



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:31 PM UTC

PDB ID : 1FZ1 / pdb_00001fz1
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM III OXIDIZED
Authors : Whittington, D.A.; Lippard, S.J.
Deposited on : 2000-10-03
Resolution : 1.96 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:

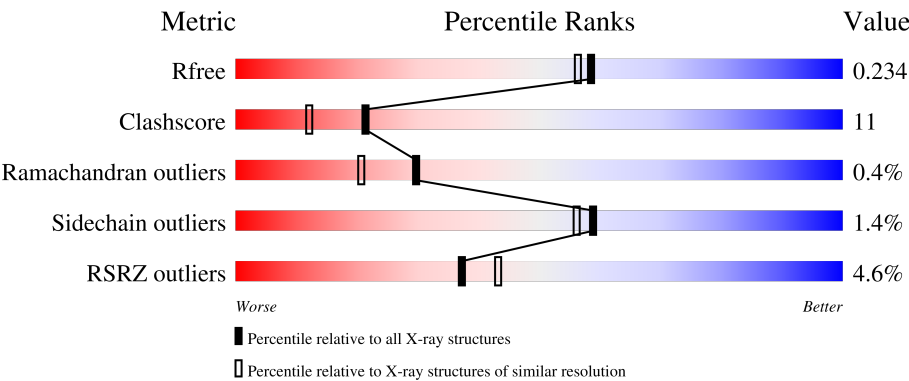
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	3% 73% 22% ..
1	B	527	2% 70% 25% ..
2	C	389	% 81% 17% .
2	D	389	7% 71% 26% ..
3	E	170	3% 79% 18% ..

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Mol	Chain	Length	Quality of chain
3	F	170	21% 72% 24% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18852 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	511	Total	C	N	O	S	0	0	0
			4185	2677	721	769	18			
1	B	511	Total	C	N	O	S	0	0	0
			4185	2677	721	769	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	0	0	0
			3193	2054	551	580	8			
2	D	387	Total	C	N	O	S	0	0	0
			3183	2048	549	578	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	0	0	0
			1368	867	246	250	5			
3	F	168	Total	C	N	O	S	0	0	0
			1386	878	250	253	5			

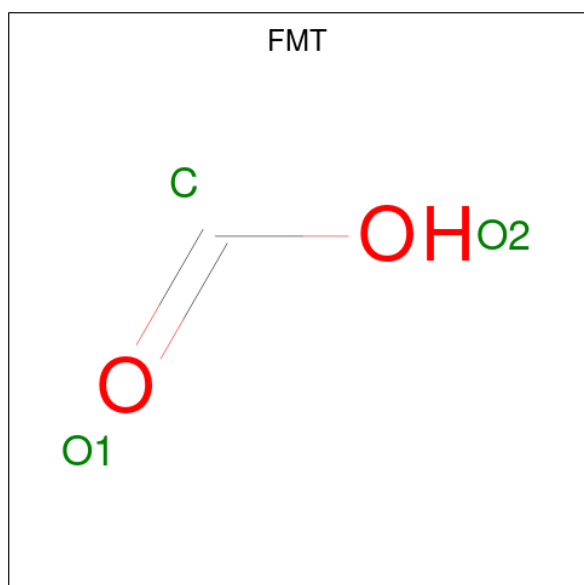
- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Ca 1 1	0	0
5	C	3	Total Ca 3 3	0	0

- Molecule 6 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	300	Total O 300 300	0	0
7	B	290	Total O 290 290	0	0

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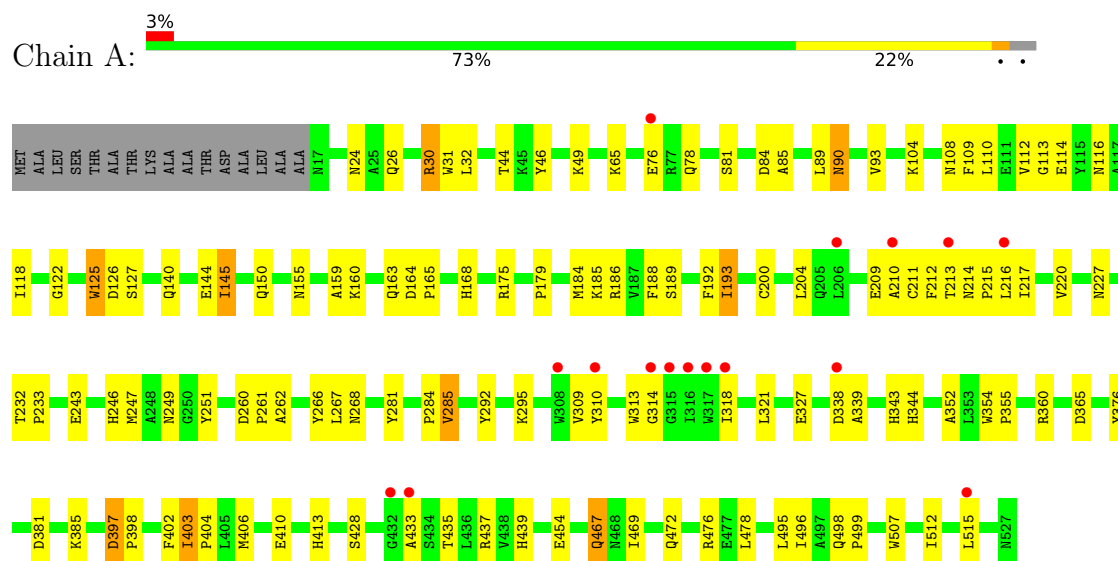
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	324	Total 324	O 324	0	0
7	D	192	Total 192	O 192	0	0
7	E	163	Total 163	O 163	0	0
7	F	72	Total 72	O 72	0	0

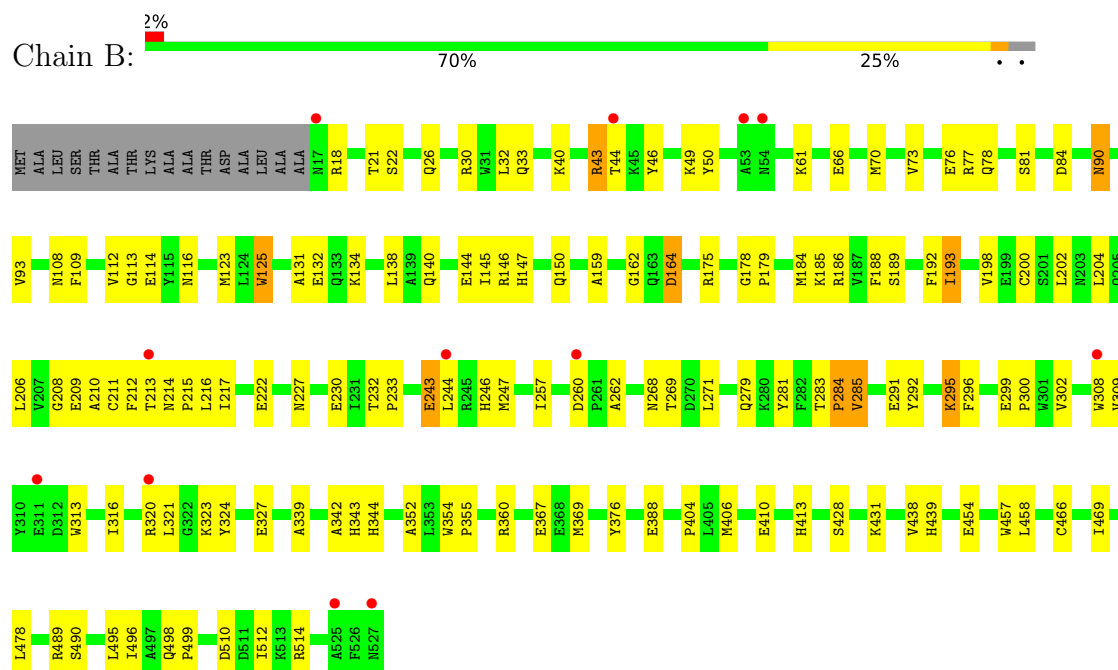
3 Residue-property plots [i](#)

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

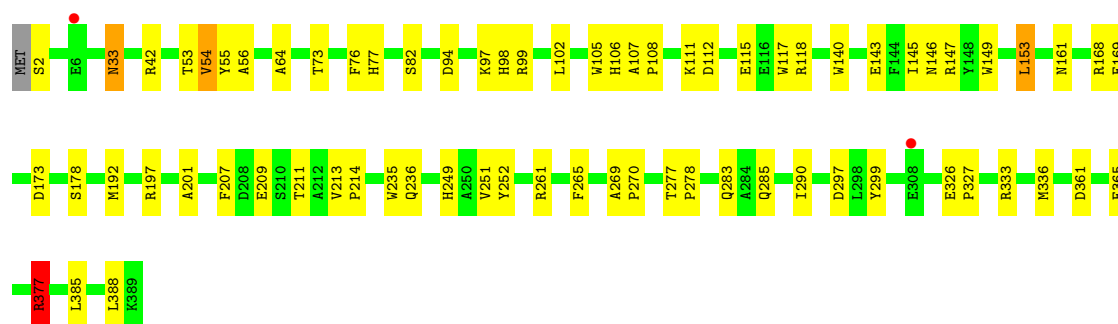


• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN



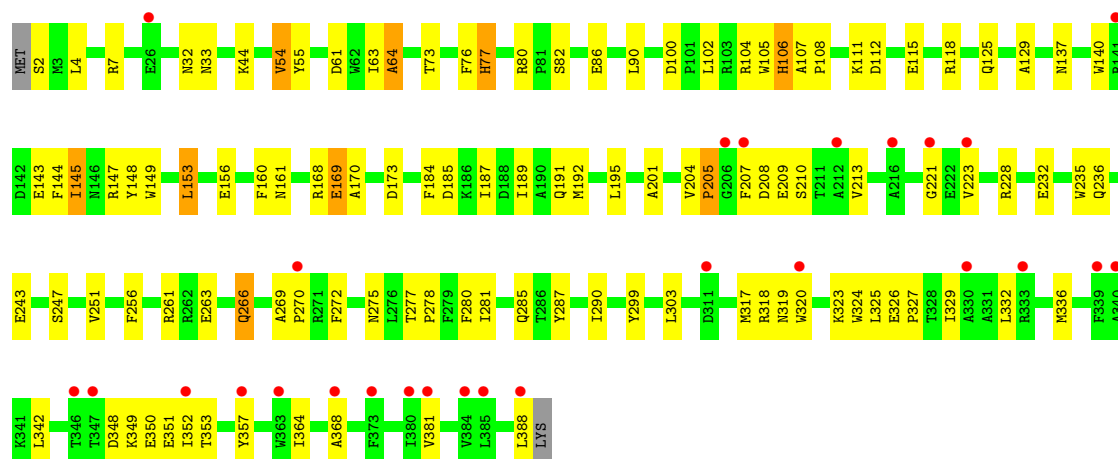
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C:  81% 17%



• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D:  71% 26% 7%



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain E:  79% 18% 3%



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F:  72% 24% 21%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.40Å 171.97Å 221.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.80 – 1.96 22.80 – 1.96	Depositor EDS
% Data completeness (in resolution range)	93.0 (22.80-1.96) 93.1 (22.80-1.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.18 (at 1.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.200 , 0.234 0.200 , 0.234	Depositor DCC
R_{free} test set	6400 reflections (3.29%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18852	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: FMT, FE, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/4310	0.90	18/5853 (0.3%)
1	B	0.36	0/4310	0.90	18/5853 (0.3%)
2	C	0.41	0/3289	0.88	14/4464 (0.3%)
2	D	0.35	0/3279	0.85	10/4453 (0.2%)
3	E	0.39	0/1396	0.87	6/1880 (0.3%)
3	F	0.31	0/1416	0.80	2/1907 (0.1%)
All	All	0.37	0/18000	0.88	68/24410 (0.3%)

There are no bond length outliers.

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ALA	N-CA-C	10.38	122.18	111.07
2	C	105	TRP	N-CA-C	-7.89	98.59	109.95
1	B	496	ILE	N-CA-C	-7.77	103.23	110.53
1	A	309	VAL	N-CA-C	7.76	117.83	110.53
1	A	164	ASP	CA-C-N	7.76	127.81	119.28
1	A	164	ASP	C-N-CA	7.76	127.81	119.28
1	B	193	ILE	N-CA-C	7.58	121.13	113.47
2	C	106	HIS	N-CA-C	7.20	119.75	111.11
1	B	309	VAL	N-CA-C	6.98	117.09	110.53
2	D	106	HIS	N-CA-C	6.96	118.52	111.07
2	C	149	TRP	N-CA-C	-6.84	103.90	111.36
1	A	339	ALA	N-CA-C	6.82	118.60	111.03
1	B	431	LYS	N-CA-C	-6.82	105.11	113.50
2	C	377	ARG	N-CA-C	6.64	118.52	111.28
3	E	130	ASP	N-CA-C	-6.61	104.15	111.36
2	D	204	VAL	CA-C-N	6.57	128.06	119.84
2	D	204	VAL	C-N-CA	6.57	128.06	119.84
1	A	266	TYR	N-CA-C	6.56	121.94	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ILE	N-CA-C	-6.55	104.11	110.72
2	D	105	TRP	N-CA-C	-6.54	100.53	109.95
1	B	285	VAL	N-CA-C	6.42	116.58	110.42
1	B	243	GLU	N-CA-C	6.35	120.13	112.38
3	F	118	TYR	N-CA-C	6.28	120.25	112.59
1	A	285	VAL	N-CA-C	6.25	116.40	110.53
3	E	118	TYR	N-CA-C	6.18	121.58	113.30
1	B	93	VAL	N-CA-C	6.14	117.09	111.81
2	C	169	GLU	N-CA-C	6.09	120.87	113.38
1	A	496	ILE	N-CA-C	-5.98	104.91	110.53
3	E	39	HIS	N-CA-C	5.93	122.51	113.61
1	A	267	LEU	N-CA-C	5.93	118.25	111.02
2	D	148	TYR	N-CA-C	5.88	117.77	111.36
2	C	236	GLN	N-CA-C	5.76	120.47	113.38
1	B	478	LEU	N-CA-C	5.73	117.99	111.11
1	A	478	LEU	N-CA-C	5.73	117.98	111.11
2	D	54	VAL	N-CA-C	5.69	116.76	109.30
1	A	397	ASP	CA-C-N	5.67	125.52	119.28
1	A	397	ASP	C-N-CA	5.67	125.52	119.28
1	B	178	GLY	CA-C-N	5.67	125.20	119.19
1	B	178	GLY	C-N-CA	5.67	125.20	119.19
1	A	243	GLU	N-CA-C	5.66	118.39	111.82
1	A	122	GLY	N-CA-C	-5.63	105.56	112.77
2	C	56	ALA	N-CA-C	-5.62	105.24	111.36
2	C	53	THR	N-CA-C	5.60	120.38	112.93
2	D	77	HIS	N-CA-C	-5.50	101.77	109.96
2	C	249	HIS	N-CA-C	5.40	119.03	112.23
2	C	299	TYR	N-CA-C	5.40	119.03	112.23
1	B	316	ILE	N-CA-C	5.33	115.47	110.30
1	A	193	ILE	N-CA-C	5.33	120.43	109.34
3	E	74	GLU	N-CA-C	5.28	117.03	111.28
2	C	265	PHE	N-CA-C	5.27	116.83	111.14
2	C	252	TYR	N-CA-C	5.27	116.71	110.97
1	A	93	VAL	N-CA-C	5.23	116.31	111.81
1	B	145	ILE	N-CA-C	-5.22	105.45	110.72
3	E	53	TYR	N-CA-C	5.18	116.93	111.28
3	F	39	HIS	N-CA-C	5.14	122.01	113.89
1	A	85	ALA	N-CA-C	5.14	116.57	111.07
3	E	79	HIS	N-CA-C	5.13	121.30	113.61
2	D	236	GLN	N-CA-C	5.10	119.66	113.38
2	C	54	VAL	N-CA-C	5.07	116.22	109.37
1	B	164	ASP	CA-C-N	5.07	124.68	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ASP	C-N-CA	5.07	124.68	119.56
2	C	77	HIS	N-CA-C	-5.05	102.57	110.10
1	B	162	GLY	N-CA-C	5.05	120.32	112.60
2	D	318	ARG	N-CA-C	-5.04	105.97	111.82
1	B	342	ALA	N-CA-C	5.03	117.15	111.11
2	D	169	GLU	N-CA-C	5.01	119.55	113.38
1	B	295	LYS	N-CA-C	-5.01	104.89	111.96
1	A	104	LYS	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4185	0	3981	88	0
1	B	4185	0	3981	120	0
2	C	3193	0	3042	48	0
2	D	3183	0	3029	88	0
3	E	1368	0	1363	24	0
3	F	1386	0	1377	40	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	C	3	0	0	0	0
6	A	3	0	1	0	0
7	A	300	0	0	6	0
7	B	290	0	0	6	0
7	C	324	0	0	6	0
7	D	192	0	0	6	0
7	E	163	0	0	1	0
7	F	72	0	0	7	0
All	All	18852	0	16774	372	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 11.

All (372) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:41:THR:HG23	3:F:43:PHE:H	1.26	1.01
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.04	0.99
1:A:78:GLN:HE22	1:A:150:GLN:HE21	0.95	0.91
1:A:435:THR:HG21	1:A:437:ARG:HE	1.38	0.87
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.55	0.87
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.21	0.86
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.57	0.85
3:E:41:THR:O	3:E:44:ARG:HD2	1.76	0.85
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.22	0.83
1:B:44:THR:HG22	1:B:46:TYR:H	1.42	0.82
1:B:268:ASN:HD21	1:B:327:GLU:H	1.24	0.82
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.61	0.80
1:A:435:THR:CG2	1:A:437:ARG:HE	1.95	0.79
3:F:40:THR:O	3:F:41:THR:HG22	1.83	0.79
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.65	0.79
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.82	0.79
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.64	0.79
1:B:209:GLU:HA	1:B:213:THR:OG1	1.83	0.79
1:A:109:PHE:HB3	1:A:184:MET:HE2	1.65	0.78
1:A:78:GLN:HE22	1:A:150:GLN:NE2	1.79	0.77
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.78	0.77
3:F:41:THR:O	3:F:44:ARG:HD2	1.83	0.77
2:C:361:ASP:OD2	2:C:377:ARG:HD3	1.84	0.76
1:A:44:THR:HG22	1:A:46:TYR:H	1.50	0.76
1:A:467:GLN:HG3	7:A:9288:HOH:O	1.84	0.76
3:E:98:MET:HE1	3:E:107:ALA:CB	2.16	0.76
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.16	0.75
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.36	0.74
1:B:406:MET:O	1:B:410:GLU:HG3	1.88	0.73
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.71	0.72
3:F:58:ALA:O	3:F:62:GLU:HG3	1.90	0.72
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.84	0.71
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.71	0.71
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.90	0.71
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.26	0.71
3:F:153:GLU:H	3:F:153:GLU:CD	1.99	0.71
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.74	0.70
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.21	0.70
2:C:336:MET:HE3	2:C:388:LEU:HG	1.74	0.70
1:A:227:ASN:HD21	1:A:295:LYS:H	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASN:HD21	1:A:327:GLU:H	1.40	0.69
3:F:57:GLU:O	3:F:61:GLU:HG3	1.93	0.69
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.39	0.69
2:C:365:GLU:HG3	7:C:5249:HOH:O	1.93	0.69
1:B:244:LEU:HG	7:B:5024:HOH:O	1.92	0.69
1:B:33:GLN:NE2	1:B:132:GLU:H	1.91	0.68
1:B:367:GLU:HG3	7:B:5031:HOH:O	1.93	0.68
1:B:33:GLN:HE22	1:B:132:GLU:H	1.42	0.67
2:D:228:ARG:O	2:D:232:GLU:HG3	1.94	0.67
1:B:413:HIS:HD2	1:B:428:SER:OG	1.77	0.67
2:D:348:ASP:OD2	2:D:350:GLU:HB3	1.93	0.67
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.60	0.67
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.78	0.67
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.10	0.67
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.76	0.66
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.78	0.65
3:F:9:ASN:OD1	3:F:11:THR:HG23	1.95	0.65
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.77	0.65
1:B:30:ARG:O	1:B:30:ARG:HD3	1.97	0.65
2:D:153:LEU:C	2:D:153:LEU:HD12	2.22	0.65
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.78	0.65
1:B:269:THR:HG23	7:B:5213:HOH:O	1.96	0.65
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.44	0.65
1:A:213:THR:O	1:A:217:ILE:HG12	1.98	0.64
3:F:13:ASP:O	3:F:16:VAL:HG22	1.97	0.64
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.97	0.63
1:A:140:GLN:O	1:A:144:GLU:HG2	1.98	0.63
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.47	0.63
3:E:98:MET:HE3	3:E:98:MET:O	1.98	0.62
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.82	0.62
1:B:227:ASN:HD21	1:B:295:LYS:H	1.46	0.62
3:E:22:LEU:HD11	3:E:31:MET:SD	2.39	0.62
1:B:489:ARG:HD2	1:B:495:LEU:O	1.99	0.62
1:B:192:PHE:O	1:B:200:CYS:HB3	2.00	0.62
1:B:269:THR:HG21	7:F:237:HOH:O	1.99	0.62
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.30	0.61
2:D:111:LYS:O	2:D:115:GLU:HG3	2.00	0.61
3:E:24:THR:HG22	3:E:27:LYS:H	1.65	0.61
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.82	0.61
3:E:101:ALA:HA	3:E:106:GLU:OE2	2.01	0.61
3:E:98:MET:HE1	3:E:107:ALA:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:O	1:B:217:ILE:HG12	2.02	0.60
2:C:333:ARG:HD2	7:C:5327:HOH:O	2.01	0.60
2:D:326:GLU:HB3	2:D:327:PRO:HD3	1.83	0.60
3:F:24:THR:HG21	7:F:214:HOH:O	2.02	0.60
3:E:59:LYS:HE2	7:E:209:HOH:O	2.02	0.60
1:A:406:MET:O	1:A:410:GLU:HG3	2.02	0.59
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.84	0.59
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.02	0.59
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.84	0.59
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.82	0.59
1:B:268:ASN:ND2	1:B:327:GLU:H	1.95	0.59
2:D:44:LYS:HG3	7:D:499:HOH:O	2.01	0.59
1:B:26:GLN:HE21	1:B:61:LYS:HD2	1.66	0.59
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.83	0.59
2:D:352:ILE:HG13	2:D:353:THR:N	2.18	0.59
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.36	0.59
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.85	0.58
1:A:209:GLU:HA	1:A:213:THR:HB	1.85	0.58
3:F:22:LEU:HD13	3:F:28:ALA:HA	1.83	0.58
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.38	0.58
2:D:324:TRP:C	2:D:327:PRO:HD2	2.28	0.58
2:C:361:ASP:OD2	2:C:377:ARG:CD	2.50	0.58
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.68	0.58
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.03	0.58
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.12	0.58
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.84	0.58
3:F:15:TRP:O	3:F:19:ILE:HG23	2.04	0.58
1:B:18:ARG:O	2:D:129:ALA:HA	2.04	0.58
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.85	0.57
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.51	0.57
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.37	0.57
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.85	0.57
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.50	0.57
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.39	0.57
3:F:41:THR:HG23	3:F:43:PHE:N	2.09	0.57
1:A:155:ASN:HD22	1:A:168:HIS:CD2	2.12	0.57
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.87	0.57
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.86	0.57
1:A:204:LEU:O	1:A:209:GLU:HG3	2.05	0.56
2:D:247:SER:HG	2:D:324:TRP:CD1	2.23	0.56
1:A:338:ASP:OD1	1:A:433:ALA:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.87	0.56
3:F:132:GLU:HG3	7:F:185:HOH:O	2.05	0.56
1:A:76:GLU:HG2	1:B:76:GLU:OE2	2.06	0.56
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.88	0.56
1:B:210:ALA:N	1:B:247:MET:HE1	2.21	0.56
1:B:243:GLU:O	1:B:247:MET:HG2	2.05	0.56
3:E:41:THR:O	3:E:44:ARG:CD	2.52	0.56
1:B:44:THR:HG21	7:B:5140:HOH:O	2.05	0.55
2:C:211:THR:O	2:C:214:PRO:HD2	2.06	0.55
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.87	0.55
1:A:227:ASN:ND2	1:A:295:LYS:H	2.04	0.55
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.72	0.55
1:A:186:ARG:HA	2:C:73:THR:OG1	2.06	0.54
1:A:185:LYS:O	1:A:189:SER:HB2	2.07	0.54
1:B:244:LEU:HB2	7:B:5176:HOH:O	2.06	0.54
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.89	0.54
1:A:268:ASN:ND2	1:A:327:GLU:H	2.06	0.53
1:B:43:ARG:HD2	1:B:43:ARG:C	2.33	0.53
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.42	0.53
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.41	0.53
1:B:212:PHE:O	1:B:215:PRO:HD2	2.09	0.53
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.73	0.53
2:C:336:MET:HE2	2:C:385:LEU:HD23	1.91	0.53
1:A:163:GLN:HG2	7:A:9078:HOH:O	2.09	0.52
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.90	0.52
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.45	0.52
1:B:206:LEU:HB2	7:B:5218:HOH:O	2.09	0.52
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.08	0.52
1:B:32:LEU:C	1:B:32:LEU:HD23	2.34	0.52
2:C:211:THR:C	2:C:214:PRO:HD2	2.35	0.52
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.44	0.52
1:B:43:ARG:HD2	1:B:43:ARG:O	2.10	0.52
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.43	0.52
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.04	0.52
2:D:324:TRP:O	2:D:327:PRO:HD2	2.10	0.52
3:E:98:MET:HE2	3:E:138:ARG:CG	2.39	0.52
3:F:61:GLU:O	3:F:121:PRO:HG2	2.08	0.52
2:D:187:ILE:O	2:D:191:GLN:HG3	2.10	0.52
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.40	0.51
1:B:109:PHE:O	1:B:112:VAL:HG12	2.10	0.51
1:B:198:VAL:O	1:B:202:LEU:HG	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.92	0.51
3:E:98:MET:HE1	3:E:107:ALA:HB1	1.89	0.51
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.10	0.51
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.92	0.51
2:D:352:ILE:CD1	2:D:388:LEU:HD11	2.40	0.51
2:C:336:MET:CE	2:C:385:LEU:HD23	2.40	0.51
1:B:227:ASN:ND2	1:B:295:LYS:H	2.07	0.51
2:C:2:SER:HB2	7:C:5189:HOH:O	2.09	0.51
1:A:160:LYS:HE3	7:A:9243:HOH:O	2.11	0.51
2:D:184:PHE:O	2:D:187:ILE:HG22	2.11	0.51
3:E:4:LEU:HG	3:E:4:LEU:O	2.11	0.50
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.93	0.50
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.09	0.50
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.12	0.50
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.47	0.50
7:D:518:HOH:O	3:F:125:VAL:HG22	2.11	0.49
2:D:213:VAL:HG23	7:D:569:HOH:O	2.12	0.49
2:D:352:ILE:HD11	2:D:388:LEU:HD11	1.94	0.49
3:E:57:GLU:O	3:E:61:GLU:HG3	2.12	0.49
7:C:5020:HOH:O	3:E:125:VAL:HG22	2.12	0.49
2:D:348:ASP:OD1	2:D:351:GLU:HG3	2.12	0.49
1:B:30:ARG:HD3	1:B:30:ARG:C	2.37	0.49
1:B:46:TYR:CD2	1:B:123:MET:HE3	2.47	0.49
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.43	0.49
2:C:97:LYS:HD2	7:C:5246:HOH:O	2.12	0.49
1:A:84:ASP:HB3	1:B:81:SER:OG	2.13	0.49
2:D:145:ILE:O	2:D:149:TRP:HB3	2.13	0.49
1:B:369:MET:HE1	1:B:388:GLU:OE2	2.13	0.48
2:D:275:ASN:C	2:D:278:PRO:HD2	2.38	0.48
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.95	0.48
3:F:33:LYS:O	3:F:37:MET:HG2	2.12	0.48
1:A:212:PHE:O	1:A:215:PRO:HD2	2.13	0.48
1:B:490:SER:OG	2:D:32:ASN:HB2	2.13	0.48
2:C:153:LEU:C	2:C:153:LEU:HD12	2.37	0.48
1:B:185:LYS:O	1:B:189:SER:HB2	2.13	0.48
2:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.48
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.97	0.48
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.79	0.48
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.31	0.48
2:D:223:VAL:HG23	7:D:577:HOH:O	2.14	0.48
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.09	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD21	1:B:230:GLU:HG3	1.94	0.48
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.97	0.47
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.44	0.47
1:B:186:ARG:HD3	1:B:186:ARG:C	2.39	0.47
1:B:227:ASN:HD21	1:B:296:PHE:H	1.62	0.47
1:A:186:ARG:HD3	1:A:186:ARG:C	2.39	0.47
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.49	0.47
1:B:188:PHE:HZ	1:B:213:THR:HG22	1.79	0.47
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.50	0.47
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.14	0.47
2:C:111:LYS:O	2:C:115:GLU:HG3	2.14	0.47
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.80	0.47
3:F:33:LYS:HE3	3:F:117:ALA:HA	1.95	0.47
1:A:314:GLY:O	1:A:318:ILE:HD11	2.15	0.47
2:C:98:HIS:HE1	2:C:178:SER:OG	1.97	0.47
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.50	0.47
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.50	0.47
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.80	0.46
1:B:232:THR:HB	1:B:233:PRO:HD3	1.97	0.46
2:C:235:TRP:CD1	2:C:235:TRP:C	2.93	0.46
1:B:125:TRP:CD1	1:B:125:TRP:C	2.93	0.46
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.14	0.46
2:D:185:ASP:O	2:D:189:ILE:HG12	2.15	0.46
1:A:116:ASN:CG	1:A:189:SER:HA	2.41	0.46
2:D:143:GLU:O	2:D:147:ARG:HB3	2.16	0.46
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.51	0.46
3:F:162:ARG:NH1	3:F:164:VAL:HG12	2.31	0.46
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.10	0.46
2:D:90:LEU:CD1	2:D:303:LEU:HD13	2.46	0.46
3:E:40:THR:C	3:E:41:THR:HG23	2.40	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.51	0.46
1:A:343:HIS:CD2	1:A:343:HIS:H	2.31	0.46
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.81	0.46
1:B:184:MET:HE2	1:B:188:PHE:CG	2.51	0.46
2:D:54:VAL:O	2:D:55:TYR:HB2	2.15	0.46
1:A:109:PHE:O	1:A:112:VAL:HG12	2.16	0.46
1:A:268:ASN:HD21	1:A:327:GLU:N	2.11	0.46
1:B:466:CYS:HB2	2:D:73:THR:HA	1.99	0.45
3:E:98:MET:HE2	3:E:138:ARG:HG2	1.97	0.45
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.16	0.45
1:B:510:ASP:O	1:B:514:ARG:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:GLN:NE2	7:A:9288:HOH:O	2.49	0.45
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.52	0.45
1:B:159:ALA:O	2:D:33:ASN:HB2	2.16	0.45
1:A:44:THR:HG21	7:A:9010:HOH:O	2.16	0.45
1:B:230:GLU:C	1:B:233:PRO:HD2	2.42	0.45
2:D:299:TYR:O	2:D:317:MET:HE1	2.16	0.45
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.98	0.45
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.52	0.45
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.99	0.45
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.51	0.45
1:A:81:SER:OG	1:B:84:ASP:HB3	2.16	0.45
2:D:192:MET:HE3	2:D:280:PHE:CE2	2.52	0.45
1:B:184:MET:HE3	1:B:184:MET:HA	1.98	0.45
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.52	0.45
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.32	0.45
2:C:143:GLU:O	2:C:147:ARG:HB3	2.17	0.45
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.98	0.45
1:A:232:THR:HB	1:A:233:PRO:HD3	1.97	0.44
1:B:184:MET:HE2	1:B:188:PHE:CB	2.47	0.44
1:A:159:ALA:O	2:C:33:ASN:HB2	2.18	0.44
1:B:116:ASN:CG	1:B:189:SER:HA	2.43	0.44
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.18	0.44
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.32	0.44
1:B:208:GLY:O	1:B:213:THR:HG23	2.17	0.44
2:C:33:ASN:C	2:C:33:ASN:ND2	2.75	0.44
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.98	0.44
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.52	0.44
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.53	0.44
2:C:54:VAL:O	2:C:55:TYR:HB2	2.17	0.44
2:C:146:ASN:O	2:C:214:PRO:HG3	2.18	0.44
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.53	0.44
2:D:140:TRP:CE2	2:D:145:ILE:HD11	2.53	0.44
2:D:324:TRP:HA	2:D:327:PRO:HD2	2.00	0.43
3:F:154:GLU:HG3	3:F:158:GLN:HE21	1.82	0.43
1:B:360:ARG:HG2	1:B:498:GLN:HB2	2.01	0.43
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.99	0.43
2:C:209:GLU:HG2	7:C:5188:HOH:O	2.18	0.43
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.51	0.43
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.16	0.43
1:A:44:THR:OG1	1:A:127:SER:HA	2.18	0.43
1:A:249:ASN:HD22	1:A:249:ASN:HA	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:GLU:O	1:B:70:MET:HG2	2.18	0.43
1:B:202:LEU:HD22	1:B:206:LEU:CD2	2.47	0.43
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.32	0.43
2:C:192:MET:HE2	2:C:283:GLN:OE1	2.18	0.43
1:A:260:ASP:OD1	1:A:261:PRO:HD2	2.18	0.43
2:D:195:LEU:C	2:D:195:LEU:HD23	2.44	0.43
2:D:209:GLU:HG2	7:D:461:HOH:O	2.19	0.43
3:E:4:LEU:O	3:E:4:LEU:CG	2.66	0.43
3:E:154:GLU:O	3:E:158:GLN:HG3	2.18	0.43
1:A:30:ARG:HD3	1:A:31:TRP:CD1	2.54	0.43
1:B:73:VAL:HG12	1:B:77:ARG:HH22	1.83	0.43
1:B:186:ARG:HA	2:D:73:THR:OG1	2.18	0.43
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.99	0.43
2:D:269:ALA:N	2:D:270:PRO:CD	2.82	0.43
2:D:332:LEU:O	2:D:336:MET:HG2	2.19	0.43
1:A:140:GLN:HG3	1:A:246:HIS:CE1	2.53	0.43
1:A:193:ILE:HD11	2:C:82:SER:HB3	2.01	0.43
1:A:402:PHE:O	1:A:403:ILE:HD12	2.18	0.43
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.47	0.43
1:A:413:HIS:HD2	1:A:428:SER:OG	2.01	0.43
1:B:323:LYS:HE2	1:B:324:TYR:CZ	2.54	0.43
1:B:292:TYR:OH	1:B:344:HIS:CD2	2.69	0.42
2:D:325:LEU:O	2:D:329:ILE:HG13	2.20	0.42
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.54	0.42
3:F:133:ARG:NH1	3:F:134:GLN:HG3	2.35	0.42
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.54	0.42
2:D:77:HIS:CG	3:F:140:MET:HG2	2.54	0.42
3:F:49:LEU:HA	7:F:178:HOH:O	2.18	0.42
2:D:277:THR:HB	2:D:278:PRO:HD3	2.01	0.42
3:F:26:GLU:HB2	7:F:213:HOH:O	2.19	0.42
1:A:192:PHE:O	1:A:200:CYS:HB3	2.19	0.42
1:B:209:GLU:C	1:B:247:MET:HE1	2.44	0.42
2:C:42:ARG:HB2	2:C:99:ARG:HG3	2.00	0.42
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.37	0.42
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.99	0.42
1:B:283:THR:HB	1:B:284:PRO:HD3	2.02	0.42
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.38	0.42
2:D:80:ARG:HG2	2:D:86:GLU:OE1	2.18	0.42
1:A:360:ARG:HG2	1:A:498:GLN:HB2	2.01	0.42
1:A:165:PRO:HG3	7:A:9076:HOH:O	2.20	0.42
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:O	1:A:114:GLU:HG2	2.19	0.42
2:D:169:GLU:O	2:D:170:ALA:C	2.61	0.42
3:F:39:HIS:HD2	7:F:225:HOH:O	2.02	0.42
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.19	0.41
2:C:277:THR:HB	2:C:278:PRO:HD3	2.01	0.41
2:D:63:ILE:O	2:D:64:ALA:C	2.62	0.41
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.56	0.41
2:D:125:GLN:HE21	2:D:125:GLN:HB3	1.74	0.41
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.56	0.41
1:B:457:TRP:CZ3	1:B:458:LEU:HD23	2.55	0.41
3:E:55:TRP:CZ2	3:E:59:LYS:HE3	2.54	0.41
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.81	0.41
1:B:210:ALA:CA	1:B:247:MET:HE1	2.50	0.41
2:D:349:LYS:HA	2:D:352:ILE:HG12	2.02	0.41
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.55	0.41
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.56	0.41
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.20	0.41
2:D:266:GLN:HA	2:D:266:GLN:HE21	1.84	0.41
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.21	0.41
2:D:349:LYS:HG3	2:D:352:ILE:HD11	2.03	0.41
1:A:184:MET:HE3	1:A:188:PHE:CD2	2.56	0.41
1:B:202:LEU:HD22	1:B:206:LEU:HD23	2.03	0.41
1:B:320:ARG:HH11	1:B:320:ARG:HB3	1.86	0.41
2:C:269:ALA:N	2:C:270:PRO:CD	2.84	0.41
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.56	0.41
1:A:210:ALA:HA	1:A:247:MET:HE1	2.03	0.41
1:A:216:LEU:O	1:A:220:VAL:HG23	2.20	0.41
1:A:365:ASP:OD2	1:A:365:ASP:C	2.63	0.41
2:C:98:HIS:HD2	2:C:297:ASP:OD1	2.03	0.41
2:D:2:SER:HB2	7:D:466:HOH:O	2.21	0.41
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.55	0.41
3:F:75:VAL:HG23	7:F:217:HOH:O	2.20	0.41
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.56	0.41
2:C:201:ALA:HA	2:C:207:PHE:HB3	2.01	0.41
2:D:195:LEU:HD23	2:D:195:LEU:O	2.21	0.41
1:A:354:TRP:N	1:A:355:PRO:CD	2.85	0.40
1:B:21:THR:HG22	1:B:22:SER:N	2.37	0.40
1:A:32:LEU:HD23	1:A:32:LEU:C	2.46	0.40
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.60	0.40
1:B:90:ASN:HD22	1:B:90:ASN:HA	1.64	0.40
1:B:114:GLU:CD	1:B:147:HIS:HB3	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.56	0.40
1:B:299:GLU:HA	1:B:300:PRO:HD3	1.98	0.40
2:D:266:GLN:HB2	2:D:281:ILE:HG21	2.03	0.40
2:D:352:ILE:CG1	2:D:353:THR:N	2.84	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	509/527 (97%)	490 (96%)	18 (4%)	1 (0%)	43	36
1	B	509/527 (97%)	489 (96%)	18 (4%)	2 (0%)	30	21
2	C	386/389 (99%)	378 (98%)	6 (2%)	2 (0%)	24	16
2	D	385/389 (99%)	365 (95%)	16 (4%)	4 (1%)	12	5
3	E	164/170 (96%)	162 (99%)	2 (1%)	0	100	100
3	F	166/170 (98%)	162 (98%)	4 (2%)	0	100	100
All	All	2119/2172 (98%)	2046 (97%)	64 (3%)	9 (0%)	30	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
2	D	64	ALA
2	D	205	PRO
2	D	221	GLY
1	A	284	PRO
2	C	64	ALA
1	B	284	PRO
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	433/442 (98%)	427 (99%)	6 (1%)	59	56
1	B	433/442 (98%)	429 (99%)	4 (1%)	70	70
2	C	322/323 (100%)	318 (99%)	4 (1%)	63	61
2	D	321/323 (99%)	315 (98%)	6 (2%)	50	45
3	E	144/147 (98%)	142 (99%)	2 (1%)	59	56
3	F	146/147 (99%)	142 (97%)	4 (3%)	39	32
All	All	1799/1824 (99%)	1773 (99%)	26 (1%)	59	56

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	90	ASN
1	A	125	TRP
1	A	310	TYR
1	A	403	ILE
1	A	467	GLN
1	B	43	ARG
1	B	90	ASN
1	B	125	TRP
1	B	279	GLN
2	C	33	ASN
2	C	153	LEU
2	C	173	ASP
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	266	GLN
3	E	24	THR
3	E	44	ARG

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Mol	Chain	Res	Type
3	F	11	THR
3	F	41	THR
3	F	164	VAL
3	F	167	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) 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	155	ASN
1	A	168	HIS
1	A	203	ASN
1	A	227	ASN
1	A	249	ASN
1	A	268	ASN
1	A	273	ASN
1	A	343	HIS
1	A	344	HIS
1	A	382	HIS
1	A	411	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	B	26	GLN
1	B	33	GLN
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	203	ASN
1	B	205	GLN
1	B	214	ASN
1	B	227	ASN

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Mol	Chain	Res	Type
1	B	249	ASN
1	B	252	GLN
1	B	268	ASN
1	B	273	ASN
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	125	GLN
2	D	161	ASN
2	D	266	GLN
2	D	285	GLN
2	D	296	GLN
3	E	45	ASN
3	E	144	ASN
3	E	158	GLN
3	E	165	HIS
3	F	7	HIS
3	F	39	HIS
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
3	F	158	GLN
3	F	167	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 9 ligands modelled in this entry, 8 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	FMT	A	9001	4	2,2,2	0.64	0	1,1,1	0.61	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 ⓘ

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	511/527 (96%)	0.16	16 (3%) 51 58	16, 27, 45, 63	0
1	B	511/527 (96%)	0.13	12 (2%) 61 68	16, 27, 45, 62	0
2	C	388/389 (99%)	-0.35	2 (0%) 87 90	13, 21, 35, 52	0
2	D	387/389 (99%)	0.65	27 (6%) 22 26	18, 33, 51, 58	0
3	E	166/170 (97%)	-0.05	5 (3%) 52 59	17, 24, 38, 56	0
3	F	168/170 (98%)	1.29	35 (20%) 2 2	30, 42, 57, 64	0
All	All	2131/2172 (98%)	0.22	97 (4%) 37 43	13, 28, 48, 64	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	4	LEU	5.3
3	F	19	ILE	4.9
2	D	352	ILE	4.4
3	E	168	SER	3.9
2	D	385	LEU	3.9
1	A	206	LEU	3.6
3	F	20	ALA	3.6
2	D	26	GLU	3.4
2	D	388	LEU	3.4
1	B	213	THR	3.4
1	A	310	TYR	3.3
2	D	384	VAL	3.2
1	A	432	GLY	3.1
3	F	71	ALA	3.1
1	A	318	ILE	3.1
1	B	244	LEU	3.0
1	A	338	ASP	2.9
3	F	100	ALA	2.9
3	F	122	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
3	F	84	GLY	2.9
3	F	170	HIS	2.8
3	F	70	ARG	2.8
1	A	316	ILE	2.8
2	D	380	ILE	2.8
2	D	373	PHE	2.7
1	A	317	TRP	2.7
1	B	54	ASN	2.7
3	F	83	PHE	2.7
1	A	210	ALA	2.6
3	F	41	THR	2.6
2	D	270	PRO	2.6
1	B	260	ASP	2.6
1	A	213	THR	2.6
1	A	216	LEU	2.5
2	D	216	ALA	2.5
3	F	17	ASN	2.5
3	F	118	TYR	2.5
2	D	340	ALA	2.5
2	D	347	THR	2.5
2	D	330	ALA	2.4
3	F	64	VAL	2.4
3	F	127	TYR	2.4
3	F	30	GLU	2.4
2	D	311	ASP	2.4
3	F	80	LYS	2.4
2	D	381	VAL	2.3
1	B	308	TRP	2.3
1	B	311	GLU	2.3
3	F	27	LYS	2.3
1	B	525	ALA	2.3
2	D	368	ALA	2.3
1	B	320	ARG	2.3
2	D	333	ARG	2.3
3	F	21	GLN	2.3
2	D	212	ALA	2.2
2	D	357	TYR	2.2
3	F	69	ALA	2.2
3	F	16	VAL	2.2
3	F	164	VAL	2.2
1	A	76	GLU	2.2
3	F	22	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	221	GLY	2.2
3	E	167	GLN	2.2
1	A	433	ALA	2.2
2	D	207	PHE	2.2
3	E	23	ASN	2.2
1	A	314	GLY	2.2
2	C	6	GLU	2.2
3	F	11	THR	2.2
1	A	315	GLY	2.2
2	D	206	GLY	2.2
1	B	17	ASN	2.1
3	F	23	ASN	2.1
2	C	308	GLU	2.1
3	E	153	GLU	2.1
3	F	110	ILE	2.1
2	D	320	TRP	2.1
3	F	76	ASP	2.1
3	F	66	VAL	2.1
3	F	67	LEU	2.1
1	B	53	ALA	2.1
1	B	44	THR	2.1
3	F	24	THR	2.1
2	D	223	VAL	2.1
3	F	161	VAL	2.1
3	F	101	ALA	2.1
2	D	141	ARG	2.1
3	F	93	GLY	2.0
1	B	527	ASN	2.0
1	A	308	TRP	2.0
1	A	515	LEU	2.0
2	D	363	TRP	2.0
3	F	28	ALA	2.0
2	D	339	PHE	2.0
3	F	72	PHE	2.0
2	D	346	THR	2.0
3	F	162	ARG	2.0

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

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
6	FMT	A	9001	3/3	0.80	0.14	40,40,45,49	0
5	CA	C	5006	1/1	0.94	0.06	52,52,52,52	0
5	CA	C	5008	1/1	0.95	0.10	44,44,44,44	0
5	CA	A	5005	1/1	0.98	0.05	37,37,37,37	0
5	CA	C	5007	1/1	0.99	0.09	36,36,36,36	0
4	FE	A	5002	1/1	0.99	0.03	36,36,36,36	0
4	FE	B	5004	1/1	0.99	0.04	36,36,36,36	0
4	FE	A	5001	1/1	1.00	0.03	25,25,25,25	0
4	FE	B	5003	1/1	1.00	0.01	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.