



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:29 AM UTC

PDB ID : 1FZ7 / pdb_00001fz7
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM III SOAKED
IN 0.9 M ETHANOL
Authors : Whittington, D.A.; Sazinsky, M.H.; 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

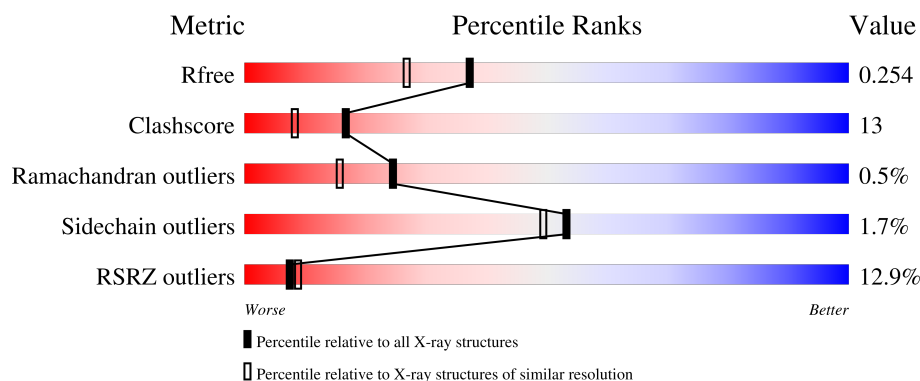
1 Overall quality at a glance

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	11% 69% 26% ..
1	B	527	8% 69% 27% ..
2	C	389	2% 76% 22% .
2	D	389	23% 63% 35% .
3	E	170	3% 76% 19% ..

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Mol	Chain	Length	Quality of chain
3	F	170	42% 57% 38%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18582 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4177	2673	719	767	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	7	0	0
			3193	2054	551	580	8			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	166	Total	C	N	O	S	0	0	0
			1368	867	246	250	5			
3	F	167	Total	C	N	O	S	0	0	0
			1377	872	248	252	5			

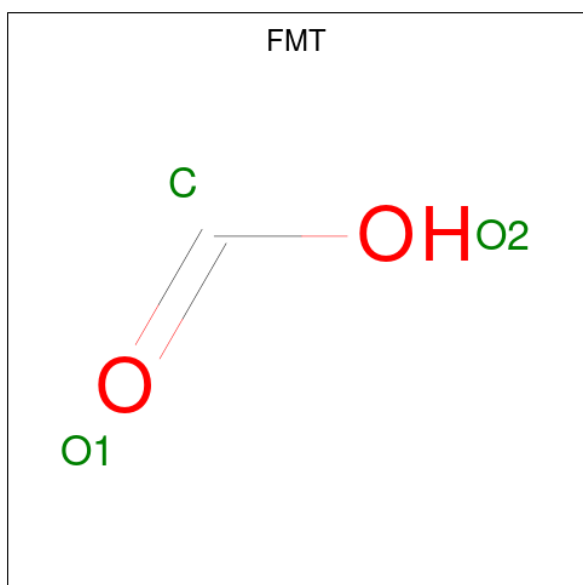
- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

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

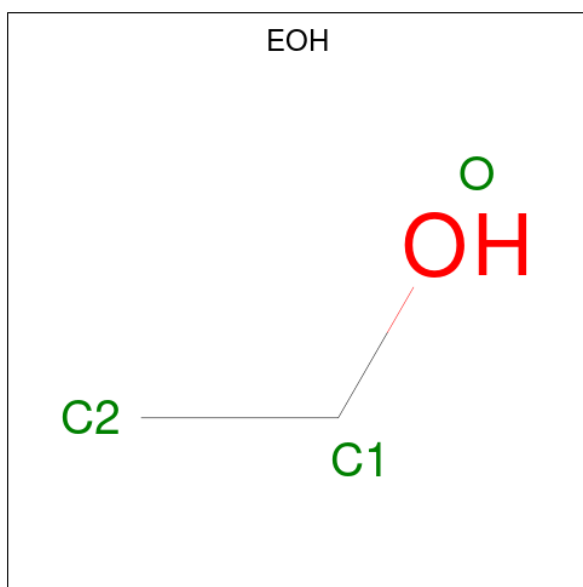
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	C	2	Total	Ca	0	0
			2	2		

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



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

- Molecule 7 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			3	2	1		

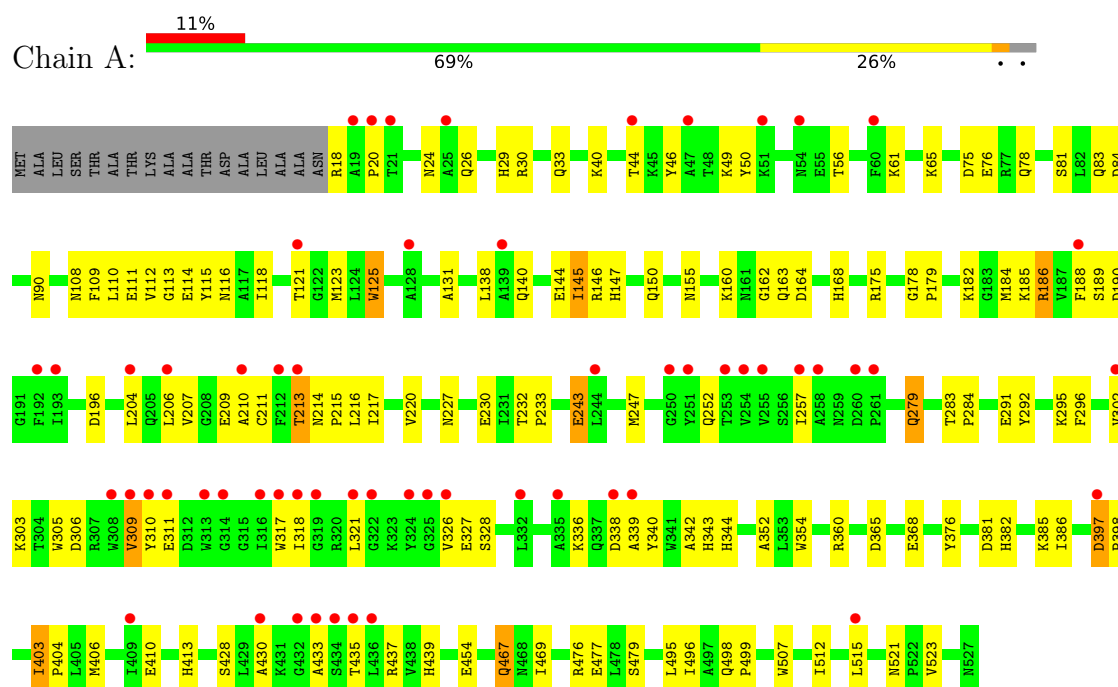
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	246	Total	O	0	0
			246	246		
8	B	225	Total	O	0	0
			225	225		
8	C	303	Total	O	0	0
			303	303		
8	D	116	Total	O	0	0
			116	116		
8	E	152	Total	O	0	0
			152	152		
8	F	42	Total	O	0	0
			42	42		

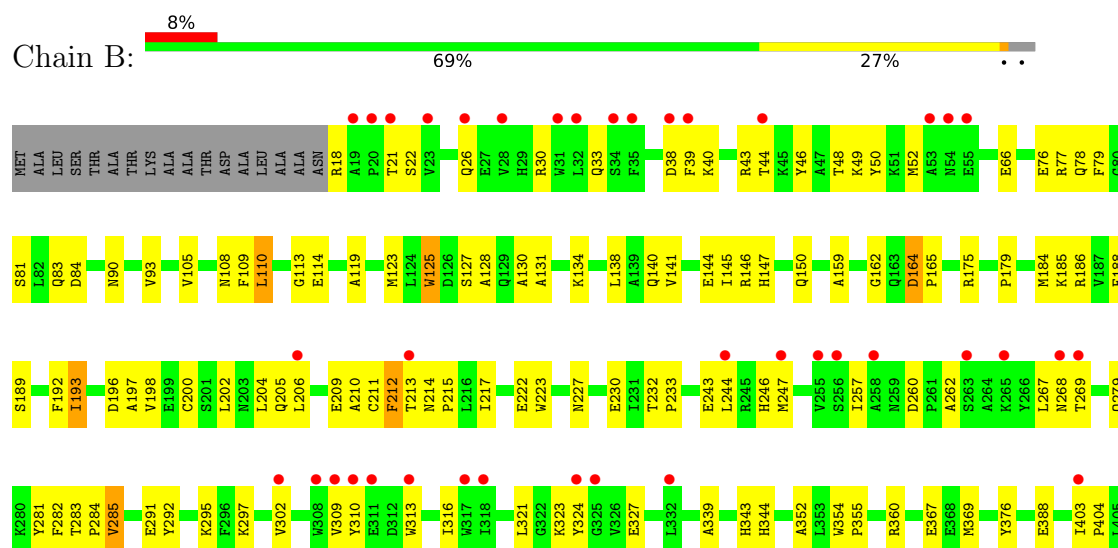
3 Residue-property plots [i](#)

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

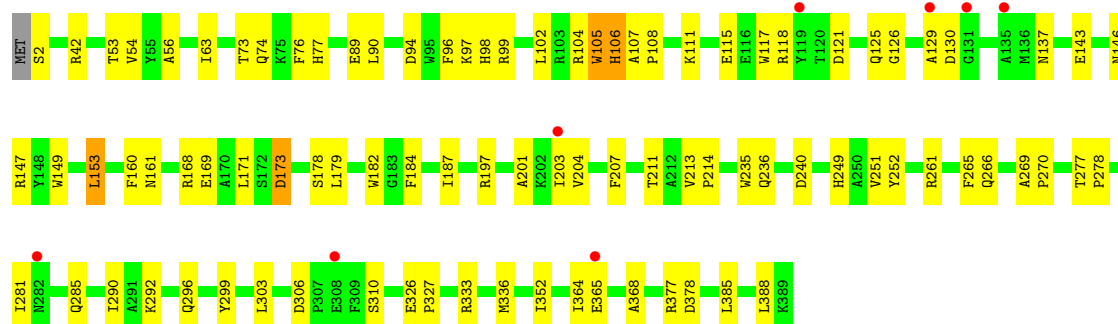
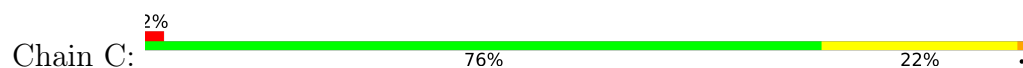


• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

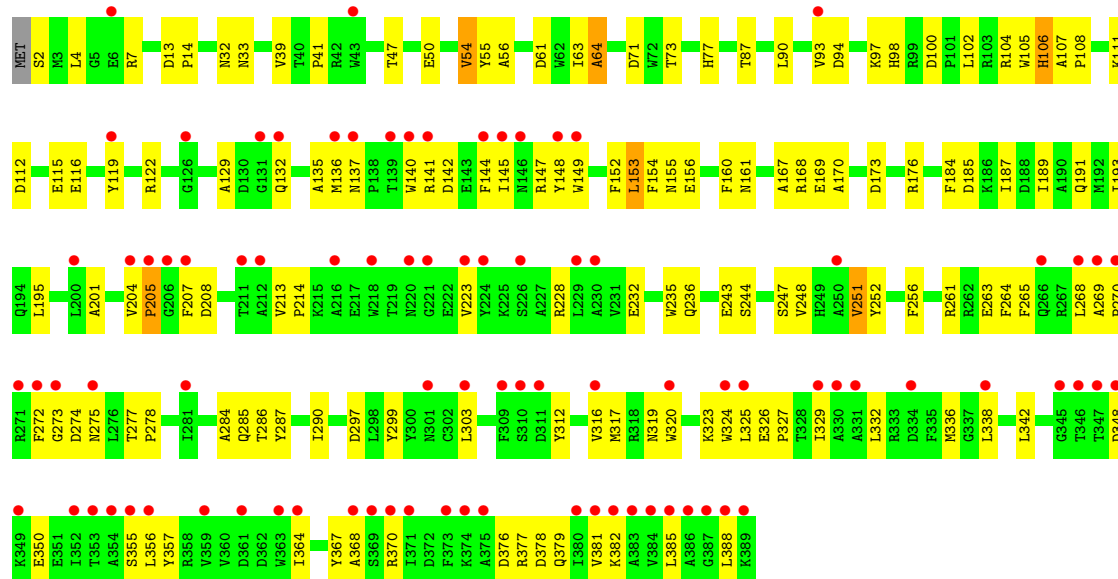




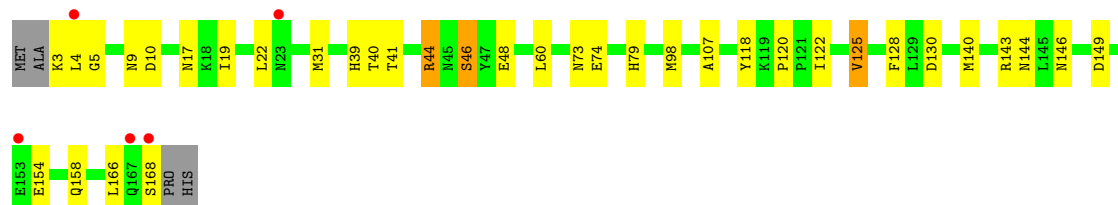
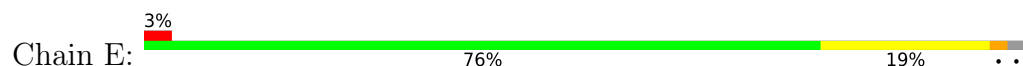
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



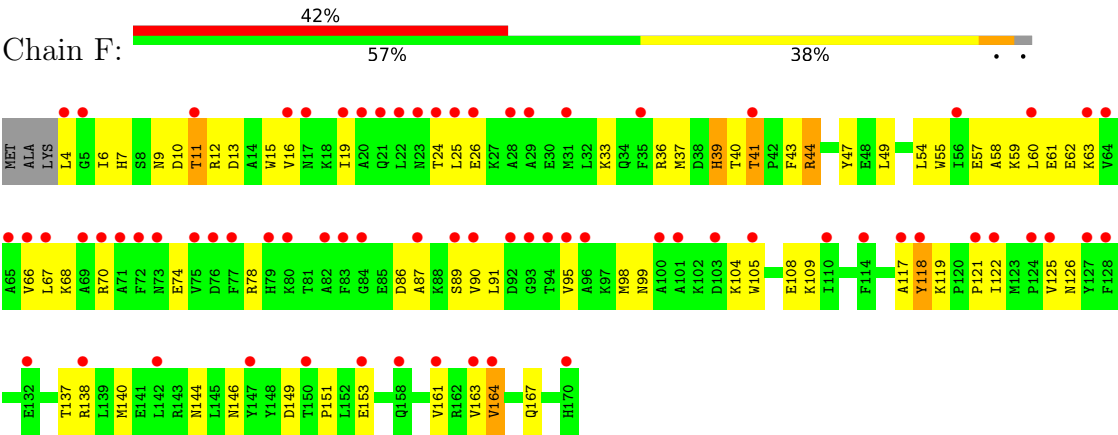
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



• 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	71.40Å 172.37Å 221.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.96 30.00 – 1.96	Depositor EDS
% Data completeness (in resolution range)	90.1 (30.00-1.96) 90.2 (30.00-1.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.19 (at 1.96Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.255 0.214 , 0.254	Depositor DCC
R_{free} test set	6226 reflections (3.24%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.4	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	18582	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% 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, EOH

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	0.37	0/4302	0.90	14/5842 (0.2%)
1	B	0.37	0/4302	0.89	16/5842 (0.3%)
2	C	0.43	0/3289	0.89	18/4464 (0.4%)
2	D	0.34	0/3289	0.85	10/4464 (0.2%)
3	E	0.41	0/1396	0.89	8/1880 (0.4%)
3	F	0.32	0/1407	0.82	2/1896 (0.1%)
All	All	0.38	0/17985	0.88	68/24388 (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	8.74	120.88	111.36
1	A	397	ASP	CA-C-N	7.14	126.98	119.05
1	A	397	ASP	C-N-CA	7.14	126.98	119.05
2	C	169	GLU	N-CA-C	6.99	121.98	113.38
1	B	164	ASP	CA-C-N	6.71	126.66	119.28
1	B	164	ASP	C-N-CA	6.71	126.66	119.28
2	D	105	TRP	N-CA-C	-6.66	100.36	109.95
1	B	193	ILE	N-CA-C	6.64	120.04	113.53
2	C	106	HIS	N-CA-C	6.61	119.04	111.11
2	C	105	TRP	N-CA-C	-6.57	100.48	109.95
2	C	149	TRP	N-CA-C	-6.52	104.25	111.36
1	A	145	ILE	N-CA-C	-6.50	104.16	110.72
1	B	309	VAL	N-CA-C	6.46	116.50	110.42
2	D	204	VAL	CA-C-N	6.44	127.89	119.84
2	D	204	VAL	C-N-CA	6.44	127.89	119.84
1	B	496	ILE	N-CA-C	-6.39	104.53	110.53
1	A	164	ASP	CA-C-N	6.38	125.96	119.19
1	A	164	ASP	C-N-CA	6.38	125.96	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	GLY	CA-C-N	6.37	125.94	119.19
1	A	178	GLY	C-N-CA	6.37	125.94	119.19
3	E	118	TYR	N-CA-C	6.35	121.80	113.30
2	C	56	ALA	N-CA-C	-6.23	104.54	111.71
2	C	236	GLN	N-CA-C	6.22	121.80	113.72
1	A	496	ILE	N-CA-C	-6.08	104.81	110.53
2	D	54	VAL	N-CA-C	6.05	117.09	108.93
1	B	431	LYS	N-CA-C	-6.04	106.07	113.50
1	A	162	GLY	N-CA-C	6.02	121.81	112.60
1	B	285	VAL	N-CA-C	6.00	116.19	110.42
3	E	130	ASP	N-CA-C	-5.98	104.84	111.36
2	C	377	ARG	N-CA-C	5.91	117.72	111.28
3	E	39	HIS	N-CA-C	5.80	122.31	113.61
1	A	243	GLU	N-CA-C	5.78	118.35	111.71
2	C	252	TYR	N-CA-C	5.78	117.27	110.97
3	E	73	ASN	N-CA-C	-5.70	103.17	110.53
1	B	93	VAL	N-CA-C	5.66	116.42	111.56
1	B	145	ILE	N-CA-C	-5.58	105.09	110.72
2	D	252	TYR	N-CA-C	5.58	117.04	111.07
1	A	339	ALA	N-CA-C	5.56	117.20	111.03
3	E	122	ILE	N-CA-C	-5.55	105.69	110.74
1	A	309	VAL	N-CA-C	5.54	115.74	110.42
3	F	39	HIS	N-CA-C	5.54	121.27	113.02
2	D	286	THR	N-CA-C	-5.52	105.34	111.36
3	E	79	HIS	N-CA-C	5.50	121.86	113.61
3	E	143	ARG	N-CA-C	5.48	117.33	111.36
1	B	490	SER	N-CA-C	5.47	117.95	111.33
1	B	316	ILE	N-CA-C	5.46	115.56	110.42
2	D	106	HIS	N-CA-C	5.46	117.66	111.11
2	C	63	ILE	N-CA-C	-5.37	98.74	107.28
1	B	162	GLY	N-CA-C	5.35	120.78	112.60
2	C	249	HIS	N-CA-C	5.32	118.93	112.23
3	F	118	TYR	N-CA-C	5.32	119.74	112.88
2	C	171	LEU	N-CA-C	5.27	119.34	113.02
2	D	56	ALA	N-CA-C	-5.27	105.62	111.36
1	B	212	PHE	N-CA-C	5.25	119.33	112.13
2	C	137	ASN	CA-C-N	5.25	124.70	119.24
2	C	137	ASN	C-N-CA	5.25	124.70	119.24
3	E	74	GLU	N-CA-C	5.23	116.98	111.28
1	A	213	THR	N-CA-C	5.22	116.65	111.07
2	C	265	PHE	N-CA-C	5.21	116.64	111.07
2	D	236	GLN	N-CA-C	5.17	119.57	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	299	TYR	N-CA-C	5.14	118.71	112.23
2	C	53	THR	N-CA-C	5.14	119.77	112.93
1	A	291	GLU	N-CA-C	5.13	116.95	111.36
2	C	54	VAL	N-CA-C	5.13	116.29	109.37
1	B	267	LEU	N-CA-C	5.07	116.50	110.97
2	D	119	TYR	N-CA-C	-5.06	105.66	111.07
1	B	310	TYR	N-CA-C	5.05	116.59	111.14
2	C	104	ARG	N-CA-C	5.01	116.48	108.41

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	4177	0	3975	116	0
1	B	4177	0	3975	123	0
2	C	3193	0	3042	66	0
2	D	3193	0	3042	109	0
3	E	1368	0	1363	23	0
3	F	1377	0	1364	60	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	0	0
5	C	2	0	0	0	0
6	A	3	0	1	0	0
7	B	3	0	5	0	0
8	A	246	0	0	9	0
8	B	225	0	0	5	0
8	C	303	0	0	5	0
8	D	116	0	0	3	0
8	E	152	0	0	1	0
8	F	42	0	0	2	0
All	All	18582	0	16767	438	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 13.

All (438) 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	1.21	1.06
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.37	1.05
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.05	0.95
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.49	0.95
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.17	0.93
3:F:40:THR:O	3:F:41:THR:HG22	1.71	0.91
1:B:44:THR:HG22	1:B:46:TYR:H	1.37	0.86
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.59	0.84
3:F:41:THR:O	3:F:44:ARG:HD2	1.77	0.84
1:B:244:LEU:HG	8:B:9096:HOH:O	1.78	0.83
1:A:44:THR:HG22	1:A:46:TYR:H	1.44	0.82
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.23	0.82
1:A:209:GLU:HA	1:A:213:THR:HB	1.60	0.81
1:B:52:MET:HE1	1:B:127:SER:HB3	1.62	0.81
1:B:209:GLU:HA	1:B:213:THR:OG1	1.80	0.81
1:A:338:ASP:OD1	1:A:433:ALA:HB2	1.82	0.79
2:C:336:MET:HE3	2:C:388:LEU:HG	1.65	0.79
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.28	0.79
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.31	0.79
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.64	0.79
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.83	0.79
1:A:184:MET:HE3	1:A:188:PHE:HB2	1.63	0.78
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.84	0.78
3:F:13:ASP:O	3:F:16:VAL:HG22	1.83	0.78
1:A:227:ASN:HD21	1:A:295:LYS:H	1.33	0.76
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.68	0.76
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.31	0.76
3:F:153:GLU:H	3:F:153:GLU:CD	1.94	0.75
1:B:268:ASN:HD21	1:B:327:GLU:H	1.32	0.75
1:A:467:GLN:HG3	8:A:9140:HOH:O	1.86	0.75
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.68	0.75
2:D:228:ARG:O	2:D:232:GLU:HG3	1.87	0.75
1:B:123:MET:HE3	1:B:197:ALA:HA	1.69	0.74
1:A:213:THR:O	1:A:217:ILE:HG12	1.87	0.74
3:E:41:THR:O	3:E:44:ARG:HD2	1.88	0.73
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.69	0.73
1:B:30:ARG:O	1:B:30:ARG:HD3	1.88	0.73
3:F:4:LEU:HD11	3:F:10:ASP:OD2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.35	0.72
1:B:413:HIS:HD2	1:B:428:SER:OG	1.72	0.71
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.73	0.70
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.72	0.70
3:F:146:ASN:HB3	3:F:149:ASP:OD2	1.91	0.70
2:C:333:ARG:HD3	8:C:5012:HOH:O	1.92	0.70
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.21	0.69
1:B:406:MET:O	1:B:410:GLU:HG3	1.92	0.69
1:B:18:ARG:O	2:D:129:ALA:HA	1.93	0.68
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.74	0.68
3:E:22:LEU:HD11	3:E:31:MET:SD	2.32	0.68
3:E:98:MET:HE1	3:E:107:ALA:CB	2.23	0.68
1:A:76:GLU:HG2	1:B:76:GLU:OE2	1.92	0.68
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.87	0.68
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.91	0.67
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.78	0.67
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.78	0.67
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.25	0.67
1:B:369:MET:HE2	8:B:9144:HOH:O	1.94	0.66
2:D:135:ALA:O	2:D:273:GLY:HA3	1.96	0.66
3:F:15:TRP:O	3:F:19:ILE:HG23	1.94	0.66
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.78	0.66
1:B:227:ASN:HD21	1:B:295:LYS:H	1.43	0.66
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.94	0.65
3:F:41:THR:HG23	3:F:43:PHE:N	2.04	0.65
2:D:184:PHE:O	2:D:187:ILE:HG22	1.96	0.65
1:A:306:ASP:HB2	8:A:9217:HOH:O	1.96	0.65
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.78	0.65
3:F:9:ASN:OD1	3:F:11:THR:HG23	1.97	0.65
1:A:186:ARG:HA	2:C:73:THR:OG1	1.97	0.65
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.78	0.65
1:A:20:PRO:HG3	2:C:129:ALA:HB2	1.79	0.64
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.45	0.64
1:B:52:MET:CE	1:B:127:SER:HB3	2.27	0.64
1:B:30:ARG:HD3	1:B:30:ARG:C	2.23	0.64
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.80	0.64
2:D:324:TRP:C	2:D:327:PRO:HD2	2.23	0.63
1:A:185:LYS:O	1:A:189:SER:HB2	1.98	0.63
1:A:310:TYR:CZ	1:A:336:LYS:HD2	2.33	0.63
2:D:269:ALA:HB1	2:D:274:ASP:OD2	1.99	0.63
1:A:227:ASN:ND2	1:A:295:LYS:H	1.96	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:GLU:O	1:B:247:MET:HG2	1.99	0.63
3:F:4:LEU:HD21	3:F:10:ASP:H	1.64	0.62
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.46	0.62
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.00	0.62
2:D:167:ALA:O	2:D:176:ARG:NH1	2.33	0.62
2:D:71:ASP:HB2	3:F:54:LEU:HD11	1.81	0.62
1:A:184:MET:HE3	1:A:188:PHE:CB	2.30	0.62
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.13	0.62
2:C:96:PHE:O	2:C:99:ARG:NH2	2.32	0.62
3:F:105:TRP:O	3:F:109:LYS:HG3	2.00	0.61
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.00	0.61
1:A:109:PHE:O	1:A:112:VAL:HG12	2.00	0.61
1:A:406:MET:O	1:A:410:GLU:HG3	1.99	0.61
2:D:153:LEU:C	2:D:153:LEU:HD12	2.26	0.61
3:F:57:GLU:O	3:F:61:GLU:HG3	2.00	0.60
3:F:58:ALA:O	3:F:62:GLU:HG3	2.01	0.60
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.66	0.60
1:B:119:ALA:HB1	2:D:168:ARG:HD2	1.83	0.60
1:B:269:THR:HG21	8:F:192:HOH:O	2.00	0.60
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.84	0.60
1:B:198:VAL:O	1:B:202:LEU:HG	2.02	0.60
1:A:84:ASP:HB3	1:B:81:SER:OG	2.01	0.59
2:C:365:GLU:HG2	8:C:5298:HOH:O	2.01	0.59
2:D:2:SER:HB2	8:D:488:HOH:O	2.02	0.59
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.68	0.59
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.86	0.59
1:B:52:MET:HE1	1:B:127:SER:CB	2.33	0.59
3:F:61:GLU:O	3:F:121:PRO:HG2	2.03	0.59
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.85	0.59
2:D:187:ILE:O	2:D:191:GLN:HG3	2.02	0.59
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.36	0.59
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.37	0.59
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.85	0.58
2:D:275:ASN:C	2:D:278:PRO:HD2	2.28	0.58
2:D:326:GLU:HB2	2:D:327:PRO:HD3	1.84	0.58
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.69	0.57
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.86	0.57
1:B:213:THR:O	1:B:217:ILE:HG12	2.04	0.57
1:B:466:CYS:HB2	2:D:73:THR:HA	1.85	0.57
1:B:489:ARG:HD2	1:B:495:LEU:O	2.05	0.57
1:B:210:ALA:N	1:B:247:MET:HE1	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:112:ASP:O	2:D:116:GLU:HG3	2.04	0.57
3:E:41:THR:O	3:E:44:ARG:CD	2.52	0.57
1:A:110:LEU:O	1:A:114:GLU:HG2	2.04	0.57
2:D:377:ARG:O	2:D:381:VAL:HG23	2.04	0.57
1:A:190:ASP:HB3	2:C:74:GLN:O	2.05	0.57
1:B:196:ASP:HB2	3:F:140:MET:SD	2.44	0.57
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.05	0.57
1:B:186:ARG:HD3	1:B:186:ARG:O	2.05	0.56
1:B:49:LYS:HE3	3:F:144:ASN:HD22	1.70	0.56
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.41	0.56
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.35	0.56
2:D:312:TYR:O	2:D:316:VAL:HG23	2.06	0.56
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.68	0.56
1:A:40:LYS:HD2	8:A:9119:HOH:O	2.06	0.56
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.35	0.56
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.02	0.56
3:E:98:MET:HE3	3:E:98:MET:O	2.06	0.56
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.88	0.56
3:F:91:LEU:O	3:F:95:VAL:HG23	2.05	0.56
2:C:89:GLU:CD	3:E:125:VAL:HG13	2.31	0.55
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.32	0.55
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.89	0.55
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.88	0.55
2:C:211:THR:O	2:C:214:PRO:HD2	2.07	0.55
1:A:196:ASP:HB2	3:E:140:MET:SD	2.46	0.54
2:C:266:GLN:HE22	2:D:132:GLN:CD	2.15	0.54
3:F:98:MET:HG3	3:F:138:ARG:HG2	1.88	0.54
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.72	0.54
2:D:263:GLU:HB3	2:D:355:SER:HB2	1.88	0.54
3:E:46:SER:OG	3:E:48:GLU:HG2	2.07	0.54
2:D:357:TYR:CE2	2:D:381:VAL:HG21	2.42	0.54
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.88	0.54
2:C:211:THR:C	2:C:214:PRO:HD2	2.33	0.54
3:E:5:GLY:H	3:E:9:ASN:HB3	1.72	0.54
1:B:186:ARG:HD3	1:B:186:ARG:C	2.33	0.54
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.23	0.54
1:A:305:TRP:CE2	1:A:309:VAL:HG21	2.43	0.54
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.22	0.54
3:F:4:LEU:CD2	3:F:10:ASP:H	2.20	0.54
1:B:212:PHE:O	1:B:215:PRO:HD2	2.08	0.54
2:D:111:LYS:O	2:D:115:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:ALA:HB2	1:B:509:LEU:HD21	1.90	0.54
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.90	0.54
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.90	0.54
2:C:98:HIS:HE1	2:C:178:SER:OG	1.92	0.53
2:D:141:ARG:CG	2:D:142:ASP:N	2.71	0.53
1:A:204:LEU:O	1:A:209:GLU:HG3	2.08	0.53
2:D:376:ASP:OD2	2:D:379:GLN:HB2	2.08	0.53
2:D:367:TYR:O	2:D:370:ARG:HB2	2.07	0.53
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.39	0.53
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.43	0.53
2:C:261:ARG:HE	2:C:285:GLN:NE2	2.00	0.53
1:B:48:THR:O	3:F:137:THR:HG23	2.09	0.52
3:F:36:ARG:NH1	3:F:119:LYS:HB3	2.24	0.52
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.18	0.52
1:B:43:ARG:HD2	1:B:43:ARG:C	2.34	0.52
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.45	0.52
1:B:185:LYS:O	1:B:189:SER:HB2	2.10	0.52
1:B:123:MET:HE1	1:B:200:CYS:SG	2.50	0.52
1:B:367:GLU:HG3	8:B:9015:HOH:O	2.09	0.52
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.45	0.52
1:A:18:ARG:O	2:C:129:ALA:HA	2.10	0.52
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.06	0.52
1:A:186:ARG:HD3	1:A:186:ARG:C	2.34	0.52
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.92	0.52
2:D:378:ASP:O	2:D:382:LYS:HG3	2.10	0.51
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.92	0.51
1:A:437:ARG:HG2	1:A:437:ARG:HH11	1.75	0.51
1:A:116:ASN:CG	1:A:189:SER:HA	2.36	0.51
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.93	0.51
1:A:76:GLU:OE1	1:B:76:GLU:HG2	2.10	0.51
1:B:192:PHE:O	1:B:200:CYS:HB3	2.11	0.51
2:C:333:ARG:HD2	8:C:5192:HOH:O	2.10	0.51
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.94	0.51
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.46	0.51
3:F:104:LYS:O	3:F:108:GLU:HG2	2.10	0.51
3:F:33:LYS:O	3:F:37:MET:HG2	2.10	0.50
1:A:29:HIS:CD2	1:A:61:LYS:HA	2.47	0.50
1:A:140:GLN:O	1:A:144:GLU:HG2	2.12	0.50
1:B:227:ASN:ND2	1:B:295:LYS:H	2.09	0.50
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.93	0.50
1:B:445:MET:HE3	1:B:523:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.92	0.50
2:D:265:PHE:O	2:D:269:ALA:HB2	2.12	0.50
3:F:19:ILE:HG22	3:F:60:LEU:HD21	1.94	0.50
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.11	0.50
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.92	0.50
3:F:24:THR:HG22	3:F:26:GLU:H	1.77	0.49
1:A:113:GLY:HA3	1:A:188:PHE:CD2	2.47	0.49
1:B:26:GLN:HG3	8:B:9084:HOH:O	2.12	0.49
2:C:90:LEU:HD13	2:C:303:LEU:HD13	1.94	0.49
2:C:111:LYS:O	2:C:115:GLU:HG3	2.12	0.49
2:D:147:ARG:HD2	2:D:148:TYR:CE1	2.47	0.49
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.47	0.49
1:B:441:TYR:HB2	3:F:161:VAL:HG23	1.93	0.49
1:A:206:LEU:HD12	1:A:317:TRP:HH2	1.77	0.49
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.95	0.49
3:F:95:VAL:HG12	3:F:99:ASN:HD21	1.77	0.49
2:C:292:LYS:O	2:C:296:GLN:HG3	2.13	0.49
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.48	0.49
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.78	0.49
1:B:186:ARG:HA	2:D:73:THR:OG1	2.12	0.49
2:D:94:ASP:HB3	2:D:97:LYS:HG3	1.94	0.49
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.12	0.49
3:F:39:HIS:CD2	3:F:49:LEU:HD12	2.47	0.49
1:B:110:LEU:O	1:B:114:GLU:HG2	2.13	0.48
1:A:413:HIS:HD2	1:A:428:SER:OG	1.97	0.48
2:C:266:GLN:NE2	2:D:132:GLN:CD	2.72	0.48
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.49	0.48
2:C:97:LYS:HD2	8:C:5101:HOH:O	2.12	0.48
1:A:83:GLN:HB3	1:B:77:ARG:NH1	2.29	0.48
2:C:143:GLU:O	2:C:147:ARG:HB3	2.13	0.48
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.12	0.48
1:B:114:GLU:CD	1:B:147:HIS:HB3	2.39	0.48
1:B:247:MET:HE2	1:B:247:MET:HA	1.95	0.48
2:C:336:MET:CE	2:C:385:LEU:HD23	2.43	0.48
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.14	0.48
2:C:306:ASP:O	2:C:310:SER:HB2	2.13	0.48
2:D:54:VAL:O	2:D:55:TYR:HB2	2.14	0.48
2:D:324:TRP:O	2:D:327:PRO:HD2	2.14	0.48
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.77	0.48
2:D:136:MET:HA	2:D:273:GLY:O	2.14	0.48
3:F:63:LYS:HZ2	3:F:67:LEU:HD11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ALA:O	2:D:274:ASP:HB3	2.14	0.47
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.78	0.47
1:A:83:GLN:HB3	1:B:77:ARG:HH12	1.79	0.47
1:A:210:ALA:HA	1:A:247:MET:HE1	1.97	0.47
1:B:230:GLU:C	1:B:233:PRO:HD2	2.39	0.47
2:D:325:LEU:O	2:D:329:ILE:HG13	2.14	0.47
3:F:16:VAL:O	3:F:19:ILE:HG12	2.15	0.47
1:B:268:ASN:ND2	1:B:327:GLU:H	2.07	0.47
2:C:235:TRP:CD1	2:C:235:TRP:C	2.92	0.47
2:C:336:MET:HE2	2:C:385:LEU:HD23	1.97	0.47
1:A:81:SER:OG	1:B:84:ASP:HB3	2.14	0.47
1:A:108:ASN:ND2	1:A:175:ARG:HH11	2.12	0.47
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.15	0.47
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.97	0.47
1:B:490:SER:OG	2:D:32:ASN:HB2	2.14	0.47
2:D:145:ILE:O	2:D:149:TRP:HB3	2.15	0.47
2:D:213:VAL:HB	2:D:214:PRO:CD	2.45	0.47
3:E:98:MET:HE1	3:E:107:ALA:HB2	1.95	0.47
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.50	0.47
1:B:260:ASP:OD2	1:B:262:ALA:HB3	2.15	0.47
2:C:2:SER:HB2	8:C:5038:HOH:O	2.14	0.47
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.96	0.47
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.15	0.47
1:B:33:GLN:HE22	1:B:130:ALA:HB1	1.80	0.47
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.98	0.46
1:B:369:MET:HE1	1:B:388:GLU:OE2	2.14	0.46
2:D:274:ASP:OD2	2:D:277:THR:HB	2.15	0.46
3:F:40:THR:O	3:F:41:THR:CG2	2.55	0.46
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.50	0.46
1:A:243:GLU:O	1:A:247:MET:HG2	2.15	0.46
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.14	0.46
1:B:165:PRO:HG3	8:B:9114:HOH:O	2.16	0.46
2:D:169:GLU:O	2:D:170:ALA:C	2.57	0.46
2:D:235:TRP:CD1	2:D:235:TRP:C	2.91	0.46
1:A:118:ILE:HD13	1:A:145:ILE:HG12	1.97	0.46
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.15	0.46
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.98	0.46
2:C:179:LEU:HD12	2:C:182:TRP:CZ3	2.51	0.46
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.97	0.46
2:C:153:LEU:C	2:C:153:LEU:HD12	2.41	0.46
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:TYR:CD2	1:A:257:ILE:HD12	2.51	0.46
1:A:125:TRP:CD1	1:A:125:TRP:C	2.94	0.46
1:A:138:LEU:HD22	2:C:160:PHE:CZ	2.50	0.46
1:B:204:LEU:HG	1:B:205:GLN:HG3	1.97	0.46
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.50	0.46
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.99	0.46
1:B:113:GLY:HA3	1:B:188:PHE:CD2	2.51	0.45
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.98	0.45
2:D:356:LEU:HD12	2:D:385:LEU:HD13	1.98	0.45
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.51	0.45
1:B:21:THR:HG22	1:B:22:SER:N	2.31	0.45
1:A:186:ARG:HD3	1:A:186:ARG:O	2.17	0.45
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.98	0.45
2:D:152:PHE:O	2:D:155:ASN:HB3	2.16	0.45
3:E:98:MET:HE1	3:E:107:ALA:HB1	1.98	0.45
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.17	0.45
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.99	0.45
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.46	0.45
2:D:148:TYR:HE2	2:D:223:VAL:HG21	1.82	0.45
2:D:336:MET:CE	2:D:356:LEU:HD11	2.47	0.45
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.64	0.45
1:B:125:TRP:CD1	1:B:125:TRP:C	2.95	0.45
2:D:153:LEU:HD12	2:D:154:PHE:N	2.31	0.45
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.78	0.45
2:D:47:THR:OG1	2:D:50:GLU:HG3	2.17	0.45
1:A:227:ASN:HD21	1:A:296:PHE:H	1.64	0.44
1:A:318:ILE:HD11	1:A:327:GLU:O	2.16	0.44
1:A:216:LEU:O	1:A:220:VAL:HG23	2.17	0.44
1:A:302:VAL:CG1	1:A:376:TYR:HE2	2.29	0.44
2:D:348:ASP:OD2	2:D:350:GLU:HB3	2.17	0.44
1:B:184:MET:CE	1:B:188:PHE:HB2	2.47	0.44
1:B:184:MET:HE1	1:B:282:PHE:CZ	2.52	0.44
1:B:484:GLU:OE1	3:F:6:ILE:HB	2.17	0.44
3:E:3:LYS:HB3	3:E:10:ASP:OD1	2.17	0.44
3:E:154:GLU:O	3:E:158:GLN:HG3	2.17	0.44
3:F:74:GLU:O	3:F:78:ARG:HG3	2.18	0.44
1:B:403:ILE:HG23	1:B:403:ILE:O	2.17	0.44
1:A:321:LEU:N	1:A:321:LEU:HD12	2.31	0.44
1:A:354:TRP:CH2	1:A:499:PRO:HD3	2.53	0.44
1:B:202:LEU:HD22	1:B:206:LEU:HD23	1.98	0.44
1:A:207:VAL:O	1:A:211:CYS:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:247:SER:O	2:D:251:VAL:HB	2.17	0.44
3:E:40:THR:C	3:E:41:THR:HG23	2.43	0.44
3:F:33:LYS:HE3	3:F:117:ALA:HA	2.00	0.44
1:A:46:TYR:CD2	1:A:123:MET:HE3	2.52	0.44
2:C:105:TRP:O	2:C:108:PRO:HD2	2.17	0.44
2:C:184:PHE:O	2:C:187:ILE:HG22	2.18	0.44
2:D:176:ARG:HG3	2:D:176:ARG:HH11	1.83	0.44
3:F:12:ARG:O	3:F:16:VAL:HG13	2.18	0.44
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.47	0.44
2:D:208:ASP:HA	8:D:497:HOH:O	2.17	0.44
2:C:364:ILE:HA	2:C:368:ALA:HB3	2.00	0.43
1:A:185:LYS:HA	1:A:189:SER:HB2	1.99	0.43
1:A:26:GLN:HG2	8:A:9192:HOH:O	2.18	0.43
1:A:318:ILE:HD13	1:A:328:SER:HA	1.99	0.43
2:D:189:ILE:HD11	2:D:284:ALA:HA	2.01	0.43
2:D:264:PHE:O	2:D:268:LEU:HG	2.18	0.43
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.33	0.43
1:A:33:GLN:HA	1:A:131:ALA:HB3	2.01	0.43
1:B:283:THR:HB	1:B:284:PRO:HD3	2.01	0.43
2:C:336:MET:HE1	2:C:352:ILE:CG2	2.48	0.43
3:F:36:ARG:CZ	3:F:119:LYS:HB3	2.48	0.43
1:B:79:PHE:O	1:B:83:GLN:HG3	2.18	0.43
1:B:209:GLU:C	1:B:247:MET:HE1	2.44	0.43
2:D:195:LEU:C	2:D:195:LEU:HD23	2.44	0.43
2:C:77:HIS:CD2	3:E:140:MET:HG2	2.53	0.43
1:B:66:GLU:HA	1:B:66:GLU:OE2	2.19	0.43
1:B:444:GLU:OE2	1:B:444:GLU:HA	2.18	0.43
2:C:203:ILE:HG13	2:C:204:VAL:HG23	2.00	0.43
1:A:182:LYS:O	2:C:73:THR:HG21	2.19	0.42
1:A:365:ASP:OD2	1:A:365:ASP:C	2.62	0.42
1:A:477:GLU:OE1	1:A:479:SER:OG	2.32	0.42
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.54	0.42
1:B:159:ALA:O	2:D:33:ASN:HB2	2.19	0.42
1:A:186:ARG:HB3	8:A:9153:HOH:O	2.19	0.42
1:B:128:ALA:O	1:B:134:LYS:HE2	2.19	0.42
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.34	0.42
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.54	0.42
2:C:266:GLN:HB2	2:C:281:ILE:HG21	2.01	0.42
2:D:185:ASP:O	2:D:189:ILE:HG12	2.19	0.42
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.85	0.42
1:A:306:ASP:O	1:A:310:TYR:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.20	0.42
2:C:240:ASP:HB2	3:E:125:VAL:CG2	2.49	0.42
2:D:244:SER:O	2:D:248:VAL:HG23	2.19	0.42
3:E:17:ASN:HB3	8:E:907:HOH:O	2.18	0.42
1:A:230:GLU:C	1:A:233:PRO:HD2	2.45	0.42
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.54	0.42
2:D:63:ILE:O	2:D:64:ALA:C	2.63	0.42
1:B:210:ALA:CA	1:B:247:MET:HE1	2.50	0.42
2:D:153:LEU:HA	2:D:193:ILE:HD12	2.02	0.42
3:F:25:LEU:HD22	3:F:68:LYS:HA	2.02	0.42
2:D:54:VAL:HG12	2:D:55:TYR:CD2	2.54	0.42
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.02	0.42
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.55	0.42
1:B:202:LEU:HD22	1:B:206:LEU:CD2	2.50	0.42
1:B:232:THR:HB	1:B:233:PRO:HD3	2.02	0.42
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.37	0.42
1:A:44:THR:HG21	8:A:9204:HOH:O	2.18	0.41
1:A:163:GLN:HG2	8:A:9037:HOH:O	2.19	0.41
1:B:105:VAL:O	1:B:109:PHE:HB2	2.20	0.41
2:D:277:THR:N	2:D:278:PRO:CD	2.83	0.41
1:A:123:MET:HB2	2:C:168:ARG:HD3	2.03	0.41
1:B:38:ASP:O	1:B:39:PHE:HB3	2.20	0.41
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.54	0.41
2:D:336:MET:C	2:D:338:LEU:H	2.28	0.41
1:A:118:ILE:HD11	1:A:145:ILE:HA	2.03	0.41
2:D:93:VAL:HG13	8:D:478:HOH:O	2.19	0.41
2:D:144:PHE:CZ	2:D:342:LEU:HD23	2.56	0.41
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.55	0.41
1:A:113:GLY:HA3	1:A:188:PHE:HD2	1.84	0.41
1:A:292:TYR:OH	1:A:344:HIS:CD2	2.65	0.41
3:F:66:VAL:HG12	3:F:70:ARG:NH2	2.36	0.41
1:B:223:TRP:CZ3	1:B:297:LYS:HA	2.55	0.41
2:C:121:ASP:O	2:C:125:GLN:HG3	2.20	0.41
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.04	0.41
2:D:357:TYR:CD2	2:D:381:VAL:HG21	2.56	0.41
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.55	0.41
1:B:50:TYR:CD1	1:B:50:TYR:N	2.89	0.41
2:D:357:TYR:CD2	2:D:377:ARG:NH2	2.89	0.41
3:F:125:VAL:HG23	3:F:126:ASN:N	2.35	0.41
2:D:39:VAL:O	2:D:41:PRO:HD3	2.21	0.41
1:A:65:LYS:HB3	2:C:117:TRP:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:OD2	1:A:146:ARG:NH1	2.54	0.41
1:A:121:THR:HG21	1:A:140:GLN:CG	2.50	0.41
1:A:382:HIS:O	1:A:386:ILE:HG13	2.20	0.41
1:B:123:MET:SD	2:D:168:ARG:NH1	2.94	0.41
1:B:283:THR:HB	1:B:284:PRO:CD	2.50	0.41
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.56	0.41
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.56	0.41
1:A:321:LEU:O	1:A:326:VAL:HB	2.21	0.41
1:A:343:HIS:H	1:A:343:HIS:CD2	2.39	0.41
2:C:277:THR:N	2:C:278:PRO:CD	2.84	0.41
2:D:213:VAL:HB	2:D:214:PRO:HD3	2.02	0.41
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.39	0.40
2:D:87:THR:HG21	2:D:169:GLU:OE1	2.21	0.40
1:A:232:THR:HB	1:A:233:PRO:HD3	2.02	0.40
1:A:430:ALA:HA	8:A:9170:HOH:O	2.20	0.40
2:D:228:ARG:HH11	2:D:228:ARG:HG2	1.86	0.40
1:A:108:ASN:O	1:A:111:GLU:HB3	2.20	0.40
2:C:126:GLY:O	2:C:130:ASP:HB2	2.21	0.40
2:D:148:TYR:CE2	2:D:338:LEU:HD13	2.56	0.40
2:D:299:TYR:O	2:D:317:MET:HE1	2.21	0.40
3:F:39:HIS:HD2	8:F:189:HOH:O	2.04	0.40
1:A:76:GLU:CD	8:A:9005:HOH:O	2.64	0.40
1:A:435:THR:HG22	3:E:168:SER:HA	2.03	0.40
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.71	0.40
1:B:140:GLN:O	1:B:141:VAL:C	2.64	0.40
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.53	0.40
2:C:146:ASN:O	2:C:214:PRO:HG3	2.22	0.40
3:F:86:ASP:HB3	3:F:89:SER:OG	2.21	0.40
1:A:115:TYR:OH	2:C:173:ASP:HA	2.22	0.40
2:D:13:ASP:HA	2:D:14:PRO:HD3	1.96	0.40
2:D:261:ARG:NE	2:D:285:GLN:HE22	2.07	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	508/527 (96%)	486 (96%)	20 (4%)	2 (0%)	30	21
1	B	508/527 (96%)	483 (95%)	24 (5%)	1 (0%)	43	36
2	C	386/389 (99%)	377 (98%)	8 (2%)	1 (0%)	36	28
2	D	386/389 (99%)	357 (92%)	25 (6%)	4 (1%)	12	5
3	E	164/170 (96%)	162 (99%)	2 (1%)	0	100	100
3	F	165/170 (97%)	156 (94%)	7 (4%)	2 (1%)	10	4
All	All	2117/2172 (98%)	2021 (96%)	86 (4%)	10 (0%)	24	16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
1	A	311	GLU
2	D	64	ALA
3	F	122	ILE
1	A	340	TYR
2	D	205	PRO
2	D	251	VAL
3	F	87	ALA
2	D	388	LEU
2	C	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%)	424 (98%)	8 (2%)	50	45
1	B	432/442 (98%)	427 (99%)	5 (1%)	63	61
2	C	322/323 (100%)	319 (99%)	3 (1%)	70	70
2	D	322/323 (100%)	317 (98%)	5 (2%)	55	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	144/147 (98%)	140 (97%)	4 (3%)	38	30
3	F	145/147 (99%)	140 (97%)	5 (3%)	32	23
All	All	1797/1824 (98%)	1767 (98%)	30 (2%)	53	49

All (30) 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	160	LYS
1	A	186	ARG
1	A	279	GLN
1	A	403	ILE
1	A	467	GLN
1	B	90	ASN
1	B	110	LEU
1	B	125	TRP
1	B	279	GLN
1	B	440	GLU
2	C	153	LEU
2	C	173	ASP
2	C	378	ASP
2	D	4	LEU
2	D	122	ARG
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
3	E	44	ARG
3	E	46	SER
3	E	125	VAL
3	E	166	LEU
3	F	11	THR
3	F	41	THR
3	F	44	ARG
3	F	164	VAL
3	F	167	GLN

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

Mol	Chain	Res	Type
1	A	41	ASN
1	A	54	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	116	ASN
1	A	129	GLN
1	A	155	ASN
1	A	168	HIS
1	A	203	ASN
1	A	205	GLN
1	A	227	ASN
1	A	249	ASN
1	A	252	GLN
1	A	268	ASN
1	A	273	ASN
1	A	279	GLN
1	A	343	HIS
1	A	344	HIS
1	A	382	HIS
1	A	412	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	472	GLN
1	B	33	GLN
1	B	42	ASN
1	B	78	GLN
1	B	90	ASN
1	B	108	ASN
1	B	133	GLN
1	B	168	HIS
1	B	203	ASN
1	B	227	ASN
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

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Mol	Chain	Res	Type
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	85	ASN
2	C	98	HIS
2	C	125	GLN
2	C	146	ASN
2	C	161	ASN
2	C	266	GLN
2	C	285	GLN
2	C	296	GLN
2	C	301	ASN
2	D	98	HIS
2	D	161	ASN
2	D	285	GLN
2	D	296	GLN
3	E	23	ASN
3	E	45	ASN
3	E	144	ASN
3	E	158	GLN
3	E	165	HIS
3	F	7	HIS
3	F	45	ASN
3	F	99	ASN
3	F	144	ASN
3	F	167	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 [i](#)

Of 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	$\# Z > 2$
7	EOH	B	9002	4	2,2,2	0.51	0	1,1,1	0.14	0
6	FMT	A	9001	4	2,2,2	0.65	0	1,1,1	0.62	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	510/527 (96%)	0.70	59 (11%) 9 11	22, 36, 62, 78	0
1	B	510/527 (96%)	0.51	44 (8%) 16 19	22, 36, 63, 78	0
2	C	388/389 (99%)	-0.10	8 (2%) 63 70	18, 26, 46, 62	0
2	D	388/389 (99%)	1.27	88 (22%) 2 2	26, 46, 68, 81	2 (0%)
3	E	166/170 (97%)	0.15	5 (3%) 52 59	20, 29, 46, 69	0
3	F	167/170 (98%)	2.03	71 (42%) 0 0	37, 56, 75, 86	0
All	All	2129/2172 (98%)	0.67	275 (12%) 7 9	18, 37, 66, 86	2 (0%)

All (275) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	ALA	6.5
3	E	4	LEU	6.0
3	F	19	ILE	5.4
3	F	72	PHE	5.0
2	D	270	PRO	4.9
2	D	384	VAL	4.8
3	F	4	LEU	4.7
1	A	19	ALA	4.5
2	D	207	PHE	4.3
1	B	53	ALA	4.2
1	A	339	ALA	4.1
2	D	382	LYS	4.1
3	F	69	ALA	4.0
3	F	101	ALA	4.0
1	A	316	ILE	4.0
3	F	93	GLY	4.0
1	A	244	LEU	4.0
3	F	77	PHE	4.0
1	A	338	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	275	ASN	3.9
3	E	167	GLN	3.9
1	B	244	LEU	3.9
1	A	432	GLY	3.9
2	D	221	GLY	3.8
3	E	168	SER	3.8
1	A	310	TYR	3.8
2	D	385	LEU	3.8
3	F	118	TYR	3.7
2	D	223	VAL	3.7
3	F	161	VAL	3.7
1	B	55	GLU	3.7
1	B	54	ASN	3.7
1	A	308	TRP	3.6
3	F	66	VAL	3.6
3	F	75	VAL	3.6
1	A	213	THR	3.6
3	F	20	ALA	3.5
3	F	67	LEU	3.6
2	D	145	ILE	3.5
3	F	65	ALA	3.5
2	D	368	ALA	3.5
1	B	403	ILE	3.4
3	F	82	ALA	3.4
2	D	380	ILE	3.4
2	D	363	TRP	3.4
1	A	20	PRO	3.4
1	A	318	ILE	3.4
1	A	317	TRP	3.4
1	B	256	SER	3.4
2	D	388	LEU	3.4
2	D	126	GLY	3.3
2	D	375	ALA	3.3
3	F	56	ILE	3.3
1	A	210	ALA	3.3
1	B	19	ALA	3.3
3	F	80	LYS	3.3
3	F	22	LEU	3.3
3	F	125	VAL	3.3
3	F	170	HIS	3.3
3	F	21	GLN	3.3
3	F	84	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	141	ARG	3.2
2	D	144	PHE	3.2
2	D	373	PHE	3.2
3	F	83	PHE	3.2
3	F	100	ALA	3.2
2	D	387	GLY	3.2
2	D	320	TRP	3.2
2	D	139	THR	3.2
1	A	326	VAL	3.2
2	D	140	TRP	3.1
3	F	71	ALA	3.1
3	F	87	ALA	3.1
3	F	127	TYR	3.1
3	F	128	PHE	3.1
1	A	322	GLY	3.1
2	D	338	LEU	3.1
1	A	212	PHE	3.1
2	D	250	ALA	3.1
2	D	361	ASP	3.1
2	D	272	PHE	3.1
1	A	435	THR	3.1
2	D	347	THR	3.1
2	D	356	LEU	3.0
2	D	93	VAL	3.0
3	F	103	ASP	3.0
2	D	386	ALA	3.0
1	A	255	VAL	3.0
3	F	41	THR	3.0
2	D	229	LEU	2.9
1	A	309	VAL	2.9
3	F	35	PHE	2.9
2	D	146	ASN	2.9
3	E	23	ASN	2.9
3	F	16	VAL	2.9
3	F	124	PRO	2.9
1	A	335	ALA	2.9
2	D	389	LYS	2.9
1	B	206	LEU	2.9
2	D	131	GLY	2.9
3	F	121	PRO	2.9
3	F	28	ALA	2.9
3	F	96	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	206	LEU	2.9
3	F	24	THR	2.8
1	A	251	TYR	2.8
2	D	212	ALA	2.8
3	F	117	ALA	2.8
1	A	260	ASP	2.8
1	A	321	LEU	2.8
2	D	218	TRP	2.8
2	D	352	ILE	2.8
2	D	381	VAL	2.8
1	A	313	TRP	2.8
1	B	265	LYS	2.8
1	B	38	ASP	2.8
3	F	89	SER	2.8
1	A	257	ILE	2.8
1	B	35	PHE	2.7
1	B	311	GLU	2.7
1	B	213	THR	2.7
1	B	269	THR	2.7
2	D	371	ILE	2.7
1	A	302	VAL	2.7
1	A	311	GLU	2.7
2	D	354	ALA	2.7
3	F	79	HIS	2.7
3	F	142	LEU	2.7
1	A	409	ILE	2.7
1	B	317	TRP	2.7
2	D	200	LEU	2.7
2	D	220	ASN	2.7
3	F	90	VAL	2.7
2	D	331	ALA	2.6
1	B	31	TRP	2.6
2	D	271	ARG	2.6
1	A	188	PHE	2.6
1	A	434	SER	2.6
1	A	258	ALA	2.6
3	F	29	ALA	2.6
3	F	73	ASN	2.6
3	F	114	PHE	2.6
1	A	325	GLY	2.6
1	A	25	ALA	2.6
2	D	316	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	247	MET	2.6
2	D	137	ASN	2.6
1	B	310	TYR	2.5
1	A	60	PHE	2.5
1	A	332	LEU	2.5
3	F	25	LEU	2.5
2	D	374	LYS	2.5
3	F	122	ILE	2.5
2	C	135	ALA	2.5
3	F	23	ASN	2.5
3	F	64	VAL	2.5
1	A	121	THR	2.5
1	B	44	THR	2.5
2	D	224	TYR	2.5
3	F	147	TYR	2.5
1	A	204	LEU	2.5
3	F	60	LEU	2.5
1	A	319	GLY	2.5
1	A	193	ILE	2.5
2	D	329	ILE	2.5
1	B	255	VAL	2.5
2	D	353	THR	2.5
1	B	20	PRO	2.5
1	B	504	ASP	2.5
2	D	119	TYR	2.5
3	F	95	VAL	2.5
2	C	131	GLY	2.4
2	D	226	SER	2.4
1	B	302	VAL	2.4
2	D	204	VAL	2.4
1	A	250	GLY	2.4
2	D	273	GLY	2.4
2	C	365	GLU	2.4
2	D	6	GLU	2.4
2	D	349	LYS	2.4
2	D	334	ASP	2.4
1	B	527	ASN	2.4
2	D	311	ASP	2.4
2	D	348	ASP	2.4
1	A	139	ALA	2.4
2	C	129	ALA	2.4
1	B	309	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	310	SER	2.4
2	D	355	SER	2.4
3	F	70	ARG	2.3
1	A	44	THR	2.3
3	F	94	THR	2.3
1	A	430	ALA	2.3
2	D	230	ALA	2.3
3	F	110	ILE	2.3
2	C	308	GLU	2.3
1	B	21	THR	2.3
1	A	54	ASN	2.3
1	B	318	ILE	2.3
1	A	254	VAL	2.3
2	C	282	ASN	2.3
3	F	17	ASN	2.3
3	F	150	THR	2.3
2	D	216	ALA	2.3
3	F	5	GLY	2.3
2	D	369	SER	2.3
1	B	32	LEU	2.3
3	F	31	MET	2.3
1	B	514	ARG	2.2
3	F	105	TRP	2.2
3	F	164	VAL	2.2
3	F	153	GLU	2.2
2	D	330	ALA	2.2
2	D	370	ARG	2.2
1	A	21	THR	2.2
2	D	211	THR	2.2
2	D	132	GLN	2.2
1	A	314	GLY	2.2
2	D	206	GLY	2.2
1	A	128	ALA	2.2
1	B	258	ALA	2.2
1	B	324	TYR	2.2
2	D	148	TYR	2.2
1	B	313	TRP	2.2
3	F	63	LYS	2.2
3	E	153	GLU	2.2
1	B	26	GLN	2.2
2	D	346	THR	2.2
3	F	76	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	263	SER	2.2
1	B	325	GLY	2.2
2	D	303	LEU	2.2
2	D	345	GLY	2.2
1	B	268	ASN	2.1
2	D	301	ASN	2.1
1	B	308	TRP	2.1
1	B	34	SER	2.1
1	A	51	LYS	2.1
1	A	261	PRO	2.1
2	D	205	PRO	2.1
1	A	192	PHE	2.1
1	B	39	PHE	2.1
1	A	324	TYR	2.1
3	F	163	VAL	2.1
3	F	26	GLU	2.1
1	A	515	LEU	2.1
2	D	268	LEU	2.1
2	D	325	LEU	2.1
2	D	269	ALA	2.1
1	A	397	ASP	2.1
3	F	92	ASP	2.1
3	F	138	ARG	2.1
1	A	253	THR	2.1
3	F	11	THR	2.1
2	D	136	MET	2.1
1	B	23	VAL	2.1
2	D	43	TRP	2.1
2	D	324	TRP	2.1
2	D	266	GLN	2.1
1	A	436	LEU	2.1
1	B	332	LEU	2.1
1	B	517	CYS	2.1
1	B	459	ALA	2.1
2	C	203	ILE	2.0
3	F	132	GLU	2.0
2	C	119	TYR	2.0
3	F	158	GLN	2.0
2	D	149	TRP	2.0
1	A	47	ALA	2.0
2	D	383	ALA	2.0
2	D	281	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	309	PHE	2.0
2	D	364	ILE	2.0
1	B	28	VAL	2.0
2	D	359	VAL	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(Å ²)	Q<0.9
6	FMT	A	9001	3/3	0.89	0.13	51,51,53,57	0
7	EOH	B	9002	3/3	0.92	0.16	46,46,47,49	0
5	CA	C	5006	1/1	0.95	0.06	65,65,65,65	0
4	FE	A	5002	1/1	0.98	0.06	49,49,49,49	0
4	FE	A	5001	1/1	0.99	0.06	42,42,42,42	0
5	CA	C	5007	1/1	0.99	0.08	40,40,40,40	0
4	FE	B	5004	1/1	0.99	0.04	44,44,44,44	0
5	CA	A	5005	1/1	0.99	0.07	40,40,40,40	0
4	FE	B	5003	1/1	1.00	0.04	34,34,34,34	0

6.5 Other polymers [i](#)

There are no such residues in this entry.