F:837:HOH:O	1.85	0.76
1:A:23:ASN:ND2	1:A:26:THR:H	1.83	0.76
1:E:264:GLN:NE2	1:E:393:SER:OG	2.19	0.76
1:B:208:ASN:HD21	1:B:210:ARG:HE	1.30	0.76
1:A:263:MET:CE	1:A:295:SER:HB3	2.15	0.75
1:D:442:ILE:HD13	4:E:1141:HOH:O	1.85	0.75
1:C:176:ARG:HH11	1:C:179:GLN:HE22	1.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:ASN:HD22	1:C:280:LEU:H	1.34	0.75
1:A:441:GLN:O	1:A:442:ILE:HG12	1.88	0.74
1:D:176:ARG:HH11	1:D:179:GLN:HE22	1.35	0.74
1:A:428:GLN:HG2	4:A:1202:HOH:O	1.87	0.74
1:B:43:HIS:HE1	1:B:406:ARG:H	1.35	0.73
1:C:100:LYS:HE3	4:C:700:HOH:O	1.87	0.73
1:E:277:ASN:HD22	1:E:280:LEU:H	1.35	0.73
1:E:290:ARG:NH2	1:E:309:GLU:HA	2.03	0.73
1:F:208:ASN:HD21	1:F:210:ARG:HE	1.37	0.73
1:F:124:ALA:HB3	4:F:683:HOH:O	1.88	0.72
1:B:43:HIS:CE1	1:B:406:ARG:H	2.07	0.72
1:F:43:HIS:HE1	1:F:406:ARG:H	1.36	0.72
1:A:43:HIS:HE1	1:A:406:ARG:H	1.36	0.71
1:E:42:ASN:HD21	1:E:154:GLU:H	1.38	0.71
1:C:93:GLU:HA	4:C:1332:HOH:O	1.90	0.71
1:A:254:GLU:HG2	1:A:404:TRP:NE1	2.04	0.70
1:E:255:ASP:O	1:E:260:LYS:HE3	1.91	0.70
1:B:208:ASN:ND2	1:B:210:ARG:HE	1.90	0.70
1:D:208:ASN:ND2	1:D:210:ARG:HE	1.89	0.70
1:F:238:LEU:HD12	4:F:1154:HOH:O	1.91	0.70
1:B:42:ASN:HD21	1:B:154:GLU:H	1.39	0.69
1:C:16:ILE:N	4:C:505:HOH:O	2.25	0.69
1:F:433:LYS:HZ1	1:F:440:GLU:CD	1.99	0.69
1:D:85:LEU:HB3	4:D:1125:HOH:O	1.92	0.69
1:F:208:ASN:ND2	1:F:210:ARG:HE	1.90	0.69
1:D:410:LYS:HE3	4:D:804:HOH:O	1.92	0.69
1:B:108:HIS:HB2	3:B:500:FES:S1	2.33	0.68
1:B:393:SER:HB3	1:B:394:PRO:CD	2.24	0.68
1:C:254:GLU:OE2	1:C:403:ARG:NH1	2.27	0.68
1:E:100:LYS:HE2	4:E:933:HOH:O	1.93	0.68
1:E:372:MET:HE1	4:E:747:HOH:O	1.93	0.68
1:F:261:GLY:HA2	1:F:400:LEU:HD11	1.74	0.68
1:C:420:LYS:HE2	4:C:987:HOH:O	1.92	0.68
1:E:43:HIS:HE1	1:E:406:ARG:H	1.41	0.68
1:F:442:ILE:O	1:F:442:ILE:CG2	2.36	0.68
1:B:372:MET:HE1	4:B:746:HOH:O	1.93	0.68
1:C:287:LEU:HD21	4:C:1258:HOH:O	1.92	0.68
1:D:282:LEU:HD12	4:D:1296:HOH:O	1.92	0.68
1:A:43:HIS:CE1	1:A:406:ARG:H	2.11	0.68
1:B:264:GLN:NE2	1:B:393:SER:OG	2.27	0.68
1:D:241:GLY:HA3	1:F:124:ALA:HB1	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:HIS:CE1	1:F:406:ARG:H	2.11	0.68
1:D:277:ASN:HD22	1:D:280:LEU:H	1.41	0.67
1:C:403:ARG:HD2	4:C:1040:HOH:O	1.92	0.67
1:E:43:HIS:CE1	1:E:406:ARG:H	2.12	0.67
1:D:85:LEU:CD2	1:D:85:LEU:H	2.08	0.67
1:E:208:ASN:ND2	1:E:210:ARG:HE	1.92	0.67
1:E:22:ASN:HD22	1:E:22:ASN:N	1.91	0.67
1:F:20:ARG:HD2	1:F:22:ASN:HD21	1.60	0.67
1:F:108:HIS:O	4:F:1344:HOH:O	2.13	0.67
1:F:94:LYS:HD3	4:F:921:HOH:O	1.95	0.66
1:B:257:ASP:HB3	4:B:1171:HOH:O	1.94	0.66
1:C:42:ASN:HD21	1:C:154:GLU:H	1.43	0.66
1:C:43:HIS:HE1	1:C:406:ARG:H	1.41	0.66
1:D:23:ASN:ND2	1:D:26:THR:H	1.93	0.66
1:E:256:ASP:HB3	4:E:1023:HOH:O	1.94	0.66
1:B:287:LEU:HD23	4:B:898:HOH:O	1.95	0.66
1:C:419:VAL:HG13	1:C:422:THR:CG2	2.25	0.66
1:B:22:ASN:HD22	1:B:22:ASN:N	1.91	0.66
1:A:208:ASN:ND2	1:A:210:ARG:HE	1.92	0.66
1:A:343:LYS:HB3	4:A:956:HOH:O	1.96	0.66
1:E:108:HIS:HB2	3:E:500:FES:S1	2.35	0.66
1:C:43:HIS:CE1	1:C:406:ARG:H	2.13	0.65
1:E:211:ILE:CG2	1:E:372:MET:HE2	2.24	0.65
1:F:211:ILE:HG23	1:F:372:MET:CE	2.26	0.65
1:A:42:ASN:HD21	1:A:154:GLU:H	1.45	0.65
1:B:441:GLN:O	1:B:442:ILE:HB	1.96	0.65
1:C:441:GLN:HG2	4:C:1332:HOH:O	1.96	0.65
1:C:442:ILE:O	1:C:442:ILE:CG2	2.32	0.65
1:B:277:ASN:HD22	1:B:280:LEU:H	1.45	0.65
1:F:433:LYS:NZ	1:F:440:GLU:OE1	2.29	0.65
1:A:442:ILE:HG21	4:B:1259:HOH:O	1.97	0.65
1:C:419:VAL:HG12	4:C:577:HOH:O	1.96	0.65
1:B:442:ILE:HG23	4:B:986:HOH:O	1.97	0.64
1:C:211:ILE:HG23	1:C:372:MET:HE3	1.77	0.64
1:B:25:LYS:NZ	4:B:1118:HOH:O	2.29	0.64
1:D:441:GLN:O	1:D:442:ILE:HB	1.96	0.64
1:C:79:ALA:C	1:C:80:LEU:HD12	2.22	0.64
1:A:283:LYS:HE3	4:A:1099:HOH:O	1.98	0.64
1:F:20:ARG:HD2	1:F:22:ASN:ND2	2.13	0.64
1:C:108:HIS:HB2	3:C:500:FES:S1	2.38	0.64
1:C:23:ASN:ND2	1:C:26:THR:H	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:HIS:HD1	1:A:228:ASN:HD21	1.44	0.63
1:D:201:MET:HE2	1:D:358:LEU:HB3	1.81	0.63
1:A:20:ARG:HD2	1:A:22:ASN:HD21	1.64	0.62
1:B:16:ILE:N	4:B:810:HOH:O	2.32	0.62
1:C:22:ASN:HD22	1:C:22:ASN:N	1.93	0.62
1:D:290:ARG:NE	1:D:308:PRO:O	2.32	0.62
1:E:211:ILE:HG23	1:E:372:MET:CE	2.24	0.62
1:E:393:SER:HB3	1:E:394:PRO:CD	2.29	0.62
1:C:419:VAL:HG13	1:C:422:THR:HG23	1.81	0.62
1:D:372:MET:HE1	4:D:770:HOH:O	1.98	0.62
1:E:16:ILE:N	4:E:1189:HOH:O	2.31	0.62
1:B:22:ASN:H	1:B:22:ASN:ND2	1.95	0.62
1:C:410:LYS:HG3	4:C:1224:HOH:O	2.00	0.62
1:E:73:VAL:HG11	1:E:100:LYS:O	1.99	0.62
1:C:201:MET:HE3	1:C:358:LEU:HB3	1.80	0.61
1:A:22:ASN:HD22	1:A:22:ASN:N	1.94	0.61
1:C:73:VAL:HG11	1:C:100:LYS:O	2.00	0.61
1:D:42:ASN:HD21	1:D:154:GLU:H	1.48	0.61
1:A:23:ASN:C	1:A:23:ASN:HD22	2.09	0.61
1:A:82:ASP:OD1	1:A:90:ARG:HG2	2.00	0.61
1:E:85:LEU:CD2	1:E:85:LEU:H	2.13	0.61
1:F:372:MET:HE1	4:F:1172:HOH:O	2.00	0.61
1:A:16:ILE:N	4:A:789:HOH:O	2.33	0.61
1:E:176:ARG:CZ	4:E:685:HOH:O	2.48	0.61
1:A:23:ASN:HD22	1:A:26:THR:H	1.49	0.61
1:E:287:LEU:H	1:E:287:LEU:HD23	1.66	0.60
1:A:255:ASP:O	1:A:260:LYS:NZ	2.30	0.60
1:D:73:VAL:HG11	1:D:100:LYS:O	2.00	0.60
1:D:410:LYS:HD3	4:D:1216:HOH:O	1.99	0.60
1:F:108:HIS:HB2	3:F:500:FES:S1	2.41	0.60
1:E:79:ALA:C	1:E:80:LEU:HD12	2.27	0.60
1:C:23:ASN:C	1:C:23:ASN:HD22	2.09	0.60
1:C:222:ILE:HB	4:C:770:HOH:O	2.02	0.60
1:E:201:MET:HE2	1:E:358:LEU:HB3	1.83	0.60
1:D:23:ASN:HD22	1:D:23:ASN:C	2.09	0.59
1:D:85:LEU:H	1:D:85:LEU:HD23	1.66	0.59
1:F:277:ASN:HD22	1:F:280:LEU:H	1.47	0.59
1:F:23:ASN:C	1:F:23:ASN:HD22	2.08	0.59
1:A:100:LYS:HE3	4:A:1208:HOH:O	2.01	0.59
1:F:42:ASN:HD21	1:F:154:GLU:H	1.51	0.59
1:A:222:ILE:HB	4:A:723:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:MET:HE3	1:A:263:MET:HA	1.85	0.59
1:A:277:ASN:HD22	1:A:280:LEU:H	1.48	0.59
1:C:287:LEU:HD23	4:C:1212:HOH:O	2.01	0.59
1:B:73:VAL:HG11	1:B:100:LYS:O	2.01	0.59
1:A:393:SER:HB2	1:A:394:PRO:CD	2.33	0.59
1:D:79:ALA:C	1:D:80:LEU:HD12	2.28	0.58
1:D:290:ARG:NH2	4:D:864:HOH:O	2.35	0.58
1:E:94:LYS:HE2	4:E:1007:HOH:O	2.03	0.58
1:F:25:LYS:HG2	4:F:1027:HOH:O	2.03	0.58
1:E:433:LYS:NZ	1:E:440:GLU:OE1	2.33	0.58
1:F:79:ALA:C	1:F:80:LEU:HD12	2.28	0.58
1:F:211:ILE:CG2	1:F:372:MET:HE2	2.28	0.58
1:B:442:ILE:O	1:B:442:ILE:CG2	2.51	0.58
1:E:42:ASN:ND2	1:E:154:GLU:H	2.02	0.58
1:D:287:LEU:HD23	1:D:287:LEU:H	1.69	0.57
1:D:43:HIS:HE1	1:D:406:ARG:H	1.50	0.57
1:D:247:ASP:OD2	1:D:247:ASP:C	2.46	0.57
1:D:442:ILE:C	4:D:1192:HOH:O	2.47	0.57
1:F:172:ARG:O	1:F:176:ARG:HG2	2.04	0.57
1:B:176:ARG:NH1	4:B:998:HOH:O	2.34	0.57
1:D:43:HIS:CE1	1:D:406:ARG:H	2.22	0.57
1:B:23:ASN:C	1:B:23:ASN:HD22	2.12	0.57
1:B:79:ALA:C	1:B:80:LEU:HD12	2.30	0.57
1:D:20:ARG:HD2	1:D:22:ASN:HD21	1.69	0.57
1:F:393:SER:HB2	1:F:394:PRO:CD	2.35	0.57
1:F:433:LYS:HD2	4:F:929:HOH:O	2.03	0.57
1:C:393:SER:HB2	1:C:394:PRO:CD	2.35	0.57
1:B:311:HIS:HE1	4:B:1030:HOH:O	1.86	0.57
1:C:129:LYS:HD3	4:C:1306:HOH:O	2.03	0.57
1:B:23:ASN:ND2	1:B:26:THR:H	2.02	0.57
1:D:16:ILE:N	4:D:748:HOH:O	2.37	0.57
1:A:125:ASN:HD21	1:B:389:ALA:HB3	1.70	0.57
1:B:222:ILE:HB	4:B:788:HOH:O	2.05	0.57
1:F:373:GLN:HG3	4:F:1146:HOH:O	2.04	0.57
1:C:372:MET:HE1	4:C:702:HOH:O	2.04	0.56
1:D:442:ILE:O	1:D:442:ILE:CG2	2.52	0.56
1:F:201:MET:HE3	1:F:358:LEU:HB3	1.87	0.56
1:A:372:MET:HE1	4:A:659:HOH:O	2.05	0.56
1:E:442:ILE:O	1:E:442:ILE:HG22	2.04	0.56
1:F:22:ASN:HD22	1:F:22:ASN:N	1.90	0.56
1:A:404:TRP:CH2	4:A:1253:HOH:O	2.47	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:LYS:HD2	1:D:25:LYS:C	2.30	0.56
1:E:424:LEU:HG	4:F:1146:HOH:O	2.05	0.56
1:A:287:LEU:HD21	4:A:1105:HOH:O	1.96	0.56
1:C:82:ASP:OD1	1:C:90:ARG:HG2	2.06	0.56
1:D:283:LYS:NZ	4:D:816:HOH:O	2.34	0.56
1:D:400:LEU:HB2	4:D:871:HOH:O	2.05	0.56
1:A:226:LYS:HD3	4:C:1323:HOH:O	2.04	0.56
1:D:20:ARG:HD2	1:D:22:ASN:ND2	2.21	0.56
1:D:194:ASP:HB3	4:D:1153:HOH:O	2.06	0.56
1:D:240:LEU:O	1:F:124:ALA:HB2	2.05	0.56
1:A:73:VAL:HG11	1:A:100:LYS:O	2.06	0.56
4:D:1030:HOH:O	1:E:226:LYS:HD3	2.04	0.56
1:A:79:ALA:C	1:A:80:LEU:HD12	2.31	0.56
1:A:20:ARG:HD2	1:A:22:ASN:ND2	2.21	0.55
1:D:194:ASP:HB3	4:D:976:HOH:O	2.04	0.55
1:F:73:VAL:HG13	1:F:100:LYS:HD2	1.88	0.55
1:C:291:HIS:HD2	4:C:1006:HOH:O	1.88	0.55
1:B:85:LEU:CD2	1:B:85:LEU:H	2.18	0.55
1:B:142:HIS:HD2	4:B:565:HOH:O	1.88	0.55
1:A:220:ALA:O	1:C:108:HIS:HD2	1.89	0.55
1:D:22:ASN:HD22	1:D:22:ASN:N	1.90	0.55
1:A:285:GLU:HA	4:A:969:HOH:O	2.07	0.55
1:C:246:SER:HB3	4:C:825:HOH:O	2.07	0.55
1:D:85:LEU:HD23	1:D:85:LEU:N	2.22	0.54
1:D:311:HIS:CD2	4:D:783:HOH:O	2.60	0.54
1:F:400:LEU:HD23	1:F:400:LEU:C	2.32	0.54
1:F:100:LYS:HE3	4:F:616:HOH:O	2.06	0.54
1:A:246:SER:OG	1:A:270:LYS:HD3	2.08	0.54
1:D:393:SER:HB2	1:D:394:PRO:CD	2.38	0.54
1:F:94:LYS:HB3	1:F:106:TRP:CG	2.43	0.54
1:B:403:ARG:NH2	4:B:590:HOH:O	2.41	0.54
1:D:125:ASN:HD21	1:E:389:ALA:HB3	1.73	0.54
1:B:393:SER:HB3	1:B:394:PRO:HD3	1.89	0.54
1:E:225:HIS:HD1	1:E:228:ASN:ND2	2.00	0.54
1:F:403:ARG:NH2	4:F:782:HOH:O	2.40	0.54
1:E:23:ASN:ND2	1:E:26:THR:H	2.06	0.53
1:F:41:ILE:O	1:F:42:ASN:HB2	2.08	0.53
1:C:22:ASN:H	1:C:22:ASN:ND2	1.94	0.53
1:D:186:PRO:HB2	4:D:866:HOH:O	2.07	0.53
1:D:290:ARG:NH2	4:D:799:HOH:O	2.41	0.53
1:E:169:LEU:HD13	4:E:1331:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:LYS:C	1:F:25:LYS:HD2	2.33	0.53
1:E:442:ILE:O	1:E:442:ILE:CG2	2.55	0.53
1:B:223:LEU:HA	1:B:226:LYS:HG2	1.90	0.53
1:F:27:GLN:HE21	1:F:34:LYS:NZ	2.05	0.53
1:F:27:GLN:NE2	1:F:34:LYS:HZ1	2.06	0.53
1:B:225:HIS:HD1	1:B:228:ASN:ND2	2.04	0.53
1:C:211:ILE:CG2	1:C:372:MET:HE3	2.39	0.53
1:E:441:GLN:O	1:E:442:ILE:HB	2.08	0.53
1:B:311:HIS:HD2	4:B:747:HOH:O	1.90	0.53
1:D:41:ILE:O	1:D:42:ASN:HB2	2.09	0.53
1:E:237:VAL:HG11	4:E:1361:HOH:O	2.08	0.53
1:E:25:LYS:HD2	1:E:25:LYS:C	2.34	0.52
4:E:846:HOH:O	1:F:277:ASN:HB2	2.08	0.52
1:D:108:HIS:HB2	3:D:500:FES:S1	2.49	0.52
1:D:290:ARG:CZ	4:D:864:HOH:O	2.57	0.52
1:B:42:ASN:ND2	1:B:154:GLU:H	2.05	0.52
1:E:27:GLN:HE21	1:E:34:LYS:HZ1	1.56	0.52
1:C:277:ASN:ND2	1:C:280:LEU:H	2.06	0.52
1:F:16:ILE:N	4:F:874:HOH:O	2.42	0.52
1:F:124:ALA:HB1	4:F:684:HOH:O	2.10	0.52
1:A:25:LYS:C	1:A:25:LYS:HD2	2.34	0.52
1:A:90:ARG:HB2	4:A:592:HOH:O	2.08	0.52
1:A:182:HIS:HA	4:A:1171:HOH:O	2.09	0.52
1:B:366:LEU:HD11	4:B:564:HOH:O	2.08	0.52
1:E:23:ASN:C	1:E:23:ASN:HD22	2.16	0.52
1:B:290:ARG:NH2	1:B:309:GLU:HA	2.25	0.51
1:A:211:ILE:CG2	1:A:372:MET:HE3	2.41	0.51
1:B:201:MET:CE	1:B:358:LEU:HB3	2.41	0.51
1:B:377:TYR:HB3	4:B:889:HOH:O	2.09	0.51
1:F:420:LYS:NZ	4:F:580:HOH:O	2.36	0.51
1:A:125:ASN:HB2	4:B:598:HOH:O	2.10	0.51
1:B:27:GLN:HE21	1:B:34:LYS:NZ	2.07	0.51
1:E:94:LYS:HD3	4:F:907:HOH:O	2.10	0.51
1:B:41:ILE:O	1:B:42:ASN:HB2	2.11	0.51
1:A:339:ASP:O	1:A:343:LYS:HG3	2.11	0.51
1:D:142:HIS:HD2	4:D:724:HOH:O	1.94	0.51
1:F:340:GLU:O	1:F:344:LYS:HG3	2.10	0.51
1:A:283:LYS:CE	4:A:1099:HOH:O	2.57	0.51
1:B:85:LEU:HD22	1:B:112:PHE:CE2	2.46	0.51
1:D:194:ASP:O	1:D:195:ASN:HB2	2.11	0.51
1:A:403:ARG:NH1	4:A:935:HOH:O	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ASP:HB2	4:B:769:HOH:O	2.10	0.50
1:D:225:HIS:HD1	1:D:228:ASN:ND2	2.03	0.50
1:F:225:HIS:HD1	1:F:228:ASN:ND2	2.05	0.50
1:E:20:ARG:HD2	1:E:22:ASN:ND2	2.26	0.50
1:F:290:ARG:NH1	1:F:309:GLU:HA	2.27	0.50
1:C:25:LYS:C	1:C:25:LYS:HD2	2.37	0.50
1:A:55:GLU:O	1:A:56:ASP:HB2	2.11	0.50
1:D:42:ASN:ND2	1:D:154:GLU:H	2.10	0.50
1:A:18:ASP:HB3	4:A:1142:HOH:O	2.12	0.49
1:C:41:ILE:O	1:C:42:ASN:HB2	2.12	0.49
1:D:121:THR:HA	1:D:131:ILE:HD13	1.93	0.49
1:A:22:ASN:H	1:A:22:ASN:ND2	1.99	0.49
1:B:27:GLN:HE21	1:B:34:LYS:HZ1	1.59	0.49
1:D:94:LYS:HB3	1:D:106:TRP:CG	2.47	0.49
1:F:23:ASN:HD22	1:F:26:THR:H	1.56	0.49
1:F:27:GLN:HE21	1:F:34:LYS:HZ1	1.61	0.49
1:F:124:ALA:CB	4:F:1344:HOH:O	2.49	0.49
1:A:108:HIS:HB2	3:A:500:FES:S1	2.52	0.49
1:D:201:MET:CE	1:D:358:LEU:HB3	2.42	0.49
1:E:85:LEU:H	1:E:85:LEU:HD23	1.76	0.49
1:E:254:GLU:O	1:E:255:ASP:O	2.30	0.49
1:F:287:LEU:HD23	1:F:287:LEU:O	2.12	0.49
1:F:202:HIS:HA	1:F:328:TYR:O	2.13	0.49
1:D:140:PRO:HG2	1:D:151:PHE:CB	2.36	0.49
1:B:442:ILE:O	1:B:442:ILE:HG22	2.10	0.49
1:C:342:ARG:HD3	4:C:889:HOH:O	2.12	0.49
1:E:311:HIS:HD2	4:E:649:HOH:O	1.95	0.49
1:F:261:GLY:CA	1:F:400:LEU:HD11	2.43	0.49
1:D:176:ARG:NH1	1:D:179:GLN:HE22	2.06	0.49
1:D:211:ILE:HG23	1:D:372:MET:HE3	1.95	0.49
1:D:227:ASP:HA	1:D:232:HIS:HE1	1.78	0.49
1:A:393:SER:HB2	1:A:394:PRO:HD3	1.95	0.48
1:B:428:GLN:NE2	4:B:1186:HOH:O	2.43	0.48
1:D:100:LYS:HE3	4:D:761:HOH:O	2.12	0.48
1:D:186:PRO:HG2	4:D:520:HOH:O	2.12	0.48
1:F:227:ASP:HB2	4:F:1290:HOH:O	2.13	0.48
1:F:311:HIS:HD2	4:F:739:HOH:O	1.97	0.48
1:E:243:LEU:HD12	4:E:1123:HOH:O	2.12	0.48
1:E:393:SER:HB3	1:E:394:PRO:HD3	1.93	0.48
1:E:41:ILE:O	1:E:42:ASN:HB2	2.14	0.48
1:B:227:ASP:HA	1:B:232:HIS:HE1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:GLN:NE2	4:C:795:HOH:O	2.40	0.48
1:E:427:LYS:HD2	1:F:206:PHE:CD1	2.49	0.48
1:C:42:ASN:ND2	1:C:154:GLU:H	2.08	0.48
1:D:420:LYS:NZ	4:D:945:HOH:O	2.34	0.48
1:E:256:ASP:N	1:E:256:ASP:OD1	2.47	0.48
1:C:253:VAL:HG13	4:C:956:HOH:O	2.13	0.48
1:D:211:ILE:CG2	1:D:372:MET:HE3	2.43	0.48
1:F:257:ASP:HB3	4:F:1305:HOH:O	2.14	0.48
1:A:41:ILE:O	1:A:42:ASN:HB2	2.13	0.47
4:D:1041:HOH:O	1:E:277:ASN:HB2	2.14	0.47
1:B:20:ARG:HD2	1:B:22:ASN:HD21	1.78	0.47
1:F:433:LYS:CD	4:F:929:HOH:O	2.60	0.47
1:A:195:ASN:ND2	4:A:1238:HOH:O	2.45	0.47
4:A:1057:HOH:O	1:B:277:ASN:HB2	2.15	0.47
1:E:20:ARG:HD2	1:E:22:ASN:HD21	1.80	0.47
1:E:27:GLN:HE21	1:E:34:LYS:NZ	2.12	0.47
1:E:270:LYS:HE2	4:E:1077:HOH:O	2.15	0.47
1:F:212:ALA:HB2	4:F:898:HOH:O	2.12	0.47
1:B:85:LEU:HD22	1:B:112:PHE:CZ	2.49	0.47
1:C:222:ILE:HG21	4:C:920:HOH:O	2.13	0.47
1:C:411:PRO:HD3	4:C:719:HOH:O	2.12	0.47
1:D:63:ILE:HG21	1:D:152:VAL:HG21	1.97	0.47
1:B:176:ARG:NH2	1:B:179:GLN:HE22	2.12	0.47
1:B:31:GLN:N	1:B:32:PRO:CD	2.77	0.47
1:F:246:SER:HB3	4:F:867:HOH:O	2.15	0.47
1:A:276:GLU:HG3	4:A:1280:HOH:O	2.15	0.47
1:C:290:ARG:NH1	1:C:309:GLU:HA	2.29	0.47
1:E:290:ARG:NH2	4:E:1086:HOH:O	2.31	0.47
1:A:201:MET:HE2	1:A:358:LEU:HB3	1.97	0.47
1:D:290:ARG:CD	4:D:864:HOH:O	2.52	0.47
1:E:142:HIS:HD2	4:E:723:HOH:O	1.97	0.47
1:A:94:LYS:NZ	4:A:1190:HOH:O	2.39	0.46
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.56	0.46
1:A:442:ILE:C	4:A:1270:HOH:O	2.58	0.46
1:C:419:VAL:CG1	1:C:422:THR:CG2	2.93	0.46
1:D:335:VAL:HG21	4:D:798:HOH:O	2.15	0.46
1:F:31:GLN:HB3	1:F:32:PRO:HD3	1.97	0.46
1:F:23:ASN:HD21	1:F:26:THR:H	1.61	0.46
1:A:225:HIS:HD1	1:A:228:ASN:ND2	2.12	0.46
1:A:424:LEU:HG	4:B:1220:HOH:O	2.15	0.46
1:C:399:LYS:O	1:C:403:ARG:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LEU:HD23	4:A:969:HOH:O	2.16	0.46
1:B:201:MET:HE2	1:B:358:LEU:HB3	1.98	0.46
1:D:22:ASN:H	1:D:22:ASN:ND2	1.93	0.46
1:E:219:ASN:HD21	1:E:264:GLN:HE22	1.64	0.46
1:B:194:ASP:O	1:B:195:ASN:HB2	2.15	0.46
1:B:339:ASP:OD1	1:B:343:LYS:HE3	2.16	0.46
1:E:285:GLU:O	1:E:286:GLY:C	2.58	0.46
1:E:290:ARG:HH21	1:E:309:GLU:HA	1.79	0.46
1:A:420:LYS:NZ	4:A:850:HOH:O	2.44	0.45
1:E:278:GLN:NE2	4:E:677:HOH:O	2.49	0.45
1:C:337:PRO:HD2	1:C:341:ASP:OD1	2.16	0.45
1:E:227:ASP:HA	1:E:232:HIS:HE1	1.82	0.45
1:E:222:ILE:HB	4:E:610:HOH:O	2.16	0.45
1:F:75:GLY:HA2	4:F:1019:HOH:O	2.16	0.45
1:F:238:LEU:CD1	4:F:1154:HOH:O	2.58	0.45
1:A:16:ILE:HG13	4:A:1292:HOH:O	2.15	0.45
1:C:264:GLN:NE2	1:C:393:SER:OG	2.49	0.45
1:F:411:PRO:HD3	4:F:849:HOH:O	2.16	0.45
1:C:311:HIS:HD2	4:C:699:HOH:O	1.98	0.45
1:D:85:LEU:CD2	1:D:85:LEU:N	2.73	0.45
1:E:97:CYS:SG	1:E:103:ILE:HG12	2.57	0.45
1:F:73:VAL:HG11	1:F:100:LYS:O	2.16	0.45
1:F:291:HIS:HD2	4:F:1257:HOH:O	1.98	0.45
1:F:332:LEU:CD1	1:F:353:TYR:HB3	2.47	0.45
1:D:25:LYS:C	1:D:25:LYS:CD	2.90	0.45
1:B:20:ARG:HD2	1:B:22:ASN:ND2	2.32	0.45
1:F:180:PHE:HZ	1:F:253:VAL:HG21	1.82	0.45
1:A:217:PHE:HB3	1:A:302:LEU:HD13	1.98	0.45
1:A:442:ILE:HD13	4:B:1259:HOH:O	2.16	0.45
1:B:340:GLU:HG3	4:B:1197:HOH:O	2.17	0.45
1:B:400:LEU:C	1:B:400:LEU:HD12	2.42	0.45
1:C:22:ASN:ND2	1:C:387:LEU:H	2.15	0.45
1:E:201:MET:CE	1:E:358:LEU:HB3	2.46	0.45
1:F:222:ILE:HB	4:F:695:HOH:O	2.16	0.45
1:F:287:LEU:HD23	1:F:287:LEU:C	2.42	0.45
1:D:176:ARG:HH11	1:D:179:GLN:NE2	2.09	0.45
1:F:22:ASN:ND2	1:F:22:ASN:N	2.61	0.45
1:F:42:ASN:ND2	1:F:154:GLU:H	2.13	0.45
1:A:25:LYS:HD2	1:A:25:LYS:O	2.17	0.44
1:A:27:GLN:HE21	1:A:34:LYS:HZ1	1.66	0.44
1:A:290:ARG:HD2	4:A:515:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:LEU:H	1:B:85:LEU:HD23	1.82	0.44
1:A:27:GLN:HE21	1:A:34:LYS:NZ	2.16	0.44
1:C:202:HIS:HA	1:C:328:TYR:O	2.18	0.44
1:E:85:LEU:HD23	1:E:85:LEU:N	2.32	0.44
1:E:277:ASN:ND2	1:E:280:LEU:H	2.11	0.44
1:F:400:LEU:C	1:F:400:LEU:CD2	2.90	0.44
1:A:343:LYS:HG2	4:A:1025:HOH:O	2.18	0.44
1:C:55:GLU:O	1:C:56:ASP:HB2	2.18	0.44
1:F:180:PHE:CD2	1:F:263:MET:HG2	2.52	0.44
1:F:433:LYS:NZ	4:F:929:HOH:O	2.25	0.44
1:A:348:ARG:NH2	4:A:631:HOH:O	2.50	0.44
1:B:85:LEU:CD2	1:B:112:PHE:CE2	3.00	0.44
1:C:94:LYS:HB3	1:C:106:TRP:CG	2.53	0.44
1:C:222:ILE:HG23	1:C:223:LEU:N	2.32	0.44
1:D:55:GLU:O	1:D:56:ASP:HB2	2.17	0.44
1:A:176:ARG:HH21	1:A:179:GLN:HE22	1.65	0.44
1:C:317:TRP:HB2	1:C:329:TRP:HB2	2.00	0.44
1:F:256:ASP:HB2	4:F:750:HOH:O	2.16	0.44
1:D:66:VAL:HA	1:D:67:PRO:HD3	1.86	0.44
1:D:442:ILE:O	1:D:442:ILE:HG22	2.16	0.44
1:E:31:GLN:HB3	1:E:32:PRO:HD3	1.99	0.44
1:E:80:LEU:HD12	1:E:80:LEU:N	2.32	0.44
1:F:393:SER:HB2	1:F:394:PRO:HD3	2.00	0.44
1:C:183:PRO:HB3	4:C:941:HOH:O	2.17	0.44
1:E:180:PHE:HZ	1:E:253:VAL:HG21	1.82	0.44
1:E:209:TRP:CG	1:E:320:PRO:HG3	2.52	0.44
1:F:310:GLU:O	1:F:311:HIS:HB2	2.17	0.44
1:A:42:ASN:HD22	1:A:153:ARG:HA	1.83	0.44
1:A:332:LEU:CD1	1:A:353:TYR:HB3	2.47	0.44
1:E:287:LEU:HD23	1:E:287:LEU:N	2.33	0.44
1:E:332:LEU:CD1	1:E:353:TYR:HB3	2.48	0.44
1:E:354:LYS:HD3	4:E:910:HOH:O	2.18	0.43
1:D:352:MET:HE3	1:D:353:TYR:CE1	2.53	0.43
1:E:273:PRO:HD3	4:E:1324:HOH:O	2.17	0.43
1:E:287:LEU:H	1:E:287:LEU:CD2	2.29	0.43
1:B:42:ASN:HD22	1:B:153:ARG:HA	1.82	0.43
1:A:140:PRO:HD2	1:A:151:PHE:HB3	2.00	0.43
1:F:348:ARG:O	1:F:352:MET:HB3	2.19	0.43
1:A:54:GLU:HB3	4:A:1024:HOH:O	2.19	0.43
1:B:226:LYS:HB2	1:B:226:LYS:NZ	2.33	0.43
1:C:27:GLN:HE21	1:C:34:LYS:NZ	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:CG2	1:B:105:CYS:SG	3.06	0.43
1:B:337:PRO:HD2	1:B:341:ASP:OD1	2.18	0.43
1:C:67:PRO:HB2	1:C:82:ASP:HB3	2.01	0.43
1:C:82:ASP:CG	1:C:90:ARG:HG2	2.43	0.43
1:E:31:GLN:N	1:E:32:PRO:CD	2.81	0.43
1:F:73:VAL:CG1	1:F:100:LYS:HD2	2.47	0.43
1:C:158:PRO:HG2	1:C:161:ASP:CG	2.43	0.43
1:E:85:LEU:CD2	1:E:112:PHE:CZ	3.01	0.43
1:F:208:ASN:HD21	1:F:210:ARG:NE	2.12	0.43
1:C:27:GLN:NE2	1:C:34:LYS:HZ1	2.17	0.43
1:D:174:PRO:O	1:D:175:GLU:C	2.61	0.43
1:D:209:TRP:CG	1:D:320:PRO:HG3	2.54	0.43
1:E:55:GLU:O	1:E:56:ASP:HB2	2.17	0.43
1:F:22:ASN:H	1:F:22:ASN:ND2	1.94	0.43
1:F:219:ASN:HD21	1:F:264:GLN:HE22	1.66	0.43
1:A:31:GLN:N	1:A:32:PRO:CD	2.82	0.43
1:A:42:ASN:ND2	1:A:154:GLU:H	2.13	0.43
1:D:106:TRP:H	1:D:106:TRP:CD1	2.36	0.43
1:D:332:LEU:CD1	1:D:353:TYR:HB3	2.49	0.43
1:E:16:ILE:HG12	4:E:1138:HOH:O	2.19	0.43
1:E:223:LEU:HG	4:E:672:HOH:O	2.19	0.43
1:C:120:VAL:O	1:C:121:THR:HB	2.18	0.43
1:B:106:TRP:CD1	1:B:106:TRP:H	2.37	0.42
1:B:180:PHE:CD2	1:B:263:MET:HG2	2.54	0.42
1:D:31:GLN:N	1:D:32:PRO:CD	2.83	0.42
1:E:85:LEU:H	1:E:85:LEU:HD22	1.84	0.42
1:C:393:SER:HB2	1:C:394:PRO:HD3	2.01	0.42
1:E:66:VAL:HA	1:E:67:PRO:HD3	1.88	0.42
1:E:310:GLU:O	1:E:311:HIS:HB2	2.18	0.42
1:C:310:GLU:O	1:C:311:HIS:HB2	2.19	0.42
1:C:428:GLN:HB3	4:C:795:HOH:O	2.19	0.42
1:E:219:ASN:HD21	1:E:264:GLN:NE2	2.17	0.42
1:F:373:GLN:NE2	4:F:898:HOH:O	2.52	0.42
1:C:346:GLN:HB2	4:C:1320:HOH:O	2.18	0.42
1:A:245:THR:HG22	4:A:939:HOH:O	2.18	0.42
1:D:85:LEU:CD2	1:D:112:PHE:CE2	3.03	0.42
1:D:128:ASP:HA	4:D:853:HOH:O	2.20	0.42
1:E:22:ASN:H	1:E:22:ASN:ND2	1.95	0.42
1:F:142:HIS:HD2	4:F:656:HOH:O	2.02	0.42
1:A:174:PRO:HA	1:A:177:SER:OG	2.20	0.42
1:C:63:ILE:HG21	1:C:152:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:LEU:CD2	1:D:112:PHE:CZ	3.03	0.42
1:C:160:GLU:HG3	1:C:161:ASP:OD2	2.20	0.42
1:D:280:LEU:HD12	4:D:1296:HOH:O	2.20	0.42
1:F:222:ILE:HG23	1:F:223:LEU:N	2.34	0.42
1:A:82:ASP:CG	1:A:90:ARG:HG2	2.45	0.42
1:A:308:PRO:HD2	1:A:312:VAL:HG11	2.02	0.42
1:A:375:PHE:CG	1:C:88:GLY:HA3	2.54	0.42
1:C:363:ASP:O	1:C:366:LEU:HB2	2.20	0.42
1:E:261:GLY:HA3	1:E:297:VAL:HG12	2.00	0.42
1:F:106:TRP:CD1	1:F:106:TRP:H	2.37	0.42
1:C:354:LYS:HB3	1:C:355:PRO:CD	2.50	0.42
1:D:280:LEU:HD21	1:F:111:THR:HG21	2.02	0.42
1:C:339:ASP:HA	1:C:342:ARG:NH1	2.34	0.41
1:C:420:LYS:NZ	4:C:871:HOH:O	2.46	0.41
1:E:85:LEU:HD22	1:E:112:PHE:CZ	2.55	0.41
1:E:420:LYS:HE2	4:E:950:HOH:O	2.19	0.41
1:F:31:GLN:N	1:F:32:PRO:CD	2.83	0.41
1:C:106:TRP:CD1	1:C:106:TRP:H	2.37	0.41
1:E:106:TRP:H	1:E:106:TRP:CD1	2.36	0.41
1:E:287:LEU:HD12	4:E:1115:HOH:O	2.19	0.41
1:E:319:VAL:HA	1:E:320:PRO:HD3	1.96	0.41
1:A:290:ARG:NH1	1:A:309:GLU:HA	2.36	0.41
1:B:16:ILE:N	4:B:607:HOH:O	2.53	0.41
1:B:85:LEU:CD2	1:B:112:PHE:CZ	3.03	0.41
1:A:28:SER:HA	4:A:952:HOH:O	2.20	0.41
1:C:140:PRO:HD2	1:C:151:PHE:HB3	2.02	0.41
1:D:23:ASN:HD22	1:D:26:THR:H	1.65	0.41
1:D:142:HIS:HE1	4:D:901:HOH:O	2.03	0.41
1:F:275:LEU:N	1:F:275:LEU:HD12	2.36	0.41
1:A:254:GLU:HG2	1:A:404:TRP:CE2	2.55	0.41
1:B:125:ASN:HD21	1:C:389:ALA:HB3	1.86	0.41
1:C:62:GLN:NE2	4:C:851:HOH:O	2.53	0.41
1:D:301:VAL:HG22	1:D:317:TRP:CD1	2.56	0.41
1:E:85:LEU:HD22	1:E:112:PHE:CE2	2.55	0.41
1:E:237:VAL:HB	1:E:288:LYS:H	1.85	0.41
1:E:254:GLU:C	1:E:255:ASP:O	2.64	0.41
1:A:88:GLY:HA3	1:B:375:PHE:CG	2.56	0.41
1:B:373:GLN:HG3	4:B:1220:HOH:O	2.20	0.41
1:E:85:LEU:CD2	1:E:112:PHE:CE2	3.03	0.41
1:E:403:ARG:NH2	4:E:581:HOH:O	2.53	0.41
1:F:442:ILE:HG21	1:F:442:ILE:HD13	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ASP:O	1:A:288:LYS:HD3	2.21	0.41
1:A:424:LEU:O	1:A:428:GLN:HG3	2.21	0.41
1:B:202:HIS:HA	1:B:328:TYR:O	2.21	0.41
1:B:217:PHE:HB3	1:B:302:LEU:HD13	2.02	0.41
1:B:246:SER:OG	1:B:270:LYS:HD3	2.19	0.41
1:C:225:HIS:HD1	1:C:228:ASN:ND2	2.08	0.41
1:E:111:THR:HG21	1:F:280:LEU:HD21	2.03	0.41
1:B:275:LEU:HD12	1:B:275:LEU:N	2.36	0.41
1:B:310:GLU:O	1:B:311:HIS:HB2	2.21	0.41
1:C:208:ASN:ND2	1:C:210:ARG:H	2.18	0.41
1:C:211:ILE:HG23	1:C:372:MET:CE	2.49	0.41
1:C:394:PRO:O	1:C:398:ARG:HG3	2.21	0.41
1:D:63:ILE:CG2	1:D:152:VAL:HG21	2.51	0.41
1:D:111:THR:HG21	1:E:280:LEU:HD21	2.01	0.41
1:F:36:ALA:HA	4:F:681:HOH:O	2.21	0.41
1:A:31:GLN:HB3	1:A:32:PRO:HD3	2.02	0.40
1:B:46:PRO:HG3	1:B:317:TRP:CD2	2.56	0.40
1:E:108:HIS:HD2	1:F:220:ALA:O	2.04	0.40
1:F:85:LEU:HD21	1:F:112:PHE:HE2	1.86	0.40
1:F:394:PRO:O	1:F:398:ARG:HG3	2.21	0.40
1:A:354:LYS:HB3	1:A:355:PRO:CD	2.51	0.40
1:C:428:GLN:HG3	4:C:1136:HOH:O	2.21	0.40
1:D:85:LEU:H	1:D:85:LEU:HD22	1.85	0.40
1:D:290:ARG:NH2	1:D:290:ARG:HG2	2.37	0.40
1:F:63:ILE:HG21	1:F:152:VAL:HG21	2.03	0.40
1:A:202:HIS:HA	1:A:328:TYR:O	2.21	0.40
1:A:211:ILE:HG23	1:A:372:MET:HE3	2.02	0.40
1:A:254:GLU:HG2	1:A:404:TRP:HE1	1.82	0.40
1:A:310:GLU:O	1:A:311:HIS:HB2	2.21	0.40
1:C:194:ASP:O	1:C:195:ASN:HB2	2.21	0.40
1:D:260:LYS:HG2	4:D:678:HOH:O	2.20	0.40
1:D:317:TRP:HB2	1:D:329:TRP:HB2	2.03	0.40
1:F:354:LYS:HB3	1:F:355:PRO:HD3	2.03	0.40
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.89	0.40
1:B:94:LYS:HE3	4:B:1039:HOH:O	2.22	0.40
1:B:237:VAL:HB	1:B:287:LEU:HA	2.03	0.40
1:B:308:PRO:HD2	1:B:312:VAL:HG11	2.02	0.40
1:C:134:THR:OG1	1:C:135:GLY:N	2.54	0.40
1:B:352:MET:SD	1:B:352:MET:C	3.05	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%)	401 (94%)	23 (5%)	1 (0%)	43	31
1	B	425/446 (95%)	403 (95%)	21 (5%)	1 (0%)	43	31
1	C	425/446 (95%)	400 (94%)	24 (6%)	1 (0%)	43	31
1	D	425/446 (95%)	401 (94%)	23 (5%)	1 (0%)	43	31
1	E	425/446 (95%)	399 (94%)	23 (5%)	3 (1%)	18	8
1	F	425/446 (95%)	400 (94%)	24 (6%)	1 (0%)	43	31
All	All	2550/2676 (95%)	2404 (94%)	138 (5%)	8 (0%)	36	25

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	255	ASP
1	E	286	GLY
1	B	300	GLY
1	C	300	GLY
1	D	300	GLY
1	E	300	GLY
1	A	300	GLY
1	F	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	373/392 (95%)	359 (96%)	14 (4%)	29	17
1	B	373/392 (95%)	364 (98%)	9 (2%)	43	31
1	C	373/392 (95%)	358 (96%)	15 (4%)	28	15
1	D	373/392 (95%)	360 (96%)	13 (4%)	32	19
1	E	373/392 (95%)	361 (97%)	12 (3%)	34	22
1	F	373/392 (95%)	362 (97%)	11 (3%)	37	25
All	All	2238/2352 (95%)	2164 (97%)	74 (3%)	33	21

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	23	ASN
1	A	25	LYS
1	A	53	LEU
1	A	90	ARG
1	A	169	LEU
1	A	223	LEU
1	A	226	LYS
1	A	283	LYS
1	A	339	ASP
1	A	340	GLU
1	A	352	MET
1	A	366	LEU
1	A	392	ILE
1	B	22	ASN
1	B	23	ASN
1	B	25	LYS
1	B	85	LEU
1	B	226	LYS
1	B	255	ASP
1	B	352	MET
1	B	366	LEU
1	B	442	ILE
1	C	22	ASN
1	C	23	ASN
1	C	25	LYS
1	C	90	ARG

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Mol	Chain	Res	Type
1	C	130	LEU
1	C	169	LEU
1	C	226	LYS
1	C	243	LEU
1	C	256	ASP
1	C	269	ASP
1	C	290	ARG
1	C	298	LEU
1	C	352	MET
1	C	366	LEU
1	C	410	LYS
1	D	22	ASN
1	D	23	ASN
1	D	25	LYS
1	D	85	LEU
1	D	103	ILE
1	D	147	MET
1	D	226	LYS
1	D	243	LEU
1	D	255	ASP
1	D	338	THR
1	D	339	ASP
1	D	352	MET
1	D	442	ILE
1	E	22	ASN
1	E	23	ASN
1	E	25	LYS
1	E	85	LEU
1	E	103	ILE
1	E	226	LYS
1	E	255	ASP
1	E	256	ASP
1	E	285	GLU
1	E	352	MET
1	E	366	LEU
1	E	440	GLU
1	F	22	ASN
1	F	23	ASN
1	F	25	LYS
1	F	85	LEU
1	F	243	LEU
1	F	256	ASP

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Mol	Chain	Res	Type
1	F	283	LYS
1	F	287	LEU
1	F	352	MET
1	F	366	LEU
1	F	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (119) 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	125	ASN
1	A	179	GLN
1	A	195	ASN
1	A	208	ASN
1	A	228	ASN
1	A	264	GLN
1	A	277	ASN
1	A	346	GLN
1	A	374	ASN
1	A	428	GLN
1	B	22	ASN
1	B	23	ASN
1	B	27	GLN
1	B	29	GLN
1	B	42	ASN
1	B	43	HIS
1	B	62	GLN
1	B	142	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

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Mol	Chain	Res	Type
1	B	374	ASN
1	B	428	GLN
1	B	441	GLN
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	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	314	GLN
1	C	346	GLN
1	C	362	ASN
1	C	374	ASN
1	C	428	GLN
1	D	22	ASN
1	D	23	ASN
1	D	27	GLN
1	D	42	ASN
1	D	43	HIS
1	D	62	GLN
1	D	74	ASN
1	D	125	ASN
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	291	HIS
1	D	311	HIS
1	D	346	GLN
1	D	351	HIS

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Mol	Chain	Res	Type
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	125	ASN
1	E	142	HIS
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	278	GLN
1	E	291	HIS
1	E	311	HIS
1	E	314	GLN
1	E	346	GLN
1	E	351	HIS
1	E	359	HIS
1	E	362	ASN
1	E	374	ASN
1	E	428	GLN
1	E	441	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	195	ASN
1	F	208	ASN
1	F	228	ASN
1	F	264	GLN
1	F	277	ASN
1	F	311	HIS
1	F	346	GLN
1	F	351	HIS

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Mol	Chain	Res	Type
1	F	374	ASN
1	F	428	GLN

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 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	C	500	1	0,4,4	-	-	-		
3	FES	E	500	1	0,4,4	-	-	-		
3	FES	A	500	1	0,4,4	-	-	-		
3	FES	B	500	1	0,4,4	-	-	-		
3	FES	D	500	1	0,4,4	-	-	-		
3	FES	F	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	C	500	1	-	-	0/1/1/1
3	FES	E	500	1	-	-	0/1/1/1
3	FES	A	500	1	-	-	0/1/1/1
3	FES	B	500	1	-	-	0/1/1/1
3	FES	D	500	1	-	-	0/1/1/1
3	FES	F	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	C	500	FES	1	0
3	E	500	FES	1	0
3	A	500	FES	1	0
3	B	500	FES	1	0
3	D	500	FES	1	0
3	F	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.