



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:57 AM UTC

PDB ID : 1ON9 / pdb_00001on9
Title : Transcarboxylase 12S crystal structure: hexamer assembly and substrate binding to a multienzyme core (with hydrolyzed methylmalonyl-coenzyme a bound)
Authors : Hall, P.R.; Wang, Y.-F.; Rivera-Hainaj, R.E.; Zheng, X.; Pustai-Carey, M.; Carey, P.R.; Yee, V.C.
Deposited on : 2003-02-27
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 : ?? (???), CSD ??CSD?? (???)
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

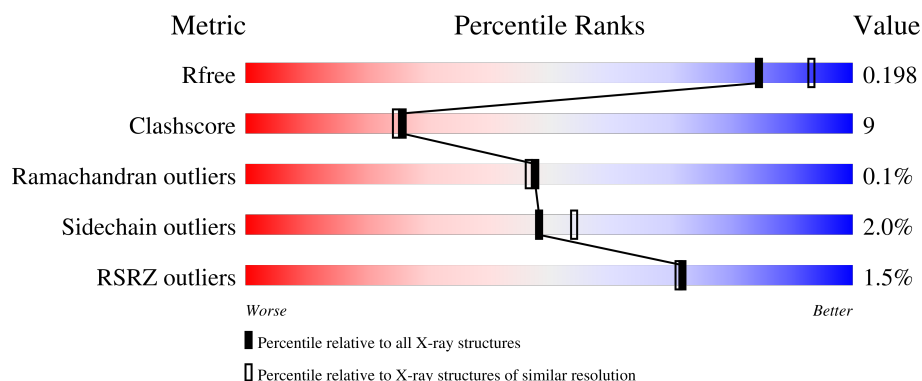
1 Overall quality at a glance

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	523	0% 78% 19% ..
1	B	523	81% 15% ..
1	C	523	3% 80% 17% ..
1	D	523	3% 75% 20% ..
1	E	523	81% 17% ..

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Mol	Chain	Length	Quality of chain
1	F	523	% 78% 19% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26869 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.

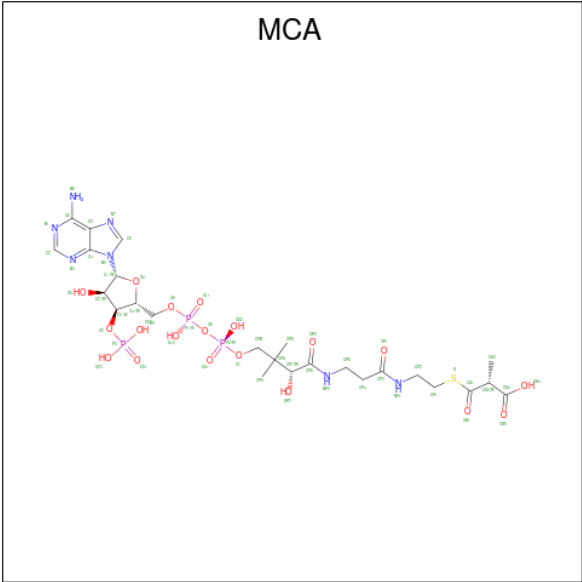
- Molecule 1 is a protein called Methylmalonyl-CoA carboxyltransferase 12S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			3900	2448	679	754	19			
1	B	516	Total	C	N	O	S	0	0	0
			3900	2448	679	754	19			
1	C	514	Total	C	N	O	S	0	0	0
			3878	2433	674	752	19			
1	D	504	Total	C	N	O	S	0	0	0
			3805	2394	660	732	19			
1	E	519	Total	C	N	O	S	0	0	0
			3925	2464	684	758	19			
1	F	516	Total	C	N	O	S	0	0	0
			3900	2448	679	754	19			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		
2	B	1	Total	Cd	0	0
			1	1		
2	C	1	Total	Cd	0	0
			1	1		

- Molecule 3 is METHYLMALONYL-COENZYME A (CCD ID: MCA) (formula: C₂₅H₄₀N₇O₁₉P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
3	C	1	Total	C	N	O	P	0	0
			26	10	5	9	2		
3	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	C	O	0	0
			8	6	2		

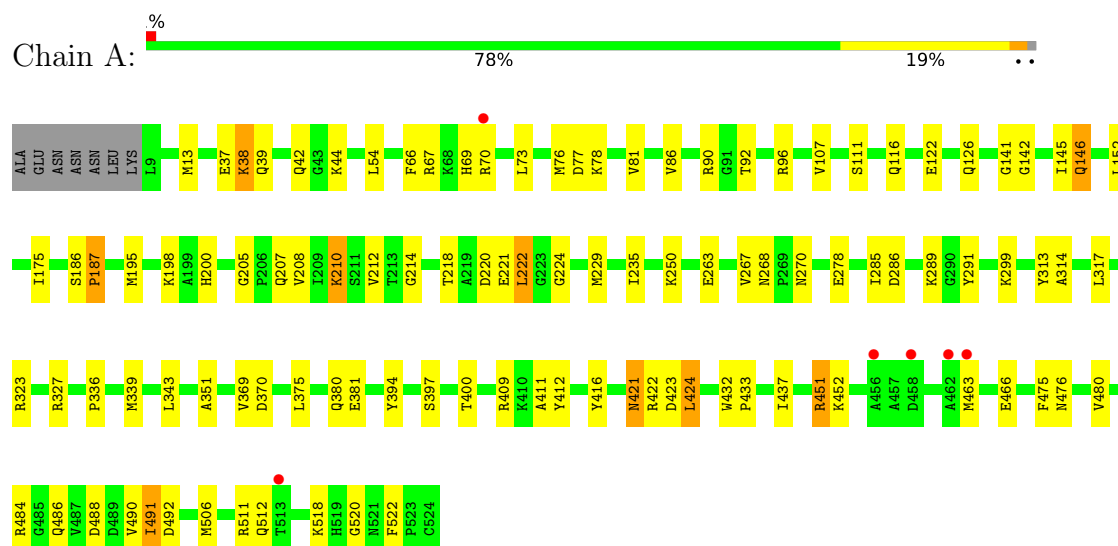
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	558	Total	O	0	0
			558	558		
5	B	616	Total	O	0	0
			616	616		
5	C	557	Total	O	0	0
			557	557		
5	D	492	Total	O	0	0
			492	492		
5	E	610	Total	O	0	0
			610	610		
5	F	557	Total	O	0	0
			557	557		

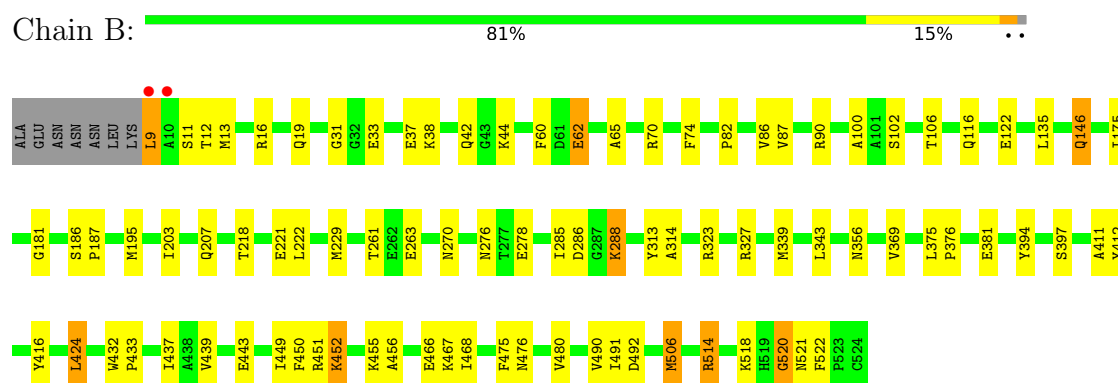
3 Residue-property plots [i](#)

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.

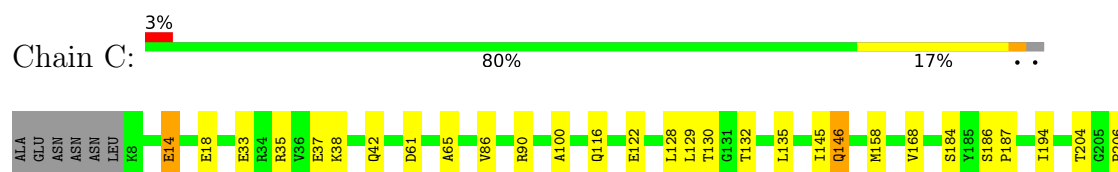
- Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

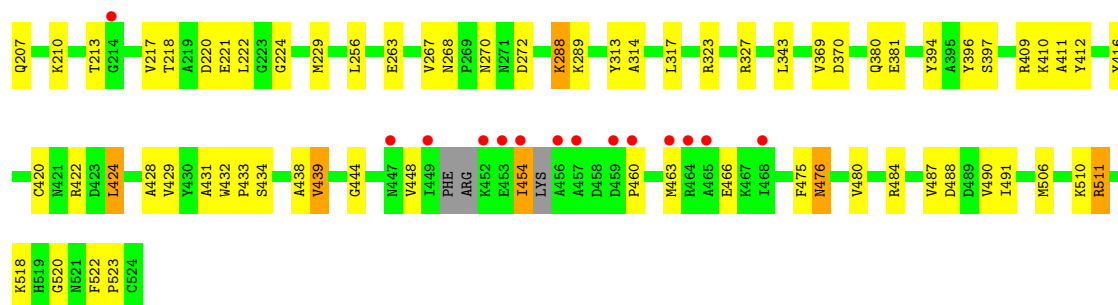


- Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

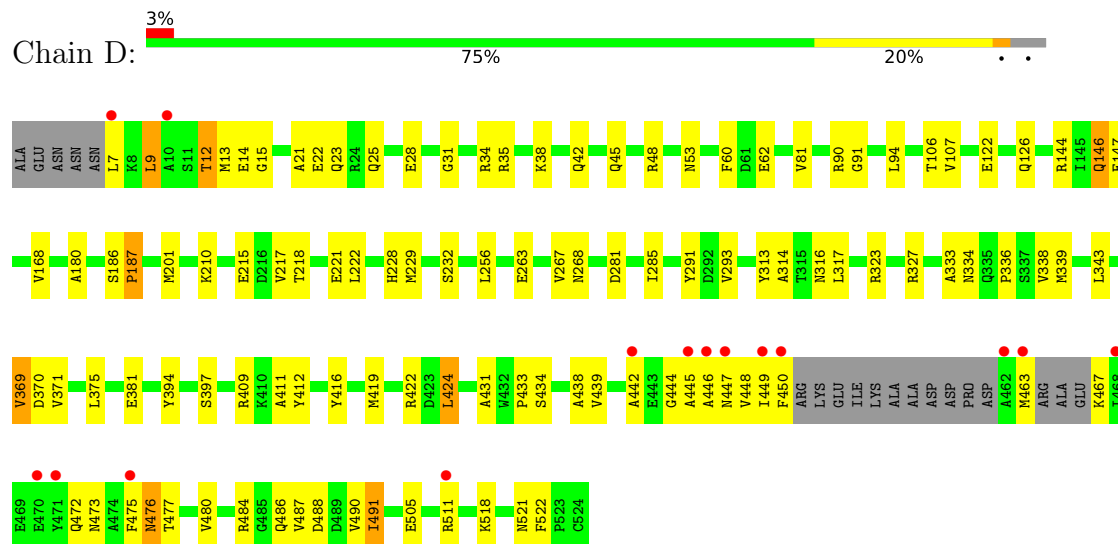


- Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

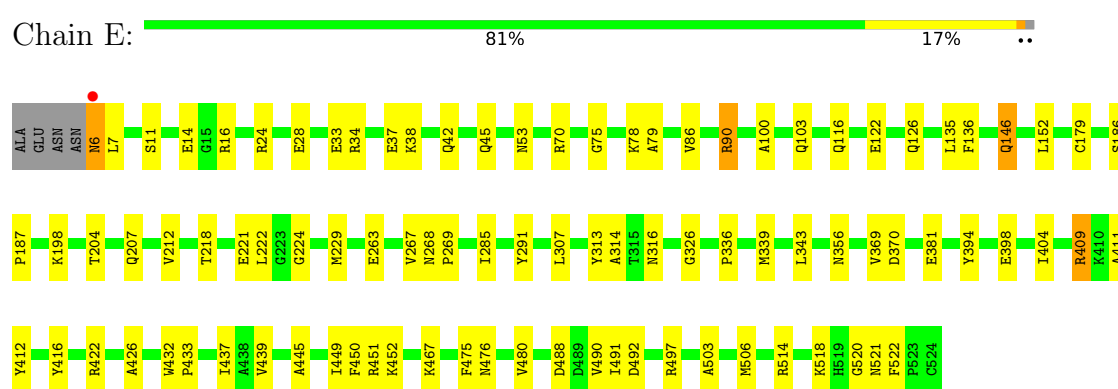




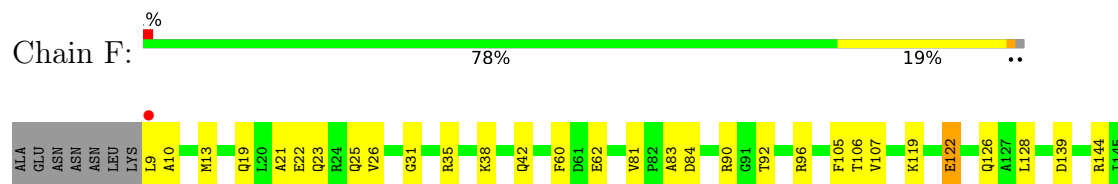
• Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit

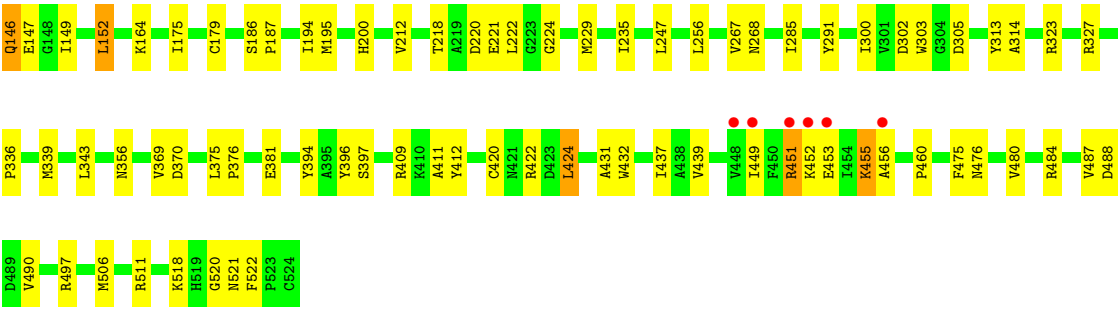


• Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit



• Molecule 1: Methylmalonyl-CoA carboxyltransferase 12S subunit





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.81Å 200.02Å 145.90Å 90.00° 102.97° 90.00°	Depositor
Resolution (Å)	29.55 – 2.00 29.55 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.55-2.00) 96.2 (29.55-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 1.88Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.152 , 0.198 0.154 , 0.198	Depositor DCC
R_{free} test set	10242 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26869	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: MPD, CD, MCA

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	0.48	0/3972	0.98	16/5378 (0.3%)
1	B	0.51	1/3972 (0.0%)	0.99	15/5378 (0.3%)
1	C	0.47	0/3947	0.98	15/5342 (0.3%)
1	D	0.47	0/3874	0.97	15/5243 (0.3%)
1	E	0.51	0/3997	0.99	13/5411 (0.2%)
1	F	0.48	0/3972	0.99	17/5378 (0.3%)
All	All	0.49	1/23734 (0.0%)	0.98	91/32130 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	506	MET	SD-CE	-6.59	1.63	1.79

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	476	ASN	N-CA-C	9.54	123.61	112.93
1	A	476	ASN	N-CA-C	8.99	122.97	112.72
1	E	476	ASN	N-CA-C	8.95	122.95	112.93
1	B	476	ASN	N-CA-C	8.92	122.92	112.93
1	B	369	VAL	N-CA-C	8.13	119.56	108.17
1	F	476	ASN	N-CA-C	8.10	121.55	112.97
1	A	369	VAL	N-CA-C	7.68	119.34	108.36
1	C	369	VAL	N-CA-C	7.64	119.28	108.36
1	E	212	VAL	N-CA-C	7.33	118.12	110.72
1	F	369	VAL	N-CA-C	7.31	118.82	108.36
1	E	369	VAL	N-CA-C	7.20	118.66	108.36
1	B	439	VAL	N-CA-C	-6.93	102.87	112.50
1	D	490	VAL	N-CA-C	-6.88	98.53	108.36
1	A	490	VAL	N-CA-C	-6.68	98.80	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	369	VAL	N-CA-C	6.65	117.88	108.36
1	E	518	LYS	N-CA-C	-6.59	104.09	111.28
1	F	518	LYS	N-CA-C	-6.52	104.25	111.36
1	C	412	TYR	N-CA-C	6.48	119.80	109.24
1	F	490	VAL	N-CA-C	-6.35	99.28	108.17
1	B	432	TRP	N-CA-C	-6.33	100.82	110.07
1	D	518	LYS	N-CA-C	-6.31	104.48	111.36
1	D	476	ASN	N-CA-C	6.26	120.54	113.02
1	C	490	VAL	N-CA-C	-6.22	99.47	108.17
1	F	412	TYR	N-CA-C	6.18	119.32	109.24
1	B	490	VAL	N-CA-C	-6.18	99.52	108.36
1	C	518	LYS	N-CA-C	-6.15	104.66	111.36
1	A	412	TYR	N-CA-C	6.12	119.22	109.24
1	C	270	ASN	N-CA-C	-6.10	97.19	107.99
1	E	432	TRP	N-CA-C	-6.08	101.28	110.39
1	A	518	LYS	N-CA-C	-6.01	104.64	111.07
1	F	432	TRP	N-CA-C	-5.91	101.53	110.39
1	E	439	VAL	N-CA-C	-5.89	104.31	112.50
1	B	412	TYR	N-CA-C	5.89	118.84	109.24
1	F	179	CYS	N-CA-C	-5.87	98.30	110.80
1	E	412	TYR	N-CA-C	5.84	119.16	109.46
1	E	490	VAL	N-CA-C	-5.83	100.01	108.17
1	D	256	LEU	N-CA-C	5.80	117.93	110.39
1	C	256	LEU	N-CA-C	5.79	117.92	110.39
1	E	492	ASP	N-CA-C	-5.79	101.00	109.50
1	D	371	VAL	CA-C-N	5.77	125.47	119.64
1	D	371	VAL	C-N-CA	5.77	125.47	119.64
1	B	518	LYS	N-CA-C	-5.76	105.08	111.36
1	B	263	GLU	N-CA-C	-5.76	100.90	110.17
1	B	270	ASN	N-CA-C	-5.73	97.85	107.99
1	C	439	VAL	N-CA-C	-5.72	104.55	112.50
1	F	343	LEU	N-CA-C	-5.72	101.22	110.32
1	A	343	LEU	N-CA-C	-5.72	101.23	110.32
1	F	256	LEU	N-CA-C	5.67	118.51	110.40
1	F	235	ILE	N-CA-C	5.67	117.00	108.96
1	D	439	VAL	N-CA-C	-5.66	104.63	112.50
1	D	281	ASP	N-CA-C	5.65	120.33	113.38
1	B	492	ASP	N-CA-C	-5.61	102.58	109.65
1	B	343	LEU	N-CA-C	-5.61	102.22	110.52
1	C	263	GLU	N-CA-C	-5.56	101.22	110.17
1	E	343	LEU	N-CA-C	-5.54	101.52	110.32
1	D	491	ILE	N-CA-C	5.53	117.61	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	GLU	N-CA-C	-5.52	101.29	110.17
1	C	224	GLY	N-CA-C	-5.51	103.97	112.85
1	C	343	LEU	N-CA-C	-5.51	101.56	110.32
1	A	212	VAL	N-CA-C	5.50	116.57	111.45
1	E	263	GLU	N-CA-C	-5.50	101.32	110.17
1	D	263	GLU	N-CA-C	-5.47	101.37	110.17
1	A	270	ASN	N-CA-C	-5.47	98.31	107.99
1	D	168	VAL	N-CA-C	-5.46	106.86	111.56
1	E	179	CYS	N-CA-C	-5.46	99.18	110.80
1	D	343	LEU	N-CA-C	-5.45	102.41	110.48
1	A	432	TRP	N-CA-C	-5.42	102.26	110.39
1	F	212	VAL	N-CA-C	5.41	116.46	111.81
1	D	180	ALA	N-CA-C	5.41	118.05	109.24
1	E	224	GLY	N-CA-C	-5.40	105.37	112.82
1	F	439	VAL	N-CA-C	-5.38	105.02	112.50
1	B	520	GLY	N-CA-C	-5.38	103.94	112.66
1	B	62	GLU	N-CA-C	5.33	118.62	110.20
1	C	432	TRP	N-CA-C	-5.30	102.33	110.07
1	A	380	GLN	N-CA-C	-5.27	105.61	111.36
1	C	65	ALA	N-CA-C	-5.26	105.55	111.28
1	A	492	ASP	N-CA-C	-5.24	101.79	109.50
1	A	235	ILE	N-CA-C	5.19	116.33	108.96
1	D	412	TYR	N-CA-C	5.18	117.69	109.24
1	B	285	ILE	N-CA-C	-5.14	104.66	111.09
1	C	194	ILE	N-CA-C	-5.13	100.36	107.80
1	A	141	GLY	N-CA-C	-5.12	108.96	115.31
1	A	491	ILE	N-CA-C	5.11	116.96	108.99
1	F	300	ILE	CB-CA-C	-5.09	105.53	111.94
1	F	224	GLY	N-CA-C	-5.08	104.73	112.51
1	F	194	ILE	N-CA-C	-5.06	100.60	107.99
1	F	305	ASP	N-CA-C	5.06	117.81	109.76
1	A	224	GLY	N-CA-C	-5.06	104.71	112.85
1	B	65	ALA	N-CA-C	-5.04	105.78	111.28
1	F	139	ASP	N-CA-C	-5.04	100.07	110.80
1	C	380	GLN	N-CA-C	-5.00	105.90	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	3900	0	3850	85	0
1	B	3900	0	3850	86	0
1	C	3878	0	3826	77	0
1	D	3805	0	3763	94	0
1	E	3925	0	3880	75	0
1	F	3900	0	3850	80	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	11	0	0
3	B	26	0	11	0	0
3	C	26	0	11	1	0
3	D	31	0	11	1	0
3	E	23	0	11	1	0
3	F	27	0	11	2	0
4	F	8	0	14	0	0
5	A	558	0	0	9	0
5	B	616	0	0	9	0
5	C	557	0	0	11	0
5	D	492	0	0	12	0
5	E	610	0	0	6	0
5	F	557	0	0	10	0
All	All	26869	0	23099	442	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 9.

All (442) 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:F:452:LYS:HD2	1:F:453:GLU:N	1.77	1.00
1:B:146:GLN:H	1:B:146:GLN:HE21	1.08	0.98
1:D:7:LEU:HD22	1:D:23:GLN:HE21	1.30	0.97
1:E:422:ARG:HH11	1:E:422:ARG:HG2	1.33	0.93
1:D:477:THR:HG22	1:D:480:VAL:HG23	1.50	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ARG:HH12	1:B:261:THR:HG21	1.36	0.90
1:E:146:GLN:H	1:E:146:GLN:HE21	1.18	0.89
1:B:286:ASP:OD1	1:B:288:LYS:HG2	1.73	0.88
1:C:146:GLN:H	1:C:146:GLN:HE21	1.19	0.88
1:D:13:MET:HB2	1:E:285:ILE:HD11	1.54	0.87
1:F:146:GLN:H	1:F:146:GLN:HE21	1.19	0.86
1:B:146:GLN:H	1:B:146:GLN:NE2	1.72	0.86
1:A:70:ARG:HH11	1:A:70:ARG:HB3	1.40	0.85
1:B:506:MET:HE3	1:B:506:MET:O	1.75	0.85
1:D:146:GLN:H	1:D:146:GLN:HE21	1.26	0.83
1:F:452:LYS:HD2	1:F:453:GLU:H	1.45	0.81
1:B:218:THR:OG1	1:B:221:GLU:HG3	1.81	0.81
1:A:145:ILE:HG13	5:D:4397:HOH:O	1.81	0.80
1:C:206:PRO:HD2	1:C:207:GLN:HE22	1.46	0.80
1:A:146:GLN:H	1:A:146:GLN:HE21	1.27	0.79
1:B:452:LYS:H	1:B:452:LYS:HZ2	1.30	0.78
1:D:218:THR:OG1	1:D:221:GLU:HG3	1.85	0.76
1:F:339:MET:HE1	1:F:375:LEU:HD22	1.67	0.76
1:E:146:GLN:H	1:E:146:GLN:NE2	1.82	0.76
1:E:16:ARG:NH1	1:F:285:ILE:HD12	2.01	0.76
1:E:316:ASN:HB3	1:E:339:MET:HE3	1.68	0.75
1:F:451:ARG:NH2	1:F:452:LYS:HG3	2.02	0.75
1:E:78:LYS:HD2	1:E:79:ALA:N	2.03	0.74
1:A:146:GLN:H	1:A:146:GLN:NE2	1.85	0.74
1:A:451:ARG:NH1	1:A:451:ARG:HB2	2.03	0.73
1:F:186:SER:HB3	1:F:187:PRO:HD3	1.69	0.73
1:A:70:ARG:HB3	1:A:70:ARG:NH1	2.02	0.73
1:F:9:LEU:HD23	1:F:19:GLN:HE22	1.52	0.73
1:A:210:LYS:HE2	1:A:214:GLY:HA2	1.71	0.73
1:C:454:ILE:HA	1:C:463:MET:HG2	1.70	0.73
1:F:146:GLN:H	1:F:146:GLN:NE2	1.87	0.72
1:F:247:LEU:HD23	5:F:6486:HOH:O	1.89	0.72
1:D:463:MET:HG3	1:D:467:LYS:HG2	1.70	0.72
1:B:146:GLN:HE21	1:B:146:GLN:N	1.87	0.72
1:C:61:ASP:HB2	5:C:7491:HOH:O	1.89	0.72
1:C:207:GLN:CD	1:C:207:GLN:H	1.97	0.72
1:C:422:ARG:HH11	1:C:422:ARG:HG2	1.52	0.72
1:D:186:SER:HB3	1:D:187:PRO:HD3	1.72	0.72
1:D:7:LEU:HD22	1:D:23:GLN:NE2	2.05	0.71
1:D:122:GLU:HG3	5:D:4413:HOH:O	1.91	0.71
1:C:454:ILE:HD13	1:C:454:ILE:H	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:SER:HB3	1:A:187:PRO:HD3	1.73	0.70
1:E:422:ARG:HG2	1:E:422:ARG:NH1	2.07	0.70
1:B:506:MET:HE2	1:C:130:THR:CB	2.22	0.70
1:B:186:SER:HB3	1:B:187:PRO:HD3	1.73	0.69
1:D:477:THR:CG2	1:D:480:VAL:HG23	2.22	0.69
1:D:12:THR:HG23	1:D:15:GLY:H	1.57	0.69
1:D:442:ALA:HB2	1:D:472:GLN:HE21	1.58	0.69
1:D:7:LEU:CD2	1:D:23:GLN:HE21	2.05	0.69
1:C:146:GLN:H	1:C:146:GLN:NE2	1.92	0.68
1:D:35:ARG:HH12	3:D:4004:MCA:P3	2.15	0.68
1:A:207:GLN:HE21	1:A:208:VAL:HG23	1.58	0.68
1:E:70:ARG:HD2	5:F:6349:HOH:O	1.92	0.68
1:E:186:SER:HB3	1:E:187:PRO:HD3	1.76	0.67
1:F:35:ARG:HH12	3:F:4006:MCA:P3	2.18	0.67
1:C:206:PRO:HD2	1:C:207:GLN:NE2	2.10	0.66
1:D:146:GLN:H	1:D:146:GLN:NE2	1.91	0.66
1:C:145:ILE:HG22	1:F:449:ILE:HD11	1.78	0.66
1:E:78:LYS:HD2	1:E:78:LYS:C	2.20	0.65
1:C:272:ASP:OD2	5:C:7501:HOH:O	2.14	0.65
1:F:394:TYR:OH	1:F:520:GLY:HA3	1.97	0.65
1:F:9:LEU:HD23	1:F:19:GLN:NE2	2.13	0.64
1:B:455:LYS:HD3	1:B:455:LYS:C	2.23	0.64
1:D:475:PHE:HA	1:D:480:VAL:HG11	1.78	0.64
1:A:422:ARG:NH2	1:A:488:ASP:OD1	2.28	0.64
1:C:122:GLU:HG3	5:C:7472:HOH:O	1.97	0.64
1:D:38:LYS:O	1:D:42:GLN:HG3	1.98	0.63
1:F:397:SER:OG	1:F:424:LEU:HD13	1.98	0.63
1:B:33:GLU:O	1:B:37:GLU:HG3	1.98	0.63
1:A:486:GLN:HG2	5:A:7460:HOH:O	1.97	0.63
1:E:218:THR:OG1	1:E:221:GLU:HG3	1.98	0.63
1:B:339:MET:CE	1:B:375:LEU:HD22	2.29	0.63
1:A:90:ARG:CD	1:C:506:MET:HG2	2.29	0.62
1:B:452:LYS:N	1:B:452:LYS:HD3	2.14	0.62
1:F:497:ARG:HD3	5:F:6205:HOH:O	1.98	0.62
1:C:411:ALA:HB1	1:C:416:TYR:CD2	2.35	0.62
1:A:90:ARG:HD2	1:C:506:MET:HG2	1.81	0.62
1:F:9:LEU:HA	1:F:19:GLN:HE22	1.63	0.62
1:F:21:ALA:O	1:F:25:GLN:HG2	1.99	0.62
1:F:455:LYS:HE2	1:F:456:ALA:HB2	1.82	0.61
1:C:222:LEU:HD11	1:F:381:GLU:HG3	1.83	0.61
1:E:445:ALA:O	1:E:449:ILE:HG12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:NZ	1:B:288:LYS:HB3	2.17	0.60
1:B:339:MET:HE3	1:B:375:LEU:HD22	1.82	0.60
1:D:394:TYR:CD2	1:D:522:PHE:HD2	2.19	0.60
1:A:451:ARG:HB2	1:A:451:ARG:HH11	1.66	0.60
1:E:34:ARG:HB3	1:E:34:ARG:HH11	1.67	0.60
1:C:289:LYS:HA	1:C:289:LYS:HE3	1.84	0.60
1:D:477:THR:HG22	1:D:480:VAL:CG2	2.28	0.59
1:A:205:GLY:HA3	1:A:207:GLN:HE22	1.67	0.59
1:B:411:ALA:HB1	1:B:416:TYR:CD2	2.38	0.59
1:C:218:THR:OG1	1:C:221:GLU:HG3	2.03	0.59
1:B:397:SER:OG	1:B:424:LEU:HD13	2.02	0.59
1:F:218:THR:OG1	1:F:221:GLU:HG3	2.03	0.58
1:F:339:MET:CE	1:F:375:LEU:HD22	2.33	0.58
1:C:90:ARG:HD3	5:C:7077:HOH:O	2.03	0.58
1:A:452:LYS:HD2	1:A:452:LYS:N	2.17	0.58
1:E:90:ARG:HG2	1:F:506:MET:HG2	1.85	0.58
1:C:33:GLU:O	1:C:37:GLU:HG3	2.03	0.58
1:F:455:LYS:HG3	1:F:456:ALA:N	2.19	0.58
1:D:397:SER:OG	1:D:424:LEU:HD13	2.04	0.58
1:F:38:LYS:O	1:F:42:GLN:HG3	2.04	0.58
1:A:229:MET:O	1:A:313:TYR:HB2	2.04	0.58
1:A:210:LYS:HE2	1:A:210:LYS:O	2.03	0.57
1:C:186:SER:HB3	1:C:187:PRO:HD3	1.86	0.57
1:B:455:LYS:HD3	1:B:456:ALA:N	2.19	0.57
1:C:454:ILE:HA	1:C:463:MET:CG	2.35	0.57
1:B:9:LEU:HD23	1:B:9:LEU:N	2.20	0.57
1:B:82:PRO:HG3	5:B:7608:HOH:O	2.05	0.57
1:A:286:ASP:HB3	1:A:289:LYS:HD3	1.87	0.57
1:B:175:ILE:HB	1:B:195:MET:HG3	1.87	0.57
5:A:7469:HOH:O	1:D:217:VAL:HB	2.04	0.57
1:B:506:MET:HE2	1:C:130:THR:HB	1.85	0.57
1:B:9:LEU:HD12	1:B:16:ARG:NE	2.20	0.56
1:C:394:TYR:OH	1:C:520:GLY:HA3	2.05	0.56
1:D:422:ARG:NH2	1:D:488:ASP:OD1	2.38	0.56
5:D:4317:HOH:O	1:E:506:MET:HE1	2.05	0.56
1:F:411:ALA:HB3	1:F:437:ILE:HA	1.87	0.56
1:F:451:ARG:CZ	1:F:452:LYS:HG3	2.35	0.56
1:A:90:ARG:HD3	5:A:7018:HOH:O	2.04	0.56
1:A:218:THR:OG1	1:A:221:GLU:HG3	2.04	0.56
1:A:198:LYS:HE2	5:A:7549:HOH:O	2.05	0.56
1:A:285:ILE:HD12	1:B:11:SER:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:MET:HG2	1:B:90:ARG:CD	2.35	0.56
1:D:444:GLY:O	1:D:448:VAL:HG23	2.06	0.56
1:E:229:MET:O	1:E:313:TYR:HB2	2.05	0.56
1:C:381:GLU:HG3	1:F:222:LEU:HD11	1.87	0.56
1:C:410:LYS:HE3	5:C:7374:HOH:O	2.04	0.56
1:A:210:LYS:HE3	5:A:7537:HOH:O	2.05	0.55
1:E:146:GLN:HE21	1:E:146:GLN:N	1.97	0.55
1:D:12:THR:HG23	1:D:15:GLY:N	2.20	0.55
1:A:394:TYR:CD2	1:A:522:PHE:HD2	2.25	0.55
1:E:422:ARG:NH2	1:E:488:ASP:OD1	2.35	0.55
1:B:506:MET:HE1	1:C:132:THR:HG21	1.88	0.55
1:A:463:MET:O	1:A:466:GLU:HB3	2.06	0.55
1:C:454:ILE:H	1:C:454:ILE:CD1	2.19	0.55
1:B:276:ASN:OD1	1:B:278:GLU:HB2	2.06	0.55
1:C:35:ARG:HH12	3:C:4003:MCA:P3	2.29	0.55
1:F:146:GLN:HE21	1:F:146:GLN:N	1.98	0.55
1:D:476:ASN:N	1:D:476:ASN:HD22	2.05	0.55
1:A:146:GLN:HE21	1:A:146:GLN:N	2.02	0.54
1:D:228:HIS:HA	1:D:232:SER:HB2	1.90	0.54
1:C:397:SER:OG	1:C:424:LEU:HD13	2.07	0.54
1:D:477:THR:HG23	1:D:480:VAL:H	1.73	0.54
1:F:31:GLY:O	1:F:35:ARG:HG3	2.07	0.54
1:C:370:ASP:CG	1:C:409:ARG:HB3	2.31	0.54
1:E:433:PRO:HD3	1:E:491:ILE:O	2.08	0.54
1:A:285:ILE:HG23	1:B:16:ARG:NH1	2.22	0.54
1:A:299:LYS:NZ	5:A:7490:HOH:O	2.38	0.54
1:D:210:LYS:HA	1:D:215:GLU:O	2.07	0.54
1:A:484:ARG:NH2	1:B:70:ARG:NH1	2.55	0.54
1:E:394:TYR:CD2	1:E:522:PHE:HD2	2.25	0.54
1:A:433:PRO:HD3	1:A:491:ILE:O	2.08	0.54
1:D:334:ASN:O	1:D:336:PRO:HD3	2.09	0.54
1:E:404:ILE:HD12	1:E:503:ALA:HB1	1.90	0.54
1:E:90:ARG:HG2	1:F:506:MET:HE3	1.89	0.53
1:E:514:ARG:HD3	5:E:4547:HOH:O	2.08	0.53
1:D:31:GLY:O	1:D:35:ARG:HD2	2.07	0.53
1:E:411:ALA:HB1	1:E:416:TYR:CD2	2.43	0.53
1:B:475:PHE:HA	1:B:480:VAL:HG11	1.89	0.53
1:D:9:LEU:HD21	1:E:433:PRO:O	2.08	0.53
1:E:34:ARG:HB3	1:E:34:ARG:NH1	2.23	0.53
1:A:339:MET:HE3	1:A:375:LEU:HD13	1.90	0.53
1:F:35:ARG:HG2	5:F:6445:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:PHE:HA	1:A:480:VAL:HG11	1.89	0.53
1:B:86:VAL:HB	1:B:116:GLN:HG3	1.91	0.53
1:E:422:ARG:HD3	1:E:426:ALA:O	2.07	0.53
1:E:38:LYS:NZ	3:E:4005:MCA:H5'1	2.23	0.53
1:C:422:ARG:HH11	1:C:422:ARG:CG	2.22	0.53
1:E:75:GLY:O	1:E:78:LYS:HE3	2.08	0.53
1:B:514:ARG:NH2	5:B:7547:HOH:O	2.41	0.52
1:A:394:TYR:OH	1:A:520:GLY:HA3	2.09	0.52
1:A:411:ALA:HB3	1:A:437:ILE:HA	1.91	0.52
1:B:433:PRO:HD3	1:B:491:ILE:O	2.10	0.52
1:A:522:PHE:HD1	1:D:522:PHE:CD1	2.26	0.52
1:B:87:VAL:HB	5:B:7559:HOH:O	2.07	0.52
1:D:90:ARG:CB	1:E:506:MET:HE3	2.40	0.52
1:B:9:LEU:HA	1:B:19:GLN:HE22	1.75	0.52
1:A:285:ILE:HD11	1:B:13:MET:N	2.24	0.52
1:E:398:GLU:HG2	5:E:4174:HOH:O	2.08	0.52
1:A:397:SER:OG	1:A:424:LEU:HD13	2.09	0.52
1:C:323:ARG:HA	1:C:327:ARG:O	2.09	0.52
1:A:86:VAL:HB	1:A:116:GLN:HG3	1.91	0.51
1:B:394:TYR:OH	1:B:520:GLY:HA3	2.09	0.51
1:A:506:MET:HG2	1:B:90:ARG:HD2	1.92	0.51
1:D:444:GLY:HA2	1:D:447:ASN:HB3	1.92	0.51
1:B:222:LEU:HD11	1:E:381:GLU:HG3	1.93	0.51
1:F:291:TYR:CZ	1:F:336:PRO:HG2	2.45	0.51
1:A:291:TYR:CZ	1:A:336:PRO:HG2	2.46	0.51
1:E:122:GLU:O	1:E:126:GLN:HG2	2.10	0.51
1:F:451:ARG:HA	5:F:6475:HOH:O	2.09	0.51
1:B:506:MET:HG2	1:C:90:ARG:CD	2.40	0.51
5:B:7492:HOH:O	1:E:521:ASN:HB3	2.09	0.51
1:C:438:ALA:HB2	1:C:476:ASN:CG	2.35	0.51
1:B:229:MET:O	1:B:313:TYR:HB2	2.11	0.51
1:D:14:GLU:HA	1:D:14:GLU:OE2	2.11	0.51
1:F:339:MET:HE1	1:F:375:LEU:CD2	2.40	0.51
1:F:394:TYR:CD2	1:F:522:PHE:HD2	2.29	0.51
1:A:370:ASP:CG	1:A:409:ARG:HB3	2.35	0.51
1:A:522:PHE:HD1	1:D:522:PHE:HD1	1.56	0.51
1:A:207:GLN:CD	1:A:207:GLN:H	2.19	0.50
1:F:370:ASP:CG	1:F:409:ARG:HB3	2.36	0.50
1:A:285:ILE:HG23	1:B:16:ARG:HH12	1.77	0.50
1:E:38:LYS:O	1:E:42:GLN:HG3	2.11	0.50
1:D:431:ALA:HB2	1:D:487:VAL:HG11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:TYR:OH	1:E:520:GLY:HA3	2.11	0.50
1:A:38:LYS:O	1:A:42:GLN:HG3	2.11	0.50
1:B:506:MET:HE1	1:C:132:THR:CG2	2.41	0.50
1:C:204:THR:HG21	1:F:376:PRO:HB3	1.93	0.50
1:D:7:LEU:HD22	5:D:4166:HOH:O	2.10	0.50
1:A:285:ILE:HD11	1:B:12:THR:C	2.36	0.50
1:C:14:GLU:O	1:C:18:GLU:HG3	2.11	0.50
1:C:454:ILE:HD13	1:C:454:ILE:N	2.25	0.50
1:D:12:THR:HG23	1:D:15:GLY:HA3	1.93	0.50
1:D:90:ARG:NE	1:E:506:MET:HG2	2.26	0.50
1:D:433:PRO:HD3	1:D:491:ILE:O	2.11	0.50
1:E:422:ARG:NH1	1:E:422:ARG:CG	2.70	0.50
1:C:86:VAL:HB	1:C:116:GLN:HG3	1.94	0.49
1:D:60:PHE:CE2	1:D:62:GLU:HB2	2.47	0.49
1:A:278:GLU:HB3	1:A:299:LYS:HE2	1.93	0.49
1:F:229:MET:O	1:F:313:TYR:HB2	2.12	0.49
5:A:7426:HOH:O	1:D:521:ASN:HB2	2.12	0.49
1:B:506:MET:HG2	1:C:90:ARG:HD2	1.94	0.49
1:A:323:ARG:HA	1:A:327:ARG:O	2.12	0.49
1:C:14:GLU:CD	1:C:14:GLU:H	2.21	0.49
1:E:291:TYR:CE2	1:E:336:PRO:HG2	2.48	0.49
1:F:19:GLN:O	1:F:23:GLN:HG2	2.12	0.49
1:A:145:ILE:HG22	1:D:449:ILE:HD11	1.95	0.49
1:B:506:MET:CE	1:C:130:THR:HB	2.42	0.49
1:E:45:GLN:NE2	1:E:53:ASN:HD22	2.09	0.49
1:E:475:PHE:HA	1:E:480:VAL:HG11	1.94	0.49
1:F:313:TYR:O	1:F:314:ALA:C	2.54	0.49
1:D:45:GLN:NE2	1:D:53:ASN:HD22	2.10	0.49
1:D:90:ARG:HD3	1:D:91:GLY:N	2.28	0.49
1:F:455:LYS:HG3	1:F:456:ALA:H	1.77	0.49
1:D:21:ALA:O	1:D:25:GLN:HG3	2.13	0.49
1:D:313:TYR:O	1:D:314:ALA:C	2.55	0.48
1:B:381:GLU:HG3	1:E:222:LEU:HD11	1.95	0.48
1:C:206:PRO:HB3	1:C:217:VAL:O	2.13	0.48
1:C:146:GLN:HE21	1:C:146:GLN:N	2.00	0.48
1:D:201:MET:O	1:D:228:HIS:NE2	2.39	0.48
1:D:486:GLN:HG2	5:D:4344:HOH:O	2.13	0.48
1:F:484:ARG:HD2	5:F:6349:HOH:O	2.12	0.48
1:A:39:GLN:NE2	1:A:44:LYS:HE2	2.28	0.48
1:A:267:VAL:O	1:A:268:ASN:C	2.57	0.48
1:C:433:PRO:HD3	1:C:491:ILE:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:229:MET:O	1:C:313:TYR:HB2	2.14	0.48
1:C:422:ARG:HD3	5:C:7252:HOH:O	2.14	0.48
1:F:422:ARG:NH2	1:F:488:ASP:OD1	2.40	0.48
1:D:122:GLU:O	1:D:126:GLN:HG2	2.14	0.47
1:D:323:ARG:HA	1:D:327:ARG:O	2.14	0.47
1:D:81:VAL:HG13	1:D:107:VAL:CG1	2.44	0.47
1:A:313:TYR:O	1:A:314:ALA:C	2.58	0.47
1:D:90:ARG:CD	1:E:506:MET:HG2	2.44	0.47
1:B:376:PRO:HB3	1:E:204:THR:HG21	1.96	0.47
1:D:316:ASN:HB3	1:D:339:MET:HE3	1.96	0.47
1:C:429:VAL:HG12	1:C:487:VAL:HG12	1.96	0.47
1:E:411:ALA:HB3	1:E:437:ILE:HA	1.97	0.47
1:B:356:ASN:ND2	5:B:7115:HOH:O	2.45	0.47
1:C:38:LYS:O	1:C:42:GLN:HG3	2.15	0.47
1:A:54:LEU:O	1:A:250:LYS:HE2	2.14	0.47
1:B:323:ARG:HA	1:B:327:ARG:O	2.15	0.47
1:D:445:ALA:O	1:D:449:ILE:HG13	2.15	0.47
5:E:4240:HOH:O	1:F:506:MET:HE1	2.14	0.47
1:F:35:ARG:CB	1:F:106:THR:HB	2.45	0.47
1:F:90:ARG:NH1	5:F:6483:HOH:O	2.48	0.47
1:E:24:ARG:O	1:E:28:GLU:HG3	2.15	0.47
1:D:146:GLN:HE21	1:D:146:GLN:N	2.04	0.46
1:A:70:ARG:HE	1:C:484:ARG:NE	2.14	0.46
1:E:316:ASN:CB	1:E:339:MET:HE3	2.43	0.46
1:B:443:GLU:HA	1:B:468:ILE:HG12	1.98	0.46
1:C:158:MET:HE1	5:C:7156:HOH:O	2.15	0.46
1:A:38:LYS:NZ	1:A:38:LYS:HB3	2.31	0.46
1:A:69:HIS:CD2	1:A:76:MET:HE3	2.51	0.46
1:B:451:ARG:HG2	1:B:451:ARG:HH11	1.81	0.46
1:B:452:LYS:H	1:B:452:LYS:HD3	1.78	0.46
1:C:220:ASP:HB2	5:C:7476:HOH:O	2.16	0.46
1:D:339:MET:HE1	5:D:4022:HOH:O	2.15	0.46
1:E:198:LYS:HD2	5:E:4226:HOH:O	2.15	0.46
1:B:207:GLN:HA	1:B:207:GLN:HE21	1.81	0.46
1:D:12:THR:HG23	1:D:15:GLY:CA	2.46	0.46
1:E:14:GLU:OE2	1:E:14:GLU:HA	2.15	0.46
1:B:74:PHE:CD1	1:E:450:PHE:HZ	2.34	0.45
1:F:455:LYS:CG	1:F:456:ALA:N	2.79	0.45
1:C:510:LYS:O	1:C:511:ARG:HD3	2.15	0.45
1:D:444:GLY:CA	1:D:447:ASN:HB3	2.46	0.45
1:E:267:VAL:O	1:E:268:ASN:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:ARG:HG2	1:C:422:ARG:NH1	2.28	0.45
1:C:428:ALA:HA	1:C:488:ASP:OD2	2.17	0.45
1:E:291:TYR:CZ	1:E:336:PRO:HG2	2.51	0.45
1:F:200:HIS:HB2	5:F:6202:HOH:O	2.16	0.45
1:C:184:SER:C	1:C:187:PRO:HD2	2.41	0.45
1:C:444:GLY:O	1:C:448:VAL:HG23	2.16	0.45
1:E:6:ASN:OD1	1:E:6:ASN:N	2.50	0.45
1:A:317:LEU:CD2	1:A:351:ALA:HB2	2.47	0.45
5:D:4449:HOH:O	1:E:506:MET:HE1	2.17	0.45
1:E:313:TYR:O	1:E:314:ALA:C	2.60	0.45
1:E:451:ARG:HD2	1:E:452:LYS:HE3	1.97	0.45
1:B:313:TYR:O	1:B:314:ALA:C	2.60	0.45
1:C:394:TYR:CD2	1:C:522:PHE:HD2	2.35	0.45
1:D:442:ALA:HB2	1:D:472:GLN:NE2	2.27	0.45
1:F:452:LYS:NZ	1:F:453:GLU:HB2	2.32	0.45
1:F:511:ARG:HH11	1:F:511:ARG:HG3	1.81	0.45
1:B:207:GLN:HA	1:B:207:GLN:NE2	2.32	0.45
1:C:100:ALA:HA	1:C:135:LEU:O	2.17	0.45
1:A:205:GLY:CA	1:A:207:GLN:HE22	2.28	0.44
1:E:86:VAL:HB	1:E:116:GLN:HG3	1.99	0.44
1:E:90:ARG:CB	1:F:506:MET:HE3	2.48	0.44
1:F:291:TYR:CE2	1:F:336:PRO:HG2	2.52	0.44
1:C:267:VAL:O	1:C:268:ASN:C	2.60	0.44
1:D:434:SER:OG	1:F:13:MET:HE1	2.17	0.44
1:F:323:ARG:HA	1:F:327:ARG:O	2.18	0.44
1:B:38:LYS:O	1:B:42:GLN:HG3	2.18	0.44
1:C:439:VAL:HA	1:F:152:LEU:HG	1.99	0.44
1:D:446:ALA:O	1:D:450:PHE:HD1	1.99	0.44
1:D:447:ASN:C	1:D:447:ASN:HD22	2.25	0.44
1:E:370:ASP:CG	1:E:409:ARG:HB3	2.41	0.44
1:B:181:GLY:HA2	1:B:203:ILE:O	2.16	0.44
1:C:313:TYR:O	1:C:314:ALA:C	2.61	0.44
1:A:67:ARG:NH2	5:A:7157:HOH:O	2.49	0.44
1:B:522:PHE:HD1	1:E:522:PHE:CD1	2.36	0.44
1:C:431:ALA:HB2	1:C:487:VAL:HG11	2.00	0.44
1:D:476:ASN:N	1:D:476:ASN:ND2	2.65	0.44
1:E:16:ARG:HH11	1:F:285:ILE:HD12	1.81	0.44
1:F:267:VAL:O	1:F:268:ASN:C	2.59	0.44
1:C:184:SER:O	1:C:187:PRO:HD2	2.18	0.44
1:F:83:ALA:HB1	1:F:119:LYS:NZ	2.33	0.44
1:B:102:SER:HB3	5:B:7559:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:GLU:OE1	1:D:215:GLU:HA	2.18	0.44
1:F:22:GLU:O	1:F:26:VAL:HG23	2.17	0.44
1:B:394:TYR:CD2	1:B:522:PHE:HD2	2.36	0.44
1:D:22:GLU:HG3	5:D:4445:HOH:O	2.18	0.43
1:D:94:LEU:HB3	5:D:4226:HOH:O	2.18	0.43
1:B:42:GLN:HB2	1:B:44:LYS:HE2	2.00	0.43
1:A:13:MET:HE1	1:C:434:SER:OG	2.18	0.43
1:A:222:LEU:HD21	1:D:381:GLU:HG3	2.01	0.43
1:F:81:VAL:HG13	1:F:107:VAL:CG1	2.48	0.43
1:A:317:LEU:HD22	1:A:351:ALA:HB2	2.00	0.43
1:B:506:MET:CE	5:B:7479:HOH:O	2.66	0.43
1:D:484:ARG:HG3	1:D:484:ARG:HH11	1.84	0.43
1:F:60:PHE:CE2	1:F:62:GLU:HB2	2.53	0.43
1:B:411:ALA:HB3	1:B:437:ILE:HA	2.00	0.43
1:C:128:LEU:CD1	1:C:168:VAL:HG11	2.49	0.43
1:F:451:ARG:HB3	5:F:6474:HOH:O	2.19	0.43
1:A:92:THR:HA	1:A:96:ARG:O	2.19	0.43
1:B:467:LYS:HD3	1:B:467:LYS:HA	1.79	0.43
1:F:451:ARG:N	5:F:6474:HOH:O	2.52	0.43
1:A:86:VAL:HB	1:A:116:GLN:CG	2.49	0.43
1:B:506:MET:HE2	1:C:130:THR:OG1	2.17	0.43
1:D:370:ASP:CG	1:D:409:ARG:HB3	2.43	0.43
1:F:396:TYR:CG	1:F:420:CYS:HB2	2.53	0.43
1:F:431:ALA:HB2	1:F:487:VAL:HG11	2.01	0.43
1:A:122:GLU:O	1:A:126:GLN:HG2	2.19	0.43
1:B:452:LYS:HB2	1:B:452:LYS:NZ	2.34	0.43
1:C:210:LYS:O	1:C:213:THR:O	2.36	0.43
1:C:475:PHE:HA	1:C:480:VAL:HG11	2.01	0.43
1:D:267:VAL:O	1:D:268:ASN:C	2.61	0.43
1:F:92:THR:HA	1:F:96:ARG:O	2.18	0.43
1:F:122:GLU:O	1:F:126:GLN:HG2	2.19	0.43
1:F:175:ILE:HB	1:F:195:MET:HG3	2.01	0.43
1:B:521:ASN:HA	1:E:356:ASN:HD21	1.83	0.42
1:D:31:GLY:HA3	1:D:106:THR:O	2.19	0.42
1:E:269:PRO:HB3	1:E:326:GLY:HA3	2.00	0.42
1:A:421:ASN:HB2	5:A:7083:HOH:O	2.19	0.42
1:A:421:ASN:HD21	1:A:423:ASP:HB2	1.84	0.42
1:D:438:ALA:HB2	1:D:476:ASN:CG	2.44	0.42
1:E:103:GLN:HG3	1:E:136:PHE:HE2	1.84	0.42
1:E:497:ARG:HD3	5:E:4182:HOH:O	2.19	0.42
1:A:77:ASP:OD1	1:A:78:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:GLU:O	1:E:37:GLU:HG3	2.19	0.42
1:E:100:ALA:HA	1:E:135:LEU:O	2.19	0.42
1:E:450:PHE:CE2	1:E:467:LYS:HD2	2.53	0.42
1:F:302:ASP:HB3	1:F:303:TRP:CD1	2.54	0.42
1:A:200:HIS:CD2	1:A:220:ASP:HA	2.55	0.42
1:B:31:GLY:HA3	1:B:106:THR:O	2.19	0.42
1:F:144:ARG:HD2	1:F:147:GLU:CD	2.44	0.42
1:A:81:VAL:HG13	1:A:107:VAL:CG1	2.50	0.42
1:B:452:LYS:N	1:B:452:LYS:CD	2.82	0.42
1:D:293:VAL:HG21	1:D:333:ALA:HB1	2.01	0.42
1:B:60:PHE:CE2	1:B:62:GLU:HB2	2.53	0.42
1:B:449:ILE:HG13	1:B:450:PHE:CD1	2.55	0.42
1:A:73:LEU:HD12	1:D:475:PHE:CZ	2.55	0.42
1:A:152:LEU:HD21	1:D:416:TYR:HD1	1.85	0.42
1:C:460:PRO:HG3	5:C:7320:HOH:O	2.20	0.42
1:D:90:ARG:HB2	1:E:506:MET:HE3	2.01	0.42
1:B:9:LEU:HD12	1:B:16:ARG:HE	1.85	0.41
1:B:100:ALA:HA	1:B:135:LEU:O	2.20	0.41
1:D:316:ASN:HA	1:D:338:VAL:HB	2.02	0.41
1:F:149:ILE:HA	1:F:152:LEU:HB2	2.02	0.41
1:A:411:ALA:HB1	1:A:416:TYR:CD2	2.54	0.41
1:D:25:GLN:HG3	5:D:4209:HOH:O	2.20	0.41
1:F:128:LEU:CD2	1:F:164:LYS:HE2	2.50	0.41
1:A:175:ILE:HB	1:A:195:MET:HG3	2.02	0.41
1:A:291:TYR:CE1	1:A:336:PRO:HG2	2.55	0.41
1:D:291:TYR:CZ	1:D:336:PRO:HG2	2.56	0.41
1:E:45:GLN:HE22	1:E:53:ASN:HD22	1.68	0.41
1:A:506:MET:HG2	1:B:90:ARG:HD3	2.01	0.41
1:B:411:ALA:HB1	1:B:416:TYR:CG	2.55	0.41
1:A:522:PHE:CD1	1:D:522:PHE:HD1	2.37	0.41
1:D:35:ARG:HH11	1:D:35:ARG:HG2	1.86	0.41
1:E:449:ILE:HG13	1:E:450:PHE:CD1	2.56	0.41
1:B:70:ARG:NH1	1:B:70:ARG:HB2	2.35	0.41
1:B:207:GLN:NE2	1:B:207:GLN:CA	2.83	0.41
1:B:506:MET:HE1	5:B:7479:HOH:O	2.19	0.41
1:D:473:ASN:N	1:D:473:ASN:HD22	2.19	0.41
1:F:475:PHE:HA	1:F:480:VAL:HG11	2.02	0.41
1:B:218:THR:HG1	1:B:221:GLU:HG3	1.80	0.41
1:C:522:PHE:HA	1:C:523:PRO:HD3	1.98	0.41
1:F:81:VAL:HG12	1:F:84:ASP:HA	2.03	0.41
1:F:451:ARG:H	1:F:451:ARG:NE	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:LYS:HA	1:C:289:LYS:CE	2.50	0.41
1:A:66:PHE:HB3	5:C:7133:HOH:O	2.21	0.41
1:A:81:VAL:HG13	1:A:107:VAL:HG12	2.03	0.41
5:C:7459:HOH:O	1:F:521:ASN:HB3	2.21	0.41
1:D:94:LEU:HD11	5:D:4193:HOH:O	2.19	0.41
1:D:186:SER:CB	1:D:187:PRO:HD3	2.48	0.41
1:D:229:MET:O	1:D:313:TYR:HB2	2.20	0.41
1:D:411:ALA:HB1	1:D:416:TYR:CD2	2.55	0.41
1:D:511:ARG:NH1	5:D:4210:HOH:O	2.54	0.41
1:E:11:SER:HA	5:E:4431:HOH:O	2.21	0.41
1:B:521:ASN:HA	1:E:356:ASN:ND2	2.36	0.41
1:A:400:THR:HG22	1:A:512:GLN:HE21	1.86	0.40
1:D:28:GLU:HG2	1:D:48:ARG:CZ	2.50	0.40
1:F:105:PHE:CZ	3:F:4006:MCA:H5'2	2.56	0.40
1:C:288:LYS:HB2	1:C:288:LYS:NZ	2.36	0.40
1:D:144:ARG:HD2	1:D:147:GLU:CD	2.46	0.40
1:D:369:VAL:HG22	1:D:419:MET:HB3	2.03	0.40
1:A:381:GLU:HG3	1:D:222:LEU:HD11	2.03	0.40
1:B:9:LEU:N	1:B:9:LEU:CD2	2.84	0.40
1:C:422:ARG:CG	1:C:422:ARG:NH1	2.81	0.40
1:F:200:HIS:CD2	1:F:220:ASP:HA	2.57	0.40
1:B:122:GLU:HG3	5:B:7545:HOH:O	2.20	0.40
1:B:522:PHE:HD1	1:E:522:PHE:HD1	1.70	0.40
1:C:396:TYR:CD2	1:C:420:CYS:HB2	2.56	0.40
1:A:111:SER:HA	1:A:142:GLY:O	2.21	0.40
1:D:285:ILE:HD13	1:D:285:ILE:HA	1.98	0.40
1:F:35:ARG:HB2	1:F:106:THR:HB	2.02	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	514/523 (98%)	497 (97%)	17 (3%)	0	100	100
1	B	514/523 (98%)	500 (97%)	14 (3%)	0	100	100
1	C	508/523 (97%)	485 (96%)	23 (4%)	0	100	100
1	D	498/523 (95%)	480 (96%)	18 (4%)	0	100	100
1	E	517/523 (99%)	498 (96%)	18 (4%)	1 (0%)	43	42
1	F	514/523 (98%)	496 (96%)	17 (3%)	1 (0%)	43	42
All	All	3065/3138 (98%)	2956 (96%)	107 (4%)	2 (0%)	48	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	10	ALA
1	E	409	ARG

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	405/411 (98%)	396 (98%)	9 (2%)	45	50
1	B	405/411 (98%)	398 (98%)	7 (2%)	53	60
1	C	403/411 (98%)	394 (98%)	9 (2%)	45	50
1	D	396/411 (96%)	387 (98%)	9 (2%)	44	49
1	E	408/411 (99%)	401 (98%)	7 (2%)	53	60
1	F	405/411 (98%)	397 (98%)	8 (2%)	48	54
All	All	2422/2466 (98%)	2373 (98%)	49 (2%)	48	54

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	38	LYS
1	A	146	GLN

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Mol	Chain	Res	Type
1	A	187	PRO
1	A	210	LYS
1	A	222	LEU
1	A	421	ASN
1	A	424	LEU
1	A	451	ARG
1	B	9	LEU
1	B	146	GLN
1	B	288	LYS
1	B	424	LEU
1	B	452	LYS
1	B	466	GLU
1	B	514	ARG
1	C	14	GLU
1	C	129	LEU
1	C	146	GLN
1	C	288	LYS
1	C	317	LEU
1	C	424	LEU
1	C	454	ILE
1	C	466	GLU
1	C	511	ARG
1	D	9	LEU
1	D	12	THR
1	D	34	ARG
1	D	146	GLN
1	D	187	PRO
1	D	317	LEU
1	D	375	LEU
1	D	424	LEU
1	D	505	GLU
1	E	6	ASN
1	E	7	LEU
1	E	90	ARG
1	E	146	GLN
1	E	152	LEU
1	E	207	GLN
1	E	307	LEU
1	F	122	GLU
1	F	146	GLN
1	F	152	LEU
1	F	356	ASN

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Mol	Chain	Res	Type
1	F	424	LEU
1	F	451	ARG
1	F	455	LYS
1	F	460	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	126	GLN
1	A	146	GLN
1	A	162	ASN
1	A	207	GLN
1	A	356	ASN
1	A	379	GLN
1	A	421	ASN
1	A	512	GLN
1	A	521	ASN
1	B	19	GLN
1	B	23	GLN
1	B	45	GLN
1	B	146	GLN
1	B	162	ASN
1	B	207	GLN
1	B	271	ASN
1	B	512	GLN
1	C	25	GLN
1	C	53	ASN
1	C	58	HIS
1	C	146	GLN
1	C	162	ASN
1	C	207	GLN
1	C	271	ASN
1	C	379	GLN
1	C	512	GLN
1	C	521	ASN
1	D	23	GLN
1	D	25	GLN
1	D	45	GLN
1	D	58	HIS
1	D	146	GLN
1	D	162	ASN

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Mol	Chain	Res	Type
1	D	207	GLN
1	D	271	ASN
1	D	447	ASN
1	D	472	GLN
1	D	473	ASN
1	D	476	ASN
1	D	512	GLN
1	E	6	ASN
1	E	23	GLN
1	E	45	GLN
1	E	53	ASN
1	E	58	HIS
1	E	146	GLN
1	E	162	ASN
1	E	268	ASN
1	E	362	ASN
1	F	58	HIS
1	F	146	GLN
1	F	162	ASN
1	F	271	ASN
1	F	512	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 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	516/523 (98%)	-0.45	6 (1%)	76 76	8, 16, 41, 62	0
1	B	516/523 (98%)	-0.61	2 (0%)	88 88	6, 14, 34, 69	0
1	C	514/523 (98%)	-0.49	14 (2%)	56 55	8, 15, 48, 96	0
1	D	504/523 (96%)	-0.29	15 (2%)	52 51	8, 19, 45, 105	0
1	E	519/523 (99%)	-0.65	1 (0%)	91 90	7, 14, 33, 51	0
1	F	516/523 (98%)	-0.48	7 (1%)	73 73	8, 16, 37, 69	0
All	All	3085/3138 (98%)	-0.50	45 (1%)	72 71	6, 16, 39, 105	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	454	ILE	4.4
1	D	462	ALA	4.2
1	C	449	ILE	4.2
1	D	449	ILE	3.8
1	F	9	LEU	3.8
1	C	464	ARG	3.6
1	C	456	ALA	3.5
1	C	465	ALA	3.1
1	C	457	ALA	3.1
1	B	10	ALA	3.0
1	D	445	ALA	2.9
1	F	449	ILE	2.9
1	B	9	LEU	2.8
1	F	451	ARG	2.7
1	D	10	ALA	2.7
1	D	463	MET	2.7
1	F	452	LYS	2.7
1	E	6	ASN	2.6
1	A	70	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	468	ILE	2.6
1	D	468	ILE	2.6
1	C	452	LYS	2.5
1	D	450	PHE	2.5
1	A	458	ASP	2.5
1	C	460	PRO	2.5
1	D	470	GLU	2.4
1	A	463	MET	2.4
1	D	446	ALA	2.4
1	D	442	ALA	2.3
1	C	214	GLY	2.3
1	F	453	GLU	2.3
1	C	453	GLU	2.2
1	D	447	ASN	2.2
1	F	448	VAL	2.2
1	A	456	ALA	2.2
1	A	513	THR	2.2
1	C	463	MET	2.1
1	C	459	ASP	2.1
1	D	7	LEU	2.1
1	D	475	PHE	2.1
1	C	447	ASN	2.1
1	A	462	ALA	2.1
1	F	456	ALA	2.1
1	D	511	ARG	2.0
1	D	471	TYR	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
3	MCA	C	4003	26/55	0.75	0.17	62,81,94,95	0
3	MCA	B	4002	26/55	0.76	0.20	82,89,92,93	0
3	MCA	D	4004	31/55	0.77	0.15	68,89,110,110	0
3	MCA	E	4005	23/55	0.79	0.15	53,65,76,76	0
3	MCA	F	4006	27/55	0.79	0.13	41,64,82,82	0
3	MCA	A	4001	27/55	0.81	0.15	62,76,85,87	0
4	MPD	F	6006	8/8	0.91	0.09	20,24,28,35	0
2	CD	B	7002	1/1	1.00	0.01	11,11,11,11	0
2	CD	C	7003	1/1	1.00	0.01	14,14,14,14	0
2	CD	A	7001	1/1	1.00	0.01	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.