



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:35 PM UTC

PDB ID : 1FZH / pdb_00001fzh
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM II PRESSURIZED WITH XENON GAS
Authors : Whittington, D.A.; Rosenzweig, A.C.; Frederick, C.A.; Lippard, S.J.
Deposited on : 2000-10-03
Resolution : 2.60 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

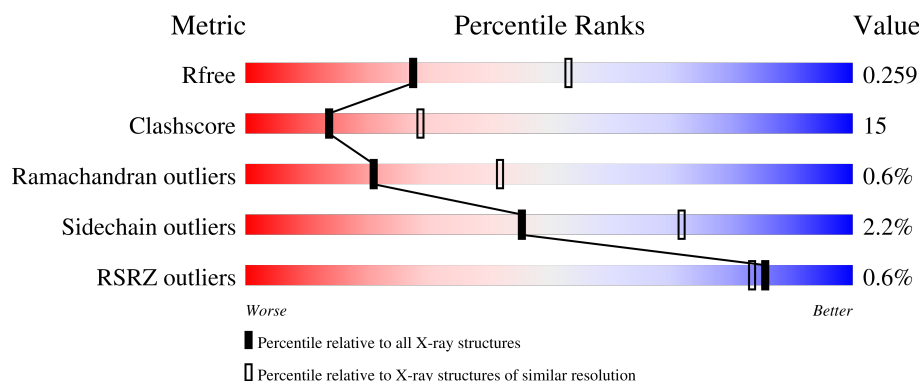
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	% 66% 27% • •
1	B	527	65% 29% • •
2	C	389	77% 21% •
2	D	389	% 66% 30% •
3	E	170	% 69% 26% • •

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Mol	Chain	Length	Quality of chain
3	F	170	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	XE	A	9006	-	-	X	-
6	XE	B	9010	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18070 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	510	Total	C	N	O	S	0	0	0
			4177	2673	719	767	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	388	Total	C	N	O	S	0	0	0
			3187	2051	548	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	165	Total	C	N	O	S	0	0	0
			1362	864	245	248	5			
3	F	167	Total	C	N	O	S	0	0	0
			1375	872	247	251	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	B	1	Total Ca 1 1	0	0
5	C	2	Total Ca 2 2	0	0

- Molecule 6 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total Xe 6 6	0	0
6	B	5	Total Xe 5 5	0	0

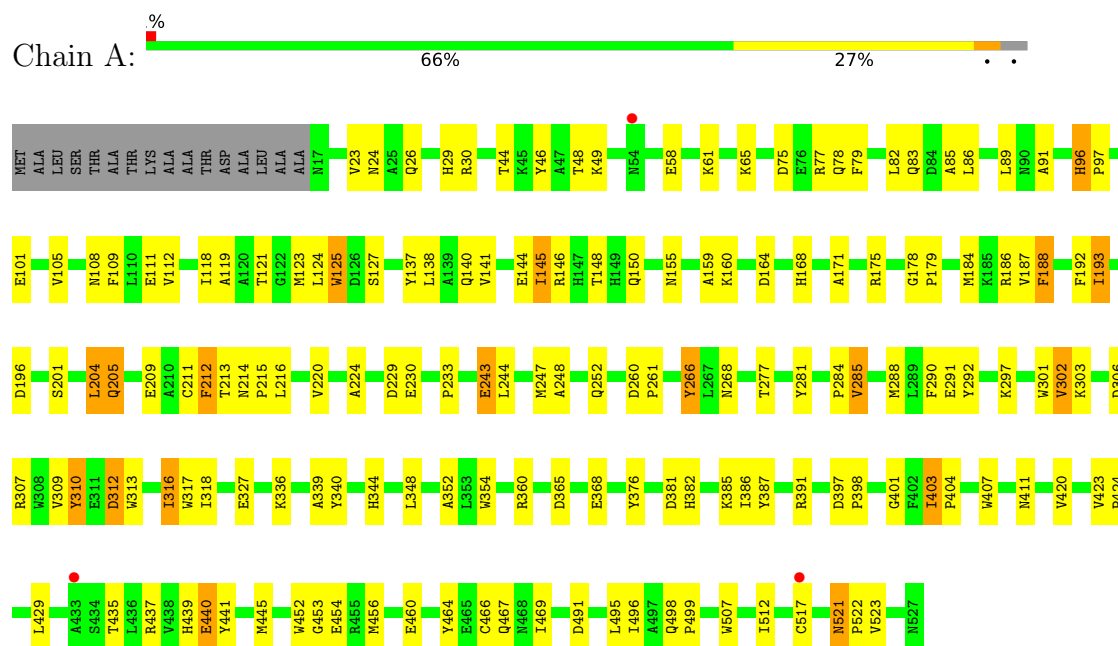
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	133	Total O 133 133	0	0
7	B	134	Total O 134 134	0	0
7	C	154	Total O 154 154	0	0
7	D	67	Total O 67 67	0	0
7	E	63	Total O 63 63	0	0
7	F	21	Total O 21 21	0	0

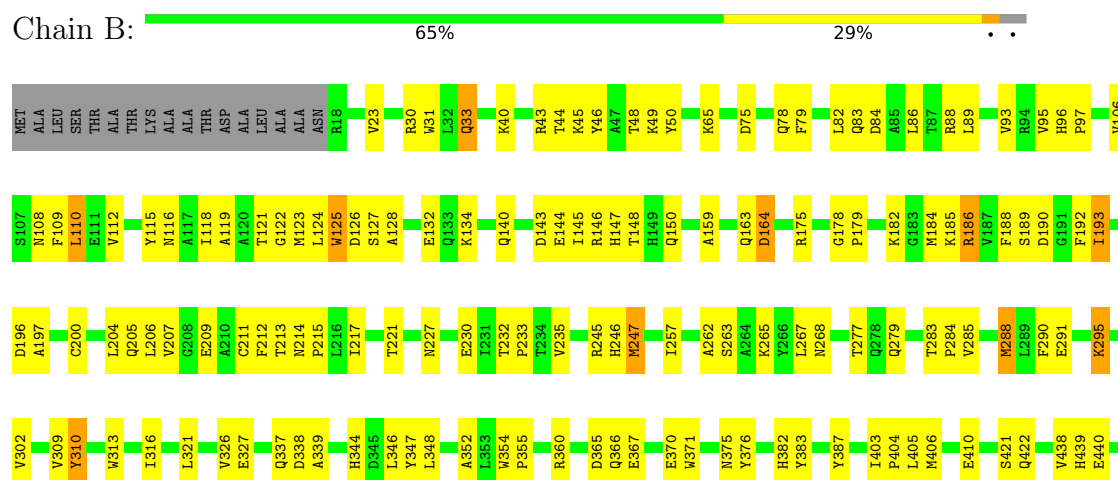
3 Residue-property plots

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



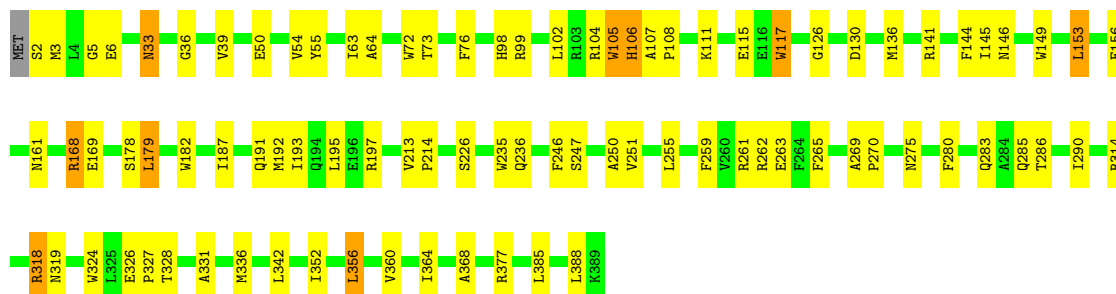
• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN





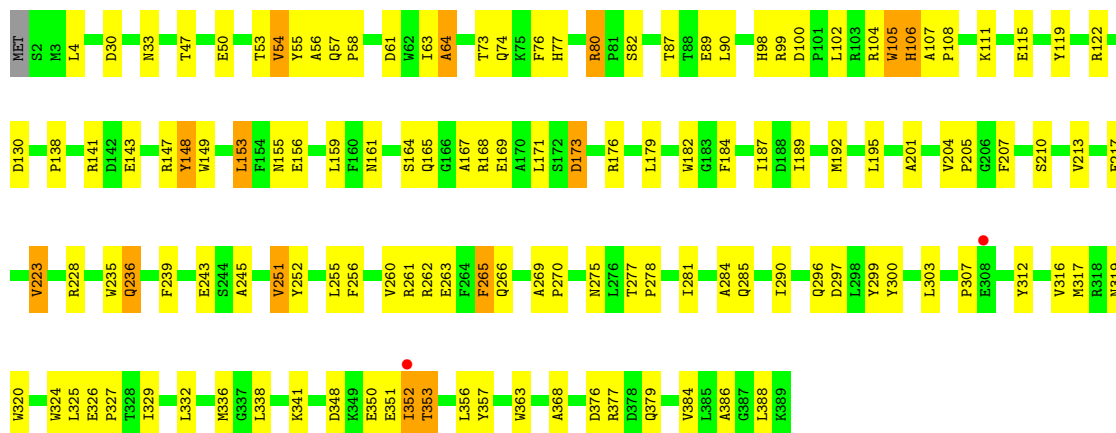
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain C: 77% 21% .



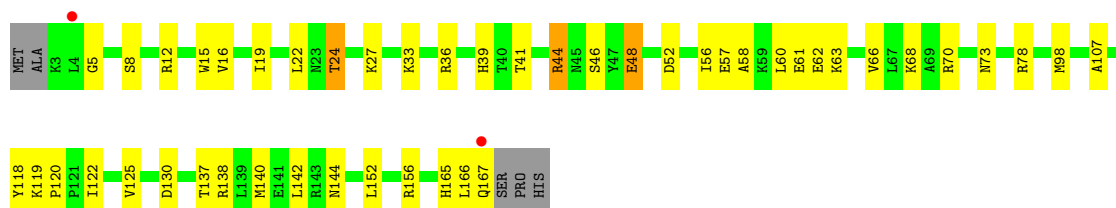
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

Chain D: 66% 30% .



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

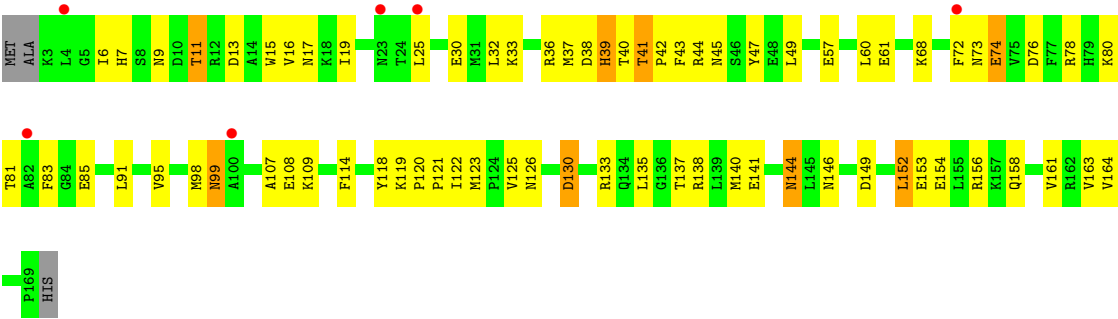
Chain E: 69% 26% . .



• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN

Chain F: 4% 56% 38% 5% .





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.27Å 174.62Å 223.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.00 – 2.60 29.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	86.3 (29.00-2.60) 86.3 (29.00-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.53 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.260 0.205 , 0.259	Depositor DCC
R_{free} test set	2958 reflections (3.62%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	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	0.92	EDS
Total number of atoms	18070	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, XE, 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	0.42	0/4310	1.01	30/5853 (0.5%)
1	B	0.44	1/4302 (0.0%)	0.96	18/5842 (0.3%)
2	C	0.47	0/3289	0.90	10/4464 (0.2%)
2	D	0.42	0/3283	0.91	16/4457 (0.4%)
3	E	0.47	0/1390	0.92	5/1872 (0.3%)
3	F	0.39	0/1404	0.83	4/1892 (0.2%)
All	All	0.44	1/17978 (0.0%)	0.94	83/24380 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	288	MET	SD-CE	-6.89	1.62	1.79

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ASP	CA-C-N	10.20	130.37	119.05
1	A	164	ASP	C-N-CA	10.20	130.37	119.05
1	B	193	ILE	N-CA-C	9.26	122.08	113.20
1	A	339	ALA	N-CA-C	9.03	123.60	112.23
1	A	178	GLY	CA-C-N	8.13	127.81	119.19
1	A	178	GLY	C-N-CA	8.13	127.81	119.19
1	B	164	ASP	CA-C-N	8.11	128.06	119.05
1	B	164	ASP	C-N-CA	8.11	128.06	119.05
1	A	309	VAL	N-CA-C	8.08	118.09	110.74
1	A	193	ILE	N-CA-C	7.81	120.68	113.10
1	A	243	GLU	N-CA-C	7.61	120.46	111.71
1	B	339	ALA	N-CA-C	7.46	121.63	112.23
2	D	54	VAL	N-CA-C	7.22	118.75	109.30
1	B	316	ILE	N-CA-C	6.84	116.85	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLN	N-CA-C	6.72	121.44	111.96
2	D	105	TRP	N-CA-C	-6.59	100.46	109.95
2	D	106	HIS	N-CA-C	6.55	118.97	111.11
1	A	145	ILE	N-CA-C	-6.53	104.39	110.53
1	B	496	ILE	N-CA-C	-6.52	104.29	110.42
3	E	130	ASP	N-CA-C	-6.52	104.25	111.36
1	B	285	VAL	N-CA-C	6.50	116.64	110.53
1	B	310	TYR	N-CA-C	6.41	118.06	111.14
1	A	397	ASP	CA-C-N	6.33	126.81	119.47
1	A	397	ASP	C-N-CA	6.33	126.81	119.47
2	C	169	GLU	N-CA-C	6.19	121.11	113.50
2	C	236	GLN	N-CA-C	6.19	120.99	113.38
2	C	106	HIS	N-CA-C	6.18	118.52	111.11
2	D	57	GLN	CA-C-N	6.16	127.53	119.84
2	D	57	GLN	C-N-CA	6.16	127.53	119.84
1	A	204	LEU	N-CA-C	6.15	117.68	110.97
2	C	104	ARG	N-CA-C	5.98	118.04	108.41
1	A	401	GLY	N-CA-C	-5.96	105.90	115.08
1	B	478	LEU	N-CA-C	5.93	118.23	111.11
2	D	56	ALA	N-CA-C	-5.90	104.98	111.82
3	E	73	ASN	N-CA-C	-5.89	102.93	110.53
1	A	85	ALA	N-CA-C	5.87	117.35	111.07
3	E	39	HIS	N-CA-C	5.83	121.71	113.02
1	B	291	GLU	N-CA-C	5.82	118.57	111.82
1	A	212	PHE	N-CA-C	5.82	120.67	112.93
1	A	291	GLU	N-CA-C	5.80	117.69	111.36
1	A	316	ILE	N-CA-C	5.77	115.96	110.42
1	A	496	ILE	N-CA-C	-5.77	105.22	110.82
1	B	212	PHE	N-CA-C	5.73	119.79	112.12
2	D	236	GLN	N-CA-C	5.72	120.32	113.23
1	A	285	VAL	N-CA-C	5.71	115.90	110.42
1	A	188	PHE	N-CA-C	5.67	119.78	112.41
1	A	96	HIS	CA-C-N	5.66	125.13	119.24
1	A	96	HIS	C-N-CA	5.66	125.13	119.24
2	C	149	TRP	N-CA-C	-5.66	105.03	111.14
2	D	53	THR	N-CA-C	5.61	119.82	112.13
3	E	118	TYR	N-CA-C	5.58	120.78	113.30
2	C	105	TRP	N-CA-C	-5.52	101.83	110.17
2	D	368	ALA	N-CA-C	5.51	117.72	111.11
1	A	397	ASP	N-CA-C	5.48	117.37	109.04
2	D	148	TYR	N-CA-C	5.47	117.05	111.14
1	A	266	TYR	N-CA-C	5.46	120.43	113.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	204	VAL	CA-C-N	5.46	126.66	119.84
2	D	204	VAL	C-N-CA	5.46	126.66	119.84
2	C	318	ARG	N-CA-C	-5.40	105.47	111.36
1	A	460	GLU	CA-C-N	5.33	125.39	119.32
1	A	460	GLU	C-N-CA	5.33	125.39	119.32
2	D	353	THR	N-CA-C	-5.32	106.85	113.55
2	C	265	PHE	N-CA-C	5.31	116.75	111.07
1	A	521	ASN	CA-C-N	5.28	125.59	119.47
1	A	521	ASN	C-N-CA	5.28	125.59	119.47
2	D	171	LEU	N-CA-C	5.28	119.43	113.15
2	D	265	PHE	N-CA-C	5.27	116.83	111.14
2	C	286	THR	N-CA-C	-5.25	105.55	111.28
3	E	48	GLU	N-CA-C	5.25	117.91	111.82
1	B	295	LYS	N-CA-C	-5.23	104.96	112.13
3	F	39	HIS	N-CA-C	5.15	122.07	114.09
1	B	309	VAL	N-CA-C	5.14	115.42	110.74
3	F	152	LEU	N-CA-C	5.14	117.55	111.33
1	B	469	ILE	N-CA-C	5.11	115.84	110.62
1	B	188	PHE	N-CA-C	5.10	118.54	112.72
3	F	130	ASP	N-CA-C	-5.09	105.91	111.82
1	B	122	GLY	N-CA-C	-5.07	106.28	112.77
3	F	99	ASN	N-CA-C	-5.06	106.36	112.54
1	A	312	ASP	N-CA-C	5.04	117.16	111.11
1	B	178	GLY	CA-C-N	5.04	125.48	120.04
1	B	178	GLY	C-N-CA	5.04	125.48	120.04
2	D	77	HIS	N-CA-C	-5.02	102.48	109.96
2	C	72	TRP	N-CA-C	-5.01	103.79	110.55

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	126	0
1	B	4177	0	3975	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	3193	0	3042	82	0
2	D	3187	0	3031	109	0
3	E	1362	0	1358	30	0
3	F	1375	0	1370	59	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	2	0	0	0	0
6	A	6	0	0	5	0
6	B	5	0	0	5	0
7	A	133	0	0	7	0
7	B	134	0	0	4	0
7	C	154	0	0	5	0
7	D	67	0	0	3	0
7	E	63	0	0	1	0
7	F	21	0	0	0	0
All	All	18070	0	16757	497	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 15.

All (497) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:HG22	1:B:46:TYR:H	1.24	0.96
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.17	0.93
3:F:41:THR:HG22	3:F:43:PHE:H	1.33	0.93
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.51	0.93
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.17	0.93
1:A:44:THR:HG22	1:A:46:TYR:H	1.38	0.89
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.56	0.88
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.56	0.86
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.58	0.84
1:A:288:MET:HE3	6:A:9002:XE:XE	2.57	0.83
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.61	0.83
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.24	0.82
3:E:24:THR:HG22	3:E:27:LYS:H	1.44	0.81
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.81	0.79
2:D:336:MET:HE2	2:D:384:VAL:HG12	1.64	0.79
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.46	0.78
1:A:23:VAL:HB	2:C:195:LEU:HD11	1.64	0.77
1:B:288:MET:HE1	1:B:346:LEU:HG	1.65	0.77
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.64	0.77
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.67	0.76
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.20	0.75
3:F:9:ASN:OD1	3:F:11:THR:HG23	1.86	0.74
2:D:138:PRO:HA	2:D:141:ARG:NH1	2.02	0.74
1:B:109:PHE:O	1:B:112:VAL:HG12	1.88	0.73
1:A:193:ILE:HD12	2:C:168:ARG:HH21	1.53	0.73
2:D:336:MET:HE2	2:D:384:VAL:CG1	2.19	0.72
3:F:41:THR:O	3:F:44:ARG:HD2	1.89	0.72
1:B:78:GLN:HE21	1:B:235:VAL:HA	1.54	0.72
2:D:122:ARG:HD3	7:D:433:HOH:O	1.89	0.72
2:C:247:SER:HG	2:C:324:TRP:CD1	2.08	0.71
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.73	0.71
2:D:138:PRO:HA	2:D:141:ARG:HH12	1.56	0.70
3:E:46:SER:OG	3:E:48:GLU:HG2	1.91	0.70
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.89	0.70
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.74	0.70
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.73	0.69
1:B:33:GLN:HE22	1:B:132:GLU:H	1.38	0.69
3:E:98:MET:HE1	3:E:107:ALA:CB	2.21	0.69
1:A:148:THR:HG21	6:A:9006:XE:XE	2.71	0.69
2:D:376:ASP:OD2	2:D:379:GLN:HG2	1.93	0.69
1:A:243:GLU:O	1:A:247:MET:HG2	1.92	0.68
2:D:312:TYR:O	2:D:316:VAL:HG23	1.93	0.68
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.42	0.68
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.76	0.68
2:D:76:PHE:HB2	2:D:80:ARG:HB3	1.76	0.68
3:F:40:THR:O	3:F:41:THR:HB	1.93	0.67
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.30	0.67
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.26	0.66
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.24	0.66
3:E:12:ARG:O	3:E:16:VAL:HG23	1.95	0.66
3:E:22:LEU:O	3:E:63:LYS:HE2	1.95	0.66
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.29	0.66
1:A:429:LEU:HG	1:A:429:LEU:O	1.96	0.65
1:B:106:VAL:O	1:B:110:LEU:HB2	1.97	0.65
1:A:381:ASP:O	1:A:385:LYS:HD2	1.95	0.65
1:B:186:ARG:HD3	1:B:186:ARG:C	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.60	0.65
1:A:317:TRP:HD1	1:A:318:ILE:HD12	1.61	0.65
3:E:57:GLU:O	3:E:61:GLU:HG3	1.96	0.65
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.79	0.64
1:B:472:GLN:OE1	3:F:6:ILE:HG23	1.97	0.64
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.80	0.64
2:D:47:THR:OG1	2:D:50:GLU:HG3	1.97	0.64
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.29	0.64
1:A:23:VAL:HB	2:C:195:LEU:CD1	2.27	0.64
2:D:338:LEU:HD12	2:D:341:LYS:HG3	1.80	0.64
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.79	0.64
1:B:290:PHE:CE2	6:B:9005:XE:XE	3.29	0.64
1:B:82:LEU:HD23	1:B:86:LEU:HD12	1.80	0.63
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.81	0.63
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.80	0.63
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.79	0.63
1:B:186:ARG:HD3	1:B:186:ARG:O	1.98	0.63
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.96	0.63
2:D:324:TRP:O	2:D:327:PRO:HD2	1.98	0.63
3:F:32:LEU:HD12	3:F:60:LEU:HD23	1.81	0.63
2:C:6:GLU:HG3	7:C:5079:HOH:O	1.99	0.62
2:C:314:ARG:O	2:C:318:ARG:HB2	1.99	0.62
1:A:365:ASP:OD2	1:A:368:GLU:HG3	1.98	0.62
2:D:153:LEU:C	2:D:153:LEU:HD12	2.24	0.62
1:A:44:THR:CG2	1:A:46:TYR:H	2.11	0.62
1:B:44:THR:OG1	1:B:127:SER:HA	1.99	0.62
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.48	0.62
1:B:288:MET:HE1	1:B:346:LEU:CG	2.28	0.62
2:C:336:MET:HE1	2:C:352:ILE:CG2	2.30	0.62
3:E:66:VAL:HG12	3:E:70:ARG:HH21	1.65	0.62
1:B:128:ALA:O	1:B:134:LYS:HE2	2.00	0.61
3:E:41:THR:O	3:E:44:ARG:HD2	1.99	0.61
1:A:121:THR:HG21	1:A:140:GLN:HG2	1.81	0.61
1:B:40:LYS:HG3	7:B:9107:HOH:O	2.00	0.61
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.65	0.61
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.34	0.61
3:F:13:ASP:O	3:F:16:VAL:HG22	2.02	0.60
1:B:159:ALA:O	2:D:33:ASN:HB2	2.02	0.60
2:C:2:SER:HB2	7:C:5113:HOH:O	2.02	0.60
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.82	0.60
1:B:406:MET:O	1:B:410:GLU:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:VAL:HB	3:F:164:VAL:HG23	1.84	0.60
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.37	0.59
2:D:275:ASN:C	2:D:278:PRO:HD2	2.27	0.59
2:C:153:LEU:C	2:C:153:LEU:HD12	2.27	0.59
2:D:82:SER:O	2:D:168:ARG:NH2	2.34	0.59
2:D:213:VAL:HG23	7:D:454:HOH:O	2.01	0.59
1:B:48:THR:O	3:F:137:THR:HG23	2.01	0.59
1:B:186:ARG:CZ	1:B:277:THR:HG23	2.33	0.59
2:D:325:LEU:O	2:D:329:ILE:HG13	2.03	0.59
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.84	0.59
2:C:33:ASN:HD22	2:C:33:ASN:H	1.50	0.59
1:A:307:ARG:HG2	1:A:312:ASP:OD2	2.03	0.58
1:B:288:MET:HE2	1:B:347:TYR:N	2.17	0.58
1:B:43:ARG:HD2	1:B:43:ARG:C	2.27	0.58
1:B:262:ALA:HA	1:B:265:LYS:HE2	1.83	0.58
1:A:105:VAL:O	1:A:109:PHE:HB2	2.03	0.58
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.86	0.58
1:A:160:LYS:HA	2:C:33:ASN:HB2	1.85	0.58
1:A:290:PHE:CE2	6:A:9004:XE:XE	3.35	0.58
1:A:204:LEU:HG	1:A:205:GLN:HG3	1.86	0.58
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.86	0.58
2:D:165:GLN:NE2	2:D:239:PHE:O	2.37	0.58
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.97	0.58
2:C:144:PHE:CZ	2:C:342:LEU:HD23	2.38	0.58
2:C:146:ASN:HD22	2:C:197:ARG:HE	1.52	0.58
1:A:517:CYS:HB3	6:A:9008:XE:XE	2.82	0.57
1:B:163:GLN:HG2	7:B:9100:HOH:O	2.04	0.57
2:D:336:MET:CE	2:D:356:LEU:HD11	2.34	0.57
3:F:153:GLU:H	3:F:153:GLU:CD	2.13	0.57
2:D:184:PHE:O	2:D:187:ILE:HG22	2.05	0.57
1:A:209:GLU:HA	1:A:213:THR:HB	1.87	0.56
1:B:468:ASN:OD1	1:B:471:GLU:HG3	2.05	0.56
2:C:33:ASN:HD22	2:C:33:ASN:N	2.03	0.56
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.40	0.56
1:B:227:ASN:HD21	1:B:295:LYS:H	1.51	0.56
2:D:299:TYR:O	2:D:317:MET:HE1	2.05	0.56
1:B:288:MET:HE2	1:B:347:TYR:CA	2.35	0.56
3:E:44:ARG:HG3	3:E:46:SER:O	2.06	0.56
1:A:91:ALA:HB1	7:A:9012:HOH:O	2.04	0.56
1:A:124:LEU:HB3	1:A:137:TYR:CE1	2.41	0.56
3:F:146:ASN:HB3	3:F:149:ASP:OD2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:81:THR:HG23	3:F:85:GLU:O	2.06	0.56
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.52	0.56
3:F:41:THR:CG2	3:F:43:PHE:H	2.13	0.56
3:F:118:TYR:HB3	3:F:123:MET:HB2	1.88	0.56
1:A:101:GLU:CD	1:A:360:ARG:HH11	2.14	0.56
2:D:143:GLU:O	2:D:147:ARG:HB3	2.05	0.56
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.05	0.56
1:B:115:TYR:OH	2:D:173:ASP:HA	2.05	0.56
2:D:351:GLU:C	2:D:353:THR:H	2.13	0.55
3:F:41:THR:HG22	3:F:43:PHE:N	2.12	0.55
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.69	0.55
3:F:33:LYS:O	3:F:37:MET:HG2	2.05	0.55
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.88	0.55
1:A:44:THR:HG22	1:A:46:TYR:N	2.16	0.55
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.72	0.55
3:E:58:ALA:O	3:E:62:GLU:HG3	2.07	0.55
1:B:185:LYS:O	1:B:189:SER:HB2	2.07	0.54
1:B:352:ALA:CA	1:B:404:PRO:HB2	2.35	0.54
1:B:44:THR:HG23	1:B:126:ASP:OD1	2.06	0.54
1:B:23:VAL:HB	2:D:195:LEU:HD21	1.90	0.54
1:B:44:THR:HG22	1:B:46:TYR:N	2.09	0.54
1:A:268:ASN:HD21	1:A:327:GLU:H	1.55	0.54
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.54	0.54
2:C:275:ASN:ND2	2:D:266:GLN:HE21	2.06	0.54
2:D:223:VAL:HG11	2:D:338:LEU:HB2	1.89	0.54
1:A:310:TYR:CE1	1:A:336:LYS:HD2	2.43	0.54
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.05	0.54
2:D:98:HIS:CD2	2:D:99:ARG:H	2.26	0.54
2:D:87:THR:HG21	2:D:169:GLU:OE1	2.07	0.53
3:F:41:THR:HG23	3:F:42:PRO:HD2	1.88	0.53
1:B:209:GLU:HA	1:B:213:THR:OG1	2.09	0.53
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.72	0.53
3:F:81:THR:CG2	3:F:85:GLU:HG3	2.39	0.53
2:C:326:GLU:HG3	7:C:5122:HOH:O	2.09	0.53
2:C:261:ARG:NE	2:C:285:GLN:HE22	1.99	0.53
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.91	0.53
2:D:352:ILE:HD11	2:D:388:LEU:HD11	1.91	0.53
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.44	0.53
2:D:235:TRP:CD1	2:D:235:TRP:C	2.87	0.52
3:F:32:LEU:HA	3:F:60:LEU:HD23	1.92	0.52
2:D:277:THR:O	2:D:281:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:MET:HE3	1:B:346:LEU:HB3	1.90	0.52
1:B:354:TRP:CH2	1:B:499:PRO:HD3	2.45	0.52
1:A:437:ARG:HG2	1:A:437:ARG:HH11	1.75	0.51
2:C:54:VAL:HG12	2:C:55:TYR:CD2	2.45	0.51
3:E:98:MET:HE1	3:E:107:ALA:HB2	1.91	0.51
2:C:261:ARG:HE	2:C:285:GLN:NE2	2.02	0.51
3:F:91:LEU:C	3:F:91:LEU:HD23	2.35	0.51
1:A:24:ASN:OD1	1:A:26:GLN:HG3	2.11	0.51
1:B:121:THR:HA	1:B:124:LEU:HD12	1.91	0.51
2:D:266:GLN:HE22	2:D:278:PRO:HB3	1.76	0.51
1:B:125:TRP:O	1:B:125:TRP:CD1	2.64	0.51
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.11	0.51
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.93	0.51
1:A:196:ASP:HB2	3:E:140:MET:SD	2.51	0.51
1:A:437:ARG:NH1	1:A:454:GLU:OE2	2.44	0.51
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.45	0.51
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.46	0.51
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.93	0.51
2:C:192:MET:HE3	2:C:280:PHE:CD2	2.46	0.51
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.46	0.50
1:B:196:ASP:HB2	3:F:140:MET:SD	2.51	0.50
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.45	0.50
3:E:41:THR:O	3:E:44:ARG:CD	2.59	0.50
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.46	0.50
1:B:43:ARG:HD2	1:B:43:ARG:O	2.10	0.50
1:B:84:ASP:OD1	1:B:88:ARG:NH2	2.44	0.50
2:C:235:TRP:CD1	2:C:235:TRP:C	2.90	0.50
3:F:15:TRP:O	3:F:19:ILE:HG23	2.11	0.50
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.12	0.50
1:A:79:PHE:O	1:A:83:GLN:HG3	2.12	0.50
2:C:356:LEU:O	2:C:360:VAL:HG23	2.12	0.50
3:E:152:LEU:O	3:E:156:ARG:HG3	2.11	0.50
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.11	0.50
1:A:382:HIS:O	1:A:386:ILE:HG13	2.11	0.50
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.94	0.50
1:B:288:MET:HE2	1:B:347:TYR:HA	1.94	0.50
2:D:149:TRP:HB2	2:D:265:PHE:CE2	2.47	0.50
1:A:248:ALA:O	1:A:252:GLN:HB2	2.12	0.49
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.12	0.49
1:B:33:GLN:NE2	1:B:132:GLU:H	2.07	0.49
2:C:111:LYS:O	2:C:115:GLU:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TRP:CD1	1:A:125:TRP:C	2.90	0.49
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.60	0.49
2:D:89:GLU:CD	3:F:125:VAL:HG13	2.37	0.49
1:A:119:ALA:O	2:C:168:ARG:HD2	2.12	0.49
1:B:193:ILE:O	2:D:168:ARG:NH1	2.44	0.49
2:D:243:GLU:HG3	2:D:320:TRP:CD1	2.47	0.49
1:B:468:ASN:CG	1:B:471:GLU:HG3	2.37	0.49
3:F:98:MET:HE1	3:F:107:ALA:O	2.12	0.49
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.08	0.49
1:A:354:TRP:CZ2	1:A:403:ILE:HD11	2.46	0.49
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.93	0.49
3:F:16:VAL:HG23	3:F:17:ASN:N	2.28	0.49
1:B:213:THR:O	1:B:217:ILE:HG12	2.12	0.49
2:D:255:LEU:HD21	2:D:363:TRP:CG	2.48	0.49
1:A:495:LEU:HB3	7:A:9081:HOH:O	2.12	0.49
1:B:30:ARG:HG2	1:B:30:ARG:HH11	1.78	0.49
2:C:226:SER:HB2	2:C:331:ALA:HA	1.95	0.49
3:E:15:TRP:CD1	3:E:56:ILE:HD13	2.48	0.49
1:B:232:THR:HB	1:B:233:PRO:HD3	1.95	0.48
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.48	0.48
1:A:121:THR:HG21	1:A:140:GLN:CG	2.43	0.48
1:A:216:LEU:O	1:A:220:VAL:HG23	2.12	0.48
1:B:82:LEU:HD23	1:B:86:LEU:CD1	2.43	0.48
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.43	0.48
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.94	0.48
1:B:466:CYS:HB2	2:D:73:THR:HA	1.95	0.48
1:A:137:TYR:O	1:A:141:VAL:HG23	2.14	0.48
1:B:33:GLN:HA	1:B:33:GLN:NE2	2.22	0.48
1:B:119:ALA:HB1	2:D:168:ARG:HD2	1.95	0.48
2:D:262:ARG:HA	2:D:266:GLN:HB3	1.94	0.48
1:A:184:MET:HE3	1:A:188:PHE:HB2	1.95	0.48
2:D:54:VAL:O	2:D:55:TYR:HB2	2.14	0.48
3:E:165:HIS:CE1	3:E:167:GLN:HG3	2.48	0.48
1:A:44:THR:OG1	1:A:127:SER:HA	2.13	0.48
2:C:263:GLU:OE2	2:C:263:GLU:HA	2.14	0.48
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.96	0.48
3:F:109:LYS:HZ2	3:F:109:LYS:HB2	1.77	0.48
1:B:95:VAL:HG12	1:B:96:HIS:N	2.29	0.48
1:B:288:MET:CE	1:B:346:LEU:HB3	2.43	0.48
2:C:179:LEU:HD12	2:C:182:TRP:CE3	2.49	0.48
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.67	0.48
3:F:57:GLU:O	3:F:61:GLU:HG3	2.14	0.48
3:F:73:ASN:O	3:F:74:GLU:C	2.57	0.48
3:F:81:THR:HG21	3:F:85:GLU:HG3	1.95	0.48
2:C:136:MET:SD	2:C:141:ARG:HB2	2.54	0.48
2:D:80:ARG:HB2	7:D:423:HOH:O	2.14	0.48
2:C:336:MET:HE3	2:C:388:LEU:HG	1.95	0.48
1:A:302:VAL:HG23	1:A:303:LYS:H	1.79	0.47
1:B:31:TRP:CH2	2:D:210:SER:HA	2.49	0.47
2:C:193:ILE:HA	7:C:5058:HOH:O	2.12	0.47
2:D:228:ARG:HG2	2:D:228:ARG:HH11	1.79	0.47
2:D:260:VAL:O	2:D:265:PHE:HD1	1.97	0.47
2:D:336:MET:HE1	2:D:356:LEU:HD11	1.95	0.47
3:E:98:MET:HE1	3:E:107:ALA:HB1	1.95	0.47
1:A:101:GLU:OE1	1:A:360:ARG:HD3	2.14	0.47
1:B:125:TRP:O	1:B:125:TRP:HD1	1.97	0.47
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.49	0.47
3:E:165:HIS:HE1	3:E:167:GLN:HG3	1.79	0.47
3:F:38:ASP:HA	3:F:45:ASN:HB2	1.95	0.47
1:A:204:LEU:O	1:A:209:GLU:HG3	2.15	0.47
1:B:489:ARG:NH1	1:B:496:ILE:O	2.46	0.47
2:D:98:HIS:CD2	2:D:99:ARG:N	2.82	0.47
3:E:15:TRP:O	3:E:19:ILE:HG13	2.14	0.47
1:B:30:ARG:HG2	1:B:30:ARG:NH1	2.29	0.47
1:B:366:GLN:O	1:B:370:GLU:HG3	2.15	0.47
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.79	0.47
1:B:125:TRP:CD1	1:B:125:TRP:C	2.92	0.47
2:C:50:GLU:OE1	2:C:99:ARG:NH1	2.48	0.47
1:B:367:GLU:HG3	7:B:9066:HOH:O	2.15	0.47
2:D:179:LEU:HD23	2:D:182:TRP:CZ3	2.50	0.47
2:D:189:ILE:HD12	2:D:284:ALA:HB2	1.96	0.47
2:D:326:GLU:HB2	2:D:327:PRO:HD3	1.96	0.47
1:A:48:THR:O	3:E:137:THR:HG23	2.14	0.47
1:A:521:ASN:CG	1:A:523:VAL:HG12	2.39	0.47
1:B:519:PHE:CD2	6:B:9010:XE:XE	3.46	0.47
1:A:77:ARG:HG3	7:A:9079:HOH:O	2.14	0.47
1:B:93:VAL:HG13	2:C:3:MET:HE3	1.97	0.47
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.97	0.47
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.50	0.47
1:A:186:ARG:CZ	1:A:277:THR:HG23	2.45	0.47
1:A:230:GLU:HG3	1:B:89:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:192:MET:HE3	2:C:280:PHE:CE2	2.50	0.47
2:D:98:HIS:O	2:D:99:ARG:HG2	2.14	0.47
1:B:93:VAL:HG11	2:C:3:MET:HG2	1.96	0.46
1:B:445:MET:HE1	1:B:527:ASN:ND2	2.30	0.46
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.50	0.46
1:B:79:PHE:HB3	1:B:83:GLN:NE2	2.30	0.46
1:B:211:CYS:HB2	1:B:313:TRP:CG	2.50	0.46
1:B:489:ARG:HB3	2:D:30:ASP:OD2	2.14	0.46
2:C:187:ILE:O	2:C:191:GLN:HG3	2.15	0.46
2:C:255:LEU:HB2	2:C:328:THR:HG21	1.96	0.46
3:F:61:GLU:O	3:F:121:PRO:HG2	2.16	0.46
1:A:82:LEU:HD23	1:A:86:LEU:HD12	1.97	0.46
2:C:336:MET:HE1	2:C:352:ILE:HG21	1.97	0.46
2:D:189:ILE:HD11	2:D:284:ALA:HA	1.96	0.46
1:A:101:GLU:CD	1:A:360:ARG:HD3	2.41	0.46
2:C:270:PRO:HB3	2:D:270:PRO:CB	2.42	0.46
2:D:155:ASN:O	2:D:159:LEU:HG	2.15	0.46
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.50	0.46
1:B:214:ASN:CG	1:B:247:MET:HE1	2.41	0.46
1:B:365:ASP:OD2	1:B:365:ASP:C	2.58	0.46
2:C:336:MET:HE1	2:C:352:ILE:HG22	1.96	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.51	0.46
1:A:224:ALA:HB1	1:A:229:ASP:HB3	1.98	0.46
1:B:44:THR:HG22	1:B:45:LYS:N	2.30	0.46
1:B:143:ASP:OD2	1:B:245:ARG:NH2	2.46	0.46
2:C:54:VAL:O	2:C:55:TYR:HB2	2.15	0.46
3:E:120:PRO:HG2	3:E:125:VAL:HG12	1.96	0.46
1:A:452:TRP:O	1:A:456:MET:HG3	2.15	0.46
1:B:23:VAL:HB	2:D:195:LEU:CD2	2.45	0.46
1:B:123:MET:HE1	1:B:200:CYS:SG	2.56	0.46
2:D:61:ASP:OD2	3:F:7:HIS:HD2	1.99	0.46
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.97	0.46
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.51	0.45
1:B:96:HIS:ND1	1:B:97:PRO:HD2	2.32	0.45
2:C:146:ASN:ND2	2:C:197:ARG:HE	2.14	0.45
1:A:186:ARG:HD3	1:A:186:ARG:C	2.40	0.45
1:A:407:TRP:CE2	1:A:411:ASN:ND2	2.85	0.45
1:B:268:ASN:HD21	1:B:327:GLU:H	1.65	0.45
2:C:98:HIS:HE1	2:C:178:SER:OG	2.00	0.45
3:F:154:GLU:HG3	3:F:158:GLN:HE21	1.82	0.45
1:A:306:ASP:OD2	1:A:336:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLU:C	1:A:233:PRO:HD2	2.42	0.45
2:C:146:ASN:HD21	2:C:197:ARG:NH2	1.99	0.45
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.47	0.45
3:F:137:THR:O	3:F:141:GLU:HG3	2.16	0.45
1:A:146:ARG:HB2	2:C:106:HIS:NE2	2.32	0.45
1:B:405:LEU:HD22	6:B:9011:XE:XE	2.95	0.45
1:A:58:GLU:HB2	7:A:9140:HOH:O	2.16	0.44
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.15	0.44
1:A:317:TRP:CD1	1:A:318:ILE:HD12	2.48	0.44
2:D:319:ASN:OD1	3:F:78:ARG:HD3	2.17	0.44
3:F:30:GLU:OE2	3:F:30:GLU:HA	2.16	0.44
3:F:152:LEU:O	3:F:156:ARG:HG3	2.17	0.44
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.52	0.44
1:A:159:ALA:O	2:C:33:ASN:HB2	2.17	0.44
1:A:244:LEU:HA	1:A:247:MET:HG3	1.98	0.44
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.65	0.44
1:B:82:LEU:HA	1:B:86:LEU:HD12	1.99	0.44
1:B:263:SER:C	1:B:265:LYS:N	2.74	0.44
1:B:109:PHE:HB3	1:B:184:MET:HE2	2.00	0.44
2:C:385:LEU:O	2:C:388:LEU:HB2	2.18	0.44
2:D:243:GLU:HG3	2:D:320:TRP:NE1	2.32	0.44
1:B:337:GLN:HG3	1:B:338:ASP:N	2.32	0.44
2:D:296:GLN:O	2:D:300:TYR:HB2	2.17	0.44
3:F:95:VAL:HG12	3:F:99:ASN:HD21	1.82	0.44
1:B:140:GLN:O	1:B:144:GLU:HG2	2.18	0.44
1:B:263:SER:C	1:B:265:LYS:H	2.25	0.44
2:D:336:MET:HB3	2:D:388:LEU:HD23	1.98	0.44
3:E:138:ARG:NH2	3:E:142:LEU:HD21	2.33	0.44
3:F:41:THR:HG23	3:F:42:PRO:CD	2.47	0.44
1:A:302:VAL:HG11	1:A:340:TYR:CE1	2.53	0.44
2:D:111:LYS:O	2:D:115:GLU:HG3	2.18	0.44
1:A:521:ASN:HA	1:A:522:PRO:HD2	1.82	0.44
1:B:30:ARG:HG2	1:B:30:ARG:O	2.18	0.44
2:D:54:VAL:HA	2:D:173:ASP:OD1	2.18	0.44
2:D:324:TRP:C	2:D:327:PRO:HD2	2.42	0.44
3:F:125:VAL:HG23	3:F:126:ASN:N	2.33	0.44
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.33	0.43
1:B:493:LYS:HE2	1:B:508:THR:HG21	2.00	0.43
2:C:259:PHE:CD1	2:C:263:GLU:HB2	2.54	0.43
1:B:371:TRP:CE2	1:B:375:ASN:ND2	2.86	0.43
1:B:438:VAL:C	3:F:164:VAL:HG22	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:LEU:HD13	2:C:290:ILE:HG23	1.99	0.43
2:C:246:PHE:O	2:C:250:ALA:HB3	2.18	0.43
1:A:192:PHE:CE2	1:A:204:LEU:HA	2.53	0.43
1:B:230:GLU:C	1:B:233:PRO:HD2	2.43	0.43
2:D:167:ALA:O	2:D:176:ARG:NH1	2.51	0.43
3:F:76:ASP:C	3:F:78:ARG:N	2.74	0.43
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.83	0.43
1:B:207:VAL:HG22	1:B:313:TRP:CZ2	2.54	0.43
1:B:227:ASN:ND2	1:B:295:LYS:H	2.16	0.43
1:A:89:LEU:HD21	1:B:230:GLU:HG3	2.00	0.43
1:A:317:TRP:HD1	1:A:318:ILE:CD1	2.30	0.43
2:D:251:VAL:HG12	2:D:252:TYR:N	2.34	0.43
3:F:119:LYS:O	3:F:120:PRO:C	2.61	0.43
1:A:187:VAL:HG12	1:A:277:THR:HG22	2.00	0.43
7:A:9022:HOH:O	3:E:144:ASN:HB3	2.17	0.43
1:B:521:ASN:OD1	1:B:523:VAL:HG12	2.19	0.43
2:D:236:GLN:OE1	2:D:236:GLN:HA	2.17	0.43
1:B:75:ASP:OD2	1:B:146:ARG:NH1	2.52	0.43
1:B:125:TRP:O	1:B:134:LYS:HG2	2.19	0.43
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.35	0.43
3:F:25:LEU:HD22	3:F:68:LYS:HA	2.01	0.43
1:A:440:GLU:HG3	1:A:441:TYR:N	2.31	0.43
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.52	0.43
2:D:105:TRP:O	2:D:108:PRO:HD2	2.19	0.43
3:F:81:THR:C	3:F:83:PHE:H	2.27	0.43
1:A:266:TYR:HB3	7:A:9022:HOH:O	2.18	0.43
1:A:491:ASP:OD2	1:A:491:ASP:C	2.61	0.43
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.19	0.42
1:B:196:ASP:O	1:B:197:ALA:C	2.62	0.42
1:B:148:THR:HG21	6:B:9007:XE:XE	2.97	0.42
1:B:489:ARG:NH1	1:B:496:ILE:HA	2.34	0.42
2:D:269:ALA:N	2:D:270:PRO:CD	2.83	0.42
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.54	0.42
1:B:118:ILE:HD13	1:B:145:ILE:HG12	2.01	0.42
2:C:126:GLY:O	2:C:130:ASP:HB2	2.19	0.42
1:A:109:PHE:O	1:A:112:VAL:HG12	2.19	0.42
1:A:212:PHE:O	1:A:216:LEU:HB2	2.20	0.42
1:B:268:ASN:ND2	1:B:327:GLU:H	2.17	0.42
1:A:420:VAL:HG13	1:A:464:TYR:CE2	2.54	0.42
1:B:33:GLN:HE21	1:B:33:GLN:CA	2.17	0.42
1:A:148:THR:CG2	6:A:9006:XE:XE	3.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASN:HD22	1:B:193:ILE:HD13	1.84	0.42
2:C:33:ASN:H	2:C:33:ASN:ND2	2.16	0.42
2:D:164:SER:O	2:D:167:ALA:HB3	2.20	0.42
3:F:114:PHE:CD2	3:F:135:LEU:HD12	2.55	0.42
1:A:96:HIS:HA	1:A:97:PRO:HD3	1.92	0.42
1:A:453:GLY:HA3	7:A:9024:HOH:O	2.20	0.41
2:D:102:LEU:CB	2:D:104:ARG:HD2	2.49	0.41
2:D:148:TYR:CD1	2:D:338:LEU:HD11	2.55	0.41
1:A:146:ARG:HB2	2:C:106:HIS:CD2	2.55	0.41
1:A:244:LEU:HD23	1:A:247:MET:HG3	2.02	0.41
1:B:217:ILE:O	1:B:221:THR:HG23	2.20	0.41
1:B:403:ILE:O	1:B:403:ILE:HG13	2.19	0.41
2:C:105:TRP:O	2:C:108:PRO:HD2	2.20	0.41
3:E:33:LYS:HE2	7:E:206:HOH:O	2.20	0.41
1:A:301:TRP:O	1:A:302:VAL:C	2.64	0.41
1:B:382:HIS:HD2	1:B:383:TYR:CE1	2.39	0.41
2:C:36:GLY:O	2:C:39:VAL:HG23	2.19	0.41
1:A:186:ARG:NH1	1:A:277:THR:HG23	2.35	0.41
1:A:212:PHE:O	1:A:216:LEU:CB	2.68	0.41
1:A:292:TYR:OH	1:A:344:HIS:HD2	2.03	0.41
1:B:112:VAL:HG23	2:D:58:PRO:HG3	2.02	0.41
1:B:519:PHE:CG	6:B:9010:XE:XE	3.52	0.41
1:A:124:LEU:HD21	1:A:201:SER:HB2	2.01	0.41
1:A:297:LYS:N	1:A:297:LYS:HD2	2.36	0.41
1:B:112:VAL:CG2	2:D:58:PRO:HG3	2.50	0.41
1:B:439:HIS:HE1	1:B:454:GLU:OE1	2.04	0.41
1:A:138:LEU:O	1:A:141:VAL:HB	2.21	0.41
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.51	0.41
1:B:190:ASP:HB3	2:D:74:GLN:HB3	2.03	0.41
2:D:351:GLU:C	2:D:353:THR:N	2.77	0.41
1:A:260:ASP:HA	1:A:261:PRO:HD3	1.95	0.41
2:C:5:GLY:HA3	7:C:5151:HOH:O	2.21	0.41
2:D:357:TYR:HE2	2:D:377:ARG:HE	1.67	0.41
1:A:171:ALA:O	1:A:175:ARG:HD3	2.20	0.41
1:A:437:ARG:HG2	1:A:437:ARG:NH1	2.35	0.41
1:A:466:CYS:HB2	2:C:73:THR:HA	2.03	0.41
1:B:65:LYS:HE2	2:D:192:MET:HE2	2.02	0.41
1:B:438:VAL:HG12	3:F:164:VAL:HG21	2.03	0.41
1:B:115:TYR:CE2	2:D:173:ASP:HB3	2.56	0.41
1:B:267:LEU:HD21	1:B:326:VAL:HG22	2.03	0.41
2:C:146:ASN:O	2:C:214:PRO:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:147:ARG:HH11	2:D:217:GLU:HB2	1.86	0.41
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.21	0.41
2:D:324:TRP:HA	2:D:327:PRO:HD2	2.03	0.41
1:A:186:ARG:HA	2:C:73:THR:OG1	2.20	0.40
1:A:348:LEU:HD23	1:A:387:TYR:CZ	2.56	0.40
1:B:147:HIS:CE1	7:B:9145:HOH:O	2.75	0.40
2:C:141:ARG:O	2:C:145:ILE:HB	2.20	0.40
1:B:192:PHE:CE2	1:B:204:LEU:HA	2.56	0.40
1:B:283:THR:HB	1:B:284:PRO:HD3	2.03	0.40
1:B:507:TRP:CD1	1:B:507:TRP:N	2.89	0.40
2:D:76:PHE:HB2	2:D:80:ARG:CB	2.49	0.40
3:E:98:MET:HE3	3:E:98:MET:HA	2.03	0.40
1:A:108:ASN:O	1:A:111:GLU:HB3	2.21	0.40
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.56	0.40
1:B:348:LEU:HD23	1:B:387:TYR:CE2	2.56	0.40
1:B:521:ASN:HA	1:B:522:PRO:HD2	1.95	0.40
2:C:156:GLU:HA	2:C:156:GLU:OE2	2.21	0.40
2:C:283:GLN:HG3	2:D:119:TYR:OH	2.21	0.40
3:E:52:ASP:O	3:E:56:ILE:HG13	2.21	0.40
1:A:244:LEU:HA	1:A:247:MET:CG	2.52	0.40
2:C:63:ILE:O	2:C:64:ALA:C	2.64	0.40
2:C:319:ASN:OD1	3:E:78:ARG:HD3	2.22	0.40
1:B:182:LYS:HA	1:B:182:LYS:HD3	1.92	0.40
1:B:421:SER:O	1:B:422:GLN:HB2	2.22	0.40
2:C:179:LEU:HD12	2:C:179:LEU:HA	1.89	0.40
2:C:262:ARG:HD3	2:D:130:ASP:OD2	2.21	0.40
2:D:63:ILE:O	2:D:64:ALA:C	2.64	0.40
3:E:36:ARG:NH2	3:E:119:LYS:HD2	2.37	0.40
3:F:32:LEU:HA	3:F:60:LEU:CD2	2.52	0.40
3:F:72:PHE:CE1	3:F:80:LYS:HB3	2.55	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%)	483 (95%)	25 (5%)	1 (0%)	43	66
1	B	508/527 (96%)	480 (94%)	28 (6%)	0	100	100
2	C	386/389 (99%)	371 (96%)	14 (4%)	1 (0%)	36	58
2	D	386/389 (99%)	356 (92%)	24 (6%)	6 (2%)	7	16
3	E	163/170 (96%)	153 (94%)	8 (5%)	2 (1%)	10	23
3	F	165/170 (97%)	143 (87%)	19 (12%)	3 (2%)	6	14
All	All	2117/2172 (98%)	1986 (94%)	118 (6%)	13 (1%)	21	42

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	74	GLU
2	D	251	VAL
3	E	5	GLY
3	F	122	ILE
2	D	64	ALA
2	D	352	ILE
3	F	144	ASN
2	D	205	PRO
2	D	386	ALA
1	A	284	PRO
2	D	307	PRO
2	C	251	VAL
3	E	122	ILE

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%)	422 (98%)	11 (2%)	42	69
1	B	432/442 (98%)	423 (98%)	9 (2%)	47	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	322/323 (100%)	315 (98%)	7 (2%)	45	72
2	D	321/323 (99%)	316 (98%)	5 (2%)	55	79
3	E	143/147 (97%)	138 (96%)	5 (4%)	32	59
3	F	145/147 (99%)	142 (98%)	3 (2%)	47	73
All	All	1796/1824 (98%)	1756 (98%)	40 (2%)	45	72

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	125	TRP
1	A	302	VAL
1	A	310	TYR
1	A	316	ILE
1	A	391	ARG
1	A	403	ILE
1	A	435	THR
1	A	440	GLU
1	A	445	MET
1	A	467	GLN
1	B	33	GLN
1	B	110	LEU
1	B	125	TRP
1	B	186	ARG
1	B	247	MET
1	B	279	GLN
1	B	310	TYR
1	B	440	GLU
1	B	445	MET
2	C	33	ASN
2	C	117	TRP
2	C	153	LEU
2	C	168	ARG
2	C	179	LEU
2	C	356	LEU
2	C	377	ARG
2	D	4	LEU
2	D	80	ARG
2	D	153	LEU
2	D	173	ASP
2	D	223	VAL

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Mol	Chain	Res	Type
3	E	8	SER
3	E	24	THR
3	E	44	ARG
3	E	68	LYS
3	E	166	LEU
3	F	11	THR
3	F	41	THR
3	F	108	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	108	ASN
1	A	133	GLN
1	A	155	ASN
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	278	GLN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	366	GLN
1	A	411	ASN
1	A	439	HIS
1	A	442	ASN
1	B	33	GLN
1	B	36	ASN
1	B	54	ASN
1	B	78	GLN
1	B	83	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	133	GLN
1	B	227	ASN

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Mol	Chain	Res	Type
1	B	249	ASN
1	B	252	GLN
1	B	259	ASN
1	B	268	ASN
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	422	GLN
1	B	439	HIS
1	B	451	GLN
1	B	516	ASN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	161	ASN
2	C	220	ASN
2	C	285	GLN
2	C	301	ASN
2	D	57	GLN
2	D	98	HIS
2	D	106	HIS
2	D	155	ASN
2	D	161	ASN
2	D	220	ASN
2	D	266	GLN
2	D	285	GLN
2	D	296	GLN
2	D	301	ASN
3	E	23	ASN
3	E	45	ASN
3	E	134	GLN
3	E	144	ASN
3	E	158	GLN
3	E	165	HIS
3	F	7	HIS
3	F	45	ASN
3	F	79	HIS

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Mol	Chain	Res	Type
3	F	99	ASN
3	F	158	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 19 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 ⓘ

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%)	-0.20	3 (0%) 85 83	17, 30, 47, 60	0
1	B	510/527 (96%)	-0.23	0 100 100	15, 30, 48, 56	0
2	C	388/389 (99%)	-0.51	0 100 100	13, 22, 36, 52	0
2	D	388/389 (99%)	0.05	2 (0%) 87 85	19, 36, 54, 66	0
3	E	165/170 (97%)	-0.34	2 (1%) 76 73	15, 26, 39, 50	0
3	F	167/170 (98%)	0.52	6 (3%) 46 40	32, 44, 60, 69	0
All	All	2129/2172 (98%)	-0.17	13 (0%) 85 83	13, 30, 50, 69	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	ALA	3.2
2	D	352	ILE	2.8
3	F	4	LEU	2.8
3	F	82	ALA	2.7
3	F	25	LEU	2.7
3	E	4	LEU	2.4
1	A	54	ASN	2.4
1	A	517	CYS	2.4
3	F	23	ASN	2.3
3	F	72	PHE	2.2
2	D	308	GLU	2.1
3	F	100	ALA	2.1
3	E	167	GLN	2.1

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
5	CA	C	5007	1/1	0.85	0.13	70,70,70,70	0
5	CA	C	5006	1/1	0.91	0.12	52,52,52,52	0
5	CA	A	5005	1/1	0.91	0.11	52,52,52,52	0
6	XE	A	9008	1/1	0.91	0.09	32,32,32,32	1
5	CA	B	5008	1/1	0.92	0.06	45,45,45,45	0
6	XE	A	9004	1/1	0.97	0.05	32,32,32,32	1
6	XE	B	9010	1/1	0.97	0.08	32,32,32,32	1
6	XE	A	9002	1/1	0.98	0.05	32,32,32,32	1
6	XE	A	9009	1/1	0.98	0.07	32,32,32,32	1
6	XE	B	9005	1/1	0.98	0.05	32,32,32,32	1
6	XE	B	9007	1/1	0.98	0.05	32,32,32,32	1
4	FE	B	5004	1/1	0.98	0.04	36,36,36,36	0
6	XE	B	9011	1/1	0.98	0.05	32,32,32,32	1
4	FE	A	5001	1/1	0.99	0.02	27,27,27,27	0
6	XE	A	9006	1/1	0.99	0.04	32,32,32,32	1
4	FE	A	5002	1/1	0.99	0.02	31,31,31,31	0
4	FE	B	5003	1/1	0.99	0.03	28,28,28,28	0
6	XE	A	9001	1/1	1.00	0.01	32,32,32,32	0
6	XE	B	9003	1/1	1.00	0.02	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.