



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:45 AM GMT

PDB ID : 2IHW
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

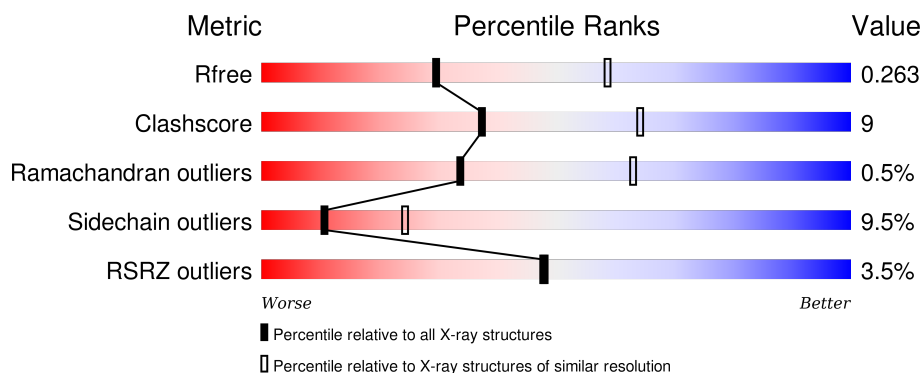
1 Overall quality at a glance

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}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>16%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	262	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	262	<div> <div>2%</div> <div> <div></div> <div>69%</div> <div>18%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	262	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>20%</div> <div>•</div> <div>11%</div> </div> </div>
1	E	262	<div> <div>4%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	262	
1	G	262	
1	H	262	

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	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	X
2	ACT	G	601	-	-	-	X
2	ACT	H	600	-	-	X	-
2	ACT	H	601	-	-	X	-
3	CL	A	602	-	-	X	-
3	CL	A	603	-	-	-	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:

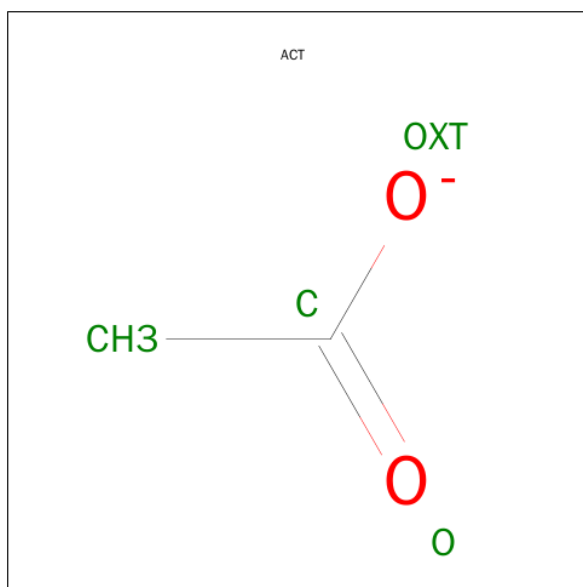
Chain	Residue	Modelled	Actual	Comment	Reference
A	160	GLY	-	CLONING ARTIFACT	UNP P11181
A	161	HIS	-	CLONING ARTIFACT	UNP P11181
B	160	GLY	-	CLONING ARTIFACT	UNP P11181
B	161	HIS	-	CLONING ARTIFACT	UNP P11181
C	160	GLY	-	CLONING ARTIFACT	UNP P11181
C	161	HIS	-	CLONING ARTIFACT	UNP P11181
D	160	GLY	-	CLONING 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

Continued on next page...

Continued from previous page...

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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

Continued on next page...

Continued from previous page...

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 (three-letter code: CL) (formula: Cl).

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

Continued on next page...

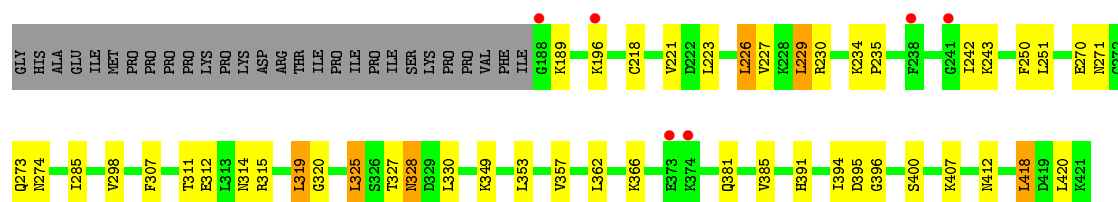
Continued from previous page...

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

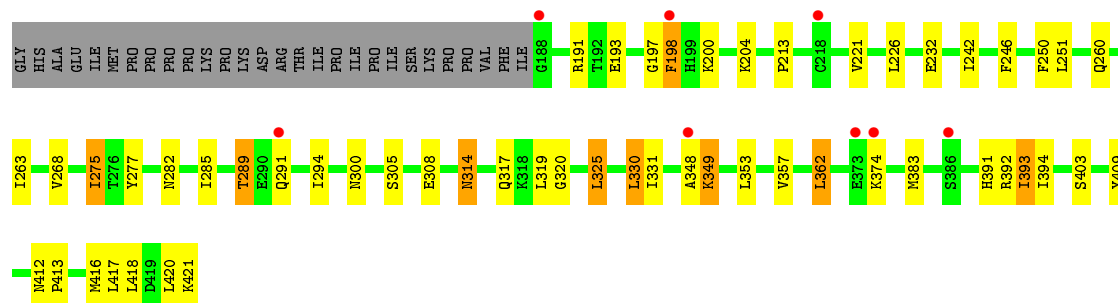
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

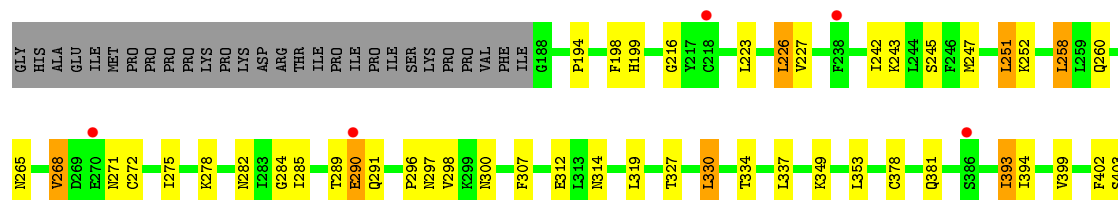
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



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

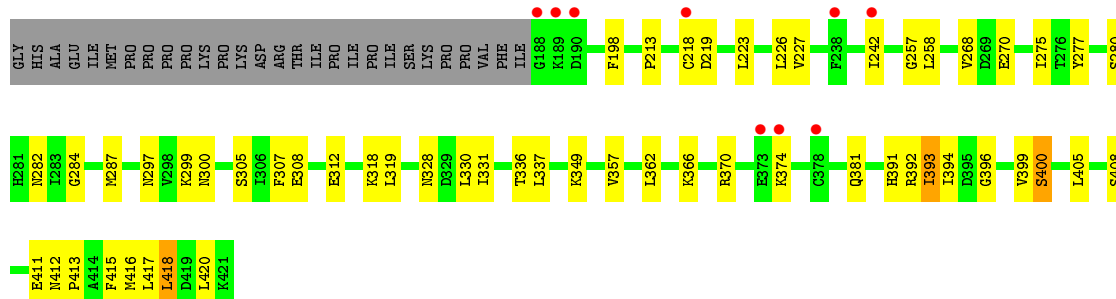


- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex

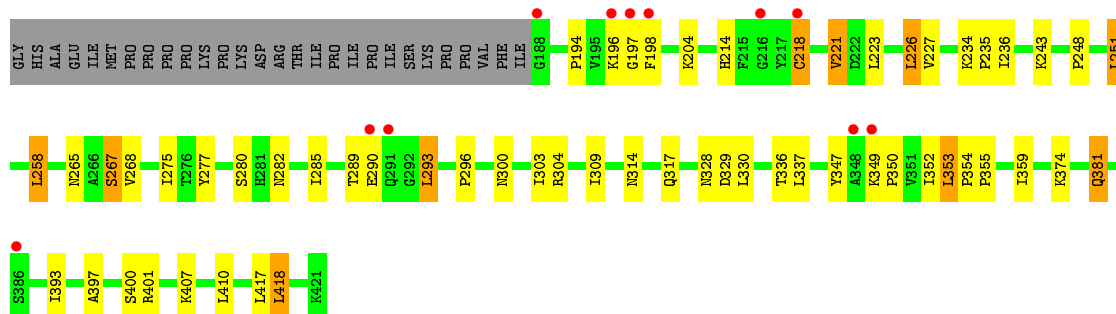




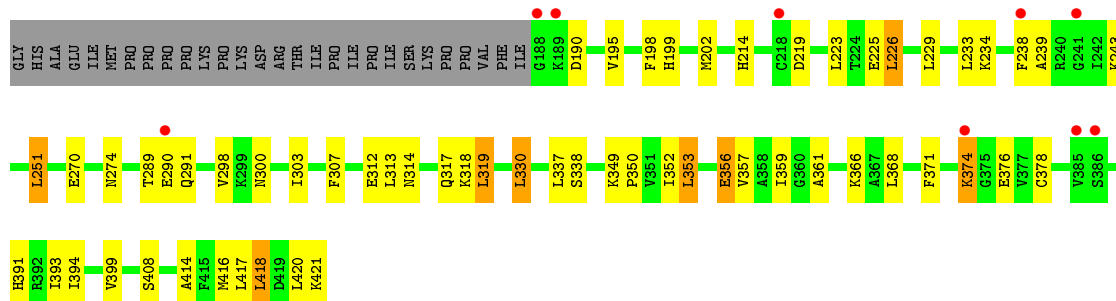
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



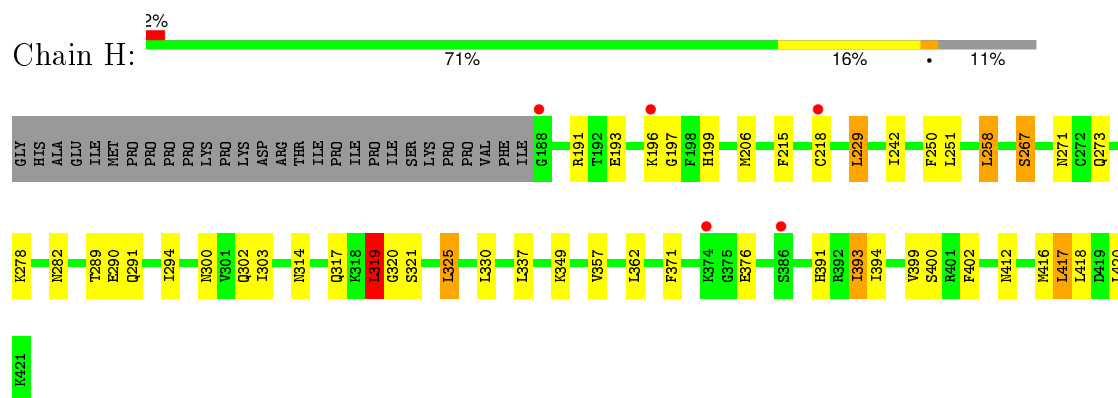
- Molecule 1: Lipoamide acyltransferase component of branched-chain alpha-keto acid dehydrogenase complex



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



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



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 40.12 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.70) 97.7 (40.12-2.70)	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 5.2.0019	Depositor
R, R_{free}	0.183 , 0.257 0.201 , 0.263	Depositor DCC
R_{free} test set	3297 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.1	EDS
Estimated twinning fraction	0.005 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 65279 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ACT

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	0.93	1/1837 (0.1%)	0.88	1/2481 (0.0%)
1	B	0.97	1/1837 (0.1%)	0.90	1/2481 (0.0%)
1	C	0.91	1/1837 (0.1%)	0.85	0/2481
1	D	0.92	1/1837 (0.1%)	0.88	1/2481 (0.0%)
1	E	0.93	1/1837 (0.1%)	0.92	2/2481 (0.1%)
1	F	1.01	4/1837 (0.2%)	0.93	5/2481 (0.2%)
1	G	0.91	2/1837 (0.1%)	0.85	1/2481 (0.0%)
1	H	1.02	1/1837 (0.1%)	0.95	5/2481 (0.2%)
All	All	0.95	12/14696 (0.1%)	0.90	16/19848 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	374	LYS	CE-NZ	14.89	1.86	1.49
1	G	188	GLY	N-CA	12.84	1.65	1.46
1	H	218	CYS	CB-SG	-6.95	1.70	1.82
1	E	218	CYS	CB-SG	-6.28	1.71	1.82
1	F	374	LYS	CD-CE	6.03	1.66	1.51
1	A	218	CYS	CB-SG	-5.91	1.72	1.81
1	D	218	CYS	CB-SG	-5.49	1.72	1.81
1	B	198	PHE	CE2-CZ	5.47	1.47	1.37
1	F	378	CYS	CB-SG	-5.46	1.73	1.81
1	C	378	CYS	CB-SG	-5.37	1.73	1.81
1	G	270	GLU	CG-CD	5.19	1.59	1.51
1	F	356	GLU	CD-OE2	5.07	1.31	1.25

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	374	LYS	CD-CE-NZ	-7.44	94.58	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	ASP	CB-CG-OD1	6.64	124.28	118.30
1	E	304	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	F	313	LEU	CA-CB-CG	5.95	128.98	115.30
1	H	417	LEU	CB-CG-CD1	-5.73	101.26	111.00
1	B	330	LEU	CA-CB-CG	5.67	128.34	115.30
1	F	353	LEU	CA-CB-CG	5.60	128.17	115.30
1	F	219	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	219	ASP	CB-CG-OD1	5.45	123.20	118.30
1	E	418	LEU	CA-CB-CG	5.23	127.34	115.30
1	H	206	MET	CG-SD-CE	5.22	108.55	100.20
1	H	319	LEU	CA-CB-CG	5.19	127.24	115.30
1	H	400	SER	N-CA-CB	-5.19	102.71	110.50
1	G	418	LEU	CA-CB-CG	5.18	127.22	115.30
1	F	202	MET	CG-SD-CE	5.12	108.40	100.20
1	H	229	LEU	CB-CG-CD1	-5.10	102.33	111.00

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	27	0
1	B	1803	0	1859	32	0
1	C	1803	0	1859	34	0
1	D	1803	0	1859	30	0
1	E	1803	0	1859	35	0
1	F	1803	0	1859	37	0
1	G	1803	0	1859	39	0
1	H	1803	0	1859	25	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
2	F	8	0	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	272	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 (272) 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:NZ	1:F:374:LYS:CE	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
2:B:600:ACT:H1	2:B:601:ACT:H2	1.61	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:NZ	1:G:374:LYS:HB2	2.03	0.73
1:G:282:ASN:HD22	1:G:300:ASN:H	1.35	0.73
1:G:393:ILE:CD1	1:G:394:ILE:HD12	2.17	0.73
1:E:267:SER:HB3	1:E:355:PRO:O	1.88	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
1:C:289:THR:C	1:C:291:GLN:H	1.92	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
2:B:600:ACT:CH3	2:B:601:ACT:H2	2.24	0.66
1:A:319:LEU:HB3	1:A:325:LEU:HD13	1.78	0.66
1:F:374:LYS:CD	1:F:374:LYS:NZ	2.59	0.66
1:B:251:LEU:HD21	1:B:285:ILE:HD11	1.76	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:F:393:ILE:HD12	1:F:394:ILE:HG13	1.77	0.65
1:E:243:LYS:H	1:E:314:ASN:HD21	1.42	0.65
1:A:227:VAL:HG21	1:A:381:GLN:HG2	1.78	0.65
1:H:282:ASN:HD22	1:H:300:ASN:H	1.44	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:600:ACT:H1	2:E:601:ACT:H3	1.79	0.64
1:G:374:LYS:HZ3	1:G:374:LYS:HB2	1.62	0.64
1:F:414:ALA:O	1:F:417:LEU:HB2	1.98	0.64
1:D:305:SER:OG	1:D:308:GLU:HG3	1.99	0.63
1:A:229:LEU:HD12	1:A:229:LEU:O	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:E:251:LEU:HD12	1:E:337:LEU:HD12	1.80	0.62
1:D:416:MET:O	1:D:420:LEU:HG	1.99	0.62
1:A:349:LYS:NZ	3:A:602:CL:CL	2.69	0.61
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: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: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:F:198:PHE:CE2	1:F:199:HIS:CE1	2.85	0.59
1:E:282:ASN:ND2	1:E:300:ASN:H	2.00	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
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:B:282:ASN:HD22	1:B:300:ASN:H	1.52	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:267:SER:HB2	1:H:278:LYS:HE3	1.86	0.56
1:G:340:ILE:HG13	1:G:341:GLY:N	2.18	0.56
2:E:600:ACT:CH3	2:E:601:ACT:CH3	2.81	0.56
1:F:289:THR:C	1:F:291:GLN:H	2.08	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:A:229:LEU:C	1:A:229:LEU:HD12	2.26	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:H:251:LEU:HD12	1:H:337:LEU:CD1	2.35	0.54
1:G:374:LYS:CB	1:G:374:LYS:NZ	2.71	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:H:320:GLY:HA2	1:H:325:LEU:HD22	1.91	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: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:D:280:SER:HB3	1:D:282:ASN:HD21	1.74	0.52
1:C:289:THR:HG22	1:C:291:GLN:N	2.25	0.52
1:H:289:THR:C	1:H:291:GLN:H	2.13	0.52
1:A:396:GLY:O	1:A:400:SER:HB2	2.10	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:G:247:MET:O	1:G:251:LEU:HB2	2.11	0.51
1:A:223:LEU:HD22	1:A:226:LEU:HD12	1.92	0.51
1:B:197:GLY:O	1:B:200:LYS:HB2	2.10	0.51
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:191:ARG:HH21	1:B:193:GLU:CD	2.14	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:242:ILE:HG23	1:H:314:ASN:HD21	1.75	0.49
1:G:370:ARG:HG2	1:G:370:ARG:HH11	1.76	0.49
1:G:289:THR:HG21	4:G:125:HOH:O	2.12	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:294:ILE:HD11	1:G:330:LEU:HD21	1.94	0.48
1:G:270:GLU:OE1	1:G:270:GLU:HA	2.13	0.48
1:G:349:LYS:NZ	3:G:603:CL:CL	2.79	0.48
1:C:289:THR:C	1:C:291:GLN:N	2.64	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: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:C:278:LYS:HD3	1:C:334:THR:HG22	1.96	0.48
1:B:263:ILE:O	1:B:263:ILE:HG12	2.14	0.48
1:A:250:PHE:CD2	1:A:362:LEU:HD13	2.48	0.48
1:F:416:MET:O	1:F:420:LEU:HG	2.14	0.48
1:E:381:GLN:HE21	1:E:381:GLN:HA	1.79	0.48
1:F:289:THR:C	1:F:291:GLN:N	2.66	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:F:238:PHE:O	1:F:239:ALA:C	2.51	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
1:C:289:THR:HG22	1:C:290:GLU:N	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:THR:CG2	1:C:290:GLU:N	2.78	0.47
1:B:403:SER:HB3	4:B:13:HOH:O	2.15	0.47
1:C:258:LEU:HD13	1:C:402:PHE:CE1	2.50	0.46
2:E:600:ACT:H1	2:E:601:ACT:H1	1.92	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
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:G:370:ARG:O	1:G:378:CYS:HB2	2.16	0.46
1:F:223:LEU:HD22	1:F:226:LEU:HD12	1.97	0.46
1:A:328:ASN:H	1:A:328:ASN:ND2	2.14	0.46
1:E:268:VAL:CG1	1:E:393:ILE:HG12	2.44	0.45
1:D:415:PHE:CD1	1:D:415:PHE:N	2.83	0.45
1:G:330:LEU:HA	1:G:330:LEU:HD12	1.79	0.45
1:C:258:LEU:HG	1:C:265:ASN:HB2	1.98	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:B:314:ASN:HD22	1:B:314:ASN:N	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:G:251:LEU:CD1	1:G:337:LEU:HD12	2.47	0.44
1:E:223:LEU:HD22	1:E:226:LEU:HD12	1.99	0.44
1:C:268:VAL:HG21	1:C:272:CYS:SG	2.57	0.44
1:A:242:ILE:HD12	1:A:311:THR:HA	1.99	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:299:LYS:NZ	1:D:328:ASN:O	2.45	0.44
1:H:258:LEU:HD13	1:H:402:PHE:CE1	2.53	0.44
1:D:284:GLY:HA2	1:D:297:ASN:HA	2.00	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
2:E:601:ACT:OXT	1:F:391:HIS:NE2	2.51	0.43
1:F:251:LEU:CD1	1:F:337:LEU:HD12	2.46	0.43
1:E:218:CYS:HB3	1:E:347:TYR:CE1	2.52	0.43
1:B:348:ALA:HB1	1:C:216:GLY:O	2.18	0.43
1:E:410:LEU:HA	1:E:410:LEU:HD23	1.86	0.43
1:A:243:LYS:H	1:A:314:ASN:HD21	1.67	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:N	1:E:236:ILE:HD13	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:319:LEU:HA	1:F:319:LEU:HD12	1.77	0.43
1:G:221:VAL:HG13	1:G:407:LYS:HG3	2.01	0.43
1:F:338:SER:O	1:F:361:ALA:HA	2.19	0.43
1:G:414:ALA:O	1:G:417:LEU:HB2	2.19	0.43
1:B:409:TYR:O	1:B:413:PRO:HA	2.18	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:G:296:PRO:HA	1:G:329:ASP:O	2.18	0.42
1:C:282:ASN:HD22	1:C:300:ASN:H	1.66	0.42
1:G:241:GLY:O	1:G:242:ILE:HD13	2.20	0.42
1:C:284:GLY:HA2	1:C:297:ASN:HA	2.01	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:E:353:LEU:O	1:E:354:PRO:C	2.58	0.42
1:G:370:ARG:HG2	1:G:370:ARG:NH1	2.34	0.42
1:B:242:ILE:HA	1:B:242:ILE:HD13	1.74	0.42
1:C:275:ILE:HD11	1:C:393:ILE:CG2	2.49	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
1:F:330:LEU:HA	1:F:330:LEU:HD12	1.91	0.42
1:A:230:ARG:NH2	1:A:234:LYS:HD3	2.34	0.42
1:C:275:ILE:HD11	1:C:393:ILE:HG22	2.02	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:E:280:SER:HB3	1:E:282:ASN:ND2	2.35	0.41
1:B:357:VAL:HB	1:B:394:ILE:HD11	2.02	0.41
1:D:415:PHE:HD1	1:D:415:PHE:N	2.18	0.41
1:G:352:ILE:O	1:G:354:PRO:HD3	2.21	0.41
1:H:320:GLY:HA2	1:H:325:LEU:CD2	2.50	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:C:252:LYS:HD2	1:C:252:LYS:HA	1.89	0.41
1:F:300:ASN:HB3	1:F:303:ILE:HG12	2.02	0.41
1:C:330:LEU:HD12	1:C:330:LEU:HA	1.90	0.41
1:G:271:ASN:HB2	1:G:273:GLN:HG2	2.03	0.41
1:H:197:GLY:C	1:H:199:HIS:N	2.75	0.41
1:F:371:PHE:HA	1:F:376:GLU:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:248:PRO:HA	1:E:309:ILE:HG21	2.03	0.41
1:D:391:HIS:ND1	1:D:391:HIS:O	2.52	0.41
1:E:300:ASN:HB3	1:E:303:ILE:HG12	2.03	0.40
1:B:357:VAL:HG21	1:B:394:ILE:HD11	2.02	0.40
1:F:243:LYS:H	1:F:314:ASN:HD21	1.68	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: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:G:369:PRO:O	1:G:370:ARG:NH1	2.54	0.40
1:B:416:MET:O	1:B:420:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	39	69
1	D	232/262 (88%)	220 (95%)	11 (5%)	1 (0%)	39	69
1	E	232/262 (88%)	223 (96%)	8 (3%)	1 (0%)	39	69
1	F	232/262 (88%)	208 (90%)	22 (10%)	2 (1%)	21	49
1	G	232/262 (88%)	214 (92%)	15 (6%)	3 (1%)	15	37
1	H	232/262 (88%)	223 (96%)	8 (3%)	1 (0%)	39	69
All	All	1856/2096 (88%)	1751 (94%)	96 (5%)	9 (0%)	34	63

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%)	180 (92%)	16 (8%)	14	32
1	B	196/222 (88%)	175 (89%)	21 (11%)	8	19
1	C	196/222 (88%)	181 (92%)	15 (8%)	16	36
1	D	196/222 (88%)	178 (91%)	18 (9%)	11	25
1	E	196/222 (88%)	178 (91%)	18 (9%)	11	25
1	F	196/222 (88%)	182 (93%)	14 (7%)	18	41
1	G	196/222 (88%)	164 (84%)	32 (16%)	3	7
1	H	196/222 (88%)	181 (92%)	15 (8%)	16	36
All	All	1568/1776 (88%)	1419 (90%)	149 (10%)	11	24

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	189	LYS
1	A	196	LYS
1	A	226	LEU
1	A	229	LEU
1	A	270	GLU
1	A	271	ASN
1	A	273	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	198	PHE
1	B	204	LYS
1	B	232	GLU
1	B	260	GLN
1	B	275	ILE
1	B	289	THR
1	B	294	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	412	ASN
1	B	417	LEU
1	B	418	LEU
1	B	421	LYS
1	C	226	LEU
1	C	243	LYS
1	C	251	LEU
1	C	258	LEU
1	C	268	VAL
1	C	271	ASN
1	C	314	ASN
1	C	319	LEU
1	C	327	THR
1	C	330	LEU
1	C	353	LEU
1	C	393	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	399	VAL
1	C	412	ASN
1	C	418	LEU
1	D	198	PHE
1	D	226	LEU
1	D	258	LEU
1	D	287	MET
1	D	318	LYS
1	D	319	LEU
1	D	330	LEU
1	D	331	ILE
1	D	362	LEU
1	D	366	LYS
1	D	374	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	196	LYS
1	E	198	PHE
1	E	204	LYS
1	E	221	VAL
1	E	226	LEU
1	E	251	LEU
1	E	258	LEU
1	E	267	SER
1	E	293	LEU
1	E	317	GLN
1	E	328	ASN
1	E	330	LEU
1	E	353	LEU
1	E	374	LYS
1	E	381	GLN
1	E	400	SER
1	E	417	LEU
1	E	418	LEU
1	F	226	LEU
1	F	234	LYS
1	F	251	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	270	GLU
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	F	421	LYS
1	G	193	GLU
1	G	198	PHE
1	G	200	LYS
1	G	228	LYS
1	G	229	LEU
1	G	251	LEU
1	G	270	GLU
1	G	272	CYS
1	G	274	ASN
1	G	275	ILE
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
1	G	364	THR
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	421	LYS
1	H	229	LEU
1	H	258	LEU
1	H	267	SER
1	H	271	ASN
1	H	273	GLN
1	H	294	ILE
1	H	317	GLN
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) 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
1	B	282	ASN
1	B	381	GLN
1	B	384	ASN
1	C	199	HIS
1	C	271	ASN
1	C	282	ASN
1	D	282	ASN
1	D	314	ASN
1	E	282	ASN
1	E	314	ASN
1	E	381	GLN
1	E	384	ASN
1	F	199	HIS
1	F	274	ASN
1	F	314	ASN
1	G	282	ASN
1	G	314	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	381	GLN
1	H	274	ASN
1	H	282	ASN
1	H	314	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 carbohydrates 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	A	600	-	1,3,3	2.41	1 (100%)	0,3,3	0.00	-
2	ACT	A	601	-	1,3,3	2.52	1 (100%)	0,3,3	0.00	-
2	ACT	B	600	-	1,3,3	2.24	1 (100%)	0,3,3	0.00	-
2	ACT	B	601	-	1,3,3	0.79	0	0,3,3	0.00	-
2	ACT	C	600	-	1,3,3	1.61	0	0,3,3	0.00	-
2	ACT	C	601	-	1,3,3	1.81	0	0,3,3	0.00	-
2	ACT	D	600	-	1,3,3	2.11	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACT	D	601	-	1,3,3	1.16	0	0,3,3	0.00	-
2	ACT	E	600	-	1,3,3	2.17	1 (100%)	0,3,3	0.00	-
2	ACT	E	601	-	1,3,3	2.00	1 (100%)	0,3,3	0.00	-
2	ACT	F	600	-	1,3,3	2.54	1 (100%)	0,3,3	0.00	-
2	ACT	F	601	-	1,3,3	2.02	1 (100%)	0,3,3	0.00	-
2	ACT	G	600	-	1,3,3	1.49	0	0,3,3	0.00	-
2	ACT	G	601	-	1,3,3	1.59	0	0,3,3	0.00	-
2	ACT	H	600	-	1,3,3	0.77	0	0,3,3	0.00	-
2	ACT	H	601	-	1,3,3	1.69	0	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACT	A	600	-	-	0/0/0/0	0/0/0/0
2	ACT	A	601	-	-	0/0/0/0	0/0/0/0
2	ACT	B	600	-	-	0/0/0/0	0/0/0/0
2	ACT	B	601	-	-	0/0/0/0	0/0/0/0
2	ACT	C	600	-	-	0/0/0/0	0/0/0/0
2	ACT	C	601	-	-	0/0/0/0	0/0/0/0
2	ACT	D	600	-	-	0/0/0/0	0/0/0/0
2	ACT	D	601	-	-	0/0/0/0	0/0/0/0
2	ACT	E	600	-	-	0/0/0/0	0/0/0/0
2	ACT	E	601	-	-	0/0/0/0	0/0/0/0
2	ACT	F	600	-	-	0/0/0/0	0/0/0/0
2	ACT	F	601	-	-	0/0/0/0	0/0/0/0
2	ACT	G	600	-	-	0/0/0/0	0/0/0/0
2	ACT	G	601	-	-	0/0/0/0	0/0/0/0
2	ACT	H	600	-	-	0/0/0/0	0/0/0/0
2	ACT	H	601	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	ACT	CH3-C	2.00	1.51	1.48
2	F	601	ACT	CH3-C	2.02	1.51	1.48
2	D	600	ACT	CH3-C	2.11	1.51	1.48
2	E	600	ACT	CH3-C	2.17	1.51	1.48
2	B	600	ACT	CH3-C	2.24	1.51	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	ACT	CH3-C	2.41	1.52	1.48
2	A	601	ACT	CH3-C	2.52	1.52	1.48
2	F	600	ACT	CH3-C	2.54	1.52	1.48

There are no bond angle outliers.

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	A	600	ACT	2	0
2	A	601	ACT	3	0
2	B	600	ACT	4	0
2	B	601	ACT	4	0
2	C	600	ACT	2	0
2	C	601	ACT	3	0
2	D	600	ACT	3	0
2	D	601	ACT	3	0
2	E	600	ACT	5	0
2	E	601	ACT	7	0
2	H	600	ACT	3	0
2	H	601	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%)	0.04	6 (2%) 59 59	42, 53, 70, 82	0
1	B	234/262 (89%)	0.08	8 (3%) 49 49	44, 52, 70, 81	0
1	C	234/262 (89%)	0.01	5 (2%) 67 68	42, 53, 67, 80	0
1	D	234/262 (89%)	-0.01	9 (3%) 44 44	40, 52, 67, 78	0
1	E	234/262 (89%)	0.11	11 (4%) 35 34	44, 52, 67, 80	0
1	F	234/262 (89%)	0.11	9 (3%) 44 44	42, 52, 66, 75	0
1	G	234/262 (89%)	0.20	12 (5%) 32 30	43, 53, 69, 79	0
1	H	234/262 (89%)	0.10	5 (2%) 67 68	44, 52, 70, 81	0
All	All	1872/2096 (89%)	0.08	65 (3%) 48 48	40, 52, 69, 82	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	188	GLY	4.3
1	G	373	GLU	4.3
1	D	188	GLY	4.1
1	A	188	GLY	4.0
1	E	198	PHE	4.0
1	G	198	PHE	3.9
1	F	188	GLY	3.9
1	B	374	LYS	3.7
1	E	291	GLN	3.6
1	B	198	PHE	3.5
1	H	188	GLY	3.4
1	G	374	LYS	3.3
1	C	270	GLU	3.2
1	H	196	LYS	3.1
1	D	189	LYS	3.0
1	G	238	PHE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	196	LYS	2.9
1	D	238	PHE	2.9
1	B	373	GLU	2.8
1	E	348	ALA	2.8
1	D	373	GLU	2.8
1	E	197	GLY	2.7
1	E	218	CYS	2.7
1	D	190	ASP	2.7
1	D	374	LYS	2.7
1	H	218	CYS	2.7
1	F	189	LYS	2.6
1	F	374	LYS	2.6
1	F	238	PHE	2.6
1	E	188	GLY	2.6
1	E	290	GLU	2.6
1	D	242	ILE	2.6
1	G	291	GLN	2.6
1	C	238	PHE	2.6
1	A	241	GLY	2.5
1	F	386	SER	2.5
1	F	218	CYS	2.5
1	C	290	GLU	2.5
1	A	373	GLU	2.5
1	G	372	ASN	2.5
1	G	348	ALA	2.5
1	B	291	GLN	2.4
1	B	348	ALA	2.4
1	G	242	ILE	2.4
1	G	290	GLU	2.3
1	C	218	CYS	2.3
1	B	386	SER	2.3
1	F	241	GLY	2.3
1	G	377	VAL	2.3
1	G	379	LYS	2.2
1	B	218	CYS	2.2
1	E	386	SER	2.2
1	D	218	CYS	2.2
1	E	216	GLY	2.2
1	D	378	CYS	2.2
1	F	290	GLU	2.2
1	F	385	VAL	2.1
1	B	188	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	386	SER	2.1
1	A	374	LYS	2.1
1	E	196	LYS	2.1
1	H	374	LYS	2.1
1	A	238	PHE	2.1
1	C	386	SER	2.0
1	E	349	LYS	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	CL	A	603	1/1	0.73	0.35	6.21	74,74,74,74	0
2	ACT	G	601	4/4	0.87	0.26	5.40	80,80,81,81	0
2	ACT	E	601	4/4	0.89	0.22	2.44	67,67,67,67	0
2	ACT	A	601	4/4	0.88	0.22	2.08	64,65,65,65	0
3	CL	C	602	1/1	0.94	0.25	1.97	59,59,59,59	0
2	ACT	G	600	4/4	0.96	0.20	1.30	61,61,61,61	0
3	CL	A	602	1/1	0.96	0.20	0.47	62,62,62,62	0
2	ACT	H	600	4/4	0.96	0.20	0.25	47,48,48,49	0
3	CL	F	602	1/1	0.98	0.20	0.09	65,65,65,65	0
2	ACT	H	601	4/4	0.93	0.16	-0.03	51,52,52,52	0
3	CL	E	602	1/1	0.97	0.21	-0.04	64,64,64,64	0
2	ACT	D	600	4/4	0.92	0.18	-0.16	58,60,60,60	0
3	CL	D	602	1/1	0.95	0.20	-0.19	75,75,75,75	0
2	ACT	E	600	4/4	0.94	0.18	-0.25	56,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ACT	F	601	4/4	0.96	0.15	-0.39	57,57,58,58	0
2	ACT	B	601	4/4	0.96	0.14	-0.59	52,53,53,54	0
2	ACT	C	600	4/4	0.97	0.14	-0.66	58,58,58,58	0
3	CL	B	602	1/1	0.96	0.13	-1.00	66,66,66,66	0
3	CL	H	602	1/1	0.97	0.14	-1.01	54,54,54,54	0
2	ACT	C	601	4/4	0.95	0.12	-1.35	63,63,63,64	0
2	ACT	F	600	4/4	0.98	0.12	-1.60	50,51,51,51	0
2	ACT	B	600	4/4	0.97	0.14	-1.82	50,51,52,53	0
2	ACT	A	600	4/4	0.98	0.09	-2.72	50,50,51,51	0
2	ACT	D	601	4/4	0.97	0.09	-2.88	56,56,56,56	0
3	CL	E	603	1/1	0.87	0.28	-	74,74,74,74	0
3	CL	G	603	1/1	0.97	0.24	-	68,68,68,68	0
3	CL	H	603	1/1	0.90	0.21	-	61,61,61,61	1
3	CL	G	602	1/1	0.96	0.07	-	63,63,63,63	1

6.5 Other polymers [i](#)

There are no such residues in this entry.