



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:51 PM UTC

PDB ID : 1FZ6 / pdb_00001fz6
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM II SOAKED IN
1 M METHANOL
Authors : Whittington, D.A.; Sazinsky, M.H.; Lippard, S.J.
Deposited on : 2000-10-03
Resolution : 2.05 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

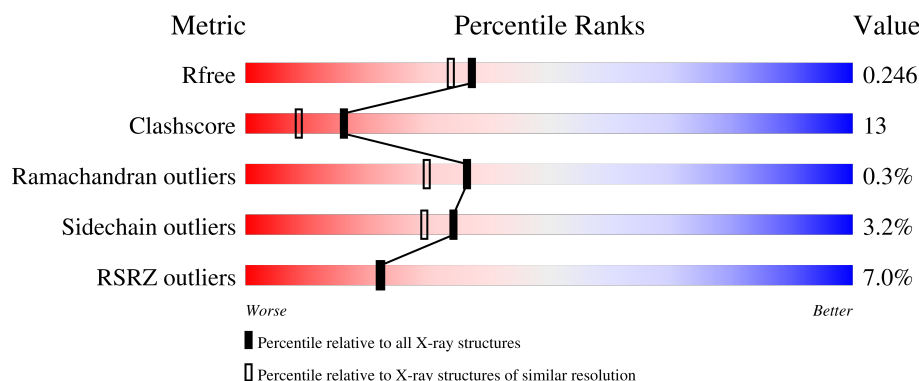
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	527	4% 69% 26% ..
1	B	527	4% 66% 27% ..
2	C	389	% 78% 19% .
2	D	389	13% 67% 29% ..
3	E	170	5% 74% 19% ...

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Mol	Chain	Length	Quality of chain
3	F	170	26% 65% 29%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18586 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 METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	40	0	0
			4177	2673	719	767	18			
1	B	510	Total	C	N	O	S	36	0	0
			4173	2671	718	766	18			

- Molecule 2 is a protein called METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	388	Total	C	N	O	S	30	0	0
			3193	2054	551	580	8			
2	D	388	Total	C	N	O	S	42	0	0
			3193	2054	551	580	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	370	ARG	ALA	conflict	UNP P18798
D	370	ARG	ALA	conflict	UNP P18798

- Molecule 3 is a protein called METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	4	0	0
			1368	867	246	250	5			
3	F	166	Total	C	N	O	S	8	0	0
			1366	866	245	250	5			

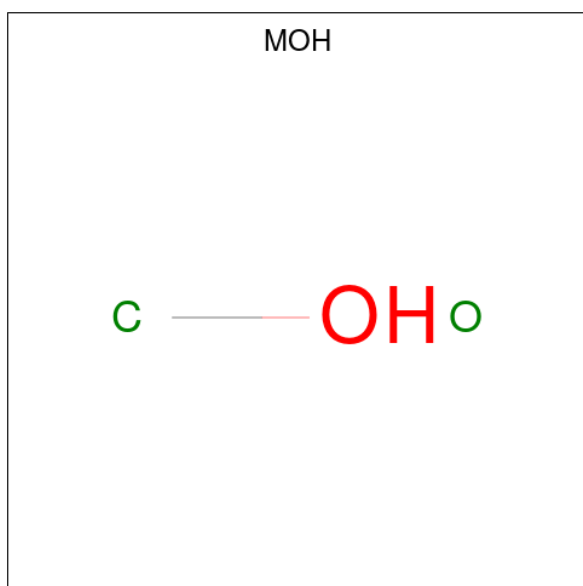
- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Fe	0	0
			2	2		
4	B	2	Total	Fe	0	0
			2	2		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		

- Molecule 6 is METHANOL (CCD ID: MOH) (formula: CH₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			2	1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	259	Total	O	0	0
			259	259		

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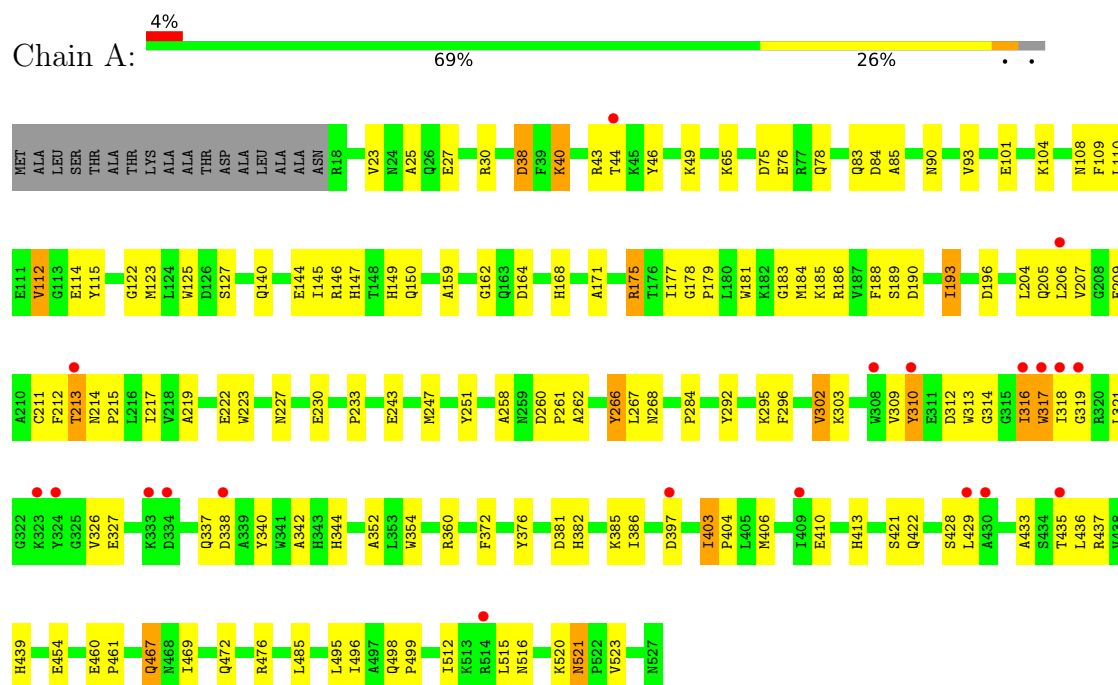
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	239	Total 239	O 239	0	0
7	C	286	Total 286	O 286	0	0
7	D	144	Total 144	O 144	0	0
7	E	125	Total 125	O 125	0	0
7	F	54	Total 54	O 54	0	0

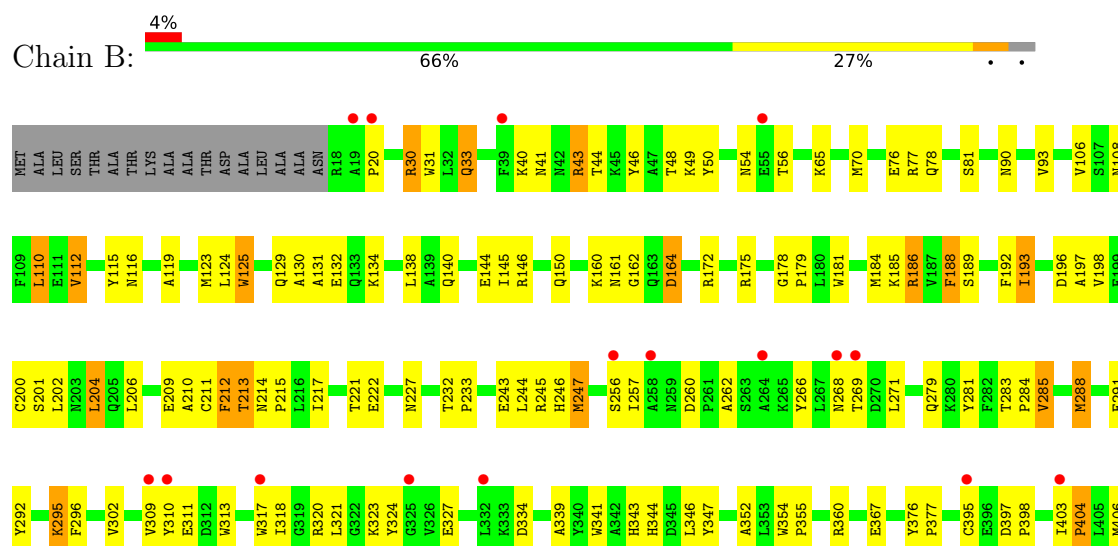
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

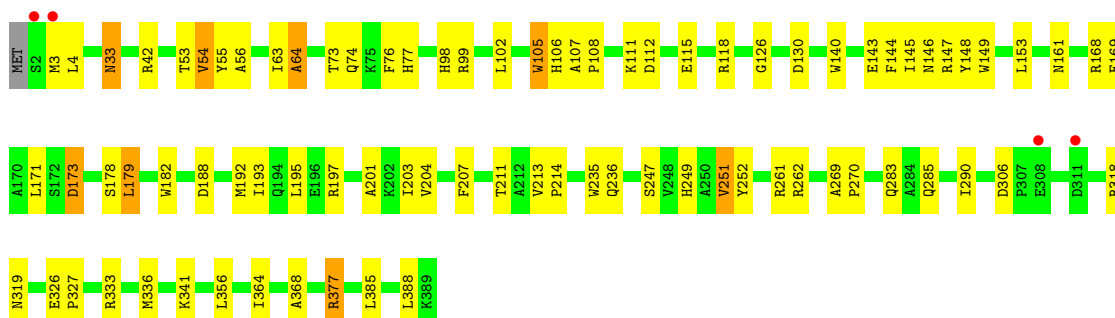
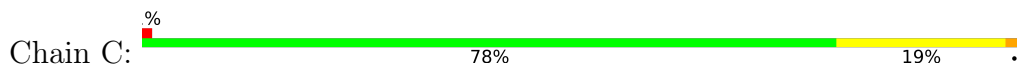


• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

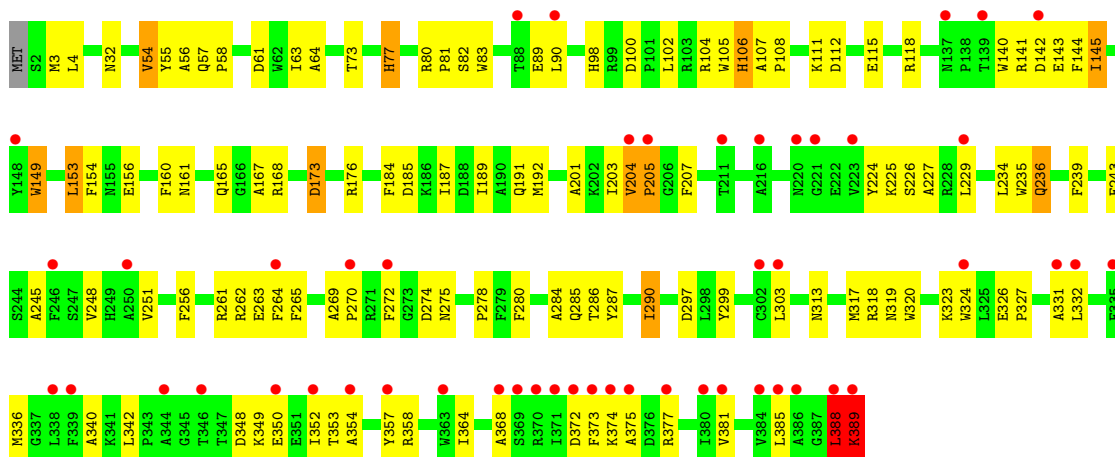




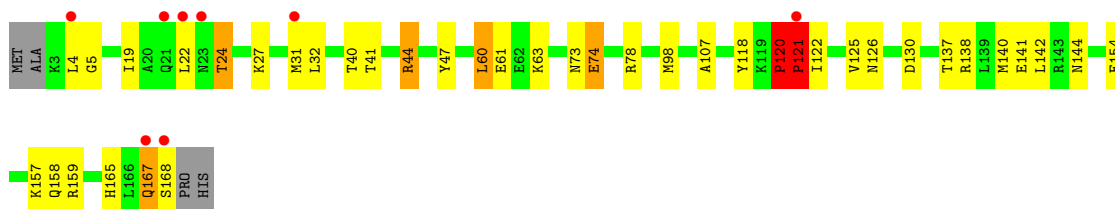
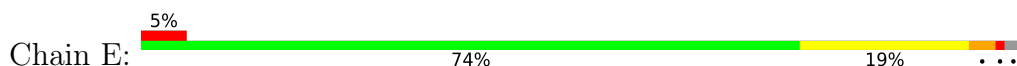
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

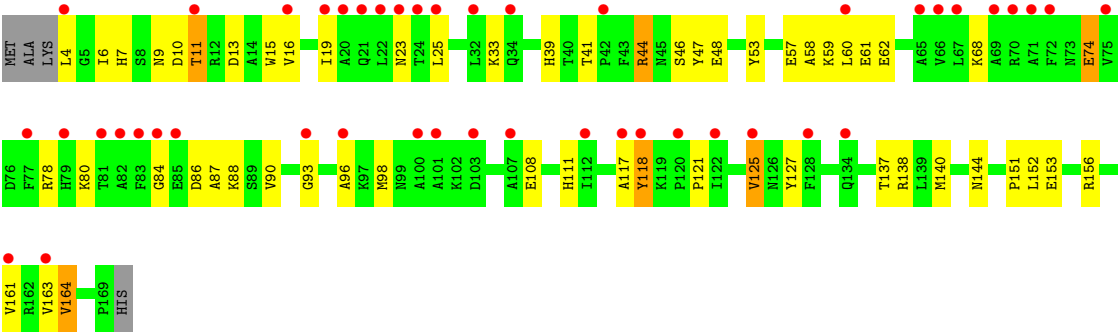


• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.67Å 171.29Å 221.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.05 29.90 – 2.05	Depositor EDS
% Data completeness (in resolution range)	89.0 (29.90-2.05) 89.1 (29.90-2.05)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.04Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.244 0.220 , 0.246	Depositor DCC
R_{free} test set	5330 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18586	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MOH, 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	0/4302	1.00	34/5842 (0.6%)
1	B	0.48	1/4298 (0.0%)	1.00	27/5837 (0.5%)
2	C	0.46	0/3289	0.91	18/4464 (0.4%)
2	D	1.21	13/3289 (0.4%)	1.13	30/4464 (0.7%)
3	E	1.26	10/1396 (0.7%)	1.47	15/1880 (0.8%)
3	F	0.41	0/1395	0.90	4/1881 (0.2%)
All	All	0.74	24/17969 (0.1%)	1.04	128/24368 (0.5%)

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
3	E	0	1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	389	LYS	CA-C	39.89	2.36	1.52
2	D	389	LYS	CB-CG	32.20	2.49	1.52
3	E	167	GLN	C-N	-29.56	0.92	1.33
2	D	388	LEU	CA-C	25.79	1.87	1.52
3	E	167	GLN	CA-C	22.71	1.80	1.52
2	D	389	LYS	CA-CB	16.55	1.86	1.53
3	E	167	GLN	C-O	-16.17	1.04	1.23
2	D	388	LEU	C-N	11.09	1.48	1.33
2	D	388	LEU	N-CA	9.20	1.58	1.46
2	D	388	LEU	C-O	-8.65	1.13	1.24
2	D	389	LYS	N-CA	8.19	1.61	1.46
1	B	288	MET	SD-CE	-7.81	1.60	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	389	LYS	CG-CD	7.55	1.75	1.52
3	E	121	PRO	CA-C	7.41	1.62	1.52
2	D	372	ASP	CA-C	6.72	1.62	1.53
3	E	121	PRO	CG-CD	6.45	1.72	1.50
2	D	374	LYS	CA-C	-6.36	1.45	1.52
3	E	121	PRO	N-CD	6.18	1.56	1.47
3	E	120	PRO	CA-CB	-6.11	1.45	1.54
2	D	374	LYS	N-CA	5.90	1.53	1.46
3	E	167	GLN	N-CA	5.76	1.53	1.46
3	E	121	PRO	N-CA	5.30	1.54	1.47
3	E	122	ILE	N-CA	5.13	1.52	1.46
2	D	375	ALA	N-CA	-5.01	1.39	1.45

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	120	PRO	CA-C-N	23.19	148.83	119.84
3	E	120	PRO	C-N-CA	23.19	148.83	119.84
2	D	389	LYS	N-CA-CB	-22.16	72.84	110.50
3	E	167	GLN	CA-C-O	-17.09	101.00	120.66
3	E	167	GLN	O-C-N	16.23	143.07	123.27
2	D	389	LYS	N-CA-C	16.11	156.10	111.00
3	E	120	PRO	C-N-CD	-16.02	59.30	125.00
2	D	389	LYS	CA-CB-CG	14.80	143.71	114.10
3	E	121	PRO	CA-N-CD	-14.66	91.47	112.00
2	D	388	LEU	CA-C-O	-14.37	99.96	120.51
2	D	373	PHE	N-CA-C	-12.78	92.48	110.50
3	E	121	PRO	N-CA-C	-12.03	87.69	112.47
2	D	389	LYS	CA-C-O	10.35	152.04	121.00
1	A	316	ILE	N-CA-C	10.17	120.16	110.30
1	A	337	GLN	OE1-CD-NE2	-9.76	112.84	122.60
3	F	39	HIS	N-CA-C	9.38	124.98	112.88
2	D	372	ASP	N-CA-C	9.33	124.18	112.24
1	B	339	ALA	N-CA-C	9.18	120.89	111.07
1	A	164	ASP	CA-C-N	8.98	129.16	119.28
1	A	164	ASP	C-N-CA	8.98	129.16	119.28
2	D	389	LYS	CB-CG-CD	8.55	130.97	111.30
1	A	316	ILE	CA-C-N	8.46	131.44	120.44
1	A	316	ILE	C-N-CA	8.46	131.44	120.44
2	D	389	LYS	CB-CA-C	8.44	126.14	110.10
1	B	397	ASP	CA-C-N	7.87	127.16	118.97
1	B	397	ASP	C-N-CA	7.87	127.16	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	373	PHE	CA-C-O	-7.84	113.02	121.56
1	B	309	VAL	N-CA-C	7.67	117.75	110.53
2	D	388	LEU	CA-C-N	7.46	135.13	121.70
2	D	388	LEU	C-N-CA	7.46	135.13	121.70
2	C	106	HIS	N-CA-C	7.42	120.02	111.11
1	B	490	SER	N-CA-C	7.34	120.21	111.33
1	A	317	TRP	N-CA-CB	-7.31	99.40	110.01
2	D	374	LYS	CA-C-N	-7.26	111.18	122.87
2	D	374	LYS	C-N-CA	-7.26	111.18	122.87
1	B	496	ILE	N-CA-C	-7.06	103.90	110.53
2	D	374	LYS	N-CA-C	-6.94	95.87	108.02
2	C	105	TRP	N-CA-C	-6.87	100.06	109.95
3	E	130	ASP	N-CA-C	-6.73	104.01	111.82
1	B	164	ASP	CA-C-N	6.72	126.68	119.28
1	B	164	ASP	C-N-CA	6.72	126.68	119.28
3	E	120	PRO	N-CA-C	6.67	118.84	110.70
1	A	337	GLN	CG-CD-NE2	6.65	126.38	116.40
1	B	193	ILE	N-CA-C	6.64	120.18	113.47
2	D	143	GLU	CA-C-N	-6.55	109.87	122.06
2	D	143	GLU	C-N-CA	-6.55	109.87	122.06
1	B	426	CYS	CA-C-N	6.52	127.99	119.84
1	B	426	CYS	C-N-CA	6.52	127.99	119.84
1	B	285	VAL	N-CA-C	6.51	116.67	110.42
1	A	212	PHE	N-CA-C	6.46	121.53	112.93
1	A	317	TRP	N-CA-C	6.45	117.97	111.07
1	B	295	LYS	N-CA-C	-6.43	103.32	112.13
2	D	105	TRP	N-CA-C	-6.42	100.71	109.95
1	A	496	ILE	N-CA-C	-6.41	104.50	110.53
2	D	56	ALA	N-CA-C	-6.37	104.41	111.36
1	A	145	ILE	N-CA-C	-6.34	104.32	110.72
3	E	74	GLU	N-CA-C	6.25	118.10	111.28
1	A	213	THR	N-CA-C	6.21	118.13	111.36
1	A	178	GLY	CA-C-N	6.16	125.72	119.19
1	A	178	GLY	C-N-CA	6.16	125.72	119.19
1	B	204	LEU	N-CA-C	6.16	117.87	111.03
3	F	118	TYR	N-CA-C	6.15	120.09	112.59
2	C	169	GLU	N-CA-C	6.08	120.86	113.38
2	D	286	THR	N-CA-C	-6.08	104.73	111.36
2	C	236	GLN	N-CA-C	6.04	120.81	113.38
1	A	397	ASP	CA-C-N	6.04	125.72	119.56
1	A	397	ASP	C-N-CA	6.04	125.72	119.56
1	B	431	LYS	N-CA-C	-5.98	106.14	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	118	TYR	N-CA-C	5.93	121.24	113.30
2	D	204	VAL	CA-C-N	5.85	127.15	119.84
2	D	204	VAL	C-N-CA	5.85	127.15	119.84
2	C	262	ARG	N-CA-C	5.84	118.53	111.40
1	B	178	GLY	CA-C-N	5.83	125.37	119.19
1	B	178	GLY	C-N-CA	5.83	125.37	119.19
2	C	149	TRP	N-CA-C	-5.81	105.03	111.36
1	A	85	ALA	N-CA-C	5.80	118.07	111.11
1	B	188	PHE	N-CA-C	5.79	120.36	112.88
2	C	53	THR	N-CA-C	5.79	120.07	112.13
1	B	20	PRO	N-CA-C	-5.77	101.45	110.50
2	D	262	ARG	N-CA-C	5.75	118.42	111.40
1	B	478	LEU	N-CA-C	5.71	117.96	111.11
1	A	309	VAL	N-CA-C	5.66	115.85	110.53
3	F	53	TYR	N-CA-C	5.66	117.44	111.28
1	B	212	PHE	N-CA-C	5.65	119.87	112.13
1	A	258	ALA	N-CA-C	5.63	117.42	111.28
2	C	249	HIS	N-CA-C	5.62	119.31	112.23
2	D	106	HIS	N-CA-C	5.61	117.84	111.11
2	D	373	PHE	N-CA-CB	-5.57	102.15	110.17
2	C	77	HIS	N-CA-C	-5.55	101.83	110.10
2	C	54	VAL	N-CA-C	5.54	116.56	109.30
1	A	266	TYR	N-CA-C	5.53	121.44	114.31
1	B	93	VAL	N-CA-C	5.53	116.56	111.81
1	B	145	ILE	N-CA-C	-5.52	105.15	110.72
3	E	121	PRO	CA-CB-CG	-5.51	94.02	104.50
2	D	318	ARG	N-CA-C	-5.51	105.36	111.36
3	F	6	ILE	N-CA-C	5.50	120.79	109.34
3	E	73	ASN	N-CA-C	-5.50	103.44	110.53
1	B	247	MET	N-CA-C	-5.49	105.20	111.07
1	A	38	ASP	N-CA-C	5.48	118.56	109.46
2	C	171	LEU	N-CA-C	5.46	119.04	112.93
2	C	252	TYR	N-CA-C	5.46	116.92	110.97
1	B	162	GLY	N-CA-C	5.45	120.93	112.60
1	A	267	LEU	N-CA-C	5.44	117.64	111.11
2	C	144	PHE	N-CA-C	5.43	119.08	112.23
1	A	193	ILE	N-CA-C	5.40	120.56	109.34
2	D	236	GLN	N-CA-C	5.29	119.89	113.38
1	A	310	TYR	N-CA-C	5.29	116.85	111.14
1	A	122	GLY	N-CA-C	-5.28	105.94	113.86
2	D	149	TRP	N-CA-C	-5.27	105.20	111.69
1	A	40	LYS	N-CA-C	5.25	117.41	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	148	TYR	N-CA-C	5.25	118.15	111.69
1	A	25	ALA	N-CA-C	5.20	116.63	111.07
1	A	205	GLN	N-CA-C	5.18	119.49	111.56
2	C	306	ASP	CA-C-N	5.16	125.46	119.47
2	C	306	ASP	C-N-CA	5.16	125.46	119.47
3	E	167	GLN	N-CA-C	-5.15	100.64	109.24
3	E	5	GLY	N-CA-C	5.14	125.37	113.18
1	A	521	ASN	CA-C-N	5.12	124.78	119.56
1	A	521	ASN	C-N-CA	5.12	124.78	119.56
1	B	266	TYR	N-CA-C	5.10	120.36	114.04
2	D	54	VAL	N-CA-C	5.09	115.80	108.93
1	B	65	LYS	N-CA-C	5.08	116.89	111.36
2	C	377	ARG	N-CA-C	5.08	117.48	111.33
1	A	460	GLU	CA-C-N	5.07	125.10	119.32
1	A	460	GLU	C-N-CA	5.07	125.10	119.32
1	A	162	GLY	N-CA-C	5.05	120.84	112.66
2	D	77	HIS	N-CA-C	-5.04	102.45	109.96
2	C	56	ALA	N-CA-C	-5.01	105.81	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	120	PRO	Mainchain

5.2 Too-close contacts [i](#)

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	4177	0	3975	105	0
1	B	4173	0	3969	134	0
2	C	3193	0	3042	61	0
2	D	3193	0	3042	111	0
3	E	1368	0	1362	38	0
3	F	1366	0	1357	45	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	2	0	0	0	0
7	A	259	0	0	6	0
7	B	239	0	0	5	0
7	C	286	0	0	3	0
7	D	144	0	0	0	0
7	E	125	0	0	2	0
7	F	54	0	0	0	0
All	All	18586	0	16747	442	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 13.

All (442) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:389:LYS:CG	2:D:389:LYS:CD	1.75	1.59
3:E:167:GLN:C	3:E:167:GLN:CA	1.80	1.54
2:D:389:LYS:CB	2:D:389:LYS:CA	1.86	1.50
2:D:388:LEU:C	2:D:388:LEU:CA	1.87	1.46
2:D:389:LYS:CB	2:D:389:LYS:N	2.07	1.17
3:E:165:HIS:CE1	3:E:167:GLN:HE21	1.66	1.13
3:E:165:HIS:HE1	3:E:167:GLN:NE2	1.48	1.12
2:D:389:LYS:C	2:D:389:LYS:HA	1.87	0.98
2:D:389:LYS:CA	2:D:389:LYS:C	2.36	0.97
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.49	0.94
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.17	0.92
2:D:389:LYS:CG	2:D:389:LYS:CB	2.49	0.91
1:A:44:THR:HG22	1:A:46:TYR:H	1.35	0.90
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.16	0.89
3:E:167:GLN:CA	3:E:168:SER:N	2.32	0.88
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.19	0.88
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.58	0.86
3:F:41:THR:O	3:F:44:ARG:HD2	1.76	0.85
1:B:44:THR:HG22	1:B:46:TYR:H	1.42	0.85
3:E:22:LEU:HD11	3:E:31:MET:SD	2.18	0.84
3:E:167:GLN:CA	3:E:167:GLN:O	2.24	0.83
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.28	0.81
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.61	0.80
3:F:4:LEU:HD21	3:F:10:ASP:H	1.47	0.80
3:E:165:HIS:HE1	3:E:167:GLN:HE21	0.79	0.79
3:E:165:HIS:CE1	3:E:167:GLN:NE2	2.38	0.79
1:B:210:ALA:HA	1:B:247:MET:HE1	1.64	0.79
3:F:153:GLU:H	3:F:153:GLU:CD	1.90	0.79
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.65	0.78
3:F:58:ALA:O	3:F:62:GLU:HG3	1.83	0.78
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.84	0.78
2:D:389:LYS:CB	2:D:389:LYS:H	1.95	0.78
1:A:338:ASP:OD2	1:A:433:ALA:HB2	1.84	0.77
1:A:313:TRP:CD1	1:A:317:TRP:CD1	2.72	0.77
3:E:98:MET:HE1	3:E:107:ALA:CB	2.16	0.76
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.83	0.75
2:C:3:MET:HG3	2:C:4:LEU:H	1.52	0.75
1:A:268:ASN:HD21	1:A:327:GLU:H	1.34	0.75
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.69	0.75
1:B:123:MET:HE3	1:B:197:ALA:HA	1.67	0.74
1:B:33:GLN:HE22	1:B:132:GLU:H	1.34	0.74
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.53	0.74
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.88	0.73
3:F:13:ASP:O	3:F:16:VAL:HG22	1.86	0.73
1:A:213:THR:O	1:A:217:ILE:HG12	1.88	0.73
3:E:24:THR:HG22	3:E:27:LYS:H	1.51	0.73
2:C:336:MET:HE3	2:C:388:LEU:HG	1.69	0.73
1:A:467:GLN:HG3	7:A:5223:HOH:O	1.89	0.72
1:A:227:ASN:HD21	1:A:295:LYS:H	1.36	0.72
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.70	0.72
2:D:388:LEU:CA	2:D:388:LEU:O	2.34	0.72
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.72	0.71
1:B:355:PRO:HG2	1:B:403:ILE:CD1	2.20	0.71
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.71	0.71
3:E:41:THR:O	3:E:44:ARG:HD2	1.91	0.70
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.76	0.69
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.40	0.69
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.72	0.69
3:F:151:PRO:HB2	3:F:153:GLU:OE1	1.93	0.69
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.75	0.69
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.07	0.69
1:B:160:LYS:HE3	1:B:161:ASN:OD1	1.94	0.68
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.23	0.68
3:E:98:MET:HE1	3:E:107:ALA:HB1	1.75	0.68
2:D:153:LEU:C	2:D:153:LEU:HD12	2.20	0.67
1:A:435:THR:HG21	1:A:437:ARG:HE	1.60	0.67
1:A:243:GLU:O	1:A:247:MET:HG2	1.95	0.67
2:D:275:ASN:C	2:D:278:PRO:HD2	2.20	0.66
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.30	0.66
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.76	0.66
1:B:213:THR:O	1:B:217:ILE:HG12	1.95	0.66
1:B:355:PRO:HG2	1:B:403:ILE:HD11	1.78	0.66
2:C:105:TRP:O	2:C:108:PRO:HD2	1.96	0.66
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.78	0.65
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.45	0.65
1:B:489:ARG:HD2	1:B:495:LEU:O	1.97	0.65
1:B:422:GLN:O	1:B:424:PRO:HD3	1.96	0.65
1:B:33:GLN:NE2	1:B:132:GLU:H	1.93	0.65
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.63	0.64
3:E:167:GLN:C	3:E:167:GLN:CB	2.68	0.64
1:A:429:LEU:HG	1:A:429:LEU:O	1.96	0.64
1:B:210:ALA:CA	1:B:247:MET:HE1	2.28	0.64
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.46	0.64
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.79	0.64
2:C:3:MET:HE2	2:C:4:LEU:HD13	1.80	0.64
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.80	0.63
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.62	0.63
3:E:61:GLU:HB3	3:E:121:PRO:HG2	1.81	0.63
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.62	0.63
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.00	0.62
1:B:70:MET:HE1	1:B:245:ARG:NH1	2.15	0.62
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.82	0.62
2:D:385:LEU:HD12	2:D:388:LEU:CD1	2.30	0.62
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.33	0.61
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.36	0.61
3:E:98:MET:HE2	3:E:138:ARG:CG	2.31	0.61
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.94	0.61
3:F:57:GLU:O	3:F:61:GLU:HG3	2.00	0.61
1:B:288:MET:HE1	1:B:346:LEU:CG	2.31	0.61
1:B:268:ASN:HD21	1:B:327:GLU:H	1.47	0.60
1:B:288:MET:HE1	1:B:346:LEU:HG	1.82	0.60
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.83	0.60
3:E:167:GLN:C	3:E:167:GLN:N	2.57	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:TRP:C	2:D:327:PRO:HD2	2.26	0.60
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.83	0.60
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	0.60
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.01	0.60
1:B:227:ASN:HD21	1:B:295:LYS:H	1.49	0.60
1:A:227:ASN:ND2	1:A:295:LYS:H	1.99	0.60
2:D:349:LYS:HA	2:D:352:ILE:HG12	1.84	0.59
1:A:65:LYS:NZ	2:C:192:MET:HE2	2.18	0.59
2:D:389:LYS:CG	2:D:389:LYS:CE	2.77	0.59
1:B:198:VAL:O	1:B:202:LEU:HG	2.02	0.59
1:B:288:MET:CE	1:B:346:LEU:HB3	2.31	0.59
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.36	0.59
1:A:104:LYS:HG2	1:A:168:HIS:CD2	2.37	0.59
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.18	0.59
1:A:185:LYS:O	1:A:189:SER:HB2	2.04	0.58
1:B:288:MET:HE2	1:B:347:TYR:N	2.18	0.58
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.84	0.58
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.03	0.58
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.86	0.58
2:D:389:LYS:HA	2:D:389:LYS:OXT	2.03	0.58
1:A:222:GLU:HA	1:A:222:GLU:OE1	2.04	0.58
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.39	0.57
2:C:3:MET:HG3	2:C:4:LEU:N	2.18	0.57
1:A:435:THR:CG2	1:A:437:ARG:HE	2.17	0.57
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.86	0.57
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.68	0.57
2:D:340:ALA:CB	2:D:389:LYS:HD3	2.35	0.57
1:A:268:ASN:ND2	1:A:327:GLU:H	2.02	0.57
2:D:187:ILE:O	2:D:191:GLN:HG3	2.04	0.57
1:A:314:GLY:C	1:A:318:ILE:HG21	2.30	0.56
2:C:111:LYS:O	2:C:115:GLU:HG3	2.05	0.56
2:D:89:GLU:CD	3:F:125:VAL:HG13	2.31	0.56
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.87	0.56
1:B:43:ARG:HD2	1:B:43:ARG:C	2.30	0.56
2:D:336:MET:HE3	2:D:388:LEU:HD11	1.88	0.56
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.95	0.56
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.14	0.56
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.56
1:A:209:GLU:HA	1:A:213:THR:HB	1.87	0.56
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.40	0.56
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:THR:OG1	1:A:127:SER:HA	2.06	0.56
1:B:43:ARG:HD2	1:B:43:ARG:O	2.06	0.56
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.36	0.56
2:D:82:SER:O	2:D:168:ARG:NH2	2.34	0.56
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.88	0.55
1:A:65:LYS:HZ3	2:C:192:MET:HE2	1.71	0.55
1:A:207:VAL:O	1:A:211:CYS:HB3	2.06	0.55
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.42	0.55
1:A:313:TRP:CD1	1:A:317:TRP:HD1	2.25	0.55
3:F:9:ASN:OD1	3:F:11:THR:HG23	2.06	0.55
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.88	0.55
3:E:167:GLN:O	3:E:167:GLN:N	2.39	0.55
2:D:224:TYR:O	2:D:227:ALA:HB3	2.07	0.55
1:B:288:MET:HE1	1:B:346:LEU:CB	2.36	0.55
1:B:193:ILE:O	2:D:168:ARG:NH1	2.40	0.55
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.39	0.55
1:A:382:HIS:O	1:A:386:ILE:HG13	2.07	0.55
1:B:175:ARG:CZ	1:B:181:TRP:CH2	2.90	0.54
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.59	0.54
2:C:235:TRP:CD1	2:C:235:TRP:C	2.86	0.54
3:F:15:TRP:O	3:F:19:ILE:HG23	2.08	0.54
1:A:84:ASP:HB3	1:B:81:SER:OG	2.08	0.54
3:F:74:GLU:O	3:F:78:ARG:HG3	2.08	0.54
1:A:140:GLN:O	1:A:144:GLU:HG2	2.08	0.53
3:E:98:MET:HE1	3:E:107:ALA:HB2	1.90	0.53
1:A:184:MET:HE3	1:A:184:MET:HA	1.90	0.53
1:B:355:PRO:HG2	1:B:403:ILE:HD12	1.91	0.53
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.43	0.53
2:C:336:MET:HE2	2:C:385:LEU:HD23	1.91	0.53
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.91	0.53
3:E:22:LEU:O	3:E:63:LYS:HE2	2.09	0.53
3:F:25:LEU:HD22	3:F:68:LYS:HA	1.91	0.53
1:B:283:THR:HB	1:B:284:PRO:HD3	1.91	0.53
2:C:333:ARG:HD2	7:C:5166:HOH:O	2.09	0.53
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.45	0.52
2:D:385:LEU:HD12	2:D:388:LEU:HD11	1.92	0.52
1:B:44:THR:HG21	7:B:9009:HOH:O	2.09	0.52
2:D:388:LEU:C	2:D:388:LEU:CB	2.78	0.52
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.93	0.52
1:B:246:HIS:CD2	1:B:246:HIS:N	2.76	0.52
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:MET:O	1:A:410:GLU:HG3	2.10	0.52
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.91	0.51
1:A:520:LYS:HB3	1:A:520:LYS:HZ2	1.74	0.51
1:B:212:PHE:O	1:B:215:PRO:HD2	2.10	0.51
1:B:288:MET:HE1	1:B:346:LEU:HB3	1.92	0.51
1:B:490:SER:OG	2:D:32:ASN:HB2	2.09	0.51
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.40	0.51
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.08	0.51
1:B:269:THR:HG23	7:B:9185:HOH:O	2.10	0.51
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.92	0.51
1:A:413:HIS:HD2	1:A:428:SER:OG	1.94	0.51
2:D:167:ALA:O	2:D:176:ARG:NH1	2.43	0.51
1:A:354:TRP:CZ2	1:A:403:ILE:HD11	2.46	0.51
2:D:58:PRO:HD2	2:D:83:TRP:HZ3	1.75	0.51
1:A:314:GLY:O	1:A:318:ILE:HG21	2.10	0.51
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.46	0.51
2:C:188:ASP:O	2:C:192:MET:HG2	2.11	0.51
1:A:413:HIS:CD2	1:A:429:LEU:HB2	2.47	0.50
1:B:186:ARG:HA	2:D:73:THR:OG1	2.11	0.50
1:A:302:VAL:HG22	1:A:376:TYR:CZ	2.46	0.50
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.12	0.50
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.12	0.50
2:C:211:THR:O	2:C:214:PRO:HD2	2.11	0.50
2:D:269:ALA:HB1	2:D:274:ASP:OD2	2.10	0.50
3:F:90:VAL:HG11	3:F:118:TYR:CZ	2.46	0.50
1:B:119:ALA:HA	2:D:167:ALA:O	2.11	0.50
1:A:159:ALA:O	2:C:33:ASN:HB2	2.12	0.50
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.43	0.50
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.93	0.50
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.77	0.50
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.94	0.50
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.94	0.50
1:B:106:VAL:O	1:B:110:LEU:HB2	2.12	0.50
1:A:76:GLU:OE1	1:B:76:GLU:HG2	2.12	0.49
2:C:3:MET:CG	2:C:4:LEU:H	2.24	0.49
2:D:389:LYS:CD	2:D:389:LYS:HG3	2.20	0.49
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.95	0.49
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.95	0.49
1:B:227:ASN:HD21	1:B:296:PHE:H	1.60	0.49
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.48	0.49
1:B:210:ALA:N	1:B:247:MET:HE1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:TRP:O	2:D:327:PRO:HD2	2.12	0.49
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.94	0.49
1:B:41:ASN:O	2:D:236:GLN:HB3	2.12	0.49
1:A:421:SER:O	1:A:422:GLN:HB2	2.13	0.49
2:C:341:LYS:HE3	7:C:5020:HOH:O	2.12	0.49
3:F:80:LYS:HE3	3:F:84:GLY:O	2.12	0.49
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.41	0.49
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.24	0.49
3:E:157:LYS:HD2	7:E:295:HOH:O	2.13	0.49
2:D:235:TRP:CD1	2:D:235:TRP:C	2.90	0.49
1:A:196:ASP:HB2	3:E:140:MET:SD	2.53	0.48
1:B:112:VAL:CG2	2:D:58:PRO:HG3	2.43	0.48
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.12	0.48
2:D:377:ARG:O	2:D:381:VAL:HG23	2.13	0.48
2:C:3:MET:CE	2:C:4:LEU:HD13	2.43	0.48
1:A:403:ILE:HD12	7:A:5094:HOH:O	2.12	0.48
1:B:112:VAL:HG21	1:B:181:TRP:HH2	1.78	0.48
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.95	0.48
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.78	0.48
2:D:111:LYS:O	2:D:115:GLU:HG3	2.13	0.48
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.49	0.48
1:B:146:ARG:HG2	1:B:150:GLN:OE1	2.14	0.48
1:B:406:MET:O	1:B:410:GLU:HG3	2.13	0.48
1:A:110:LEU:O	1:A:114:GLU:HG2	2.14	0.48
1:A:193:ILE:HD12	2:C:168:ARG:HH21	1.79	0.48
1:B:367:GLU:HG3	7:B:9131:HOH:O	2.13	0.48
3:F:46:SER:OG	3:F:48:GLU:HG2	2.14	0.48
1:A:219:ALA:O	1:A:223:TRP:HD1	1.97	0.47
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.32	0.47
1:B:466:CYS:HB2	2:D:73:THR:HA	1.95	0.47
2:D:326:GLU:HB2	2:D:327:PRO:HD3	1.96	0.47
1:B:78:GLN:NE2	1:B:150:GLN:HE21	2.05	0.47
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.49	0.47
2:D:234:LEU:HD13	2:D:248:VAL:HG22	1.95	0.47
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.80	0.47
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.95	0.47
1:B:124:LEU:HD21	1:B:201:SER:HB2	1.95	0.47
2:D:226:SER:HB2	2:D:331:ALA:HA	1.96	0.47
3:E:138:ARG:NH2	3:E:142:LEU:HD21	2.30	0.47
1:B:48:THR:O	3:F:137:THR:HG23	2.14	0.47
1:B:414:PRO:O	1:B:426:CYS:SG	2.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:211:THR:C	2:C:214:PRO:HD2	2.40	0.47
2:C:333:ARG:HD3	7:C:5024:HOH:O	2.13	0.47
2:C:146:ASN:O	2:C:214:PRO:HG3	2.15	0.47
1:A:520:LYS:HB3	1:A:520:LYS:NZ	2.30	0.47
1:B:140:GLN:O	1:B:144:GLU:HG2	2.15	0.47
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.49	0.47
1:B:355:PRO:CG	1:B:403:ILE:HD11	2.44	0.47
2:D:349:LYS:HE2	2:D:385:LEU:HD21	1.96	0.47
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.96	0.47
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.45	0.47
2:C:336:MET:CE	2:C:385:LEU:HD23	2.45	0.47
1:B:184:MET:HE3	1:B:184:MET:HA	1.97	0.47
1:A:186:ARG:HD3	1:A:186:ARG:C	2.40	0.46
3:E:98:MET:HE3	3:E:98:MET:O	2.15	0.46
1:A:171:ALA:O	1:A:175:ARG:HD2	2.15	0.46
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.46
1:B:444:GLU:OE2	1:B:444:GLU:HA	2.15	0.46
2:C:146:ASN:HB2	2:C:207:PHE:CZ	2.51	0.46
1:B:192:PHE:O	1:B:200:CYS:HB3	2.16	0.46
2:D:185:ASP:O	2:D:189:ILE:HG12	2.16	0.46
3:F:19:ILE:HG21	3:F:60:LEU:HD12	1.98	0.46
1:A:302:VAL:HG11	1:A:340:TYR:CE1	2.50	0.46
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.12	0.46
1:A:302:VAL:HG22	1:A:376:TYR:OH	2.16	0.46
1:A:227:ASN:HD21	1:A:296:PHE:H	1.63	0.46
2:C:54:VAL:O	2:C:55:TYR:HB2	2.16	0.46
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.51	0.46
1:B:116:ASN:CG	1:B:189:SER:HA	2.41	0.45
1:B:123:MET:HE1	1:B:200:CYS:SG	2.55	0.45
1:A:321:LEU:O	1:A:326:VAL:HB	2.16	0.45
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.79	0.45
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.16	0.45
1:B:175:ARG:CZ	1:B:181:TRP:CZ2	2.99	0.45
1:B:227:ASN:ND2	1:B:295:LYS:H	2.14	0.45
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.98	0.45
2:C:269:ALA:N	2:C:270:PRO:CD	2.80	0.45
2:D:349:LYS:HG3	2:D:352:ILE:HD11	1.97	0.45
1:B:334:ASP:HB2	7:B:9103:HOH:O	2.16	0.45
2:C:192:MET:HE2	2:C:283:GLN:OE1	2.17	0.45
1:A:109:PHE:O	1:A:112:VAL:HG12	2.17	0.45
2:C:247:SER:O	2:C:251:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:154:GLU:O	3:E:158:GLN:HG3	2.17	0.45
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.99	0.45
2:D:189:ILE:HD11	2:D:284:ALA:HA	1.99	0.45
2:D:313:ASN:HB3	2:D:317:MET:HE2	1.99	0.45
3:F:98:MET:HE1	3:F:111:HIS:HB2	1.99	0.45
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.52	0.45
3:E:125:VAL:HG23	3:E:126:ASN:N	2.31	0.45
3:F:152:LEU:O	3:F:156:ARG:HG3	2.16	0.45
1:A:303:LYS:HB2	1:A:303:LYS:HE3	1.83	0.44
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.52	0.44
2:C:98:HIS:HE1	2:C:178:SER:OG	1.99	0.44
1:B:115:TYR:OH	2:D:173:ASP:HA	2.17	0.44
1:B:341:TRP:CE2	1:B:431:LYS:HD3	2.53	0.44
1:B:524:LYS:O	1:B:527:ASN:HB2	2.18	0.44
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.99	0.44
3:F:4:LEU:HD11	3:F:10:ASP:OD2	2.17	0.44
2:C:179:LEU:HD12	2:C:182:TRP:CZ3	2.52	0.44
2:D:352:ILE:HD12	2:D:388:LEU:HD11	1.99	0.44
1:A:512:ILE:O	1:A:515:LEU:HB2	2.17	0.44
1:B:317:TRP:CE3	1:B:320:ARG:NH2	2.85	0.44
3:F:88:LYS:HB2	3:F:127:TYR:CE2	2.53	0.44
1:A:101:GLU:CD	1:A:360:ARG:HD3	2.42	0.44
2:D:80:ARG:HD2	2:D:81:PRO:O	2.18	0.44
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.99	0.44
2:D:225:LYS:O	2:D:229:LEU:HG	2.18	0.44
1:A:435:THR:HG22	1:A:436:LEU:N	2.32	0.44
1:A:472:GLN:NE2	7:A:5223:HOH:O	2.51	0.44
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.47	0.44
3:F:61:GLU:O	3:F:121:PRO:HG2	2.17	0.44
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.53	0.43
1:B:196:ASP:HB2	3:F:140:MET:SD	2.58	0.43
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.18	0.43
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.52	0.43
1:B:209:GLU:C	1:B:247:MET:HE1	2.42	0.43
2:D:141:ARG:HG2	2:D:142:ASP:N	2.33	0.43
2:D:189:ILE:HD12	2:D:284:ALA:HB2	2.00	0.43
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.81	0.43
2:C:126:GLY:O	2:C:130:ASP:HB2	2.19	0.43
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.53	0.43
1:B:54:ASN:HB3	1:B:129:GLN:HB2	2.00	0.43
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ILE:HG12	1:A:485:LEU:HB2	2.01	0.43
1:A:372:PHE:O	1:A:376:TYR:N	2.45	0.43
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.00	0.43
2:D:98:HIS:HD2	2:D:297:ASP:OD1	2.02	0.43
1:B:292:TYR:OH	1:B:344:HIS:HD2	2.02	0.43
1:B:483:ALA:HB2	1:B:509:LEU:HD21	2.00	0.43
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.52	0.43
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.54	0.43
2:D:203:ILE:HG13	2:D:204:VAL:HG23	2.01	0.43
1:A:312:ASP:O	1:A:316:ILE:HB	2.19	0.42
1:B:125:TRP:CD1	1:B:125:TRP:C	2.97	0.42
2:D:57:GLN:HA	2:D:58:PRO:HD3	1.89	0.42
3:E:40:THR:C	3:E:41:THR:HG23	2.44	0.42
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.67	0.42
2:D:165:GLN:OE1	2:D:239:PHE:HA	2.20	0.42
1:B:30:ARG:HD3	1:B:31:TRP:CD1	2.55	0.42
1:B:56:THR:HG21	1:B:256:SER:OG	2.18	0.42
2:D:63:ILE:O	2:D:64:ALA:C	2.62	0.42
1:A:318:ILE:HG23	1:A:319:GLY:N	2.35	0.42
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.01	0.42
2:C:63:ILE:O	2:C:64:ALA:C	2.62	0.42
2:D:145:ILE:O	2:D:149:TRP:HB3	2.20	0.42
2:D:336:MET:HE3	2:D:388:LEU:CD1	2.50	0.42
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.54	0.42
1:B:54:ASN:C	1:B:130:ALA:HB2	2.44	0.42
2:C:143:GLU:O	2:C:147:ARG:HB3	2.20	0.42
2:D:58:PRO:HD2	2:D:83:TRP:CZ3	2.54	0.42
1:A:93:VAL:HG11	2:D:3:MET:HG2	2.01	0.42
1:A:190:ASP:HB3	2:C:74:GLN:O	2.20	0.42
1:A:260:ASP:OD1	1:A:261:PRO:HD2	2.20	0.42
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.17	0.42
1:B:437:ARG:NH1	1:B:454:GLU:OE2	2.52	0.42
1:A:230:GLU:C	1:A:233:PRO:HD2	2.45	0.42
1:B:33:GLN:HA	1:B:131:ALA:HB3	2.02	0.42
1:B:244:LEU:HB2	7:B:9224:HOH:O	2.19	0.42
1:B:283:THR:HB	1:B:284:PRO:CD	2.49	0.42
1:A:109:PHE:HB3	1:A:184:MET:SD	2.60	0.42
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.55	0.42
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.20	0.42
3:F:41:THR:O	3:F:44:ARG:CD	2.59	0.42
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.02	0.42
1:B:186:ARG:HD3	1:B:186:ARG:C	2.45	0.42
1:B:317:TRP:HE3	1:B:320:ARG:NH2	2.17	0.42
2:D:184:PHE:O	2:D:187:ILE:HG22	2.20	0.42
2:C:33:ASN:N	2:C:33:ASN:HD22	2.17	0.41
3:E:4:LEU:O	3:E:4:LEU:CG	2.68	0.41
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.35	0.41
1:B:172:ARG:HD3	2:D:55:TYR:C	2.46	0.41
2:D:77:HIS:CG	3:F:140:MET:HG2	2.55	0.41
3:F:93:GLY:O	3:F:96:ALA:HB3	2.20	0.41
1:A:40:LYS:HD2	7:A:5122:HOH:O	2.20	0.41
2:D:192:MET:HE3	2:D:280:PHE:CE2	2.55	0.41
2:D:354:ALA:O	2:D:358:ARG:HG3	2.20	0.41
3:F:59:LYS:HA	3:F:59:LYS:HD3	1.86	0.41
1:A:266:TYR:HB3	7:A:5058:HOH:O	2.19	0.41
3:E:137:THR:O	3:E:141:GLU:HG3	2.21	0.41
1:B:232:THR:HB	1:B:233:PRO:HD3	2.03	0.41
2:C:193:ILE:O	2:C:197:ARG:HG3	2.20	0.41
2:D:349:LYS:CE	2:D:385:LEU:HD21	2.51	0.41
3:E:32:LEU:HD13	3:E:60:LEU:HB3	2.03	0.41
3:E:74:GLU:O	3:E:78:ARG:HG3	2.21	0.41
1:B:460:GLU:OE1	1:B:463:ARG:HD3	2.21	0.41
2:D:264:PHE:HD2	2:D:265:PHE:CD1	2.39	0.41
2:D:389:LYS:CD	2:D:389:LYS:HG2	2.20	0.41
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.51	0.41
1:B:30:ARG:HD3	1:B:31:TRP:NE1	2.36	0.41
1:B:217:ILE:O	1:B:221:THR:HG23	2.21	0.41
1:B:288:MET:HB2	1:B:288:MET:HE3	1.78	0.41
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.56	0.41
2:D:385:LEU:CD1	2:D:388:LEU:CD1	2.97	0.41
2:D:389:LYS:CA	2:D:389:LYS:HB2	2.25	0.41
3:E:4:LEU:O	3:E:4:LEU:HD12	2.20	0.41
1:A:23:VAL:HA	1:A:27:GLU:OE2	2.20	0.41
1:A:381:ASP:HA	1:A:385:LYS:HE2	2.03	0.41
2:D:144:PHE:CD1	2:D:144:PHE:N	2.89	0.41
2:D:153:LEU:HG	2:D:154:PHE:CD1	2.56	0.41
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.54	0.40
1:B:243:GLU:O	1:B:247:MET:HG2	2.21	0.40
1:B:355:PRO:CD	1:B:403:ILE:HD11	2.51	0.40
3:F:86:ASP:O	3:F:87:ALA:C	2.64	0.40
1:A:43:ARG:HD2	1:A:43:ARG:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:HIS:CE1	7:A:5219:HOH:O	2.74	0.40
1:A:204:LEU:O	1:A:209:GLU:HG3	2.21	0.40
1:B:185:LYS:O	1:B:189:SER:HB2	2.22	0.40
1:A:115:TYR:OH	2:C:173:ASP:HA	2.21	0.40
1:A:183:GLY:HA2	1:A:422:GLN:HB2	2.03	0.40
3:F:98:MET:HG3	3:F:138:ARG:CG	2.51	0.40
2:D:340:ALA:HA	2:D:389:LYS:HD3	2.03	0.40
2:D:352:ILE:HG13	2:D:353:THR:N	2.35	0.40
3:E:24:THR:HG23	7:E:183:HOH:O	2.22	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	508/527 (96%)	487 (96%)	21 (4%)	0	100	100
1	B	508/527 (96%)	479 (94%)	28 (6%)	1 (0%)	43	37
2	C	386/389 (99%)	372 (96%)	12 (3%)	2 (0%)	24	16
2	D	386/389 (99%)	362 (94%)	21 (5%)	3 (1%)	16	9
3	E	164/170 (96%)	159 (97%)	4 (2%)	1 (1%)	21	13
3	F	164/170 (96%)	153 (93%)	11 (7%)	0	100	100
All	All	2116/2172 (97%)	2012 (95%)	97 (5%)	7 (0%)	36	30

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	121	PRO
1	B	40	LYS
2	D	388	LEU

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Mol	Chain	Res	Type
2	C	64	ALA
2	D	251	VAL
2	C	251	VAL
2	D	205	PRO

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	432/442 (98%)	421 (98%)	11 (2%)	42	39
1	B	431/442 (98%)	413 (96%)	18 (4%)	26	20
2	C	322/323 (100%)	314 (98%)	8 (2%)	42	39
2	D	322/323 (100%)	314 (98%)	8 (2%)	42	39
3	E	144/147 (98%)	139 (96%)	5 (4%)	32	27
3	F	144/147 (98%)	137 (95%)	7 (5%)	22	15
All	All	1795/1824 (98%)	1738 (97%)	57 (3%)	34	29

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	38	ASP
1	A	90	ASN
1	A	112	VAL
1	A	175	ARG
1	A	206	LEU
1	A	302	VAL
1	A	310	TYR
1	A	403	ILE
1	A	467	GLN
1	A	516	ASN
1	B	30	ARG
1	B	33	GLN
1	B	43	ARG

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Mol	Chain	Res	Type
1	B	90	ASN
1	B	110	LEU
1	B	112	VAL
1	B	125	TRP
1	B	186	ARG
1	B	213	THR
1	B	222	GLU
1	B	279	GLN
1	B	310	TYR
1	B	311	GLU
1	B	377	PRO
1	B	395	CYS
1	B	398	PRO
1	B	404	PRO
1	B	427	PRO
2	C	33	ASN
2	C	153	LEU
2	C	173	ASP
2	C	179	LEU
2	C	195	LEU
2	C	318	ARG
2	C	356	LEU
2	C	377	ARG
2	D	4	LEU
2	D	145	ILE
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	290	ILE
2	D	388	LEU
2	D	389	LYS
3	E	24	THR
3	E	44	ARG
3	E	60	LEU
3	E	120	PRO
3	E	121	PRO
3	F	11	THR
3	F	23	ASN
3	F	44	ARG
3	F	74	GLU
3	F	108	GLU
3	F	125	VAL

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Mol	Chain	Res	Type
3	F	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	129	GLN
1	A	155	ASN
1	A	161	ASN
1	A	168	HIS
1	A	203	ASN
1	A	227	ASN
1	A	249	ASN
1	A	268	ASN
1	A	272	ASN
1	A	273	ASN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	382	HIS
1	A	411	ASN
1	A	412	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	B	33	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	150	GLN
1	B	168	HIS
1	B	205	GLN
1	B	214	ASN
1	B	227	ASN
1	B	249	ASN
1	B	252	GLN
1	B	268	ASN

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Mol	Chain	Res	Type
1	B	273	ASN
1	B	278	GLN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	411	ASN
1	B	413	HIS
1	B	439	HIS
1	B	451	GLN
1	B	486	HIS
1	B	516	ASN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	125	GLN
2	C	146	ASN
2	C	161	ASN
2	C	285	GLN
2	C	293	GLN
2	C	301	ASN
2	D	98	HIS
2	D	161	ASN
2	D	285	GLN
2	D	289	GLN
2	D	296	GLN
2	D	301	ASN
3	E	45	ASN
3	E	144	ASN
3	E	158	GLN
3	E	165	HIS
3	E	167	GLN
3	F	7	HIS
3	F	45	ASN
3	F	144	ASN
3	F	167	GLN

5.3.3 RNA ⓘ

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 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\# Z > 2$
6	MOH	B	9001	4	1,1,1	0.49	0	-		

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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	167:GLN	C	168:SER	N	0.92

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	510/527 (96%)	0.37	20 (3%)	43	44	19, 32, 49, 63	10 (1%)
1	B	510/527 (96%)	0.38	21 (4%)	41	41	18, 33, 50, 62	9 (1%)
2	C	388/389 (99%)	-0.15	4 (1%)	79	81	11, 25, 39, 54	7 (1%)
2	D	388/389 (99%)	0.97	50 (12%)	7	7	18, 40, 61, 79	10 (2%)
3	E	166/170 (97%)	0.27	8 (4%)	35	36	21, 30, 44, 59	1 (0%)
3	F	166/170 (97%)	1.66	45 (27%)	1	1	27, 49, 67, 75	2 (1%)
All	All	2128/2172 (97%)	0.48	148 (6%)	22	22	11, 33, 55, 79	39 (1%)

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	389	LYS	5.9
2	D	352	ILE	5.7
1	A	319	GLY	5.6
3	F	19	ILE	4.5
3	F	67	LEU	4.5
3	F	4	LEU	4.5
3	E	121	PRO	4.4
3	F	71	ALA	4.4
2	D	380	ILE	4.4
1	A	317	TRP	4.3
2	D	385	LEU	4.3
3	F	83	PHE	4.2
3	F	65	ALA	4.0
3	F	84	GLY	3.8
1	B	527	ASN	3.8
3	F	25	LEU	3.6
2	D	381	VAL	3.6
3	F	60	LEU	3.6
1	B	403	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
3	F	72	PHE	3.5
2	D	373	PHE	3.4
3	F	20	ALA	3.4
2	D	388	LEU	3.4
2	D	250	ALA	3.4
1	A	310	TYR	3.3
2	D	331	ALA	3.3
2	C	3	MET	3.3
3	F	118	TYR	3.3
1	A	318	ILE	3.3
2	D	354	ALA	3.3
1	A	338	ASP	3.3
3	E	167	GLN	3.2
3	F	21	GLN	3.2
2	C	2	SER	3.1
2	D	270	PRO	3.1
2	D	338	LEU	3.1
3	F	117	ALA	3.1
3	F	69	ALA	3.1
2	D	205	PRO	3.0
2	D	384	VAL	3.0
1	A	316	ILE	3.0
3	F	128	PHE	3.0
1	B	264	ALA	3.0
3	F	93	GLY	3.0
2	D	302	CYS	2.9
3	E	4	LEU	2.9
3	F	77	PHE	2.9
3	F	101	ALA	2.9
3	F	16	VAL	2.9
3	E	23	ASN	2.9
1	B	504	ASP	2.9
3	F	103	ASP	2.9
2	D	223	VAL	2.8
3	F	161	VAL	2.8
1	A	44	THR	2.8
3	F	122	ILE	2.8
2	D	137	ASN	2.8
1	B	19	ALA	2.8
2	D	363	TRP	2.8
2	D	220	ASN	2.8
3	F	70	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	350	GLU	2.8
2	D	370	ARG	2.7
3	F	23	ASN	2.7
3	F	85	GLU	2.7
2	D	335	PHE	2.7
2	D	216	ALA	2.7
2	D	139	THR	2.7
3	E	22	LEU	2.7
2	D	386	ALA	2.6
1	A	435	THR	2.6
2	D	264	PHE	2.6
3	F	66	VAL	2.6
3	F	24	THR	2.6
2	D	246	PHE	2.6
3	F	120	PRO	2.6
1	B	268	ASN	2.6
2	D	88	THR	2.6
2	D	90	LEU	2.6
2	D	372	ASP	2.6
1	B	39	PHE	2.5
1	B	256	SER	2.5
1	A	308	TRP	2.5
1	B	258	ALA	2.5
3	F	11	THR	2.5
1	A	213	THR	2.4
1	A	429	LEU	2.4
1	B	55	GLU	2.4
3	F	22	LEU	2.4
2	D	339	PHE	2.4
2	D	374	LYS	2.4
2	D	142	ASP	2.4
2	D	272	PHE	2.4
3	F	125	VAL	2.4
3	F	163	VAL	2.4
3	E	168	SER	2.4
2	D	211	THR	2.4
3	F	82	ALA	2.3
2	D	221	GLY	2.3
2	D	204	VAL	2.3
1	B	269	THR	2.3
2	D	346	THR	2.3
1	A	430	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	148	TYR	2.3
2	D	368	ALA	2.3
2	C	311	ASP	2.3
1	A	409	ILE	2.3
1	B	309	VAL	2.3
1	B	395	CYS	2.3
1	A	324	TYR	2.3
3	F	32	LEU	2.3
1	A	397	ASP	2.3
1	B	317	TRP	2.3
3	F	134	GLN	2.2
2	D	303	LEU	2.2
3	F	79	HIS	2.2
1	A	514	ARG	2.2
2	D	371	ILE	2.2
1	A	334	ASP	2.2
1	B	325	GLY	2.2
1	B	332	LEU	2.2
2	D	332	LEU	2.2
3	E	21	GLN	2.2
2	C	308	GLU	2.2
2	D	344	ALA	2.2
3	F	100	ALA	2.2
2	D	357	TYR	2.2
1	A	333	LYS	2.2
2	D	229	LEU	2.1
1	A	323	LYS	2.1
3	F	34	GLN	2.1
1	A	206	LEU	2.1
3	F	81	THR	2.1
2	D	324	TRP	2.1
3	F	75	VAL	2.1
1	B	525	ALA	2.1
3	E	31	MET	2.1
1	B	310	TYR	2.1
3	F	42	PRO	2.1
2	D	369	SER	2.1
3	F	107	ALA	2.1
2	D	377	ARG	2.0
1	B	441	TYR	2.0
3	F	112	ILE	2.0
2	D	375	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
3	F	96	ALA	2.0
1	B	517	CYS	2.0
1	B	20	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	B	5005	1/1	0.84	0.12	68,68,68,68	0
5	CA	C	5007	1/1	0.84	0.12	77,77,77,77	0
6	MOH	B	9001	2/2	0.86	0.19	43,43,43,45	0
5	CA	A	5006	1/1	0.97	0.13	45,45,45,45	0
4	FE	A	5001	1/1	0.99	0.04	30,30,30,30	0
4	FE	A	5002	1/1	0.99	0.03	42,42,42,42	0
4	FE	B	5003	1/1	0.99	0.02	30,30,30,30	0
4	FE	B	5004	1/1	0.99	0.06	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.