



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:51 AM UTC

PDB ID : 2IHW / pdb_00002ihw
Title : Crystal structure of a cubic core of the dihydrolipoamide acyltransferase (E2b) component in the branched-chain alpha-ketoacid dehydrogenase complex (BCKDC), apo form
Authors : Kato, M.; Wynn, R.M.; Chuang, J.L.; Brautigam, C.A.; Custorio, M.; Chuang, D.T.
Deposited on : 2006-09-27
Resolution : 2.70 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

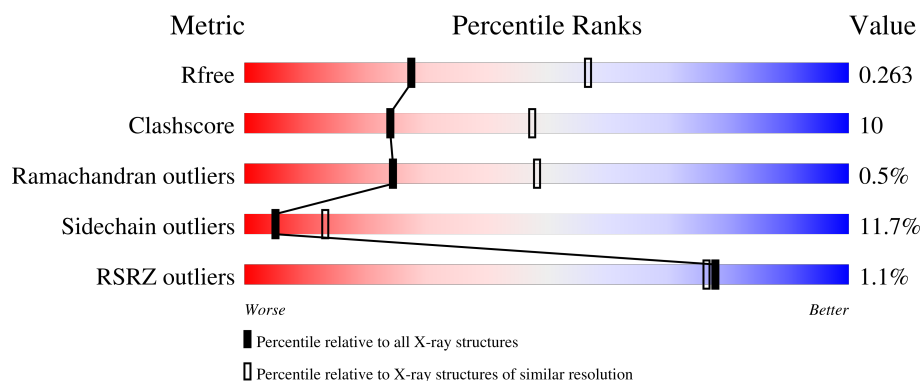
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	262	
1	B	262	
1	C	262	
1	D	262	

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Mol	Chain	Length	Quality of chain
1	E	262	 % 63% 21% 5% 11%
1	F	262	 64% 20% 5% 11%
1	G	262	 3% 57% 27% 5% 11%
1	H	262	 % 68% 18% 5% 11%

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
2	ACT	A	600	-	-	X	-
2	ACT	A	601	-	-	X	-
2	ACT	B	600	-	-	X	-
2	ACT	B	601	-	-	X	-
2	ACT	C	600	-	-	X	-
2	ACT	C	601	-	-	X	-
2	ACT	D	600	-	-	X	-
2	ACT	D	601	-	-	X	-
2	ACT	E	600	-	-	X	-
2	ACT	E	601	-	-	X	-
2	ACT	H	600	-	-	X	-
2	ACT	H	601	-	-	X	-
3	CL	A	602	-	-	X	-
3	CL	B	602	-	-	X	-
3	CL	D	602	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14638 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 Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	B	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	C	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	D	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	E	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	F	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	G	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			
1	H	234	Total	C	N	O	S	0	0	0
			1803	1158	306	330	9			

There are 16 discrepancies between the modelled and reference sequences:

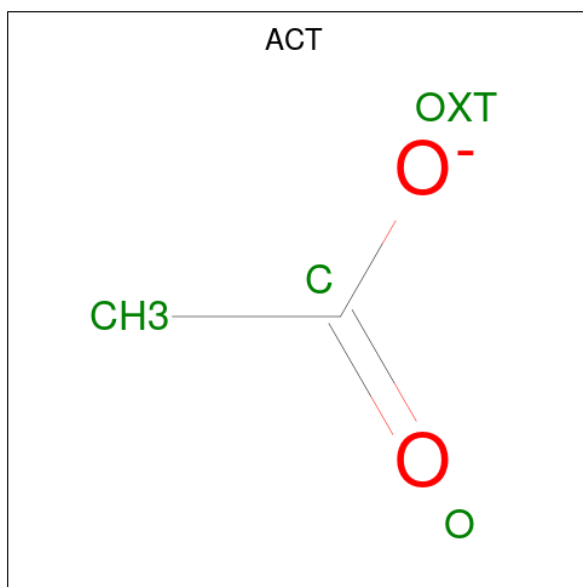
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	GLY	-	cloning artifact	UNP P11181
A	161	HIS	-	cloning artifact	UNP P11181
B	160	GLY	-	cloning artifact	UNP P11181
B	161	HIS	-	cloning artifact	UNP P11181
C	160	GLY	-	cloning artifact	UNP P11181
C	161	HIS	-	cloning artifact	UNP P11181
D	160	GLY	-	cloning artifact	UNP P11181
D	161	HIS	-	cloning artifact	UNP P11181
E	160	GLY	-	cloning artifact	UNP P11181
E	161	HIS	-	cloning artifact	UNP P11181
F	160	GLY	-	cloning artifact	UNP P11181
F	161	HIS	-	cloning artifact	UNP P11181

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Chain	Residue	Modelled	Actual	Comment	Reference
G	160	GLY	-	cloning artifact	UNP P11181
G	161	HIS	-	cloning artifact	UNP P11181
H	160	GLY	-	cloning artifact	UNP P11181
H	161	HIS	-	cloning artifact	UNP P11181

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Cl 2 2	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	2	Total Cl 2 2	0	0
3	F	1	Total Cl 1 1	0	0
3	G	2	Total Cl 2 2	0	0
3	H	2	Total Cl 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0
4	B	18	Total O 18 18	0	0

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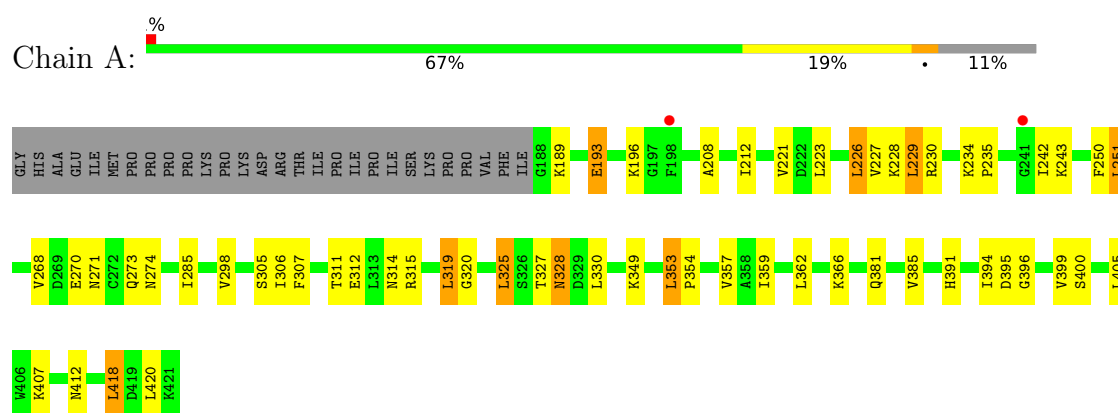
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	16	Total 16	O 16	0	0
4	D	19	Total 19	O 19	0	0
4	E	17	Total 17	O 17	0	0
4	F	19	Total 19	O 19	0	0
4	G	8	Total 8	O 8	0	0
4	H	23	Total 23	O 23	0	0

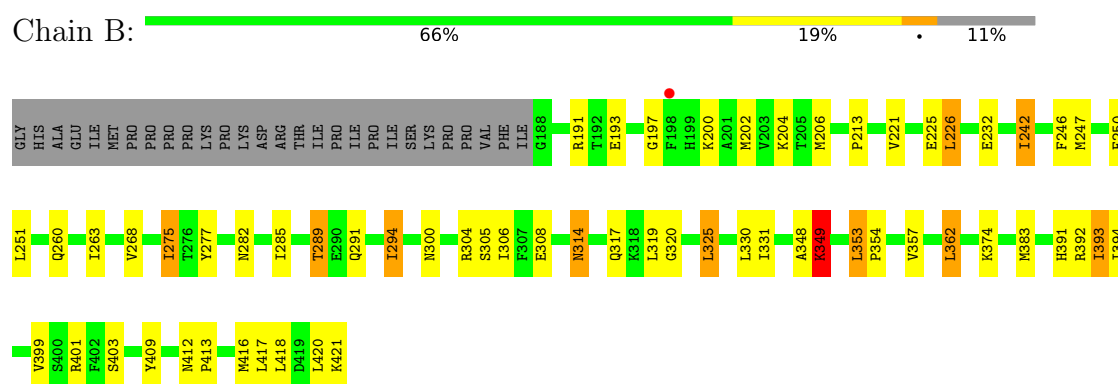
3 Residue-property plots

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.

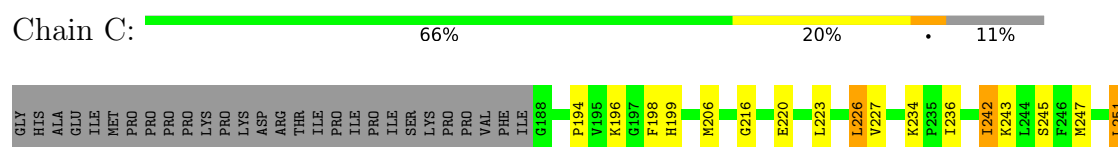
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

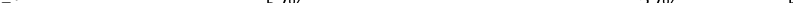


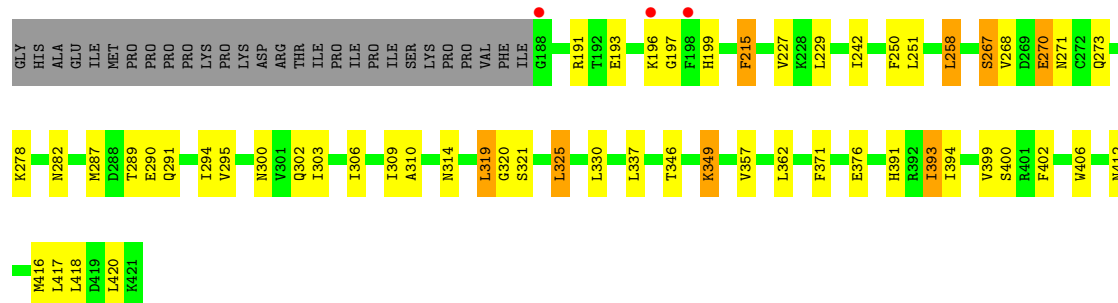
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



- Chain G: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	194.65Å 194.65Å 171.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.70) 97.8 (50.00-2.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.257 0.201 , 0.263	Depositor DCC
R_{free} test set	3301 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 25.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.005 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14638	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: ACT, CL

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	1.09	0/1837	1.21	9/2481 (0.4%)
1	B	1.15	1/1837 (0.1%)	1.19	4/2481 (0.2%)
1	C	1.08	1/1837 (0.1%)	1.17	5/2481 (0.2%)
1	D	1.14	1/1837 (0.1%)	1.21	7/2481 (0.3%)
1	E	1.13	3/1837 (0.2%)	1.24	6/2481 (0.2%)
1	F	1.15	2/1837 (0.1%)	1.25	13/2481 (0.5%)
1	G	1.06	1/1837 (0.1%)	1.23	9/2481 (0.4%)
1	H	1.23	2/1837 (0.1%)	1.26	7/2481 (0.3%)
All	All	1.13	11/14696 (0.1%)	1.22	60/19848 (0.3%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	188	GLY	N-CA	12.35	1.65	1.45
1	F	374	LYS	CE-NZ	12.31	1.86	1.49
1	H	346	THR	CA-C	7.49	1.56	1.52
1	E	221	VAL	CA-CB	6.51	1.64	1.54
1	H	227	VAL	CA-CB	5.72	1.60	1.54
1	F	303	ILE	CA-CB	5.42	1.60	1.54
1	C	399	VAL	CA-CB	5.32	1.61	1.54
1	B	206	MET	CA-C	5.29	1.59	1.52
1	E	339	ASN	CA-C	-5.21	1.47	1.53
1	E	357	VAL	CA-C	5.16	1.58	1.52
1	D	212	ILE	CA-C	-5.05	1.49	1.53

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	329	ASP	N-CA-C	-9.39	101.95	113.50
1	D	393	ILE	CB-CA-C	-7.67	102.52	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	406	TRP	N-CA-C	-7.19	103.44	111.28
1	C	236	ILE	N-CA-C	-6.85	106.11	112.96
1	F	407	LYS	N-CA-C	-6.57	104.04	111.14
1	C	402	PHE	N-CA-C	-6.43	104.20	111.14
1	A	359	ILE	CA-C-N	-6.32	116.75	121.61
1	A	359	ILE	C-N-CA	-6.32	116.75	121.61
1	H	349	LYS	CA-C-N	-6.28	114.16	120.31
1	H	349	LYS	C-N-CA	-6.28	114.16	120.31
1	F	212	ILE	CB-CA-C	-6.23	103.61	110.78
1	F	345	GLY	N-CA-C	6.15	117.80	111.95
1	D	315	ARG	N-CA-C	-6.09	104.72	111.36
1	A	405	LEU	N-CA-C	-6.00	104.08	111.40
1	H	215	PHE	CA-C-N	-5.95	117.03	122.80
1	H	215	PHE	C-N-CA	-5.95	117.03	122.80
1	C	196	LYS	N-CA-C	5.90	118.82	109.50
1	G	332	GLY	N-CA-C	5.88	123.96	114.90
1	E	345	GLY	N-CA-C	5.84	121.45	112.81
1	G	419	ASP	N-CA-C	5.55	120.21	113.38
1	A	212	ILE	CB-CA-C	-5.54	104.81	111.18
1	E	247	MET	CA-C-N	-5.52	113.21	119.28
1	E	247	MET	C-N-CA	-5.52	113.21	119.28
1	G	412	ASN	CA-C-N	5.50	125.21	119.82
1	G	412	ASN	C-N-CA	5.50	125.21	119.82
1	A	208	ALA	N-CA-C	-5.45	105.50	111.82
1	C	242	ILE	N-CA-C	5.43	115.92	107.99
1	B	349	LYS	CA-C-N	-5.42	115.00	120.31
1	B	349	LYS	C-N-CA	-5.42	115.00	120.31
1	F	374	LYS	CD-CE-NZ	-5.41	94.58	111.90
1	D	195	VAL	N-CA-C	-5.41	101.70	108.84
1	A	193	GLU	N-CA-C	5.40	116.97	108.23
1	F	393	ILE	N-CA-C	5.39	118.91	113.47
1	F	215	PHE	CA-C-N	-5.38	117.58	122.80
1	F	215	PHE	C-N-CA	-5.38	117.58	122.80
1	B	401	ARG	N-CA-C	-5.34	105.53	111.36
1	H	406	TRP	N-CA-C	-5.33	105.36	111.07
1	D	331	ILE	N-CA-CB	-5.31	106.02	112.07
1	D	270	GLU	CA-C-N	-5.29	114.18	122.65
1	D	270	GLU	C-N-CA	-5.29	114.18	122.65
1	E	248	PRO	N-CA-C	-5.26	106.55	113.65
1	E	285	ILE	CB-CA-C	-5.23	104.19	110.99
1	A	399	VAL	CB-CA-C	-5.23	105.08	112.14
1	A	395	ASP	CA-C-N	5.22	125.75	120.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ASP	C-N-CA	5.22	125.75	120.00
1	D	242	ILE	N-CA-C	5.20	115.97	108.48
1	F	399	VAL	CB-CA-C	-5.15	105.19	112.14
1	H	270	GLU	N-CA-C	5.15	116.58	110.97
1	C	329	ASP	N-CA-C	-5.13	106.53	112.89
1	F	295	VAL	CA-C-N	-5.13	115.44	120.52
1	F	295	VAL	C-N-CA	-5.13	115.44	120.52
1	B	294	ILE	CB-CA-C	5.09	118.33	110.50
1	G	328	ASN	N-CA-C	5.07	119.33	113.20
1	E	290	GLU	N-CA-C	-5.06	107.08	113.20
1	F	353	LEU	CB-CA-C	-5.06	105.88	110.44
1	G	271	ASN	N-CA-C	5.05	120.07	112.94
1	G	274	ASN	N-CA-C	5.05	116.92	108.99
1	F	212	ILE	N-CA-C	5.05	113.43	107.77
1	G	285	ILE	CB-CA-C	-5.04	103.62	110.42
1	H	400	SER	N-CA-CB	-5.03	102.71	110.01

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	1803	0	1859	32	0
1	B	1803	0	1859	34	0
1	C	1803	0	1859	37	0
1	D	1803	0	1859	32	0
1	E	1803	0	1859	36	0
1	F	1803	0	1859	41	0
1	G	1803	0	1859	44	0
1	H	1803	0	1859	27	0
2	A	8	0	6	3	0
2	B	8	0	6	4	0
2	C	8	0	6	3	0
2	D	8	0	6	3	0
2	E	8	0	6	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	8	0	6	0	0
2	G	8	0	6	0	0
2	H	8	0	6	3	0
3	A	2	0	0	2	0
3	B	1	0	0	2	0
3	C	1	0	0	1	0
3	D	1	0	0	2	0
3	E	2	0	0	1	0
3	F	1	0	0	1	0
3	G	2	0	0	1	0
3	H	2	0	0	1	0
4	A	18	0	0	0	0
4	B	18	0	0	3	0
4	C	16	0	0	3	0
4	D	19	0	0	0	0
4	E	17	0	0	1	0
4	F	19	0	0	2	0
4	G	8	0	0	1	0
4	H	23	0	0	1	0
All	All	14638	0	14920	294	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 10.

All (294) 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:374:LYS:CE	1:F:374:LYS:NZ	1.86	1.38
1:G:393:ILE:HD13	1:G:394:ILE:HD12	1.36	1.08
1:B:320:GLY:HA2	1:B:325:LEU:HD22	1.49	0.95
1:B:349:LYS:NZ	3:B:602:CL:CL	2.39	0.93
2:A:600:ACT:H1	2:A:601:ACT:H2	1.50	0.91
2:B:600:ACT:H1	2:B:601:ACT:CH3	2.02	0.89
1:C:349:LYS:NZ	3:C:602:CL:CL	2.42	0.88
1:G:282:ASN:ND2	1:G:300:ASN:H	1.72	0.87
1:B:289:THR:HG22	1:B:291:GLN:H	1.36	0.86
1:H:251:LEU:HD12	1:H:337:LEU:HD12	1.61	0.83
1:B:305:SER:OG	1:B:308:GLU:HG3	1.78	0.83
1:H:250:PHE:CD2	1:H:362:LEU:HD13	2.14	0.82
2:D:600:ACT:H3	2:D:601:ACT:H3	1.60	0.82
1:F:198:PHE:HE2	1:F:199:HIS:CE1	1.98	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:600:ACT:H1	2:B:601:ACT:H2	1.61	0.81
1:E:194:PRO:HA	1:F:274:ASN:HD22	1.46	0.78
1:C:198:PHE:CE1	1:C:199:HIS:CE1	2.71	0.78
2:E:600:ACT:H1	2:E:601:ACT:CH3	2.14	0.77
1:F:349:LYS:NZ	3:F:602:CL:CL	2.54	0.77
1:C:289:THR:C	1:C:291:GLN:H	1.92	0.76
1:H:196:LYS:O	1:H:199:HIS:HB2	1.86	0.76
1:G:393:ILE:HD13	1:G:394:ILE:CD1	2.15	0.75
1:B:320:GLY:HA2	1:B:325:LEU:CD2	2.17	0.75
1:D:282:ASN:HD22	1:D:300:ASN:H	1.34	0.74
1:G:374:LYS:HB2	1:G:374:LYS:NZ	2.03	0.73
1:G:282:ASN:HD22	1:G:300:ASN:H	1.35	0.73
1:E:267:SER:HB3	1:E:355:PRO:O	1.88	0.73
1:G:393:ILE:CD1	1:G:394:ILE:HD12	2.17	0.73
3:H:602:CL:CL	4:H:77:HOH:O	2.43	0.72
1:A:357:VAL:HB	1:A:394:ILE:HD11	1.69	0.72
1:H:282:ASN:ND2	1:H:300:ASN:H	1.85	0.72
1:H:319:LEU:HB3	1:H:325:LEU:HD13	1.70	0.72
3:A:602:CL:CL	4:B:100:HOH:O	2.46	0.71
2:D:600:ACT:H3	2:D:601:ACT:CH3	2.20	0.71
3:D:602:CL:CL	4:E:63:HOH:O	2.47	0.70
1:C:251:LEU:HD13	1:C:337:LEU:HD12	1.73	0.70
1:C:414:ALA:O	1:C:417:LEU:HB2	1.92	0.69
2:E:600:ACT:CH3	2:E:601:ACT:H3	2.23	0.69
1:E:268:VAL:HG11	1:E:393:ILE:HG12	1.74	0.69
2:D:600:ACT:CH3	2:D:601:ACT:H3	2.23	0.68
1:A:418:LEU:HD22	1:F:307:PHE:HB2	1.76	0.68
1:D:349:LYS:NZ	3:D:602:CL:CL	2.65	0.67
1:C:198:PHE:CZ	1:C:199:HIS:CE1	2.82	0.67
1:A:221:VAL:HG22	1:A:407:LYS:HG3	1.77	0.67
1:G:393:ILE:HD12	1:G:393:ILE:H	1.59	0.66
1:A:320:GLY:HA2	1:A:325:LEU:HD22	1.76	0.66
1:A:319:LEU:HB3	1:A:325:LEU:HD13	1.78	0.66
2:B:600:ACT:CH3	2:B:601:ACT:H2	2.24	0.66
1:B:251:LEU:HD21	1:B:285:ILE:HD11	1.76	0.66
1:F:374:LYS:NZ	1:F:374:LYS:CD	2.59	0.66
2:B:600:ACT:H1	2:B:601:ACT:H1	1.77	0.65
1:E:251:LEU:CD1	1:E:337:LEU:HD12	2.26	0.65
1:E:243:LYS:H	1:E:314:ASN:HD21	1.42	0.65
1:F:393:ILE:HD12	1:F:394:ILE:HG13	1.77	0.65
1:A:227:VAL:HG21	1:A:381:GLN:HG2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:282:ASN:HD22	1:H:300:ASN:H	1.44	0.64
2:E:600:ACT:H1	2:E:601:ACT:H3	1.79	0.64
1:F:414:ALA:O	1:F:417:LEU:HB2	1.98	0.64
1:G:374:LYS:HB2	1:G:374:LYS:HZ3	1.62	0.64
1:D:305:SER:OG	1:D:308:GLU:HG3	1.99	0.63
1:A:229:LEU:O	1:A:229:LEU:HD12	1.99	0.63
1:F:251:LEU:HD12	1:F:337:LEU:HD12	1.80	0.63
1:E:194:PRO:CA	1:F:274:ASN:HD22	2.09	0.63
1:E:282:ASN:HD22	1:E:300:ASN:H	1.47	0.63
1:E:289:THR:HG22	1:E:290:GLU:H	1.63	0.62
1:A:349:LYS:NZ	3:A:602:CL:CL	2.69	0.62
1:D:416:MET:O	1:D:420:LEU:HG	1.99	0.62
1:E:251:LEU:HD12	1:E:337:LEU:HD12	1.80	0.62
1:B:282:ASN:ND2	1:B:300:ASN:H	1.98	0.61
1:D:282:ASN:ND2	1:D:300:ASN:H	1.98	0.61
1:D:213:PRO:HG2	1:D:392:ARG:HG3	1.83	0.61
1:A:320:GLY:CA	1:A:325:LEU:HD22	2.31	0.61
1:G:280:SER:HB3	1:G:300:ASN:OD1	1.99	0.61
1:H:242:ILE:HG23	1:H:314:ASN:ND2	2.15	0.61
1:H:371:PHE:HA	1:H:376:GLU:O	2.01	0.61
2:C:600:ACT:H1	2:C:601:ACT:H3	1.83	0.60
1:B:268:VAL:HG11	1:B:393:ILE:HG12	1.82	0.60
1:G:251:LEU:HD21	1:G:285:ILE:HD11	1.83	0.60
1:A:251:LEU:HD21	1:A:285:ILE:HD11	1.82	0.60
1:A:229:LEU:HD12	1:A:229:LEU:C	2.26	0.60
1:A:274:ASN:HD22	1:C:194:PRO:HA	1.66	0.60
2:C:600:ACT:CH3	2:C:601:ACT:H3	2.33	0.59
1:B:275:ILE:HD13	1:B:277:TYR:CE1	2.38	0.59
1:D:370:ARG:HG2	1:D:370:ARG:HH11	1.66	0.59
1:F:289:THR:C	1:F:291:GLN:H	2.08	0.59
1:G:243:LYS:H	1:G:314:ASN:HD21	1.48	0.59
1:C:260:GLN:HG3	1:C:405:LEU:HD21	1.85	0.59
1:G:322:ALA:O	1:G:324:GLN:HG2	2.02	0.59
1:E:282:ASN:ND2	1:E:300:ASN:H	2.00	0.59
1:F:198:PHE:CE2	1:F:199:HIS:CE1	2.85	0.59
2:A:600:ACT:H1	2:A:601:ACT:CH3	2.31	0.58
1:B:289:THR:HG22	1:B:291:GLN:N	2.14	0.58
1:F:225:GLU:HB2	4:F:110:HOH:O	2.03	0.58
1:D:268:VAL:HG11	1:D:393:ILE:HG12	1.86	0.58
1:F:229:LEU:HD23	1:F:233:LEU:HD12	1.87	0.57
1:C:227:VAL:HG21	1:C:381:GLN:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:305:SER:O	1:G:309:ILE:HG13	2.05	0.57
1:H:251:LEU:CD1	1:H:337:LEU:HD12	2.33	0.57
1:H:289:THR:C	1:H:291:GLN:H	2.13	0.57
1:B:282:ASN:HD22	1:B:300:ASN:H	1.52	0.56
1:F:368:LEU:HD23	4:F:75:HOH:O	2.05	0.56
1:D:213:PRO:CG	1:D:392:ARG:HG3	2.35	0.56
1:G:340:ILE:HG13	1:G:341:GLY:N	2.18	0.56
1:H:267:SER:HB2	1:H:278:LYS:HE3	1.86	0.56
2:E:600:ACT:CH3	2:E:601:ACT:CH3	2.81	0.56
1:E:221:VAL:HB	1:E:407:LYS:HG3	1.88	0.56
1:E:194:PRO:HA	1:F:274:ASN:ND2	2.21	0.56
1:C:289:THR:C	1:C:291:GLN:N	2.64	0.55
1:B:191:ARG:HH21	1:B:193:GLU:CD	2.14	0.55
1:B:357:VAL:CG2	1:B:394:ILE:HD11	2.36	0.55
1:D:312:GLU:OE1	1:D:312:GLU:HA	2.05	0.55
1:G:374:LYS:NZ	1:G:374:LYS:CB	2.71	0.54
1:H:251:LEU:HD12	1:H:337:LEU:CD1	2.35	0.54
1:B:247:MET:HE3	1:B:251:LEU:HD11	1.89	0.54
1:E:336:THR:HB	1:E:359:ILE:HG13	1.90	0.54
1:E:293:LEU:HD13	2:E:601:ACT:O	2.07	0.54
1:B:221:VAL:HG12	1:B:383:MET:O	2.08	0.53
1:D:227:VAL:HG21	1:D:381:GLN:HG2	1.89	0.53
1:E:234:LYS:HB2	1:E:235:PRO:HD3	1.91	0.53
1:E:349:LYS:NZ	3:E:602:CL:CL	2.78	0.53
1:F:289:THR:C	1:F:291:GLN:N	2.66	0.53
1:A:298:VAL:HG13	1:A:312:GLU:HG2	1.90	0.53
1:C:403:SER:HB3	4:C:11:HOH:O	2.09	0.53
1:H:320:GLY:HA2	1:H:325:LEU:HD22	1.91	0.53
1:G:371:PHE:HA	1:G:376:GLU:O	2.09	0.52
1:C:251:LEU:CD1	1:C:337:LEU:HD12	2.39	0.52
1:B:213:PRO:HG2	1:B:392:ARG:HG3	1.91	0.52
1:B:289:THR:CG2	1:B:291:GLN:H	2.18	0.52
1:C:289:THR:HG22	1:C:291:GLN:N	2.25	0.52
1:D:280:SER:HB3	1:D:282:ASN:HD21	1.74	0.52
1:A:396:GLY:O	1:A:400:SER:HB2	2.10	0.52
1:F:238:PHE:O	1:F:239:ALA:C	2.51	0.52
1:E:350:PRO:HB2	1:E:359:ILE:HD13	1.91	0.52
1:D:270:GLU:OE1	1:D:270:GLU:HA	2.09	0.51
1:A:223:LEU:HD22	1:A:226:LEU:HD12	1.92	0.51
1:G:247:MET:O	1:G:251:LEU:HB2	2.11	0.51
1:B:197:GLY:O	1:B:200:LYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:VAL:HB	1:D:394:ILE:HD11	1.93	0.51
1:D:411:GLU:O	1:D:413:PRO:HD3	2.10	0.51
1:E:296:PRO:HA	1:E:329:ASP:O	2.12	0.50
1:C:245:SER:HB2	4:C:103:HOH:O	2.11	0.50
1:G:198:PHE:CD1	1:G:291:GLN:HB2	2.46	0.50
1:B:226:LEU:CD1	1:B:246:PHE:HD1	2.25	0.50
1:B:319:LEU:HB3	1:B:325:LEU:HD13	1.92	0.50
1:D:242:ILE:HG13	1:D:307:PHE:CE1	2.46	0.50
1:E:275:ILE:HD13	1:E:277:TYR:CZ	2.46	0.50
1:C:298:VAL:HG13	1:C:312:GLU:HG2	1.93	0.49
1:A:312:GLU:OE2	1:A:315:ARG:NH2	2.38	0.49
1:A:362:LEU:HD23	1:A:385:VAL:HG23	1.94	0.49
1:G:289:THR:HG21	4:G:125:HOH:O	2.12	0.49
1:G:370:ARG:HH11	1:G:370:ARG:HG2	1.76	0.49
1:H:242:ILE:HG23	1:H:314:ASN:HD21	1.75	0.49
1:D:396:GLY:O	1:D:400:SER:HB2	2.13	0.49
1:F:298:VAL:HG13	1:F:312:GLU:HG2	1.95	0.49
1:A:420:LEU:HB3	1:F:420:LEU:HB3	1.95	0.49
1:F:357:VAL:HG11	1:F:393:ILE:HD11	1.93	0.49
1:H:393:ILE:HD12	1:H:394:ILE:N	2.28	0.49
1:C:242:ILE:HG13	1:C:307:PHE:CE1	2.48	0.48
1:G:270:GLU:OE1	1:G:270:GLU:HA	2.13	0.48
1:G:294:ILE:HD11	1:G:330:LEU:HD21	1.94	0.48
1:G:349:LYS:NZ	3:G:603:CL:CL	2.79	0.48
1:A:307:PHE:HB2	1:F:418:LEU:HD22	1.94	0.48
2:H:600:ACT:CH3	2:H:601:ACT:H3	2.44	0.48
1:B:263:ILE:HG12	1:B:263:ILE:O	2.14	0.48
1:C:278:LYS:HD3	1:C:334:THR:HG22	1.96	0.48
1:D:280:SER:HB3	1:D:282:ASN:ND2	2.27	0.48
1:D:370:ARG:HG2	1:D:370:ARG:NH1	2.27	0.48
1:A:250:PHE:CD2	1:A:362:LEU:HD13	2.48	0.48
1:G:287:MET:HE1	1:G:317:GLN:HA	1.96	0.48
1:E:381:GLN:HA	1:E:381:GLN:HE21	1.79	0.48
1:F:416:MET:O	1:F:420:LEU:HG	2.14	0.48
1:D:223:LEU:O	1:D:227:VAL:HG23	2.14	0.47
1:E:223:LEU:O	1:E:227:VAL:HG23	2.13	0.47
1:B:250:PHE:CD2	1:B:362:LEU:HD13	2.49	0.47
1:F:214:HIS:CD2	1:F:352:ILE:HG13	2.49	0.47
1:C:223:LEU:HD22	1:C:226:LEU:HD12	1.95	0.47
1:D:275:ILE:HG13	1:F:195:VAL:HG22	1.97	0.47
2:A:601:ACT:O	1:B:391:HIS:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:353:LEU:O	1:E:354:PRO:C	2.58	0.47
1:D:357:VAL:HB	1:D:394:ILE:CD1	2.45	0.47
1:G:198:PHE:HB3	1:G:291:GLN:HB3	1.96	0.47
1:B:403:SER:HB3	4:B:13:HOH:O	2.15	0.47
1:C:289:THR:CG2	1:C:290:GLU:N	2.78	0.47
1:C:258:LEU:HD13	1:C:402:PHE:CE1	2.50	0.46
1:C:247:MET:O	1:C:251:LEU:HD22	2.15	0.46
1:C:393:ILE:HD12	1:C:394:ILE:HG13	1.97	0.46
2:E:600:ACT:H1	2:E:601:ACT:H1	1.92	0.46
1:A:391:HIS:CE1	1:C:206:MET:HE3	2.51	0.46
1:E:397:ALA:O	1:E:401:ARG:HG3	2.16	0.46
1:G:396:GLY:O	1:G:400:SER:HB2	2.16	0.46
1:A:328:ASN:ND2	1:A:328:ASN:H	2.14	0.46
1:F:223:LEU:HD22	1:F:226:LEU:HD12	1.97	0.46
1:G:370:ARG:O	1:G:378:CYS:HB2	2.16	0.46
1:D:415:PHE:N	1:D:415:PHE:CD1	2.83	0.45
1:E:268:VAL:CG1	1:E:393:ILE:HG12	2.44	0.45
1:C:289:THR:HG22	1:C:290:GLU:N	2.30	0.45
1:C:258:LEU:HG	1:C:265:ASN:HB2	1.98	0.45
1:G:330:LEU:HD12	1:G:330:LEU:HA	1.79	0.45
1:H:349:LYS:HD3	1:H:349:LYS:O	2.16	0.45
1:D:257:GLY:HA2	1:D:405:LEU:HD23	1.98	0.45
1:D:277:TYR:O	1:F:190:ASP:HA	2.16	0.45
1:C:247:MET:HE3	1:C:251:LEU:HD22	1.98	0.45
1:B:314:ASN:N	1:B:314:ASN:HD22	2.14	0.45
1:C:285:ILE:O	1:C:296:PRO:HD2	2.17	0.45
3:B:602:CL:CL	4:C:93:HOH:O	2.58	0.45
1:A:242:ILE:HD12	1:A:311:THR:HA	1.99	0.44
1:C:268:VAL:HG21	1:C:272:CYS:SG	2.57	0.44
1:E:223:LEU:HD22	1:E:226:LEU:HD12	1.99	0.44
1:G:251:LEU:CD1	1:G:337:LEU:HD12	2.47	0.44
1:H:197:GLY:C	1:H:199:HIS:H	2.25	0.44
1:A:305:SER:O	1:A:306:ILE:C	2.57	0.44
1:A:353:LEU:O	1:A:354:PRO:C	2.61	0.44
1:D:383:MET:HE2	1:D:383:MET:HB3	1.94	0.44
2:H:600:ACT:H3	2:H:601:ACT:CH3	2.47	0.44
1:H:416:MET:O	1:H:420:LEU:HG	2.17	0.44
1:D:284:GLY:HA2	1:D:297:ASN:HA	2.00	0.44
1:H:258:LEU:HD13	1:H:402:PHE:CE1	2.53	0.44
1:A:391:HIS:NE2	2:C:601:ACT:H1	2.33	0.44
1:D:336:THR:O	1:D:337:LEU:HD23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:416:MET:O	1:G:417:LEU:C	2.61	0.44
1:A:229:LEU:C	1:A:229:LEU:CD1	2.91	0.44
1:G:238:PHE:C	1:G:240:ARG:H	2.26	0.44
2:E:601:ACT:OXT	1:F:391:HIS:NE2	2.51	0.43
1:B:348:ALA:HB1	1:C:216:GLY:O	2.18	0.43
1:E:218:CYS:HB3	1:E:347:TYR:CE1	2.52	0.43
1:F:251:LEU:CD1	1:F:337:LEU:HD12	2.46	0.43
1:G:409:TYR:O	1:G:416:MET:HE2	2.17	0.43
1:A:243:LYS:H	1:A:314:ASN:HD21	1.67	0.43
1:E:410:LEU:HD23	1:E:410:LEU:HA	1.86	0.43
1:F:350:PRO:HG2	1:F:359:ILE:HG23	1.99	0.43
1:A:391:HIS:O	1:A:391:HIS:ND1	2.50	0.43
1:E:236:ILE:HD13	1:E:236:ILE:N	2.33	0.43
1:H:215:PHE:HB2	1:H:391:HIS:CD2	2.54	0.43
1:F:391:HIS:O	1:F:391:HIS:ND1	2.47	0.43
1:H:197:GLY:C	1:H:199:HIS:N	2.75	0.43
1:B:409:TYR:O	1:B:413:PRO:HA	2.18	0.43
1:C:339:ASN:O	1:C:340:ILE:C	2.59	0.43
1:F:319:LEU:HA	1:F:319:LEU:HD12	1.77	0.43
1:F:338:SER:O	1:F:361:ALA:HA	2.19	0.43
1:G:221:VAL:HG13	1:G:407:LYS:HG3	2.01	0.43
1:G:414:ALA:O	1:G:417:LEU:HB2	2.19	0.43
1:E:285:ILE:O	1:E:296:PRO:HD2	2.19	0.43
1:H:394:ILE:CG2	1:H:399:VAL:HG23	2.49	0.43
1:C:198:PHE:CZ	1:C:199:HIS:HE1	2.33	0.43
1:H:302:GLN:HG2	1:H:303:ILE:HG23	2.00	0.43
1:D:416:MET:O	1:D:417:LEU:C	2.62	0.42
1:C:282:ASN:HD22	1:C:300:ASN:H	1.66	0.42
1:G:296:PRO:HA	1:G:329:ASP:O	2.18	0.42
1:C:284:GLY:HA2	1:C:297:ASN:HA	2.01	0.42
1:F:212:ILE:HG23	1:F:390:ASP:CG	2.44	0.42
1:G:241:GLY:O	1:G:242:ILE:HD13	2.20	0.42
1:G:208:ALA:O	1:G:211:LYS:HG3	2.18	0.42
1:H:191:ARG:NH1	1:H:193:GLU:OE2	2.48	0.42
1:B:242:ILE:HD13	1:B:242:ILE:HA	1.74	0.42
1:G:370:ARG:HG2	1:G:370:ARG:NH1	2.34	0.42
1:C:275:ILE:HD11	1:C:393:ILE:CG2	2.49	0.42
1:A:230:ARG:NH2	1:A:234:LYS:HD3	2.34	0.42
1:F:330:LEU:HD12	1:F:330:LEU:HA	1.91	0.42
1:G:251:LEU:HD12	1:G:251:LEU:HA	1.58	0.42
2:H:600:ACT:H3	2:H:601:ACT:H3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ILE:HD11	1:C:393:ILE:HG22	2.02	0.42
1:E:206:MET:HE3	1:F:391:HIS:CE1	2.55	0.42
1:E:214:HIS:CD2	1:E:352:ILE:HG13	2.55	0.41
1:A:234:LYS:N	1:A:235:PRO:CD	2.83	0.41
1:B:353:LEU:O	1:B:354:PRO:C	2.63	0.41
1:A:271:ASN:C	1:A:271:ASN:HD22	2.27	0.41
1:B:357:VAL:HB	1:B:394:ILE:HD11	2.02	0.41
1:D:415:PHE:N	1:D:415:PHE:HD1	2.18	0.41
1:E:280:SER:HB3	1:E:282:ASN:ND2	2.35	0.41
1:G:352:ILE:O	1:G:354:PRO:HD3	2.21	0.41
1:B:357:VAL:HB	1:B:394:ILE:CD1	2.51	0.41
1:E:258:LEU:HG	1:E:265:ASN:HB2	2.03	0.41
1:H:320:GLY:HA2	1:H:325:LEU:CD2	2.50	0.41
1:C:252:LYS:HD2	1:C:252:LYS:HA	1.89	0.41
1:C:330:LEU:HD12	1:C:330:LEU:HA	1.90	0.41
1:F:300:ASN:HB3	1:F:303:ILE:HG12	2.02	0.41
1:G:271:ASN:HB2	1:G:273:GLN:HG2	2.03	0.41
1:F:371:PHE:HA	1:F:376:GLU:O	2.21	0.41
1:D:391:HIS:O	1:D:391:HIS:ND1	2.52	0.41
1:E:248:PRO:HA	1:E:309:ILE:HG21	2.03	0.41
1:H:309:ILE:O	1:H:310:ALA:C	2.64	0.41
1:B:357:VAL:HG21	1:B:394:ILE:HD11	2.02	0.40
1:D:237:ALA:O	1:D:238:PHE:C	2.64	0.40
1:E:300:ASN:HB3	1:E:303:ILE:HG12	2.03	0.40
1:F:243:LYS:H	1:F:314:ASN:HD21	1.68	0.40
1:F:313:LEU:O	1:F:314:ASN:C	2.64	0.40
1:G:285:ILE:O	1:G:296:PRO:HD2	2.21	0.40
1:E:350:PRO:HG2	1:E:359:ILE:HG23	2.03	0.40
1:F:407:LYS:O	1:F:408:SER:C	2.65	0.40
1:H:357:VAL:CG2	1:H:394:ILE:HD11	2.52	0.40
1:B:394:ILE:HA	4:B:98:HOH:O	2.21	0.40
1:B:416:MET:O	1:B:420:LEU:HG	2.21	0.40
1:G:217:TYR:CD1	1:G:217:TYR:C	3.00	0.40
1:G:369:PRO:O	1:G:370:ARG:NH1	2.54	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	232/262 (88%)	223 (96%)	9 (4%)	0	100	100
1	B	232/262 (88%)	224 (97%)	8 (3%)	0	100	100
1	C	232/262 (88%)	216 (93%)	15 (6%)	1 (0%)	30	54
1	D	232/262 (88%)	220 (95%)	11 (5%)	1 (0%)	30	54
1	E	232/262 (88%)	223 (96%)	8 (3%)	1 (0%)	30	54
1	F	232/262 (88%)	208 (90%)	22 (10%)	2 (1%)	14	35
1	G	232/262 (88%)	214 (92%)	15 (6%)	3 (1%)	9	25
1	H	232/262 (88%)	223 (96%)	8 (3%)	1 (0%)	30	54
All	All	1856/2096 (88%)	1751 (94%)	96 (5%)	9 (0%)	24	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	290	GLU
1	D	418	LEU
1	E	197	GLY
1	G	239	ALA
1	G	356	GLU
1	F	356	GLU
1	H	290	GLU
1	F	290	GLU
1	G	331	ILE

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	196/222 (88%)	177 (90%)	19 (10%)	8	20
1	B	196/222 (88%)	169 (86%)	27 (14%)	3	9
1	C	196/222 (88%)	177 (90%)	19 (10%)	8	20
1	D	196/222 (88%)	174 (89%)	22 (11%)	6	15
1	E	196/222 (88%)	169 (86%)	27 (14%)	3	9
1	F	196/222 (88%)	178 (91%)	18 (9%)	8	22
1	G	196/222 (88%)	163 (83%)	33 (17%)	2	6
1	H	196/222 (88%)	177 (90%)	19 (10%)	8	20
All	All	1568/1776 (88%)	1384 (88%)	184 (12%)	5	13

All (184) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LYS
1	A	193	GLU
1	A	196	LYS
1	A	226	LEU
1	A	228	LYS
1	A	229	LEU
1	A	251	LEU
1	A	268	VAL
1	A	270	GLU
1	A	273	GLN
1	A	319	LEU
1	A	325	LEU
1	A	327	THR
1	A	328	ASN
1	A	330	LEU
1	A	353	LEU
1	A	366	LYS
1	A	412	ASN
1	A	418	LEU
1	B	202	MET
1	B	204	LYS
1	B	225	GLU
1	B	226	LEU
1	B	232	GLU
1	B	242	ILE

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Mol	Chain	Res	Type
1	B	260	GLN
1	B	275	ILE
1	B	289	THR
1	B	294	ILE
1	B	304	ARG
1	B	306	ILE
1	B	314	ASN
1	B	317	GLN
1	B	325	LEU
1	B	330	LEU
1	B	331	ILE
1	B	349	LYS
1	B	353	LEU
1	B	362	LEU
1	B	374	LYS
1	B	393	ILE
1	B	399	VAL
1	B	412	ASN
1	B	417	LEU
1	B	418	LEU
1	B	421	LYS
1	C	220	GLU
1	C	226	LEU
1	C	234	LYS
1	C	243	LYS
1	C	251	LEU
1	C	258	LEU
1	C	268	VAL
1	C	271	ASN
1	C	306	ILE
1	C	313	LEU
1	C	319	LEU
1	C	327	THR
1	C	330	LEU
1	C	353	LEU
1	C	393	ILE
1	C	399	VAL
1	C	407	LYS
1	C	412	ASN
1	C	418	LEU
1	D	198	PHE
1	D	226	LEU

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Mol	Chain	Res	Type
1	D	234	LYS
1	D	258	LEU
1	D	287	MET
1	D	290	GLU
1	D	294	ILE
1	D	306	ILE
1	D	318	LYS
1	D	319	LEU
1	D	330	LEU
1	D	331	ILE
1	D	362	LEU
1	D	364	THR
1	D	366	LYS
1	D	393	ILE
1	D	399	VAL
1	D	400	SER
1	D	408	SER
1	D	412	ASN
1	D	417	LEU
1	D	418	LEU
1	E	189	LYS
1	E	193	GLU
1	E	196	LYS
1	E	198	PHE
1	E	204	LYS
1	E	221	VAL
1	E	226	LEU
1	E	229	LEU
1	E	236	ILE
1	E	251	LEU
1	E	258	LEU
1	E	267	SER
1	E	283	ILE
1	E	290	GLU
1	E	293	LEU
1	E	306	ILE
1	E	317	GLN
1	E	328	ASN
1	E	330	LEU
1	E	353	LEU
1	E	359	ILE
1	E	374	LYS

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Mol	Chain	Res	Type
1	E	393	ILE
1	E	400	SER
1	E	417	LEU
1	E	418	LEU
1	E	421	LYS
1	F	205	THR
1	F	226	LEU
1	F	234	LYS
1	F	251	LEU
1	F	268	VAL
1	F	270	GLU
1	F	287	MET
1	F	290	GLU
1	F	304	ARG
1	F	317	GLN
1	F	318	LYS
1	F	319	LEU
1	F	330	LEU
1	F	353	LEU
1	F	366	LYS
1	F	399	VAL
1	F	408	SER
1	F	418	LEU
1	G	189	LYS
1	G	193	GLU
1	G	200	LYS
1	G	204	LYS
1	G	228	LYS
1	G	229	LEU
1	G	251	LEU
1	G	270	GLU
1	G	274	ASN
1	G	275	ILE
1	G	280	SER
1	G	290	GLU
1	G	306	ILE
1	G	312	GLU
1	G	318	LYS
1	G	327	THR
1	G	328	ASN
1	G	330	LEU
1	G	353	LEU

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Mol	Chain	Res	Type
1	G	364	THR
1	G	365	ILE
1	G	366	LYS
1	G	370	ARG
1	G	374	LYS
1	G	376	GLU
1	G	377	VAL
1	G	384	ASN
1	G	386	SER
1	G	393	ILE
1	G	399	VAL
1	G	408	SER
1	G	412	ASN
1	G	418	LEU
1	H	229	LEU
1	H	258	LEU
1	H	267	SER
1	H	268	VAL
1	H	270	GLU
1	H	271	ASN
1	H	273	GLN
1	H	287	MET
1	H	294	ILE
1	H	295	VAL
1	H	306	ILE
1	H	319	LEU
1	H	321	SER
1	H	325	LEU
1	H	330	LEU
1	H	393	ILE
1	H	412	ASN
1	H	417	LEU
1	H	418	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	ASN
1	A	273	GLN
1	A	274	ASN
1	A	314	ASN
1	A	328	ASN

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Mol	Chain	Res	Type
1	B	282	ASN
1	B	328	ASN
1	B	381	GLN
1	C	199	HIS
1	C	282	ASN
1	C	384	ASN
1	D	274	ASN
1	D	282	ASN
1	D	314	ASN
1	D	339	ASN
1	E	265	ASN
1	E	282	ASN
1	E	314	ASN
1	E	339	ASN
1	E	381	GLN
1	E	384	ASN
1	F	199	HIS
1	F	274	ASN
1	F	314	ASN
1	F	384	ASN
1	G	282	ASN
1	G	314	ASN
1	G	339	ASN
1	G	372	ASN
1	G	381	GLN
1	H	282	ASN
1	H	324	GLN
1	H	381	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 28 ligands modelled in this entry, 12 are monoatomic - leaving 16 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
2	ACT	D	601	-	3,3,3	0.77	0	3,3,3	1.67	1 (33%)
2	ACT	H	601	-	3,3,3	0.91	0	3,3,3	1.59	1 (33%)
2	ACT	A	600	-	3,3,3	0.84	0	3,3,3	1.48	1 (33%)
2	ACT	F	601	-	3,3,3	0.97	0	3,3,3	1.22	0
2	ACT	G	601	-	3,3,3	0.89	0	3,3,3	1.25	0
2	ACT	B	601	-	3,3,3	0.75	0	3,3,3	1.22	0
2	ACT	G	600	-	3,3,3	0.78	0	3,3,3	1.61	0
2	ACT	H	600	-	3,3,3	1.16	0	3,3,3	1.26	0
2	ACT	E	600	-	3,3,3	0.78	0	3,3,3	1.59	1 (33%)
2	ACT	F	600	-	3,3,3	1.19	0	3,3,3	1.85	1 (33%)
2	ACT	C	601	-	3,3,3	0.91	0	3,3,3	1.78	2 (66%)
2	ACT	C	600	-	3,3,3	0.76	0	3,3,3	1.24	0
2	ACT	E	601	-	3,3,3	1.04	0	3,3,3	1.28	0
2	ACT	B	600	-	3,3,3	0.61	0	3,3,3	1.69	1 (33%)
2	ACT	A	601	-	3,3,3	0.72	0	3,3,3	1.98	2 (66%)
2	ACT	D	600	-	3,3,3	1.06	0	3,3,3	1.56	1 (33%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	ACT	OXT-C-O	-2.66	112.16	122.03
2	A	601	ACT	OXT-C-O	-2.50	112.76	122.03
2	A	601	ACT	OXT-C-CH3	2.34	124.86	115.05
2	B	600	ACT	OXT-C-CH3	2.27	124.56	115.05
2	C	601	ACT	OXT-C-O	-2.24	113.71	122.03
2	D	600	ACT	OXT-C-O	-2.23	113.74	122.03
2	D	601	ACT	OXT-C-CH3	2.21	124.31	115.05
2	C	601	ACT	OXT-C-CH3	2.12	123.93	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	ACT	OXT-C-CH3	2.11	123.92	115.05
2	H	601	ACT	OXT-C-CH3	2.04	123.59	115.05
2	A	600	ACT	OXT-C-CH3	2.03	123.56	115.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	ACT	3	0
2	H	601	ACT	3	0
2	A	600	ACT	2	0
2	B	601	ACT	4	0
2	H	600	ACT	3	0
2	E	600	ACT	5	0
2	C	601	ACT	3	0
2	C	600	ACT	2	0
2	E	601	ACT	7	0
2	B	600	ACT	4	0
2	A	601	ACT	3	0
2	D	600	ACT	3	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	234/262 (89%)	-0.03	2 (0%) 81 80	42, 53, 70, 82	0
1	B	234/262 (89%)	-0.06	1 (0%) 88 87	44, 52, 70, 81	0
1	C	234/262 (89%)	0.02	1 (0%) 88 87	42, 53, 67, 80	0
1	D	234/262 (89%)	-0.07	3 (1%) 75 73	40, 52, 67, 78	0
1	E	234/262 (89%)	-0.07	3 (1%) 75 73	44, 52, 67, 80	0
1	F	234/262 (89%)	-0.02	0 100 100	42, 52, 66, 75	0
1	G	234/262 (89%)	0.19	7 (2%) 52 49	43, 53, 69, 79	0
1	H	234/262 (89%)	0.00	3 (1%) 75 73	44, 52, 70, 81	0
All	All	1872/2096 (89%)	-0.00	20 (1%) 78 76	40, 52, 69, 82	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	198	PHE	3.6
1	H	198	PHE	3.4
1	H	188	GLY	3.0
1	G	198	PHE	2.9
1	G	377	VAL	2.8
1	B	198	PHE	2.6
1	G	291	GLN	2.5
1	A	198	PHE	2.5
1	C	322	ALA	2.5
1	D	198	PHE	2.4
1	G	238	PHE	2.4
1	E	291	GLN	2.4
1	G	292	GLY	2.3
1	G	188	GLY	2.3
1	D	196	LYS	2.2
1	E	290	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	196	LYS	2.2
1	A	241	GLY	2.0
1	D	190	ASP	2.0
1	G	289	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(Å ²)	Q<0.9
2	ACT	G	601	4/4	0.75	0.23	80,80,81,81	0
2	ACT	A	601	4/4	0.77	0.21	64,65,65,65	0
2	ACT	E	601	4/4	0.84	0.16	67,67,67,67	0
2	ACT	H	601	4/4	0.85	0.14	51,52,52,52	0
2	ACT	C	601	4/4	0.87	0.14	63,63,63,64	0
2	ACT	D	600	4/4	0.88	0.16	58,60,60,60	0
3	CL	G	602	1/1	0.88	0.13	63,63,63,63	1
2	ACT	D	601	4/4	0.92	0.10	56,56,56,56	0
2	ACT	A	600	4/4	0.92	0.10	50,50,51,51	0
2	ACT	F	601	4/4	0.92	0.12	57,57,58,58	0
2	ACT	G	600	4/4	0.93	0.13	61,61,61,61	0
2	ACT	E	600	4/4	0.93	0.13	56,57,57,57	0
2	ACT	F	600	4/4	0.94	0.09	50,51,51,51	0
2	ACT	H	600	4/4	0.94	0.12	47,48,48,49	0
2	ACT	B	601	4/4	0.94	0.12	52,53,53,54	0
3	CL	E	603	1/1	0.94	0.16	74,74,74,74	0
2	ACT	B	600	4/4	0.94	0.09	50,51,52,53	0
3	CL	A	603	1/1	0.95	0.14	74,74,74,74	0
3	CL	B	602	1/1	0.95	0.08	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	C	600	4/4	0.96	0.11	58,58,58,58	0
3	CL	D	602	1/1	0.96	0.08	75,75,75,75	0
3	CL	H	602	1/1	0.96	0.06	54,54,54,54	0
3	CL	F	602	1/1	0.97	0.08	65,65,65,65	0
3	CL	E	602	1/1	0.97	0.09	64,64,64,64	0
3	CL	G	603	1/1	0.97	0.06	68,68,68,68	0
3	CL	C	602	1/1	0.97	0.13	59,59,59,59	0
3	CL	A	602	1/1	0.98	0.11	62,62,62,62	0
3	CL	H	603	1/1	0.98	0.18	61,61,61,61	1

6.5 Other polymers [i](#)

There are no such residues in this entry.