



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:24 AM UTC

PDB ID : 1FZI / pdb_00001fzi
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM I PRESSURIZED WITH XENON GAS
Authors : Whittington, D.A.; Rosenzweig, A.C.; Frederick, C.A.; Lippard, S.J.
Deposited on : 2000-10-03
Resolution : 3.30 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:

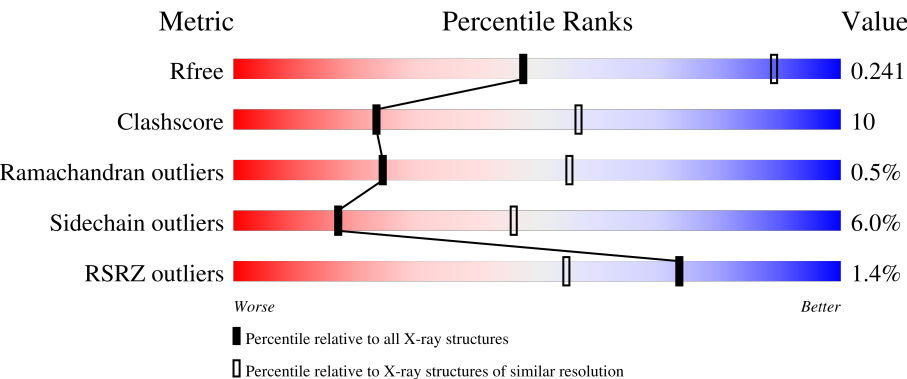
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	2% 71% 22% • •
1	B	527	2% 69% 25% • •
2	C	389	% 76% 20% • •
2	D	389	% 72% 23% • •
3	E	170	74% 19% • 5%

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Mol	Chain	Length	Quality of chain
3	F	170	% 74% 18% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17388 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	512	Total	C	N	O	S	0	0	0
			4186	2679	721	768	18			
1	B	512	Total	C	N	O	S	0	0	0
			4186	2679	721	768	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	384	Total	C	N	O	S	0	0	0
			3167	2038	547	575	7			
2	D	384	Total	C	N	O	S	0	0	0
			3167	2038	547	575	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	370	ARG	ALA	conflict	UNP P22869
D	370	ARG	ALA	conflict	UNP P22869

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	162	Total	C	N	O	S	0	0	0
			1336	847	240	244	5			
3	F	162	Total	C	N	O	S	0	0	0
			1336	847	240	244	5			

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

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

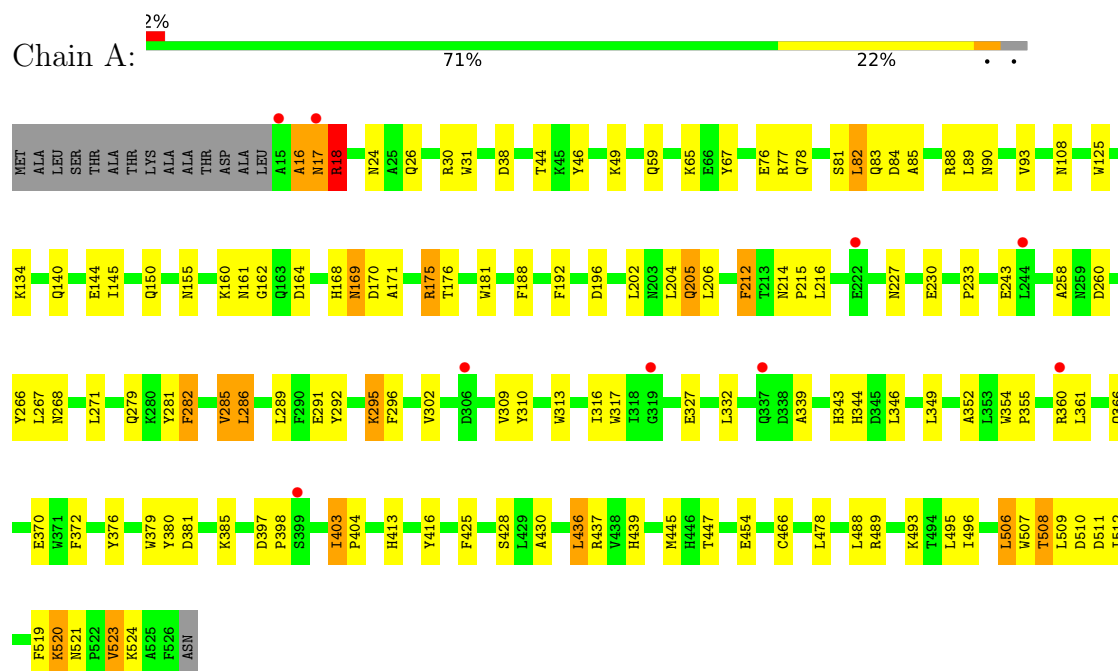
- Molecule 5 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	Xe 3	0	0
5	B	3	Total 3	Xe 3	0	0

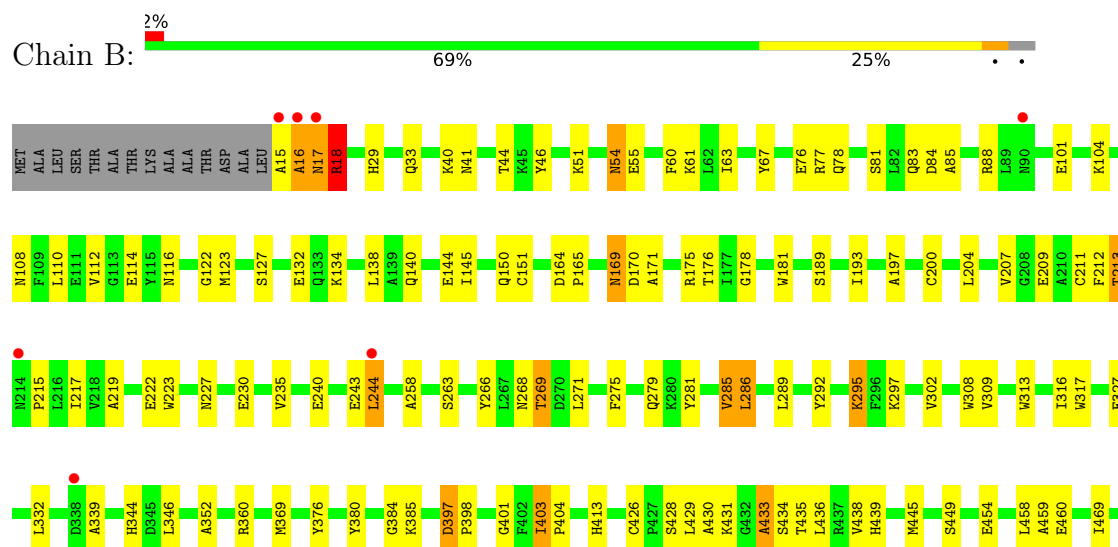
3 Residue-property plots

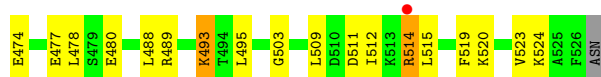
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

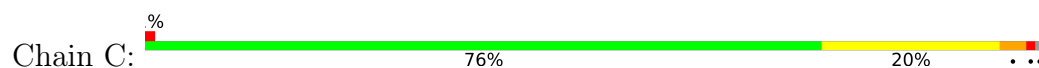


• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

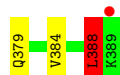
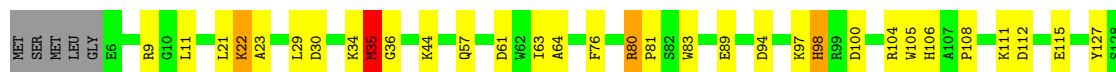




• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



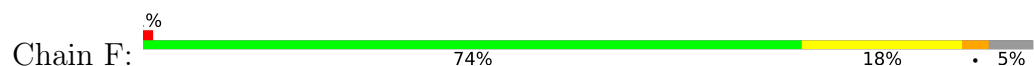
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

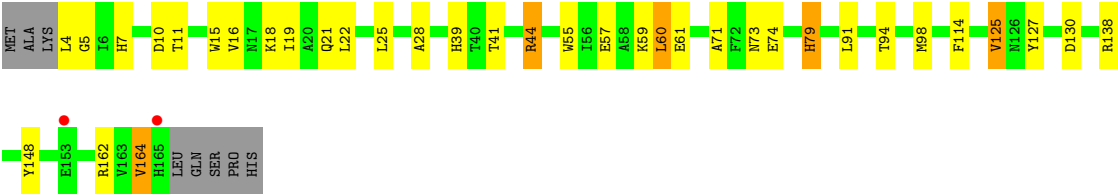


• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN



• 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	61.70Å 109.60Å 330.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.30 12.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	68.9 (12.00-3.30) 67.3 (12.00-3.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.99 (at 3.28Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.253 0.214 , 0.241	Depositor DCC
R_{free} test set	1129 reflections (4.47%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.637	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 26.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	17388	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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: XE, 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	0.57	0/4311	1.02	26/5856 (0.4%)
1	B	0.59	0/4311	1.05	26/5856 (0.4%)
2	C	0.60	1/3263 (0.0%)	0.98	25/4430 (0.6%)
2	D	0.57	0/3263	0.97	19/4430 (0.4%)
3	E	0.59	0/1364	0.99	10/1838 (0.5%)
3	F	0.61	0/1364	1.04	10/1838 (0.5%)
All	All	0.58	1/17876 (0.0%)	1.01	116/24248 (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
1	A	0	1
1	B	0	1
2	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	136	MET	SD-CE	-5.49	1.65	1.79

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	21	GLN	OE1-CD-NE2	-9.81	112.79	122.60
3	F	21	GLN	OE1-CD-NE2	-9.75	112.85	122.60
1	A	339	ALA	N-CA-C	9.26	121.14	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ALA	N-CA-C	9.16	120.96	110.97
1	B	316	ILE	N-CA-C	9.11	119.14	110.30
1	B	54	ASN	N-CA-C	-9.05	99.28	110.41
2	C	133	ILE	CB-CA-C	-8.32	99.26	112.16
2	D	105	TRP	N-CA-C	-7.69	98.88	109.95
2	D	144	PHE	N-CA-C	7.66	119.41	111.14
1	A	295	LYS	N-CA-C	-7.65	101.17	111.96
2	D	236	GLN	N-CA-C	7.48	122.41	113.28
3	F	5	GLY	N-CA-C	7.29	124.55	112.30
1	A	258	ALA	N-CA-C	7.26	120.24	111.82
1	B	426	CYS	CA-C-N	7.25	127.58	119.32
1	B	426	CYS	C-N-CA	7.25	127.58	119.32
2	C	104	ARG	N-CA-C	7.23	120.51	108.73
1	A	243	GLU	N-CA-C	7.12	119.05	111.28
1	A	16	ALA	N-CA-C	7.11	121.05	110.52
1	A	430	ALA	N-CA-C	7.10	120.25	110.24
1	B	266	TYR	N-CA-C	6.98	122.69	114.04
1	B	295	LYS	N-CA-C	-6.89	102.24	111.96
2	C	103	ARG	CA-C-N	-6.74	113.81	122.77
2	C	103	ARG	C-N-CA	-6.74	113.81	122.77
1	B	433	ALA	N-CA-C	6.67	125.01	110.80
1	B	478	LEU	N-CA-C	6.66	119.10	111.11
3	E	21	GLN	CG-CD-NE2	6.66	126.39	116.40
3	F	21	GLN	CG-CD-NE2	6.63	126.35	116.40
3	F	79	HIS	N-CA-C	6.58	122.28	113.72
2	C	63	ILE	N-CA-C	-6.56	96.84	107.28
1	B	258	ALA	N-CA-C	6.56	119.25	111.71
1	A	266	TYR	N-CA-C	6.48	122.67	114.31
1	A	285	VAL	N-CA-C	6.47	116.64	110.42
3	E	130	ASP	N-CA-C	-6.47	104.30	111.36
2	C	144	PHE	N-CA-C	6.44	118.09	111.14
2	C	146	ASN	N-CA-C	6.40	117.92	111.07
2	D	252	TYR	N-CA-C	6.39	117.94	110.97
1	A	309	VAL	N-CA-C	6.38	117.01	110.82
1	A	205	GLN	N-CA-C	6.36	119.45	111.24
1	A	93	VAL	N-CA-C	6.35	117.27	111.81
2	C	54	VAL	N-CA-C	6.35	117.50	108.93
1	B	85	ALA	N-CA-C	6.28	118.64	111.11
1	B	122	GLY	N-CA-C	-6.28	104.73	112.77
1	B	403	ILE	N-CA-C	-6.28	100.14	107.61
1	A	316	ILE	N-CA-C	6.22	116.27	110.42
3	E	73	ASN	N-CA-C	-6.18	102.55	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	169	GLU	N-CA-C	6.15	120.95	113.38
1	A	380	TYR	N-CA-C	6.15	117.65	111.07
1	B	285	VAL	N-CA-C	6.13	116.31	110.42
1	B	145	ILE	N-CA-C	-6.07	104.59	110.72
3	F	130	ASP	N-CA-C	-6.00	104.86	111.82
3	F	162	ARG	N-CA-C	-5.98	97.97	108.20
1	A	282	PHE	N-CA-C	5.94	118.72	111.82
3	E	118	TYR	N-CA-C	5.94	121.26	113.30
1	A	145	ILE	N-CA-C	-5.87	104.80	110.72
1	B	430	ALA	N-CA-C	5.85	118.55	110.35
2	C	169	GLU	N-CA-C	5.83	120.54	113.38
1	A	267	LEU	N-CA-C	5.82	118.09	111.11
2	D	142	ASP	N-CA-C	5.81	117.69	111.36
2	D	106	HIS	N-CA-C	5.81	118.08	111.11
1	B	431	LYS	N-CA-C	-5.80	106.21	113.28
2	D	98	HIS	N-CA-C	5.78	118.39	110.24
1	B	243	GLU	N-CA-C	5.78	118.36	111.71
1	B	397	ASP	N-CA-C	5.76	117.79	109.04
2	C	265	PHE	N-CA-C	5.71	117.31	111.14
2	C	236	GLN	N-CA-C	5.70	120.51	113.50
1	A	212	PHE	N-CA-C	5.65	119.87	112.13
2	C	149	TRP	N-CA-C	-5.65	105.20	111.36
2	D	388	LEU	N-CA-C	5.64	122.81	110.80
2	C	225	LYS	N-CA-C	5.63	117.89	111.02
2	C	142	ASP	N-CA-C	5.62	118.34	111.82
2	D	249	HIS	N-CA-C	5.59	119.27	112.23
1	A	291	GLU	N-CA-C	5.58	117.45	111.36
2	C	106	HIS	N-CA-C	5.53	116.98	111.07
3	F	71	ALA	N-CA-C	5.46	117.04	111.14
2	C	249	HIS	N-CA-C	5.46	119.10	112.23
3	E	149	ASP	N-CA-C	5.45	117.30	111.36
2	C	299	TYR	N-CA-C	5.42	118.11	111.82
2	D	63	ILE	N-CA-C	-5.42	98.66	107.28
1	A	162	GLY	N-CA-C	5.40	120.87	112.60
2	D	306	ASP	CA-C-N	5.40	125.74	119.47
2	D	306	ASP	C-N-CA	5.40	125.74	119.47
2	C	56	ALA	N-CA-C	-5.38	105.58	111.82
2	D	153	LEU	CA-CB-CG	5.37	135.09	116.30
1	A	17	ASN	N-CA-C	-5.37	99.37	110.80
1	A	496	ILE	N-CA-C	-5.37	105.49	110.53
1	A	85	ALA	N-CA-C	5.34	117.52	111.11
3	F	39	HIS	N-CA-C	5.33	121.60	113.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ASP	CA-C-N	5.32	124.83	119.19
1	A	164	ASP	C-N-CA	5.32	124.83	119.19
3	E	122	ILE	N-CA-C	-5.28	105.94	110.74
3	E	162	ARG	N-CA-C	-5.27	100.14	108.73
2	D	83	TRP	N-CA-C	-5.25	100.13	109.06
1	B	212	PHE	N-CA-C	5.24	119.31	112.13
3	F	74	GLU	N-CA-C	5.23	116.67	111.07
1	B	503	GLY	N-CA-C	5.22	120.42	114.67
2	D	265	PHE	N-CA-C	5.22	116.77	111.14
3	E	38	ASP	N-CA-C	5.22	117.05	111.36
3	E	39	HIS	N-CA-C	5.21	122.12	113.89
1	B	178	GLY	N-CA-C	5.20	122.95	112.34
2	C	105	TRP	N-CA-C	-5.18	101.80	109.94
2	C	153	LEU	CA-CB-CG	5.18	134.43	116.30
1	A	196	ASP	N-CA-C	-5.17	102.74	110.23
2	D	134	ARG	N-CA-C	5.15	117.57	111.33
2	C	137	ASN	CA-C-N	5.13	124.75	119.05
2	C	137	ASN	C-N-CA	5.13	124.75	119.05
1	B	309	VAL	N-CA-C	5.12	116.22	111.45
1	A	38	ASP	N-CA-C	5.12	117.91	109.76
2	C	145	ILE	CB-CA-C	-5.11	105.28	111.87
2	C	252	TYR	N-CA-C	5.10	116.53	110.97
2	D	149	TRP	N-CA-C	-5.10	105.81	111.36
1	B	193	ILE	N-CA-C	5.08	119.91	109.34
1	B	104	LYS	N-CA-C	-5.08	105.64	111.07
2	D	268	LEU	N-CA-C	5.07	119.59	113.41
1	B	213	THR	N-CA-C	5.06	117.18	111.11
3	F	73	ASN	N-CA-C	-5.05	104.01	110.53
2	C	148	TYR	N-CA-C	5.02	117.52	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	67	TYR	Sidechain
1	B	67	TYR	Sidechain
2	C	299	TYR	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	4186	0	3985	97	0
1	B	4186	0	3985	112	0
2	C	3167	0	3014	77	0
2	D	3167	0	3014	77	0
3	E	1336	0	1326	21	0
3	F	1336	0	1326	19	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	3	0	0	1	0
5	B	3	0	0	0	0
All	All	17388	0	16650	347	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 10.

All (347) 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:133:ILE:HG21	2:D:203:ILE:HD12	1.45	0.97
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.45	0.94
3:E:41:THR:O	3:E:44:ARG:HD2	1.70	0.91
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.19	0.88
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.19	0.86
1:B:512:ILE:HA	1:B:515:LEU:HD12	1.56	0.86
1:B:84:ASP:OD1	1:B:88:ARG:NH2	2.09	0.85
3:E:22:LEU:HD13	3:E:28:ALA:HA	1.58	0.85
2:C:136:MET:HE1	2:C:145:ILE:CD1	2.07	0.84
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.28	0.82
1:A:83:GLN:HB3	1:B:77:ARG:NH2	1.94	0.81
2:D:267:ARG:HH22	2:D:347:THR:HG21	1.46	0.81
2:C:225:LYS:CE	2:C:225:LYS:HA	2.10	0.80
1:A:84:ASP:OD1	1:A:88:ARG:NH2	2.15	0.79
2:D:357:TYR:HD1	2:D:377:ARG:HH12	1.30	0.78
2:C:136:MET:HE1	2:C:145:ILE:HD11	1.66	0.78
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:41:THR:O	3:F:44:ARG:HD2	1.84	0.77
1:B:123:MET:HB2	2:D:168:ARG:HD3	1.65	0.76
1:B:16:ALA:HA	2:C:362:ASP:CG	2.11	0.75
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.32	0.75
2:D:357:TYR:HD1	2:D:377:ARG:NH1	1.85	0.74
1:A:519:PHE:O	1:A:520:LYS:HE2	1.87	0.74
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.35	0.74
1:B:16:ALA:H	2:C:362:ASP:HB3	1.53	0.74
2:C:44:LYS:H	2:C:44:LYS:HD3	1.53	0.73
2:C:194:GLN:HE22	2:C:197:ARG:HH11	1.34	0.73
1:A:360:ARG:HH22	1:A:506:LEU:HD21	1.54	0.73
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.89	0.73
2:C:44:LYS:HD3	2:C:44:LYS:N	2.04	0.72
2:C:221:GLY:O	2:C:225:LYS:HG2	1.90	0.72
1:A:84:ASP:HB3	1:B:81:SER:OG	1.88	0.72
3:E:43:PHE:CZ	3:E:109:LYS:HE2	2.25	0.72
1:B:175:ARG:HD3	1:B:181:TRP:CE2	2.25	0.72
3:F:79:HIS:HD2	3:F:127:TYR:OH	1.72	0.72
1:A:44:THR:HG22	1:A:46:TYR:H	1.55	0.70
1:A:83:GLN:HB3	1:B:77:ARG:HH21	1.54	0.70
3:E:79:HIS:HD2	3:E:127:TYR:OH	1.75	0.70
2:D:357:TYR:CD1	2:D:377:ARG:NH1	2.60	0.70
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.75	0.69
1:A:24:ASN:OD1	1:A:26:GLN:HG2	1.92	0.69
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.73	0.69
3:E:138:ARG:HG3	3:E:138:ARG:HH11	1.58	0.68
2:D:258:GLN:HE21	2:D:261:ARG:HH21	1.41	0.68
3:E:138:ARG:NH1	3:E:142:LEU:HD11	2.08	0.68
1:A:17:ASN:O	1:A:18:ARG:HB2	1.93	0.67
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.77	0.67
2:C:136:MET:HE1	2:C:145:ILE:HD12	1.77	0.67
1:B:175:ARG:HG3	1:B:176:THR:N	2.10	0.67
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.41	0.67
1:A:413:HIS:HD2	1:A:428:SER:OG	1.78	0.67
1:A:493:LYS:NZ	1:A:508:THR:HG23	2.10	0.67
1:B:17:ASN:O	1:B:18:ARG:HB2	1.93	0.67
1:B:108:ASN:HD21	1:B:175:ARG:HH21	1.42	0.67
1:A:521:ASN:HB3	1:A:524:LYS:HD3	1.77	0.66
1:B:15:ALA:N	2:C:288:PHE:HE2	1.94	0.66
2:C:349:LYS:HD2	2:C:389:LYS:HE3	1.77	0.66
2:D:194:GLN:HE22	2:D:197:ARG:HH11	1.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:HG22	1:B:46:TYR:H	1.61	0.66
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.61	0.65
1:B:227:ASN:HD21	1:B:295:LYS:H	1.45	0.65
1:B:15:ALA:N	2:C:288:PHE:CE2	2.64	0.65
1:B:477:GLU:O	1:B:480:GLU:HG2	1.95	0.65
2:C:194:GLN:HE22	2:C:197:ARG:NH1	1.95	0.65
2:C:258:GLN:HE21	2:C:261:ARG:HH21	1.45	0.64
2:C:266:GLN:HE22	2:C:278:PRO:HA	1.62	0.64
1:A:354:TRP:CZ2	1:A:403:ILE:HD11	2.32	0.64
1:A:268:ASN:HD21	1:A:327:GLU:H	1.46	0.63
2:D:127:TYR:HE2	2:D:133:ILE:HG22	1.63	0.63
1:B:489:ARG:HD2	1:B:495:LEU:O	1.98	0.63
1:B:269:THR:HB	3:F:148:TYR:CE1	2.34	0.62
2:D:133:ILE:CG2	2:D:203:ILE:HD12	2.26	0.62
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.35	0.62
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.65	0.62
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.94	0.61
1:A:16:ALA:HB3	2:D:292:LYS:NZ	2.15	0.61
1:B:413:HIS:HD2	1:B:428:SER:OG	1.82	0.61
2:C:225:LYS:HD3	2:C:228:ARG:HH21	1.65	0.61
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.83	0.61
1:B:269:THR:HB	3:F:148:TYR:HE1	1.65	0.61
1:A:16:ALA:CB	2:D:292:LYS:NZ	2.64	0.61
1:B:403:ILE:HG12	1:B:515:LEU:HD22	1.82	0.60
2:C:259:PHE:CE1	2:C:356:LEU:HD13	2.36	0.60
1:A:18:ARG:NH1	2:C:133:ILE:HD11	2.16	0.60
1:B:268:ASN:HD21	1:B:327:GLU:H	1.50	0.60
3:E:101:ALA:HB3	3:E:138:ARG:HH12	1.66	0.59
2:D:336:MET:HE3	2:D:388:LEU:HD22	1.85	0.59
1:A:493:LYS:NZ	1:A:510:ASP:H	2.00	0.59
1:B:15:ALA:HB2	2:C:367:TYR:HE1	1.67	0.59
1:B:213:THR:O	1:B:217:ILE:HG12	2.01	0.59
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.85	0.59
1:A:354:TRP:CE2	1:A:403:ILE:HD11	2.38	0.59
1:B:175:ARG:HD3	1:B:181:TRP:CZ2	2.37	0.59
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.38	0.58
1:B:16:ALA:N	2:C:362:ASP:HB3	2.18	0.58
1:B:16:ALA:HA	2:C:362:ASP:OD2	2.02	0.58
2:C:136:MET:HE3	2:C:274:ASP:HB2	1.86	0.58
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.37	0.58
2:C:349:LYS:CE	2:C:389:LYS:HE3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:PRO:HA	2:D:111:LYS:HE3	1.85	0.57
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.87	0.57
2:C:96:PHE:O	2:C:99:ARG:NH2	2.38	0.57
2:C:136:MET:HE2	2:C:140:TRP:HD1	1.70	0.57
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.22	0.57
1:A:360:ARG:HH22	1:A:506:LEU:CD2	2.17	0.57
1:A:108:ASN:HD21	1:A:175:ARG:HH21	1.53	0.57
1:A:175:ARG:HG2	1:A:176:THR:N	2.17	0.57
2:C:61:ASP:OD1	3:E:7:HIS:HD2	1.88	0.57
3:F:98:MET:O	3:F:138:ARG:NH1	2.38	0.57
2:D:336:MET:HB3	2:D:388:LEU:HA	1.87	0.56
1:A:202:LEU:HD23	1:A:206:LEU:HD23	1.86	0.56
1:A:216:LEU:HD11	5:A:9005:XE:XE	2.84	0.56
1:B:140:GLN:O	1:B:144:GLU:HG2	2.06	0.56
2:C:388:LEU:CG	2:C:389:LYS:HD3	2.36	0.56
1:B:123:MET:HE1	1:B:200:CYS:SG	2.45	0.56
2:C:225:LYS:HA	2:C:225:LYS:HE3	1.84	0.56
1:B:435:THR:HG23	1:B:449:SER:O	2.05	0.56
3:F:19:ILE:HG12	3:F:60:LEU:HD13	1.86	0.56
3:F:15:TRP:HA	3:F:18:LYS:HG2	1.86	0.56
1:B:445:MET:HE3	1:B:523:VAL:HG13	1.86	0.55
1:A:436:LEU:HD21	1:A:447:THR:HG23	1.87	0.55
2:D:179:LEU:HD12	2:D:182:TRP:CE3	2.42	0.55
1:A:16:ALA:HA	2:C:129:ALA:O	2.07	0.55
2:C:225:LYS:CD	2:C:228:ARG:HH21	2.19	0.55
2:C:118:ARG:NH2	2:D:111:LYS:HD2	2.21	0.55
1:B:40:LYS:HE2	1:B:41:ASN:ND2	2.22	0.55
2:D:141:ARG:HA	2:D:145:ILE:HD12	1.88	0.55
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.42	0.55
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.72	0.54
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.42	0.54
1:B:44:THR:CG2	1:B:127:SER:HA	2.37	0.54
3:E:43:PHE:CE1	3:E:109:LYS:HE2	2.42	0.54
1:A:508:THR:HG22	1:A:511:ASP:H	1.71	0.54
1:B:401:GLY:HA2	1:B:514:ARG:NE	2.22	0.54
3:E:138:ARG:HH11	3:E:138:ARG:CG	2.20	0.54
2:C:26:GLU:CD	2:C:26:GLU:H	2.14	0.54
1:B:54:ASN:O	1:B:55:GLU:HB2	2.07	0.54
1:A:81:SER:OG	1:B:84:ASP:HB3	2.06	0.54
1:A:360:ARG:HE	1:A:489:ARG:NH2	2.06	0.54
1:B:369:MET:HE2	1:B:384:GLY:HA2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:LEU:HG	3:F:10:ASP:H	1.73	0.54
1:B:110:LEU:O	1:B:114:GLU:HG2	2.07	0.53
2:D:267:ARG:HH22	2:D:347:THR:CG2	2.20	0.53
2:C:376:ASP:HB3	2:C:379:GLN:HB3	1.90	0.53
1:A:493:LYS:CE	1:A:508:THR:HG23	2.39	0.53
1:B:219:ALA:HA	1:B:222:GLU:CD	2.33	0.53
2:D:333:ARG:HH11	2:D:333:ARG:HG2	1.73	0.53
2:D:194:GLN:HE22	2:D:197:ARG:NH1	2.06	0.53
1:B:33:GLN:HE22	1:B:132:GLU:H	1.56	0.53
2:D:336:MET:HE2	2:D:384:VAL:HG12	1.90	0.53
3:E:154:GLU:HA	3:E:157:LYS:HD3	1.91	0.53
1:A:230:GLU:C	1:A:233:PRO:HD2	2.34	0.53
2:C:378:ASP:O	2:C:382:LYS:HG2	2.09	0.53
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.98	0.53
2:D:170:ALA:O	2:D:176:ARG:NH2	2.42	0.52
2:D:336:MET:CE	2:D:356:LEU:HD21	2.40	0.52
2:C:349:LYS:CD	2:C:389:LYS:HE3	2.38	0.52
3:F:41:THR:O	3:F:44:ARG:CD	2.55	0.52
3:F:15:TRP:HA	3:F:18:LYS:CG	2.39	0.52
2:D:98:HIS:HE1	2:D:178:SER:OG	1.93	0.52
2:D:376:ASP:HB3	2:D:379:GLN:HB3	1.92	0.52
2:C:388:LEU:HG	2:C:389:LYS:HD3	1.91	0.51
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.92	0.51
1:B:169:ASN:O	2:D:35:MET:O	2.29	0.51
1:A:268:ASN:CG	1:A:327:GLU:HG2	2.36	0.51
1:A:416:TYR:HB3	1:A:447:THR:HG21	1.93	0.51
1:B:33:GLN:NE2	1:B:132:GLU:H	2.08	0.51
1:A:493:LYS:HZ1	1:A:510:ASP:H	1.57	0.51
1:B:63:ILE:HG23	2:D:191:GLN:CD	2.36	0.51
2:D:233:GLY:HA2	2:D:237:GLU:HG2	1.91	0.51
1:A:108:ASN:ND2	1:A:175:ARG:HH21	2.09	0.51
1:B:512:ILE:HA	1:B:515:LEU:CD1	2.34	0.51
2:D:94:ASP:HB3	2:D:97:LYS:HG3	1.92	0.51
2:D:150:GLY:O	2:D:153:LEU:HB3	2.11	0.51
1:B:108:ASN:ND2	1:B:175:ARG:HH21	2.09	0.51
1:A:268:ASN:ND2	1:A:327:GLU:H	2.09	0.50
1:A:381:ASP:HA	1:A:385:LYS:HD3	1.94	0.50
2:C:78:GLY:O	3:E:115:ARG:HD3	2.12	0.50
1:B:380:TYR:CE1	1:B:385:LYS:HD3	2.46	0.50
1:B:511:ASP:O	1:B:514:ARG:HG3	2.11	0.50
2:D:374:LYS:O	2:D:374:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:259:PHE:CE1	2:D:356:LEU:HD13	2.46	0.50
2:D:22:LYS:HE2	2:D:23:ALA:N	2.27	0.50
2:C:98:HIS:HE1	2:C:178:SER:OG	1.95	0.49
2:D:336:MET:HE1	2:D:356:LEU:HD21	1.93	0.49
3:F:79:HIS:CD2	3:F:127:TYR:OH	2.61	0.49
2:C:100:ASP:OD1	2:C:104:ARG:HG2	2.11	0.49
2:D:22:LYS:HE2	2:D:22:LYS:C	2.37	0.49
1:B:227:ASN:ND2	1:B:295:LYS:H	2.08	0.49
2:D:361:ASP:O	2:D:365:GLU:HG2	2.11	0.49
1:A:212:PHE:O	1:A:215:PRO:HD2	2.13	0.49
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.48	0.49
1:A:313:TRP:HA	1:A:317:TRP:HB3	1.94	0.49
1:B:18:ARG:NH1	2:D:133:ILE:HD11	2.28	0.49
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.46	0.49
1:A:413:HIS:CD2	1:A:428:SER:OG	2.64	0.49
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.47	0.49
1:B:171:ALA:O	1:B:175:ARG:HG2	2.12	0.48
2:C:225:LYS:HE3	2:C:225:LYS:CA	2.43	0.48
1:B:15:ALA:HB1	2:C:362:ASP:O	2.13	0.48
3:E:44:ARG:HG3	3:E:46:SER:O	2.13	0.48
2:D:34:LYS:O	2:D:35:MET:O	2.32	0.48
1:B:169:ASN:HA	2:D:35:MET:HA	1.96	0.48
1:A:140:GLN:O	1:A:144:GLU:HG2	2.13	0.48
1:A:493:LYS:HZ1	1:A:508:THR:HG23	1.77	0.48
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.95	0.48
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.14	0.47
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.95	0.47
2:D:361:ASP:OD2	2:D:377:ARG:NH1	2.48	0.47
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.63	0.47
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.97	0.47
1:B:519:PHE:C	1:B:520:LYS:HD2	2.40	0.47
1:A:30:ARG:HD2	1:A:31:TRP:NE1	2.29	0.47
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.62	0.47
2:C:6:GLU:HG2	2:C:7:ARG:N	2.29	0.47
2:D:269:ALA:N	2:D:270:PRO:CD	2.78	0.47
1:B:401:GLY:C	1:B:515:LEU:HD23	2.40	0.47
2:D:133:ILE:HG13	2:D:134:ARG:N	2.30	0.47
1:B:15:ALA:O	1:B:16:ALA:HB3	2.15	0.47
1:A:436:LEU:CD2	1:A:447:THR:HG23	2.45	0.46
1:A:227:ASN:HD21	1:A:296:PHE:H	1.62	0.46
2:C:225:LYS:CE	2:C:225:LYS:CA	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.98	0.46
1:A:160:LYS:NZ	1:A:161:ASN:HD21	2.14	0.46
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.50	0.46
1:B:230:GLU:OE2	2:D:9:ARG:HD3	2.16	0.46
1:A:16:ALA:CB	2:C:129:ALA:O	2.64	0.46
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.80	0.46
1:A:227:ASN:HD21	1:A:295:LYS:H	1.63	0.46
1:B:101:GLU:CD	1:B:360:ARG:HD3	2.41	0.46
1:B:209:GLU:HA	1:B:213:THR:HB	1.97	0.46
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.97	0.46
2:D:44:LYS:HA	2:D:44:LYS:HD3	1.68	0.46
1:A:16:ALA:HB2	2:D:292:LYS:NZ	2.31	0.46
1:B:401:GLY:HA2	1:B:514:ARG:HE	1.80	0.46
1:A:16:ALA:HB3	2:D:292:LYS:HZ2	1.79	0.46
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.80	0.46
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.50	0.46
1:B:493:LYS:HB2	1:B:493:LYS:NZ	2.30	0.46
1:B:110:LEU:HD23	1:B:151:CYS:SG	2.56	0.46
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.67	0.45
1:B:15:ALA:HB2	2:C:367:TYR:CE1	2.50	0.45
2:C:33:ASN:HD22	2:C:33:ASN:H	1.64	0.45
2:D:159:LEU:HG	2:D:248:VAL:HG13	1.98	0.45
1:A:366:GLN:O	1:A:370:GLU:HG3	2.17	0.45
2:D:111:LYS:O	2:D:115:GLU:HG3	2.16	0.45
1:A:169:ASN:HD22	1:A:170:ASP:N	2.14	0.45
2:D:233:GLY:HA2	2:D:237:GLU:CG	2.46	0.45
2:C:44:LYS:HE2	2:C:45:ARG:NH2	2.31	0.45
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.52	0.45
1:B:313:TRP:HA	1:B:317:TRP:HB3	1.99	0.45
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.47	0.45
1:A:77:ARG:NH1	1:B:83:GLN:HB3	2.32	0.45
1:B:169:ASN:HD22	1:B:170:ASP:N	2.14	0.45
1:B:268:ASN:OD1	1:B:327:GLU:HG2	2.17	0.45
2:C:266:GLN:HE21	2:C:266:GLN:HA	1.82	0.45
2:C:388:LEU:HB3	2:C:389:LYS:HZ2	1.82	0.45
2:D:159:LEU:HD23	2:D:186:LYS:HE3	1.98	0.45
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.25	0.44
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.91	0.44
2:D:203:ILE:HG13	2:D:204:VAL:HG23	2.00	0.44
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.43	0.44
2:D:57:GLN:OE1	2:D:176:ARG:NH2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:HH22	2:D:134:ARG:HG3	1.81	0.44
1:B:123:MET:SD	2:D:168:ARG:NH1	2.91	0.44
2:D:196:GLU:HG3	2:D:276:LEU:HD13	2.00	0.44
1:B:512:ILE:CA	1:B:515:LEU:HD12	2.39	0.44
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.53	0.44
1:A:360:ARG:HH21	1:A:489:ARG:CZ	2.31	0.44
2:D:223:VAL:HG13	2:D:335:PHE:HA	2.00	0.44
1:A:372:PHE:HB3	1:A:379:TRP:CD2	2.53	0.44
2:C:33:ASN:HD22	2:C:33:ASN:N	2.14	0.44
2:C:194:GLN:NE2	2:C:197:ARG:HH11	2.10	0.44
1:A:282:PHE:HB3	1:A:286:LEU:HD22	2.00	0.44
1:A:445:MET:HE3	1:A:523:VAL:HG13	2.00	0.44
1:B:17:ASN:HD21	2:D:134:ARG:NH1	2.16	0.44
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.53	0.44
1:A:360:ARG:NH1	2:C:29:LEU:HG	2.32	0.43
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.30	0.43
1:B:489:ARG:NH2	2:D:29:LEU:HB3	2.33	0.43
2:C:150:GLY:O	2:C:153:LEU:HB3	2.18	0.43
2:C:239:PHE:HB2	3:E:126:ASN:HA	1.99	0.43
1:B:165:PRO:HG2	2:D:30:ASP:HB3	1.99	0.43
1:B:15:ALA:O	1:B:16:ALA:CB	2.66	0.43
2:D:377:ARG:HH11	2:D:377:ARG:HB2	1.83	0.43
1:B:488:LEU:HD11	1:B:509:LEU:HD22	2.01	0.43
2:C:258:GLN:NE2	2:C:261:ARG:HH21	2.13	0.43
2:D:127:TYR:CE2	2:D:133:ILE:HG22	2.49	0.43
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.53	0.43
1:A:227:ASN:ND2	1:A:295:LYS:H	2.16	0.43
1:A:521:ASN:HD22	1:A:524:LYS:HZ3	1.66	0.43
1:B:116:ASN:CG	1:B:189:SER:HA	2.44	0.43
2:D:339:PHE:HA	2:D:342:LEU:HD22	1.99	0.43
1:A:188:PHE:CD1	1:A:192:PHE:CZ	3.07	0.43
1:A:360:ARG:NH2	1:A:506:LEU:HG	2.34	0.43
2:C:44:LYS:NZ	2:C:45:ARG:H	2.17	0.43
3:E:32:LEU:HD13	3:E:60:LEU:HB3	2.00	0.43
1:B:29:HIS:ND1	1:B:61:LYS:HG3	2.34	0.42
1:A:134:LYS:HD3	2:C:161:ASN:HD21	1.84	0.42
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.11	0.42
3:E:153:GLU:CD	3:E:153:GLU:H	2.28	0.42
1:B:18:ARG:HH22	2:D:134:ARG:CG	2.33	0.42
1:A:268:ASN:ND2	1:A:327:GLU:HG2	2.33	0.42
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.92	0.42
1:A:16:ALA:CA	2:C:129:ALA:O	2.67	0.42
1:B:15:ALA:HB1	2:C:362:ASP:C	2.45	0.42
1:B:439:HIS:CE1	1:B:454:GLU:OE1	2.70	0.42
1:B:493:LYS:NZ	1:B:493:LYS:CB	2.83	0.42
2:C:357:TYR:CD1	2:C:377:ARG:NH1	2.87	0.42
2:C:136:MET:CE	2:C:140:TRP:HD1	2.32	0.42
1:A:171:ALA:O	1:A:175:ARG:HB3	2.20	0.41
1:A:360:ARG:NE	1:A:489:ARG:NH2	2.67	0.41
2:D:240:ASP:HB2	3:F:125:VAL:CG2	2.50	0.41
1:A:76:GLU:HB3	1:B:76:GLU:OE1	2.21	0.41
1:B:123:MET:HE3	1:B:197:ALA:HA	2.02	0.41
3:F:94:THR:HG21	3:F:114:PHE:CD1	2.55	0.41
1:A:343:HIS:CD2	1:A:343:HIS:H	2.38	0.41
1:A:466:CYS:HB2	2:C:73:THR:HA	2.02	0.41
1:A:495:LEU:HD11	1:A:512:ILE:HG13	2.02	0.41
3:F:57:GLU:O	3:F:61:GLU:HG3	2.21	0.41
1:B:63:ILE:HG23	2:D:191:GLN:OE1	2.21	0.41
1:B:215:PRO:HB2	1:B:308:TRP:CE2	2.56	0.41
2:C:389:LYS:HE2	2:C:389:LYS:HB2	1.70	0.41
2:D:80:ARG:HD2	2:D:81:PRO:O	2.20	0.41
1:B:78:GLN:HE21	1:B:235:VAL:HA	1.85	0.41
1:B:207:VAL:HG11	1:B:275:PHE:HA	2.02	0.41
1:B:268:ASN:CG	1:B:327:GLU:HG2	2.46	0.41
1:A:425:PHE:HZ	1:A:447:THR:HG22	1.86	0.41
1:B:16:ALA:CB	2:D:129:ALA:O	2.69	0.41
1:B:286:LEU:HA	1:B:286:LEU:HD13	1.69	0.41
2:C:263:GLU:HB3	2:C:355:SER:HB2	2.02	0.41
2:C:357:TYR:OH	2:C:382:LYS:NZ	2.51	0.41
2:D:89:GLU:CD	3:F:125:VAL:HG13	2.45	0.41
3:E:79:HIS:CD2	3:E:127:TYR:OH	2.64	0.41
1:A:78:GLN:O	1:A:82:LEU:HD22	2.21	0.41
1:A:108:ASN:HD21	1:A:175:ARG:NH2	2.16	0.41
1:A:354:TRP:NE1	1:A:403:ILE:HD11	2.36	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.75	0.40
1:A:204:LEU:HG	1:A:205:GLN:HG3	2.03	0.40
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.56	0.40
2:C:235:TRP:CD1	2:C:235:TRP:C	2.99	0.40
1:B:60:PHE:HZ	1:B:244:LEU:HD11	1.87	0.40
3:E:32:LEU:HA	3:E:60:LEU:HD13	2.03	0.40
1:B:459:ALA:C	1:B:460:GLU:HG3	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:ARG:HE	1:B:515:LEU:HG	1.86	0.40
2:C:269:ALA:N	2:C:270:PRO:CD	2.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	510/527 (97%)	491 (96%)	18 (4%)	1 (0%)	43	71
1	B	510/527 (97%)	489 (96%)	17 (3%)	4 (1%)	16	45
2	C	382/389 (98%)	369 (97%)	12 (3%)	1 (0%)	36	65
2	D	382/389 (98%)	369 (97%)	9 (2%)	4 (1%)	12	40
3	E	160/170 (94%)	158 (99%)	2 (1%)	0	100	100
3	F	160/170 (94%)	158 (99%)	2 (1%)	0	100	100
All	All	2104/2172 (97%)	2034 (97%)	60 (3%)	10 (0%)	24	55

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	B	16	ALA
1	B	18	ARG
2	D	35	MET
1	B	433	ALA
1	B	434	SER
2	D	36	GLY
2	D	64	ALA
2	C	251	VAL
2	D	251	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/442 (98%)	405 (94%)	27 (6%)	16	44
1	B	432/442 (98%)	407 (94%)	25 (6%)	18	47
2	C	319/323 (99%)	300 (94%)	19 (6%)	17	46
2	D	319/323 (99%)	300 (94%)	19 (6%)	17	46
3	E	140/147 (95%)	131 (94%)	9 (6%)	16	44
3	F	140/147 (95%)	132 (94%)	8 (6%)	18	47
All	All	1782/1824 (98%)	1675 (94%)	107 (6%)	17	46

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	59	GLN
1	A	82	LEU
1	A	89	LEU
1	A	125	TRP
1	A	169	ASN
1	A	175	ARG
1	A	260	ASP
1	A	271	LEU
1	A	279	GLN
1	A	286	LEU
1	A	289	LEU
1	A	310	TYR
1	A	332	LEU
1	A	346	LEU
1	A	349	LEU
1	A	361	LEU
1	A	403	ILE
1	A	436	LEU
1	A	437	ARG
1	A	478	LEU
1	A	488	LEU

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Mol	Chain	Res	Type
1	A	506	LEU
1	A	508	THR
1	A	509	LEU
1	A	520	LYS
1	A	523	VAL
1	B	17	ASN
1	B	18	ARG
1	B	51	LYS
1	B	112	VAL
1	B	138	LEU
1	B	169	ASN
1	B	204	LEU
1	B	240	GLU
1	B	244	LEU
1	B	263	SER
1	B	269	THR
1	B	271	LEU
1	B	279	GLN
1	B	286	LEU
1	B	289	LEU
1	B	332	LEU
1	B	346	LEU
1	B	429	LEU
1	B	436	LEU
1	B	458	LEU
1	B	469	ILE
1	B	474	GLU
1	B	493	LYS
1	B	514	ARG
1	B	524	LYS
2	C	21	LEU
2	C	29	LEU
2	C	33	ASN
2	C	44	LYS
2	C	67	LEU
2	C	93	VAL
2	C	133	ILE
2	C	153	LEU
2	C	159	LEU
2	C	168	ARG
2	C	171	LEU
2	C	173	ASP

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Mol	Chain	Res	Type
2	C	179	LEU
2	C	225	LYS
2	C	229	LEU
2	C	266	GLN
2	C	303	LEU
2	C	356	LEU
2	C	389	LYS
2	D	11	LEU
2	D	21	LEU
2	D	22	LYS
2	D	35	MET
2	D	80	ARG
2	D	153	LEU
2	D	159	LEU
2	D	171	LEU
2	D	173	ASP
2	D	225	LYS
2	D	276	LEU
2	D	303	LEU
2	D	308	GLU
2	D	333	ARG
2	D	342	LEU
2	D	347	THR
2	D	356	LEU
2	D	377	ARG
2	D	388	LEU
3	E	25	LEU
3	E	44	ARG
3	E	60	LEU
3	E	102	LYS
3	E	125	VAL
3	E	135	LEU
3	E	138	ARG
3	E	161	VAL
3	E	162	ARG
3	F	11	THR
3	F	16	VAL
3	F	25	LEU
3	F	44	ARG
3	F	60	LEU
3	F	91	LEU
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 (77) 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	133	GLN
1	A	155	ASN
1	A	161	ASN
1	A	168	HIS
1	A	169	ASN
1	A	203	ASN
1	A	227	ASN
1	A	249	ASN
1	A	268	ASN
1	A	273	ASN
1	A	279	GLN
1	A	337	GLN
1	A	343	HIS
1	A	344	HIS
1	A	413	HIS
1	A	422	GLN
1	A	439	HIS
1	A	486	HIS
1	A	521	ASN
1	B	17	ASN
1	B	59	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	133	GLN
1	B	161	ASN
1	B	168	HIS
1	B	169	ASN
1	B	203	ASN
1	B	227	ASN
1	B	249	ASN

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Mol	Chain	Res	Type
1	B	259	ASN
1	B	268	ASN
1	B	273	ASN
1	B	279	GLN
1	B	343	HIS
1	B	344	HIS
1	B	382	HIS
1	B	411	ASN
1	B	412	ASN
1	B	413	HIS
1	B	439	HIS
1	B	442	ASN
1	B	472	GLN
1	B	486	HIS
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	194	GLN
2	C	258	GLN
2	C	266	GLN
2	C	283	GLN
2	C	285	GLN
2	C	301	ASN
2	D	98	HIS
2	D	161	ASN
2	D	194	GLN
2	D	258	GLN
2	D	283	GLN
2	D	285	GLN
2	D	301	ASN
3	E	7	HIS
3	E	39	HIS
3	E	45	ASN
3	E	79	HIS
3	E	144	ASN
3	F	7	HIS
3	F	45	ASN
3	F	79	HIS
3	F	134	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

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](#)

There are no chain breaks in this entry.

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	512/527 (97%)	0.08	9 (1%) 67 49	0, 7, 42, 83	0
1	B	512/527 (97%)	0.06	8 (1%) 70 52	0, 8, 44, 120	0
2	C	384/389 (98%)	-0.05	5 (1%) 75 56	0, 5, 33, 116	0
2	D	384/389 (98%)	-0.02	5 (1%) 75 56	0, 5, 38, 92	0
3	E	162/170 (95%)	0.05	0 100 100	0, 5, 34, 72	0
3	F	162/170 (95%)	-0.00	2 (1%) 76 58	0, 5, 32, 54	0
All	All	2116/2172 (97%)	0.02	29 (1%) 73 55	0, 6, 41, 120	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	ALA	4.7
1	A	244	LEU	3.9
2	C	225	LYS	3.4
1	B	90	ASN	3.3
2	D	350	GLU	3.3
1	B	338	ASP	3.2
1	B	15	ALA	3.1
1	A	360	ARG	3.0
1	A	17	ASN	2.9
1	B	214	ASN	2.9
1	B	514	ARG	2.8
1	B	244	LEU	2.8
1	B	16	ALA	2.8
1	B	17	ASN	2.8
2	D	389	LYS	2.6
2	C	389	LYS	2.6
1	A	319	GLY	2.6
2	C	382	LYS	2.6
3	F	165	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	337	GLN	2.6
1	A	306	ASP	2.4
1	A	222	GLU	2.4
2	D	201	ALA	2.3
2	C	301	ASN	2.3
1	A	399	SER	2.2
2	D	322	GLY	2.2
2	C	247	SER	2.2
3	F	153	GLU	2.1
2	D	308	GLU	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	XE	A	9005	1/1	0.60	0.16	10,10,10,10	1
4	FE	B	5004	1/1	0.66	0.22	15,15,15,15	0
4	FE	A	5002	1/1	0.88	0.15	10,10,10,10	0
5	XE	A	9006	1/1	0.92	0.05	15,15,15,15	1
5	XE	B	9003	1/1	0.97	0.07	15,15,15,15	1
5	XE	B	9002	1/1	0.98	0.17	10,10,10,10	0
4	FE	B	5003	1/1	0.98	0.04	15,15,15,15	0
5	XE	B	9004	1/1	0.98	0.06	10,10,10,10	1
5	XE	A	9001	1/1	0.99	0.15	10,10,10,10	0
4	FE	A	5001	1/1	0.99	0.06	10,10,10,10	0

6.5 Other polymers ⓘ

There are no such residues in this entry.