



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:07 pm BST

PDB ID : 5GN0  
Title : Structure of TAZ-TEAD complex  
Authors : Kaan, H.Y.K.; Song, H.  
Deposited on : 2016-07-18  
Resolution : 2.90 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](mailto: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.

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

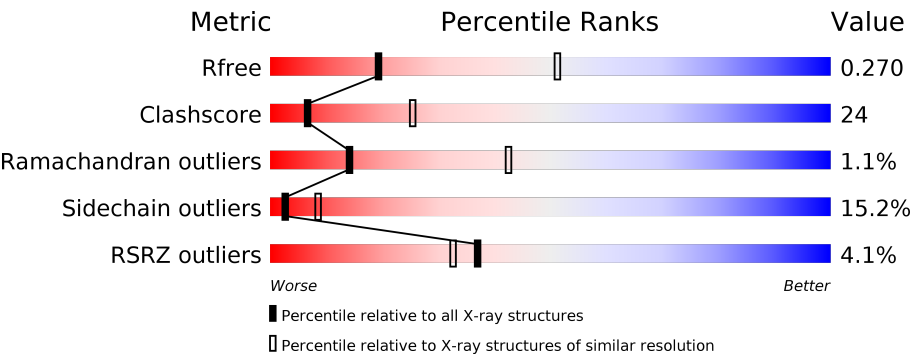
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

# 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 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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	225	<div><div>2%</div><div><div></div><div>52%</div><div>38%</div><div>8%</div><div>.</div></div></div>
1	B	225	<div><div>5%</div><div><div></div><div>62%</div><div>31%</div><div>6%</div><div>.</div></div></div>
1	C	225	<div><div>%</div><div><div></div><div>68%</div><div>24%</div><div>7%</div><div>.</div></div></div>
1	D	225	<div><div>4%</div><div><div></div><div>61%</div><div>32%</div><div>5%</div><div>.</div></div></div>
2	E	35	<div><div>17%</div><div><div></div><div>37%</div><div>43%</div><div>11%</div><div>9%</div></div></div>
2	F	35	<div><div>20%</div><div><div></div><div>43%</div><div>23%</div><div>20%</div><div>14%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	G	35	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>37%</div><div>43%</div><div>14%</div><div>6%</div></div></div>
2	H	35	<div><div><div></div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>51%</div><div>31%</div><div>9%</div><div>9%</div></div></div>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8228 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 Transcriptional enhancer factor TEF-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1775	1144	297	324	10			
1	B	222	Total	C	N	O	S	0	0	0
			1780	1147	294	329	10			
1	C	222	Total	C	N	O	S	0	0	0
			1781	1147	295	329	10			
1	D	221	Total	C	N	O	S	0	0	0
			1797	1154	298	335	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	ASP	-	expression tag	UNP Q62296
A	204	LEU	-	expression tag	UNP Q62296
A	205	ASN	-	expression tag	UNP Q62296
A	206	TRP	-	expression tag	UNP Q62296
A	207	ILE	-	expression tag	UNP Q62296
A	208	SER	-	expression tag	UNP Q62296
A	209	MET	-	expression tag	UNP Q62296
B	203	ASP	-	expression tag	UNP Q62296
B	204	LEU	-	expression tag	UNP Q62296
B	205	ASN	-	expression tag	UNP Q62296
B	206	TRP	-	expression tag	UNP Q62296
B	207	ILE	-	expression tag	UNP Q62296
B	208	SER	-	expression tag	UNP Q62296
B	209	MET	-	expression tag	UNP Q62296
C	203	ASP	-	expression tag	UNP Q62296
C	204	LEU	-	expression tag	UNP Q62296
C	205	ASN	-	expression tag	UNP Q62296
C	206	TRP	-	expression tag	UNP Q62296
C	207	ILE	-	expression tag	UNP Q62296
C	208	SER	-	expression tag	UNP Q62296
C	209	MET	-	expression tag	UNP Q62296

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Chain	Residue	Modelled	Actual	Comment	Reference
D	203	ASP	-	expression tag	UNP Q62296
D	204	LEU	-	expression tag	UNP Q62296
D	205	ASN	-	expression tag	UNP Q62296
D	206	TRP	-	expression tag	UNP Q62296
D	207	ILE	-	expression tag	UNP Q62296
D	208	SER	-	expression tag	UNP Q62296
D	209	MET	-	expression tag	UNP Q62296

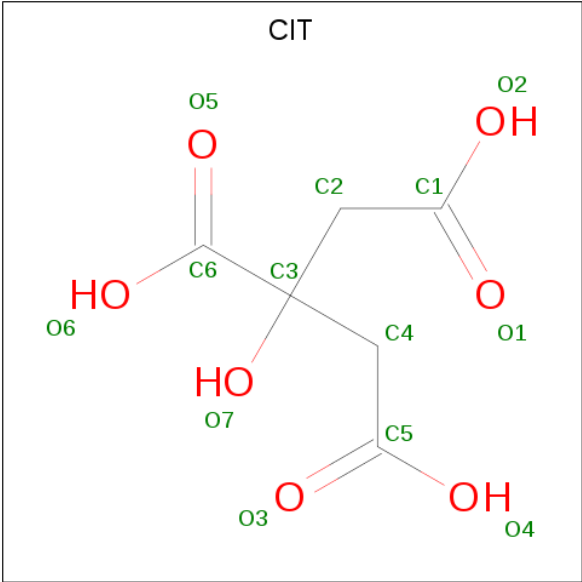
- Molecule 2 is a protein called WW domain-containing transcription regulator protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	32	Total	C	N	O	0	0	0
			250	164	40	46			
2	F	30	Total	C	N	O	0	0	0
			231	154	38	39			
2	G	33	Total	C	N	O	0	0	0
			264	171	42	50			
2	H	32	Total	C	N	O	0	0	0
			252	165	41	45			

There are 4 discrepancies between the modelled and reference sequences:

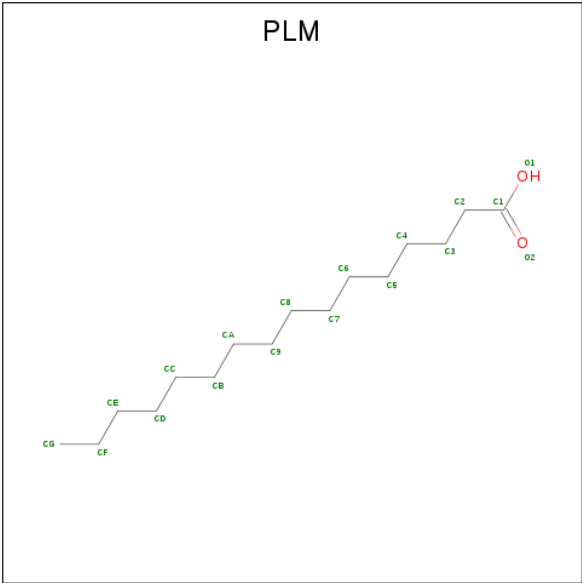
Chain	Residue	Modelled	Actual	Comment	Reference
E	23	PRO	-	expression tag	UNP Q9EPK5
F	23	PRO	-	expression tag	UNP Q9EPK5
G	23	PRO	-	expression tag	UNP Q9EPK5
H	23	PRO	-	expression tag	UNP Q9EPK5

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			18	16	2		
4	C	1	Total	C	O	0	0
			18	16	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			17	16	1		

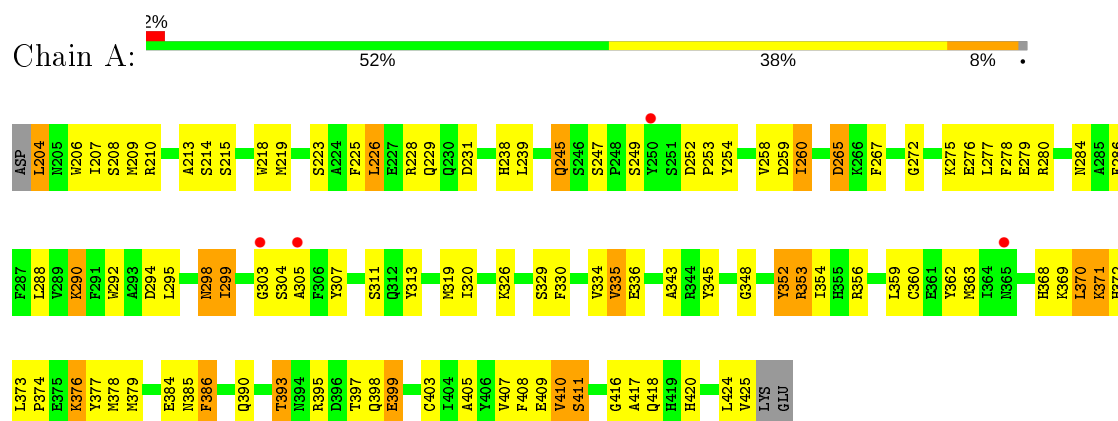
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	7	Total	O	0	0
			7	7		
5	C	4	Total	O	0	0
			4	4		
5	D	2	Total	O	0	0
			2	2		
5	F	1	Total	O	0	0
			1	1		

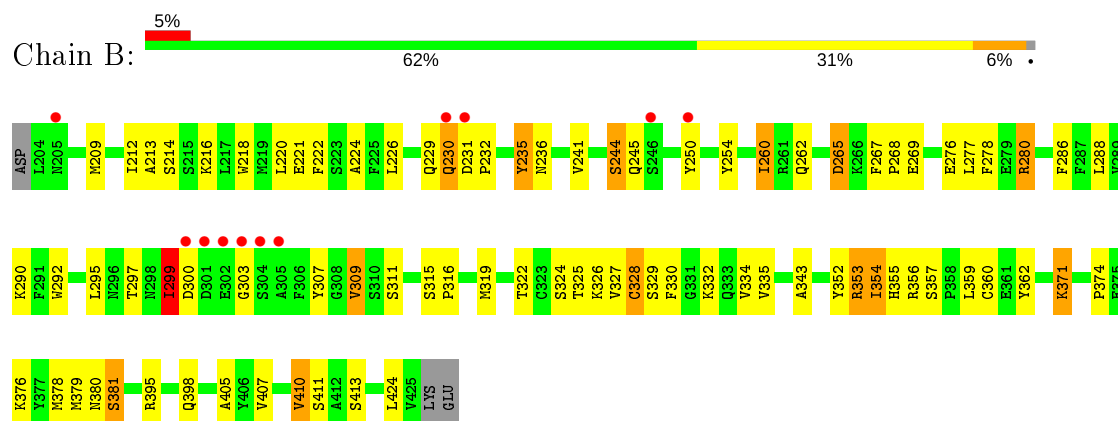
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

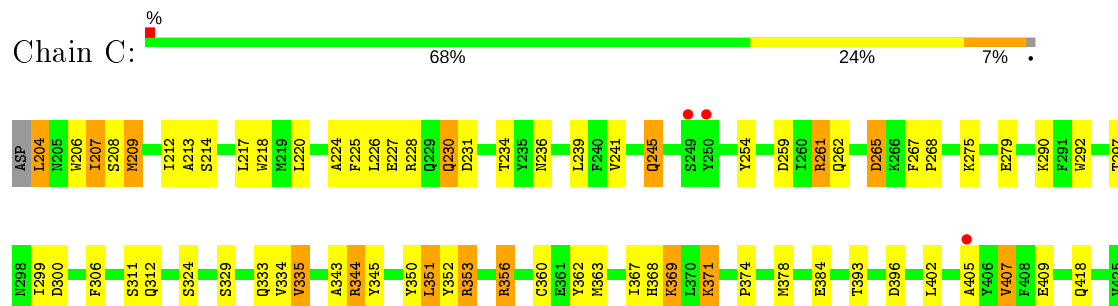
#### • Molecule 1: Transcriptional enhancer factor TEF-3



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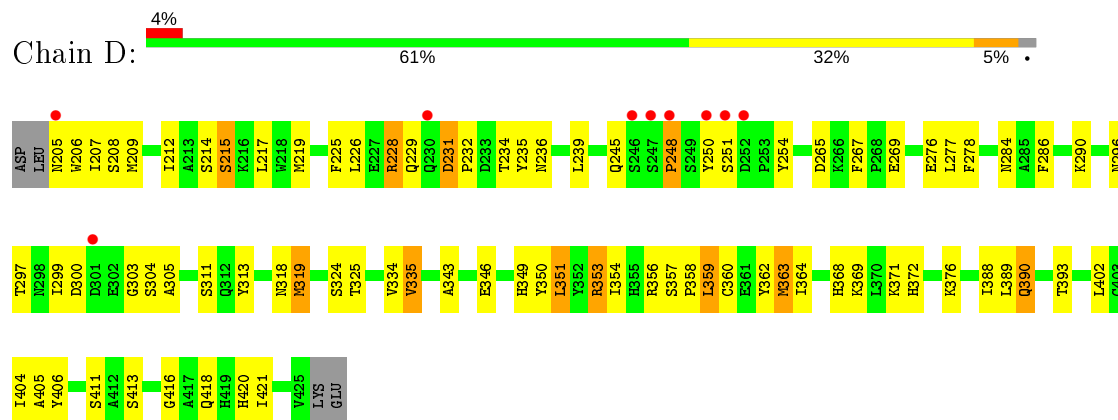
#### • Molecule 1: Transcriptional enhancer factor TEF-3



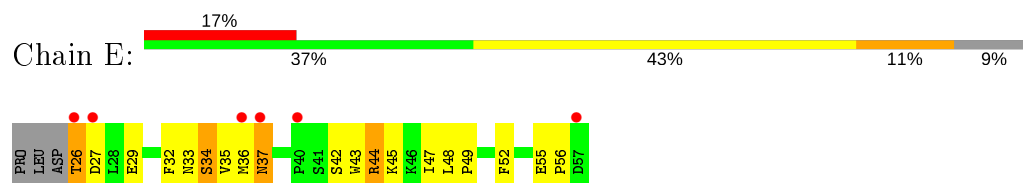


LYS  
GLU

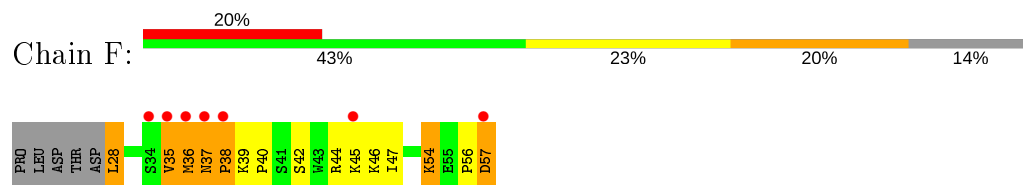
- Molecule 1: Transcriptional enhancer factor TEF-3



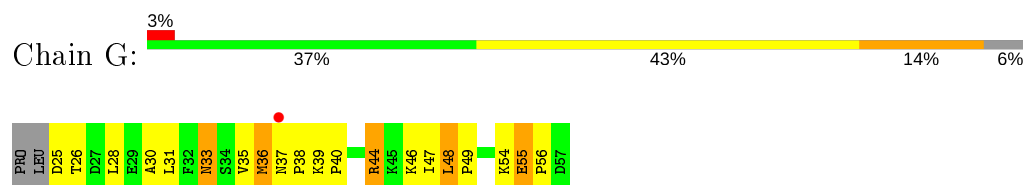
- Molecule 2: WW domain-containing transcription regulator protein 1



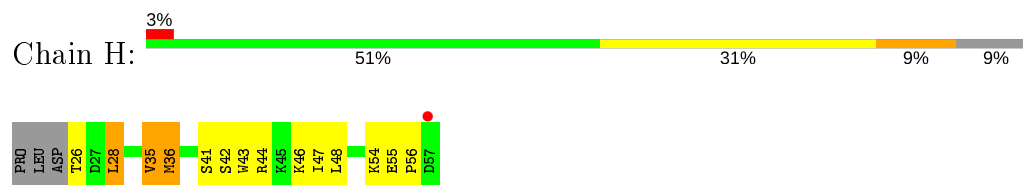
- Molecule 2: WW domain-containing transcription regulator protein 1



- Molecule 2: WW domain-containing transcription regulator protein 1



- Molecule 2: WW domain-containing transcription regulator protein 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.66Å 120.90Å 196.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.90) 98.6 (29.98-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.63 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.200 , 0.260 0.217 , 0.270	Depositor DCC
$R_{free}$ test set	2131 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	1.361	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	8228	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PLM, CIT

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	1.19	0/1824	0.87	1/2480 (0.0%)
1	B	1.29	0/1829	0.90	2/2486 (0.1%)
1	C	1.35	0/1829	0.88	1/2485 (0.0%)
1	D	1.38	0/1846	0.89	4/2505 (0.2%)
2	E	0.91	0/258	0.83	0/351
2	F	1.09	0/239	0.81	0/325
2	G	1.13	0/272	1.00	1/369 (0.3%)
2	H	1.16	0/260	0.87	0/353
All	All	1.28	0/8357	0.89	9/11354 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	299	ILE	N-CA-C	7.26	130.59	111.00
1	D	357	SER	C-N-CD	-6.33	106.67	120.60
1	A	303	GLY	N-CA-C	-5.95	98.24	113.10
2	G	55	GLU	C-N-CD	-5.90	107.62	120.60
1	C	351	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	355	HIS	N-CA-C	5.63	126.19	111.00
1	D	416	GLY	N-CA-C	5.56	127.01	113.10
1	D	265	ASP	CB-CA-C	-5.34	99.71	110.40
1	D	335	VAL	CB-CA-C	-5.25	101.42	111.40

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	1775	0	1671	106	0
1	B	1780	0	1675	75	0
1	C	1781	0	1681	65	0
1	D	1797	0	1701	60	0
2	E	250	0	235	24	0
2	F	231	0	220	22	0
2	G	264	0	250	27	0
2	H	252	0	242	15	0
3	B	13	0	5	4	0
3	C	13	0	5	2	0
4	B	18	0	31	2	0
4	C	18	0	31	2	0
4	D	17	0	31	5	0
5	A	5	0	0	0	0
5	B	7	0	0	0	0
5	C	4	0	0	0	0
5	D	2	0	0	0	0
5	F	1	0	0	0	0
All	All	8228	0	7778	376	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 24.

All (376) 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)
2:E:47:ILE:C	2:E:48:LEU:HD23	1.51	1.31
2:E:47:ILE:O	2:E:48:LEU:HD23	1.24	1.26
1:A:370:LEU:CD1	1:A:379:MET:HG2	1.73	1.17
1:A:379:MET:HE3	1:A:410:VAL:HG21	1.28	1.15
2:F:37:ASN:CB	2:F:38:PRO:HD3	1.74	1.14
1:B:231:ASP:HB2	1:B:232:PRO:HD3	1.18	1.13
1:A:370:LEU:HD11	1:A:379:MET:CG	1.83	1.08
1:C:262:GLN:OE1	2:F:47:ILE:N	1.90	1.05
2:F:37:ASN:HB3	2:F:38:PRO:CD	1.87	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:SER:OG	2:F:45:LYS:HB2	1.57	1.02
1:A:370:LEU:HD11	1:A:379:MET:HG2	1.04	1.01
2:F:42:SER:OG	2:F:45:LYS:HD2	1.62	1.00
1:A:379:MET:HE2	1:A:410:VAL:HG11	1.41	0.99
1:B:231:ASP:HB2	1:B:232:PRO:CD	1.93	0.99
1:A:326:LYS:HE2	1:A:336:GLU:OE1	1.63	0.98
2:E:47:ILE:O	2:E:48:LEU:CD2	2.12	0.96
1:B:226:LEU:HD13	1:B:307:TYR:CE2	2.00	0.96
1:B:335:VAL:HG21	1:B:362:TYR:OH	1.65	0.95
2:F:37:ASN:HB3	2:F:38:PRO:HD3	0.98	0.95
1:A:374:PRO:HG2	1:A:378:MET:SD	2.09	0.93
1:B:362:TYR:OH	4:B:502:PLM:O2	1.87	0.92
2:G:44:ARG:HG3	2:G:44:ARG:HH21	1.32	0.91
1:A:376:LYS:NZ	1:A:411:SER:O	2.04	0.90
1:B:231:ASP:CB	1:B:232:PRO:HD3	2.00	0.90
1:A:379:MET:CE	1:A:410:VAL:HG11	2.02	0.88
1:B:334:VAL:HG12	1:B:335:VAL:HG13	1.55	0.88
1:B:231:ASP:CB	1:B:232:PRO:CD	2.52	0.87
1:B:381:SER:OG	2:G:38:PRO:HB3	1.75	0.87
1:B:295:LEU:O	1:B:371:LYS:HE3	1.73	0.86
2:E:44:ARG:HG3	2:E:44:ARG:HH21	1.38	0.86
2:F:42:SER:OG	2:F:45:LYS:CD	2.25	0.85
1:A:330:PHE:CE1	1:A:385:ASN:ND2	2.44	0.85
1:A:372:HIS:O	1:A:373:LEU:HD12	1.77	0.85
1:A:370:LEU:CD1	1:A:379:MET:CG	2.45	0.85
1:D:376:LYS:NZ	1:D:411:SER:O	2.09	0.84
1:A:226:LEU:HD12	1:A:305:ALA:HB1	1.60	0.83
2:F:42:SER:HG	2:F:45:LYS:HB2	1.41	0.83
1:A:379:MET:CE	1:A:410:VAL:HG21	2.08	0.83
1:C:360:CYS:HB2	1:C:362:TYR:CE1	2.13	0.83
1:B:220:LEU:O	1:B:221:GLU:HG2	1.80	0.82
2:F:37:ASN:CB	2:F:38:PRO:CD	2.51	0.81
1:C:290:LYS:NZ	1:C:409:GLU:OE2	2.13	0.81
1:D:390:GLN:OE1	1:D:406:TYR:OH	1.99	0.81
1:C:212:ILE:H	1:C:245:GLN:HE22	1.25	0.81
1:D:231:ASP:CB	1:D:232:PRO:CD	2.61	0.79
2:E:33:ASN:O	2:E:34:SER:HB2	1.83	0.79
1:B:376:LYS:NZ	1:B:411:SER:O	2.15	0.79
1:D:325:THR:HG21	4:D:501:PLM:H52	1.64	0.79
2:G:37:ASN:N	2:G:38:PRO:HD3	1.98	0.79
1:D:231:ASP:HB3	1:D:232:PRO:CD	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ASP:HB3	1:D:232:PRO:HD2	1.64	0.78
1:B:380:ASN:OD1	1:B:410:VAL:HG23	1.83	0.77
1:D:209:MET:HE2	1:D:254:TYR:CE2	2.20	0.77
1:B:262:GLN:O	2:G:46:LYS:HE2	1.83	0.77
1:C:367:ILE:O	1:C:371:LYS:HB2	1.85	0.77
1:A:275:LYS:O	1:A:279:GLU:CG	2.33	0.77
1:B:300:ASP:OD1	1:B:303:GLY:HA2	1.86	0.76
1:A:326:LYS:CE	1:A:336:GLU:OE1	2.34	0.76
1:A:226:LEU:CD1	1:A:305:ALA:CB	2.65	0.75
2:E:47:ILE:C	2:E:48:LEU:CD2	2.45	0.75
1:A:298:ASN:O	1:A:298:ASN:ND2	2.19	0.75
1:B:267:PHE:HB3	1:B:268:PRO:CD	2.17	0.75
1:D:300:ASP:OD1	1:D:303:GLY:HA2	1.87	0.74
1:A:370:LEU:O	1:A:370:LEU:HD12	1.88	0.73
1:C:275:LYS:O	1:C:279:GLU:HG3	1.89	0.73
1:A:272:GLY:N	1:A:276:GLU:OE1	2.16	0.72
1:C:362:TYR:HB3	2:E:26:THR:HB	1.71	0.72
1:A:226:LEU:CD1	1:A:305:ALA:HB1	2.20	0.71
1:A:265:ASP:OD1	1:A:265:ASP:N	2.20	0.71
1:A:326:LYS:HG2	1:A:336:GLU:OE1	1.91	0.70
1:C:297:THR:O	1:C:371:LYS:NZ	2.24	0.70
2:G:35:VAL:O	2:G:36:MET:HB2	1.92	0.70
1:A:258:VAL:O	1:A:425:VAL:HG22	1.91	0.69
1:B:378:MET:O	1:B:381:SER:HB2	1.91	0.69
1:A:260:ILE:HG13	1:A:424:LEU:HB3	1.75	0.68
2:F:42:SER:OG	2:F:45:LYS:CB	2.39	0.68
1:D:231:ASP:HB2	1:D:234:THR:HB	1.74	0.68
1:D:356:ARG:O	1:D:358:PRO:HD3	1.94	0.68
2:H:28:LEU:C	2:H:28:LEU:HD23	2.14	0.67
1:A:353:ARG:O	1:A:353:ARG:HD3	1.93	0.67
1:C:231:ASP:HB2	1:C:234:THR:OG1	1.95	0.67
1:C:300:ASP:OD2	1:C:368:HIS:HD2	1.78	0.66
1:A:226:LEU:HD21	1:A:299:ILE:HB	1.77	0.66
1:B:267:PHE:CZ	1:B:405:ALA:HB1	2.31	0.66
1:D:351:LEU:N	1:D:351:LEU:HD13	2.11	0.66
1:C:262:GLN:O	2:F:46:LYS:HE2	1.94	0.65
2:G:37:ASN:H	2:G:38:PRO:HD3	1.59	0.65
1:C:236:ASN:HB3	1:C:299:ILE:HD11	1.76	0.65
1:B:360:CYS:HB2	1:B:362:TYR:CE1	2.32	0.65
1:C:360:CYS:CB	1:C:362:TYR:CE1	2.80	0.65
3:C:501:CIT:C6	3:C:501:CIT:O1	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:44:ARG:HH21	2:G:44:ARG:CG	2.09	0.64
2:G:28:LEU:HD12	2:G:28:LEU:N	2.10	0.64
1:B:226:LEU:HD13	1:B:307:TYR:CZ	2.33	0.64
1:B:343:ALA:HB2	1:B:352:TYR:CZ	2.33	0.64
3:B:501:CIT:O5	3:B:501:CIT:O3	2.14	0.64
1:A:373:LEU:HG	1:A:374:PRO:HD3	1.80	0.64
1:B:267:PHE:HB3	1:B:268:PRO:HD2	1.78	0.64
1:B:309:VAL:HG12	1:B:357:SER:HB3	1.80	0.64
2:F:42:SER:CB	2:F:45:LYS:HD2	2.28	0.64
2:E:48:LEU:HB3	2:E:49:PRO:HD2	1.80	0.63
1:B:343:ALA:HB2	1:B:352:TYR:CE2	2.32	0.63
1:A:275:LYS:O	1:A:279:GLU:HG2	1.99	0.62
1:C:224:ALA:HB3	1:C:241:VAL:HG22	1.81	0.62
2:E:36:MET:O	2:E:37:ASN:CB	2.48	0.62
1:A:334:VAL:HG12	1:A:335:VAL:HG22	1.81	0.62
1:A:295:LEU:HD12	1:A:410:VAL:CG2	2.30	0.62
1:B:213:ALA:HB2	1:B:218:TRP:HB2	1.82	0.62
2:G:46:LYS:HB2	2:G:48:LEU:HD11	1.82	0.61
1:B:297:THR:OG1	1:B:299:ILE:HG13	1.99	0.61
1:B:213:ALA:CB	1:B:218:TRP:HB3	2.31	0.61
1:D:217:LEU:HD23	1:D:402:LEU:HD12	1.81	0.61
1:D:226:LEU:HD11	1:D:305:ALA:CB	2.30	0.61
1:D:209:MET:CE	1:D:254:TYR:CE2	2.84	0.60
2:F:28:LEU:C	2:F:28:LEU:HD23	2.21	0.60
1:B:213:ALA:HB1	1:B:218:TRP:HB3	1.82	0.60
2:H:35:VAL:O	2:H:35:VAL:HG22	2.02	0.60
1:B:265:ASP:OD1	1:B:265:ASP:N	2.27	0.60
1:A:369:LYS:O	1:A:373:LEU:HD13	2.02	0.60
1:A:226:LEU:HD12	1:A:305:ALA:CB	2.30	0.60
1:C:360:CYS:HB2	1:C:362:TYR:CZ	2.37	0.60
2:G:35:VAL:O	2:G:36:MET:CB	2.49	0.60
2:G:36:MET:O	2:G:37:ASN:HB3	2.02	0.60
1:B:381:SER:OG	2:G:38:PRO:CB	2.49	0.60
1:D:359:LEU:CD2	1:D:363:MET:HG3	2.32	0.60
1:A:384:GLU:HG2	2:E:43:TRP:HD1	1.67	0.59
1:C:343:ALA:HB1	1:C:350:TYR:HB3	1.83	0.59
1:D:231:ASP:HB2	1:D:234:THR:CB	2.31	0.59
1:A:294:ASP:OD2	1:A:416:GLY:N	2.34	0.59
1:B:335:VAL:HG21	1:B:362:TYR:CZ	2.38	0.59
1:C:334:VAL:HG12	1:C:335:VAL:CG2	2.33	0.58
1:D:418:GLN:HB3	2:H:56:PRO:HG2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ARG:NH2	1:B:398:GLN:O	2.36	0.58
1:A:384:GLU:HG2	2:E:43:TRP:CD1	2.39	0.58
1:A:295:LEU:HD12	1:A:410:VAL:HG21	1.86	0.58
1:C:369:LYS:HD2	2:E:32:PHE:CE2	2.39	0.58
1:A:204:LEU:HD12	1:A:214:SER:O	2.04	0.58
1:B:262:GLN:O	2:G:46:LYS:CE	2.52	0.58
1:B:260:ILE:HG13	1:B:424:LEU:HD13	1.84	0.58
1:C:290:LYS:NZ	1:C:409:GLU:CD	2.58	0.57
1:A:226:LEU:HD11	1:A:305:ALA:CB	2.33	0.57
1:D:226:LEU:HD11	1:D:305:ALA:HB1	1.85	0.57
2:G:37:ASN:N	2:G:38:PRO:CD	2.65	0.57
2:G:44:ARG:HG3	2:G:44:ARG:NH2	2.11	0.57
1:A:298:ASN:C	1:A:298:ASN:HD22	2.08	0.57
1:C:350:TYR:N	1:C:350:TYR:CD1	2.73	0.57
2:E:47:ILE:HG22	2:E:47:ILE:O	2.04	0.56
2:G:39:LYS:CB	2:G:40:PRO:HD2	2.34	0.56
1:A:275:LYS:O	1:A:279:GLU:HG3	2.03	0.56
1:B:220:LEU:C	1:B:221:GLU:HG2	2.24	0.56
1:C:209:MET:HE2	1:C:254:TYR:CE2	2.40	0.56
1:C:217:LEU:HD23	1:C:402:LEU:HD12	1.86	0.56
1:C:225:PHE:HB3	1:C:239:LEU:HD23	1.87	0.56
1:C:204:LEU:HD23	1:C:214:SER:O	2.06	0.56
1:A:290:LYS:NZ	2:E:52:PHE:O	2.38	0.56
1:C:265:ASP:N	1:C:265:ASP:OD1	2.32	0.56
1:D:346:GLU:O	1:D:349:HIS:CE1	2.59	0.56
1:D:359:LEU:CD2	1:D:363:MET:CG	2.84	0.56
1:B:235:TYR:CD1	1:B:235:TYR:N	2.73	0.55
1:B:209:MET:HE2	1:B:254:TYR:CE2	2.41	0.55
1:D:297:THR:OG1	1:D:299:ILE:HG13	2.06	0.55
2:F:57:ASP:N	2:F:57:ASP:OD1	2.39	0.55
1:B:300:ASP:OD2	1:B:307:TYR:OH	2.12	0.55
2:F:35:VAL:HG22	2:F:35:VAL:O	2.04	0.55
2:G:28:LEU:O	2:G:31:LEU:HB2	2.07	0.55
1:B:278:PHE:HA	1:B:286:PHE:CZ	2.42	0.55
1:A:229:GLN:NE2	1:A:231:ASP:O	2.40	0.55
1:A:343:ALA:HB2	1:A:352:TYR:CE2	2.42	0.55
1:B:212:ILE:H	1:B:245:GLN:HE22	1.54	0.55
1:B:213:ALA:CB	1:B:218:TRP:CB	2.84	0.55
1:B:213:ALA:HB2	1:B:218:TRP:CB	2.37	0.54
1:A:215:SER:OG	1:A:284:ASN:ND2	2.39	0.54
2:H:28:LEU:HD22	2:H:28:LEU:H	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:44:ARG:NH2	2:E:44:ARG:HG3	2.16	0.53
1:A:209:MET:HE2	1:A:254:TYR:CE2	2.43	0.53
1:A:290:LYS:HG2	1:A:407:VAL:HG23	1.91	0.53
1:A:252:ASP:HB3	1:A:253:PRO:HD2	1.90	0.53
1:B:295:LEU:O	1:B:371:LYS:CE	2.54	0.53
1:A:370:LEU:C	1:A:370:LEU:HD12	2.29	0.52
1:D:388:ILE:HD12	4:D:501:PLM:H82	1.91	0.52
2:E:48:LEU:N	2:E:48:LEU:HD23	2.03	0.52
1:D:228:ARG:HB3	1:D:299:ILE:CG2	2.40	0.52
2:E:44:ARG:CG	2:E:44:ARG:HH21	2.10	0.52
1:A:208:SER:HB2	1:A:213:ALA:O	2.10	0.52
2:H:43:TRP:HA	2:H:46:LYS:HD2	1.92	0.52
1:B:209:MET:CE	1:B:254:TYR:CE2	2.92	0.52
1:C:334:VAL:HG12	1:C:335:VAL:HG22	1.90	0.52
1:A:373:LEU:HG	1:A:374:PRO:CD	2.40	0.52
1:A:370:LEU:HD12	1:A:379:MET:CG	2.36	0.52
2:G:28:LEU:CD1	2:G:28:LEU:N	2.73	0.51
1:B:376:LYS:CG	1:B:379:MET:HE3	2.40	0.51
1:D:351:LEU:N	1:D:351:LEU:CD1	2.73	0.51
2:F:36:MET:CB	2:F:40:PRO:HG3	2.41	0.51
1:D:411:SER:HB2	2:H:55:GLU:OE1	2.11	0.51
1:D:346:GLU:HB3	1:D:351:LEU:CD2	2.41	0.51
1:A:267:PHE:CZ	1:A:405:ALA:HB1	2.46	0.51
1:B:226:LEU:CD1	1:B:307:TYR:CZ	2.94	0.50
4:D:501:PLM:O2	4:D:501:PLM:H42	2.10	0.50
1:A:228:ARG:HB2	1:A:299:ILE:HG22	1.93	0.50
1:A:360:CYS:O	1:A:363:MET:HB2	2.10	0.50
2:H:41:SER:OG	2:H:44:ARG:HG3	2.12	0.50
1:C:353:ARG:HD3	3:C:501:CIT:O7	2.11	0.50
1:D:231:ASP:CB	1:D:232:PRO:HD2	2.34	0.50
1:D:231:ASP:CG	1:D:232:PRO:HD3	2.32	0.50
1:D:278:PHE:HA	1:D:286:PHE:CZ	2.47	0.50
1:D:359:LEU:HD22	1:D:363:MET:HB3	1.93	0.50
1:C:292:TRP:HA	1:C:409:GLU:O	2.12	0.50
1:D:236:ASN:HB3	1:D:299:ILE:HD13	1.93	0.50
1:C:226:LEU:HD12	1:C:306:PHE:O	2.11	0.50
1:B:226:LEU:HD13	1:B:307:TYR:CD2	2.44	0.50
1:B:354:ILE:HG22	1:B:354:ILE:O	2.11	0.50
1:D:346:GLU:O	1:D:349:HIS:ND1	2.45	0.50
1:A:213:ALA:HB2	1:A:218:TRP:CD1	2.47	0.49
1:B:216:LYS:O	1:B:315:SER:OG	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ARG:HD3	3:B:501:CIT:O6	2.12	0.49
1:D:229:GLN:HG3	1:D:235:TYR:CE2	2.47	0.49
1:B:322:THR:HG23	1:B:395:ARG:HG3	1.93	0.49
1:A:362:TYR:C	1:A:362:TYR:CD1	2.85	0.49
1:A:370:LEU:HD12	1:A:379:MET:HG2	1.80	0.49
1:B:322:THR:CG2	1:B:395:ARG:HG3	2.42	0.49
1:C:231:ASP:HB2	1:C:234:THR:CB	2.42	0.49
1:C:418:GLN:HB3	2:F:56:PRO:HG2	1.94	0.49
1:B:218:TRP:CZ3	1:B:245:GLN:O	2.66	0.49
1:A:209:MET:CE	1:A:254:TYR:CE2	2.95	0.49
1:A:228:ARG:HB3	1:A:299:ILE:CG2	2.41	0.49
1:C:362:TYR:HB3	2:E:26:THR:CB	2.42	0.49
1:D:362:TYR:CE1	2:H:28:LEU:HB3	2.47	0.49
1:A:207:ILE:HG22	1:A:207:ILE:O	2.12	0.49
1:A:370:LEU:CD1	1:A:379:MET:HG3	2.36	0.49
1:A:417:ALA:C	1:A:418:GLN:HG2	2.33	0.49
1:C:208:SER:CB	1:C:213:ALA:O	2.61	0.49
1:D:212:ILE:HD11	1:D:421:ILE:HD13	1.93	0.49
1:A:295:LEU:CD1	1:A:410:VAL:CG2	2.91	0.49
1:B:229:GLN:HG2	1:B:231:ASP:O	2.13	0.49
1:B:230:GLN:HG3	1:B:236:ASN:HD21	1.78	0.49
1:C:206:TRP:CE2	1:C:207:ILE:HG12	2.48	0.49
1:C:378:MET:HG2	2:E:35:VAL:HB	1.94	0.49
1:A:386:PHE:CD1	1:A:386:PHE:C	2.85	0.48
1:C:209:MET:HE2	1:C:254:TYR:CD2	2.48	0.48
1:B:374:PRO:HD2	1:B:378:MET:SD	2.52	0.48
1:A:352:TYR:CD1	1:A:352:TYR:N	2.81	0.48
1:A:238:HIS:HE1	1:A:294:ASP:O	1.97	0.48
1:B:221:GLU:O	1:B:311:SER:HA	2.13	0.48
1:B:226:LEU:HD23	1:B:297:THR:HG21	1.96	0.48
2:E:44:ARG:NH2	2:E:44:ARG:CG	2.72	0.48
1:A:228:ARG:CB	1:A:299:ILE:CG2	2.92	0.48
3:B:501:CIT:O3	3:B:501:CIT:C6	2.61	0.48
1:A:295:LEU:HD12	1:A:410:VAL:HG22	1.96	0.48
1:A:393:THR:HG22	1:A:399:GLU:O	2.14	0.48
1:D:318:ASN:C	1:D:319:MET:HG2	2.34	0.48
1:A:286:PHE:HB3	1:A:424:LEU:HD12	1.95	0.47
1:B:315:SER:OG	1:B:316:PRO:HD2	2.15	0.47
1:B:222:PHE:CD1	1:B:222:PHE:C	2.87	0.47
1:A:260:ILE:HG13	1:A:424:LEU:HD13	1.95	0.47
1:A:288:LEU:HB2	1:A:424:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:GLU:OE1	1:C:356:ARG:NH1	2.46	0.47
1:D:346:GLU:HB3	1:D:351:LEU:HD21	1.97	0.47
4:D:501:PLM:H71	4:D:501:PLM:H41	1.60	0.47
1:A:219:MET:HE3	1:A:313:TYR:HE1	1.79	0.47
1:A:295:LEU:CD1	1:A:410:VAL:HG21	2.45	0.47
1:C:208:SER:HB3	1:C:213:ALA:O	2.14	0.47
1:D:313:TYR:N	1:D:313:TYR:CD1	2.82	0.47
1:B:231:ASP:CG	1:B:232:PRO:CD	2.83	0.47
1:A:278:PHE:C	1:A:278:PHE:CD1	2.88	0.46
1:A:307:TYR:HB3	1:A:359:LEU:HD22	1.97	0.46
2:G:47:ILE:O	2:G:47:ILE:HG22	2.14	0.46
1:A:320:ILE:HG21	1:A:395:ARG:HD3	1.97	0.46
1:B:297:THR:O	1:B:371:LYS:NZ	2.42	0.46
1:C:300:ASP:OD1	1:C:371:LYS:NZ	2.41	0.46
1:C:343:ALA:HB2	1:C:352:TYR:CZ	2.50	0.46
1:A:371:LYS:NZ	1:A:371:LYS:HB3	2.29	0.46
1:B:231:ASP:CG	1:B:232:PRO:HD2	2.36	0.46
1:D:389:LEU:HD12	1:D:404:ILE:O	2.16	0.46
1:A:290:LYS:HG2	1:A:407:VAL:CG2	2.45	0.46
2:G:48:LEU:HB3	2:G:49:PRO:HD2	1.97	0.46
1:B:221:GLU:OE2	1:B:244:SER:OG	2.33	0.46
1:B:360:CYS:CB	1:B:362:TYR:CE1	2.97	0.46
4:B:502:PLM:HD1	4:B:502:PLM:HG3	1.50	0.46
2:G:44:ARG:NH2	2:G:44:ARG:CG	2.73	0.45
1:C:292:TRP:CD1	1:C:409:GLU:HB3	2.50	0.45
1:C:343:ALA:HB2	1:C:352:TYR:CE2	2.51	0.45
1:D:353:ARG:C	1:D:353:ARG:HD3	2.36	0.45
1:A:259:ASP:HA	1:A:425:VAL:HG23	1.97	0.45
1:A:377:TYR:OH	2:F:39:LYS:CB	2.64	0.45
2:H:35:VAL:O	2:H:35:VAL:HG13	2.17	0.45
2:H:47:ILE:O	2:H:47:ILE:HG22	2.16	0.45
1:A:330:PHE:HE1	1:A:385:ASN:ND2	2.04	0.45
1:A:353:ARG:C	1:A:353:ARG:HD3	2.37	0.44
1:D:353:ARG:C	1:D:353:ARG:CD	2.85	0.44
1:D:267:PHE:CZ	1:D:405:ALA:HB1	2.52	0.44
2:H:28:LEU:N	2:H:28:LEU:CD2	2.79	0.44
2:E:29:GLU:HG3	2:E:29:GLU:O	2.16	0.44
1:B:226:LEU:HD21	1:B:299:ILE:HB	1.99	0.44
1:C:345:TYR:CD1	1:C:345:TYR:C	2.90	0.44
1:D:214:SER:OG	1:D:215:SER:N	2.51	0.44
1:D:359:LEU:HD23	1:D:363:MET:CG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TRP:CG	2:G:55:GLU:HG3	2.52	0.44
1:C:344:ARG:NH1	1:D:351:LEU:O	2.50	0.44
1:A:280:ARG:NH1	1:A:280:ARG:HG2	2.32	0.44
1:C:267:PHE:HB3	1:C:268:PRO:HD2	1.99	0.44
1:C:374:PRO:HD2	1:C:378:MET:SD	2.58	0.44
1:A:225:PHE:HB3	1:A:239:LEU:HD23	1.99	0.44
1:A:373:LEU:CB	1:A:374:PRO:CD	2.95	0.44
1:A:280:ARG:CG	1:A:280:ARG:HH11	2.31	0.44
1:A:292:TRP:HA	1:A:409:GLU:O	2.18	0.44
1:D:229:GLN:HG3	1:D:235:TYR:CD2	2.52	0.44
1:B:297:THR:HG23	1:B:297:THR:O	2.16	0.43
1:C:290:LYS:CG	1:C:407:VAL:HG22	2.48	0.43
1:C:352:TYR:N	1:C:352:TYR:CD1	2.85	0.43
1:A:206:TRP:O	1:A:210:ARG:HD2	2.18	0.43
1:C:267:PHE:CZ	1:C:405:ALA:HB1	2.52	0.43
1:C:262:GLN:O	2:F:46:LYS:CE	2.64	0.43
1:D:231:ASP:CG	1:D:232:PRO:CD	2.85	0.43
1:A:208:SER:CB	1:A:213:ALA:O	2.66	0.43
1:A:245:GLN:H	1:A:245:GLN:HG3	1.54	0.43
1:C:300:ASP:OD2	1:C:371:LYS:HE2	2.18	0.43
1:C:290:LYS:HZ3	1:C:409:GLU:CD	2.22	0.43
1:B:376:LYS:HA	1:B:379:MET:CE	2.49	0.43
2:H:55:GLU:HA	2:H:56:PRO:HD2	1.84	0.43
1:D:343:ALA:HB1	1:D:350:TYR:HB3	2.00	0.43
1:D:334:VAL:HG12	1:D:335:VAL:CG2	2.49	0.42
2:G:55:GLU:HA	2:G:56:PRO:HD2	1.81	0.42
1:D:300:ASP:OD1	1:D:303:GLY:CA	2.63	0.42
2:H:26:THR:HG22	2:H:26:THR:O	2.18	0.42
1:A:378:MET:HE3	2:F:37:ASN:O	2.19	0.42
1:A:386:PHE:HE1	1:A:408:PHE:CE1	2.37	0.42
1:D:388:ILE:CD1	4:D:501:PLM:H82	2.48	0.42
2:F:54:LYS:HE2	2:F:54:LYS:HB3	1.65	0.42
1:A:219:MET:CE	1:A:313:TYR:CE1	3.03	0.42
1:A:397:THR:O	1:A:398:GLN:HB2	2.20	0.42
2:G:48:LEU:CB	2:G:49:PRO:CD	2.98	0.42
1:D:226:LEU:CD1	1:D:305:ALA:HB1	2.49	0.42
1:A:374:PRO:HG2	1:A:378:MET:CE	2.48	0.42
1:D:362:TYR:HE1	2:H:28:LEU:HB3	1.85	0.42
1:A:376:LYS:O	1:A:379:MET:HB2	2.20	0.42
1:C:290:LYS:HZ1	1:C:409:GLU:CD	2.15	0.42
1:C:290:LYS:HE2	1:C:409:GLU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:353:ARG:NH1	1:D:346:GLU:OE2	2.51	0.42
1:A:290:LYS:HA	1:A:407:VAL:HG22	2.02	0.42
1:C:363:MET:O	1:C:367:ILE:HG13	2.20	0.42
1:D:231:ASP:CB	1:D:232:PRO:HD3	2.47	0.42
1:A:353:ARG:C	1:A:353:ARG:CD	2.85	0.41
1:B:218:TRP:CH2	1:B:245:GLN:O	2.73	0.41
1:D:225:PHE:HB3	1:D:239:LEU:HD23	2.02	0.41
1:C:334:VAL:HG12	1:C:335:VAL:HG23	2.00	0.41
1:C:212:ILE:H	1:C:245:GLN:NE2	2.05	0.41
1:D:207:ILE:HD13	1:D:248:PRO:HG3	2.02	0.41
2:E:52:PHE:O	2:E:52:PHE:CD1	2.73	0.41
1:C:213:ALA:HB2	1:C:218:TRP:CD1	2.55	0.41
1:A:345:TYR:OH	1:A:348:GLY:HA2	2.20	0.41
2:E:55:GLU:HG3	2:E:56:PRO:HD2	2.02	0.41
1:C:396:ASP:N	1:C:396:ASP:OD1	2.53	0.41
1:A:288:LEU:CB	1:A:424:LEU:HD21	2.51	0.41
4:C:502:PLM:H71	4:C:502:PLM:HA2	1.86	0.41
1:A:219:MET:HE2	1:A:313:TYR:CE1	2.56	0.41
1:D:205:ASN:O	1:D:208:SER:OG	2.38	0.41
1:B:330:PHE:CE2	2:G:31:LEU:HD23	2.56	0.41
1:B:328:CYS:HB3	1:B:332:LYS:O	2.21	0.41
1:B:376:LYS:HG3	1:B:379:MET:CE	2.51	0.41
1:D:364:ILE:HG22	1:D:368:HIS:HD2	1.86	0.41
1:C:230:GLN:HB2	1:C:230:GLN:HE21	1.78	0.41
1:C:369:LYS:HD2	2:E:32:PHE:CZ	2.56	0.41
1:C:259:ASP:OD1	1:C:261:ARG:HB2	2.21	0.41
1:C:363:MET:HG3	4:C:502:PLM:H22	2.02	0.41
2:F:28:LEU:O	2:F:28:LEU:HG	2.21	0.41
2:G:30:ALA:O	2:G:33:ASN:HB3	2.21	0.41
2:G:39:LYS:CB	2:G:40:PRO:CD	2.99	0.41
1:C:290:LYS:CG	1:C:407:VAL:CG2	2.99	0.40
1:A:286:PHE:CD2	1:A:403:CYS:HB3	2.57	0.40
1:A:299:ILE:HG13	1:A:299:ILE:H	1.54	0.40
1:D:219:MET:O	1:D:245:GLN:NE2	2.42	0.40
1:B:288:LEU:HD11	1:B:407:VAL:HG23	2.03	0.40
3:B:501:CIT:O6	3:B:501:CIT:C1	2.69	0.40
2:H:28:LEU:CG	2:H:28:LEU:O	2.70	0.40
1:A:228:ARG:CB	1:A:299:ILE:HG22	2.52	0.40
1:B:224:ALA:HB3	1:B:241:VAL:HG22	2.04	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	220/225 (98%)	214 (97%)	5 (2%)	1 (0%)	29	61
1	B	220/225 (98%)	215 (98%)	5 (2%)	0	100	100
1	C	220/225 (98%)	213 (97%)	7 (3%)	0	100	100
1	D	219/225 (97%)	209 (95%)	9 (4%)	1 (0%)	29	61
2	E	30/35 (86%)	26 (87%)	1 (3%)	3 (10%)	0	1
2	F	28/35 (80%)	23 (82%)	2 (7%)	3 (11%)	0	1
2	G	31/35 (89%)	27 (87%)	3 (10%)	1 (3%)	4	16
2	H	30/35 (86%)	25 (83%)	3 (10%)	2 (7%)	1	3
All	All	998/1040 (96%)	952 (95%)	35 (4%)	11 (1%)	14	42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	37	ASN
2	F	36	MET
2	F	38	PRO
2	H	35	VAL
2	E	34	SER
2	F	37	ASN
2	E	42	SER
2	G	36	MET
1	A	299	ILE
1	D	248	PRO
2	H	36	MET

### 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	189/208 (91%)	158 (84%)	31 (16%)	2	7
1	B	191/208 (92%)	162 (85%)	29 (15%)	3	8
1	C	191/208 (92%)	167 (87%)	24 (13%)	4	13
1	D	196/208 (94%)	167 (85%)	29 (15%)	3	9
2	E	27/34 (79%)	23 (85%)	4 (15%)	3	9
2	F	24/34 (71%)	19 (79%)	5 (21%)	1	3
2	G	30/34 (88%)	24 (80%)	6 (20%)	1	4
2	H	28/34 (82%)	23 (82%)	5 (18%)	2	5
All	All	876/968 (90%)	743 (85%)	133 (15%)	3	8

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	LEU
1	A	223	SER
1	A	226	LEU
1	A	245	GLN
1	A	247	SER
1	A	249	SER
1	A	260	ILE
1	A	265	ASP
1	A	277	LEU
1	A	290	LYS
1	A	298	ASN
1	A	304	SER
1	A	311	SER
1	A	319	MET
1	A	329	SER
1	A	335	VAL
1	A	352	TYR
1	A	353	ARG
1	A	354	ILE
1	A	356	ARG
1	A	368	HIS
1	A	370	LEU
1	A	371	LYS
1	A	376	LYS

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Mol	Chain	Res	Type
1	A	386	PHE
1	A	390	GLN
1	A	393	THR
1	A	399	GLU
1	A	410	VAL
1	A	411	SER
1	A	420	HIS
1	B	214	SER
1	B	230	GLN
1	B	235	TYR
1	B	244	SER
1	B	250	TYR
1	B	260	ILE
1	B	265	ASP
1	B	269	GLU
1	B	276	GLU
1	B	277	LEU
1	B	280	ARG
1	B	290	LYS
1	B	299	ILE
1	B	309	VAL
1	B	319	MET
1	B	324	SER
1	B	325	THR
1	B	326	LYS
1	B	327	VAL
1	B	328	CYS
1	B	329	SER
1	B	353	ARG
1	B	354	ILE
1	B	356	ARG
1	B	359	LEU
1	B	371	LYS
1	B	381	SER
1	B	410	VAL
1	B	413	SER
1	C	204	LEU
1	C	207	ILE
1	C	209	MET
1	C	220	LEU
1	C	228	ARG
1	C	230	GLN

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Mol	Chain	Res	Type
1	C	245	GLN
1	C	261	ARG
1	C	265	ASP
1	C	311	SER
1	C	312	GLN
1	C	324	SER
1	C	329	SER
1	C	333	GLN
1	C	335	VAL
1	C	344	ARG
1	C	351	LEU
1	C	353	ARG
1	C	356	ARG
1	C	369	LYS
1	C	371	LYS
1	C	384	GLU
1	C	393	THR
1	C	407	VAL
1	D	206	TRP
1	D	215	SER
1	D	228	ARG
1	D	231	ASP
1	D	250	TYR
1	D	251	SER
1	D	269	GLU
1	D	276	GLU
1	D	277	LEU
1	D	284	ASN
1	D	290	LYS
1	D	296	ASN
1	D	304	SER
1	D	311	SER
1	D	319	MET
1	D	324	SER
1	D	351	LEU
1	D	353	ARG
1	D	354	ILE
1	D	359	LEU
1	D	360	CYS
1	D	363	MET
1	D	369	LYS
1	D	371	LYS

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Mol	Chain	Res	Type
1	D	372	HIS
1	D	390	GLN
1	D	393	THR
1	D	413	SER
1	D	420	HIS
2	E	26	THR
2	E	27	ASP
2	E	44	ARG
2	E	45	LYS
2	F	28	LEU
2	F	35	VAL
2	F	44	ARG
2	F	54	LYS
2	F	57	ASP
2	G	25	ASP
2	G	26	THR
2	G	33	ASN
2	G	44	ARG
2	G	48	LEU
2	G	54	LYS
2	H	28	LEU
2	H	36	MET
2	H	42	SER
2	H	48	LEU
2	H	54	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	HIS
1	A	298	ASN
1	A	385	ASN
1	A	390	GLN
1	B	230	GLN
1	B	236	ASN
1	B	245	GLN
1	B	296	ASN
1	B	312	GLN
1	B	390	GLN
1	B	415	HIS
1	C	230	GLN
1	C	236	ASN

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Mol	Chain	Res	Type
1	C	245	GLN
1	C	368	HIS
1	C	418	GLN
1	D	230	GLN
1	D	296	ASN
1	D	312	GLN
1	D	368	HIS

### 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 ⓘ

5 ligands are modelled in this entry.

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
3	CIT	B	501	-	3,12,12	1.51	1 (33%)	3,17,17	2.04	1 (33%)
3	CIT	C	501	-	3,12,12	0.78	0	3,17,17	1.87	2 (66%)
4	PLM	D	501	1	16,16,17	0.27	0	15,15,17	0.73	0
4	PLM	C	502	-	14,17,17	0.07	0	13,17,17	0.89	0
4	PLM	B	502	-	14,17,17	0.17	0	13,17,17	0.99	0

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
3	CIT	B	501	-	-	3/6/16/16	-
3	CIT	C	501	-	-	6/6/16/16	-
4	PLM	D	501	1	-	10/13/14/15	-
4	PLM	C	502	-	-	11/13/15/15	-
4	PLM	B	502	-	-	8/13/15/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	CIT	C2-C3	2.60	1.58	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CIT	C3-C2-C1	3.14	120.02	114.98
3	C	501	CIT	C3-C2-C1	2.30	118.66	114.98
3	C	501	CIT	C4-C3-C2	2.17	115.12	109.33

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	CIT	C1-C2-C3-O7
3	B	501	CIT	C1-C2-C3-C6
3	C	501	CIT	C1-C2-C3-C6
3	C	501	CIT	C2-C3-C4-C5
3	C	501	CIT	O7-C3-C4-C5
3	C	501	CIT	C6-C3-C4-C5
4	C	502	PLM	C1-C2-C3-C4
4	B	502	PLM	C1-C2-C3-C4
4	D	501	PLM	C4-C5-C6-C7
4	B	502	PLM	CB-CC-CD-CE
4	C	502	PLM	C9-CA-CB-CC
3	B	501	CIT	C1-C2-C3-C4
3	C	501	CIT	C1-C2-C3-O7
4	D	501	PLM	CA-CB-CC-CD

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Mol	Chain	Res	Type	Atoms
4	B	502	PLM	C6-C7-C8-C9
4	D	501	PLM	C2-C3-C4-C5
4	C	502	PLM	C2-C3-C4-C5
4	B	502	PLM	C7-C8-C9-CA
4	D	501	PLM	C8-C9-CA-CB
4	D	501	PLM	C6-C7-C8-C9
4	D	501	PLM	CC-CD-CE-CF
4	D	501	PLM	C3-C4-C5-C6
4	D	501	PLM	C7-C8-C9-CA
4	C	502	PLM	CB-CC-CD-CE
4	C	502	PLM	C7-C8-C9-CA
4	C	502	PLM	CC-CD-CE-CF
4	B	502	PLM	C5-C6-C7-C8
4	C	502	PLM	CA-CB-CC-CD
4	B	502	PLM	C3-C4-C5-C6
4	D	501	PLM	C5-C6-C7-C8
4	B	502	PLM	CC-CD-CE-CF
4	D	501	PLM	C1-C2-C3-C4
4	C	502	PLM	C4-C5-C6-C7
4	C	502	PLM	C3-C4-C5-C6
3	C	501	CIT	C1-C2-C3-C4
4	B	502	PLM	CD-CE-CF-CG
4	C	502	PLM	CD-CE-CF-CG
4	C	502	PLM	C6-C7-C8-C9

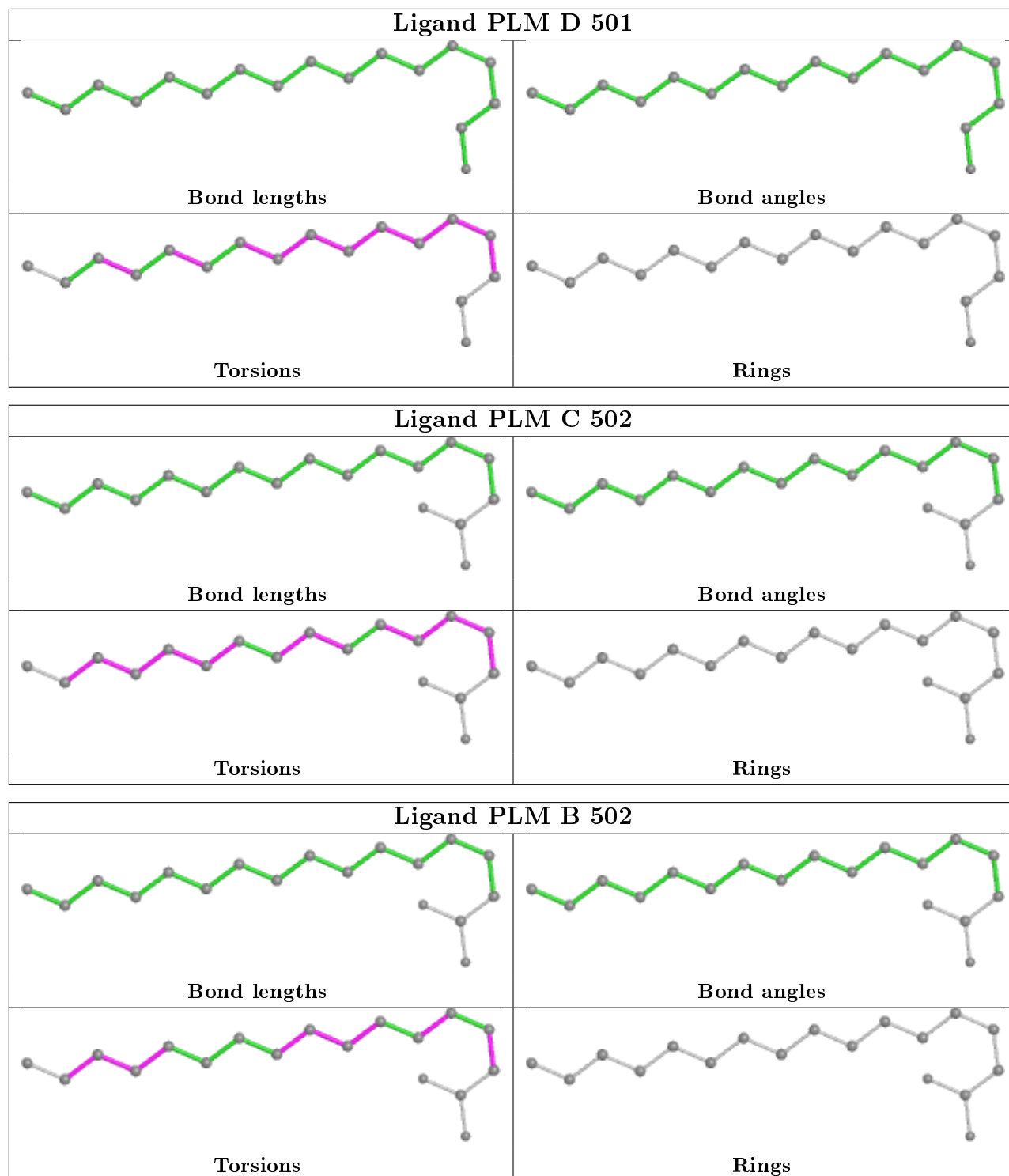
There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	CIT	4	0
3	C	501	CIT	2	0
4	D	501	PLM	5	0
4	C	502	PLM	2	0
4	B	502	PLM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	222/225 (98%)	0.17	4 (1%) 68 67	25, 61, 98, 126	0
1	B	222/225 (98%)	0.06	11 (4%) 28 25	19, 44, 83, 111	0
1	C	222/225 (98%)	-0.11	3 (1%) 75 75	27, 45, 70, 92	0
1	D	221/225 (98%)	0.05	9 (4%) 37 32	23, 41, 86, 116	0
2	E	32/35 (91%)	1.01	6 (18%) 1 0	30, 81, 110, 121	0
2	F	30/35 (85%)	0.86	7 (23%) 0 0	34, 80, 139, 148	0
2	G	33/35 (94%)	0.08	1 (3%) 50 45	37, 58, 77, 101	0
2	H	32/35 (91%)	0.12	1 (3%) 49 44	40, 51, 104, 121	0
All	All	1014/1040 (97%)	0.10	42 (4%) 37 32	19, 48, 97, 148	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	38	PRO	6.3
1	D	205	ASN	3.9
1	B	246	SER	3.9
1	B	302	GLU	3.9
2	E	57	ASP	3.8
1	B	301	ASP	3.5
1	A	305	ALA	3.5
1	D	250	TYR	3.4
2	F	36	MET	3.3
1	B	250	TYR	3.2
2	F	35	VAL	3.1
2	F	34	SER	3.0
2	E	40	PRO	3.0
2	F	57	ASP	3.0
1	D	301	ASP	2.9
1	D	251	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	H	57	ASP	2.9
1	B	205	ASN	2.9
1	B	300	ASP	2.9
2	F	37	ASN	2.9
2	E	27	ASP	2.9
1	B	303	GLY	2.8
1	A	303	GLY	2.7
1	C	249	SER	2.7
1	D	252	ASP	2.7
1	A	250	TYR	2.6
1	B	305	ALA	2.5
2	E	36	MET	2.5
2	F	45	LYS	2.4
2	G	37	ASN	2.4
1	D	230	GLN	2.4
1	D	247	SER	2.4
2	E	26	THR	2.4
1	D	246	SER	2.4
1	B	231	ASP	2.3
1	B	304	SER	2.3
1	B	230	GLN	2.3
2	E	37	ASN	2.2
1	C	250	TYR	2.2
1	A	365	ASN	2.2
1	D	248	PRO	2.2
1	C	405	ALA	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 [\(i\)](#)

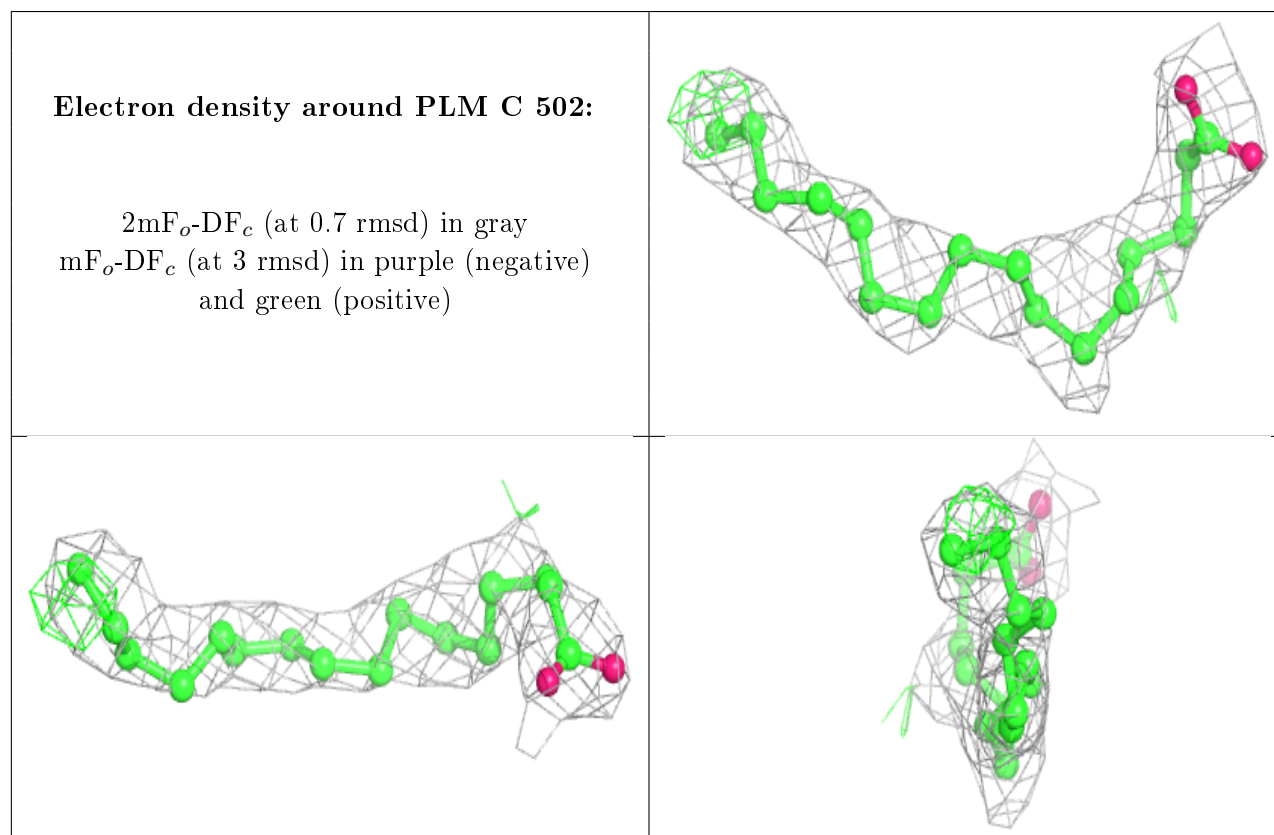
There are no carbohydrates in this entry.

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

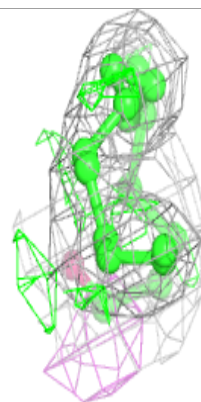
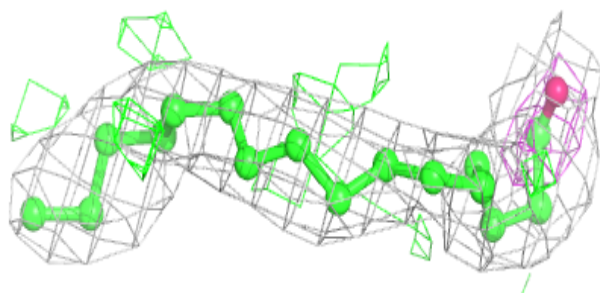
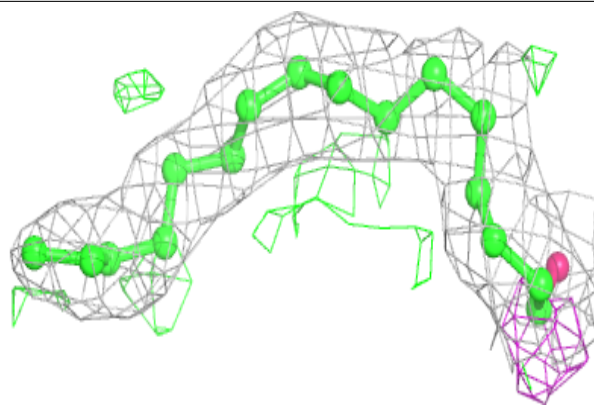
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PLM	C	502	18/18	0.73	0.38	59,70,90,94	0
3	CIT	C	501	13/13	0.78	0.20	34,44,60,62	0
4	PLM	D	501	17/18	0.82	0.40	34,52,75,77	0
3	CIT	B	501	13/13	0.82	0.19	32,43,50,51	0
4	PLM	B	502	18/18	0.84	0.47	56,62,89,94	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

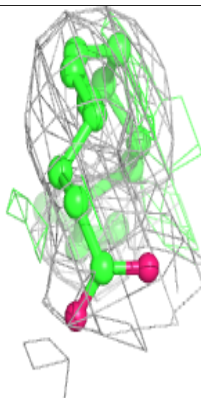
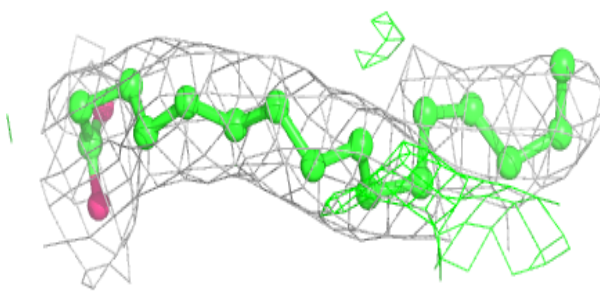
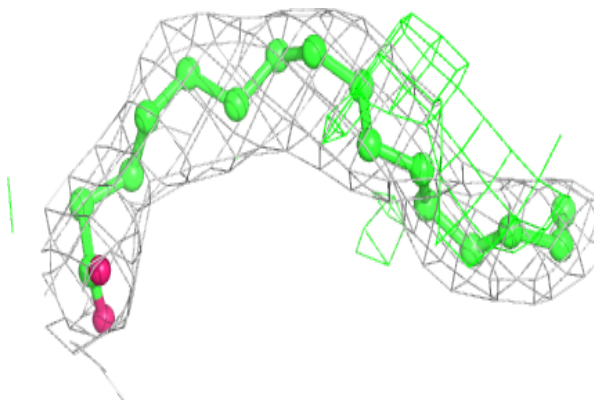


**Electron density around PLM D 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PLM B 502:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.