



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:47 AM UTC

PDB ID : 6LE5 / pdb_00006le5
Title : Crystal structure of the mitochondrial calcium uptake 1 and 2 heterodimer (MICU1-MICU2 heterodimer) in an apo state
Authors : Park, J.; Lee, Y.; Park, T.; Kang, J.Y.; Jin, M.; Yang, J.; Eom, S.H.
Deposited on : 2019-11-24
Resolution : 3.10 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

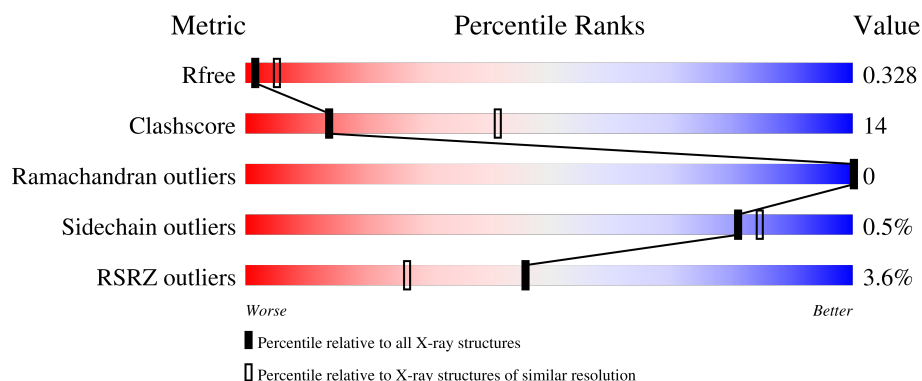
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

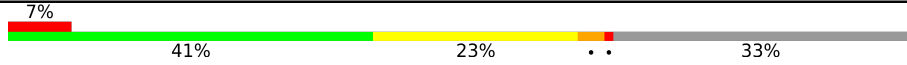
The reported resolution of this entry is 3.10 Å.

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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	348	
1	D	348	
1	E	348	
1	G	348	
2	B	325	

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Mol	Chain	Length	Quality of chain
2	C	325	60%24%14%
2	F	325	% 63%22%14%
2	H	325	2% 63%26%10%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 17392 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 Calcium uptake protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1759	1121	300	330	8			
1	D	304	Total	C	N	O	S	0	0	0
			2358	1510	390	444	14			
1	E	304	Total	C	N	O	S	0	0	0
			2380	1521	398	447	14			
1	G	236	Total	C	N	O	S	0	0	0
			1743	1113	296	327	7			

- Molecule 2 is a protein called Calcium uptake protein 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	289	Total	C	N	O	S	Se	0	0	0
			2341	1509	394	422	3	13			
2	C	280	Total	C	N	O	S	Se	0	0	0
			2258	1452	375	416	3	12			
2	F	279	Total	C	N	O	S	Se	0	0	0
			2208	1420	370	404	3	11			
2	H	291	Total	C	N	O	S	Se	0	0	0
			2345	1513	393	423	3	13			

There are 28 discrepancies between the modelled and reference sequences:

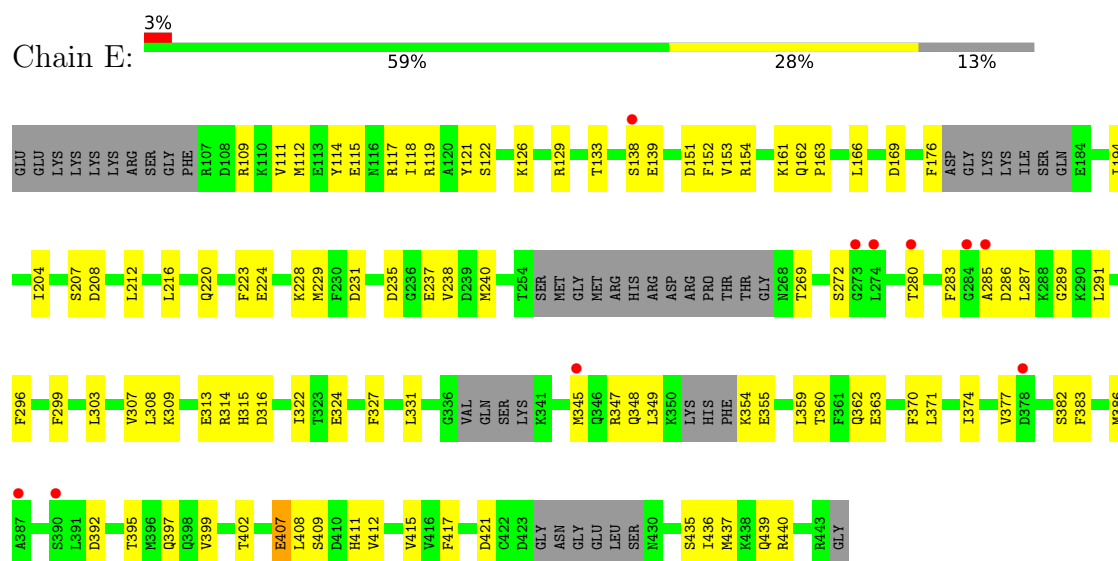
Chain	Residue	Modelled	Actual	Comment	Reference
B	77	HIS	-	expression tag	UNP Q8IYU8
B	78	HIS	-	expression tag	UNP Q8IYU8
B	79	HIS	-	expression tag	UNP Q8IYU8
B	80	HIS	-	expression tag	UNP Q8IYU8
B	81	HIS	-	expression tag	UNP Q8IYU8
B	82	HIS	-	expression tag	UNP Q8IYU8
B	83	MSE	-	expression tag	UNP Q8IYU8
C	77	HIS	-	expression tag	UNP Q8IYU8

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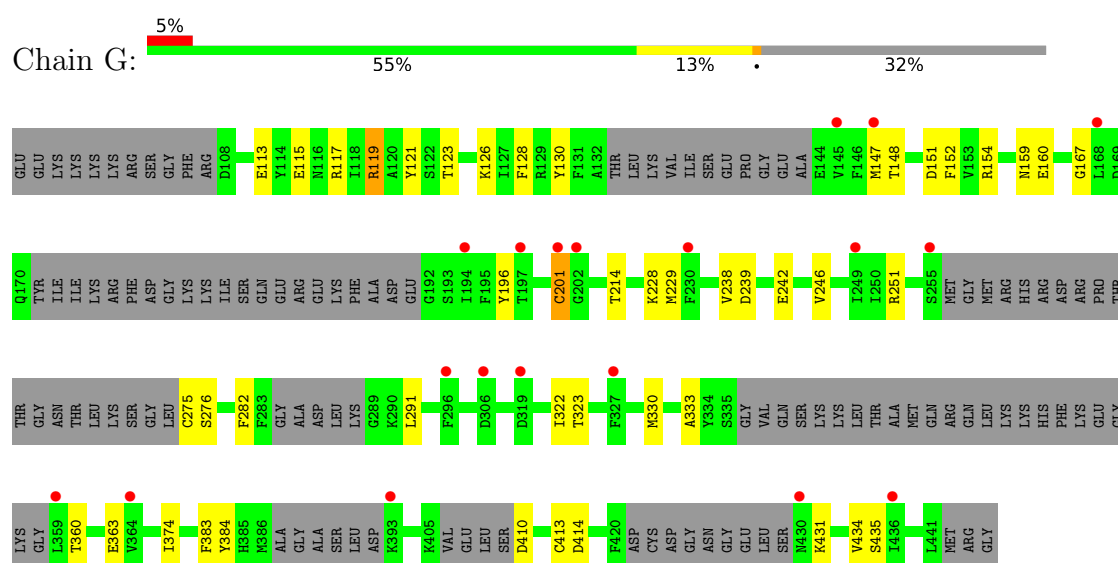
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Chain	Residue	Modelled	Actual	Comment	Reference
C	78	HIS	-	expression tag	UNP Q8IYU8
C	79	HIS	-	expression tag	UNP Q8IYU8
C	80	HIS	-	expression tag	UNP Q8IYU8
C	81	HIS	-	expression tag	UNP Q8IYU8
C	82	HIS	-	expression tag	UNP Q8IYU8
C	83	MSE	-	expression tag	UNP Q8IYU8
F	77	HIS	-	expression tag	UNP Q8IYU8
F	78	HIS	-	expression tag	UNP Q8IYU8
F	79	HIS	-	expression tag	UNP Q8IYU8
F	80	HIS	-	expression tag	UNP Q8IYU8
F	81	HIS	-	expression tag	UNP Q8IYU8
F	82	HIS	-	expression tag	UNP Q8IYU8
F	83	MSE	-	expression tag	UNP Q8IYU8
H	77	HIS	-	expression tag	UNP Q8IYU8
H	78	HIS	-	expression tag	UNP Q8IYU8
H	79	HIS	-	expression tag	UNP Q8IYU8
H	80	HIS	-	expression tag	UNP Q8IYU8
H	81	HIS	-	expression tag	UNP Q8IYU8
H	82	HIS	-	expression tag	UNP Q8IYU8
H	83	MSE	-	expression tag	UNP Q8IYU8

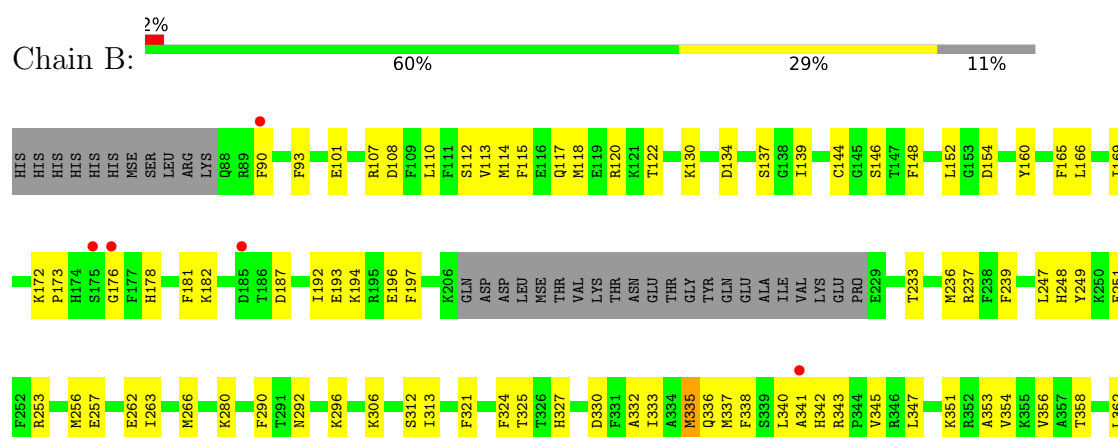
• Molecule 1: Calcium uptake protein 1, mitochondrial



• Molecule 1: Calcium uptake protein 1, mitochondrial

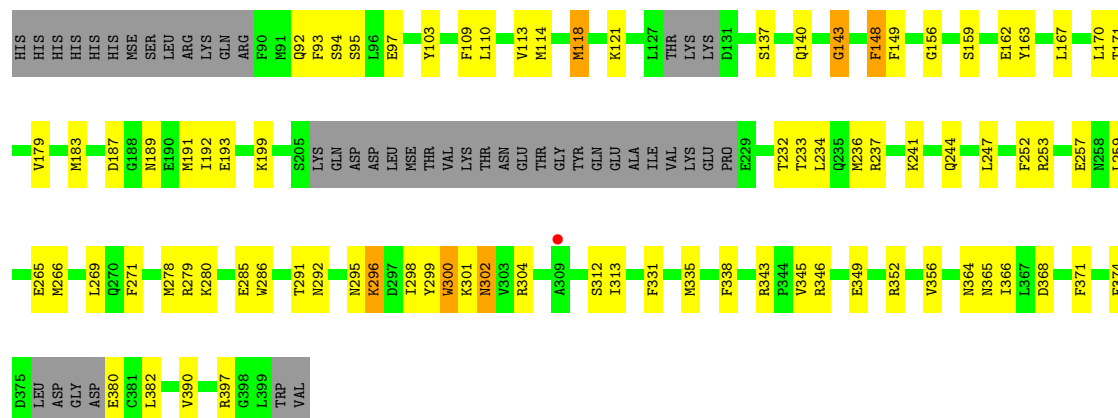


• Molecule 2: Calcium uptake protein 2, mitochondrial

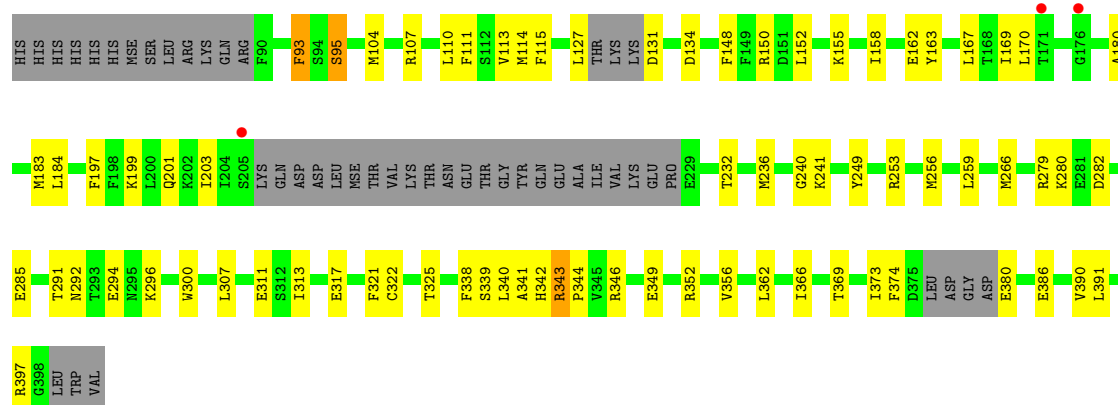




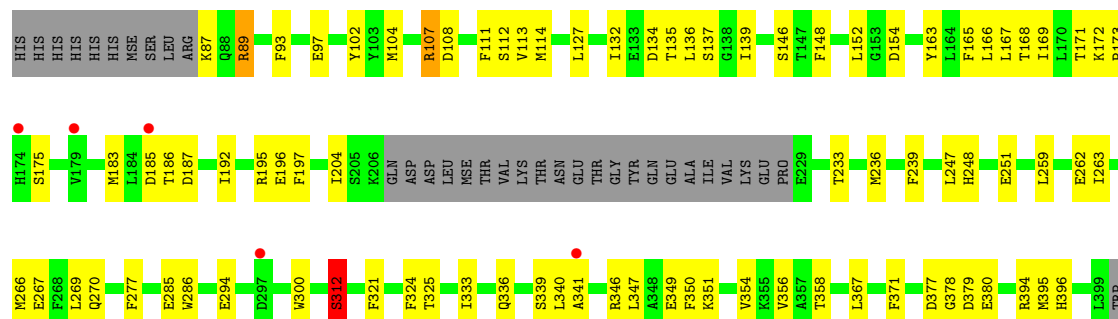
• Molecule 2: Calcium uptake protein 2, mitochondrial



• Molecule 2: Calcium uptake protein 2, mitochondrial



• Molecule 2: Calcium uptake protein 2, mitochondrial



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.97Å 173.72Å 148.00Å 90.00° 93.88° 90.00°	Depositor
Resolution (Å)	50.01 – 3.10 50.01 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.01-3.10) 99.9 (50.01-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.293 , 0.332 0.287 , 0.328	Depositor DCC
R_{free} test set	2802 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 83.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17392	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.7988e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.58	2/1787 (0.1%)	1.27	29/2411 (1.2%)
1	D	0.27	1/2401 (0.0%)	0.56	0/3239
1	E	0.33	2/2421 (0.1%)	0.63	3/3261 (0.1%)
1	G	0.18	0/1771	0.55	1/2395 (0.0%)
2	B	0.19	0/2379	0.64	7/3166 (0.2%)
2	C	0.23	0/2294	0.66	11/3054 (0.4%)
2	F	0.29	1/2243 (0.0%)	0.66	7/2994 (0.2%)
2	H	0.22	0/2383	0.59	2/3172 (0.1%)
All	All	0.30	6/17679 (0.0%)	0.71	60/23692 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	G	0	1
2	H	0	2
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	347	ARG	CA-C	5.81	1.60	1.52
2	F	340	LEU	C-O	-5.69	1.16	1.24
1	A	432	GLU	N-CA	5.68	1.53	1.45
1	A	147	MET	CA-C	-5.24	1.46	1.53
1	E	347	ARG	N-CA	-5.21	1.40	1.46
1	D	108	ASP	CA-C	5.07	1.59	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	ASP	N-CA-C	-17.13	83.60	109.81
1	A	324	GLU	CB-CA-C	14.70	139.68	110.42
1	A	324	GLU	CA-C-N	13.61	140.24	120.38
1	A	324	GLU	C-N-CA	13.61	140.24	120.38
1	A	324	GLU	N-CA-C	-13.55	81.93	110.80
2	F	344	PRO	CB-CA-C	-12.10	96.39	111.64
1	G	201	CYS	CB-CA-C	11.95	134.21	110.42
1	A	232	LEU	N-CA-C	10.44	128.74	113.40
1	A	232	LEU	CA-C-N	10.31	137.51	120.70
1	A	232	LEU	C-N-CA	10.31	137.51	120.70
1	A	433	PHE	N-CA-C	-9.11	101.04	110.97
1	A	233	ASN	N-CA-CB	-8.94	94.08	110.88
1	A	233	ASN	CB-CA-C	8.45	123.38	110.37
2	F	343	ARG	N-CA-C	8.44	128.47	109.81
2	B	187	ASP	N-CA-C	-7.96	97.89	109.59
1	A	146	PHE	CB-CA-C	-7.92	95.61	109.64
2	C	296	LYS	CB-CA-C	-7.86	95.21	110.46
2	B	395	MSE	N-CA-C	7.77	119.53	111.14
1	A	432	GLU	CA-C-O	7.60	127.20	118.77
2	C	300	TRP	CB-CA-C	-7.55	94.20	109.99
2	C	296	LYS	N-CA-C	7.30	121.09	111.75
2	C	300	TRP	N-CA-C	7.26	121.90	112.89
2	B	312	SER	N-CA-C	7.17	121.56	111.52
2	F	344	PRO	N-CA-C	7.09	121.95	111.03
1	A	394	VAL	N-CA-C	-6.70	105.95	111.91
2	F	93	PHE	CB-CA-C	6.67	121.77	109.70
1	A	432	GLU	CA-C-N	6.63	129.40	120.65
1	A	432	GLU	C-N-CA	6.63	129.40	120.65
2	B	383	SER	N-CA-C	-6.48	98.63	108.67
1	A	146	PHE	N-CA-C	6.40	118.56	110.24
1	E	139	GLU	N-CA-C	-6.39	95.69	109.81
2	B	187	ASP	CB-CA-C	6.06	119.35	110.26
1	E	139	GLU	CB-CA-C	6.04	122.07	110.17
1	A	433	PHE	N-CA-CB	-5.95	101.22	109.91
1	A	160	GLU	CB-CA-C	5.92	118.88	110.24
1	A	204	ILE	CA-C-N	5.90	133.48	122.74
1	A	204	ILE	C-N-CA	5.90	133.48	122.74
2	H	312	SER	CB-CA-C	-5.81	101.12	109.84
1	A	434	VAL	N-CA-C	5.79	117.22	110.62
1	A	436	ILE	N-CA-CB	5.77	121.22	110.77
1	A	203	LEU	CB-CA-C	-5.71	100.53	109.84
2	F	93	PHE	N-CA-C	-5.70	99.14	108.76
2	C	143	GLY	N-CA-C	-5.66	103.84	111.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	LEU	N-CA-C	5.65	118.74	109.76
1	E	402	THR	CB-CA-C	-5.50	99.78	109.02
1	A	315	HIS	N-CA-C	5.47	117.68	111.11
2	H	312	SER	N-CA-C	5.42	118.21	110.24
2	C	302	ASN	N-CA-C	-5.41	107.33	114.04
2	C	94	SER	N-CA-C	-5.33	105.47	112.72
1	A	435	SER	CA-C-N	-5.33	111.56	120.30
1	A	435	SER	C-N-CA	-5.33	111.56	120.30
2	B	335	MSE	N-CA-C	-5.26	106.99	113.41
2	C	118	MSE	CB-CA-C	-5.21	101.18	111.91
1	A	231	ASP	CB-CA-C	5.12	116.09	109.28
2	F	339	SER	N-CA-C	5.08	116.82	111.28
2	F	340	LEU	CB-CA-C	5.08	121.03	110.32
2	B	376	LEU	N-CA-C	-5.07	101.85	109.15
2	C	94	SER	CB-CA-C	-5.03	105.03	111.22
2	C	148	PHE	CA-C-N	5.00	131.09	121.54
2	C	148	PHE	C-N-CA	5.00	131.09	121.54

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	ARG	Sidechain
1	A	315	HIS	Peptide
1	A	321	ARG	Peptide
1	A	324	GLU	Peptide
1	A	431	LYS	Mainchain
1	G	119	ARG	Sidechain
2	H	107	ARG	Sidechain
2	H	89	ARG	Sidechain

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	1759	0	1548	82	0
1	D	2358	0	2222	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2380	0	2264	78	0
1	G	1743	0	1529	32	0
2	B	2341	0	2252	74	0
2	C	2258	0	2127	60	0
2	F	2208	0	2044	55	0
2	H	2345	0	2250	62	0
All	All	17392	0	16236	486	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 14.

All (486) 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:331:LEU:HD22	1:A:437:MET:HE1	1.16	1.12
1:D:371:LEU:HD21	1:D:437:MET:HB3	1.39	1.02
1:A:147:MET:SD	1:A:152:PHE:HA	2.03	0.97
1:A:119:ARG:HH11	1:A:158:PRO:HA	1.29	0.97
1:G:196:TYR:HA	1:G:201:CYS:O	1.67	0.95
2:B:120:ARG:HE	2:B:122:THR:HG22	1.32	0.91
2:F:180:ALA:O	2:F:184:LEU:HD23	1.77	0.85
2:C:189:ASN:HB3	2:C:191:MSE:HE3	1.60	0.83
2:H:146:SER:O	2:H:262:GLU:HG2	1.80	0.82
2:B:324:PHE:HA	2:B:358:THR:HG21	1.61	0.81
1:D:397:GLN:NE2	1:D:413:CYS:SG	2.53	0.81
1:A:147:MET:SD	1:A:152:PHE:CA	2.70	0.80
1:E:133:THR:HG23	1:E:151:ASP:OD2	1.82	0.79
1:E:349:LEU:HD13	1:E:354:LYS:HD2	1.64	0.79
2:B:335:MSE:HE1	2:B:345:VAL:HG21	1.66	0.78
1:A:331:LEU:CD2	1:A:437:MET:HE1	2.06	0.78
1:D:397:GLN:OE1	1:D:408:LEU:HB2	1.83	0.77
2:B:118:MSE:HE3	2:B:120:ARG:HD3	1.65	0.77
2:H:333:ILE:HA	2:H:336:GLN:HB2	1.66	0.76
1:A:147:MET:HB2	1:A:151:ASP:HB3	1.66	0.76
2:C:335:MSE:HE1	2:C:345:VAL:HG11	1.68	0.76
2:H:324:PHE:HA	2:H:358:THR:HG21	1.68	0.75
1:A:148:THR:H	1:A:151:ASP:HB2	1.51	0.75
1:A:146:PHE:CB	1:A:204:ILE:O	2.34	0.74
1:G:410:ASP:N	1:G:413:CYS:HG	1.84	0.74
2:C:265:GLU:O	2:C:269:LEU:HD23	1.87	0.74
2:C:143:GLY:O	2:C:148:PHE:HB2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASP:O	1:A:212:LEU:HB2	1.88	0.73
1:A:331:LEU:HD22	1:A:437:MET:CE	2.08	0.73
1:E:228:LYS:HA	1:E:231:ASP:OD1	1.89	0.71
1:E:324:GLU:HB3	1:E:345:MET:HE1	1.72	0.71
2:C:291:THR:HG21	2:C:390:VAL:HG13	1.73	0.71
2:F:307:LEU:HD11	2:F:369:THR:HG23	1.72	0.70
1:D:374:ILE:HD13	1:D:438:LYS:HG2	1.74	0.69
1:D:339:SER:HA	1:D:342:LEU:HB3	1.74	0.69
1:E:359:LEU:HD12	1:E:363:GLU:OE1	1.92	0.69
1:E:109:ARG:H	1:E:109:ARG:HD3	1.56	0.69
1:D:216:LEU:HD21	1:D:303:LEU:HD22	1.74	0.68
1:A:221:ARG:HH22	2:B:330:ASP:CG	2.02	0.68
1:G:113:GLU:O	1:G:117:ARG:HG2	1.94	0.68
1:D:366:ASN:HB3	1:D:406:VAL:HG11	1.75	0.68
1:D:119:ARG:NH1	1:D:154:ARG:O	2.27	0.67
2:B:172:LYS:HG3	2:B:173:PRO:HD2	1.76	0.67
2:B:146:SER:O	2:B:262:GLU:CD	2.37	0.67
1:E:163:PRO:HB2	1:E:166:LEU:HB2	1.75	0.67
1:E:138:SER:HA	1:E:176:PHE:HA	1.77	0.66
2:F:150:ARG:HG2	2:F:266:MSE:HE3	1.77	0.66
2:B:139:ILE:HD11	2:B:233:THR:HA	1.76	0.66
2:C:265:GLU:O	2:C:269:LEU:CD2	2.44	0.66
2:C:352:ARG:NH1	1:D:228:LYS:O	2.28	0.66
1:E:112:MET:HE1	1:E:161:LYS:HB2	1.78	0.65
1:E:119:ARG:NH1	1:E:154:ARG:O	2.29	0.65
2:B:292:ASN:OD1	2:B:296:LYS:NZ	2.28	0.65
1:E:231:ASP:HB2	1:E:237:GLU:O	1.96	0.65
2:H:248:HIS:HB3	2:H:251:GLU:HG2	1.78	0.65
1:D:163:PRO:HB2	1:D:166:LEU:HB2	1.78	0.65
1:A:367:PHE:O	1:A:371:LEU:HB2	1.97	0.65
2:H:104:MSE:HB2	2:H:108:ASP:HB2	1.79	0.64
1:E:238:VAL:O	1:E:291:LEU:N	2.26	0.64
2:H:136:LEU:HD13	2:H:236:MSE:HE2	1.78	0.64
1:D:280:THR:HG23	1:D:285:ALA:HA	1.79	0.63
1:A:323:THR:O	1:A:325:ARG:N	2.32	0.63
1:D:231:ASP:HB2	1:D:237:GLU:O	1.98	0.63
2:H:350:PHE:O	2:H:354:VAL:HG23	1.97	0.63
1:E:397:GLN:NE2	1:E:408:LEU:O	2.32	0.63
1:A:221:ARG:NH2	2:B:330:ASP:OD1	2.30	0.62
2:C:298:ILE:O	2:C:302:ASN:HB2	1.99	0.62
1:A:116:ASN:OD1	1:A:159:ASN:ND2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:THR:O	1:A:324:GLU:C	2.41	0.62
1:G:360:THR:HG23	1:G:363:GLU:H	1.64	0.61
1:A:252:SER:HB2	2:B:341:ALA:HB2	1.80	0.61
2:C:301:LYS:HG3	2:C:304:ARG:HE	1.64	0.61
2:B:166:LEU:HA	2:B:169:ILE:HD12	1.80	0.61
1:A:146:PHE:HB2	1:A:204:ILE:O	2.02	0.60
1:D:374:ILE:HA	1:D:377:VAL:HG12	1.82	0.60
1:A:334:TYR:HD1	1:A:440:ARG:HG2	1.66	0.60
1:G:414:ASP:OD1	1:G:414:ASP:N	2.35	0.60
1:G:384:TYR:CE2	2:H:183:MSE:HG3	2.36	0.60
1:E:314:ARG:HG2	1:E:314:ARG:O	2.00	0.60
1:E:280:THR:O	1:E:280:THR:HG22	2.00	0.60
2:C:343:ARG:HH22	1:D:230:PHE:HE1	1.49	0.60
1:E:315:HIS:HB2	1:E:322:ILE:HD11	1.84	0.60
1:E:407:GLU:HA	1:E:407:GLU:OE2	2.01	0.59
1:A:306:ASP:O	1:A:310:LEU:HG	2.02	0.59
1:E:111:VAL:O	1:E:115:GLU:HG3	2.02	0.59
1:E:133:THR:HG23	1:E:151:ASP:CG	2.27	0.59
1:E:435:SER:O	1:E:439:GLN:NE2	2.34	0.59
2:B:120:ARG:HG3	2:B:122:THR:H	1.68	0.59
2:C:93:PHE:CD2	2:C:95:SER:HB2	2.37	0.59
1:A:119:ARG:NH1	1:A:158:PRO:HA	2.08	0.59
1:A:371:LEU:HD11	1:A:437:MET:SD	2.42	0.59
1:D:362:GLN:OE1	1:D:362:GLN:N	2.32	0.59
2:H:113:VAL:HG23	2:H:114:MSE:HG2	1.85	0.58
1:D:133:THR:HG23	1:D:151:ASP:OD2	2.03	0.58
2:C:92:GLN:O	2:C:92:GLN:NE2	2.36	0.58
1:A:282:PHE:HB3	1:A:291:LEU:HD22	1.84	0.58
2:F:93:PHE:CE2	2:F:95:SER:OG	2.50	0.58
1:D:374:ILE:HD11	1:D:434:VAL:HA	1.84	0.58
2:H:377:ASP:N	2:H:378:GLY:HA3	2.18	0.58
2:B:333:ILE:O	2:B:337:MSE:HG2	2.04	0.57
1:A:231:ASP:OD1	1:A:234:GLY:CA	2.52	0.57
1:D:321:ARG:HD3	1:D:321:ARG:N	2.19	0.57
1:G:119:ARG:HH22	1:G:160:GLU:H	1.51	0.57
2:B:354:VAL:HG11	2:B:362:LEU:HD22	1.87	0.57
2:F:346:ARG:HB2	2:F:349:GLU:OE1	2.04	0.57
1:G:119:ARG:NH1	1:G:154:ARG:O	2.38	0.57
1:A:231:ASP:OD1	1:A:235:ASP:O	2.22	0.57
2:F:292:ASN:HA	2:F:296:LYS:HD3	1.86	0.57
2:B:192:ILE:HG23	2:B:247:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:347:LEU:HA	2:H:371:PHE:CZ	2.40	0.56
2:F:280:LYS:HE3	2:F:311:GLU:O	2.05	0.56
2:F:291:THR:HG21	2:F:390:VAL:HG13	1.86	0.56
2:C:295:ASN:O	2:C:299:TYR:CD1	2.59	0.56
1:E:371:LEU:HD11	1:E:440:ARG:HB3	1.87	0.56
2:H:173:PRO:HG2	2:H:395:MSE:HE1	1.87	0.56
1:E:133:THR:HB	1:E:166:LEU:HD13	1.88	0.56
2:B:118:MSE:CE	2:B:120:ARG:HD3	2.35	0.56
1:E:121:TYR:HB2	2:H:294:GLU:HG2	1.86	0.56
1:A:146:PHE:CB	1:A:204:ILE:C	2.79	0.56
1:A:146:PHE:HB2	1:A:204:ILE:H	1.71	0.56
1:E:283:PHE:O	1:E:289:GLY:HA3	2.06	0.56
2:B:166:LEU:HD23	2:B:169:ILE:HD12	1.88	0.55
2:H:139:ILE:HD11	2:H:233:THR:HA	1.88	0.55
2:C:371:PHE:CE2	2:C:382:LEU:HB2	2.42	0.55
2:B:248:HIS:O	2:B:251:GLU:HG2	2.06	0.55
2:B:280:LYS:HG2	2:B:313:ILE:HD11	1.88	0.55
2:B:332:ALA:O	2:B:336:GLN:N	2.33	0.55
1:A:146:PHE:HB3	1:A:204:ILE:C	2.31	0.55
1:A:252:SER:CB	2:B:341:ALA:HB2	2.35	0.55
2:F:343:ARG:HH21	2:F:343:ARG:HG2	1.71	0.55
2:H:134:ASP:HA	2:H:137:SER:HB3	1.89	0.55
1:A:147:MET:SD	1:A:152:PHE:CB	2.95	0.55
2:C:253:ARG:O	2:C:257:GLU:HG2	2.07	0.54
1:G:214:THR:HG21	1:G:251:ARG:HG3	1.87	0.54
1:A:146:PHE:CA	1:A:204:ILE:O	2.55	0.54
2:C:280:LYS:HE2	2:C:365:ASN:HB2	1.89	0.54
2:C:364:ASN:O	2:C:368:ASP:HB3	2.08	0.54
2:H:262:GLU:O	2:H:266:MSE:HG2	2.08	0.54
1:A:334:TYR:HE1	1:A:440:ARG:NH1	2.05	0.54
2:B:114:MSE:HG3	2:B:266:MSE:HE2	1.89	0.54
2:C:109:PHE:O	2:C:113:VAL:HG23	2.08	0.54
1:A:145:VAL:HG12	1:A:145:VAL:O	2.08	0.54
2:F:294:GLU:HG2	1:G:121:TYR:HB2	1.89	0.54
1:E:386:MET:HB3	2:F:203:ILE:HA	1.90	0.54
1:E:417:PHE:HB3	1:E:421:ASP:OD1	2.08	0.54
1:A:147:MET:HE1	1:A:209:TYR:CD1	2.43	0.53
1:E:240:MET:HE1	1:E:287:LEU:HG	1.89	0.53
2:H:172:LYS:HB3	2:H:175:SER:HB2	1.89	0.53
1:A:371:LEU:CD1	1:A:437:MET:SD	2.95	0.53
1:D:236:GLY:O	1:D:293:ILE:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:SER:HB3	1:E:412:VAL:HG13	1.90	0.53
2:C:110:LEU:HD13	2:C:266:MSE:SE	2.58	0.53
1:D:109:ARG:O	1:D:112:MET:N	2.41	0.53
1:E:359:LEU:HD11	1:E:412:VAL:HG12	1.91	0.53
1:A:239:ASP:OD2	1:A:242:GLU:HG3	2.08	0.53
1:A:433:PHE:CE1	1:A:437:MET:HG3	2.43	0.53
1:A:334:TYR:O	1:A:335:SER:CB	2.56	0.53
1:A:433:PHE:CD1	1:A:433:PHE:C	2.85	0.53
1:D:397:GLN:OE1	1:D:397:GLN:HA	2.08	0.53
1:G:147:MET:HE3	1:G:152:PHE:HA	1.91	0.52
2:F:150:ARG:CG	2:F:266:MSE:HE3	2.38	0.52
2:F:313:ILE:HG21	2:F:366:ILE:HD11	1.89	0.52
2:B:262:GLU:O	2:B:266:MSE:HG2	2.10	0.52
1:G:115:GLU:O	1:G:119:ARG:HG3	2.09	0.52
1:A:305:HIS:ND1	1:A:365:GLU:OE2	2.34	0.52
1:A:334:TYR:CD1	1:A:440:ARG:HG2	2.44	0.52
1:D:214:THR:HG21	1:D:251:ARG:HB2	1.91	0.52
2:F:321:PHE:O	2:F:325:THR:HG23	2.10	0.52
2:F:104:MSE:HB3	2:F:158:ILE:HB	1.92	0.52
1:A:231:ASP:OD1	1:A:234:GLY:N	2.44	0.51
2:F:111:PHE:HD1	2:F:115:PHE:HE2	1.57	0.51
1:E:153:VAL:HG22	1:E:307:VAL:HG13	1.92	0.51
1:E:228:LYS:O	2:F:352:ARG:NH1	2.38	0.51
1:A:324:GLU:O	1:A:327:PHE:N	2.36	0.51
1:E:395:THR:O	1:E:399:VAL:HG23	2.11	0.51
2:F:110:LEU:HD13	2:F:266:MSE:HE3	1.93	0.51
2:H:351:LYS:HG2	2:H:367:LEU:HD21	1.92	0.51
1:E:327:PHE:CG	1:E:359:LEU:HD23	2.45	0.51
2:F:322:CYS:O	2:F:325:THR:OG1	2.22	0.51
1:E:114:TYR:CZ	1:E:118:ILE:HD11	2.46	0.51
2:B:371:PHE:CE1	2:B:382:LEU:HB2	2.46	0.51
1:A:147:MET:SD	1:A:152:PHE:HB2	2.50	0.50
2:B:341:ALA:O	2:B:342:HIS:C	2.53	0.50
1:A:147:MET:HB2	1:A:151:ASP:CB	2.39	0.50
1:E:122:SER:OG	1:E:126:LYS:HD2	2.11	0.50
2:B:335:MSE:CE	2:B:345:VAL:HG21	2.39	0.50
2:B:120:ARG:HG3	2:B:122:THR:N	2.26	0.50
2:F:386:GLU:O	2:F:390:VAL:HG23	2.11	0.50
1:G:228:LYS:HD2	2:H:356:VAL:HG23	1.93	0.50
2:H:97:GLU:HG3	2:H:102:TYR:CE1	2.47	0.50
2:C:187:ASP:HB2	2:C:189:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:146:SER:O	2:H:262:GLU:CG	2.55	0.50
2:C:331:PHE:O	2:C:335:MSE:HG2	2.12	0.50
1:D:286:ASP:OD1	1:D:286:ASP:N	2.37	0.50
1:E:129:ARG:HD3	1:E:269:THR:HA	1.94	0.50
1:E:370:PHE:CE1	1:E:377:VAL:HG21	2.47	0.50
2:H:114:MSE:HG3	2:H:266:MSE:HE2	1.94	0.50
2:B:192:ILE:HG13	2:B:196:GLU:HB2	1.93	0.50
1:D:151:ASP:OD1	1:D:154:ARG:NH2	2.32	0.50
1:D:409:SER:O	1:D:412:VAL:HG22	2.11	0.50
1:G:128:PHE:CE1	1:G:147:MET:HG3	2.47	0.50
1:A:224:GLU:HA	1:A:293:ILE:HD12	1.94	0.49
1:A:231:ASP:OD1	1:A:235:ASP:N	2.45	0.49
2:C:167:LEU:O	2:C:171:THR:HG22	2.11	0.49
2:B:335:MSE:HE1	2:B:345:VAL:HG11	1.93	0.49
2:C:179:VAL:O	2:C:183:MSE:HG2	2.12	0.49
2:H:107:ARG:NH2	2:H:154:ASP:OD2	2.46	0.49
2:H:286:TRP:O	2:H:394:ARG:NH1	2.45	0.49
2:C:97:GLU:HB3	2:C:103:TYR:HB2	1.94	0.49
2:C:295:ASN:HB2	2:C:299:TYR:CE1	2.47	0.49
1:D:238:VAL:O	1:D:291:LEU:N	2.27	0.49
1:A:123:THR:HG23	1:A:126:LYS:H	1.77	0.49
2:B:93:PHE:O	2:B:120:ARG:NH2	2.46	0.49
2:F:110:LEU:HD13	2:F:266:MSE:CE	2.42	0.49
2:H:195:ARG:NH1	2:H:196:GLU:OE2	2.46	0.49
2:F:341:ALA:O	2:F:342:HIS:C	2.53	0.49
1:A:158:PRO:HG2	1:A:333:ALA:O	2.13	0.49
2:C:313:ILE:HG21	2:C:366:ILE:HD11	1.95	0.49
1:D:312:PHE:CE2	1:D:361:PHE:HB2	2.47	0.49
2:F:148:PHE:O	2:F:152:LEU:HG	2.13	0.49
1:E:348:GLN:O	1:E:349:LEU:HD23	2.13	0.48
2:C:295:ASN:O	2:C:299:TYR:HD1	1.96	0.48
1:D:291:LEU:HD22	1:D:296:PHE:HB2	1.94	0.48
1:A:237:GLU:HA	1:A:292:THR:HA	1.96	0.48
2:F:325:THR:HG22	2:F:391:LEU:HD21	1.95	0.48
2:B:113:VAL:HG21	2:B:263:ILE:HD12	1.96	0.48
2:F:199:LYS:O	2:F:203:ILE:N	2.42	0.48
1:G:242:GLU:O	1:G:246:VAL:HG23	2.13	0.48
1:G:330:MET:HA	1:G:333:ALA:HB2	1.96	0.48
2:H:336:GLN:O	2:H:340:LEU:N	2.41	0.48
1:D:360:THR:OG1	1:D:361:PHE:N	2.46	0.48
1:A:433:PHE:HE1	1:A:437:MET:HG3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:343:ARG:HG2	2:F:343:ARG:NH2	2.28	0.48
2:H:321:PHE:O	2:H:325:THR:HG23	2.14	0.48
1:D:323:THR:HB	1:D:326:GLN:HB2	1.94	0.48
1:E:194:ILE:HD11	1:E:299:PHE:CE1	2.49	0.48
1:G:128:PHE:HE1	1:G:147:MET:HG3	1.79	0.48
2:B:321:PHE:O	2:B:325:THR:HG23	2.13	0.48
2:C:352:ARG:O	2:C:356:VAL:HG12	2.14	0.47
2:F:110:LEU:O	2:F:114:MSE:HG2	2.14	0.47
2:F:294:GLU:CD	2:F:294:GLU:H	2.22	0.47
1:D:150:GLU:OE1	1:D:150:GLU:N	2.42	0.47
1:E:440:ARG:HD2	1:E:440:ARG:HA	1.65	0.47
2:H:87:LYS:C	2:H:89:ARG:H	2.21	0.47
2:H:89:ARG:NH2	2:H:112:SER:O	2.47	0.47
2:F:107:ARG:O	2:F:111:PHE:CD2	2.67	0.47
1:E:360:THR:HG22	1:E:363:GLU:CD	2.38	0.47
2:F:241:LYS:H	2:F:241:LYS:HD2	1.79	0.47
2:F:285:GLU:HA	2:F:300:TRP:CH2	2.49	0.47
2:C:137:SER:O	2:C:140:GLN:HG2	2.13	0.47
1:A:239:ASP:CG	1:A:242:GLU:HG3	2.40	0.47
2:B:115:PHE:CD2	2:B:118:MSE:SE	3.17	0.47
1:D:133:THR:HG23	1:D:151:ASP:CG	2.39	0.47
1:D:156:ILE:HD12	1:D:442:MET:HE1	1.97	0.47
2:F:369:THR:O	2:F:373:ILE:HG13	2.15	0.47
1:D:309:LYS:O	1:D:313:GLU:HG2	2.15	0.47
1:E:207:SER:HB3	1:E:272:SER:HB2	1.96	0.47
2:F:374:PHE:HE2	2:F:390:VAL:HG21	1.78	0.47
1:G:148:THR:HG23	1:G:151:ASP:H	1.80	0.47
2:H:186:THR:OG1	2:H:187:ASP:N	2.47	0.47
1:A:119:ARG:HH11	1:A:158:PRO:CA	2.16	0.47
2:B:90:PHE:CZ	2:B:160:TYR:HB2	2.50	0.47
2:B:236:MSE:HE2	2:B:236:MSE:HB3	1.86	0.47
2:F:113:VAL:HG12	2:F:397:ARG:NH1	2.30	0.47
2:B:114:MSE:HE3	2:B:114:MSE:HB3	1.85	0.47
2:B:148:PHE:CZ	2:B:152:LEU:HD11	2.49	0.47
1:D:274:LEU:O	1:D:275:CYS:SG	2.73	0.47
2:H:192:ILE:HG23	2:H:247:LEU:HB3	1.97	0.46
2:C:118:MSE:O	2:C:121:LYS:NZ	2.48	0.46
1:D:227:PHE:CE2	1:D:238:VAL:HG12	2.51	0.46
2:H:163:TYR:CZ	2:H:167:LEU:HD11	2.49	0.46
2:B:115:PHE:HD2	2:B:118:MSE:SE	2.48	0.46
2:B:165:PHE:CE2	2:B:169:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:PHE:CZ	2:B:397:ARG:HB3	2.51	0.46
2:B:327:HIS:HB2	2:B:358:THR:HG22	1.97	0.46
1:D:211:PHE:O	1:D:215:VAL:HG23	2.15	0.46
2:F:127:LEU:O	2:F:131:ASP:N	2.48	0.46
1:A:396:MET:O	1:A:399:VAL:N	2.48	0.46
2:B:337:MSE:O	2:B:340:LEU:O	2.33	0.46
2:C:271:PHE:HB2	2:C:278:MSE:HE2	1.96	0.46
2:F:150:ARG:HG2	2:F:266:MSE:CE	2.45	0.46
2:F:232:THR:O	2:F:236:MSE:HG3	2.14	0.46
1:A:242:GLU:O	1:A:246:VAL:HG23	2.15	0.46
2:H:165:PHE:CE2	2:H:169:ILE:HD11	2.50	0.46
2:H:259:LEU:O	2:H:262:GLU:HB2	2.15	0.46
2:H:294:GLU:CD	2:H:294:GLU:H	2.24	0.46
1:A:253:GLN:HE22	2:B:340:LEU:HB2	1.81	0.46
1:A:309:LYS:O	1:A:313:GLU:CB	2.63	0.46
1:E:382:SER:O	1:E:386:MET:HG2	2.16	0.46
1:E:436:ILE:HA	1:E:439:GLN:HE21	1.81	0.46
2:F:134:ASP:OD2	2:F:155:LYS:HG2	2.15	0.46
1:G:130:TYR:HA	1:G:167:GLY:O	2.15	0.46
1:A:147:MET:N	1:A:204:ILE:O	2.49	0.46
2:C:113:VAL:O	2:C:397:ARG:HD3	2.15	0.46
2:C:352:ARG:HH22	1:D:233:ASN:C	2.23	0.46
1:G:383:PHE:HB2	2:H:183:MSE:SE	2.65	0.46
1:D:153:VAL:HG21	1:D:310:LEU:HB2	1.98	0.46
2:F:338:PHE:O	2:F:342:HIS:O	2.34	0.46
1:D:153:VAL:HG22	1:D:307:VAL:HG13	1.98	0.45
2:C:247:LEU:HD11	2:C:252:PHE:HB2	1.99	0.45
1:E:360:THR:HG22	1:E:363:GLU:OE1	2.15	0.45
1:A:221:ARG:O	1:A:225:ILE:HG13	2.17	0.45
1:D:374:ILE:HD12	1:D:437:MET:HB2	1.98	0.45
1:D:430:ASN:C	1:D:432:GLU:H	2.24	0.45
1:E:283:PHE:O	1:E:289:GLY:CA	2.64	0.45
1:A:167:GLY:O	1:A:169:ASP:N	2.50	0.45
1:D:227:PHE:CD2	1:D:293:ILE:HG12	2.51	0.45
1:E:417:PHE:O	1:E:421:ASP:OD1	2.35	0.45
2:F:197:PHE:O	2:F:201:GLN:HG3	2.16	0.45
2:H:89:ARG:NH1	2:H:93:PHE:HE2	2.13	0.45
1:D:322:ILE:N	1:D:359:LEU:O	2.50	0.45
1:A:162:GLN:HB3	1:A:163:PRO:HD2	1.99	0.45
2:H:146:SER:C	2:H:262:GLU:HG2	2.41	0.45
2:H:379:ASP:O	2:H:380:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:ILE:CG2	2:B:247:LEU:HB3	2.46	0.45
2:C:278:MSE:O	2:C:312:SER:OG	2.29	0.45
1:E:383:PHE:HB3	2:F:183:MSE:SE	2.67	0.45
2:B:110:LEU:HD22	2:B:266:MSE:SE	2.67	0.45
2:B:306:LYS:O	2:B:372:LYS:HD2	2.16	0.45
2:C:269:LEU:HD22	2:C:269:LEU:N	2.32	0.45
1:A:224:GLU:HG2	1:A:293:ILE:HD13	2.00	0.44
1:A:227:PHE:HD2	1:A:293:ILE:HB	1.81	0.44
1:D:442:MET:O	1:D:443:ARG:HG2	2.17	0.44
1:E:129:ARG:HD2	1:E:169:ASP:OD1	2.17	0.44
1:E:229:MET:HE3	1:E:229:MET:HB3	1.77	0.44
2:C:156:GLY:HA2	2:C:233:THR:HG21	1.98	0.44
2:C:170:LEU:HD21	2:C:259:LEU:HG	2.00	0.44
1:E:308:LEU:HD23	1:E:308:LEU:HA	1.81	0.44
1:E:355:GLU:O	1:E:355:GLU:HG2	2.17	0.44
1:G:431:LYS:O	1:G:435:SER:OG	2.35	0.44
1:A:119:ARG:HH21	1:A:131:PHE:HZ	1.65	0.44
2:B:178:HIS:NE2	2:B:182:LYS:HE2	2.32	0.44
1:D:136:VAL:HA	1:D:174:LYS:HB2	1.98	0.44
1:G:148:THR:O	1:G:151:ASP:N	2.51	0.44
2:C:301:LYS:HG2	2:C:304:ARG:HH21	1.81	0.44
1:D:194:ILE:O	1:D:197:THR:HG23	2.18	0.44
1:E:151:ASP:OD1	1:E:154:ARG:NH2	2.35	0.44
2:H:148:PHE:CZ	2:H:152:LEU:HD11	2.51	0.44
2:B:172:LYS:NZ	2:B:176:GLY:O	2.51	0.44
2:B:365:ASN:O	2:B:369:THR:OG1	2.34	0.44
2:H:192:ILE:HD11	2:H:197:PHE:HA	2.00	0.44
2:H:285:GLU:HA	2:H:300:TRP:HH2	1.83	0.44
1:A:210:ILE:O	1:A:214:THR:HG23	2.18	0.44
2:C:338:PHE:CE2	2:C:349:GLU:HG2	2.52	0.44
1:G:147:MET:CE	1:G:152:PHE:HA	2.46	0.44
2:H:266:MSE:O	2:H:270:GLN:HG2	2.18	0.44
1:A:433:PHE:C	1:A:433:PHE:HD1	2.26	0.44
2:B:351:LYS:HG2	2:B:367:LEU:HD21	2.00	0.44
1:D:200:GLU:O	1:D:202:GLY:N	2.50	0.44
2:F:249:TYR:O	2:F:253:ARG:N	2.44	0.44
2:H:168:THR:HG21	2:H:204:ILE:HG21	2.00	0.44
1:A:278:LEU:HD12	1:A:281:TYR:HB3	2.00	0.44
1:A:400:ALA:HA	1:A:404:ALA:HB3	2.00	0.44
1:G:123:THR:HG23	1:G:126:LYS:H	1.83	0.44
1:E:223:PHE:CD2	1:E:296:PHE:HE2	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:HIS:O	1:E:415:VAL:HG23	2.18	0.43
2:H:127:LEU:HD21	2:H:132:ILE:HG23	1.99	0.43
1:A:371:LEU:HG	1:A:437:MET:SD	2.58	0.43
1:D:227:PHE:CE1	1:D:246:VAL:HG11	2.54	0.43
1:A:116:ASN:N	1:A:116:ASN:HD22	2.14	0.43
2:C:159:SER:OG	2:C:162:GLU:HG3	2.18	0.43
1:E:371:LEU:HD21	1:E:437:MET:O	2.17	0.43
2:F:279:ARG:HB3	2:F:282:ASP:OD2	2.19	0.43
2:B:93:PHE:CE2	2:B:112:SER:HA	2.53	0.43
2:C:114:MSE:HE1	2:C:266:MSE:SE	2.68	0.43
2:B:181:PHE:CG	2:B:249:TYR:HD1	2.37	0.43
1:E:231:ASP:OD2	1:E:235:ASP:O	2.36	0.43
2:H:107:ARG:HD2	2:H:111:PHE:CZ	2.54	0.43
2:B:139:ILE:HD12	2:B:236:MSE:HB2	2.00	0.43
2:C:148:PHE:O	2:C:149:PHE:HB2	2.18	0.43
2:C:271:PHE:CE1	2:C:286:TRP:HD1	2.36	0.43
1:D:208:ASP:O	1:D:212:LEU:HG	2.18	0.43
1:D:395:THR:O	1:D:399:VAL:HG23	2.19	0.43
2:F:169:ILE:HG23	2:F:256:MSE:HG2	2.00	0.43
1:E:133:THR:CG2	1:E:151:ASP:OD2	2.60	0.43
2:H:267:GLU:OE2	2:H:394:ARG:NH2	2.51	0.43
2:B:192:ILE:HD11	2:B:196:GLU:C	2.44	0.43
2:B:347:LEU:HA	2:B:371:PHE:CZ	2.54	0.43
2:C:352:ARG:HH12	1:D:234:GLY:HA2	1.82	0.43
1:D:397:GLN:CD	1:D:413:CYS:SG	3.02	0.43
2:H:135:THR:HG23	2:H:233:THR:HG23	2.00	0.43
1:D:188:PHE:HD2	1:D:201:CYS:O	2.02	0.43
1:E:231:ASP:CG	1:E:235:ASP:O	2.61	0.43
2:H:346:ARG:HB2	2:H:349:GLU:OE1	2.19	0.43
1:A:321:ARG:O	1:A:323:THR:CB	2.67	0.42
1:A:372:LYS:HE2	1:A:372:LYS:HA	2.00	0.42
2:C:192:ILE:HG12	2:C:193:GLU:H	1.84	0.42
2:C:292:ASN:HA	2:C:296:LYS:HE3	2.00	0.42
1:D:392:ASP:N	1:D:395:THR:OG1	2.50	0.42
1:E:152:PHE:HB2	1:E:204:ILE:HD12	2.01	0.42
1:E:154:ARG:NE	1:E:162:GLN:OE1	2.46	0.42
1:E:327:PHE:CZ	1:E:331:LEU:HD11	2.54	0.42
2:B:338:PHE:HB3	2:B:343:ARG:O	2.18	0.42
1:D:220:GLN:O	1:D:224:GLU:HG3	2.19	0.42
1:E:117:ARG:HB3	2:H:294:GLU:HG3	2.02	0.42
2:B:107:ARG:NH1	2:B:154:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:ASP:HA	2:B:137:SER:HB3	2.01	0.42
1:D:398:GLN:OE1	1:D:398:GLN:HA	2.19	0.42
1:G:239:ASP:H	1:G:242:GLU:HB2	1.84	0.42
2:F:170:LEU:HD21	2:F:259:LEU:HG	2.02	0.42
1:G:229:MET:HE3	1:G:229:MET:HB3	1.83	0.42
2:H:185:ASP:OD2	2:H:196:GLU:HG3	2.20	0.42
2:B:280:LYS:NZ	2:B:368:ASP:OD2	2.52	0.42
2:C:244:GLN:OE1	1:E:286:ASP:HB2	2.19	0.42
2:C:346:ARG:NH1	2:C:380:GLU:O	2.53	0.42
1:D:324:GLU:H	1:D:324:GLU:HG2	1.62	0.42
1:E:377:VAL:HG23	1:E:399:VAL:HG12	2.01	0.42
1:E:409:SER:O	1:E:412:VAL:HG22	2.20	0.42
2:B:117:GLN:C	2:B:118:MSE:HG3	2.43	0.42
2:B:146:SER:O	2:B:262:GLU:CG	2.68	0.42
2:C:285:GLU:HA	2:C:300:TRP:CH2	2.55	0.42
2:H:89:ARG:NH1	2:H:93:PHE:CE2	2.87	0.42
2:B:114:MSE:SE	2:B:266:MSE:HE2	2.70	0.42
2:B:144:CYS:HA	2:B:237:ARG:HH21	1.83	0.42
2:B:169:ILE:HG23	2:B:256:MSE:HE3	2.02	0.42
2:C:192:ILE:HG22	2:C:247:LEU:HB3	2.02	0.42
1:D:337:VAL:HG13	1:D:337:VAL:O	2.19	0.42
2:H:166:LEU:HD23	2:H:169:ILE:HD12	2.01	0.42
2:H:197:PHE:HB2	2:H:239:PHE:CZ	2.54	0.42
1:A:313:GLU:O	1:A:317:PRO:HG3	2.20	0.42
2:B:107:ARG:NH2	2:C:279:ARG:HB2	2.34	0.42
2:C:269:LEU:HD22	2:C:269:LEU:H	1.85	0.42
2:C:374:PHE:HE2	2:C:390:VAL:HG21	1.84	0.42
1:E:392:ASP:HA	1:E:417:PHE:CZ	2.55	0.42
1:E:408:LEU:HD23	1:E:408:LEU:HA	1.84	0.42
2:H:339:SER:C	2:H:341:ALA:H	2.28	0.42
1:G:275:CYS:HB2	1:G:276:SER:H	1.58	0.42
1:A:125:ASP:O	1:A:129:ARG:HG3	2.20	0.41
2:B:108:ASP:O	2:B:112:SER:OG	2.28	0.41
1:E:280:THR:HG23	1:E:285:ALA:HA	2.02	0.41
1:E:315:HIS:O	1:E:316:ASP:HB2	2.20	0.41
2:C:162:GLU:HB3	2:C:234:LEU:HD12	2.02	0.41
1:D:315:HIS:HB3	1:D:326:GLN:OE1	2.20	0.41
2:F:236:MSE:HA	2:F:240:GLY:O	2.20	0.41
2:F:321:PHE:HA	2:F:362:LEU:HD21	2.02	0.41
2:H:113:VAL:HG21	2:H:263:ILE:HD12	2.02	0.41
2:B:193:GLU:HG3	2:B:194:LYS:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:362:GLN:OE1	1:E:362:GLN:N	2.43	0.41
2:H:114:MSE:HE2	2:H:270:GLN:HG3	2.03	0.41
2:C:232:THR:O	2:C:236:MSE:HG3	2.20	0.41
2:F:338:PHE:CE2	2:F:349:GLU:HG2	2.55	0.41
1:G:238:VAL:O	1:G:291:LEU:N	2.35	0.41
1:A:372:LYS:O	1:A:374:ILE:HG22	2.21	0.41
1:D:440:ARG:C	1:D:442:MET:H	2.28	0.41
2:F:163:TYR:CZ	2:F:167:LEU:HD11	2.56	0.41
1:E:216:LEU:HD21	1:E:303:LEU:HD22	2.03	0.41
1:E:309:LYS:O	1:E:313:GLU:HG2	2.21	0.41
2:F:352:ARG:O	2:F:356:VAL:HG23	2.21	0.41
2:F:380:GLU:O	2:F:380:GLU:HG3	2.20	0.41
1:G:322:ILE:O	1:G:323:THR:HG22	2.20	0.41
2:H:247:LEU:HD12	2:H:251:GLU:OE2	2.21	0.41
1:A:115:GLU:OE1	1:A:161:LYS:HA	2.20	0.41
1:A:226:ALA:O	1:A:230:PHE:HD1	2.03	0.41
2:C:233:THR:O	2:C:237:ARG:HB2	2.21	0.41
1:A:368:PHE:HA	1:A:371:LEU:HB3	2.01	0.41
2:C:191:MSE:HE2	2:C:191:MSE:HB3	1.93	0.41
1:D:138:SER:H	1:D:175:ARG:HB2	1.86	0.41
1:E:280:THR:O	1:E:280:THR:CG2	2.68	0.41
2:H:171:THR:HG23	2:H:396:HIS:HA	2.01	0.41
2:H:259:LEU:O	2:H:263:ILE:HG12	2.21	0.41
1:A:229:MET:HE3	1:A:229:MET:HB3	1.87	0.41
2:C:163:TYR:CZ	2:C:167:LEU:HD11	2.56	0.41
2:C:199:LYS:HD2	2:C:199:LYS:HA	1.86	0.41
1:E:228:LYS:HB3	2:F:356:VAL:HG22	2.02	0.41
1:A:109:ARG:HD2	1:A:112:MET:SD	2.60	0.40
2:B:197:PHE:HB2	2:B:239:PHE:CZ	2.56	0.40
1:E:208:ASP:O	1:E:212:LEU:HG	2.20	0.40
1:E:220:GLN:O	1:E:224:GLU:HG3	2.21	0.40
2:F:279:ARG:O	2:F:282:ASP:HB2	2.21	0.40
1:G:282:PHE:CG	1:G:291:LEU:HD22	2.56	0.40
1:G:374:ILE:HD11	1:G:434:VAL:HG13	2.02	0.40
1:A:316:ASP:CB	1:A:326:GLN:HE22	2.34	0.40
2:B:130:LYS:HB3	2:B:130:LYS:HE3	1.82	0.40
2:B:165:PHE:O	2:B:169:ILE:HG13	2.21	0.40
1:D:276:SER:C	1:D:278:LEU:H	2.29	0.40
2:H:277:PHE:HB3	2:H:312:SER:HB2	2.03	0.40
2:B:253:ARG:O	2:B:257:GLU:HG2	2.21	0.40
2:B:353:ALA:HA	2:B:356:VAL:HG12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:159:ASN:O	1:G:160:GLU:HG2	2.20	0.40
2:B:107:ARG:NH2	2:B:154:ASP:OD2	2.54	0.40
1:D:441:LEU:HD23	1:D:441:LEU:HA	1.98	0.40
1:E:374:ILE:HA	1:E:377:VAL:HG12	2.03	0.40
2:F:313:ILE:HG23	2:F:317:GLU:HB2	2.02	0.40
2:H:269:LEU:HD13	2:H:269:LEU:HA	1.85	0.40
1:A:227:PHE:CD2	1:A:293:ILE:HB	2.55	0.40
2:F:162:GLU:OE2	2:F:232:THR:HG21	2.22	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	214/348 (62%)	189 (88%)	25 (12%)	0	100	100
1	D	294/348 (84%)	274 (93%)	20 (7%)	0	100	100
1	E	292/348 (84%)	276 (94%)	16 (6%)	0	100	100
1	G	218/348 (63%)	192 (88%)	26 (12%)	0	100	100
2	B	285/325 (88%)	277 (97%)	8 (3%)	0	100	100
2	C	272/325 (84%)	259 (95%)	13 (5%)	0	100	100
2	F	271/325 (83%)	260 (96%)	11 (4%)	0	100	100
2	H	287/325 (88%)	275 (96%)	12 (4%)	0	100	100
All	All	2133/2692 (79%)	2002 (94%)	131 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	166/309 (54%)	163 (98%)	3 (2%)	51	73
1	D	243/309 (79%)	242 (100%)	1 (0%)	84	86
1	E	247/309 (80%)	246 (100%)	1 (0%)	84	86
1	G	162/309 (52%)	162 (100%)	0	100	100
2	B	244/282 (86%)	243 (100%)	1 (0%)	84	86
2	C	235/282 (83%)	234 (100%)	1 (0%)	84	86
2	F	223/282 (79%)	222 (100%)	1 (0%)	84	86
2	H	243/282 (86%)	242 (100%)	1 (0%)	84	86
All	All	1763/2364 (75%)	1754 (100%)	9 (0%)	81	85

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	VAL
1	A	433	PHE
1	A	436	ILE
2	B	101	GLU
2	C	241	LYS
1	D	440	ARG
1	E	407	GLU
2	F	95	SER
2	H	312	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	159	ASN
1	A	253	GLN
1	A	300	GLN
1	A	315	HIS

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Mol	Chain	Res	Type
1	A	326	GLN
1	A	366	ASN
2	B	327	HIS
2	C	98	HIS
1	D	170	GLN
1	D	245	GLN
1	D	268	ASN
1	E	305	HIS
1	E	373	ASN
1	E	439	GLN
2	F	189	ASN
1	G	385	HIS

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](#)

There are no ligands in this entry.

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	234/348 (67%)	0.90	26 (11%) 10 5	68, 102, 136, 158	0
1	D	304/348 (87%)	0.39	8 (2%) 57 36	38, 82, 120, 130	0
1	E	304/348 (87%)	0.30	10 (3%) 49 29	30, 67, 116, 131	0
1	G	236/348 (67%)	0.84	19 (8%) 18 10	68, 103, 138, 156	0
2	B	276/325 (84%)	0.22	5 (1%) 67 47	32, 61, 97, 115	0
2	C	267/325 (82%)	0.21	1 (0%) 88 76	37, 69, 102, 128	0
2	F	266/325 (81%)	0.22	3 (1%) 78 59	31, 68, 107, 124	0
2	H	278/325 (85%)	0.05	5 (1%) 67 47	31, 56, 97, 121	0
All	All	2165/2692 (80%)	0.37	77 (3%) 46 26	30, 75, 122, 158	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	328	GLY	7.2
1	D	429	SER	6.0
1	G	249	ILE	4.5
1	A	375	ASN	3.7
1	A	359	LEU	3.7
1	G	327	PHE	3.6
2	H	179	VAL	3.5
1	G	359	LEU	3.5
1	G	230	PHE	3.3
1	G	436	ILE	3.3
1	D	138	SER	3.2
1	E	284	GLY	3.2
1	A	156	ILE	3.2
1	A	152	PHE	3.1
1	A	128	PHE	3.0
1	G	296	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	418	ALA	2.9
2	B	341	ALA	2.9
1	G	197	THR	2.8
1	G	255	SER	2.8
1	G	319	ASP	2.8
1	A	235	ASP	2.7
1	G	306	ASP	2.7
1	A	435	SER	2.7
2	F	176	GLY	2.7
1	A	149	PRO	2.6
1	D	420	PHE	2.6
1	G	364	VAL	2.6
1	A	393	LYS	2.6
1	A	327	PHE	2.6
1	A	132	ALA	2.6
2	F	205	SER	2.6
1	A	153	VAL	2.6
1	A	157	THR	2.5
1	E	345	MET	2.5
1	E	273	GLY	2.5
1	A	195	PHE	2.5
1	A	198	LEU	2.5
1	G	145	VAL	2.5
1	G	202	GLY	2.5
1	D	390	SER	2.5
1	G	194	ILE	2.4
1	G	201	CYS	2.4
1	A	145	VAL	2.4
1	D	415	VAL	2.4
1	G	393	LYS	2.4
1	E	390	SER	2.4
1	E	138	SER	2.3
1	G	147	MET	2.3
2	B	185	ASP	2.3
1	D	176	PHE	2.3
2	H	297	ASP	2.3
1	A	377	VAL	2.3
2	C	309	ALA	2.3
1	D	406	VAL	2.3
1	E	280	THR	2.2
1	A	159	ASN	2.2
1	E	274	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	176	GLY	2.2
2	H	174	HIS	2.2
1	A	203	LEU	2.2
1	A	433	PHE	2.2
2	F	171	THR	2.1
1	A	436	ILE	2.1
1	A	168	LEU	2.1
1	E	378	ASP	2.1
2	H	185	ASP	2.1
1	A	333	ALA	2.1
1	G	168	LEU	2.1
2	B	175	SER	2.0
1	G	430	ASN	2.0
1	E	285	ALA	2.0
2	H	341	ALA	2.0
1	E	387	ALA	2.0
1	A	146	PHE	2.0
2	B	90	PHE	2.0
1	A	322	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.