



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 1FZ3 / pdb_00001fz3
Title : METHANE MONOOXYGENASE HYDROXYLASE, FORM III SOAK AT
PH 6.2 (0.1 M PIPES)
Authors : Whittington, D.A.; Lippard, S.J.
Deposited on : 2000-10-03
Resolution : 2.03 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:

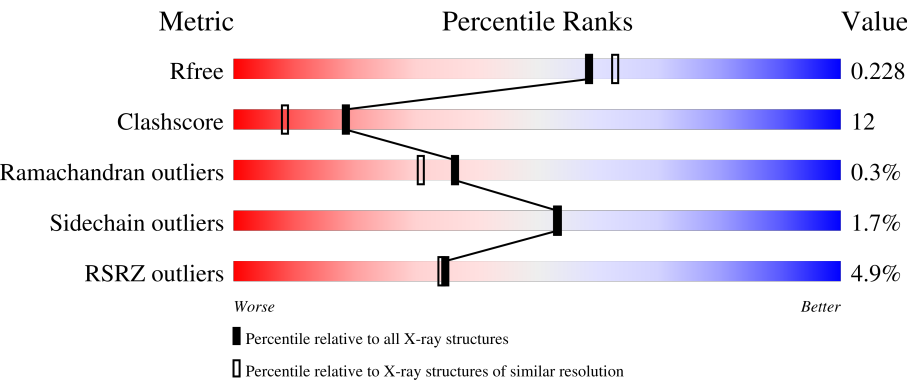
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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% 72% 23% ..
1	B	527	3% 70% 26% ..
2	C	389	% 75% 24% .
2	D	389	7% 68% 29% .
3	E	170	4% 76% 20% ..

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Mol	Chain	Length	Quality of chain
3	F	170	21% 68% 28% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18782 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	388	Total	C	N	O	S	0	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	168	Total	C	N	O	S	0	0	0
			1386	878	250	253	5			

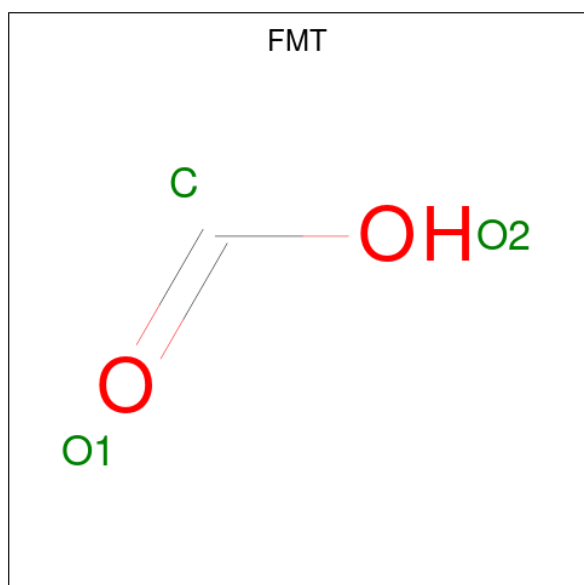
- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

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	2	Total Ca 2 2	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	269	Total O 269 269	0	0
7	B	273	Total O 273 273	0	0

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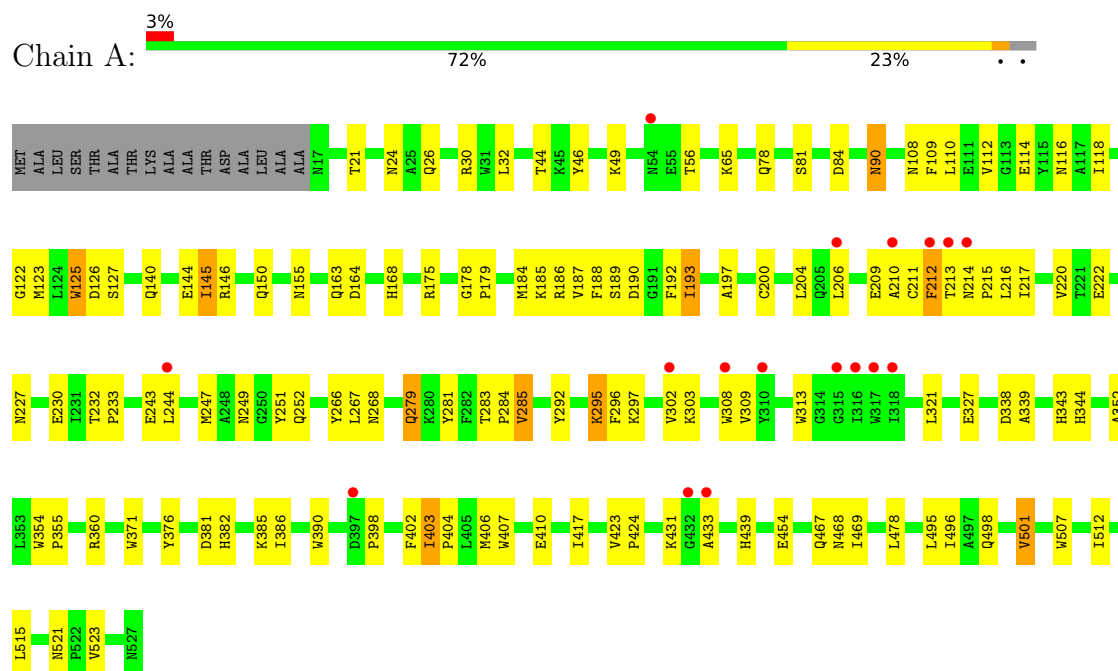
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	327	Total 327	O 327	0	0
7	D	165	Total 165	O 165	0	0
7	E	159	Total 159	O 159	0	0
7	F	69	Total 69	O 69	0	0

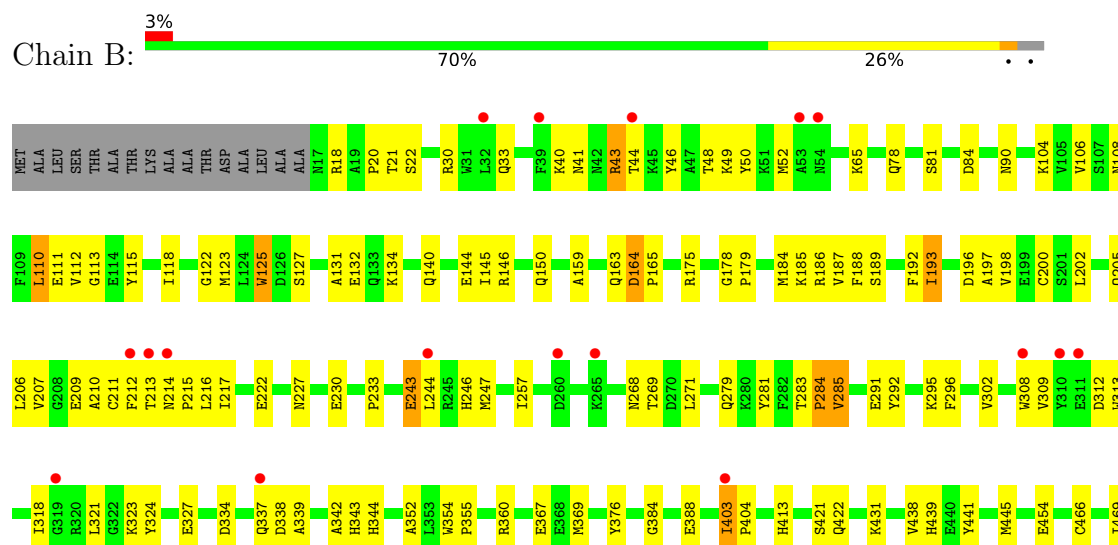
3 Residue-property plots [i](#)

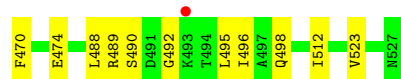
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

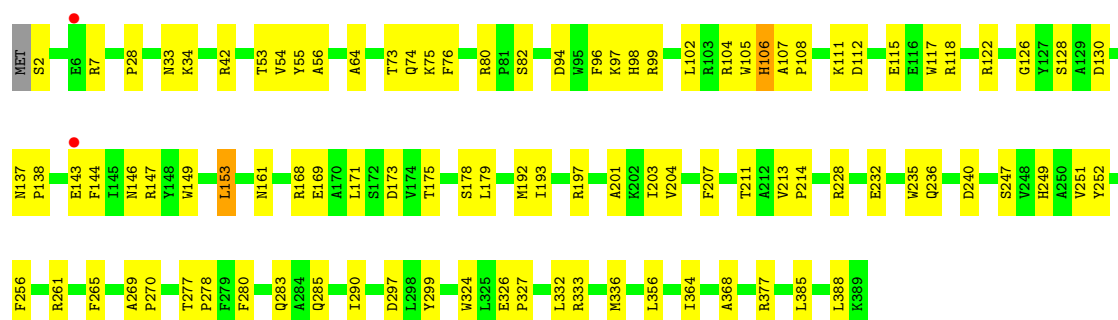
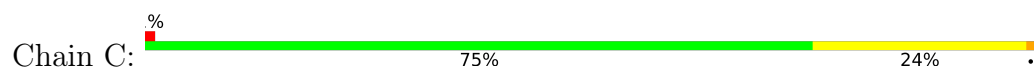


• Molecule 1: METHANE MONOOXYGENASE COMPONENT A, ALPHA CHAIN

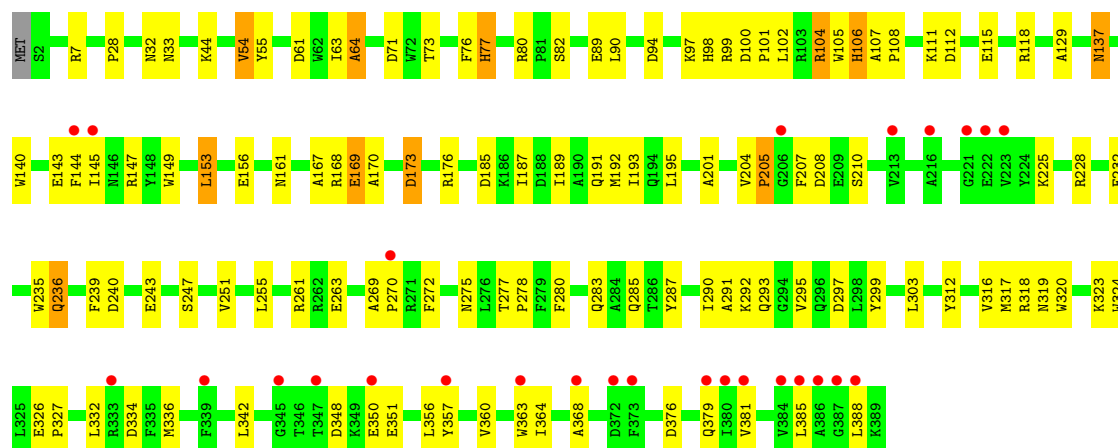




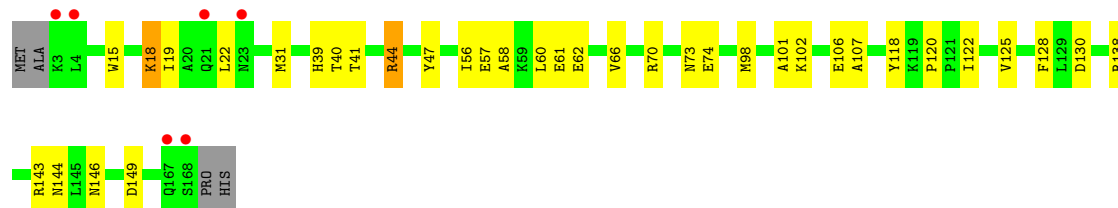
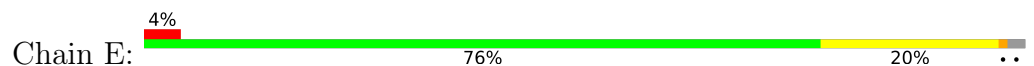
• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN



• Molecule 2: METHANE MONOOXYGENASE COMPONENT A, BETA CHAIN

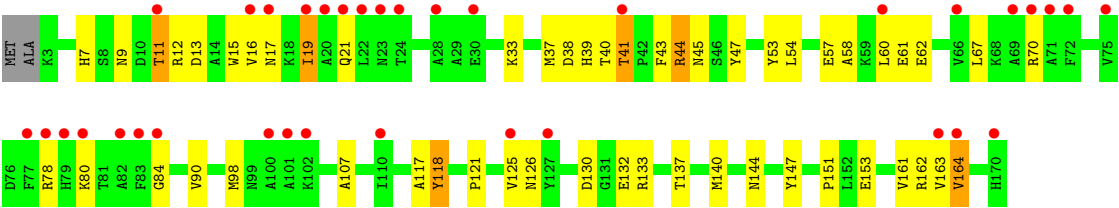


• Molecule 3: METHANE MONOOXYGENASE COMPONENT A, GAMMA CHAIN



• 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	71.37Å 172.12Å 221.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 2.03 29.99 – 2.03	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.99-2.03) 92.8 (29.99-2.03)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.09 (at 2.03Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.196 , 0.228 0.196 , 0.228	Depositor DCC
R_{free} test set	5809 reflections (3.31%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.4	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	18782	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, FMT, FE

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/4310	0.91	19/5853 (0.3%)
1	B	0.36	0/4310	0.90	16/5853 (0.3%)
2	C	0.41	0/3289	0.87	16/4464 (0.4%)
2	D	0.35	0/3289	0.85	12/4464 (0.3%)
3	E	0.39	0/1396	0.89	7/1880 (0.4%)
3	F	0.32	0/1416	0.80	3/1907 (0.2%)
All	All	0.36	0/18010	0.88	73/24421 (0.3%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ALA	N-CA-C	9.81	121.73	111.14
1	A	164	ASP	CA-C-N	7.61	127.66	119.28
1	A	164	ASP	C-N-CA	7.61	127.66	119.28
2	C	106	HIS	N-CA-C	7.59	120.21	111.11
2	D	204	VAL	CA-C-N	7.59	129.32	119.84
2	D	204	VAL	C-N-CA	7.59	129.32	119.84
1	B	431	LYS	N-CA-C	-7.37	104.31	113.38
2	C	105	TRP	N-CA-C	-7.28	99.18	110.17
1	A	266	TYR	N-CA-C	7.19	122.72	113.88
1	B	285	VAL	N-CA-C	7.19	117.32	110.42
3	E	122	ILE	N-CA-C	-7.07	104.30	110.74
1	A	339	ALA	N-CA-C	7.05	118.62	111.07
3	F	39	HIS	N-CA-C	6.97	122.77	112.94
1	B	193	ILE	N-CA-C	6.94	120.48	113.47
1	A	309	VAL	N-CA-C	6.85	116.97	110.53
1	B	496	ILE	N-CA-C	-6.68	104.25	110.53
1	A	285	VAL	N-CA-C	6.58	117.37	110.72
2	C	236	GLN	N-CA-C	6.57	121.46	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ILE	N-CA-C	6.39	119.93	113.47
1	A	178	GLY	CA-C-N	6.38	125.95	119.19
1	A	178	GLY	C-N-CA	6.38	125.95	119.19
2	D	105	TRP	N-CA-C	-6.37	100.78	109.95
2	C	149	TRP	N-CA-C	-6.26	104.54	111.36
3	E	130	ASP	N-CA-C	-6.21	104.59	111.36
1	A	243	GLU	N-CA-C	6.15	118.96	111.82
2	C	169	GLU	N-CA-C	6.10	120.88	113.38
1	B	164	ASP	CA-C-N	6.09	125.98	119.28
1	B	164	ASP	C-N-CA	6.09	125.98	119.28
1	B	309	VAL	N-CA-C	6.05	116.83	110.72
2	C	252	TYR	N-CA-C	5.93	117.44	110.97
3	E	118	TYR	N-CA-C	5.93	121.25	113.30
1	A	212	PHE	N-CA-C	5.91	120.22	112.13
1	A	122	GLY	N-CA-C	-5.88	105.24	112.77
3	E	39	HIS	N-CA-C	5.85	122.39	113.61
1	A	267	LEU	N-CA-C	5.85	118.16	111.02
2	C	249	HIS	N-CA-C	5.84	119.59	112.23
1	A	145	ILE	N-CA-C	-5.74	104.92	110.72
2	D	54	VAL	N-CA-C	5.69	116.61	108.93
2	D	77	HIS	N-CA-C	-5.62	101.72	110.10
3	F	118	TYR	N-CA-C	5.58	120.78	113.30
1	B	312	ASP	N-CA-C	5.51	117.14	111.03
3	E	73	ASN	N-CA-C	-5.49	103.44	110.53
2	D	106	HIS	N-CA-C	5.49	117.70	111.11
1	B	243	GLU	N-CA-C	5.48	119.06	112.38
3	E	143	ARG	N-CA-C	5.47	117.32	111.36
2	D	104	ARG	N-CA-C	5.45	117.19	108.41
2	C	193	ILE	N-CA-C	-5.45	105.41	110.53
1	B	178	GLY	CA-C-N	5.42	124.93	119.19
1	B	178	GLY	C-N-CA	5.42	124.93	119.19
2	D	236	GLN	N-CA-C	5.41	119.99	113.17
2	D	169	GLU	N-CA-C	5.38	119.91	113.23
1	A	496	ILE	N-CA-C	-5.38	105.47	110.53
2	C	53	THR	N-CA-C	5.37	120.07	112.93
2	C	377	ARG	N-CA-C	5.34	117.52	111.11
2	C	56	ALA	N-CA-C	-5.31	105.57	111.36
2	C	299	TYR	N-CA-C	5.30	118.91	112.23
2	C	265	PHE	N-CA-C	5.29	116.85	111.14
1	B	342	ALA	N-CA-C	5.25	117.40	111.11
2	C	171	LEU	N-CA-C	5.23	119.29	113.02
1	B	205	GLN	N-CA-C	5.22	119.13	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	318	ARG	N-CA-C	-5.22	105.59	111.28
1	A	431	LYS	N-CA-C	-5.21	106.77	113.23
3	F	147	TYR	N-CA-C	5.21	116.95	111.28
1	A	501	VAL	N-CA-C	5.21	117.18	111.77
2	C	104	ARG	N-CA-C	5.15	116.71	108.41
1	A	295	LYS	N-CA-C	-5.13	105.86	112.68
2	C	144	PHE	N-CA-C	5.11	117.75	111.82
1	A	478	LEU	N-CA-C	5.10	117.23	111.11
1	B	122	GLY	N-CA-C	-5.06	106.29	112.77
2	D	137	ASN	CA-C-N	5.05	124.83	119.28
2	D	137	ASN	C-N-CA	5.05	124.83	119.28
3	E	74	GLU	N-CA-C	5.03	116.76	111.28
1	B	104	LYS	N-CA-C	-5.00	105.91	111.36

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	97	0
1	B	4185	0	3981	127	0
2	C	3193	0	3042	65	0
2	D	3193	0	3042	101	0
3	E	1368	0	1363	25	0
3	F	1386	0	1377	51	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	A	269	0	0	3	0
7	B	273	0	0	9	0
7	C	327	0	0	5	0
7	D	165	0	0	4	0
7	E	159	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	69	0	0	2	0
All	All	18782	0	16787	413	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 12.

All (413) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:336:MET:HE3	2:C:388:LEU:HG	1.43	0.98
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.11	0.94
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.51	0.90
1:A:78:GLN:HE22	1:A:150:GLN:HE21	1.09	0.89
1:B:209:GLU:HA	1:B:213:THR:HB	1.53	0.88
1:B:123:MET:HE3	1:B:197:ALA:HA	1.56	0.87
1:A:44:THR:HG22	1:A:46:TYR:H	1.39	0.87
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.57	0.86
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.21	0.85
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.56	0.85
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.62	0.82
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.27	0.80
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.64	0.79
3:E:98:MET:HE1	3:E:107:ALA:CB	2.13	0.79
3:E:41:THR:O	3:E:44:ARG:HD2	1.83	0.78
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.66	0.78
1:A:209:GLU:HA	1:A:213:THR:OG1	1.84	0.78
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.84	0.77
1:B:44:THR:HG22	1:B:46:TYR:H	1.50	0.77
2:D:140:TRP:NE1	2:D:145:ILE:HD11	2.00	0.77
3:F:41:THR:O	3:F:44:ARG:HD2	1.84	0.76
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.69	0.75
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.30	0.75
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.69	0.75
1:A:268:ASN:HD21	1:A:327:GLU:H	1.34	0.75
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.87	0.74
1:A:184:MET:HE2	1:A:188:PHE:HB2	1.68	0.74
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.17	0.74
3:F:41:THR:CG2	3:F:43:PHE:H	2.00	0.73
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.37	0.72
1:A:227:ASN:HD21	1:A:295:LYS:H	1.38	0.71
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:58:ALA:O	3:F:62:GLU:HG3	1.90	0.71
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.37	0.71
1:A:210:ALA:HA	1:A:247:MET:HE1	1.73	0.70
1:B:367:GLU:HG3	7:B:5010:HOH:O	1.91	0.70
1:B:244:LEU:HG	7:B:5100:HOH:O	1.92	0.70
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.72	0.70
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.74	0.69
2:C:146:ASN:ND2	2:C:197:ARG:HH21	1.90	0.69
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.21	0.69
3:F:13:ASP:O	3:F:16:VAL:HG22	1.93	0.69
3:F:41:THR:HG22	3:F:43:PHE:H	1.56	0.68
3:F:57:GLU:O	3:F:61:GLU:HG3	1.92	0.68
2:C:76:PHE:HZ	2:C:168:ARG:HH12	1.42	0.67
1:B:445:MET:HE3	1:B:523:VAL:HG22	1.75	0.67
1:B:227:ASN:HD21	1:B:295:LYS:H	1.42	0.67
2:C:336:MET:HE2	2:C:385:LEU:HD23	1.77	0.67
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.60	0.66
1:A:244:LEU:HG	7:A:9115:HOH:O	1.95	0.66
2:C:333:ARG:HD2	7:C:5162:HOH:O	1.95	0.66
3:F:15:TRP:O	3:F:19:ILE:HG23	1.95	0.66
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.88	0.65
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.77	0.65
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.79	0.65
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.61	0.65
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.32	0.65
1:A:140:GLN:O	1:A:144:GLU:HG2	1.97	0.64
1:B:489:ARG:HD2	1:B:495:LEU:O	1.97	0.64
2:D:153:LEU:C	2:D:153:LEU:HD12	2.23	0.64
2:D:228:ARG:O	2:D:232:GLU:HG3	1.97	0.64
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.63	0.64
1:B:30:ARG:O	1:B:30:ARG:HD3	1.98	0.63
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.81	0.63
1:B:243:GLU:O	1:B:247:MET:HG2	1.99	0.63
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.82	0.63
1:A:406:MET:O	1:A:410:GLU:HG3	1.98	0.63
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.00	0.62
1:A:338:ASP:OD1	1:A:433:ALA:HB2	1.99	0.62
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.83	0.62
1:B:268:ASN:CG	1:B:327:GLU:HG2	2.25	0.61
2:C:270:PRO:HB3	2:D:270:PRO:HB3	1.81	0.61
1:B:213:THR:O	1:B:217:ILE:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:LEU:HD11	1:B:512:ILE:HG13	1.82	0.61
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.82	0.61
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.82	0.61
1:B:495:LEU:HD11	1:B:512:ILE:CG1	2.31	0.61
1:B:192:PHE:O	1:B:200:CYS:HB3	2.02	0.60
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.84	0.60
2:C:247:SER:HG	2:C:324:TRP:CD1	2.19	0.60
2:D:326:GLU:HB2	2:D:327:PRO:HD3	1.82	0.60
1:B:125:TRP:HE1	2:D:161:ASN:ND2	1.99	0.60
1:A:108:ASN:HD21	1:A:175:ARG:HH11	1.48	0.60
1:B:33:GLN:HE22	1:B:132:GLU:H	1.48	0.60
3:E:98:MET:HE1	3:E:107:ALA:HB2	1.82	0.60
1:A:403:ILE:HD13	1:A:515:LEU:HD11	1.83	0.59
1:B:244:LEU:HB2	7:B:5172:HOH:O	2.02	0.59
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.85	0.59
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.91	0.59
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.83	0.59
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.03	0.59
3:E:146:ASN:HB3	3:E:149:ASP:OD2	2.02	0.59
2:D:44:LYS:HG3	7:D:491:HOH:O	2.02	0.59
1:A:227:ASN:ND2	1:A:295:LYS:H	2.00	0.59
3:E:98:MET:HE1	3:E:107:ALA:HB1	1.84	0.59
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.84	0.58
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.68	0.58
1:B:369:MET:HE2	7:B:5162:HOH:O	2.04	0.58
1:A:279:GLN:HG2	1:A:283:THR:OG1	2.03	0.58
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.86	0.58
1:B:227:ASN:HD21	1:B:296:PHE:H	1.52	0.57
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.34	0.57
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.38	0.57
2:D:111:LYS:O	2:D:115:GLU:HG3	2.03	0.57
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.50	0.57
3:F:61:GLU:O	3:F:121:PRO:HG2	2.05	0.57
1:A:204:LEU:O	1:A:209:GLU:HG3	2.04	0.57
1:B:227:ASN:ND2	1:B:295:LYS:H	2.02	0.57
1:A:360:ARG:HG2	1:A:498:GLN:HB2	1.86	0.57
1:B:313:TRP:CZ2	1:B:318:ILE:HD11	2.39	0.56
3:F:9:ASN:OD1	3:F:11:THR:HG23	2.05	0.56
1:A:56:THR:HG23	1:A:252:GLN:HE21	1.71	0.56
1:B:269:THR:HG21	7:F:940:HOH:O	2.06	0.56
3:E:41:THR:O	3:E:44:ARG:CD	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:33:LYS:O	3:F:37:MET:HG2	2.05	0.56
1:B:33:GLN:NE2	1:B:132:GLU:H	2.03	0.56
3:E:98:MET:HE3	3:E:98:MET:O	2.06	0.56
1:B:18:ARG:O	2:D:129:ALA:HA	2.05	0.56
1:B:44:THR:HG21	7:B:5112:HOH:O	2.06	0.56
2:D:192:MET:HE3	2:D:280:PHE:CD2	2.41	0.56
1:A:302:VAL:HG13	1:A:376:TYR:CE2	2.41	0.55
3:F:19:ILE:HG21	3:F:60:LEU:HD12	1.88	0.55
1:B:159:ALA:O	2:D:33:ASN:HB2	2.07	0.55
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.72	0.55
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.98	0.55
3:F:153:GLU:H	3:F:153:GLU:CD	2.15	0.55
1:A:268:ASN:HD21	1:A:327:GLU:N	2.03	0.55
1:B:50:TYR:CD2	1:B:257:ILE:HD12	2.42	0.55
2:C:175:THR:O	2:C:179:LEU:HD13	2.07	0.55
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.89	0.55
1:B:164:ASP:CG	1:B:489:ARG:HH22	2.15	0.54
2:D:225:LYS:HE2	2:D:334:ASP:OD2	2.07	0.54
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.89	0.54
2:C:34:LYS:HD3	7:C:5283:HOH:O	2.07	0.54
2:C:228:ARG:O	2:C:232:GLU:HG3	2.08	0.54
1:A:186:ARG:HA	2:C:73:THR:OG1	2.07	0.54
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.07	0.54
2:D:140:TRP:O	2:D:145:ILE:HD13	2.08	0.54
1:A:44:THR:OG1	1:A:127:SER:HA	2.07	0.54
1:B:20:PRO:HG2	7:B:5143:HOH:O	2.08	0.54
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.56	0.54
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.42	0.54
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.42	0.54
2:D:145:ILE:O	2:D:149:TRP:HB3	2.08	0.54
3:F:61:GLU:HB3	3:F:121:PRO:HD3	1.90	0.53
1:B:140:GLN:HG3	1:B:246:HIS:CE1	2.42	0.53
1:B:212:PHE:O	1:B:215:PRO:HD2	2.08	0.53
2:C:211:THR:C	2:C:214:PRO:HD2	2.33	0.53
3:F:19:ILE:HD12	3:F:19:ILE:C	2.33	0.53
3:F:162:ARG:NH1	3:F:164:VAL:HG12	2.24	0.53
2:C:94:ASP:HB3	2:C:97:LYS:HG3	1.91	0.53
2:D:261:ARG:HE	2:D:285:GLN:NE2	2.07	0.53
3:E:101:ALA:HA	3:E:106:GLU:OE2	2.09	0.53
1:A:213:THR:O	1:A:217:ILE:HG12	2.10	0.52
2:D:90:LEU:CD1	2:D:303:LEU:HD13	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:58:ALA:O	3:E:62:GLU:HG3	2.10	0.52
1:B:43:ARG:HD2	1:B:43:ARG:C	2.34	0.52
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.42	0.52
3:F:41:THR:HG23	3:F:43:PHE:H	1.73	0.52
1:A:184:MET:HE2	1:A:188:PHE:CB	2.38	0.52
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.45	0.52
3:E:57:GLU:O	3:E:61:GLU:HG3	2.08	0.52
1:A:184:MET:HE2	1:A:188:PHE:CG	2.45	0.52
1:B:210:ALA:N	1:B:247:MET:HE1	2.25	0.52
1:A:268:ASN:ND2	1:A:327:GLU:H	2.04	0.52
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.92	0.52
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.93	0.52
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.91	0.52
2:D:235:TRP:CD1	2:D:235:TRP:C	2.88	0.52
1:B:268:ASN:HD21	1:B:327:GLU:H	1.56	0.52
1:B:164:ASP:OD1	1:B:489:ARG:NH2	2.43	0.51
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.44	0.51
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.45	0.51
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.38	0.51
2:C:211:THR:O	2:C:214:PRO:HD2	2.10	0.51
1:B:123:MET:HE1	1:B:200:CYS:SG	2.50	0.51
1:B:247:MET:HE2	1:B:247:MET:HA	1.92	0.51
2:D:71:ASP:HB2	3:F:54:LEU:HD11	1.93	0.51
2:C:336:MET:CE	2:C:385:LEU:HD23	2.40	0.51
1:A:186:ARG:HD3	1:A:186:ARG:C	2.34	0.51
1:B:369:MET:HE1	1:B:388:GLU:OE2	2.11	0.51
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.11	0.51
2:D:269:ALA:HB3	2:D:270:PRO:HD3	1.92	0.51
1:B:185:LYS:O	1:B:189:SER:HB2	2.11	0.51
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.44	0.51
1:A:297:LYS:HG2	1:A:371:TRP:CE2	2.46	0.50
1:B:323:LYS:HE2	1:B:324:TYR:CE1	2.45	0.50
1:B:441:TYR:HB2	3:F:161:VAL:HG23	1.92	0.50
2:C:97:LYS:HD2	7:C:5103:HOH:O	2.10	0.50
1:A:109:PHE:O	1:A:112:VAL:HG12	2.10	0.50
1:B:48:THR:O	3:F:137:THR:HG23	2.12	0.50
1:B:360:ARG:HG2	1:B:498:GLN:HB2	1.94	0.50
1:B:230:GLU:C	1:B:233:PRO:HD2	2.36	0.50
2:C:269:ALA:HB3	2:C:270:PRO:HD3	1.92	0.50
1:B:43:ARG:HD2	1:B:43:ARG:O	2.12	0.50
2:C:96:PHE:O	2:C:99:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:82:SER:O	2:D:168:ARG:NH2	2.44	0.50
2:D:137:ASN:HB3	2:D:272:PHE:HB3	1.93	0.50
3:F:40:THR:O	3:F:41:THR:HB	2.11	0.50
1:B:186:ARG:HD3	1:B:186:ARG:C	2.37	0.50
1:A:144:GLU:HA	1:A:144:GLU:OE2	2.12	0.49
3:E:66:VAL:HG12	3:E:70:ARG:HH21	1.75	0.49
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.95	0.49
1:A:108:ASN:HD21	1:A:175:ARG:HD3	1.76	0.49
2:D:324:TRP:C	2:D:327:PRO:HD2	2.37	0.49
1:B:222:GLU:OE1	2:D:7:ARG:HD3	2.13	0.49
2:C:153:LEU:C	2:C:153:LEU:HD12	2.37	0.49
2:D:247:SER:O	2:D:251:VAL:HB	2.13	0.49
1:A:185:LYS:O	1:A:189:SER:HB2	2.13	0.49
1:B:268:ASN:OD1	1:B:327:GLU:HG2	2.13	0.49
2:D:54:VAL:O	2:D:55:TYR:HB2	2.13	0.49
1:A:179:PRO:HB3	1:A:469:ILE:HD13	1.94	0.49
1:B:33:GLN:HA	1:B:131:ALA:HB3	1.95	0.49
1:B:52:MET:CE	1:B:127:SER:HB3	2.43	0.49
2:C:277:THR:HB	2:C:278:PRO:HD3	1.94	0.49
3:F:98:MET:HE1	3:F:107:ALA:O	2.13	0.49
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.48	0.48
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.95	0.48
2:C:235:TRP:CD1	2:C:235:TRP:C	2.91	0.48
1:A:206:LEU:HD11	1:A:321:LEU:HD11	1.95	0.48
1:B:193:ILE:HD11	2:D:82:SER:HB3	1.95	0.48
2:C:364:ILE:HA	2:C:368:ALA:HB3	1.95	0.48
3:E:18:LYS:HB2	3:E:18:LYS:NZ	2.28	0.48
1:B:106:VAL:O	1:B:110:LEU:HB2	2.13	0.48
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.42	0.48
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.48	0.48
1:A:163:GLN:HG2	7:A:9175:HOH:O	2.14	0.48
2:D:381:VAL:O	2:D:385:LEU:HB2	2.14	0.48
2:D:332:LEU:O	2:D:336:MET:HG2	2.14	0.48
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.12	0.47
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.14	0.47
7:C:5122:HOH:O	3:E:125:VAL:HG22	2.14	0.47
3:E:102:LYS:HG2	3:E:106:GLU:OE1	2.13	0.47
2:D:89:GLU:OE2	3:F:125:VAL:HG13	2.13	0.47
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.49	0.47
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.32	0.47
2:D:195:LEU:O	2:D:195:LEU:HD23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:356:LEU:HD12	2:D:385:LEU:HD13	1.96	0.47
1:A:123:MET:HE2	1:A:197:ALA:HA	1.96	0.47
1:A:344:HIS:HE1	1:A:376:TYR:CD2	2.32	0.47
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.50	0.47
1:B:439:HIS:HE1	1:B:454:GLU:OE1	1.97	0.47
1:A:227:ASN:HD21	1:A:296:PHE:H	1.60	0.47
3:F:130:ASP:OD1	3:F:133:ARG:NH1	2.48	0.47
2:D:101:PRO:HG2	2:D:293:GLN:HB3	1.95	0.47
2:D:275:ASN:C	2:D:278:PRO:HD2	2.40	0.47
7:D:497:HOH:O	3:F:125:VAL:HG22	2.14	0.47
2:C:98:HIS:HE1	2:C:178:SER:OG	1.97	0.46
2:C:126:GLY:O	2:C:130:ASP:HB2	2.15	0.46
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.51	0.46
1:B:209:GLU:HA	1:B:213:THR:CB	2.35	0.46
2:C:7:ARG:HG3	2:C:7:ARG:HH11	1.81	0.46
1:B:30:ARG:HD3	1:B:30:ARG:C	2.40	0.46
1:B:206:LEU:HB2	7:B:5239:HOH:O	2.16	0.46
2:C:54:VAL:O	2:C:55:TYR:HB2	2.16	0.46
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.80	0.46
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.97	0.46
2:C:75:LYS:HB3	2:C:80:ARG:O	2.15	0.46
2:C:336:MET:HE3	2:C:388:LEU:CG	2.29	0.46
3:F:17:ASN:O	3:F:21:GLN:HG2	2.15	0.46
2:C:111:LYS:O	2:C:115:GLU:HG3	2.15	0.46
1:B:41:ASN:O	2:D:236:GLN:HB3	2.16	0.46
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.15	0.46
1:A:230:GLU:C	1:A:233:PRO:HD2	2.42	0.46
2:C:2:SER:HB2	7:C:5256:HOH:O	2.15	0.46
2:D:185:ASP:O	2:D:189:ILE:HG12	2.16	0.46
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.98	0.45
1:B:186:ARG:HD3	1:B:186:ARG:O	2.16	0.45
2:D:187:ILE:O	2:D:191:GLN:HG3	2.16	0.45
1:B:466:CYS:HB2	2:D:73:THR:HA	1.99	0.45
1:A:21:THR:HG22	2:C:128:SER:CB	2.46	0.45
1:B:125:TRP:CD1	1:B:125:TRP:C	2.94	0.45
1:B:337:GLN:HG3	1:B:338:ASP:N	2.32	0.45
1:A:186:ARG:HD3	1:A:186:ARG:O	2.17	0.45
1:B:123:MET:SD	2:D:168:ARG:NH1	2.89	0.45
1:B:198:VAL:O	1:B:202:LEU:HG	2.16	0.45
1:B:413:HIS:HE1	7:B:5261:HOH:O	1.99	0.45
2:C:203:ILE:HG13	2:C:204:VAL:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:HIS:O	1:A:386:ILE:HG13	2.17	0.45
1:B:65:LYS:HE2	2:D:192:MET:HE2	1.99	0.45
1:B:140:GLN:HG3	1:B:246:HIS:CD2	2.51	0.45
1:B:334:ASP:HA	1:B:337:GLN:HG2	1.99	0.45
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.52	0.45
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.99	0.45
2:D:169:GLU:O	2:D:170:ALA:C	2.58	0.45
3:E:40:THR:C	3:E:41:THR:HG23	2.42	0.45
1:A:65:LYS:HB3	2:C:117:TRP:CG	2.52	0.44
1:B:186:ARG:HA	2:D:73:THR:OG1	2.16	0.44
1:A:81:SER:OG	1:B:84:ASP:HB3	2.16	0.44
1:A:146:ARG:HB2	2:C:106:HIS:CE1	2.53	0.44
1:A:216:LEU:O	1:A:220:VAL:HG23	2.16	0.44
2:D:143:GLU:O	2:D:147:ARG:HB3	2.17	0.44
2:D:277:THR:HB	2:D:278:PRO:HD3	1.98	0.44
1:B:196:ASP:HB2	3:F:140:MET:SD	2.58	0.44
3:F:41:THR:HG22	3:F:43:PHE:N	2.30	0.44
1:A:118:ILE:HD13	1:A:145:ILE:HG12	2.00	0.44
3:E:98:MET:HE2	3:E:138:ARG:CG	2.47	0.44
3:F:33:LYS:HE3	3:F:117:ALA:CB	2.48	0.44
3:E:44:ARG:HD3	3:E:47:TYR:CZ	2.52	0.44
3:F:12:ARG:O	3:F:16:VAL:HG13	2.17	0.44
1:A:163:GLN:O	2:C:28:PRO:HA	2.18	0.44
1:A:206:LEU:HB2	7:A:9036:HOH:O	2.18	0.44
1:B:384:GLY:O	1:B:388:GLU:HG3	2.18	0.44
2:D:239:PHE:HB2	3:F:126:ASN:HA	1.99	0.44
2:D:192:MET:HE3	2:D:280:PHE:HD2	1.83	0.44
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.53	0.44
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.52	0.44
1:B:21:THR:HG22	1:B:22:SER:N	2.32	0.44
1:B:115:TYR:OH	2:D:173:ASP:HA	2.17	0.44
2:C:261:ARG:NE	2:C:285:GLN:HE22	2.02	0.44
2:D:192:MET:HE3	2:D:280:PHE:CE2	2.52	0.44
1:A:193:ILE:HD11	2:C:82:SER:HB3	1.99	0.43
2:D:360:VAL:O	2:D:364:ILE:HG13	2.17	0.43
2:C:143:GLU:O	2:C:147:ARG:HB3	2.18	0.43
1:A:44:THR:HG23	1:A:126:ASP:OD1	2.18	0.43
2:C:98:HIS:HD2	2:C:297:ASP:OD1	2.00	0.43
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.53	0.43
2:D:348:ASP:OD1	2:D:351:GLU:HG3	2.18	0.43
3:F:132:GLU:HG3	7:F:1113:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LYS:HD2	2:C:117:TRP:HB2	2.00	0.43
1:A:216:LEU:HA	1:A:308:TRP:CH2	2.53	0.43
2:D:240:ASP:HB2	3:F:125:VAL:CG2	2.47	0.43
1:A:212:PHE:O	1:A:215:PRO:HD2	2.18	0.43
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.82	0.43
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.53	0.43
3:E:22:LEU:HD21	3:E:31:MET:SD	2.58	0.43
1:A:184:MET:HE3	1:A:184:MET:HA	2.00	0.43
2:D:326:GLU:HG3	7:D:441:HOH:O	2.18	0.43
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.66	0.43
1:A:190:ASP:HB3	2:C:74:GLN:O	2.18	0.43
1:B:196:ASP:O	1:B:197:ALA:C	2.62	0.43
1:B:33:GLN:HA	1:B:33:GLN:HE21	1.83	0.43
2:D:193:ILE:HA	7:D:553:HOH:O	2.19	0.43
2:D:243:GLU:HB2	2:D:320:TRP:CZ2	2.53	0.43
1:A:84:ASP:HB3	1:B:81:SER:OG	2.18	0.42
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.54	0.42
2:C:240:ASP:OD1	3:E:125:VAL:HG21	2.19	0.42
3:F:40:THR:HG22	3:F:53:TYR:CD1	2.54	0.42
1:A:402:PHE:O	1:A:403:ILE:HD12	2.19	0.42
2:D:269:ALA:N	2:D:270:PRO:CD	2.82	0.42
2:D:326:GLU:CB	2:D:327:PRO:HD3	2.49	0.42
2:C:192:MET:HE3	2:C:280:PHE:CD2	2.54	0.42
1:A:32:LEU:C	1:A:32:LEU:HD23	2.45	0.42
1:B:488:LEU:HD13	1:B:492:GLY:O	2.19	0.42
1:B:490:SER:OG	2:D:32:ASN:HB2	2.19	0.42
2:D:299:TYR:O	2:D:317:MET:HE1	2.19	0.42
1:A:439:HIS:CE1	1:A:454:GLU:OE1	2.69	0.42
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.30	0.42
2:D:63:ILE:O	2:D:64:ALA:C	2.61	0.42
2:D:324:TRP:O	2:D:327:PRO:HD2	2.19	0.42
1:A:343:HIS:CD2	1:A:343:HIS:H	2.37	0.42
1:B:140:GLN:O	1:B:144:GLU:HG2	2.20	0.42
2:D:167:ALA:O	2:D:176:ARG:NH1	2.51	0.42
1:A:222:GLU:OE1	2:C:7:ARG:NH1	2.52	0.42
1:A:417:ILE:HG13	1:A:468:ASN:HB2	2.02	0.42
1:B:207:VAL:O	1:B:211:CYS:HB3	2.20	0.42
2:D:77:HIS:CD2	3:F:140:MET:HG2	2.55	0.42
2:D:140:TRP:CE2	2:D:145:ILE:HD11	2.54	0.42
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.20	0.42
1:B:421:SER:O	1:B:422:GLN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:146:ASN:HD21	2:C:197:ARG:NH2	2.06	0.42
2:D:376:ASP:OD2	2:D:379:GLN:HB2	2.20	0.42
2:C:192:MET:HE2	2:C:283:GLN:OE1	2.19	0.42
1:B:283:THR:HB	1:B:284:PRO:HD3	2.01	0.41
1:B:118:ILE:HD13	1:B:145:ILE:HG12	2.02	0.41
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.55	0.41
1:B:438:VAL:HB	3:F:164:VAL:CG2	2.50	0.41
2:D:192:MET:HE2	2:D:283:GLN:OE1	2.20	0.41
3:E:15:TRP:CD1	3:E:56:ILE:HD13	2.55	0.41
3:F:19:ILE:HG21	3:F:60:LEU:CD1	2.50	0.41
2:C:146:ASN:O	2:C:214:PRO:HG3	2.20	0.41
1:A:116:ASN:CG	1:A:189:SER:HA	2.46	0.41
1:A:232:THR:HB	1:A:233:PRO:HD3	2.01	0.41
1:B:113:GLY:HA2	1:B:188:PHE:HB3	2.01	0.41
3:F:38:ASP:HA	3:F:45:ASN:HB2	2.02	0.41
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.55	0.41
1:B:163:GLN:O	2:D:28:PRO:HA	2.20	0.41
3:E:66:VAL:CG1	3:E:70:ARG:HH21	2.34	0.41
1:A:249:ASN:HD22	1:A:249:ASN:HA	1.68	0.41
1:B:184:MET:HE3	1:B:187:VAL:HG23	2.02	0.41
1:B:355:PRO:HG2	1:B:403:ILE:HD12	2.01	0.41
2:D:336:MET:HE3	2:D:388:LEU:HD21	2.02	0.41
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.85	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.61	0.41
1:A:390:TRP:HE1	1:A:407:TRP:CG	2.39	0.41
1:B:470:PHE:O	1:B:474:GLU:HB2	2.20	0.41
2:D:94:ASP:HB3	2:D:97:LYS:HG3	2.02	0.41
2:D:98:HIS:CD2	2:D:99:ARG:N	2.89	0.41
1:A:184:MET:HE3	1:A:187:VAL:CG2	2.51	0.41
1:A:192:PHE:O	1:A:200:CYS:HB3	2.20	0.41
1:B:209:GLU:C	1:B:247:MET:HE1	2.46	0.41
2:D:208:ASP:OD2	2:D:210:SER:HB3	2.20	0.41
2:D:240:ASP:HB2	3:F:125:VAL:HG21	2.02	0.41
2:D:255:LEU:HD21	2:D:363:TRP:CG	2.56	0.41
2:D:291:ALA:O	2:D:295:VAL:HG23	2.21	0.41
3:F:67:LEU:HD23	3:F:70:ARG:HH21	1.86	0.41
1:A:125:TRP:CD1	1:A:125:TRP:C	2.99	0.41
1:B:108:ASN:O	1:B:111:GLU:HB3	2.21	0.41
1:B:184:MET:HE3	1:B:187:VAL:CG2	2.51	0.41
2:D:312:TYR:O	2:D:316:VAL:HG23	2.21	0.41
3:E:15:TRP:O	3:E:19:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LEU:O	1:A:114:GLU:HG2	2.20	0.40
1:B:246:HIS:CD2	1:B:246:HIS:N	2.88	0.40
2:C:256:PHE:HA	2:C:332:LEU:HD21	2.03	0.40
1:A:303:LYS:HE3	1:A:303:LYS:HB2	1.92	0.40
1:A:360:ARG:NH2	1:A:501:VAL:O	2.54	0.40
1:A:403:ILE:HD13	1:A:515:LEU:CD1	2.48	0.40
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.94	0.40
1:B:140:GLN:HG3	1:B:246:HIS:NE2	2.35	0.40
2:D:140:TRP:NE1	2:D:145:ILE:CD1	2.81	0.40
1:B:165:PRO:HG3	7:B:5025:HOH:O	2.22	0.40
1:B:227:ASN:ND2	1:B:296:PHE:H	2.17	0.40
2:C:137:ASN:HA	2:C:138:PRO:HD3	1.94	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%)	487 (96%)	21 (4%)	1 (0%)	43	40
1	B	509/527 (97%)	484 (95%)	23 (4%)	2 (0%)	30	22
2	C	386/389 (99%)	374 (97%)	10 (3%)	2 (0%)	24	17
2	D	386/389 (99%)	367 (95%)	17 (4%)	2 (0%)	24	17
3	E	164/170 (96%)	161 (98%)	3 (2%)	0	100	100
3	F	166/170 (98%)	160 (96%)	6 (4%)	0	100	100
All	All	2120/2172 (98%)	2033 (96%)	80 (4%)	7 (0%)	36	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS

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Mol	Chain	Res	Type
2	D	64	ALA
2	D	205	PRO
2	C	64	ALA
1	A	284	PRO
2	C	251	VAL
1	B	284	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	433/442 (98%)	427 (99%)	6 (1%)	59	61
1	B	433/442 (98%)	426 (98%)	7 (2%)	55	56
2	C	322/323 (100%)	317 (98%)	5 (2%)	55	56
2	D	322/323 (100%)	317 (98%)	5 (2%)	55	56
3	E	144/147 (98%)	142 (99%)	2 (1%)	59	61
3	F	146/147 (99%)	141 (97%)	5 (3%)	32	28
All	All	1800/1824 (99%)	1770 (98%)	30 (2%)	53	53

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	279	GLN
1	A	403	ILE
1	A	467	GLN
1	B	43	ARG
1	B	90	ASN
1	B	110	LEU
1	B	112	VAL
1	B	125	TRP
1	B	279	GLN

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Mol	Chain	Res	Type
1	B	403	ILE
2	C	33	ASN
2	C	122	ARG
2	C	153	LEU
2	C	173	ASP
2	C	356	LEU
2	D	80	ARG
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
2	D	292	LYS
3	E	18	LYS
3	E	44	ARG
3	F	11	THR
3	F	19	ILE
3	F	41	THR
3	F	44	ARG
3	F	164	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	78	GLN
1	A	83	GLN
1	A	90	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	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	413	HIS
1	A	439	HIS
1	A	442	ASN

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Mol	Chain	Res	Type
1	A	486	HIS
1	B	33	GLN
1	B	78	GLN
1	B	90	ASN
1	B	100	ASN
1	B	108	ASN
1	B	133	GLN
1	B	168	HIS
1	B	203	ASN
1	B	205	GLN
1	B	214	ASN
1	B	227	ASN
1	B	249	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	439	HIS
1	B	451	GLN
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	285	GLN
2	D	293	GLN
2	D	296	GLN
2	D	301	ASN
3	E	45	ASN
3	E	134	GLN

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Mol	Chain	Res	Type
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	111	HIS
3	F	144	ASN
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 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	FMT	A	9001	4	2,2,2	0.64	0	1,1,1	0.60	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

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%)	0.07	17 (3%) 49 48	17, 28, 49, 65	0
1	B	511/527 (96%)	0.10	18 (3%) 47 46	19, 30, 50, 66	0
2	C	388/389 (99%)	-0.46	2 (0%) 87 87	14, 21, 36, 55	0
2	D	388/389 (99%)	0.60	27 (6%) 22 21	21, 36, 55, 71	0
3	E	166/170 (97%)	-0.12	6 (3%) 46 45	17, 25, 40, 61	0
3	F	168/170 (98%)	1.32	35 (20%) 2 2	30, 45, 62, 68	0
All	All	2132/2172 (98%)	0.16	105 (4%) 35 34	14, 30, 52, 71	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	168	SER	5.6
3	E	4	LEU	3.8
3	F	101	ALA	3.8
2	D	384	VAL	3.7
3	F	20	ALA	3.6
1	A	318	ILE	3.6
1	A	310	TYR	3.6
1	A	213	THR	3.5
3	F	19	ILE	3.4
1	B	403	ILE	3.3
2	D	385	LEU	3.3
2	D	386	ALA	3.3
1	A	317	TRP	3.1
1	B	214	ASN	3.0
1	B	311	GLU	3.0
1	A	433	ALA	3.0
1	B	310	TYR	3.0
1	A	244	LEU	3.0
3	F	23	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	164	VAL	3.0
2	D	387	GLY	3.0
1	B	493	LYS	3.0
3	F	100	ALA	2.9
3	F	170	HIS	2.9
2	D	223	VAL	2.9
3	F	83	PHE	2.9
1	B	54	ASN	2.9
2	D	380	ILE	2.9
1	A	432	GLY	2.9
2	D	388	LEU	2.8
3	F	72	PHE	2.8
3	F	24	THR	2.8
3	F	80	LYS	2.7
1	A	316	ILE	2.7
3	F	17	ASN	2.7
1	B	308	TRP	2.7
3	F	82	ALA	2.7
1	B	213	THR	2.7
3	F	16	VAL	2.6
3	E	23	ASN	2.6
2	D	270	PRO	2.6
3	E	167	GLN	2.6
1	A	210	ALA	2.6
2	D	372	ASP	2.6
3	F	163	VAL	2.5
3	F	127	TYR	2.5
1	B	212	PHE	2.5
1	A	212	PHE	2.5
1	B	39	PHE	2.5
3	F	77	PHE	2.5
2	D	206	GLY	2.5
1	A	214	ASN	2.5
1	B	260	ASP	2.4
3	F	41	THR	2.4
3	F	75	VAL	2.4
3	F	79	HIS	2.4
2	C	143	GLU	2.3
3	F	60	LEU	2.3
2	D	345	GLY	2.3
1	B	337	GLN	2.3
2	D	357	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	315	GLY	2.3
2	D	144	PHE	2.3
2	C	6	GLU	2.3
1	A	206	LEU	2.3
1	B	244	LEU	2.3
3	F	28	ALA	2.3
3	F	84	GLY	2.3
1	A	308	TRP	2.3
2	D	363	TRP	2.3
2	D	339	PHE	2.2
1	A	54	ASN	2.2
1	B	319	GLY	2.2
2	D	216	ALA	2.2
2	D	222	GLU	2.2
3	F	66	VAL	2.2
1	B	53	ALA	2.2
3	F	30	GLU	2.2
3	F	21	GLN	2.2
3	F	78	ARG	2.2
3	F	102	LYS	2.2
2	D	347	THR	2.2
1	A	302	VAL	2.2
3	F	70	ARG	2.2
1	B	265	LYS	2.2
2	D	145	ILE	2.1
2	D	373	PHE	2.1
2	D	381	VAL	2.1
3	E	21	GLN	2.1
3	F	71	ALA	2.1
2	D	333	ARG	2.1
3	F	110	ILE	2.1
2	D	213	VAL	2.1
3	F	69	ALA	2.1
1	B	32	LEU	2.1
3	F	22	LEU	2.1
2	D	350	GLU	2.1
2	D	379	GLN	2.1
3	F	11	THR	2.1
2	D	221	GLY	2.1
3	F	125	VAL	2.1
3	E	3	LYS	2.1
2	D	368	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	397	ASP	2.0
1	B	44	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	FMT	A	9001	3/3	0.79	0.17	41,41,48,53	0
5	CA	C	5006	1/1	0.96	0.06	51,51,51,51	0
5	CA	C	5007	1/1	0.98	0.09	35,35,35,35	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	39,39,39,39	0
5	CA	A	5005	1/1	0.99	0.08	46,46,46,46	0
4	FE	B	5003	1/1	1.00	0.03	25,25,25,25	0
4	FE	A	5001	1/1	1.00	0.02	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.