



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:11 AM UTC

PDB ID : 1D09 / pdb_00001d09
Title : ASPARTATE TRANSCARBAMOYLASE COMPLEXED WITH N-PHOSPHONACETYL-L-ASPARTATE (PALA)
Authors : Jin, L.; Stec, B.; Lipscomb, W.N.; Kantrowitz, E.R.
Deposited on : 1999-09-09
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

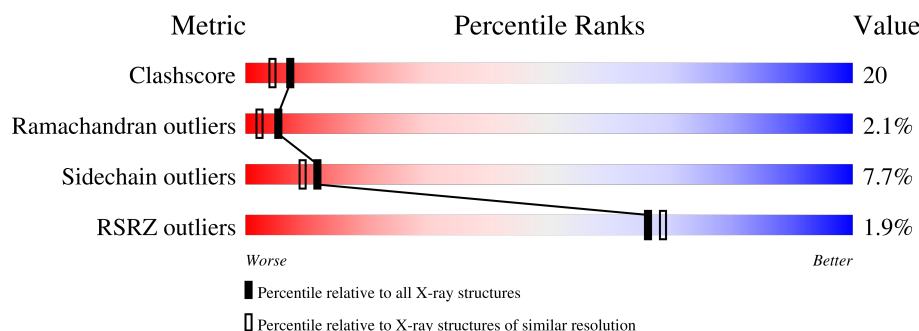
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	310	56% 37% 6%
1	C	310	60% 33% 7%
2	B	153	5% 31% 55% 13% •
2	D	153	7% 46% 43% 10% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7883 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 ASPARTATE CARBAMOYLTRANSFERASE CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2415	1527	423	456	9			

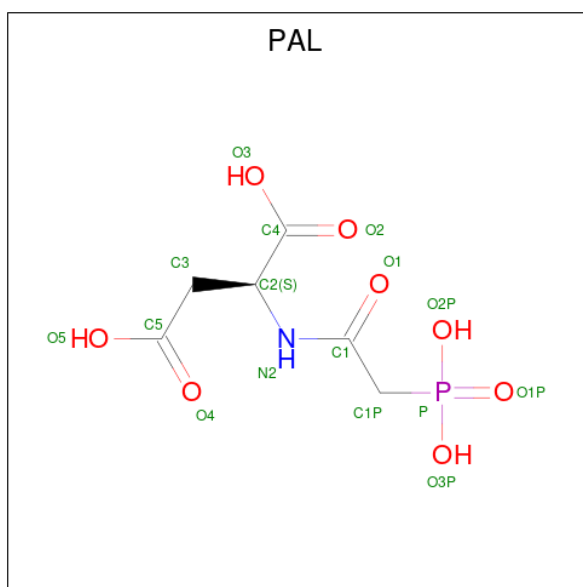
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	GLN	GLU	conflict	UNP P0A786
A	149	GLN	GLU	conflict	UNP P0A786
A	108	GLN	GLU	conflict	UNP P0A786
C	147	GLN	GLU	conflict	UNP P0A786
C	149	GLN	GLU	conflict	UNP P0A786
C	108	GLN	GLU	conflict	UNP P0A786

- Molecule 2 is a protein called ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			
2	D	153	Total	C	N	O	S	0	0	0
			1201	752	213	230	6			

- Molecule 3 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (CCD ID: PAL) (formula: $C_6H_{10}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	6	1	8	1		
3	C	1	Total	C	N	O	P	0	0
			16	6	1	8	1		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

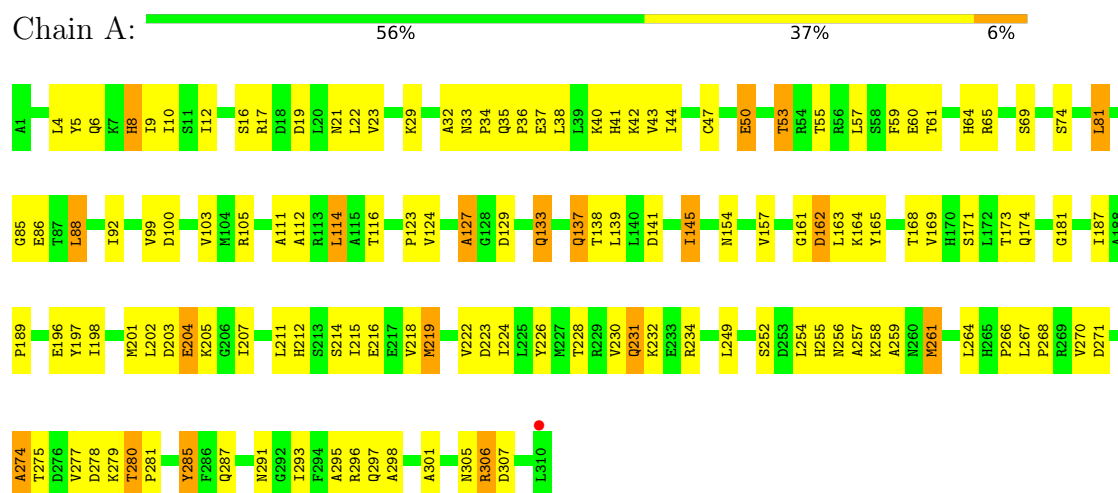
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	128	Total	O	0	0
			128	128		
5	B	110	Total	O	0	0
			110	110		
5	C	305	Total	O	0	0
			305	305		
5	D	74	Total	O	0	0
			74	74		

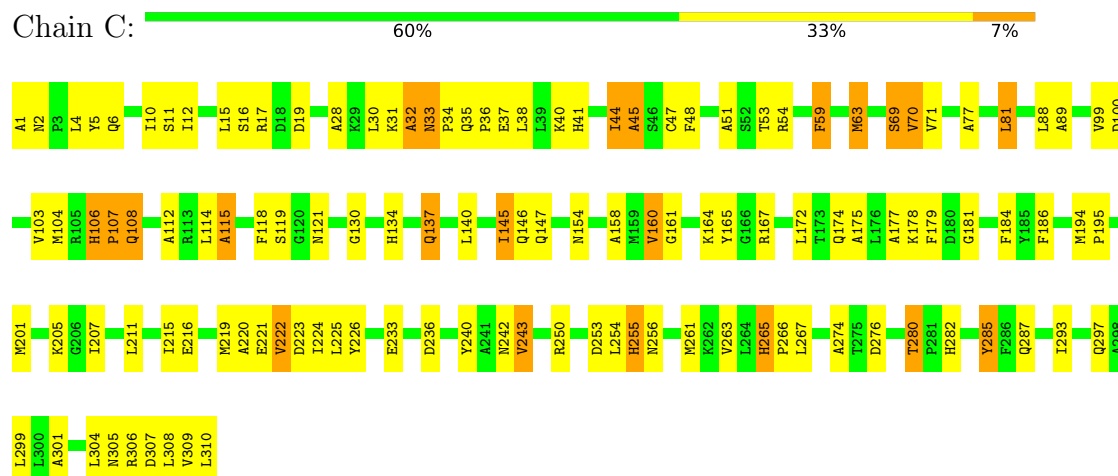
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE CATALYTIC CHAIN

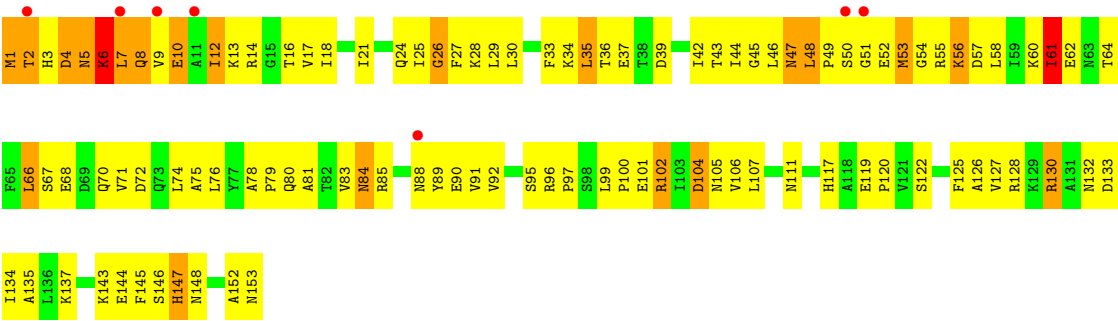


• Molecule 1: ASPARTATE CARBAMOYLTRANSFERASE CATALYTIC CHAIN

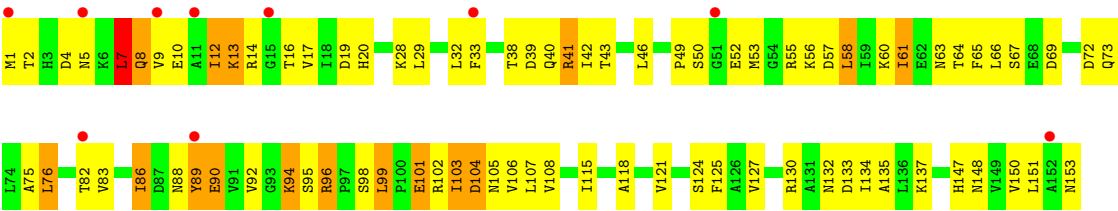


• Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN





● Molecule 2: ASPARTATE CARBAMOYLTRANSFERASE REGULATORY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	122.24Å 122.24Å 156.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.10 8.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.10) 91.2 (8.00-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.91 (at 2.05Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.203 , 0.234 0.230 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.14 , 56.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7883	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: PAL, ZN

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	1.39	12/2461 (0.5%)	1.49	35/3339 (1.0%)
1	C	1.52	19/2461 (0.8%)	1.53	40/3339 (1.2%)
2	B	1.07	2/1219 (0.2%)	1.31	13/1647 (0.8%)
2	D	1.04	0/1219	1.30	6/1647 (0.4%)
All	All	1.34	33/7360 (0.4%)	1.45	94/9972 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	32	ALA	CA-CB	-8.26	1.40	1.53
1	C	44	ILE	CA-C	8.02	1.62	1.52
1	C	222	VAL	CA-CB	-7.97	1.45	1.54
1	C	89	ALA	CA-CB	-7.94	1.41	1.53
1	C	45	ALA	CA-CB	-7.72	1.42	1.53
1	C	108	GLN	CA-C	-7.60	1.43	1.52
1	C	59	PHE	CA-C	-7.58	1.43	1.52
1	A	37	GLU	CA-C	-6.92	1.44	1.52
1	A	274	ALA	CA-CB	-6.90	1.41	1.53
1	A	261	MET	SD-CE	-6.87	1.62	1.79
2	B	61	ILE	CA-CB	6.64	1.62	1.53
1	C	115	ALA	CA-CB	-6.56	1.43	1.53
1	A	298	ALA	CA-CB	-6.45	1.43	1.53
1	A	145	ILE	CA-CB	6.43	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	ALA	CA-CB	-6.07	1.43	1.53
1	C	145	ILE	CA-CB	5.72	1.61	1.54
1	C	99	VAL	CA-C	-5.71	1.47	1.52
1	A	295	ALA	CA-CB	-5.67	1.44	1.53
1	C	63	MET	SD-CE	5.62	1.93	1.79
1	C	48	PHE	C-O	-5.54	1.17	1.24
1	C	160	VAL	CA-CB	5.49	1.62	1.54
1	C	106	HIS	C-O	-5.48	1.19	1.24
1	C	265	HIS	C-O	-5.43	1.17	1.24
1	A	127	ALA	CA-CB	-5.41	1.45	1.53
1	A	219	MET	SD-CE	-5.30	1.66	1.79
1	A	103	VAL	CA-CB	-5.29	1.47	1.54
1	A	215	ILE	CA-CB	-5.28	1.47	1.54
1	C	28	ALA	CA-CB	-5.25	1.45	1.53
1	C	53	THR	CA-C	5.22	1.57	1.52
1	A	34	PRO	CA-C	-5.13	1.46	1.52
1	A	32	ALA	CA-CB	-5.04	1.45	1.53
2	B	45	GLY	CA-C	-5.04	1.48	1.52
1	C	299	LEU	C-O	-5.03	1.18	1.24

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	7	LEU	N-CA-C	10.43	124.29	110.53
1	C	265	HIS	CA-C-N	9.77	130.03	119.28
1	C	265	HIS	C-N-CA	9.77	130.03	119.28
1	A	157	VAL	N-CA-C	8.42	120.05	107.75
1	C	88	LEU	N-CA-C	-8.15	101.96	112.23
2	B	48	LEU	CA-C-N	8.01	129.85	119.84
2	B	48	LEU	C-N-CA	8.01	129.85	119.84
1	A	137	GLN	N-CA-C	-7.95	100.98	111.24
1	C	69	SER	N-CA-C	-7.71	98.19	110.14
2	B	12	ILE	N-CA-C	7.48	120.37	108.85
1	A	33	ASN	CA-C-N	7.40	127.44	119.89
1	A	33	ASN	C-N-CA	7.40	127.44	119.89
1	C	297	GLN	N-CA-C	-7.34	102.97	110.97
1	C	236	ASP	N-CA-C	-7.28	99.47	110.39
1	C	242	ASN	N-CA-C	7.11	121.39	113.21
1	A	35	GLN	CA-C-N	7.11	128.73	119.84
1	A	35	GLN	C-N-CA	7.11	128.73	119.84
1	C	119	SER	N-CA-C	7.11	122.05	112.88
1	A	81	LEU	N-CA-C	-7.09	103.63	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	255	HIS	N-CA-C	6.85	118.75	111.28
1	C	100	ASP	N-CA-C	6.82	121.84	112.90
1	A	215	ILE	N-CA-C	-6.75	103.73	110.62
2	D	104	ASP	N-CA-C	6.68	120.57	109.95
2	D	118	ALA	N-CA-C	6.66	118.54	111.28
1	A	306	ARG	N-CA-C	6.55	118.22	111.14
2	D	7	LEU	N-CA-C	6.54	124.73	110.80
1	C	177	ALA	N-CA-C	-6.50	105.35	113.28
1	C	215	ILE	N-CA-C	-6.41	104.25	110.72
1	C	106	HIS	CA-C-N	6.34	126.89	120.04
1	C	106	HIS	C-N-CA	6.34	126.89	120.04
1	C	77	ALA	CA-C-N	-6.23	113.23	122.83
1	C	77	ALA	C-N-CA	-6.23	113.23	122.83
1	A	61	THR	N-CA-C	-6.23	104.41	111.07
1	A	189	PRO	N-CA-C	-6.20	101.73	111.34
2	D	148	ASN	N-CA-C	-6.19	104.44	111.07
1	A	111	ALA	N-CA-C	-6.17	104.64	111.36
2	B	68	GLU	N-CA-C	-6.12	103.92	111.33
1	C	263	VAL	CB-CA-C	-6.10	103.58	110.96
1	C	147	GLN	N-CA-C	6.08	120.31	113.01
2	B	53	MET	N-CA-C	-6.03	99.80	109.39
1	A	10	ILE	CB-CA-C	-6.01	104.37	111.94
1	A	231	GLN	CA-C-N	6.01	128.65	120.54
1	A	231	GLN	C-N-CA	6.01	128.65	120.54
1	C	33	ASN	CA-C-N	6.01	126.36	119.93
1	C	33	ASN	C-N-CA	6.01	126.36	119.93
1	C	287	GLN	N-CA-C	-5.93	104.90	111.36
1	C	280	THR	N-CA-C	-5.86	102.02	110.40
1	A	99	VAL	N-CA-CB	-5.85	105.67	112.34
1	C	51	ALA	N-CA-C	5.80	118.42	110.24
2	D	101	GLU	N-CA-C	-5.78	104.90	111.14
1	C	99	VAL	N-CA-C	5.71	115.50	108.53
1	A	88	LEU	N-CA-C	-5.71	105.14	111.36
1	A	287	GLN	N-CA-C	-5.68	104.70	111.69
1	A	296	ARG	N-CA-C	5.66	118.66	111.69
1	C	285	TYR	N-CA-C	5.66	118.22	111.71
1	C	223	ASP	N-CA-C	-5.64	106.57	113.50
2	B	78	ALA	CA-C-N	5.63	126.88	119.84
2	B	78	ALA	C-N-CA	5.63	126.88	119.84
1	C	221	GLU	N-CA-C	5.58	120.10	113.12
1	C	70	VAL	CB-CA-C	-5.58	101.91	110.50
1	C	53	THR	N-CA-C	-5.56	104.52	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	GLU	N-CA-C	-5.53	101.00	109.41
1	A	114	LEU	CA-CB-CG	5.52	135.63	116.30
1	C	103	VAL	N-CA-C	-5.50	99.96	107.99
1	C	161	GLY	N-CA-C	5.49	116.92	111.21
1	C	134	HIS	N-CA-C	-5.48	97.70	109.81
2	B	126	ALA	N-CA-C	-5.46	100.81	109.76
1	C	107	PRO	CA-C-N	-5.43	114.79	122.94
1	C	107	PRO	C-N-CA	-5.43	114.79	122.94
1	A	187	ILE	CB-CA-C	-5.36	104.84	111.32
1	A	50	GLU	CA-C-O	-5.30	115.43	121.58
2	B	104	ASP	N-CA-C	5.29	118.33	110.14
1	C	184	PHE	N-CA-C	5.28	117.50	108.90
2	D	86	ILE	N-CA-C	5.25	115.33	107.51
1	A	85	GLY	N-CA-C	5.22	123.12	115.08
1	C	10	ILE	CB-CA-C	-5.21	105.65	111.80
1	A	280	THR	N-CA-C	-5.19	104.16	110.13
2	B	45	GLY	N-CA-C	-5.19	102.77	110.71
1	A	8	HIS	ND1-CE1-NE2	5.17	113.57	108.40
1	A	162	ASP	N-CA-C	-5.17	98.14	107.75
2	B	119	GLU	N-CA-C	5.16	117.63	110.20
1	A	133	GLN	N-CA-C	5.13	117.96	109.85
1	A	103	VAL	N-CA-C	-5.12	100.37	107.80
1	C	137	GLN	N-CA-C	-5.10	105.63	111.14
2	B	132	ASN	N-CA-C	-5.09	103.15	111.04
1	A	259	ALA	N-CA-C	5.08	117.56	111.71
1	C	118	PHE	N-CA-C	5.08	120.11	113.30
1	A	279	LYS	N-CA-C	5.08	118.51	112.72
1	C	99	VAL	CB-CA-C	-5.06	103.52	110.91
1	A	44	ILE	N-CA-C	5.06	115.25	108.17
1	A	53	THR	N-CA-C	-5.02	106.29	112.72
1	C	36	PRO	N-CA-C	5.02	121.09	113.81
1	A	47	CYS	CA-C-N	-5.01	116.10	122.77
1	A	47	CYS	C-N-CA	-5.01	116.10	122.77

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	TYR	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2415	0	2422	72	0
1	C	2415	0	2422	64	0
2	B	1201	0	1219	93	0
2	D	1201	0	1219	81	0
3	A	16	0	6	0	0
3	C	16	0	6	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	128	0	0	3	0
5	B	110	0	0	6	1
5	C	305	0	0	2	0
5	D	74	0	0	0	0
All	All	7883	0	7294	298	1

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 20.

All (298) 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:D:42:ILE:HG12	2:D:61:ILE:HG22	1.33	1.09
2:B:99:LEU:HD12	2:B:100:PRO:HD2	1.32	1.06
2:B:10:GLU:HA	2:D:8:GLN:HG3	1.49	0.94
2:D:99:LEU:HD11	2:D:134:ILE:HD13	1.50	0.91
2:B:53:MET:HG3	2:B:56:LYS:HB3	1.55	0.88
2:B:7:LEU:HG	2:B:8:GLN:N	1.88	0.88
2:D:99:LEU:HD22	2:D:127:VAL:HG11	1.56	0.87
1:C:35:GLN:NE2	1:C:310:LEU:HD22	1.90	0.87
1:C:106:HIS:ND1	1:C:107:PRO:HD2	1.93	0.82
2:D:1:MET:HB3	2:D:90:GLU:HG2	1.61	0.82
2:B:34:LYS:HB3	2:B:37:GLU:HG3	1.62	0.81
1:A:219:MET:HE2	1:A:261:MET:HE2	1.63	0.81
1:A:133:GLN:HE22	1:A:174:GLN:HE22	1.29	0.80
2:B:7:LEU:HG	2:B:8:GLN:H	1.50	0.77
1:C:38:LEU:HD11	1:C:308:LEU:HD11	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:SER:HB2	1:A:216:GLU:HG2	1.67	0.75
2:B:47:ASN:HD22	2:B:55:ARG:HD3	1.52	0.75
1:A:219:MET:CE	1:A:261:MET:HE2	2.18	0.74
2:D:40:GLN:NE2	2:D:63:ASN:HB2	2.03	0.73
2:D:99:LEU:HD11	2:D:134:ILE:CD1	2.18	0.73
2:B:81:ALA:O	2:B:96:ARG:HG3	1.89	0.73
2:D:38:THR:HG22	2:D:40:GLN:HG2	1.72	0.72
2:B:67:SER:OG	2:B:70:GLN:HG3	1.89	0.72
2:B:134:ILE:O	2:B:147:HIS:HB3	1.90	0.72
2:D:58:LEU:HD21	2:D:60:LYS:HE3	1.69	0.72
2:B:30:LEU:HD11	2:B:44:ILE:HG12	1.72	0.71
2:B:137:LYS:HE2	5:B:1351:HOH:O	1.91	0.70
2:D:16:THR:OG1	2:D:65:PHE:HA	1.91	0.70
1:A:257:ALA:HB1	1:A:261:MET:HE3	1.74	0.69
2:D:14:ARG:NH2	2:D:65:PHE:HE2	1.90	0.69
2:D:58:LEU:C	2:D:58:LEU:HD23	2.17	0.69
2:B:107:LEU:HD22	2:B:152:ALA:HB2	1.75	0.68
1:A:137:GLN:HG2	1:A:168:THR:HG22	1.74	0.68
2:B:46:LEU:HD12	2:D:42:ILE:HB	1.74	0.67
1:A:201:MET:O	1:A:205:LYS:HG3	1.95	0.67
2:D:14:ARG:HA	2:D:86:ILE:O	1.93	0.66
1:A:218:VAL:O	1:A:222:VAL:HG13	1.95	0.66
2:D:17:VAL:HG21	2:D:86:ILE:HD12	1.77	0.66
2:B:1:MET:SD	2:B:1:MET:N	2.69	0.66
2:D:103:ILE:HD13	2:D:104:ASP:N	2.10	0.66
1:A:141:ASP:O	1:A:145:ILE:HG13	1.96	0.65
2:D:130:ARG:HE	2:D:135:ALA:HB2	1.61	0.65
2:B:130:ARG:HB2	2:B:135:ALA:HB2	1.79	0.65
1:C:130:GLY:O	1:C:167:ARG:HD3	1.98	0.64
1:C:137:GLN:O	1:C:140:LEU:HG	1.98	0.64
1:C:106:HIS:ND1	1:C:107:PRO:CD	2.61	0.64
2:D:83:VAL:HG23	2:D:95:SER:HB2	1.79	0.64
1:C:106:HIS:CE1	1:C:107:PRO:HD2	2.33	0.63
2:D:115:ILE:O	2:D:115:ILE:HG13	1.97	0.62
2:B:50:SER:OG	2:B:56:LYS:HG2	1.98	0.62
2:B:99:LEU:HD11	2:B:127:VAL:HG11	1.81	0.61
2:B:84:ASN:N	2:B:84:ASN:HD22	1.99	0.61
1:A:161:GLY:HA3	1:A:228:THR:OG1	2.00	0.61
2:B:99:LEU:HD12	2:B:100:PRO:CD	2.19	0.61
2:B:47:ASN:ND2	2:B:55:ARG:HD3	2.15	0.61
2:B:117:HIS:HB2	5:B:1396:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASN:OD1	1:A:181:GLY:HA3	2.00	0.61
2:B:9:VAL:HG12	2:D:8:GLN:OE1	2.00	0.60
2:D:82:THR:HG22	2:D:96:ARG:CZ	2.31	0.60
2:B:128:ARG:NH2	2:B:130:ARG:HG3	2.16	0.60
1:A:219:MET:HE3	1:A:219:MET:HA	1.84	0.60
2:B:71:VAL:HG13	2:B:83:VAL:HG21	1.84	0.59
1:C:154:ASN:HA	1:C:181:GLY:O	2.02	0.59
2:B:17:VAL:HG13	2:B:60:LYS:HG2	1.85	0.59
2:B:143:LYS:HB2	2:B:145:PHE:CZ	2.38	0.59
2:D:32:LEU:O	2:D:33:PHE:HD1	1.85	0.58
2:B:49:PRO:HA	2:B:54:GLY:O	2.02	0.58
1:C:47:CYS:O	1:C:104:MET:HA	2.03	0.58
2:D:102:ARG:NH1	2:D:124:SER:OG	2.37	0.58
2:B:55:ARG:HG3	2:B:55:ARG:HH11	1.68	0.58
2:B:83:VAL:C	2:B:84:ASN:HD22	2.12	0.57
2:D:103:ILE:HD13	2:D:103:ILE:C	2.30	0.57
1:C:274:ALA:HA	5:C:1555:HOH:O	2.03	0.57
2:D:32:LEU:O	2:D:33:PHE:CD1	2.58	0.57
1:A:306:ARG:HH12	1:A:307:ASP:CG	2.13	0.57
2:B:66:LEU:HD12	2:B:71:VAL:HG22	1.86	0.57
2:D:76:LEU:HG	2:D:99:LEU:HD21	1.86	0.57
1:A:196:GLU:HG3	5:A:1314:HOH:O	2.03	0.56
1:C:309:VAL:HG13	1:C:309:VAL:O	2.06	0.56
1:A:81:LEU:HA	1:A:86:GLU:HB3	1.87	0.56
2:B:25:ILE:O	2:B:27:PHE:N	2.39	0.56
2:B:8:GLN:HB2	2:D:10:GLU:HA	1.88	0.56
2:D:106:VAL:HG23	2:D:107:LEU:HG	1.88	0.56
2:B:6:LYS:HD2	2:B:6:LYS:N	2.21	0.56
2:B:25:ILE:O	2:B:28:LYS:N	2.39	0.56
1:C:17:ARG:NH2	1:C:179:PHE:HA	2.20	0.56
2:D:82:THR:HG22	2:D:96:ARG:NH1	2.21	0.56
2:B:39:ASP:HB3	2:D:55:ARG:NH1	2.20	0.56
2:D:50:SER:OG	2:D:53:MET:HB2	2.05	0.56
1:A:293:ILE:O	1:A:297:GLN:HG3	2.06	0.56
2:B:66:LEU:O	2:B:85:ARG:NH2	2.40	0.55
1:C:265:HIS:ND1	1:C:266:PRO:HD2	2.21	0.55
2:B:42:ILE:HG12	2:B:61:ILE:HG23	1.88	0.55
1:C:114:LEU:HD11	2:D:121:VAL:HG11	1.88	0.55
2:D:13:LYS:HA	2:D:89:TYR:CD2	2.41	0.54
2:D:40:GLN:O	2:D:42:ILE:HG13	2.06	0.54
2:D:94:LYS:HZ1	2:D:96:ARG:HH21	1.54	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:HB2	2:D:9:VAL:O	2.08	0.54
1:C:5:TYR:CD1	1:C:306:ARG:HA	2.43	0.54
1:A:174:GLN:HA	1:A:201:MET:HE1	1.89	0.54
2:B:47:ASN:ND2	2:D:39:ASP:HB2	2.22	0.54
2:B:111:ASN:O	2:B:117:HIS:HE1	1.90	0.54
2:D:12:ILE:N	2:D:12:ILE:HD13	2.23	0.54
2:B:24:GLN:HG3	2:B:28:LYS:HE3	1.90	0.53
2:D:94:LYS:NZ	2:D:96:ARG:HH21	2.07	0.53
1:C:1:ALA:HA	1:C:306:ARG:O	2.09	0.53
2:D:102:ARG:HB2	2:D:125:PHE:O	2.07	0.53
1:C:38:LEU:HD11	1:C:308:LEU:CD1	2.37	0.53
1:A:197:TYR:CE1	1:A:198:ILE:HD11	2.44	0.53
1:C:160:VAL:HG21	1:C:225:LEU:HD11	1.90	0.53
2:D:130:ARG:NE	2:D:135:ALA:HB2	2.22	0.53
1:A:12:ILE:O	1:A:12:ILE:HG22	2.07	0.52
2:B:21:ILE:CG2	2:B:25:ILE:HB	2.39	0.52
1:C:219:MET:HE3	1:C:254:LEU:HA	1.91	0.52
2:B:91:VAL:O	2:B:91:VAL:HG13	2.10	0.52
2:B:67:SER:HG	2:B:70:GLN:HG3	1.73	0.52
2:B:81:ALA:O	2:B:97:PRO:HD2	2.09	0.52
2:B:3:HIS:CD2	5:B:1387:HOH:O	2.63	0.52
2:B:14:ARG:HG2	2:B:88:ASN:H	1.75	0.52
1:A:211:LEU:O	1:A:212:HIS:CD2	2.63	0.51
1:A:270:VAL:HA	5:A:1416:HOH:O	2.10	0.51
1:A:226:TYR:CZ	1:A:266:PRO:HD3	2.45	0.51
2:B:18:ILE:O	2:B:58:LEU:HD12	2.09	0.51
2:B:33:PHE:CE2	2:B:74:LEU:HD23	2.46	0.51
2:D:4:ASP:HB3	2:D:9:VAL:HG21	1.93	0.51
1:C:280:THR:C	1:C:282:HIS:H	2.18	0.51
1:A:254:LEU:HD22	1:A:261:MET:HE1	1.92	0.51
2:B:4:ASP:O	2:B:5:ASN:HB2	2.11	0.50
1:C:104:MET:HE1	1:C:115:ALA:HB2	1.94	0.50
1:C:114:LEU:CD1	2:D:121:VAL:HG11	2.41	0.50
1:A:50:GLU:HB3	1:A:105:ARG:HG2	1.93	0.50
2:B:25:ILE:HG22	2:B:29:LEU:HG	1.94	0.50
2:B:106:VAL:HG12	2:B:107:LEU:HD23	1.93	0.50
1:A:40:LYS:O	1:A:41:HIS:HB2	2.11	0.50
1:A:138:THR:OG1	1:A:171:SER:HB3	2.12	0.50
2:D:52:GLU:HG3	2:D:53:MET:SD	2.52	0.50
2:B:5:ASN:C	2:B:6:LYS:HD2	2.37	0.50
1:C:220:ALA:HB2	1:C:256:ASN:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:40:GLN:O	2:D:42:ILE:N	2.44	0.50
2:B:9:VAL:HB	2:D:7:LEU:O	2.12	0.49
2:D:29:LEU:HD22	2:D:33:PHE:CE2	2.47	0.49
2:D:103:ILE:CD1	2:D:106:VAL:HG22	2.42	0.49
2:B:29:LEU:O	2:B:35:LEU:HD12	2.12	0.49
5:A:1422:HOH:O	2:B:120:PRO:HG3	2.11	0.49
1:A:230:VAL:O	1:A:232:LYS:N	2.44	0.49
1:A:12:ILE:O	1:A:12:ILE:CG2	2.60	0.49
2:B:21:ILE:HG22	2:B:25:ILE:HB	1.95	0.49
2:B:61:ILE:HB	2:B:64:THR:HB	1.95	0.49
1:C:164:LYS:HE2	1:C:165:TYR:CZ	2.47	0.49
1:A:8:HIS:CE1	1:A:123:PRO:HA	2.49	0.48
1:C:70:VAL:HG12	1:C:71:VAL:N	2.27	0.48
1:C:266:PRO:O	1:C:267:LEU:HB2	2.13	0.48
2:D:4:ASP:CG	2:D:5:ASN:N	2.72	0.48
1:A:164:LYS:HD3	1:A:165:TYR:CE2	2.49	0.48
1:A:223:ASP:O	1:A:224:ILE:HD13	2.14	0.48
2:B:107:LEU:HD23	2:B:107:LEU:N	2.28	0.48
1:C:301:ALA:O	1:C:305:ASN:HB2	2.14	0.48
2:D:50:SER:O	2:D:53:MET:N	2.46	0.48
2:D:125:PHE:HA	2:D:137:LYS:O	2.13	0.48
2:B:46:LEU:HD23	2:B:57:ASP:OD1	2.14	0.47
2:B:102:ARG:HA	2:B:125:PHE:O	2.14	0.47
1:A:162:ASP:HB2	1:A:230:VAL:HA	1.96	0.47
2:B:62:GLU:C	2:B:64:THR:H	2.22	0.47
1:A:249:LEU:HD11	1:A:254:LEU:HD21	1.96	0.47
2:B:2:THR:O	2:B:3:HIS:CG	2.68	0.47
2:B:122:SER:N	5:B:1409:HOH:O	2.44	0.47
1:A:23:VAL:HG11	1:A:139:LEU:HD13	1.97	0.47
1:A:255:HIS:ND1	1:A:256:ASN:N	2.62	0.47
2:B:48:LEU:HA	2:B:49:PRO:HD2	1.60	0.47
1:C:35:GLN:NE2	1:C:310:LEU:CD2	2.70	0.47
2:D:49:PRO:O	2:D:56:LYS:HG2	2.15	0.47
1:A:43:VAL:HG22	1:A:69:SER:HB2	1.96	0.47
2:B:107:LEU:CD2	2:B:152:ALA:HB2	2.44	0.47
2:D:40:GLN:HE21	2:D:63:ASN:HB2	1.76	0.46
2:D:58:LEU:C	2:D:58:LEU:CD2	2.88	0.46
1:C:2:ASN:OD1	1:C:4:LEU:N	2.45	0.46
1:C:44:ILE:HG21	1:C:63:MET:HE2	1.96	0.46
1:C:104:MET:HE1	1:C:115:ALA:CB	2.45	0.46
2:D:13:LYS:HG3	2:D:88:ASN:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:108:VAL:H	2:D:153:ASN:CG	2.23	0.46
1:C:6:GLN:HA	1:C:6:GLN:NE2	2.30	0.46
1:A:197:TYR:HB3	2:B:144:GLU:HG2	1.97	0.46
1:A:8:HIS:ND1	1:A:124:VAL:N	2.53	0.46
2:B:16:THR:HG22	2:B:17:VAL:N	2.31	0.46
1:C:81:LEU:C	1:C:81:LEU:HD23	2.41	0.46
2:D:83:VAL:CG2	2:D:95:SER:HB2	2.44	0.46
1:C:45:ALA:HA	1:C:71:VAL:O	2.15	0.46
1:C:40:LYS:O	1:C:41:HIS:HB2	2.16	0.45
1:A:267:LEU:HB3	1:A:268:PRO:HA	1.99	0.45
2:B:48:LEU:O	2:B:56:LYS:HG3	2.16	0.45
1:A:112:ALA:O	1:A:116:THR:HG23	2.16	0.45
2:B:4:ASP:O	2:B:5:ASN:CB	2.64	0.45
2:B:85:ARG:O	2:B:92:VAL:HG22	2.16	0.45
2:B:91:VAL:HG21	5:B:1403:HOH:O	2.17	0.45
1:C:175:ALA:O	1:C:178:LYS:HB2	2.17	0.45
1:C:106:HIS:CG	1:C:107:PRO:CD	3.00	0.45
1:C:255:HIS:CE1	5:C:1329:HOH:O	2.69	0.45
1:A:306:ARG:HG2	1:A:306:ARG:HH11	1.81	0.45
2:D:4:ASP:CG	2:D:5:ASN:H	2.25	0.45
1:A:261:MET:SD	1:A:261:MET:C	3.00	0.45
1:C:32:ALA:C	1:C:34:PRO:HD3	2.41	0.45
2:D:147:HIS:O	2:D:151:LEU:HG	2.17	0.44
1:C:158:ALA:HB2	1:C:222:VAL:HG11	1.99	0.44
2:B:79:PRO:O	2:B:97:PRO:HG2	2.17	0.44
1:C:17:ARG:CZ	1:C:179:PHE:HA	2.48	0.44
2:D:46:LEU:HA	2:D:57:ASP:OD1	2.18	0.44
1:A:291:ASN:HD22	1:A:291:ASN:HA	1.57	0.44
2:B:34:LYS:C	2:B:36:THR:H	2.25	0.44
2:B:104:ASP:O	2:B:106:VAL:HG23	2.17	0.44
2:D:1:MET:HA	2:D:90:GLU:OE1	2.17	0.44
2:D:67:SER:C	2:D:69:ASP:H	2.26	0.44
2:B:25:ILE:O	2:B:26:GLY:C	2.61	0.44
1:C:15:LEU:O	1:C:178:LYS:HE2	2.18	0.44
1:A:211:LEU:C	1:A:212:HIS:CD2	2.95	0.44
1:C:30:LEU:HD23	1:C:30:LEU:HA	1.56	0.44
1:C:186:PHE:HB2	1:C:211:LEU:HD23	1.99	0.44
1:C:33:ASN:ND2	1:C:35:GLN:HE22	2.15	0.43
2:D:150:VAL:O	2:D:153:ASN:ND2	2.51	0.43
1:A:129:ASP:OD1	1:A:129:ASP:N	2.51	0.43
1:A:219:MET:HE1	1:A:261:MET:HE2	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:ILE:HD13	2:B:14:ARG:O	2.18	0.43
1:C:280:THR:C	1:C:282:HIS:N	2.77	0.43
1:A:50:GLU:CD	1:A:234:ARG:HH22	2.26	0.43
1:C:145:ILE:O	1:C:146:GLN:C	2.62	0.43
2:D:10:GLU:N	2:D:10:GLU:CD	2.77	0.43
2:B:46:LEU:O	2:B:48:LEU:N	2.51	0.43
2:B:88:ASN:C	2:B:89:TYR:CD2	2.97	0.43
1:C:226:TYR:OH	1:C:266:PRO:HG3	2.19	0.43
2:D:16:THR:CG2	2:D:17:VAL:N	2.82	0.43
2:B:133:ASP:HB3	5:B:1369:HOH:O	2.19	0.43
2:D:19:ASP:O	2:D:20:HIS:HB2	2.18	0.43
2:D:32:LEU:O	2:D:32:LEU:HG	2.19	0.43
1:A:275:THR:O	1:A:278:ASP:HB2	2.18	0.43
1:C:174:GLN:HG2	1:C:201:MET:HE2	2.00	0.43
1:A:145:ILE:HG12	1:A:264:LEU:HD11	2.01	0.43
1:A:306:ARG:NH1	1:A:307:ASP:CG	2.76	0.43
1:C:4:LEU:HD23	1:C:4:LEU:HA	1.78	0.42
1:A:16:SER:O	1:A:17:ARG:C	2.62	0.42
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.72	0.42
1:A:280:THR:HB	1:A:281:PRO:HD2	2.01	0.42
2:B:51:GLY:O	2:B:54:GLY:N	2.52	0.42
1:C:205:LYS:HA	1:C:205:LYS:HD3	1.78	0.42
1:A:274:ALA:O	1:A:277:VAL:HG23	2.19	0.42
2:B:137:LYS:HA	2:B:144:GLU:HA	2.02	0.42
1:C:33:ASN:ND2	1:C:35:GLN:NE2	2.67	0.42
1:C:205:LYS:HB2	1:C:207:ILE:HG12	2.00	0.42
2:D:13:LYS:HD3	2:D:89:TYR:OH	2.19	0.42
2:B:88:ASN:C	2:B:90:GLU:H	2.27	0.42
1:C:16:SER:O	1:C:19:ASP:HB2	2.18	0.42
1:C:35:GLN:CD	1:C:310:LEU:CD2	2.93	0.42
1:A:198:ILE:O	1:A:202:LEU:HG	2.20	0.42
2:B:66:LEU:HB3	2:B:71:VAL:HG23	2.01	0.42
2:B:101:GLU:HG3	2:B:102:ARG:HG2	2.01	0.42
1:A:163:LEU:HA	1:A:169:VAL:HG21	2.02	0.42
2:B:75:ALA:HA	2:B:79:PRO:HA	2.02	0.42
1:C:31:LYS:O	1:C:31:LYS:HG2	2.20	0.42
2:D:73:GLN:CD	2:D:106:VAL:HG11	2.45	0.42
1:A:60:GLU:O	1:A:64:HIS:CD2	2.73	0.41
1:C:224:ILE:HD13	1:C:224:ILE:HA	1.90	0.41
1:A:5:TYR:CE2	1:A:6:GLN:HG2	2.56	0.41
1:C:114:LEU:HD11	2:D:121:VAL:CG1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:THR:HG21	1:A:127:ALA:HB1	2.02	0.41
2:B:21:ILE:HB	2:B:57:ASP:HB3	2.02	0.41
2:B:66:LEU:C	2:B:85:ARG:HH22	2.29	0.41
2:B:111:ASN:O	2:B:117:HIS:CE1	2.71	0.41
2:D:88:ASN:ND2	2:D:89:TYR:CE1	2.88	0.41
1:A:19:ASP:O	1:A:22:LEU:HB3	2.20	0.41
1:A:88:LEU:O	1:A:92:ILE:HG12	2.21	0.41
1:A:9:ILE:HG23	1:A:9:ILE:HD12	1.81	0.41
1:A:173:THR:HG21	1:A:198:ILE:CG2	2.51	0.41
1:A:258:LYS:HE3	1:A:258:LYS:HB2	1.90	0.41
1:C:11:SER:O	1:C:12:ILE:C	2.60	0.41
1:A:138:THR:OG1	1:A:171:SER:CB	2.69	0.41
2:B:146:SER:C	2:B:148:ASN:N	2.75	0.41
1:A:270:VAL:HG12	1:A:271:ASP:N	2.36	0.41
2:B:102:ARG:HB2	2:B:102:ARG:NH1	2.36	0.41
2:D:61:ILE:HD13	2:D:61:ILE:N	2.35	0.41
2:D:66:LEU:HD23	2:D:66:LEU:HA	1.78	0.41
2:D:72:ASP:O	2:D:75:ALA:HB3	2.21	0.41
1:A:301:ALA:O	1:A:305:ASN:HB2	2.21	0.41
2:D:16:THR:HG22	2:D:17:VAL:N	2.36	0.41
1:C:250:ARG:NH2	1:C:276:ASP:CG	2.78	0.41
2:D:13:LYS:O	2:D:86:ILE:HG22	2.21	0.41
2:D:40:GLN:O	2:D:41:ARG:C	2.64	0.41
2:D:90:GLU:OE1	2:D:90:GLU:HA	2.20	0.41
1:A:42:LYS:HA	1:A:100:ASP:OD2	2.21	0.41
1:C:265:HIS:HA	1:C:266:PRO:HD3	1.90	0.41
2:D:104:ASP:O	2:D:105:ASN:HB2	2.21	0.40
1:A:53:THR:O	1:A:57:LEU:HB2	2.20	0.40
2:B:48:LEU:HG	2:B:56:LYS:HE2	2.03	0.40
1:C:240:TYR:O	1:C:243:VAL:HG22	2.20	0.40
1:C:293:ILE:HA	1:C:293:ILE:HD13	1.75	0.40
1:A:4:LEU:O	1:A:5:TYR:C	2.62	0.40
2:D:103:ILE:CG2	2:D:107:LEU:HD12	2.51	0.40
1:A:139:LEU:HD23	1:A:139:LEU:HA	1.97	0.40
1:A:203:ASP:O	1:A:204:GLU:C	2.63	0.40
1:C:15:LEU:O	1:C:178:LYS:CE	2.70	0.40
2:D:127:VAL:HG13	2:D:134:ILE:HG21	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1392:HOH:O	5:B:1392:HOH:O[3_565]	1.60	0.60

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	308/310 (99%)	283 (92%)	22 (7%)	3 (1%)	12	9
1	C	308/310 (99%)	291 (94%)	17 (6%)	0	100	100
2	B	151/153 (99%)	111 (74%)	30 (20%)	10 (7%)	1	0
2	D	151/153 (99%)	114 (76%)	31 (20%)	6 (4%)	2	0
All	All	918/926 (99%)	799 (87%)	100 (11%)	19 (2%)	5	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	GLN
2	B	2	THR
2	B	5	ASN
2	B	105	ASN
2	D	7	LEU
2	D	41	ARG
2	B	13	LYS
2	B	26	GLY
2	B	130	ARG
2	D	132	ASN
2	B	6	LYS
2	D	8	GLN
2	B	10	GLU
2	B	47	ASN
2	B	35	LEU
1	A	252	SER
2	D	13	LYS

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Mol	Chain	Res	Type
2	D	92	VAL
1	A	36	PRO

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	261/261 (100%)	252 (97%)	9 (3%)	32	35
1	C	261/261 (100%)	243 (93%)	18 (7%)	14	12
2	B	137/137 (100%)	120 (88%)	17 (12%)	4	2
2	D	137/137 (100%)	120 (88%)	17 (12%)	4	2
All	All	796/796 (100%)	735 (92%)	61 (8%)	12	9

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	38	LEU
1	A	59	PHE
1	A	65	ARG
1	A	74	SER
1	A	114	LEU
1	A	204	GLU
1	A	207	ILE
1	A	285	TYR
2	B	1	MET
2	B	4	ASP
2	B	6	LYS
2	B	8	GLN
2	B	43	THR
2	B	52	GLU
2	B	56	LYS
2	B	61	ILE
2	B	66	LEU
2	B	72	ASP

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Mol	Chain	Res	Type
2	B	76	LEU
2	B	80	GLN
2	B	84	ASN
2	B	95	SER
2	B	102	ARG
2	B	147	HIS
2	B	153	ASN
1	C	37	GLU
1	C	54	ARG
1	C	59	PHE
1	C	69	SER
1	C	81	LEU
1	C	108	GLN
1	C	121	ASN
1	C	172	LEU
1	C	194	MET
1	C	195	PRO
1	C	216	GLU
1	C	233	GLU
1	C	243	VAL
1	C	253	ASP
1	C	261	MET
1	C	285	TYR
1	C	304	LEU
1	C	307	ASP
2	D	2	THR
2	D	12	ILE
2	D	28	LYS
2	D	43	THR
2	D	58	LEU
2	D	61	ILE
2	D	64	THR
2	D	76	LEU
2	D	89	TYR
2	D	90	GLU
2	D	94	LYS
2	D	96	ARG
2	D	98	SER
2	D	99	LEU
2	D	101	GLU
2	D	103	ILE
2	D	133	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	64	HIS
1	A	174	GLN
2	B	47	ASN
2	B	73	GLN
2	B	80	GLN
2	B	84	ASN
2	B	105	ASN
2	B	117	HIS
2	B	148	ASN
2	B	153	ASN
1	C	6	GLN
1	C	21	ASN
1	C	33	ASN
1	C	35	GLN
1	C	146	GLN
1	C	291	ASN
2	D	40	GLN
2	D	88	ASN
2	D	105	ASN
2	D	117	HIS
2	D	153	ASN

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](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PAL	C	1312	-	15,15,15	2.10	3 (20%)	20,21,21	2.76	8 (40%)
3	PAL	A	1311	-	15,15,15	1.64	4 (26%)	20,21,21	1.68	4 (20%)

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	PAL	C	1312	-	-	0/17/17/17	-
3	PAL	A	1311	-	-	2/17/17/17	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1312	PAL	P-O2P	-4.94	1.43	1.55
3	C	1312	PAL	P-C1P	-4.75	1.72	1.79
3	A	1311	PAL	P-O3P	3.39	1.62	1.55
3	A	1311	PAL	P-O2P	-3.09	1.48	1.55
3	A	1311	PAL	O2-C4	2.27	1.28	1.22
3	A	1311	PAL	P-O1P	2.25	1.54	1.50
3	C	1312	PAL	O5-C5	-2.24	1.23	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1312	PAL	O2P-P-C1P	6.65	120.80	106.84
3	C	1312	PAL	O3P-P-C1P	6.03	119.49	106.84
3	C	1312	PAL	O2P-P-O1P	-5.08	99.25	112.39
3	C	1312	PAL	O3P-P-O2P	-4.54	95.04	107.96
3	A	1311	PAL	O2P-P-C1P	4.49	116.26	106.84
3	A	1311	PAL	O3P-P-O1P	-3.77	102.64	112.39
3	A	1311	PAL	C4-C2-N2	2.82	117.11	110.57
3	C	1312	PAL	O3P-P-O1P	-2.30	106.45	112.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1312	PAL	O2-C4-C2	-2.29	114.87	122.26
3	C	1312	PAL	C1P-C1-N2	-2.28	113.03	115.19
3	A	1311	PAL	O3P-P-C1P	-2.23	102.16	106.84
3	C	1312	PAL	O3-C4-C2	2.23	121.04	113.51

There are no chirality outliers.

All (2) torsion outliers are listed below:

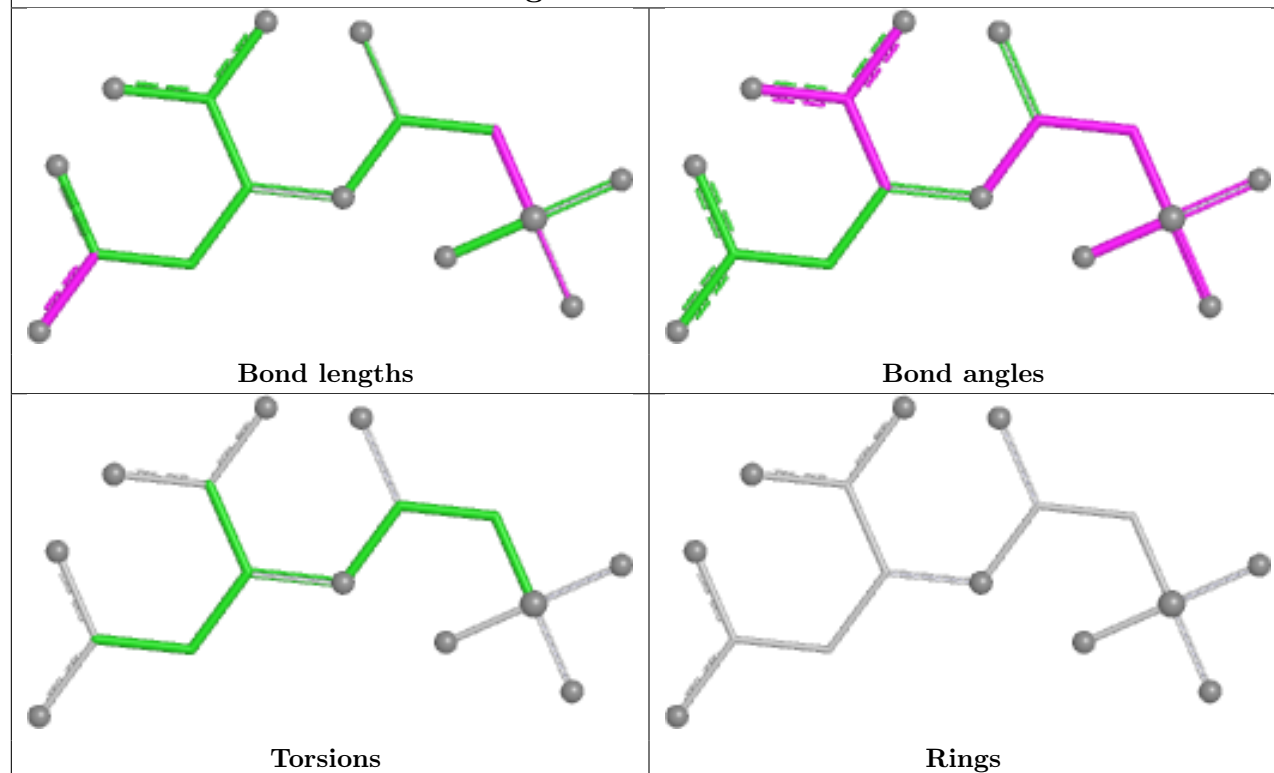
Mol	Chain	Res	Type	Atoms
3	A	1311	PAL	C1-C1P-P-O1P
3	A	1311	PAL	C1-C1P-P-O3P

There are no ring outliers.

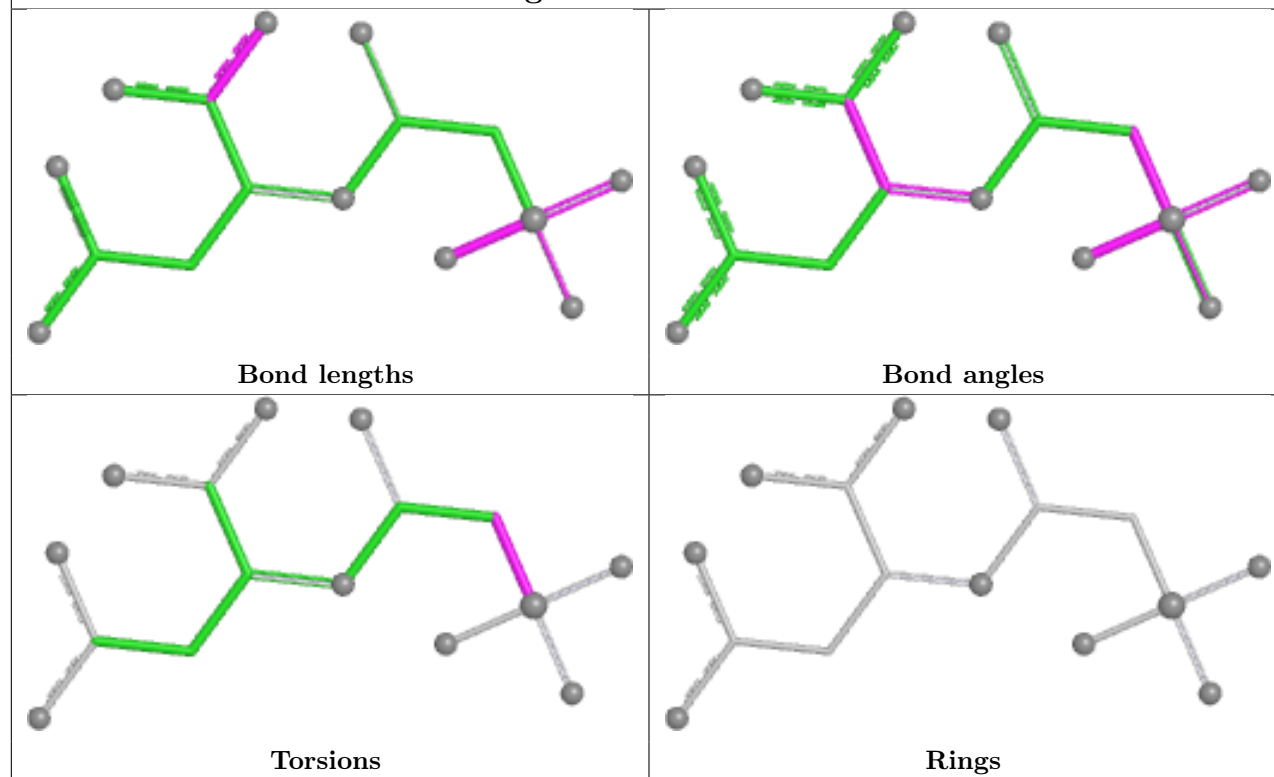
No monomer is involved in short contacts.

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.

Ligand PAL C 1312



Ligand PAL A 1311



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	310/310 (100%)	-0.51	1 (0%) 90 91	4, 23, 50, 96	0
1	C	310/310 (100%)	-0.63	0 100 100	4, 18, 45, 64	0
2	B	153/153 (100%)	0.47	7 (4%) 37 39	12, 55, 84, 98	1 (0%)
2	D	153/153 (100%)	0.54	10 (6%) 25 26	15, 57, 88, 100	1 (0%)
All	All	926/926 (100%)	-0.21	18 (1%) 66 69	4, 27, 77, 100	2 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	9	VAL	5.1
2	B	9	VAL	3.6
2	B	2	THR	3.6
2	B	50	SER	3.0
2	B	51	GLY	2.9
2	B	7	LEU	2.8
2	D	152	ALA	2.8
2	D	51	GLY	2.7
2	B	11	ALA	2.6
2	B	88	ASN	2.5
2	D	5	ASN	2.4
2	D	82	THR	2.3
2	D	11	ALA	2.3
2	D	33	PHE	2.3
1	A	310	LEU	2.3
2	D	1	MET	2.1
2	D	89	TYR	2.1
2	D	15	GLY	2.1

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](#)

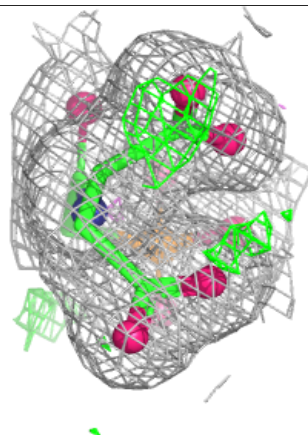
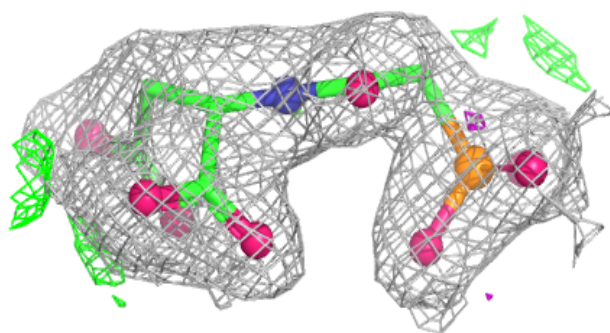
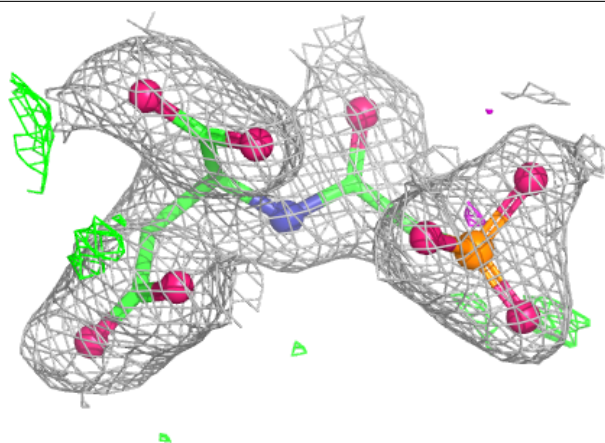
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PAL	A	1311	16/16	0.96	0.06	4,14,25,29	0
3	PAL	C	1312	16/16	0.97	0.06	2,16,24,30	0
4	ZN	B	1313	1/1	0.98	0.02	26,26,26,26	0
4	ZN	D	1314	1/1	0.99	0.02	23,23,23,23	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.

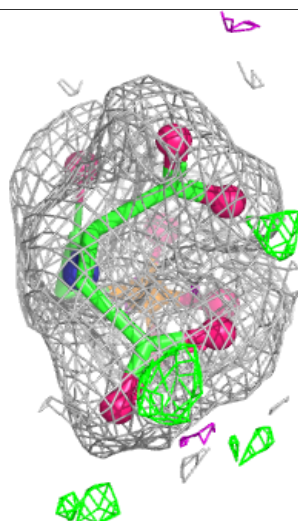
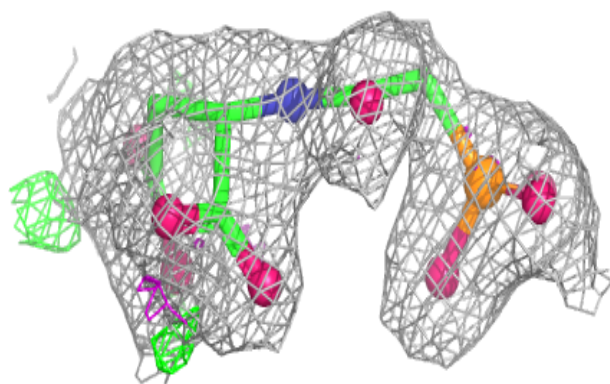
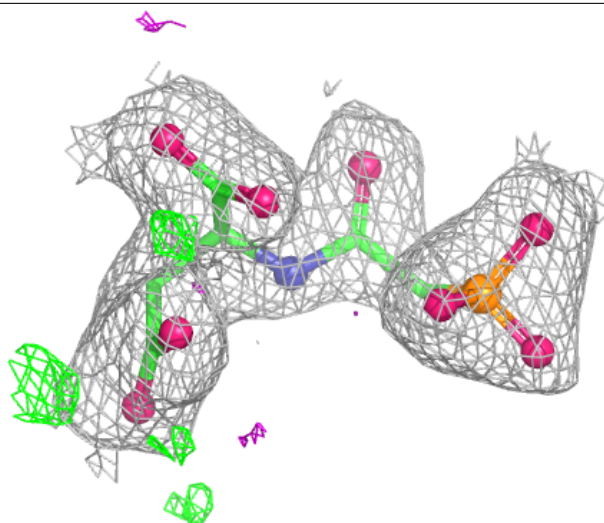
Electron density around PAL A 1311:

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



Electron density around PAL C 1312:

$2mF_o-DF_c$ (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.