



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:23 PM UTC

PDB ID : 5GN0 / pdb_00005gn0
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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

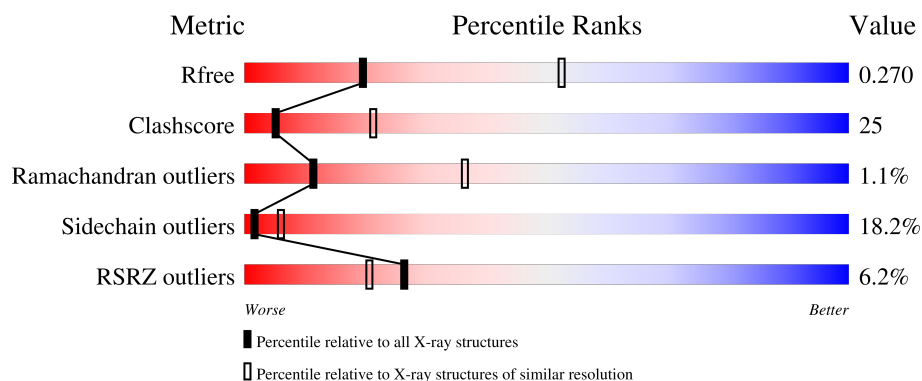
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	225	6% 47% 38% 13% ..
1	B	225	4% 52% 38% 7% ..
1	C	225	2% 58% 31% 10% .
1	D	225	5% 51% 37% 9% ..
2	E	35	11% 34% 40% 17% 9%

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Mol	Chain	Length	Quality of chain
2	F	35	26% 43% 20% 20% • 14%
2	G	35	11% 34% 40% 17% • 6%
2	H	35	17% 40% 40% 9% • 9%

2 Entry composition

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

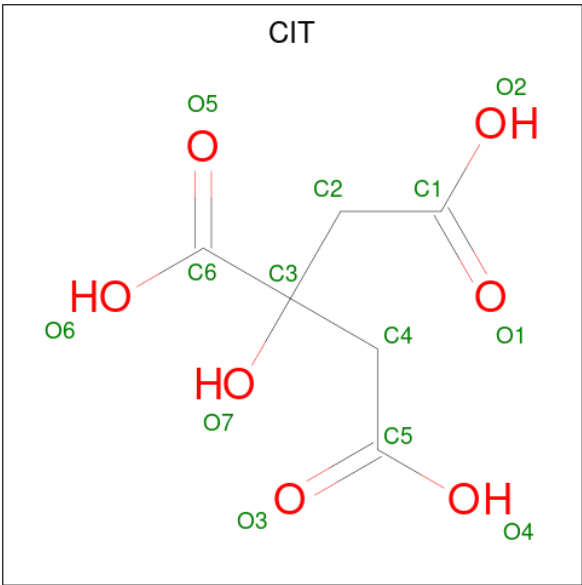
- Molecule 2 is a protein called WW domain-containing transcription regulator protein 1.

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:

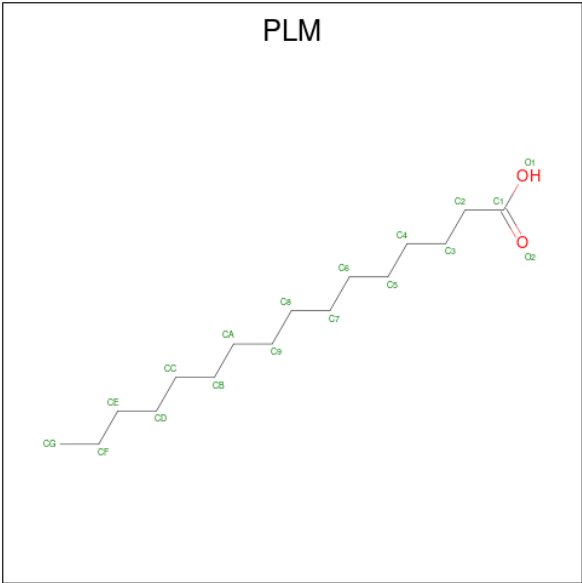
Chain	Residue	Modelled	Actual	Comment	Reference
E	23	PRO	-	expression tag	UNP Q9EPK5
F	23	PRO	-	expression tag	UNP Q9EPK5
G	23	PRO	-	expression tag	UNP Q9EPK5
H	23	PRO	-	expression tag	UNP Q9EPK5

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



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 (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



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		

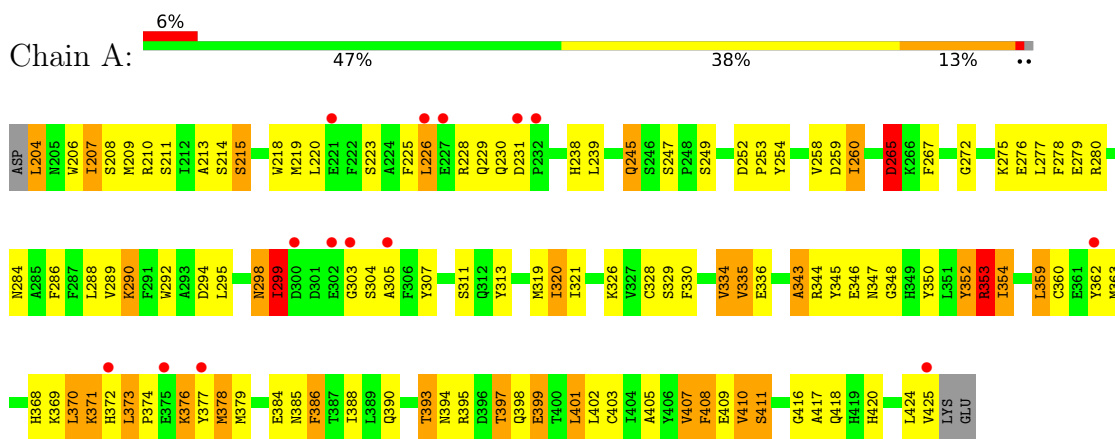
- Molecule 5 is water.

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		

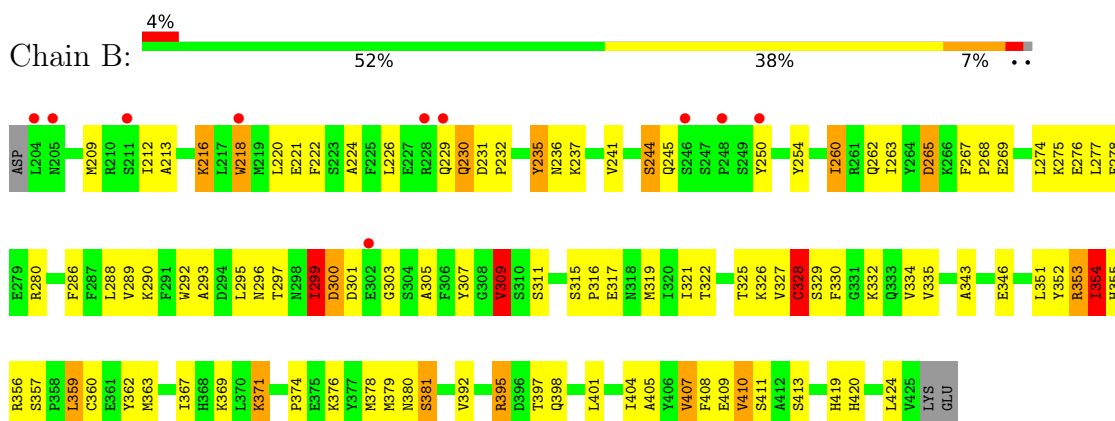
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

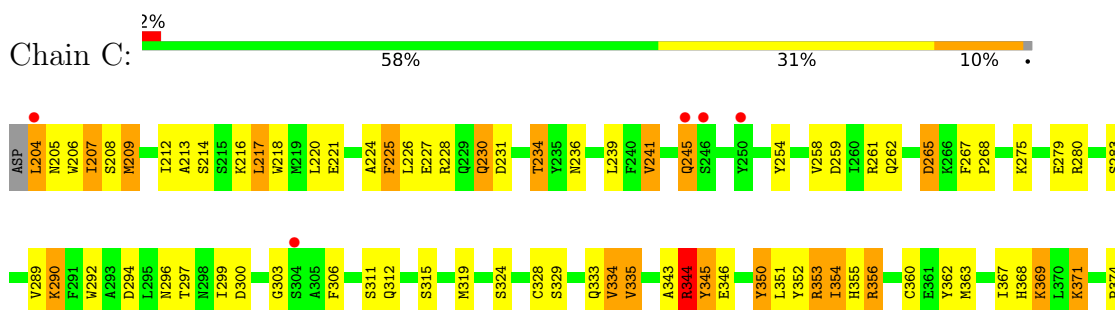
- Molecule 1: Transcriptional enhancer factor TEF-3



- Molecule 1: Transcriptional enhancer factor TEF-3



- Molecule 1: Transcriptional enhancer factor TEF-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.66Å 120.90Å 196.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 30.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.90) 98.5 (30.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	1.361	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8228	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	1.61	5/1824 (0.3%)	1.22	16/2480 (0.6%)
1	B	1.76	8/1829 (0.4%)	1.27	20/2486 (0.8%)
1	C	1.85	11/1829 (0.6%)	1.19	13/2485 (0.5%)
1	D	1.87	16/1846 (0.9%)	1.25	21/2505 (0.8%)
2	E	1.21	0/258	1.28	1/351 (0.3%)
2	F	1.46	0/239	1.12	2/325 (0.6%)
2	G	1.47	0/272	1.34	4/369 (1.1%)
2	H	1.57	1/260 (0.4%)	1.34	6/353 (1.7%)
All	All	1.74	41/8357 (0.5%)	1.24	83/11354 (0.7%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	ILE	C-O	-6.46	1.17	1.24
1	D	388	ILE	C-O	-5.96	1.18	1.24
1	C	346	GLU	C-O	-5.93	1.16	1.24
1	C	289	VAL	C-O	-5.87	1.17	1.24
1	D	241	VAL	C-O	-5.84	1.18	1.23
1	C	388	ILE	C-O	-5.71	1.18	1.24
1	D	289	VAL	C-O	-5.68	1.18	1.24
1	A	289	VAL	C-O	-5.67	1.18	1.24
1	D	319	MET	C-O	-5.67	1.17	1.23
1	D	224	ALA	C-O	-5.61	1.17	1.24
1	D	392	VAL	C-O	-5.47	1.17	1.24
1	D	411	SER	CA-C	-5.44	1.46	1.52
1	B	309	VAL	C-O	-5.40	1.18	1.24
1	C	241	VAL	C-O	-5.37	1.18	1.23
1	C	258	VAL	C-O	-5.35	1.18	1.24
1	C	404	ILE	C-O	-5.35	1.18	1.24
1	D	326	LYS	C-O	-5.33	1.17	1.24
1	B	404	ILE	C-O	-5.32	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	ARG	C-O	-5.31	1.17	1.23
1	D	223	SER	C-O	-5.31	1.17	1.23
1	C	350	TYR	C-O	-5.31	1.17	1.24
2	H	36	MET	CA-C	-5.31	1.45	1.52
1	D	375	GLU	C-O	-5.29	1.17	1.23
1	A	350	TYR	C-O	-5.28	1.17	1.24
1	B	289	VAL	C-O	-5.28	1.18	1.24
1	C	294	ASP	C-O	-5.27	1.17	1.24
1	C	379	MET	C-O	-5.26	1.18	1.24
1	A	211	SER	C-O	-5.26	1.17	1.24
1	A	346	GLU	C-O	-5.23	1.17	1.23
1	D	407	VAL	C-O	-5.23	1.18	1.24
1	C	296	ASN	C-O	-5.17	1.18	1.23
1	C	344	ARG	C-O	-5.16	1.18	1.24
1	D	337	LYS	C-O	-5.15	1.17	1.24
1	B	420	HIS	C-O	-5.12	1.17	1.23
1	B	346	GLU	C-O	-5.12	1.17	1.23
1	D	358	PRO	CA-C	-5.09	1.47	1.52
1	B	407	VAL	C-O	-5.09	1.18	1.24
1	D	325	THR	C-O	-5.06	1.18	1.24
1	B	392	VAL	C-O	-5.04	1.18	1.24
1	D	391	VAL	C-O	-5.03	1.18	1.24
1	D	309	VAL	C-O	-5.00	1.18	1.23

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	355	HIS	N-CA-C	13.66	126.19	111.03
1	B	299	ILE	N-CA-C	10.22	130.59	109.34
1	B	301	ASP	N-CA-C	-9.32	101.20	111.36
1	D	355	HIS	N-CA-C	8.66	124.47	111.04
1	A	378	MET	N-CA-C	-8.56	101.89	111.82
1	A	343	ALA	N-CA-C	8.37	121.85	110.55
1	B	263	ILE	N-CA-C	8.18	120.75	112.90
1	C	408	PHE	N-CA-C	7.95	121.84	109.52
1	D	343	ALA	N-CA-C	7.80	122.03	110.48
1	B	408	PHE	N-CA-C	7.57	121.81	109.85
1	A	408	PHE	N-CA-C	7.55	121.22	109.52
1	C	205	ASN	N-CA-C	-7.22	104.33	113.43
1	B	397	THR	N-CA-C	7.22	122.25	113.38
1	B	305	ALA	N-CA-C	7.00	119.77	110.53
2	E	41	SER	N-CA-C	6.96	121.36	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	36	MET	CA-C-N	-6.87	115.46	122.74
2	H	36	MET	C-N-CA	-6.87	115.46	122.74
1	A	328	CYS	N-CA-C	6.83	119.55	108.41
1	C	415	HIS	N-CA-C	6.71	120.78	112.59
1	D	265	ASP	CB-CA-C	-6.67	99.71	110.79
1	D	354	ILE	N-CA-C	-6.64	98.06	107.75
1	A	354	ILE	N-CA-C	-6.52	98.35	107.80
1	B	274	LEU	N-CA-C	6.49	118.36	111.28
2	H	38	PRO	N-CA-C	6.41	122.43	111.03
1	A	303	GLY	N-CA-C	-6.30	98.24	113.18
1	B	300	ASP	N-CA-CB	-6.30	101.70	110.65
2	G	28	LEU	N-CA-C	-6.28	105.37	113.16
1	C	334	VAL	CB-CA-C	-6.25	105.56	111.06
1	B	293	ALA	N-CA-C	6.24	119.72	110.48
1	A	347	ASN	N-CA-C	6.22	120.00	111.54
1	C	225	PHE	N-CA-C	6.18	118.17	108.96
1	C	328	CYS	N-CA-C	6.13	119.39	109.40
1	C	354	ILE	N-CA-C	-6.07	97.63	107.28
1	A	353	ARG	N-CA-C	6.06	117.75	108.42
1	A	220	LEU	N-CA-C	5.97	117.59	111.14
1	B	328	CYS	N-CA-C	5.95	119.10	109.40
1	B	354	ILE	N-CA-C	-5.89	97.92	107.28
1	D	347	ASN	N-CA-C	5.87	119.67	111.74
1	D	416	GLY	N-CA-C	5.83	127.01	113.18
1	C	396	ASP	N-CA-C	5.79	117.67	111.36
1	D	296	ASN	N-CA-C	5.78	118.62	108.56
2	F	38	PRO	N-CA-C	-5.74	100.65	112.47
1	D	328	CYS	N-CA-C	5.71	118.53	109.50
2	F	32	PHE	N-CA-C	5.63	118.35	111.82
1	C	345	TYR	N-CA-C	5.61	118.68	109.76
1	C	303	GLY	N-CA-C	5.57	119.65	112.18
1	B	296	ASN	N-CA-C	5.56	118.19	108.52
1	B	395	ARG	N-CA-C	5.56	117.02	111.07
1	D	293	ALA	N-CA-C	5.55	118.97	110.20
1	C	216	LYS	N-CA-C	5.55	121.07	113.97
1	D	396	ASP	N-CA-C	5.50	117.14	111.03
1	A	334	VAL	CB-CA-C	-5.49	106.23	111.44
1	D	397	THR	N-CA-C	5.47	118.17	111.82
1	A	397	THR	N-CA-C	5.46	119.94	113.28
1	A	373	LEU	CA-C-N	5.46	124.65	118.97
1	A	373	LEU	C-N-CA	5.46	124.65	118.97
1	A	265	ASP	N-CA-C	5.42	117.19	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	315	SER	CA-C-N	5.42	124.76	118.85
1	D	315	SER	C-N-CA	5.42	124.76	118.85
2	H	36	MET	N-CA-C	-5.41	99.28	110.80
2	G	26	THR	O-C-N	5.37	128.78	122.34
1	A	394	ASN	N-CA-C	-5.33	100.49	108.96
1	B	216	LYS	N-CA-C	5.32	120.05	113.50
1	D	353	ARG	N-CA-C	5.30	116.91	108.79
1	D	266	LYS	N-CA-C	5.23	119.64	113.16
1	C	355	HIS	N-CA-C	5.22	117.02	108.52
2	G	48	LEU	CA-C-N	5.21	125.11	119.85
2	G	48	LEU	C-N-CA	5.21	125.11	119.85
1	D	335	VAL	CB-CA-C	-5.19	101.42	110.71
1	B	419	HIS	N-CA-C	5.18	116.72	108.79
2	H	34	SER	N-CA-C	-5.16	101.78	109.11
1	D	319	MET	N-CA-C	5.15	115.33	108.38
1	D	333	GLN	N-CA-C	5.14	117.67	109.96
1	B	300	ASP	N-CA-C	-5.12	107.55	112.97
1	B	401	LEU	N-CA-C	5.11	116.66	111.14
1	B	218	TRP	N-CA-C	5.09	117.74	109.24
1	A	215	SER	N-CA-C	-5.08	107.03	113.18
1	B	317	GLU	N-CA-C	5.07	117.96	110.46
1	D	408	PHE	N-CA-C	5.04	117.34	109.52
1	D	334	VAL	CB-CA-C	-5.04	106.65	111.44
1	C	280	ARG	N-CA-C	5.03	116.61	111.03
1	D	225	PHE	N-CA-C	5.02	116.62	109.14
2	H	37	ASN	N-CA-C	-5.02	98.57	108.71

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	113	0
1	B	1780	0	1675	79	0
1	C	1781	0	1681	65	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1797	0	1701	66	0
2	E	250	0	235	23	0
2	F	231	0	220	23	0
2	G	264	0	250	28	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	393	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 25.

All (393) 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	1.36
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
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
2:F:42:SER:OG	2:F:45:LYS:HB2	1.57	1.02
1:A:379:MET:HE3	1:A:410:VAL:HG21	1.38	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HH21	2:G:44:ARG:HG3	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	0.89
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:E:47:ILE:C	2:E:48:LEU:CD2	2.45	0.85
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:379:MET:HE2	1:A:410:VAL:HG11	1.57	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:370:LEU:O	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
2:H:28:LEU:HD23	2:H:28:LEU:C	2.14	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
1:A:219:MET:HE3	1:A:313:TYR:HE1	1.55	0.69
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
2:G:35:VAL:O	2:G:36:MET:HB2	1.92	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
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:B:300:ASP:OD2	1:B:307:TYR:OH	2.12	0.66
1:D:209:MET:HE2	1:D:254:TYR:CE2	2.30	0.66
1:D:351:LEU:N	1:D:351:LEU:HD13	2.11	0.66
1:B:209:MET:HE3	1:B:254:TYR:CE2	2.31	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
2:F:28:LEU:C	2:F:28:LEU:HD23	2.21	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
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:O3	3:B:501:CIT:O5	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:363:MET:HE1	1:D:386:PHE:HZ	1.63	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
1:A:219:MET:HE3	1:A:313:TYR:CE1	2.35	0.62
1:A:298:ASN:C	1:A:298:ASN:HD22	2.08	0.62
1:C:290:LYS:NZ	1:C:409:GLU:CD	2.58	0.62
2:E:36:MET:O	2:E:37:ASN:CB	2.48	0.62
1:A:295:LEU:HD12	1:A:410:VAL:CG2	2.30	0.62
1:A:334:VAL:HG12	1:A:335:VAL:HG22	1.81	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:B:220:LEU:C	1:B:221:GLU:HG2	2.24	0.61
1:D:363:MET:HE1	1:D:386:PHE:CZ	2.36	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	0.61
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
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:295:LEU:HD12	1:A:379:MET:HE3	1.83	0.59
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
2:G:36:MET:O	2:G:37:ASN:HB3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:GLN:HB3	2:H:56:PRO:HG2	1.84	0.58
1:A:384:GLU:HG2	2:E:43:TRP:CD1	2.39	0.58
1:B:280:ARG:NH2	1:B:398:GLN:O	2.36	0.58
1:A:295:LEU:HD12	1:A:410:VAL:HG21	1.86	0.58
1:A:295:LEU:CD1	1:A:379:MET:HE3	2.33	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:A:378:MET:HE3	2:F:37:ASN:O	2.03	0.58
1:B:260:ILE:HG13	1:B:424:LEU:HD13	1.84	0.58
1:B:262:GLN:O	2:G:46:LYS:CE	2.52	0.58
1:A:226:LEU:HD11	1:A:305:ALA:CB	2.33	0.57
1:C:315:SER:OG	1:C:319:MET:HE2	2.05	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:C:350:TYR:N	1:C:350:TYR:CD1	2.73	0.57
1:A:370:LEU:HD12	1:A:370:LEU:C	2.29	0.57
1:B:376:LYS:HA	1:B:379:MET:HE3	1.85	0.57
1:C:209:MET:HE2	1:C:254:TYR:CE2	2.39	0.57
2:E:47:ILE:O	2:E:47:ILE:HG22	2.04	0.56
1:A:275:LYS:O	1:A:279:GLU:HG3	2.03	0.56
2:G:39:LYS:CB	2:G:40:PRO:HD2	2.34	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:OD1	1:C:265:ASP:N	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:N	1:B:235:TYR:CD1	2.73	0.55
1:D:297:THR:OG1	1:D:299:ILE:HG13	2.06	0.55
2:F:57:ASP:OD1	2:F:57:ASP:N	2.39	0.55
2:F:35:VAL:O	2:F:35:VAL:HG22	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:D:231:ASP:CG	1:D:232:PRO:HD3	2.32	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:A:379:MET:HE1	1:A:410:VAL:HG11	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ALA:HB2	1:B:218:TRP:CB	2.37	0.54
1:A:362:TYR:CD1	1:A:362:TYR:C	2.85	0.54
1:A:215:SER:OG	1:A:284:ASN:ND2	2.39	0.54
2:H:28:LEU:H	2:H:28:LEU:HD22	1.73	0.54
1:A:417:ALA:C	1:A:418:GLN:HG2	2.33	0.54
1:A:386:PHE:C	1:A:386:PHE:CD1	2.85	0.53
2:E:44:ARG:HG3	2:E:44:ARG:NH2	2.16	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:D:388:ILE:HD12	4:D:501:PLM:H82	1.91	0.52
1:D:228:ARG:HB3	1:D:299:ILE:CG2	2.40	0.52
1:B:222:PHE:CD1	1:B:222:PHE:C	2.87	0.52
1:D:318:ASN:C	1:D:319:MET:HG2	2.34	0.52
2:E:44:ARG:HH21	2:E:44:ARG:CG	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:370:LEU:HD12	1:A:379:MET:CG	2.36	0.52
1:A:373:LEU:HG	1:A:374:PRO:CD	2.40	0.52
2:G:28:LEU:N	2:G:28:LEU:CD1	2.73	0.51
1:B:231:ASP:CG	1:B:232:PRO:CD	2.83	0.51
1:A:278:PHE:CD1	1:A:278:PHE:C	2.88	0.51
1:D:351:LEU:N	1:D:351:LEU:CD1	2.73	0.51
1:D:411:SER:HB2	2:H:55:GLU:OE1	2.11	0.51
2:F:36:MET:CB	2:F:40:PRO:HG3	2.41	0.51
1:D:346:GLU:HB3	1:D:351:LEU:CD2	2.41	0.51
1:B:209:MET:HE3	1:B:254:TYR:CD2	2.45	0.51
1:B:231:ASP:CG	1:B:232:PRO:HD2	2.36	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
1:B:297:THR:O	1:B:371:LYS:NZ	2.42	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:353:ARG:HD3	1:D:353:ARG:C	2.36	0.50
1:B:226:LEU:HD13	1:B:307:TYR:CD2	2.44	0.50
1:B:354:ILE:O	1:B:354:ILE:HG22	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
1:B:353:ARG:HD3	3:B:501:CIT:O6	2.12	0.49
1:B:376:LYS:CG	1:B:379:MET:HE3	2.42	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: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:O	1:A:207:ILE:HG22	2.12	0.49
1:A:353:ARG:HD3	1:A:353:ARG:C	2.37	0.49
1:A:370:LEU:CD1	1:A:379:MET:HG3	2.36	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:D:353:ARG:C	1:D:353:ARG:CD	2.85	0.49
1:C:345:TYR:CD1	1:C:345:TYR:C	2.90	0.49
1:C:290:LYS:HZ3	1:C:409:GLU:CD	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:231:ASP:CG	1:D:232:PRO:CD	2.85	0.48
1:C:209:MET:HE2	1:C:254:TYR:CD2	2.49	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: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:D:209:MET:HE3	1:D:209:MET:HB3	1.72	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
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:295:LEU:CD1	1:A:410:VAL:HG21	2.45	0.47
1:B:369:LYS:NZ	2:G:29:GLU:OE1	2.29	0.47
1:C:208:SER:HB3	1:C:213:ALA:O	2.14	0.47
1:D:209:MET:HE1	1:D:423:ARG:NH2	2.30	0.47
1:D:313:TYR:N	1:D:313:TYR:CD1	2.82	0.47
1:A:307:TYR:HB3	1:A:359:LEU:HD22	1.97	0.46
1:A:320:ILE:HG21	1:A:395:ARG:HD3	1.97	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:353:ARG:C	1:A:353:ARG:CD	2.85	0.46
1:A:371:LYS:NZ	1:A:371:LYS:HB3	2.29	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:HG3	4:B:502:PLM:HD1	1.50	0.46
2:G:44:ARG:CG	2:G:44:ARG:NH2	2.73	0.45
2:G:47:ILE:O	2:G:47:ILE:HG22	2.14	0.45
1:C:292:TRP:CD1	1:C:409:GLU:HB3	2.50	0.45
1:A:209:MET:HE3	1:A:254:TYR:CE2	2.52	0.45
1:C:343:ALA:HB2	1:C:352:TYR:CE2	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:225:PHE:C	1:A:225:PHE:CD1	2.95	0.44
1:B:226:LEU:HD21	1:B:299:ILE:HB	1.99	0.44
1:C:290:LYS:HZ1	1:C:409:GLU:CD	2.18	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
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:HH11	1:A:280:ARG:CG	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:O	1:B:297:THR:HG23	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:A:214:SER:OG	1:A:401:LEU:O	2.30	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: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
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: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:HB3	2:F:54:LYS:HE2	1.65	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:206:TRP:CD1	1:D:206:TRP:C	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:HD21	1:B:363:MET:HE3	2.00	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:HE2	1:C:409:GLU:HB2	2.00	0.42
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:A:379:MET:HE2	1:A:410:VAL:CG1	2.40	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: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:A:288:LEU:CB	1:A:424:LEU:HD21	2.51	0.41
1:A:370:LEU:CD1	1:A:370:LEU:C	2.92	0.41
4:C:502:PLM:HA2	4:C:502:PLM:H71	1.86	0.41
1:A:209:MET:HE3	1:A:254:TYR:CD2	2.56	0.41
1:D:205:ASN:O	1:D:208:SER:OG	2.38	0.41
1:B:328:CYS:HB3	1:B:332:LYS:O	2.21	0.41
1:B:330:PHE:CE2	2:G:31:LEU:HD23	2.56	0.41
1:B:376:LYS:HG3	1:B:379:MET:CE	2.51	0.41
1:C:230:GLN:HE21	1:C:230:GLN:HB2	1.78	0.41
1:C:369:LYS:HD2	2:E:32:PHE:CZ	2.56	0.41
1:D:350:TYR:C	1:D:351:LEU:HD13	2.45	0.41
1:D:364:ILE:HG22	1:D:368:HIS:HD2	1.86	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
2:F:28:LEU:C	2:F:28:LEU:CD2	2.85	0.40
1:B:376:LYS:HA	1:B:379:MET:CE	2.49	0.40
1:A:286:PHE:CD2	1:A:403:CYS:HB3	2.57	0.40
1:A:299:ILE:H	1:A:299:ILE:HG13	1.54	0.40
1:D:219:MET:O	1:D:245:GLN:NE2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:52:PHE:CD1	2:E:52:PHE:C	3.00	0.40
2:H:28:LEU:O	2:H:28:LEU:CG	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 [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	220/225 (98%)	214 (97%)	5 (2%)	1 (0%)	24	54
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%)	24	54
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%)	3	13
2	H	30/35 (86%)	25 (83%)	3 (10%)	2 (7%)	1	3
All	All	998/1040 (96%)	952 (95%)	35 (4%)	11 (1%)	11	36

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

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Mol	Chain	Res	Type
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 [i](#)

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%)	149 (79%)	40 (21%)	1	4
1	B	191/208 (92%)	160 (84%)	31 (16%)	2	8
1	C	191/208 (92%)	160 (84%)	31 (16%)	2	8
1	D	196/208 (94%)	165 (84%)	31 (16%)	2	8
2	E	27/34 (79%)	20 (74%)	7 (26%)	0	2
2	F	24/34 (71%)	19 (79%)	5 (21%)	1	4
2	G	30/34 (88%)	23 (77%)	7 (23%)	1	3
2	H	28/34 (82%)	21 (75%)	7 (25%)	0	2
All	All	876/968 (90%)	717 (82%)	159 (18%)	2	6

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	LEU
1	A	207	ILE
1	A	223	SER
1	A	226	LEU
1	A	230	GLN
1	A	245	GLN
1	A	247	SER
1	A	249	SER

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Mol	Chain	Res	Type
1	A	260	ILE
1	A	265	ASP
1	A	277	LEU
1	A	290	LYS
1	A	298	ASN
1	A	299	ILE
1	A	304	SER
1	A	311	SER
1	A	319	MET
1	A	320	ILE
1	A	321	ILE
1	A	329	SER
1	A	335	VAL
1	A	352	TYR
1	A	353	ARG
1	A	354	ILE
1	A	359	LEU
1	A	368	HIS
1	A	370	LEU
1	A	371	LYS
1	A	376	LYS
1	A	386	PHE
1	A	388	ILE
1	A	390	GLN
1	A	393	THR
1	A	399	GLU
1	A	401	LEU
1	A	402	LEU
1	A	407	VAL
1	A	410	VAL
1	A	411	SER
1	A	420	HIS
1	B	230	GLN
1	B	235	TYR
1	B	237	LYS
1	B	244	SER
1	B	250	TYR
1	B	260	ILE
1	B	265	ASP
1	B	269	GLU
1	B	275	LYS
1	B	276	GLU

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Mol	Chain	Res	Type
1	B	277	LEU
1	B	290	LYS
1	B	299	ILE
1	B	309	VAL
1	B	319	MET
1	B	325	THR
1	B	326	LYS
1	B	327	VAL
1	B	328	CYS
1	B	329	SER
1	B	351	LEU
1	B	353	ARG
1	B	354	ILE
1	B	356	ARG
1	B	359	LEU
1	B	367	ILE
1	B	371	LYS
1	B	381	SER
1	B	409	GLU
1	B	410	VAL
1	B	413	SER
1	C	204	LEU
1	C	207	ILE
1	C	209	MET
1	C	217	LEU
1	C	220	LEU
1	C	221	GLU
1	C	228	ARG
1	C	230	GLN
1	C	234	THR
1	C	245	GLN
1	C	265	ASP
1	C	283	SER
1	C	290	LYS
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

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Mol	Chain	Res	Type
1	C	353	ARG
1	C	354	ILE
1	C	356	ARG
1	C	369	LYS
1	C	371	LYS
1	C	384	GLU
1	C	388	ILE
1	C	393	THR
1	C	407	VAL
1	C	420	HIS
1	D	206	TRP
1	D	207	ILE
1	D	215	SER
1	D	228	ARG
1	D	231	ASP
1	D	251	SER
1	D	260	ILE
1	D	269	GLU
1	D	276	GLU
1	D	277	LEU
1	D	290	LYS
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
1	D	372	HIS
1	D	390	GLN
1	D	393	THR
1	D	407	VAL
1	D	409	GLU
1	D	410	VAL
1	D	413	SER
1	D	420	HIS
2	E	26	THR

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Mol	Chain	Res	Type
2	E	27	ASP
2	E	28	LEU
2	E	44	ARG
2	E	45	LYS
2	E	47	ILE
2	E	48	LEU
2	F	28	LEU
2	F	35	VAL
2	F	46	LYS
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	46	LYS
2	G	48	LEU
2	G	54	LYS
2	H	28	LEU
2	H	33	ASN
2	H	36	MET
2	H	42	SER
2	H	47	ILE
2	H	48	LEU
2	H	54	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	236	ASN
1	A	238	HIS
1	A	298	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	349	HIS
1	B	372	HIS
1	B	415	HIS
1	C	230	GLN

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Mol	Chain	Res	Type
1	C	236	ASN
1	C	242	HIS
1	C	245	GLN
1	C	368	HIS
1	C	418	GLN
1	D	230	GLN
1	D	284	ASN
1	D	296	ASN
1	D	312	GLN
1	D	333	GLN
1	D	368	HIS
1	D	398	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	501	-	12,12,12	1.57	4 (33%)	17,17,17	1.80	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PLM	C	502	-	17,17,17	0.52	0	17,17,17	1.11	2 (11%)
3	CIT	B	501	-	12,12,12	1.60	2 (16%)	17,17,17	1.84	7 (41%)
4	PLM	D	501	1	15,16,17	0.26	0	14,15,17	0.68	0
4	PLM	B	502	-	17,17,17	0.52	0	17,17,17	1.26	2 (11%)

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	C	501	-	-	6/16/16/16	-
4	PLM	C	502	-	-	12/15/15/15	-
3	CIT	B	501	-	-	7/16/16/16	-
4	PLM	D	501	1	-	10/14/14/15	-
4	PLM	B	502	-	-	10/15/15/15	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	CIT	C2-C3	3.73	1.58	1.54
3	C	501	CIT	O3-C5	2.35	1.29	1.22
3	B	501	CIT	O5-C6	2.32	1.29	1.22
3	C	501	CIT	O5-C6	2.23	1.29	1.22
3	C	501	CIT	C3-C6	-2.20	1.51	1.53
3	C	501	CIT	C2-C1	2.18	1.57	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CIT	O1-C1-C2	-3.43	113.25	122.95
3	C	501	CIT	C2-C3-C6	-3.05	103.28	110.03
3	B	501	CIT	O7-C3-C6	3.02	113.25	108.96
3	B	501	CIT	C4-C3-C6	-2.85	103.74	110.03
3	C	501	CIT	O7-C3-C4	-2.82	102.95	109.38
3	C	501	CIT	O3-C5-C4	-2.75	115.17	122.95
3	B	501	CIT	O2-C1-C2	2.60	122.58	114.35
3	C	501	CIT	O5-C6-C3	-2.58	117.10	122.09
3	B	501	CIT	C2-C3-C6	2.51	115.58	110.03
4	B	502	PLM	C3-C2-C1	-2.39	108.28	114.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	501	CIT	O7-C3-C4	-2.37	103.97	109.38
3	C	501	CIT	C4-C3-C2	2.26	115.12	109.31
4	B	502	PLM	O2-C1-C2	-2.24	115.99	123.09
4	C	502	PLM	C3-C2-C1	-2.24	108.67	114.51
3	B	501	CIT	C3-C2-C1	2.23	120.02	113.92
4	C	502	PLM	O2-C1-C2	-2.18	116.18	123.09
3	C	501	CIT	C4-C3-C6	2.08	114.64	110.03

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	D	501	PLM	C4-C5-C6-C7
3	B	501	CIT	C1-C2-C3-O7
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	B	501	CIT	C1-C2-C3-C6
3	C	501	CIT	C1-C2-C3-O7
3	C	501	CIT	C1-C2-C3-C6
4	B	502	PLM	C6-C7-C8-C9
4	D	501	PLM	CA-CB-CC-CD
4	D	501	PLM	CC-CD-CE-CF
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	B	502	PLM	C1-C2-C3-C4
4	C	502	PLM	C1-C2-C3-C4
4	D	501	PLM	C8-C9-CA-CB
4	D	501	PLM	C6-C7-C8-C9
4	C	502	PLM	CB-CC-CD-CE
4	D	501	PLM	C3-C4-C5-C6
4	D	501	PLM	C7-C8-C9-CA
4	C	502	PLM	C7-C8-C9-CA
4	C	502	PLM	CC-CD-CE-CF
4	C	502	PLM	CA-CB-CC-CD
4	B	502	PLM	C5-C6-C7-C8
3	B	501	CIT	C2-C3-C6-O6
4	B	502	PLM	C3-C4-C5-C6

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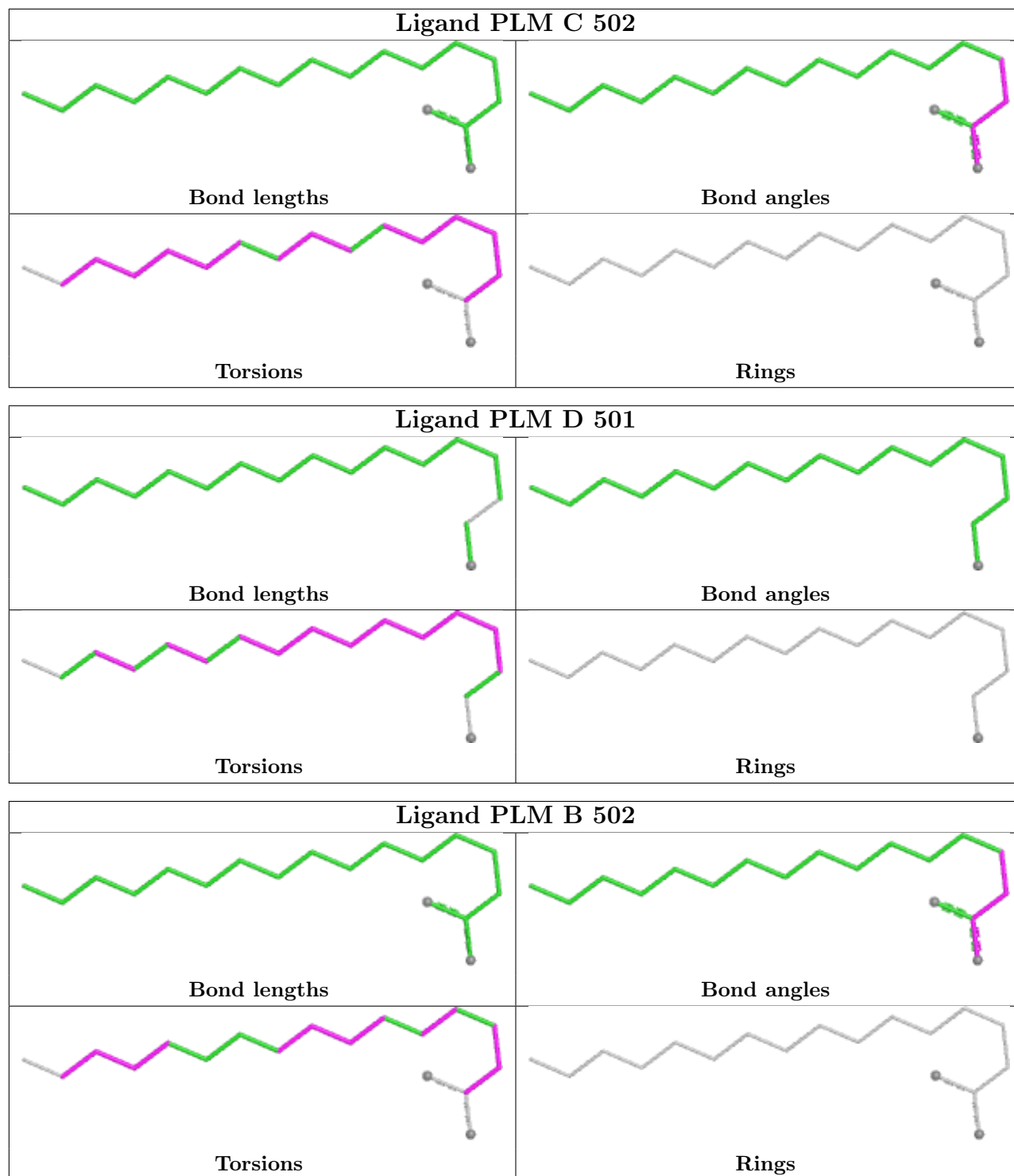
Mol	Chain	Res	Type	Atoms
4	D	501	PLM	C5-C6-C7-C8
3	B	501	CIT	C2-C3-C6-O5
3	B	501	CIT	C4-C3-C6-O6
4	D	501	PLM	C1-C2-C3-C4
4	B	502	PLM	CC-CD-CE-CF
4	C	502	PLM	C4-C5-C6-C7
3	B	501	CIT	C4-C3-C6-O5
4	C	502	PLM	C3-C4-C5-C6
4	B	502	PLM	O2-C1-C2-C3
4	B	502	PLM	CD-CE-CF-CG
3	C	501	CIT	C1-C2-C3-C4
4	B	502	PLM	O1-C1-C2-C3
4	C	502	PLM	O2-C1-C2-C3
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	C	501	CIT	2	0
4	C	502	PLM	2	0
3	B	501	CIT	4	0
4	D	501	PLM	5	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 [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	222/225 (98%)	0.63	14 (6%)	26 20	25, 61, 98, 126	0
1	B	222/225 (98%)	0.31	10 (4%)	38 30	19, 44, 83, 111	0
1	C	222/225 (98%)	0.26	5 (2%)	61 52	27, 45, 70, 92	0
1	D	221/225 (98%)	0.29	11 (4%)	34 27	23, 41, 86, 116	0
2	E	32/35 (91%)	1.07	4 (12%)	8 7	30, 81, 110, 121	0
2	F	30/35 (85%)	1.38	9 (30%)	1 1	34, 80, 139, 148	0
2	G	33/35 (94%)	0.76	4 (12%)	8 7	37, 58, 77, 101	0
2	H	32/35 (91%)	0.75	6 (18%)	3 3	40, 51, 104, 121	0
All	All	1014/1040 (97%)	0.45	63 (6%)	26 21	19, 48, 97, 148	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	28	LEU	5.0
2	F	35	VAL	4.5
2	F	38	PRO	4.3
1	A	362	TYR	4.3
2	F	33	ASN	4.2
2	F	36	MET	4.2
2	H	34	SER	4.1
2	H	26	THR	3.9
1	B	250	TYR	3.9
1	A	231	ASP	3.7
1	B	205	ASN	3.7
2	H	28	LEU	3.4
2	E	36	MET	3.4
2	E	40	PRO	3.2
1	A	372	HIS	3.2
1	D	230	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	300	ASP	3.0
1	B	302	GLU	2.9
1	B	204	LEU	2.8
1	B	248	PRO	2.8
1	B	211	SER	2.7
1	D	229	GLN	2.7
1	C	204	LEU	2.7
1	C	246	SER	2.7
1	A	425	VAL	2.7
1	D	302	GLU	2.7
2	E	26	THR	2.6
1	A	302	GLU	2.6
1	A	375	GLU	2.6
2	H	35	VAL	2.6
2	F	40	PRO	2.6
1	A	377	TYR	2.6
2	F	37	ASN	2.5
2	F	34	SER	2.5
1	A	226	LEU	2.5
1	D	281	GLY	2.5
2	G	25	ASP	2.5
1	D	231	ASP	2.4
1	D	280	ARG	2.4
1	A	221	GLU	2.4
1	B	246	SER	2.4
1	A	232	PRO	2.4
1	C	245	GLN	2.4
1	D	206	TRP	2.4
1	A	227	GLU	2.3
1	A	305	ALA	2.3
1	B	228	ARG	2.3
1	B	218	TRP	2.3
1	D	249	SER	2.3
1	D	250	TYR	2.3
2	H	27	ASP	2.2
1	D	205	ASN	2.2
1	C	250	TYR	2.2
2	G	41	SER	2.2
2	G	40	PRO	2.1
2	F	39	LYS	2.1
1	A	303	GLY	2.1
2	E	28	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	362	TYR	2.1
2	G	36	MET	2.0
1	B	229	GLN	2.0
1	C	304	SER	2.0
2	H	36	MET	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](#)

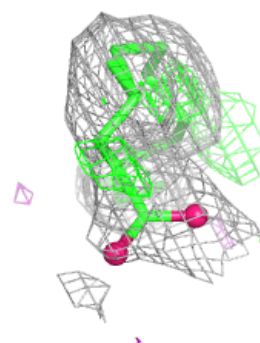
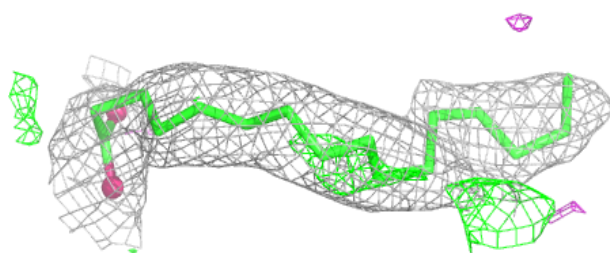
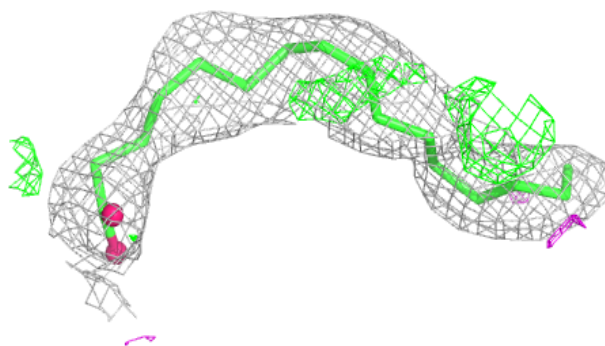
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CIT	C	501	13/13	0.81	0.15	34,44,60,62	0
3	CIT	B	501	13/13	0.82	0.15	32,43,50,51	0
4	PLM	B	502	18/18	0.88	0.24	56,62,89,94	0
4	PLM	D	501	17/18	0.89	0.18	34,52,75,77	0
4	PLM	C	502	18/18	0.90	0.19	59,70,90,94	0

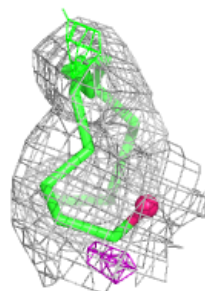
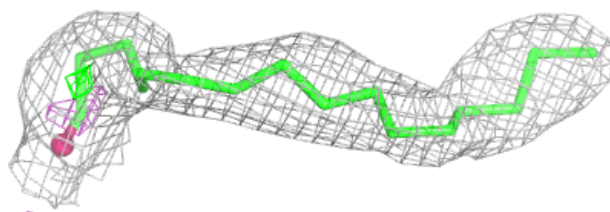
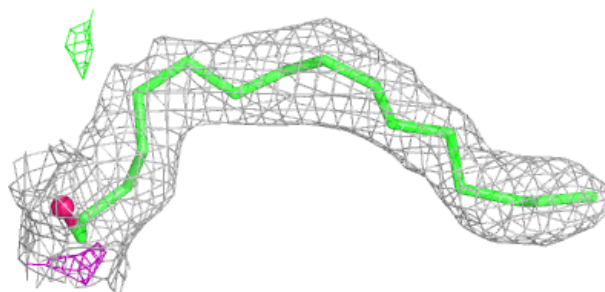
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

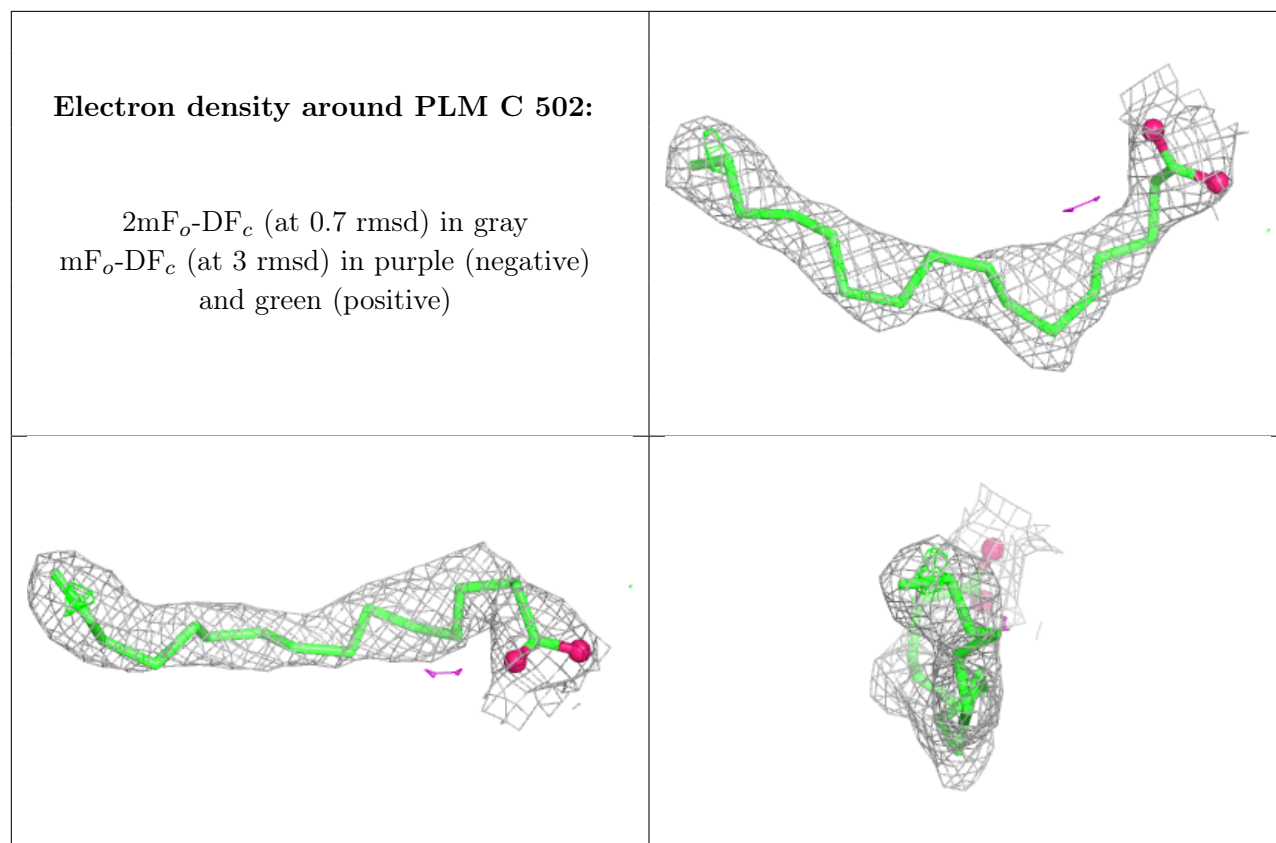
Electron density around PLM B 502:

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

**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)





6.5 Other polymers [i](#)

There are no such residues in this entry.