



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:34 PM UTC

PDB ID : 1XVC / pdb_00001xvc
Title : soluble methane monooxygenase hydroxylase: 8-bromooctanol soaked structure
Authors : Sazinsky, M.H.; Lippard, S.J.
Deposited on : 2004-10-27
Resolution : 2.00 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

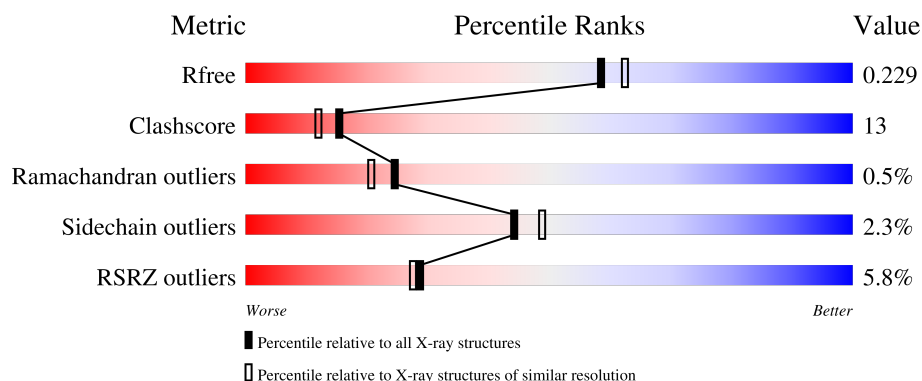
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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% 69% 26% ..
1	B	527	2% 70% 24% ..
2	C	389	80% 18% .
2	D	389	11% 67% 30% ..
3	E	170	5% 71% 24% ...

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Mol	Chain	Length	Quality of chain
3	F	170	28% 56% 38% . .

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
8	FMT	B	2064	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 18280 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
			4150	2656	712	764	18			
1	B	510	Total	C	N	O	S	0	0	0
			4137	2646	711	762	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
			3163	2036	545	574	8			
2	D	387	Total	C	N	O	S	0	0	0
			3141	2022	541	570	8			

- 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
			1364	864	245	250	5			
3	F	166	Total	C	N	O	S	0	0	0
			1358	860	243	250	5			

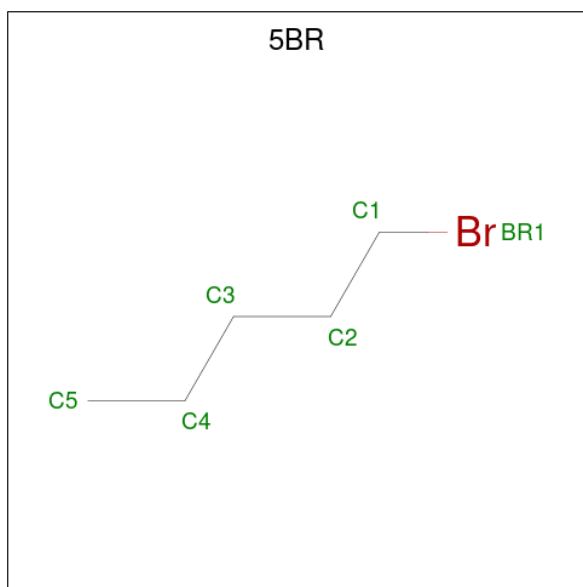
- Molecule 4 is FE (III) ION (CCD ID: FE) (formula: Fe).

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 BROMIDE ION (CCD ID: BR) (formula: Br).

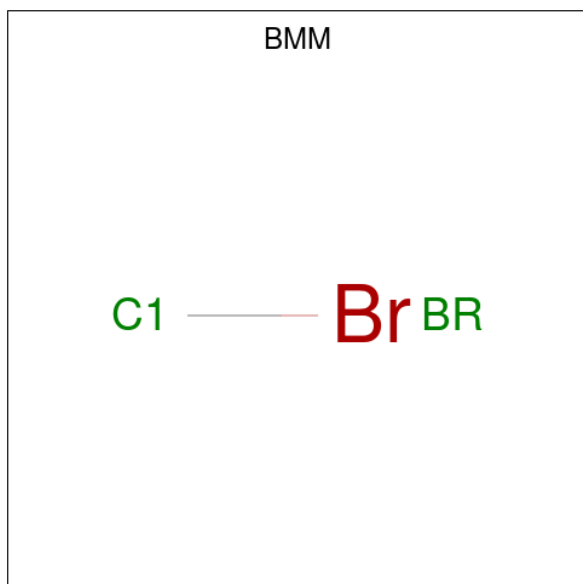
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Br 1	0	0
5	B	1	Total 1	Br 1	0	0

- Molecule 6 is 1-BROMOPENTANE (CCD ID: 5BR) (formula: $C_5H_{11}Br$).



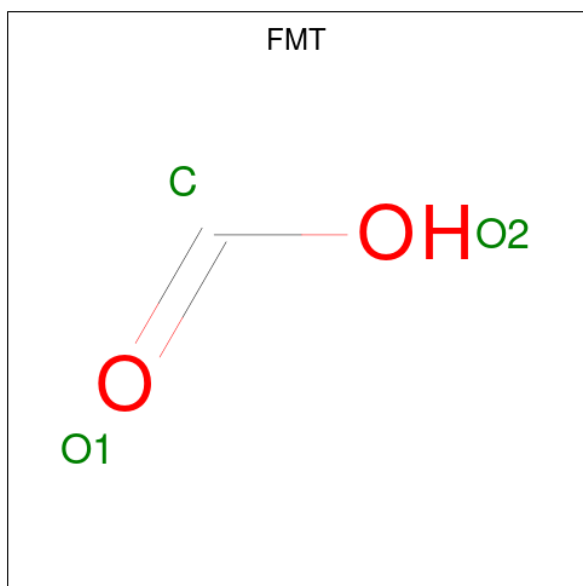
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 6	Br 1	C 5	0	0

- Molecule 7 is BROMOMETHANE (CCD ID: BMM) (formula: CH_3Br).



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

- Molecule 8 is FORMIC ACID (CCD ID: FMT) (formula: CH_2O_2).



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

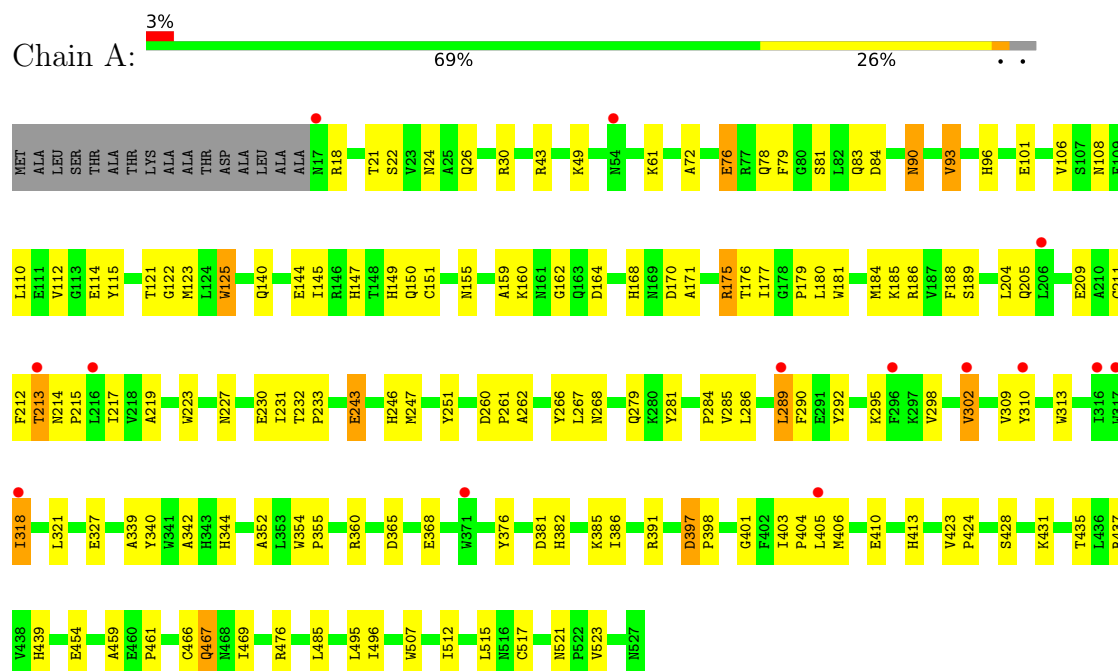
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	223	Total	O	0	0
			223	223		
9	B	214	Total	O	0	0
			214	214		
9	C	249	Total	O	0	0
			249	249		
9	D	120	Total	O	0	0
			120	120		
9	E	106	Total	O	0	0
			106	106		
9	F	38	Total	O	0	0
			38	38		

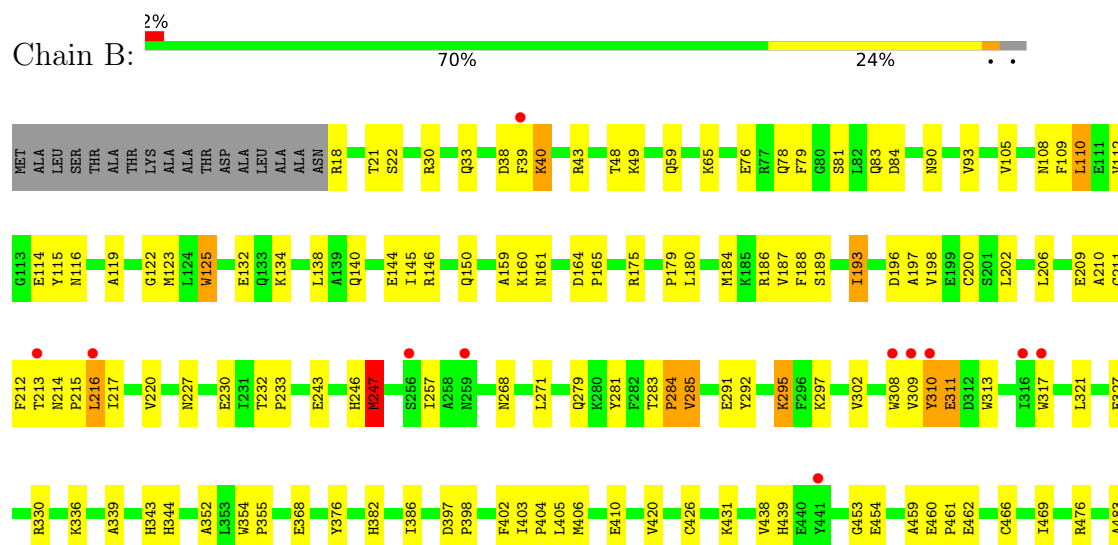
3 Residue-property plots

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



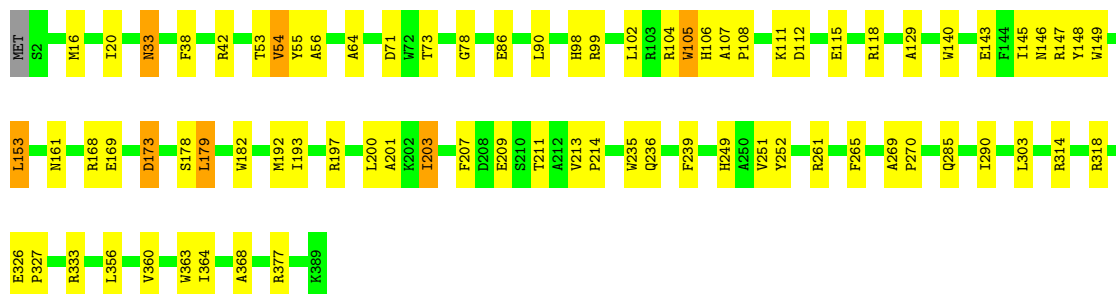
- Molecule 1: Methane monooxygenase component A alpha chain





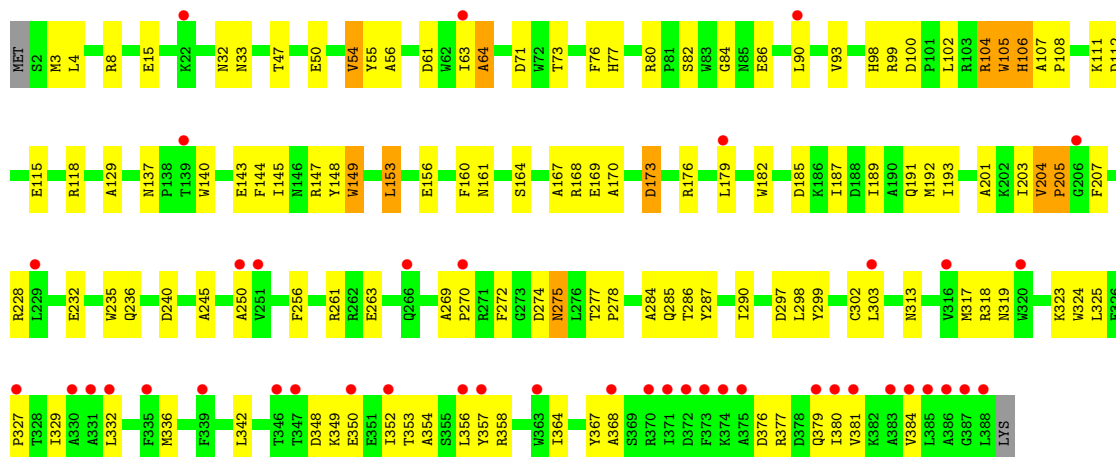
- Molecule 2: Methane monooxygenase component A beta chain

Chain C: 80% 18%



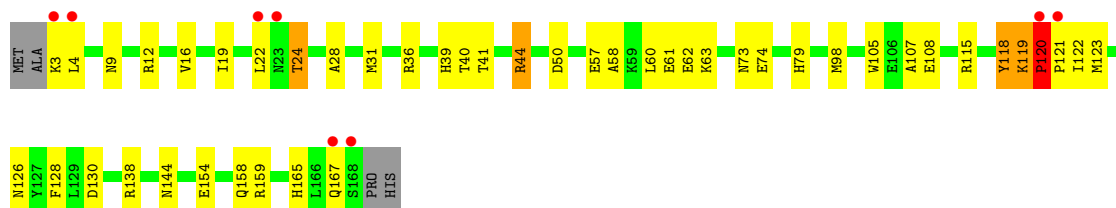
- Molecule 2: Methane monooxygenase component A beta chain

Chain D: 11% 67% 30%



- Molecule 3: Methane monooxygenase component A gamma chain

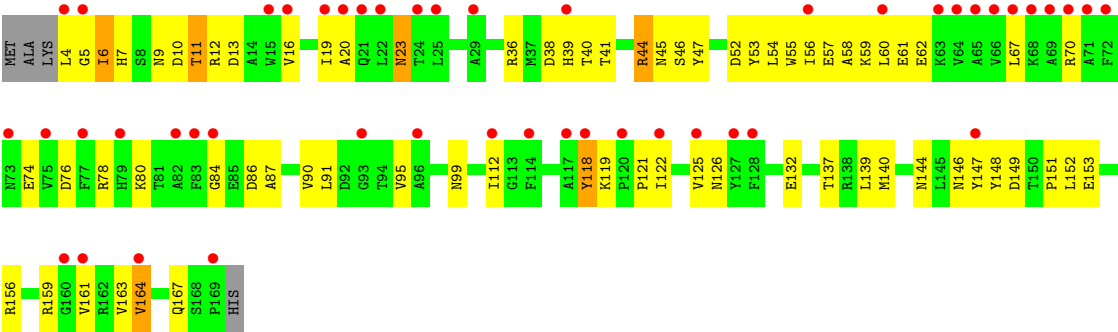
Chain E: 5% 71% 24%



- Molecule 3: Methane monooxygenase component A gamma chain

Chain F: 28% 56% 38%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.41Å 171.03Å 221.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.79 – 2.00 29.79 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (29.79-2.00) 92.1 (29.79-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.206 , 0.234 0.203 , 0.229	Depositor DCC
R_{free} test set	5913 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å ²)	29.5	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.7	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	18280	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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, BMM, BR, 5BR

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	0/4275	0.92	19/5812 (0.3%)
1	B	0.37	0/4262	0.91	18/5796 (0.3%)
2	C	0.41	0/3259	0.90	13/4430 (0.3%)
2	D	0.36	0/3237	0.86	15/4406 (0.3%)
3	E	0.40	0/1392	1.03	11/1876 (0.6%)
3	F	0.32	0/1387	0.82	3/1873 (0.2%)
All	All	0.38	0/17812	0.90	79/24193 (0.3%)

There are no bond length outliers.

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	119	LYS	CA-C-N	11.97	132.71	120.38
3	E	119	LYS	C-N-CA	11.97	132.71	120.38
3	E	120	PRO	N-CA-C	11.59	124.84	110.70
1	B	339	ALA	N-CA-C	8.88	121.04	111.36
3	E	130	ASP	N-CA-C	-8.02	102.62	111.36
1	A	339	ALA	N-CA-C	7.97	119.97	111.28
1	B	496	ILE	N-CA-C	-7.91	103.10	110.53
2	D	204	VAL	CA-C-N	7.65	129.40	119.84
2	D	204	VAL	C-N-CA	7.65	129.40	119.84
1	A	164	ASP	CA-C-N	7.61	127.25	119.56
1	A	164	ASP	C-N-CA	7.61	127.25	119.56
2	C	105	TRP	N-CA-C	-7.17	99.63	109.95
1	B	431	LYS	N-CA-C	-7.03	104.51	113.23
2	C	149	TRP	N-CA-C	-6.99	103.75	111.36
3	E	118	TYR	N-CA-C	6.80	122.42	113.30
2	D	105	TRP	N-CA-C	-6.78	99.93	110.17
3	E	120	PRO	CA-C-N	-6.72	111.44	119.84
3	E	120	PRO	C-N-CA	-6.72	111.44	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	106	HIS	N-CA-C	6.67	119.12	111.11
1	B	243	GLU	N-CA-C	6.65	119.36	111.71
3	E	73	ASN	N-CA-C	-6.64	102.24	110.41
1	A	266	TYR	N-CA-C	6.59	122.40	113.97
2	C	236	GLN	N-CA-C	6.56	121.45	113.38
1	A	145	ILE	N-CA-C	-6.24	104.42	110.72
1	A	309	VAL	N-CA-C	6.15	116.31	110.53
1	A	243	GLU	N-CA-C	6.14	118.77	111.71
2	C	252	TYR	N-CA-C	6.08	117.60	110.97
1	B	164	ASP	CA-C-N	6.05	125.60	119.19
1	B	164	ASP	C-N-CA	6.05	125.60	119.19
3	E	39	HIS	N-CA-C	6.01	122.63	113.61
1	A	397	ASP	CA-C-N	5.93	125.81	119.28
1	A	397	ASP	C-N-CA	5.93	125.81	119.28
1	B	93	VAL	N-CA-C	5.93	116.66	111.56
3	E	79	HIS	N-CA-C	5.93	121.24	113.30
1	A	213	THR	N-CA-C	5.88	117.38	110.97
1	B	426	CYS	CA-C-N	5.88	126.02	119.32
1	B	426	CYS	C-N-CA	5.88	126.02	119.32
2	D	137	ASN	CA-C-N	5.87	125.35	119.24
2	D	137	ASN	C-N-CA	5.87	125.35	119.24
1	A	122	GLY	N-CA-C	-5.86	105.27	112.77
1	B	247	MET	N-CA-C	-5.77	104.89	111.07
2	D	149	TRP	N-CA-C	-5.71	105.13	111.36
2	C	54	VAL	N-CA-C	5.70	117.06	109.37
1	A	496	ILE	N-CA-C	-5.65	105.22	110.53
2	C	265	PHE	N-CA-C	5.62	117.21	111.14
2	D	236	GLN	N-CA-C	5.60	120.11	113.28
1	B	295	LYS	N-CA-C	-5.59	104.47	112.13
3	F	39	HIS	N-CA-C	5.56	121.95	113.61
3	E	74	GLU	N-CA-C	5.54	117.32	111.28
1	B	145	ILE	N-CA-C	-5.51	105.15	110.72
2	D	106	HIS	N-CA-C	5.50	117.71	111.11
3	F	118	TYR	N-CA-C	5.47	119.49	112.26
1	B	65	LYS	N-CA-C	5.46	117.23	111.28
2	C	169	GLU	N-CA-C	5.46	120.09	113.38
2	D	286	THR	N-CA-C	-5.44	105.35	111.28
2	C	104	ARG	N-CA-C	5.43	117.09	108.67
1	B	59	GLN	N-CA-C	5.39	117.24	111.36
1	B	285	VAL	N-CA-C	5.38	116.15	110.72
2	D	275	ASN	N-CA-C	-5.37	106.78	113.38
1	A	267	LEU	N-CA-C	5.33	117.52	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	GLN	N-CA-C	5.31	119.68	111.56
3	F	147	TYR	N-CA-C	5.30	117.74	111.33
1	B	193	ILE	N-CA-C	5.24	120.23	109.34
1	A	431	LYS	N-CA-C	-5.22	106.75	113.23
2	C	249	HIS	N-CA-C	5.21	118.80	112.23
2	D	54	VAL	N-CA-C	5.20	115.95	108.93
2	D	56	ALA	N-CA-C	-5.20	105.79	111.82
1	A	162	GLY	N-CA-C	5.18	120.53	112.60
2	C	148	TYR	N-CA-C	5.18	118.06	111.69
2	D	104	ARG	N-CA-C	5.17	116.74	108.41
2	C	56	ALA	N-CA-C	-5.17	105.64	111.28
1	A	212	PHE	N-CA-C	5.14	119.20	111.96
1	A	340	TYR	N-CA-C	5.13	119.79	111.37
1	B	122	GLY	N-CA-C	-5.12	106.51	113.37
2	D	148	TYR	N-CA-C	5.12	117.99	111.69
1	B	309	VAL	N-CA-C	5.08	115.30	110.53
2	D	318	ARG	N-CA-C	-5.04	105.79	111.28
1	A	93	VAL	N-CA-C	5.01	116.11	111.45
2	C	53	THR	N-CA-C	5.01	119.59	112.93

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	4150	0	3914	122	0
1	B	4137	0	3888	127	0
2	C	3163	0	2986	67	0
2	D	3141	0	2947	97	0
3	E	1364	0	1352	44	0
3	F	1358	0	1335	65	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	6	0	9	1	0
7	B	2	0	0	1	0
8	B	3	0	2	0	0
9	A	223	0	0	5	0
9	B	214	0	0	2	0
9	C	249	0	0	4	0
9	D	120	0	0	1	0
9	E	106	0	0	4	0
9	F	38	0	0	1	0
All	All	18280	0	16433	454	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 (454) 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:A:78:GLN:HE22	1:A:150:GLN:HE21	1.13	0.92
1:A:403:ILE:HD12	1:A:405:LEU:HD13	1.52	0.89
1:B:78:GLN:HE22	1:B:150:GLN:HE21	1.14	0.88
2:D:364:ILE:HA	2:D:368:ALA:HB3	1.57	0.87
1:B:352:ALA:HA	1:B:404:PRO:HB2	1.57	0.86
2:D:102:LEU:HD12	2:D:290:ILE:HG23	1.58	0.86
3:E:105:TRP:HA	9:E:275:HOH:O	1.74	0.86
2:C:261:ARG:HE	2:C:285:GLN:HE22	1.23	0.85
1:B:209:GLU:HA	1:B:213:THR:HB	1.59	0.84
1:A:352:ALA:HA	1:A:404:PRO:HB2	1.58	0.83
2:D:100:ASP:OD1	2:D:104:ARG:HD3	1.79	0.83
1:B:214:ASN:HB3	1:B:215:PRO:HD3	1.61	0.82
1:A:467:GLN:H	1:A:467:GLN:HE21	1.25	0.82
2:D:352:ILE:HD12	2:D:353:THR:N	1.95	0.82
1:A:155:ASN:HD22	1:A:168:HIS:HD2	1.28	0.81
3:F:41:THR:O	3:F:44:ARG:HD2	1.81	0.80
1:A:467:GLN:HE22	2:C:71:ASP:H	1.30	0.80
2:D:261:ARG:HE	2:D:285:GLN:HE22	1.28	0.80
1:B:268:ASN:HD21	1:B:327:GLU:H	1.31	0.79
1:A:268:ASN:HD21	1:A:327:GLU:H	1.31	0.79
1:A:110:LEU:HD22	1:A:151:CYS:SG	2.23	0.78
3:F:80:LYS:HE2	3:F:84:GLY:HA2	1.64	0.78
1:A:209:GLU:HA	1:A:213:THR:HB	1.68	0.76
3:F:146:ASN:HB3	3:F:149:ASP:OD2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:102:LEU:CD1	2:C:290:ILE:HG23	2.16	0.76
1:A:214:ASN:HB3	1:A:215:PRO:HD3	1.69	0.74
2:C:102:LEU:HD12	2:C:290:ILE:HG23	1.68	0.74
2:D:325:LEU:O	2:D:329:ILE:HG12	1.89	0.73
1:A:381:ASP:HA	1:A:385:LYS:HE2	1.71	0.72
1:A:467:GLN:H	1:A:467:GLN:NE2	1.87	0.72
1:A:76:GLU:HG3	1:B:76:GLU:CG	2.20	0.72
1:B:123:MET:HE3	1:B:197:ALA:HA	1.70	0.72
3:F:153:GLU:H	3:F:153:GLU:CD	1.96	0.72
2:D:167:ALA:O	2:D:176:ARG:NH1	2.22	0.71
3:E:19:ILE:HG12	3:E:60:LEU:HD13	1.73	0.70
1:A:289:LEU:HD22	1:A:290:PHE:CD2	2.25	0.70
2:C:326:GLU:HB3	2:C:327:PRO:HD3	1.72	0.70
3:F:58:ALA:O	3:F:62:GLU:HG3	1.92	0.69
1:A:292:TYR:OH	1:A:344:HIS:HD2	1.74	0.69
1:A:175:ARG:HG3	1:A:181:TRP:CD2	2.28	0.69
3:E:120:PRO:HA	3:E:123:MET:O	1.93	0.68
1:A:318:ILE:HD13	1:A:318:ILE:O	1.94	0.68
1:B:292:TYR:OH	1:B:344:HIS:HD2	1.76	0.68
1:A:18:ARG:HG2	2:C:129:ALA:O	1.94	0.68
2:C:146:ASN:HD21	2:C:197:ARG:HH21	1.40	0.68
1:A:435:THR:HG21	1:A:437:ARG:HE	1.58	0.68
1:B:382:HIS:O	1:B:386:ILE:HG12	1.94	0.68
1:A:428:SER:HB3	9:A:1813:HOH:O	1.92	0.67
1:B:210:ALA:HA	1:B:247:MET:HE1	1.76	0.67
3:F:55:TRP:HE3	3:F:56:ILE:HD12	1.58	0.67
1:A:435:THR:CG2	1:A:437:ARG:HE	2.07	0.67
3:E:98:MET:HE1	3:E:107:ALA:CB	2.25	0.67
1:A:476:ARG:HD3	3:E:4:LEU:HG	1.77	0.67
1:B:283:THR:HB	1:B:284:PRO:HD3	1.77	0.67
2:D:107:ALA:HB3	2:D:108:PRO:HD3	1.76	0.67
2:D:319:ASN:OD1	3:F:78:ARG:HD3	1.95	0.66
1:B:33:GLN:HE22	1:B:132:GLU:H	1.41	0.66
1:B:402:PHE:C	1:B:403:ILE:HD12	2.19	0.66
1:A:110:LEU:HD21	1:A:114:GLU:OE2	1.96	0.66
3:F:9:ASN:OD1	3:F:11:THR:HG23	1.94	0.66
3:F:13:ASP:O	3:F:16:VAL:HG22	1.95	0.66
2:D:102:LEU:CD1	2:D:290:ILE:HG23	2.25	0.66
1:B:439:HIS:HB3	3:F:161:VAL:HG21	1.78	0.66
2:D:187:ILE:O	2:D:191:GLN:HG3	1.95	0.66
2:D:261:ARG:HE	2:D:285:GLN:NE2	1.92	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:324:TRP:C	2:D:327:PRO:HD2	2.20	0.66
3:F:4:LEU:HD11	3:F:10:ASP:OD2	1.95	0.66
3:E:22:LEU:O	3:E:63:LYS:HE2	1.96	0.65
3:F:52:ASP:O	3:F:56:ILE:HD13	1.96	0.65
1:A:184:MET:HE3	1:A:184:MET:HA	1.78	0.65
2:C:333:ARG:HD3	9:C:520:HOH:O	1.96	0.65
3:E:120:PRO:O	3:E:121:PRO:C	2.36	0.65
2:C:200:LEU:HA	2:C:203:ILE:CD1	2.27	0.64
3:E:120:PRO:HD3	3:E:128:PHE:CG	2.32	0.64
1:A:76:GLU:HG3	1:B:76:GLU:HG3	1.77	0.64
3:E:98:MET:HE3	3:E:98:MET:O	1.97	0.64
1:B:33:GLN:NE2	1:B:132:GLU:H	1.96	0.63
1:B:216:LEU:HD23	1:B:220:VAL:HG23	1.80	0.63
3:E:41:THR:O	3:E:44:ARG:HD2	1.97	0.63
3:E:98:MET:HE2	3:E:138:ARG:CG	2.28	0.63
1:A:213:THR:O	1:A:217:ILE:HG12	1.98	0.63
1:B:398:PRO:HG3	1:B:507:TRP:CD1	2.34	0.63
2:C:360:VAL:O	2:C:364:ILE:HD13	1.98	0.63
1:A:439:HIS:HE1	1:A:454:GLU:OE1	1.82	0.62
1:A:406:MET:O	1:A:410:GLU:HG3	2.00	0.62
2:C:201:ALA:HA	2:C:207:PHE:HB3	1.81	0.62
1:B:78:GLN:NE2	1:B:150:GLN:HE21	1.93	0.61
1:B:179:PRO:HB3	1:B:469:ILE:HD13	1.82	0.61
1:A:268:ASN:ND2	1:A:327:GLU:H	1.97	0.61
1:B:302:VAL:HG13	1:B:376:TYR:HE2	1.64	0.61
3:F:19:ILE:HD12	3:F:20:ALA:N	2.15	0.61
1:B:227:ASN:HD21	1:B:295:LYS:H	1.47	0.61
1:B:439:HIS:HB3	3:F:161:VAL:CG2	2.31	0.61
1:B:108:ASN:HD21	1:B:175:ARG:HH11	1.47	0.61
2:D:153:LEU:C	2:D:153:LEU:HD12	2.27	0.60
2:D:90:LEU:HD13	2:D:303:LEU:HD13	1.83	0.60
1:A:401:GLY:HA2	1:A:515:LEU:HD21	1.84	0.60
1:B:108:ASN:HD21	1:B:175:ARG:HD3	1.67	0.59
2:D:102:LEU:HB2	2:D:104:ARG:HD2	1.83	0.59
3:E:165:HIS:HE1	3:E:167:GLN:HE21	1.48	0.59
1:A:467:GLN:NE2	2:C:71:ASP:H	1.98	0.59
3:E:165:HIS:HE1	3:E:167:GLN:NE2	2.00	0.59
1:B:403:ILE:HD13	1:B:515:LEU:HD13	1.85	0.59
3:E:4:LEU:HA	9:E:274:HOH:O	2.02	0.59
1:A:78:GLN:NE2	1:A:150:GLN:HE21	1.92	0.59
2:D:352:ILE:HD12	2:D:352:ILE:C	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:HD21	1:A:175:ARG:HE	1.49	0.58
1:A:101:GLU:CD	1:A:360:ARG:HD3	2.28	0.58
3:E:22:LEU:HD11	3:E:31:MET:SD	2.43	0.58
1:B:160:LYS:HE3	1:B:161:ASN:OD1	2.03	0.58
2:D:256:PHE:HA	2:D:332:LEU:HD21	1.85	0.58
3:F:151:PRO:HB2	3:F:153:GLU:OE1	2.02	0.58
2:C:146:ASN:ND2	2:C:197:ARG:HH21	2.01	0.58
2:D:111:LYS:O	2:D:115:GLU:HG3	2.02	0.58
2:C:105:TRP:O	2:C:108:PRO:HD2	2.04	0.58
1:B:439:HIS:HD2	3:F:163:VAL:HA	1.69	0.57
2:D:357:TYR:CE1	2:D:381:VAL:HG11	2.39	0.57
2:D:192:MET:HA	2:D:192:MET:HE2	1.87	0.57
2:C:333:ARG:HD2	9:C:609:HOH:O	2.03	0.57
2:D:323:LYS:HB2	3:F:78:ARG:HH11	1.69	0.57
3:E:57:GLU:O	3:E:61:GLU:HG3	2.02	0.57
1:B:206:LEU:HD23	1:B:271:LEU:HD13	1.87	0.57
2:D:61:ASP:OD1	3:F:7:HIS:HD2	1.87	0.57
3:E:98:MET:HE1	3:E:107:ALA:HB2	1.86	0.57
1:B:291:GLU:OE1	1:B:343:HIS:HE1	1.87	0.56
3:F:57:GLU:O	3:F:61:GLU:HG3	2.05	0.56
1:B:216:LEU:HA	1:B:308:TRP:CH2	2.41	0.56
2:D:176:ARG:HG3	2:D:176:ARG:HH11	1.70	0.56
2:D:201:ALA:HA	2:D:207:PHE:HB3	1.87	0.55
1:B:210:ALA:CA	1:B:247:MET:HE1	2.37	0.55
2:C:213:VAL:HB	2:C:214:PRO:HD3	1.89	0.55
2:D:313:ASN:HB3	2:D:317:MET:HE2	1.89	0.55
2:C:112:ASP:OD1	2:D:118:ARG:NH2	2.39	0.55
1:A:125:TRP:HE1	2:C:161:ASN:ND2	2.04	0.55
1:B:49:LYS:HD3	3:F:140:MET:HB3	1.89	0.55
2:C:261:ARG:HE	2:C:285:GLN:NE2	1.99	0.55
1:B:403:ILE:HD11	1:B:507:TRP:CZ3	2.42	0.54
1:A:140:GLN:O	1:A:144:GLU:HG2	2.07	0.54
1:B:33:GLN:HE21	1:B:33:GLN:HA	1.72	0.54
3:F:80:LYS:CE	3:F:84:GLY:HA2	2.34	0.54
1:B:212:PHE:O	1:B:215:PRO:HD2	2.08	0.54
2:C:318:ARG:NH2	9:C:586:HOH:O	2.40	0.54
3:E:4:LEU:HG	3:E:4:LEU:O	2.07	0.54
1:B:403:ILE:HD11	1:B:507:TRP:HZ3	1.73	0.53
2:D:47:THR:OG1	2:D:50:GLU:HG3	2.08	0.53
1:A:24:ASN:OD1	1:A:26:GLN:HG2	2.08	0.53
1:A:398:PRO:HG3	1:A:507:TRP:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:MET:HE1	1:B:200:CYS:SG	2.48	0.53
2:D:324:TRP:O	2:D:327:PRO:HD2	2.08	0.53
1:A:147:HIS:CE1	9:A:1850:HOH:O	2.60	0.53
2:C:107:ALA:HB3	2:C:108:PRO:HD3	1.90	0.53
2:C:118:ARG:NH2	2:D:112:ASP:OD1	2.39	0.53
2:C:209:GLU:HG2	9:C:576:HOH:O	2.09	0.53
1:B:403:ILE:HD13	1:B:515:LEU:CD1	2.38	0.53
2:C:363:TRP:CE3	2:C:364:ILE:HD12	2.43	0.53
3:F:19:ILE:HD12	3:F:19:ILE:C	2.33	0.53
2:C:42:ARG:HB2	2:C:99:ARG:HG3	1.90	0.53
1:B:184:MET:HE2	1:B:188:PHE:HB2	1.90	0.52
2:C:235:TRP:CD1	2:C:235:TRP:C	2.88	0.52
2:D:376:ASP:OD2	2:D:379:GLN:HG2	2.09	0.52
3:E:120:PRO:HD3	3:E:128:PHE:CD2	2.45	0.52
3:F:91:LEU:O	3:F:95:VAL:HG23	2.09	0.52
2:D:245:ALA:HB3	2:D:299:TYR:OH	2.09	0.52
2:D:329:ILE:CD1	2:D:380:ILE:HG23	2.39	0.52
3:E:165:HIS:CE1	3:E:167:GLN:HE21	2.27	0.52
1:A:108:ASN:HD21	1:A:175:ARG:NE	2.08	0.52
1:B:268:ASN:ND2	1:B:327:GLU:H	2.04	0.52
2:D:98:HIS:HD2	2:D:297:ASP:OD1	1.92	0.52
1:A:223:TRP:CE2	1:A:298:VAL:HB	2.45	0.52
2:D:143:GLU:O	2:D:147:ARG:HB3	2.10	0.52
1:A:260:ASP:OD2	1:A:262:ALA:HB3	2.09	0.51
1:B:206:LEU:HD11	1:B:321:LEU:HD11	1.92	0.51
2:C:140:TRP:NE1	2:C:145:ILE:HD11	2.24	0.51
2:D:179:LEU:HD23	2:D:182:TRP:CE3	2.46	0.51
1:A:186:ARG:HA	2:C:73:THR:OG1	2.10	0.51
1:B:210:ALA:N	1:B:247:MET:HE1	2.25	0.51
1:B:213:THR:O	1:B:217:ILE:HG12	2.10	0.51
1:B:460:GLU:N	1:B:461:PRO:HD3	2.26	0.51
3:F:61:GLU:O	3:F:121:PRO:HG2	2.10	0.51
1:A:289:LEU:HD23	1:A:289:LEU:C	2.36	0.51
1:A:413:HIS:HD2	1:A:428:SER:OG	1.92	0.51
3:E:98:MET:HE2	3:E:138:ARG:HG2	1.91	0.51
2:C:153:LEU:C	2:C:153:LEU:HD12	2.35	0.51
2:C:211:THR:C	2:C:214:PRO:HD2	2.36	0.51
2:D:235:TRP:CD1	2:D:235:TRP:C	2.89	0.51
3:E:36:ARG:CZ	3:E:119:LYS:HB3	2.41	0.51
2:C:314:ARG:O	2:C:318:ARG:HB2	2.11	0.51
1:B:186:ARG:HA	2:D:73:THR:OG1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HA	1:B:308:TRP:HH2	1.76	0.51
3:E:24:THR:HG23	9:E:190:HOH:O	2.11	0.51
3:F:44:ARG:HD3	3:F:47:TYR:CZ	2.46	0.51
1:B:196:ASP:HB2	3:F:140:MET:SD	2.51	0.51
1:A:18:ARG:O	2:C:129:ALA:HA	2.11	0.51
1:A:110:LEU:O	1:A:110:LEU:HD23	2.11	0.51
1:A:72:ALA:O	1:A:76:GLU:OE1	2.29	0.50
1:A:461:PRO:HG2	3:E:159:ARG:CZ	2.41	0.50
1:B:125:TRP:HE1	2:D:161:ASN:ND2	2.09	0.50
3:E:41:THR:O	3:E:44:ARG:CD	2.59	0.50
2:C:111:LYS:O	2:C:115:GLU:HG3	2.11	0.50
1:B:186:ARG:HD3	1:B:186:ARG:C	2.37	0.50
2:C:200:LEU:HA	2:C:203:ILE:HD11	1.92	0.50
1:B:302:VAL:HG13	1:B:376:TYR:CE2	2.46	0.50
1:B:405:LEU:HD12	1:B:406:MET:N	2.27	0.50
1:B:461:PRO:HG2	3:F:159:ARG:CZ	2.42	0.50
1:A:286:LEU:O	1:A:289:LEU:HB3	2.12	0.50
1:A:106:VAL:HG22	6:A:1628:5BR:H22	1.93	0.50
1:B:484:GLU:OE1	3:F:6:ILE:HB	2.11	0.50
3:E:58:ALA:O	3:E:62:GLU:HG3	2.11	0.50
1:A:123:MET:HB2	2:C:168:ARG:HD3	1.94	0.50
1:A:231:ILE:HD12	1:A:231:ILE:N	2.27	0.50
1:B:119:ALA:HB1	2:D:168:ARG:HD2	1.93	0.50
1:B:281:TYR:O	1:B:284:PRO:HD2	2.12	0.50
1:A:108:ASN:ND2	1:A:175:ARG:HH21	2.09	0.49
2:D:323:LYS:HB2	3:F:78:ARG:NH1	2.27	0.49
3:F:44:ARG:HG3	3:F:46:SER:O	2.12	0.49
3:F:12:ARG:HG2	3:F:56:ILE:HD11	1.92	0.49
1:A:382:HIS:O	1:A:386:ILE:HG13	2.11	0.49
1:A:180:LEU:HD13	9:A:1803:HOH:O	2.11	0.49
1:A:204:LEU:O	1:A:209:GLU:HG3	2.12	0.49
1:B:302:VAL:CG1	1:B:376:TYR:HE2	2.25	0.49
3:E:98:MET:HE1	3:E:107:ALA:HB1	1.94	0.49
1:B:313:TRP:HA	1:B:317:TRP:HB3	1.94	0.49
1:A:81:SER:OG	1:B:84:ASP:HB3	2.11	0.49
2:C:161:ASN:HB3	2:C:235:TRP:CE2	2.47	0.49
1:A:84:ASP:HB3	1:B:81:SER:OG	2.13	0.49
1:A:318:ILE:HD13	1:A:318:ILE:C	2.37	0.49
1:A:352:ALA:O	1:A:405:LEU:HD12	2.13	0.49
9:B:2164:HOH:O	2:D:187:ILE:HD12	2.11	0.49
2:C:16:MET:O	2:C:20:ILE:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:54:VAL:O	2:C:55:TYR:HB2	2.12	0.49
1:B:438:VAL:HB	3:F:164:VAL:HG22	1.95	0.49
2:D:54:VAL:O	2:D:55:TYR:HB2	2.13	0.49
3:E:120:PRO:C	3:E:122:ILE:N	2.68	0.49
1:A:114:GLU:CD	1:A:147:HIS:HB3	2.38	0.48
3:F:36:ARG:NH1	3:F:119:LYS:HB3	2.27	0.48
1:A:177:ILE:HG12	1:A:485:LEU:HB2	1.95	0.48
1:B:344:HIS:HE1	1:B:376:TYR:CD2	2.30	0.48
1:A:302:VAL:HG22	1:A:376:TYR:OH	2.14	0.48
3:F:19:ILE:HG21	3:F:60:LEU:HD12	1.96	0.48
1:A:211:CYS:HB2	1:A:313:TRP:CD1	2.48	0.48
1:A:227:ASN:HD21	1:A:295:LYS:H	1.60	0.48
1:A:302:VAL:HG22	1:A:376:TYR:CZ	2.49	0.48
1:B:209:GLU:C	1:B:247:MET:HE1	2.39	0.48
9:D:500:HOH:O	3:F:125:VAL:HG22	2.13	0.48
3:F:12:ARG:O	3:F:16:VAL:HG13	2.14	0.48
1:A:495:LEU:HD11	1:A:512:ILE:HG13	1.94	0.47
1:B:180:LEU:HD13	7:B:1266:BMM:C1	2.44	0.47
1:B:18:ARG:O	2:D:129:ALA:HA	2.14	0.47
3:E:40:THR:C	3:E:41:THR:HG23	2.39	0.47
3:E:118:TYR:O	3:E:119:LYS:C	2.56	0.47
1:A:521:ASN:OD1	1:A:523:VAL:HG12	2.14	0.47
1:A:125:TRP:HE1	2:C:161:ASN:HD22	1.63	0.47
2:D:161:ASN:HB3	2:D:235:TRP:CE2	2.49	0.47
3:F:95:VAL:HG12	3:F:99:ASN:ND2	2.29	0.47
2:D:377:ARG:O	2:D:381:VAL:HG23	2.15	0.47
1:B:146:ARG:HB2	2:D:106:HIS:CE1	2.49	0.47
1:B:257:ILE:C	1:B:257:ILE:HD12	2.40	0.47
1:B:354:TRP:CG	1:B:355:PRO:HD3	2.50	0.47
3:F:125:VAL:HG23	3:F:126:ASN:N	2.28	0.47
1:A:76:GLU:OE2	1:B:76:GLU:OE2	2.33	0.47
1:B:211:CYS:HB2	1:B:313:TRP:CD1	2.50	0.47
1:B:344:HIS:HE1	1:B:376:TYR:CE2	2.33	0.47
2:D:105:TRP:O	2:D:108:PRO:HD2	2.14	0.47
3:E:22:LEU:HD21	3:E:31:MET:CE	2.44	0.47
1:A:186:ARG:HD3	1:A:186:ARG:C	2.39	0.47
2:D:348:ASP:OD2	2:D:350:GLU:HB2	2.15	0.47
1:B:281:TYR:CZ	1:B:285:VAL:HG21	2.50	0.47
2:C:179:LEU:HD22	2:C:182:TRP:CZ3	2.50	0.47
1:A:365:ASP:OD2	1:A:368:GLU:HG3	2.15	0.46
1:B:116:ASN:CG	1:B:189:SER:HA	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:MET:HE3	1:B:187:VAL:CG2	2.45	0.46
2:C:143:GLU:O	2:C:147:ARG:HB3	2.15	0.46
2:D:336:MET:CE	2:D:356:LEU:HD11	2.45	0.46
1:A:251:TYR:CD2	1:A:321:LEU:HD21	2.49	0.46
2:C:211:THR:O	2:C:214:PRO:HD2	2.15	0.46
2:D:277:THR:HB	2:D:278:PRO:HD3	1.98	0.46
1:A:108:ASN:HD21	1:A:175:ARG:HH21	1.61	0.46
1:B:206:LEU:HD11	1:B:321:LEU:CD1	2.46	0.46
1:A:403:ILE:HD11	1:A:517:CYS:SG	2.55	0.46
1:B:134:LYS:HD3	2:D:161:ASN:HD21	1.81	0.46
2:D:298:LEU:O	2:D:302:CYS:HB2	2.15	0.46
1:A:49:LYS:HD3	3:E:144:ASN:HD22	1.81	0.46
1:B:140:GLN:O	1:B:144:GLU:HG2	2.16	0.46
1:B:184:MET:HE2	1:B:188:PHE:CG	2.50	0.46
1:B:216:LEU:HD23	1:B:216:LEU:C	2.41	0.46
3:E:3:LYS:HG2	3:E:9:ASN:HA	1.98	0.46
3:E:120:PRO:O	3:E:122:ILE:N	2.49	0.46
1:A:115:TYR:OH	2:C:173:ASP:HA	2.16	0.46
1:B:115:TYR:OH	2:D:173:ASP:HA	2.16	0.46
2:C:203:ILE:HD13	2:C:203:ILE:H	1.81	0.46
2:D:145:ILE:O	2:D:149:TRP:HB3	2.16	0.46
1:A:149:HIS:CE1	2:C:105:TRP:HB2	2.51	0.46
1:B:459:ALA:C	1:B:461:PRO:HD3	2.41	0.46
2:C:86:GLU:HB2	3:E:120:PRO:HG2	1.97	0.46
1:A:232:THR:HB	1:A:233:PRO:HD3	1.98	0.45
1:B:402:PHE:O	1:B:403:ILE:HD12	2.16	0.45
3:F:23:ASN:N	3:F:23:ASN:HD22	2.14	0.45
1:A:171:ALA:O	1:A:175:ARG:HB3	2.16	0.45
1:A:467:GLN:HE21	1:A:467:GLN:N	2.04	0.45
2:D:63:ILE:O	2:D:64:ALA:C	2.57	0.45
2:D:80:ARG:HG2	2:D:86:GLU:OE1	2.17	0.45
1:B:125:TRP:HE1	2:D:161:ASN:HD22	1.64	0.45
2:D:156:GLU:HA	2:D:156:GLU:OE2	2.17	0.45
3:F:4:LEU:HD21	3:F:10:ASP:H	1.82	0.45
1:A:24:ASN:OD1	1:A:26:GLN:CG	2.65	0.45
1:A:219:ALA:O	1:A:223:TRP:HD1	1.99	0.45
3:F:40:THR:O	3:F:41:THR:OG1	2.33	0.45
3:F:74:GLU:O	3:F:78:ARG:HG3	2.17	0.45
1:B:79:PHE:O	1:B:83:GLN:HG3	2.15	0.45
1:B:310:TYR:CE1	1:B:336:LYS:HD2	2.52	0.45
2:D:185:ASP:O	2:D:189:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:95:VAL:HG12	3:F:99:ASN:HD21	1.82	0.45
2:C:140:TRP:HE1	2:C:145:ILE:HD11	1.82	0.45
1:A:403:ILE:CD1	1:A:405:LEU:HD13	2.36	0.45
2:D:8:ARG:NH2	2:D:15:GLU:HB3	2.32	0.45
2:D:169:GLU:O	2:D:170:ALA:C	2.58	0.45
1:B:43:ARG:HD2	1:B:43:ARG:C	2.42	0.45
1:B:123:MET:SD	2:D:168:ARG:NH1	2.90	0.45
1:A:108:ASN:HD21	1:A:175:ARG:NH2	2.16	0.44
2:C:98:HIS:HE1	2:C:178:SER:OG	2.00	0.44
2:C:153:LEU:HA	2:C:193:ILE:HD12	1.98	0.44
1:B:144:GLU:OE2	1:B:144:GLU:HA	2.17	0.44
2:C:192:MET:HE2	2:C:192:MET:HA	1.99	0.44
1:A:21:THR:HG22	1:A:22:SER:N	2.32	0.44
1:A:284:PRO:HB3	1:A:342:ALA:HB1	1.99	0.44
1:B:466:CYS:HB2	2:D:73:THR:HA	1.99	0.44
3:F:40:THR:HG22	3:F:53:TYR:CE1	2.52	0.44
2:D:153:LEU:HA	2:D:193:ILE:HD12	1.99	0.44
1:B:403:ILE:HG22	1:B:405:LEU:HG	2.00	0.44
1:A:170:ASP:HA	2:C:38:PHE:HE2	1.82	0.44
2:C:269:ALA:N	2:C:270:PRO:CD	2.81	0.44
2:C:363:TRP:HE3	2:C:364:ILE:HD12	1.82	0.44
1:A:179:PRO:HB3	1:A:469:ILE:HD13	2.00	0.44
1:B:105:VAL:O	1:B:109:PHE:HB2	2.18	0.44
3:F:23:ASN:HD22	3:F:23:ASN:C	2.24	0.44
1:A:121:THR:HG21	1:A:140:GLN:CG	2.48	0.44
1:A:185:LYS:O	1:A:189:SER:HB2	2.18	0.44
1:B:193:ILE:HD11	2:D:82:SER:HB3	2.00	0.44
2:C:86:GLU:O	3:E:120:PRO:HG2	2.17	0.44
1:A:281:TYR:CZ	1:A:285:VAL:HG21	2.53	0.44
1:B:159:ALA:O	2:D:33:ASN:HB2	2.18	0.44
3:E:12:ARG:O	3:E:16:VAL:HG23	2.18	0.44
1:A:61:LYS:NZ	9:A:1831:HOH:O	2.50	0.43
1:B:193:ILE:HB	2:D:168:ARG:CZ	2.48	0.43
1:B:227:ASN:ND2	1:B:295:LYS:H	2.16	0.43
1:B:483:ALA:HB2	1:B:509:LEU:HD21	1.99	0.43
1:B:21:THR:HG22	1:B:22:SER:N	2.34	0.43
1:B:186:ARG:HD3	1:B:186:ARG:O	2.18	0.43
1:B:439:HIS:HE1	1:B:454:GLU:OE1	2.01	0.43
1:A:93:VAL:HG11	2:D:3:MET:HG2	2.00	0.43
3:E:154:GLU:O	3:E:158:GLN:HG3	2.18	0.43
1:A:175:ARG:HG3	1:A:181:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:ALA:HB3	2:D:270:PRO:HD3	2.00	0.43
3:E:44:ARG:NH2	3:E:50:ASP:OD1	2.52	0.43
1:B:110:LEU:O	1:B:114:GLU:HG2	2.19	0.43
1:B:397:ASP:HA	1:B:398:PRO:HD3	1.89	0.43
3:E:108:GLU:CD	9:E:275:HOH:O	2.61	0.43
1:A:302:VAL:HG13	1:A:376:TYR:HE2	1.83	0.43
1:A:397:ASP:HA	1:A:398:PRO:HD3	1.82	0.43
3:F:132:GLU:HG3	9:F:900:HOH:O	2.18	0.43
1:A:352:ALA:O	1:A:405:LEU:CD1	2.67	0.43
1:B:49:LYS:HD3	3:F:144:ASN:HD22	1.84	0.43
3:F:55:TRP:CZ2	3:F:59:LYS:HE2	2.54	0.43
2:C:269:ALA:HB3	2:C:270:PRO:HD3	2.01	0.43
2:D:77:HIS:HB3	3:F:139:LEU:HD23	2.01	0.43
3:F:152:LEU:O	3:F:156:ARG:HG3	2.18	0.43
1:A:96:HIS:HB2	2:C:20:ILE:HD12	2.00	0.43
1:B:138:LEU:HD22	2:D:160:PHE:CZ	2.54	0.43
1:B:230:GLU:C	1:B:233:PRO:HD2	2.44	0.43
2:D:263:GLU:OE2	2:D:263:GLU:HA	2.17	0.43
3:E:4:LEU:O	3:E:4:LEU:CG	2.67	0.43
1:A:246:HIS:CD2	1:A:246:HIS:N	2.87	0.42
1:B:420:VAL:HG21	1:B:453:GLY:O	2.19	0.42
3:E:22:LEU:HB3	3:E:28:ALA:HB2	2.00	0.42
3:F:38:ASP:OD1	3:F:45:ASN:OD1	2.37	0.42
1:A:230:GLU:C	1:A:233:PRO:HD2	2.44	0.42
2:C:364:ILE:HA	2:C:368:ALA:HB3	2.01	0.42
1:A:159:ALA:O	2:C:33:ASN:HB2	2.19	0.42
1:B:403:ILE:HD12	1:B:403:ILE:N	2.32	0.42
3:F:61:GLU:HB3	3:F:121:PRO:HD3	2.01	0.42
1:A:110:LEU:CD2	1:A:114:GLU:OE2	2.67	0.42
1:B:246:HIS:CD2	1:B:246:HIS:N	2.87	0.42
2:C:146:ASN:HD21	2:C:197:ARG:NH2	2.14	0.42
2:D:144:PHE:CE2	2:D:342:LEU:HD23	2.54	0.42
2:D:269:ALA:N	2:D:270:PRO:CD	2.83	0.42
3:F:23:ASN:N	3:F:23:ASN:ND2	2.67	0.42
1:A:459:ALA:C	1:A:461:PRO:HD3	2.45	0.42
1:B:38:ASP:O	1:B:39:PHE:HB3	2.20	0.42
2:D:76:PHE:HZ	2:D:168:ARG:HH12	1.65	0.42
1:A:43:ARG:C	1:A:43:ARG:HD2	2.44	0.42
1:A:175:ARG:HG2	1:A:176:THR:N	2.31	0.42
1:B:406:MET:O	1:B:410:GLU:HG3	2.19	0.42
1:B:476:ARG:HG3	1:B:476:ARG:HH11	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASN:ND2	1:A:175:ARG:HE	2.17	0.42
2:C:78:GLY:O	3:E:115:ARG:HD3	2.19	0.42
3:F:153:GLU:CD	3:F:153:GLU:N	2.72	0.42
1:B:49:LYS:CE	3:F:144:ASN:HD22	2.32	0.42
2:D:250:ALA:HA	2:D:367:TYR:CD2	2.55	0.42
1:A:354:TRP:CG	1:A:355:PRO:HD3	2.55	0.42
1:B:108:ASN:ND2	1:B:175:ARG:HH11	2.13	0.42
1:B:39:PHE:O	1:B:40:LYS:C	2.63	0.42
2:C:270:PRO:HB3	2:D:270:PRO:HB3	2.00	0.42
1:A:243:GLU:O	1:A:247:MET:HG2	2.20	0.41
1:B:462:GLU:HG3	3:F:112:ILE:HD11	2.01	0.41
3:F:23:ASN:HD22	3:F:23:ASN:H	1.66	0.41
1:B:232:THR:HB	1:B:233:PRO:HD3	2.02	0.41
2:D:140:TRP:HB2	2:D:272:PHE:CD2	2.55	0.41
3:F:90:VAL:HG11	3:F:118:TYR:CE2	2.55	0.41
1:A:79:PHE:O	1:A:83:GLN:HG3	2.19	0.41
1:A:160:LYS:HA	2:C:33:ASN:HB2	2.02	0.41
1:B:48:THR:O	3:F:137:THR:HG23	2.21	0.41
1:B:125:TRP:CE2	2:D:164:SER:HB3	2.56	0.41
1:A:96:HIS:HB2	2:C:20:ILE:CD1	2.50	0.41
1:A:466:CYS:HB2	2:C:73:THR:HA	2.02	0.41
2:D:93:VAL:O	2:D:93:VAL:HG12	2.19	0.41
2:D:189:ILE:HD11	2:D:287:TYR:CD1	2.55	0.41
1:A:260:ASP:OD1	1:A:261:PRO:HD2	2.21	0.41
1:A:110:LEU:HD23	1:A:110:LEU:C	2.45	0.41
1:B:330:ARG:NH1	3:F:148:TYR:HB2	2.36	0.41
2:D:352:ILE:HD12	2:D:353:THR:CA	2.50	0.41
2:D:354:ALA:O	2:D:358:ARG:HG3	2.21	0.41
3:F:86:ASP:O	3:F:87:ALA:C	2.63	0.41
1:B:125:TRP:CD1	1:B:125:TRP:C	2.99	0.41
2:C:146:ASN:HB2	2:C:207:PHE:CZ	2.55	0.41
2:C:239:PHE:HB2	3:E:126:ASN:HA	2.03	0.41
2:D:228:ARG:O	2:D:232:GLU:HG3	2.21	0.41
1:A:289:LEU:C	1:A:289:LEU:CD2	2.93	0.41
1:A:302:VAL:HG13	9:A:1763:HOH:O	2.20	0.41
1:B:198:VAL:O	1:B:202:LEU:HG	2.21	0.41
1:B:490:SER:OG	2:D:32:ASN:HB2	2.21	0.41
2:D:71:ASP:HB2	3:F:54:LEU:HD11	2.03	0.41
2:D:349:LYS:O	2:D:352:ILE:HG13	2.20	0.41
2:D:352:ILE:CD1	2:D:353:THR:N	2.75	0.41
1:A:90:ASN:HD22	1:A:90:ASN:HA	1.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE2	1:A:188:PHE:HB2	2.02	0.40
1:B:108:ASN:HD21	1:B:175:ARG:CD	2.33	0.40
1:B:297:LYS:NZ	1:B:368:GLU:OE2	2.54	0.40
2:C:90:LEU:HD13	2:C:303:LEU:HD13	2.03	0.40
3:F:76:ASP:C	3:F:78:ARG:N	2.77	0.40
1:B:165:PRO:HG3	9:B:2146:HOH:O	2.21	0.40
1:B:405:LEU:HD12	1:B:405:LEU:C	2.46	0.40
2:D:203:ILE:HG13	2:D:204:VAL:HG23	2.02	0.40
1:B:109:PHE:O	1:B:112:VAL:HG12	2.22	0.40
2:D:240:ASP:HB2	3:F:125:VAL:CG2	2.51	0.40
3:F:67:LEU:HD23	3:F:70:ARG:HH21	1.87	0.40
1:A:423:VAL:HA	1:A:424:PRO:HD3	1.94	0.40
1:A:495:LEU:HD11	1:A:512:ILE:CG1	2.52	0.40
1:B:291:GLU:OE1	1:B:343:HIS:CE1	2.72	0.40
2:D:189:ILE:HD11	2:D:284:ALA:HA	2.03	0.40
2:D:275:ASN:C	2:D:278:PRO:HD2	2.47	0.40
2:D:63:ILE:HD11	2:D:84:GLY:HA2	2.04	0.40
2:D:98:HIS:CD2	2:D:99:ARG:N	2.89	0.40
2:D:145:ILE:HD11	2:D:274:ASP:OD2	2.21	0.40
2:D:332:LEU:HB3	2:D:384:VAL:CG1	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/527 (97%)	482 (95%)	27 (5%)	0	100	100
1	B	508/527 (96%)	479 (94%)	26 (5%)	3 (1%)	21	17
2	C	386/389 (99%)	374 (97%)	10 (3%)	2 (0%)	24	21
2	D	385/389 (99%)	364 (94%)	19 (5%)	2 (0%)	24	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	164/170 (96%)	161 (98%)	2 (1%)	1 (1%)	21	17
3	F	164/170 (96%)	154 (94%)	7 (4%)	3 (2%)	6	3
All	All	2116/2172 (97%)	2014 (95%)	91 (4%)	11 (0%)	24	21

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	LYS
3	E	120	PRO
1	B	311	GLU
2	D	205	PRO
3	F	122	ILE
2	C	64	ALA
2	D	64	ALA
3	F	6	ILE
2	C	251	VAL
1	B	284	PRO
3	F	5	GLY

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	425/442 (96%)	412 (97%)	13 (3%)	35	37
1	B	422/442 (96%)	413 (98%)	9 (2%)	47	52
2	C	315/323 (98%)	308 (98%)	7 (2%)	45	50
2	D	311/323 (96%)	307 (99%)	4 (1%)	61	68
3	E	143/147 (97%)	140 (98%)	3 (2%)	47	52
3	F	142/147 (97%)	137 (96%)	5 (4%)	32	32
All	All	1758/1824 (96%)	1717 (98%)	41 (2%)	44	49

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	76	GLU
1	A	90	ASN
1	A	112	VAL
1	A	125	TRP
1	A	175	ARG
1	A	279	GLN
1	A	289	LEU
1	A	302	VAL
1	A	310	TYR
1	A	318	ILE
1	A	391	ARG
1	A	467	GLN
1	B	30	ARG
1	B	90	ASN
1	B	110	LEU
1	B	125	TRP
1	B	216	LEU
1	B	247	MET
1	B	279	GLN
1	B	310	TYR
1	B	311	GLU
2	C	33	ASN
2	C	153	LEU
2	C	173	ASP
2	C	179	LEU
2	C	203	ILE
2	C	356	LEU
2	C	377	ARG
2	D	4	LEU
2	D	153	LEU
2	D	173	ASP
2	D	205	PRO
3	E	24	THR
3	E	44	ARG
3	E	120	PRO
3	F	11	THR
3	F	23	ASN
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 (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	41	ASN
1	A	78	GLN
1	A	90	ASN
1	A	100	ASN
1	A	108	ASN
1	A	155	ASN
1	A	161	ASN
1	A	168	HIS
1	A	203	ASN
1	A	268	ASN
1	A	273	ASN
1	A	279	GLN
1	A	344	HIS
1	A	375	ASN
1	A	382	HIS
1	A	411	ASN
1	A	413	HIS
1	A	439	HIS
1	A	442	ASN
1	A	467	GLN
1	A	472	GLN
1	A	486	HIS
1	A	516	ASN
1	B	33	GLN
1	B	42	ASN
1	B	78	GLN
1	B	90	ASN
1	B	108	ASN
1	B	155	ASN
1	B	168	HIS
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

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Mol	Chain	Res	Type
1	B	439	HIS
1	B	451	GLN
1	B	486	HIS
1	B	516	ASN
1	B	527	ASN
2	C	33	ASN
2	C	98	HIS
2	C	146	ASN
2	C	155	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	23	ASN
3	E	45	ASN
3	E	144	ASN
3	E	158	GLN
3	E	165	HIS
3	E	167	GLN
3	F	7	HIS
3	F	23	ASN
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

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z > 2$
8	FMT	B	2064	-	2,2,2	5.31	2 (100%)	1,1,1	1.47	0
6	5BR	A	1628	-	5,5,5	0.50	0	4,4,4	0.54	0
7	BMM	B	1266	-	0,1,1	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	5BR	A	1628	-	-	1/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	2064	FMT	O1-C	5.53	1.52	1.22
8	B	2064	FMT	O2-C	5.09	1.54	1.28

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1628	5BR	C1-C2-C3-C4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1628	5BR	1	0
7	B	1266	BMM	1	0

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	511/527 (96%)	0.11	14 (2%) 56 55	22, 33, 54, 66	0
1	B	510/527 (96%)	0.12	11 (2%) 62 61	22, 34, 53, 68	0
2	C	388/389 (99%)	-0.40	0 100 100	19, 26, 42, 56	0
2	D	387/389 (99%)	0.78	43 (11%) 10 9	24, 42, 65, 76	0
3	E	166/170 (97%)	0.05	8 (4%) 35 34	21, 31, 45, 61	0
3	F	166/170 (97%)	1.63	47 (28%) 1 1	40, 54, 71, 80	0
All	All	2128/2172 (97%)	0.26	123 (5%) 29 27	19, 34, 60, 80	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	120	PRO	7.5
2	D	380	ILE	5.2
2	D	352	ILE	4.9
2	D	385	LEU	4.7
3	F	4	LEU	4.7
2	D	375	ALA	4.2
3	F	19	ILE	4.1
3	F	82	ALA	4.1
2	D	388	LEU	4.0
3	F	83	PHE	3.7
3	E	121	PRO	3.6
2	D	332	LEU	3.4
3	F	161	VAL	3.4
1	B	308	TRP	3.4
2	D	384	VAL	3.4
3	F	56	ILE	3.4
3	F	67	LEU	3.1
3	F	77	PHE	3.1
2	D	386	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
3	F	20	ALA	3.0
3	F	75	VAL	3.0
2	D	372	ASP	3.0
3	F	117	ALA	3.0
3	E	168	SER	3.0
1	A	318	ILE	3.0
3	F	128	PHE	3.0
2	D	331	ALA	3.0
3	F	70	ARG	3.0
1	A	302	VAL	3.0
3	E	23	ASN	2.9
3	F	16	VAL	2.9
3	F	118	TYR	2.9
2	D	368	ALA	2.9
3	F	25	LEU	2.9
1	A	289	LEU	2.8
1	A	213	THR	2.8
3	F	120	PRO	2.8
3	F	127	TYR	2.8
3	F	60	LEU	2.8
2	D	387	GLY	2.8
3	F	24	THR	2.8
2	D	363	TRP	2.8
3	F	22	LEU	2.8
3	F	71	ALA	2.7
1	B	216	LEU	2.7
2	D	373	PHE	2.7
3	E	22	LEU	2.7
1	A	17	ASN	2.7
1	B	317	TRP	2.7
3	F	84	GLY	2.7
1	B	309	VAL	2.7
3	F	122	ILE	2.7
1	A	317	TRP	2.7
1	A	310	TYR	2.6
2	D	381	VAL	2.6
1	A	371	TRP	2.6
3	F	69	ALA	2.6
2	D	357	TYR	2.6
2	D	347	THR	2.6
2	D	339	PHE	2.5
3	E	4	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	320	TRP	2.5
2	D	371	ILE	2.5
3	F	5	GLY	2.5
3	F	114	PHE	2.5
2	D	374	LYS	2.5
3	F	66	VAL	2.4
1	B	441	TYR	2.4
3	E	167	GLN	2.4
2	D	251	VAL	2.4
1	A	206	LEU	2.4
2	D	356	LEU	2.4
2	D	266	GLN	2.4
3	F	72	PHE	2.4
3	F	29	ALA	2.3
3	F	64	VAL	2.3
3	F	147	TYR	2.3
1	A	54	ASN	2.3
2	D	316	VAL	2.3
3	F	21	GLN	2.3
1	A	216	LEU	2.3
3	F	63	LYS	2.3
3	F	112	ILE	2.3
3	F	164	VAL	2.3
3	F	79	HIS	2.2
2	D	346	THR	2.2
2	D	179	LEU	2.2
1	B	256	SER	2.2
1	A	296	PHE	2.2
1	A	405	LEU	2.2
3	F	15	TRP	2.2
1	B	316	ILE	2.2
2	D	139	THR	2.2
2	D	335	PHE	2.2
3	F	169	PRO	2.2
2	D	330	ALA	2.2
1	A	316	ILE	2.1
2	D	250	ALA	2.1
2	D	303	LEU	2.1
1	B	310	TYR	2.1
2	D	206	GLY	2.1
3	F	39	HIS	2.1
2	D	370	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	3	LYS	2.1
2	D	350	GLU	2.1
3	F	73	ASN	2.1
3	F	160	GLY	2.1
1	B	39	PHE	2.1
2	D	22	LYS	2.1
3	F	68	LYS	2.1
2	D	383	ALA	2.1
2	D	90	LEU	2.1
2	D	229	LEU	2.1
1	B	259	ASN	2.1
3	F	125	VAL	2.1
2	D	379	GLN	2.0
2	D	270	PRO	2.0
2	D	327	PRO	2.0
3	F	93	GLY	2.0
2	D	63	ILE	2.0
3	F	65	ALA	2.0
3	F	96	ALA	2.0
1	B	213	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	5BR	A	1628	6/6	0.88	0.29	73,73,73,73	0
8	FMT	B	2064	3/3	0.88	0.12	30,30,35,35	0
7	BMM	B	1266	2/2	0.95	0.17	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	BR	B	1701	1/1	0.97	0.10	63,63,63,63	0
5	BR	A	1028	1/1	0.97	0.14	81,81,81,81	0
4	FE	B	1328	1/1	0.99	0.02	38,38,38,38	0
4	FE	A	1330	1/1	0.99	0.02	28,28,28,28	0
4	FE	A	935	1/1	0.99	0.02	39,39,39,39	0
4	FE	B	1327	1/1	1.00	0.01	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.