



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:46 AM UTC

PDB ID : 1I5O / pdb_00001i5o
Title : CRYSTAL STRUCTURE OF MUTANT R105A OF E. COLI ASPARTATE
TRANSCARBAMOYLASE
Authors : Macol, C.P.; Tsuruta, H.; Stec, B.; Kantrowitz, E.R.
Deposited on : 2001-02-28
Resolution : 2.80 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

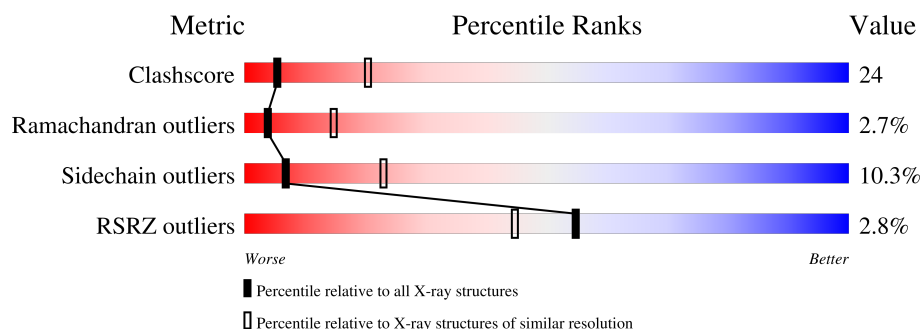
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	
1	C	310	
2	B	153	
2	D	153	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7534 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 TRANSCARBAMOYLASE CATALYTIC CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2409	1524	420	456	9			
1	C	310	Total	C	N	O	S	0	0	0
			2409	1524	420	456	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	ALA	ARG	engineered mutation	UNP P0A786
C	105	ALA	ARG	engineered mutation	UNP P0A786

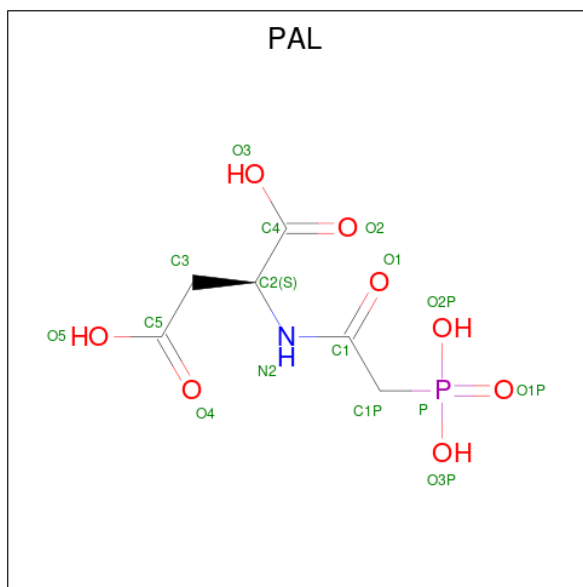
- Molecule 2 is a protein called ASPARTATE TRANSCARBAMOYLASE REGULATORY CHAIN.

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 ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is N-(PHOSPHONACETYL)-L-ASPARTIC ACID (CCD ID: PAL) (formula: C₆H₁₀NO₈P).



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

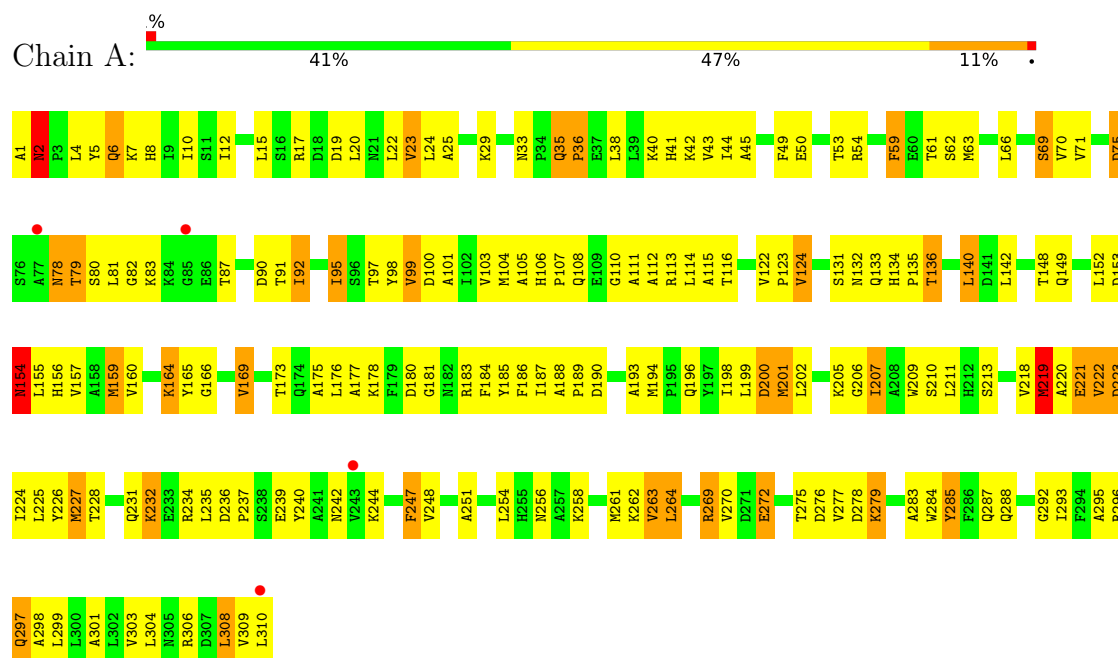
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	84	Total	O	0	0
			84	84		
5	B	55	Total	O	0	0
			55	55		
5	C	104	Total	O	0	0
			104	104		
5	D	53	Total	O	0	0
			53	53		

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.

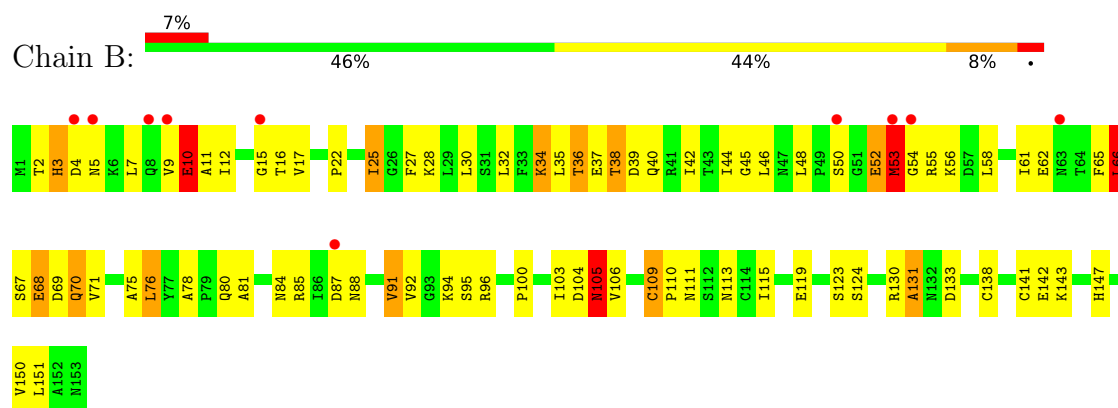
• Molecule 1: ASPARTATE TRANSCARBAMOYLASE CATALYTIC CHAIN



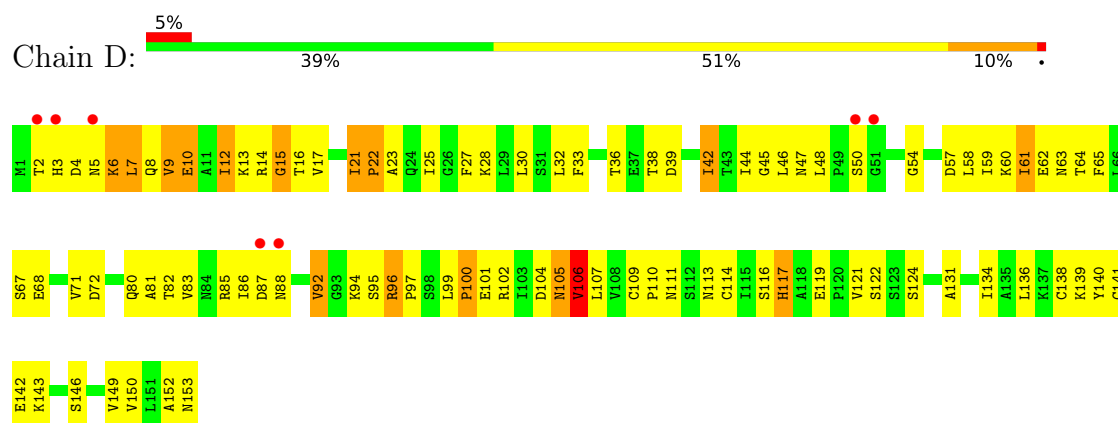
• Molecule 1: ASPARTATE TRANSCARBAMOYLASE CATALYTIC CHAIN



• Molecule 2: ASPARTATE TRANSCARBAMOYLASE REGULATORY CHAIN



• Molecule 2: ASPARTATE TRANSCARBAMOYLASE 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	122.25Å 122.25Å 142.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.80 10.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	77.0 (10.00-2.80) 90.4 (10.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 2.76Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.155 , 0.212 0.199 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7534	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.06	3/2455 (0.1%)	1.43	40/3332 (1.2%)
1	C	1.11	4/2455 (0.2%)	1.47	37/3332 (1.1%)
2	B	0.88	0/1219	1.30	11/1647 (0.7%)
2	D	0.85	0/1219	1.34	13/1647 (0.8%)
All	All	1.02	7/7348 (0.1%)	1.41	101/9958 (1.0%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	94	VAL	CA-CB	8.26	1.63	1.54
1	C	201	MET	SD-CE	7.85	1.99	1.79
1	A	132	ASN	CA-C	7.09	1.56	1.52
1	C	263	VAL	CA-CB	-5.33	1.48	1.54
1	A	219	MET	SD-CE	5.16	1.92	1.79
1	A	122	VAL	CA-CB	5.06	1.60	1.54
1	C	46	SER	CA-C	5.01	1.59	1.53

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	33	ASN	CA-C-N	14.50	134.71	119.78
1	C	33	ASN	C-N-CA	14.50	134.71	119.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLN	CA-C-N	11.76	131.56	119.56
1	A	35	GLN	C-N-CA	11.76	131.56	119.56
2	D	21	ILE	N-CA-C	-11.29	98.92	108.63
1	C	218	VAL	N-CA-C	10.06	122.56	112.90
1	C	255	HIS	N-CA-C	9.40	122.70	111.33
1	A	272	GLU	N-CA-C	9.15	121.26	111.28
2	B	119	GLU	N-CA-C	9.11	122.86	110.29
1	A	99	VAL	N-CA-C	8.96	122.01	109.29
1	C	180	ASP	N-CA-C	8.77	123.13	110.24
2	D	6	LYS	N-CA-C	-8.71	102.09	112.89
1	A	61	THR	N-CA-C	-7.92	102.58	111.14
1	A	220	ALA	N-CA-C	7.73	121.19	111.69
1	C	236	ASP	N-CA-C	-7.55	99.65	110.08
1	C	61	THR	N-CA-C	-7.30	103.25	111.14
2	B	109	CYS	CA-C-N	7.17	126.79	119.19
2	B	109	CYS	C-N-CA	7.17	126.79	119.19
1	C	122	VAL	CA-C-N	7.12	127.38	119.90
1	C	122	VAL	C-N-CA	7.12	127.38	119.90
1	C	196	GLN	N-CA-C	7.07	123.04	111.37
1	A	293	ILE	N-CA-C	7.07	117.15	110.30
1	C	78	ASN	N-CA-C	-7.04	104.67	113.18
1	A	222	VAL	N-CA-C	6.98	119.19	109.55
1	A	15	LEU	N-CA-C	6.89	119.35	108.67
2	D	109	CYS	CA-C-N	6.79	127.35	119.47
2	D	109	CYS	C-N-CA	6.79	127.35	119.47
1	C	265	HIS	CA-C-N	6.75	127.01	119.32
1	C	265	HIS	C-N-CA	6.75	127.01	119.32
1	C	50	GLU	N-CA-C	-6.74	97.42	108.41
2	D	62	GLU	N-CA-C	6.67	120.15	110.42
2	D	106	VAL	N-CA-C	6.51	117.26	110.62
1	A	279	LYS	N-CA-C	6.49	120.94	112.89
2	B	105	ASN	N-CA-C	6.47	124.58	110.80
1	C	193	ALA	N-CA-C	6.43	119.98	109.76
1	A	188	ALA	N-CA-C	6.41	113.99	108.22
1	C	106	HIS	CA-C-N	6.40	126.11	119.64
1	C	106	HIS	C-N-CA	6.40	126.11	119.64
1	C	207	ILE	N-CA-C	6.39	117.31	107.99
1	A	33	ASN	CA-C-N	6.31	126.53	119.90
1	A	33	ASN	C-N-CA	6.31	126.53	119.90
1	C	88	LEU	N-CA-C	-6.31	103.92	111.69
1	A	298	ALA	N-CA-C	-6.30	104.32	111.07
1	A	292	GLY	N-CA-C	-6.29	104.99	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	ASP	N-CA-C	-6.29	104.57	112.93
1	C	241	ALA	N-CA-C	6.16	118.79	111.71
2	B	15	GLY	N-CA-C	6.14	119.57	111.52
1	C	287	GLN	N-CA-C	-6.10	104.75	111.82
1	A	247	PHE	N-CA-C	6.07	121.15	111.81
1	C	2	ASN	CA-C-N	6.04	127.39	119.84
1	C	2	ASN	C-N-CA	6.04	127.39	119.84
1	A	70	VAL	N-CA-C	6.02	117.42	108.46
1	A	180	ASP	N-CA-C	6.02	119.63	109.76
1	A	263	VAL	CB-CA-C	-6.00	102.91	111.31
2	D	8	GLN	N-CA-C	5.91	119.28	109.46
1	C	133	GLN	N-CA-C	5.91	118.46	109.95
1	A	92	ILE	CB-CA-C	-5.88	104.34	112.04
1	C	222	VAL	N-CA-C	5.84	117.15	109.21
1	A	104	MET	N-CA-C	5.83	118.97	109.06
1	C	152	LEU	N-CA-C	-5.81	106.16	113.72
1	A	36	PRO	N-CA-C	5.79	121.36	113.84
2	D	109	CYS	N-CA-C	5.74	117.77	109.04
1	A	154	ASN	N-CA-C	5.69	122.92	110.80
1	A	193	ALA	N-CA-C	5.68	118.88	110.48
1	C	242	ASN	N-CA-C	5.62	117.21	111.14
1	A	50	GLU	N-CA-C	-5.61	99.37	108.52
2	B	38	THR	N-CA-C	5.58	117.27	110.41
1	A	295	ALA	N-CA-C	-5.58	105.35	111.82
1	A	132	ASN	N-CA-C	5.55	116.94	108.12
1	A	309	VAL	N-CA-C	5.51	120.79	109.34
1	C	71	VAL	N-CA-C	-5.44	100.64	108.42
1	C	184	PHE	N-CA-C	5.44	118.27	109.40
1	C	175	ALA	N-CA-C	-5.43	105.27	111.14
2	D	42	ILE	N-CA-C	-5.42	102.06	109.55
2	B	75	ALA	N-CA-C	5.32	118.87	112.38
1	A	23	VAL	N-CA-C	-5.32	105.32	110.42
1	A	206	GLY	N-CA-C	-5.32	105.66	114.48
1	A	223	ASP	N-CA-C	-5.31	105.87	112.93
2	B	66	LEU	N-CA-C	5.31	117.87	109.96
1	C	288	GLN	N-CA-C	-5.31	105.39	111.07
1	A	2	ASN	N-CA-C	5.29	121.49	109.81
2	B	106	VAL	CA-C-O	5.27	123.57	119.46
1	A	131	SER	N-CA-C	-5.26	106.62	112.57
1	A	87	THR	N-CA-C	5.26	118.06	110.28
1	A	242	ASN	N-CA-C	-5.22	105.27	111.69
2	B	4	ASP	N-CA-C	-5.21	101.75	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	117	HIS	N-CA-C	5.20	117.69	111.71
2	D	15	GLY	N-CA-C	5.18	118.33	110.97
1	C	269	ARG	N-CA-C	-5.17	102.81	110.46
2	B	150	VAL	N-CA-C	5.17	116.51	110.62
1	A	2	ASN	CA-C-N	5.16	124.61	119.24
1	A	2	ASN	C-N-CA	5.16	124.61	119.24
2	D	21	ILE	CB-CA-C	-5.14	106.16	110.94
1	A	164	LYS	N-CA-C	5.12	116.55	111.07
1	C	164	LYS	N-CA-C	5.11	116.66	111.14
1	C	31	LYS	N-CA-C	-5.07	106.35	112.54
1	C	286	PHE	N-CA-C	-5.07	105.41	112.45
1	A	269	ARG	N-CA-C	-5.05	102.58	110.42
2	D	22	PRO	N-CA-C	5.04	118.77	110.55
1	C	282	HIS	N-CA-C	-5.02	107.00	113.23
1	A	207	ILE	N-CA-C	5.00	115.79	108.58

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	226	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	2409	0	2414	123	0
1	C	2409	0	2414	105	0
2	B	1201	0	1219	63	0
2	D	1201	0	1219	75	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	B	16	0	6	2	0
5	A	84	0	0	5	0
5	B	55	0	0	3	0
5	C	104	0	0	6	0
5	D	53	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7534	0	7272	347	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 (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ILE:HD11	1:C:116:THR:HG21	1.47	0.96
1:C:23:VAL:HG11	1:C:139:LEU:HD13	1.50	0.91
2:B:45:GLY:HA3	2:B:48:LEU:HD11	1.56	0.87
2:D:9:VAL:HB	2:D:60:LYS:HZ1	1.39	0.87
2:B:133:ASP:HB2	2:B:147:HIS:HE1	1.40	0.85
1:C:45:ALA:HB2	1:C:99:VAL:HG11	1.58	0.85
1:C:4:LEU:HD12	1:C:302:LEU:HD13	1.59	0.84
2:D:96:ARG:HH21	2:D:96:ARG:HB2	1.41	0.83
2:B:105:ASN:HA	2:B:123:SER:OG	1.79	0.83
1:A:4:LEU:HA	1:A:7:LYS:HD3	1.60	0.82
1:C:254:LEU:HD11	1:C:277:VAL:HG13	1.62	0.81
1:C:232:LYS:HE2	1:C:232:LYS:H	1.45	0.81
1:C:164:LYS:HA	1:C:195:PRO:HD3	1.60	0.81
2:D:17:VAL:HG13	2:D:58:LEU:HD21	1.62	0.80
2:D:9:VAL:HB	2:D:60:LYS:NZ	1.95	0.80
1:A:29:LYS:HB3	1:A:310:LEU:HG	1.63	0.79
2:B:38:THR:HG22	2:B:42:ILE:HD11	1.64	0.79
2:B:133:ASP:HB2	2:B:147:HIS:CE1	2.17	0.79
1:C:279:LYS:H	1:C:279:LYS:HD2	1.48	0.78
2:D:45:GLY:HA3	2:D:48:LEU:HD11	1.66	0.77
1:A:10:ILE:HD11	1:A:116:THR:HG21	1.65	0.77
2:B:10:GLU:HA	2:D:7:LEU:O	1.84	0.76
1:A:160:VAL:HG21	1:A:225:LEU:HD11	1.66	0.76
1:C:31:LYS:HE3	1:C:291:ASN:ND2	2.01	0.75
1:A:19:ASP:O	1:A:23:VAL:HG23	1.87	0.75
2:B:30:LEU:HA	2:B:35:LEU:HD12	1.68	0.74
2:D:14:ARG:HA	2:D:87:ASP:HA	1.70	0.74
2:B:12:ILE:HD11	2:B:62:GLU:HB2	1.71	0.73
1:A:261:MET:HE1	1:A:263:VAL:HG22	1.68	0.73
1:A:189:PRO:HG3	1:A:247:PHE:CE2	2.24	0.72
1:C:189:PRO:HG3	1:C:192:LEU:HD12	1.70	0.72
1:A:209:TRP:HZ3	1:A:211:LEU:HG	1.54	0.71
2:D:111:ASN:O	2:D:117:HIS:HE1	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:GLY:HA2	5:A:371:HOH:O	1.92	0.70
1:C:242:ASN:HB2	5:C:322:HOH:O	1.92	0.70
1:A:116:THR:HG22	1:A:124:VAL:HG13	1.74	0.69
1:C:160:VAL:HG11	1:C:215:ILE:HD11	1.74	0.69
1:C:160:VAL:HG22	1:C:187:ILE:HB	1.75	0.69
1:A:219:MET:HG3	1:A:256:ASN:HB2	1.74	0.68
1:C:164:LYS:HE3	1:C:165:TYR:CZ	2.28	0.68
1:A:308:LEU:HD23	1:A:308:LEU:H	1.58	0.68
1:C:108:GLN:HA	2:D:113:ASN:ND2	2.09	0.68
1:A:45:ALA:HB2	1:A:99:VAL:HG11	1.77	0.67
1:C:185:TYR:CD2	1:C:218:VAL:HG11	2.28	0.67
2:B:38:THR:CG2	2:B:42:ILE:HD11	2.24	0.67
2:D:85:ARG:HB3	2:D:92:VAL:HG22	1.77	0.67
1:A:8:HIS:CD2	1:A:116:THR:HB	2.30	0.67
1:C:254:LEU:HD13	1:C:280:THR:HG21	1.77	0.67
2:B:91:VAL:HG21	4:B:998:PAL:O1	1.94	0.66
1:C:168:THR:HG23	5:C:343:HOH:O	1.95	0.66
2:D:12:ILE:HD13	2:D:12:ILE:H	1.60	0.66
1:C:44:ILE:HG13	1:C:101:ALA:HB3	1.77	0.66
1:C:136:THR:HG23	1:C:296:ARG:HH11	1.59	0.65
1:C:188:ALA:HB1	1:C:189:PRO:HD2	1.78	0.65
2:D:114:CYS:SG	2:D:116:SER:OG	2.45	0.65
1:A:160:VAL:CG2	1:A:225:LEU:HD11	2.26	0.65
1:A:269:ARG:HA	1:A:272:GLU:OE2	1.97	0.64
1:A:299:LEU:O	1:A:303:VAL:HG23	1.98	0.64
1:A:223:ASP:O	1:A:261:MET:HA	1.97	0.64
1:A:8:HIS:NE2	1:A:116:THR:HB	2.11	0.64
1:A:157:VAL:HG21	1:A:176:LEU:HD13	1.81	0.63
2:B:3:HIS:ND1	2:B:10:GLU:HB3	2.13	0.63
2:D:96:ARG:HB2	2:D:96:ARG:NH2	2.12	0.63
1:C:1:ALA:HB2	1:C:306:ARG:NH2	2.13	0.63
1:C:132:ASN:OD1	1:C:133:GLN:HG2	1.98	0.62
1:A:8:HIS:CE1	1:A:123:PRO:HA	2.34	0.62
1:C:185:TYR:CE2	1:C:218:VAL:HG11	2.35	0.62
1:A:275:THR:HG22	1:A:279:LYS:NZ	2.15	0.62
1:A:69:SER:HA	5:A:317:HOH:O	2.00	0.61
1:C:71:VAL:HA	5:C:315:HOH:O	1.99	0.61
1:C:170:HIS:CE1	1:C:195:PRO:HG3	2.36	0.61
1:C:203:ASP:HA	5:C:397:HOH:O	1.99	0.61
1:A:254:LEU:HD11	1:A:277:VAL:HG13	1.82	0.61
2:D:146:SER:HB3	2:D:149:VAL:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:GLN:NE2	1:C:234:ARG:HG3	2.17	0.60
2:B:65:PHE:HE2	2:B:85:ARG:HG3	1.66	0.60
1:A:106:HIS:ND1	1:A:107:PRO:HD2	2.16	0.60
2:D:67:SER:O	2:D:71:VAL:HG23	2.02	0.60
2:D:139:LYS:HD3	2:D:140:TYR:CZ	2.37	0.59
2:B:10:GLU:HG2	2:D:5:ASN:HD21	1.67	0.59
1:A:261:MET:SD	1:A:261:MET:C	2.86	0.59
1:C:13:ASN:HD21	1:C:174:GLN:NE2	1.99	0.59
1:C:24:LEU:HD12	1:C:152:LEU:HD11	1.85	0.59
2:D:83:VAL:HB	2:D:95:SER:HB2	1.85	0.59
2:D:10:GLU:O	2:D:60:LYS:HE2	2.03	0.58
1:A:156:HIS:CD2	1:A:183:ARG:HD3	2.38	0.58
2:B:28:LYS:O	2:B:32:LEU:HB2	2.03	0.58
2:B:42:ILE:HB	2:D:46:LEU:HB2	1.85	0.58
2:B:67:SER:O	2:B:71:VAL:HG23	2.04	0.58
1:A:201:MET:HE3	1:A:205:LYS:HD3	1.84	0.58
1:C:75:ASP:CG	1:C:76:SER:H	2.11	0.58
2:B:76:LEU:HD22	2:B:151:LEU:HD11	1.86	0.58
1:C:231:GLN:HE22	1:C:234:ARG:HG3	1.68	0.58
1:A:42:LYS:HA	1:A:100:ASP:OD2	2.04	0.57
1:C:189:PRO:CG	1:C:192:LEU:HD12	2.34	0.57
2:B:22:PRO:HG2	2:B:25:ILE:HG13	1.87	0.57
1:C:160:VAL:HG21	1:C:215:ILE:HG12	1.86	0.57
1:A:148:THR:HG21	1:A:262:LYS:HG3	1.86	0.57
1:C:114:LEU:HD11	2:D:119:GLU:HB2	1.87	0.57
2:B:66:LEU:HD23	2:B:66:LEU:N	2.20	0.56
1:C:138:THR:O	1:C:141:ASP:HB2	2.05	0.56
1:C:140:LEU:HD22	1:C:292:GLY:HA2	1.88	0.56
2:D:136:LEU:HD12	2:D:150:VAL:HG21	1.87	0.56
1:A:285:TYR:O	1:A:288:GLN:HB3	2.06	0.56
1:C:132:ASN:HD21	2:D:142:GLU:HG3	1.71	0.56
1:C:137:GLN:O	1:C:140:LEU:HG	2.06	0.56
2:D:16:THR:OG1	2:D:65:PHE:HA	2.05	0.56
1:A:154:ASN:HA	1:A:181:GLY:O	2.05	0.56
2:D:116:SER:HA	2:D:121:VAL:HG21	1.87	0.56
1:A:106:HIS:CG	1:A:107:PRO:HD2	2.41	0.56
1:A:66:LEU:HG	1:A:297:GLN:HE21	1.71	0.55
1:A:63:MET:HE2	1:A:103:VAL:HG21	1.87	0.55
2:D:6:LYS:O	2:D:7:LEU:HG	2.05	0.55
1:C:5:TYR:O	1:C:7:LYS:HG2	2.06	0.55
1:A:44:ILE:HD13	1:A:63:MET:HG2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:VAL:O	1:A:222:VAL:HG23	2.07	0.54
1:A:149:GLN:HE21	1:A:224:ILE:HD11	1.73	0.54
2:D:99:LEU:HD11	2:D:134:ILE:HD13	1.89	0.54
2:B:80:GLN:NE2	2:B:96:ARG:HH12	2.05	0.54
2:D:71:VAL:HG13	2:D:83:VAL:HG21	1.89	0.54
1:C:114:LEU:HD11	2:D:119:GLU:CB	2.38	0.54
1:A:239:GLU:HB3	5:A:339:HOH:O	2.07	0.54
2:B:130:ARG:HG2	2:B:131:ALA:H	1.72	0.54
1:A:159:MET:HE3	1:A:173:THR:OG1	2.08	0.53
1:A:308:LEU:HD23	1:A:308:LEU:N	2.23	0.53
1:C:24:LEU:HD11	1:C:142:LEU:HB3	1.89	0.53
1:C:130:GLY:O	1:C:167:ARG:HD3	2.08	0.53
1:A:202:LEU:HD22	1:A:207:ILE:HG21	1.91	0.53
1:A:275:THR:HG22	1:A:279:LYS:HZ2	1.74	0.53
2:D:13:LYS:O	2:D:86:ILE:HG22	2.09	0.53
1:A:111:ALA:HA	2:B:115:ILE:HG12	1.89	0.53
1:A:92:ILE:HG21	1:A:115:ALA:O	2.09	0.53
1:A:201:MET:HE2	1:A:202:LEU:HA	1.90	0.53
1:C:293:ILE:O	1:C:297:GLN:HG3	2.09	0.52
1:A:116:THR:HG22	1:A:124:VAL:CG1	2.39	0.52
1:A:142:LEU:HD23	1:A:152:LEU:HD22	1.90	0.52
1:A:189:PRO:HG3	1:A:247:PHE:HE2	1.74	0.52
2:D:42:ILE:HD12	2:D:42:ILE:H	1.75	0.52
1:C:233:GLU:C	1:C:235:LEU:H	2.17	0.52
1:A:8:HIS:ND1	1:A:123:PRO:HA	2.25	0.52
2:B:78:ALA:HB1	2:B:81:ALA:HB2	1.91	0.52
2:B:48:LEU:O	2:B:56:LYS:HG2	2.10	0.51
1:A:184:PHE:HB3	1:A:186:PHE:CE1	2.46	0.51
2:D:16:THR:HG1	2:D:65:PHE:HA	1.75	0.51
1:A:275:THR:O	1:A:278:ASP:HB2	2.09	0.51
1:C:249:LEU:HD23	1:C:277:VAL:HG11	1.91	0.51
1:A:25:ALA:O	1:A:29:LYS:HG3	2.10	0.51
1:A:101:ALA:HB2	1:A:304:LEU:HD21	1.91	0.51
2:B:91:VAL:CG2	4:B:998:PAL:O1	2.58	0.51
2:D:25:ILE:O	2:D:28:LYS:HB2	2.10	0.51
2:D:99:LEU:CD1	2:D:134:ILE:HD13	2.41	0.51
2:D:38:THR:CG2	2:D:42:ILE:HD11	2.41	0.51
2:B:50:SER:HB2	2:B:56:LYS:HD3	1.92	0.51
2:D:22:PRO:HD3	2:D:80:GLN:HE22	1.74	0.51
1:A:44:ILE:CD1	1:A:63:MET:HG2	2.41	0.51
2:D:12:ILE:HD13	2:D:12:ILE:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ARG:HH22	1:C:252:SER:HB2	1.76	0.50
1:C:269:ARG:HA	1:C:272:GLU:OE1	2.12	0.50
2:B:76:LEU:HD21	2:B:147:HIS:HD2	1.76	0.50
1:C:13:ASN:HD21	1:C:174:GLN:HE22	1.58	0.50
2:D:59:ILE:HG22	2:D:61:ILE:HG12	1.93	0.50
2:D:30:LEU:HD22	2:D:36:THR:CG2	2.42	0.50
1:A:196:GLN:O	1:A:200:ASP:HB2	2.12	0.50
2:B:11:ALA:O	2:D:7:LEU:HD22	2.11	0.50
1:C:23:VAL:HG11	1:C:139:LEU:CD1	2.33	0.50
2:B:36:THR:HG21	2:D:27:PHE:CG	2.46	0.50
1:C:1:ALA:HB2	1:C:306:ARG:CZ	2.42	0.50
1:C:272:GLU:CD	1:C:272:GLU:H	2.19	0.50
2:B:27:PHE:CD1	2:D:36:THR:HG21	2.46	0.50
2:D:81:ALA:O	2:D:97:PRO:HD3	2.11	0.50
1:A:79:THR:C	1:A:81:LEU:H	2.20	0.50
1:A:97:THR:O	1:A:98:TYR:HD1	1.95	0.50
1:C:140:LEU:HD22	1:C:292:GLY:CA	2.42	0.50
1:A:201:MET:HE2	1:A:201:MET:C	2.37	0.49
2:B:94:LYS:HD3	5:B:1039:HOH:O	2.11	0.49
1:C:239:GLU:HA	5:C:322:HOH:O	2.12	0.49
2:D:17:VAL:CG1	2:D:58:LEU:HD21	2.37	0.49
1:A:264:LEU:HB3	1:A:288:GLN:NE2	2.27	0.49
2:D:58:LEU:HD13	2:D:60:LYS:NZ	2.27	0.49
2:D:124:SER:HB3	2:D:139:LYS:HD2	1.93	0.49
1:C:47:CYS:O	1:C:104:MET:HA	2.12	0.49
1:A:2:ASN:HB3	1:A:308:LEU:HD22	1.94	0.49
2:B:52:GLU:O	2:B:53:MET:HB2	2.12	0.49
1:A:17:ARG:HD2	1:A:178:LYS:O	2.12	0.49
1:C:76:SER:HA	1:C:79:THR:HB	1.95	0.49
1:C:125:LEU:HD22	1:C:299:LEU:HD23	1.95	0.49
1:A:140:LEU:HD23	1:A:140:LEU:C	2.38	0.49
1:A:80:SER:C	1:A:82:GLY:H	2.20	0.49
1:C:279:LYS:H	1:C:279:LYS:CD	2.24	0.49
2:D:101:GLU:HG3	2:D:102:ARG:N	2.27	0.49
2:B:130:ARG:HG2	2:B:131:ALA:N	2.28	0.48
1:A:53:THR:O	1:A:54:ARG:C	2.55	0.48
2:B:16:THR:HG21	2:B:66:LEU:HG	1.95	0.48
2:B:61:ILE:HD11	2:B:66:LEU:HD21	1.96	0.48
1:C:184:PHE:O	1:C:209:TRP:HA	2.14	0.48
1:A:134:HIS:N	1:A:135:PRO:HD3	2.29	0.48
1:A:156:HIS:HB3	1:A:185:TYR:HE1	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:GLU:CD	2:B:68:GLU:H	2.21	0.48
1:C:1:ALA:HB2	1:C:306:ARG:HH22	1.78	0.48
2:B:65:PHE:CE2	2:B:85:ARG:HG3	2.47	0.48
2:B:76:LEU:HD12	2:B:103:ILE:CD1	2.44	0.48
2:D:111:ASN:O	2:D:117:HIS:CE1	2.60	0.48
2:D:32:LEU:HB2	2:D:33:PHE:CD2	2.49	0.47
1:C:79:THR:HG22	1:C:81:LEU:H	1.80	0.47
1:C:87:THR:HB	2:D:119:GLU:OE2	2.13	0.47
1:A:251:ALA:O	1:A:254:LEU:HB2	2.14	0.47
1:A:20:LEU:O	1:A:24:LEU:HG	2.14	0.47
1:A:166:GLY:O	1:A:169:VAL:HG22	2.15	0.47
1:C:139:LEU:HD23	1:C:139:LEU:HA	1.50	0.47
2:D:15:GLY:N	2:D:86:ILE:O	2.48	0.46
1:A:175:ALA:HA	1:A:178:LYS:HD2	1.97	0.46
2:D:14:ARG:HB2	2:D:63:ASN:OD1	2.15	0.46
1:A:38:LEU:HD21	1:A:301:ALA:HB1	1.97	0.46
1:A:221:GLU:HG2	5:A:391:HOH:O	2.15	0.46
1:C:201:MET:SD	1:C:201:MET:C	2.98	0.46
1:A:227:MET:HE3	1:A:227:MET:HB3	1.79	0.46
1:A:269:ARG:HH12	1:A:278:ASP:CG	2.23	0.46
1:A:153:ASP:O	1:A:155:LEU:N	2.48	0.46
2:D:21:ILE:HB	2:D:57:ASP:HB2	1.96	0.46
1:A:189:PRO:HG3	1:A:247:PHE:CD2	2.50	0.46
2:B:17:VAL:CG2	2:B:84:ASN:HB2	2.45	0.46
2:D:44:ILE:N	2:D:44:ILE:HD12	2.30	0.46
2:D:82:THR:HB	2:D:94:LYS:HE2	1.97	0.46
2:B:58:LEU:HD23	2:B:58:LEU:C	2.40	0.46
2:D:38:THR:HG22	2:D:42:ILE:HD11	1.98	0.46
1:A:205:LYS:HB3	1:A:207:ILE:HG13	1.97	0.46
1:A:251:ALA:HB3	1:A:276:ASP:HB3	1.98	0.46
2:B:76:LEU:HD12	2:B:103:ILE:HD13	1.97	0.46
1:A:232:LYS:O	1:A:235:LEU:HB2	2.16	0.45
1:C:5:TYR:CE1	1:C:6:GLN:HG2	2.51	0.45
2:D:46:LEU:O	2:D:47:ASN:HB2	2.15	0.45
1:C:44:ILE:HD12	1:C:44:ILE:N	2.31	0.45
1:A:78:ASN:O	1:A:80:SER:N	2.49	0.45
1:A:194:MET:HB3	5:A:324:HOH:O	2.15	0.45
1:A:231:GLN:OE1	1:A:231:GLN:HA	2.17	0.45
1:A:236:ASP:H	1:A:239:GLU:HG2	1.82	0.45
1:C:20:LEU:HD23	1:C:20:LEU:HA	1.54	0.45
2:B:67:SER:C	2:B:69:ASP:N	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:VAL:HG12	1:A:223:ASP:N	2.31	0.45
1:C:298:ALA:O	1:C:302:LEU:HG	2.16	0.45
1:A:40:LYS:HE3	1:A:41:HIS:NE2	2.32	0.45
1:A:108:GLN:HB3	2:B:113:ASN:O	2.17	0.45
2:B:141:CYS:O	2:B:142:GLU:HB2	2.16	0.45
1:C:20:LEU:O	1:C:24:LEU:HG	2.17	0.45
2:D:15:GLY:HA2	2:D:64:THR:H	1.81	0.45
1:A:235:LEU:HD13	1:A:240:TYR:HD2	1.82	0.45
2:B:109:CYS:SG	2:B:111:ASN:HB3	2.56	0.45
1:C:154:ASN:HA	1:C:181:GLY:O	2.17	0.45
2:D:138:CYS:SG	2:D:140:TYR:HB2	2.57	0.45
1:A:20:LEU:N	1:A:20:LEU:HD23	2.32	0.45
2:D:30:LEU:HD22	2:D:36:THR:HG22	1.99	0.45
1:C:66:LEU:HD23	1:C:66:LEU:HA	1.73	0.44
1:C:12:ILE:C	1:C:14:ASP:H	2.25	0.44
1:C:114:LEU:HD12	2:D:121:VAL:HG11	2.00	0.44
1:A:154:ASN:HA	1:A:181:GLY:C	2.41	0.44
1:A:251:ALA:HA	1:A:254:LEU:HD12	1.99	0.44
1:A:5:TYR:O	1:A:6:GLN:HB2	2.17	0.44
1:A:59:PHE:O	1:A:62:SER:HB2	2.18	0.44
1:C:8:HIS:HB2	1:C:10:ILE:CD1	2.47	0.44
1:C:270:VAL:HG23	1:C:271:ASP:N	2.32	0.44
2:D:141:CYS:SG	2:D:143:LYS:HB2	2.57	0.44
1:A:164:LYS:HD3	1:A:165:TYR:CE2	2.53	0.44
2:B:12:ILE:CD1	2:B:62:GLU:HB2	2.46	0.44
2:B:104:ASP:C	2:B:105:ASN:OD1	2.61	0.44
1:C:265:HIS:HA	1:C:266:PRO:HD2	1.82	0.44
2:B:30:LEU:HD11	2:B:44:ILE:HG12	2.00	0.44
1:C:232:LYS:H	1:C:232:LYS:CE	2.24	0.44
1:A:63:MET:CE	1:A:103:VAL:HG21	2.48	0.43
1:A:198:ILE:HD13	1:A:198:ILE:HA	1.87	0.43
2:D:146:SER:O	2:D:149:VAL:N	2.49	0.43
1:A:35:GLN:HG3	1:A:310:LEU:HD22	2.00	0.43
1:C:86:GLU:HG2	1:C:87:THR:N	2.32	0.43
1:A:66:LEU:CD2	1:A:297:GLN:NE2	2.82	0.43
1:C:114:LEU:CD1	2:D:119:GLU:HG3	2.48	0.43
1:A:136:THR:OG1	1:A:296:ARG:NE	2.51	0.43
1:A:177:ALA:HB1	1:A:201:MET:HE1	2.00	0.43
1:A:232:LYS:H	1:A:232:LYS:HG3	1.43	0.43
1:A:199:LEU:HD22	1:A:209:TRP:CE2	2.54	0.43
2:B:9:VAL:HG12	2:D:7:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:THR:O	1:A:95:ILE:HG12	2.19	0.43
2:B:54:GLY:O	2:B:55:ARG:HG3	2.19	0.43
1:A:66:LEU:CG	1:A:297:GLN:HE21	2.32	0.43
1:C:39:LEU:HD23	1:C:39:LEU:HA	1.81	0.43
2:B:22:PRO:HG2	2:B:25:ILE:CG1	2.49	0.42
2:D:105:ASN:OD1	2:D:122:SER:HB3	2.19	0.42
1:A:4:LEU:CD1	1:A:22:LEU:HD23	2.48	0.42
1:C:31:LYS:HE3	1:C:291:ASN:HD21	1.81	0.42
1:C:170:HIS:O	1:C:174:GLN:HG3	2.19	0.42
1:C:114:LEU:HD11	2:D:119:GLU:HG3	2.01	0.42
2:D:136:LEU:HD12	2:D:150:VAL:CG2	2.49	0.42
1:A:133:GLN:HB3	1:A:135:PRO:HD3	2.01	0.42
1:C:127:ALA:O	1:C:134:HIS:CD2	2.73	0.42
2:D:104:ASP:O	2:D:106:VAL:N	2.50	0.42
1:A:201:MET:HE2	1:A:201:MET:O	2.20	0.42
1:C:308:LEU:HD13	1:C:310:LEU:HD12	2.02	0.42
1:A:272:GLU:CD	1:A:272:GLU:H	2.28	0.42
2:B:10:GLU:CG	2:D:5:ASN:HD21	2.31	0.42
2:B:69:ASP:O	2:B:70:GLN:C	2.62	0.42
1:A:112:ALA:O	1:A:115:ALA:HB3	2.20	0.42
1:C:240:TYR:O	1:C:244:LYS:HB2	2.19	0.42
1:C:250:ARG:NH2	1:C:252:SER:HB2	2.34	0.42
1:C:163:LEU:HG	1:C:188:ALA:HB2	2.01	0.42
1:C:166:GLY:O	1:C:170:HIS:CD2	2.73	0.41
1:C:194:MET:HA	1:C:195:PRO:HD2	1.87	0.41
1:C:279:LYS:HD2	1:C:279:LYS:N	2.25	0.41
2:D:72:ASP:HB3	2:D:100:PRO:HB3	2.02	0.41
1:A:81:LEU:HA	1:A:83:LYS:NZ	2.36	0.41
2:B:138:CYS:O	2:B:142:GLU:HA	2.21	0.41
1:C:299:LEU:HD12	1:C:299:LEU:HA	1.90	0.41
1:A:5:TYR:CD2	1:A:306:ARG:HA	2.55	0.41
1:A:35:GLN:HA	1:A:36:PRO:HD3	1.81	0.41
1:C:162:ASP:CG	1:C:192:LEU:HD22	2.45	0.41
1:A:45:ALA:HA	1:A:71:VAL:O	2.20	0.41
2:B:67:SER:C	2:B:69:ASP:H	2.28	0.41
2:B:92:VAL:HG12	2:B:92:VAL:O	2.21	0.41
1:C:114:LEU:O	1:C:118:PHE:HD1	2.04	0.41
1:A:49:PHE:HB2	1:A:105:ALA:O	2.21	0.41
2:B:34:LYS:HB3	2:B:37:GLU:HG2	2.02	0.41
2:B:39:ASP:HB3	5:B:1022:HOH:O	2.20	0.41
1:C:249:LEU:HA	1:C:249:LEU:HD12	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASN:HA	1:C:294:PHE:HD2	1.85	0.41
1:A:4:LEU:HG	1:A:22:LEU:HD23	2.03	0.41
2:B:109:CYS:HA	2:B:110:PRO:HD3	1.70	0.41
2:B:143:LYS:HD3	5:B:1046:HOH:O	2.21	0.41
1:C:8:HIS:HB2	1:C:10:ILE:HD12	2.02	0.41
1:C:233:GLU:C	1:C:235:LEU:N	2.77	0.41
1:C:308:LEU:HA	1:C:308:LEU:HD23	1.51	0.41
1:A:209:TRP:CZ3	1:A:211:LEU:HG	2.44	0.41
1:A:225:LEU:HG	1:A:263:VAL:HG13	2.03	0.41
1:A:277:VAL:O	1:A:283:ALA:HB2	2.21	0.41
1:C:159:MET:CE	1:C:172:LEU:HD23	2.51	0.41
1:C:196:GLN:HG3	5:C:367:HOH:O	2.21	0.41
2:B:87:ASP:O	2:B:88:ASN:HB3	2.21	0.40
1:A:114:LEU:O	1:A:115:ALA:C	2.65	0.40
2:B:46:LEU:HD12	2:D:42:ILE:HB	2.02	0.40
1:C:156:HIS:ND1	1:C:221:GLU:O	2.54	0.40
2:D:101:GLU:HB3	5:D:450:HOH:O	2.21	0.40
2:D:106:VAL:HG23	2:D:107:LEU:HG	2.02	0.40
1:A:1:ALA:CB	1:A:306:ARG:HG2	2.51	0.40
1:A:113:ARG:O	1:A:114:LEU:C	2.64	0.40
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.66	0.40
1:A:209:TRP:HZ3	1:A:211:LEU:CG	2.28	0.40
1:A:284:TRP:CE2	1:A:287:GLN:HG2	2.57	0.40
2:B:80:GLN:HA	2:B:96:ARG:HH11	1.86	0.40
1:C:108:GLN:HG2	5:D:417:HOH:O	2.21	0.40
1:C:274:ALA:HB3	1:C:277:VAL:HG23	2.04	0.40
2:D:50:SER:O	2:D:54:GLY:N	2.54	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	308/310 (99%)	269 (87%)	34 (11%)	5 (2%)	7	27
1	C	308/310 (99%)	269 (87%)	36 (12%)	3 (1%)	12	38
2	B	151/153 (99%)	117 (78%)	26 (17%)	8 (5%)	1	5
2	D	151/153 (99%)	123 (82%)	19 (13%)	9 (6%)	1	3
All	All	918/926 (99%)	778 (85%)	115 (12%)	25 (3%)	4	15

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	154	ASN
2	B	5	ASN
2	B	10	GLU
2	B	105	ASN
2	B	131	ALA
2	D	9	VAL
2	D	105	ASN
2	D	131	ALA
1	A	270	VAL
1	C	132	ASN
2	D	23	ALA
1	A	75	ASP
2	B	2	THR
2	B	53	MET
1	C	85	GLY
2	D	7	LEU
1	A	244	LYS
2	B	7	LEU
2	B	100	PRO
2	D	3	HIS
2	D	10	GLU
2	D	152	ALA
1	C	134	HIS
2	D	100	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	260/260 (100%)	226 (87%)	34 (13%)	4	14
1	C	260/260 (100%)	239 (92%)	21 (8%)	11	33
2	B	137/137 (100%)	122 (89%)	15 (11%)	6	21
2	D	137/137 (100%)	125 (91%)	12 (9%)	9	29
All	All	794/794 (100%)	712 (90%)	82 (10%)	7	23

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	6	GLN
1	A	12	ILE
1	A	43	VAL
1	A	59	PHE
1	A	69	SER
1	A	75	ASP
1	A	78	ASN
1	A	90	ASP
1	A	95	ILE
1	A	124	VAL
1	A	136	THR
1	A	140	LEU
1	A	159	MET
1	A	169	VAL
1	A	187	ILE
1	A	190	ASP
1	A	200	ASP
1	A	201	MET
1	A	210	SER
1	A	213	SER
1	A	219	MET
1	A	221	GLU
1	A	227	MET
1	A	228	THR
1	A	232	LYS
1	A	234	ARG
1	A	237	PRO
1	A	248	VAL
1	A	258	LYS
1	A	264	LEU

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Mol	Chain	Res	Type
1	A	285	TYR
1	A	297	GLN
1	A	308	LEU
2	B	3	HIS
2	B	10	GLU
2	B	25	ILE
2	B	34	LYS
2	B	36	THR
2	B	40	GLN
2	B	52	GLU
2	B	53	MET
2	B	66	LEU
2	B	68	GLU
2	B	70	GLN
2	B	76	LEU
2	B	91	VAL
2	B	95	SER
2	B	124	SER
1	C	7	LYS
1	C	10	ILE
1	C	38	LEU
1	C	59	PHE
1	C	74	SER
1	C	90	ASP
1	C	98	TYR
1	C	159	MET
1	C	171	SER
1	C	205	LYS
1	C	216	GLU
1	C	218	VAL
1	C	227	MET
1	C	231	GLN
1	C	232	LYS
1	C	238	SER
1	C	256	ASN
1	C	279	LYS
1	C	285	TYR
1	C	305	ASN
1	C	309	VAL
2	D	2	THR
2	D	4	ASP
2	D	12	ILE

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Mol	Chain	Res	Type
2	D	39	ASP
2	D	61	ILE
2	D	68	GLU
2	D	88	ASN
2	D	92	VAL
2	D	96	ARG
2	D	106	VAL
2	D	110	PRO
2	D	153	ASN

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	2	ASN
1	A	13	ASN
1	A	21	ASN
1	A	108	GLN
1	A	149	GLN
1	A	246	GLN
1	A	260	ASN
1	A	297	GLN
1	A	305	ASN
2	B	8	GLN
2	B	24	GLN
2	B	40	GLN
2	B	73	GLN
2	B	80	GLN
2	B	84	ASN
2	B	147	HIS
1	C	13	ASN
1	C	33	ASN
1	C	108	GLN
1	C	154	ASN
1	C	231	GLN
1	C	291	ASN
2	D	111	ASN
2	D	117	HIS
2	D	153	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
4	PAL	B	998	-	15,15,15	2.63	4 (26%)	20,21,21	1.14	1 (5%)

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
4	PAL	B	998	-	-	12/17/17/17	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	998	PAL	P-C1P	7.68	1.91	1.79
4	B	998	PAL	P-O1P	4.58	1.59	1.50
4	B	998	PAL	P-O2P	2.60	1.60	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	998	PAL	P-O3P	2.10	1.59	1.55

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	PAL	O3P-P-C1P	2.99	113.11	106.84

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	998	PAL	C1-C1P-P-O1P
4	B	998	PAL	C4-C2-C3-C5
4	B	998	PAL	C1-C1P-P-O2P
4	B	998	PAL	N2-C2-C3-C5
4	B	998	PAL	C2-C3-C5-O5
4	B	998	PAL	C2-C3-C5-O4
4	B	998	PAL	C1-C1P-P-O3P
4	B	998	PAL	N2-C2-C4-O3
4	B	998	PAL	N2-C2-C4-O2
4	B	998	PAL	C3-C2-C4-O2
4	B	998	PAL	O1-C1-C1P-P
4	B	998	PAL	C3-C2-C4-O3

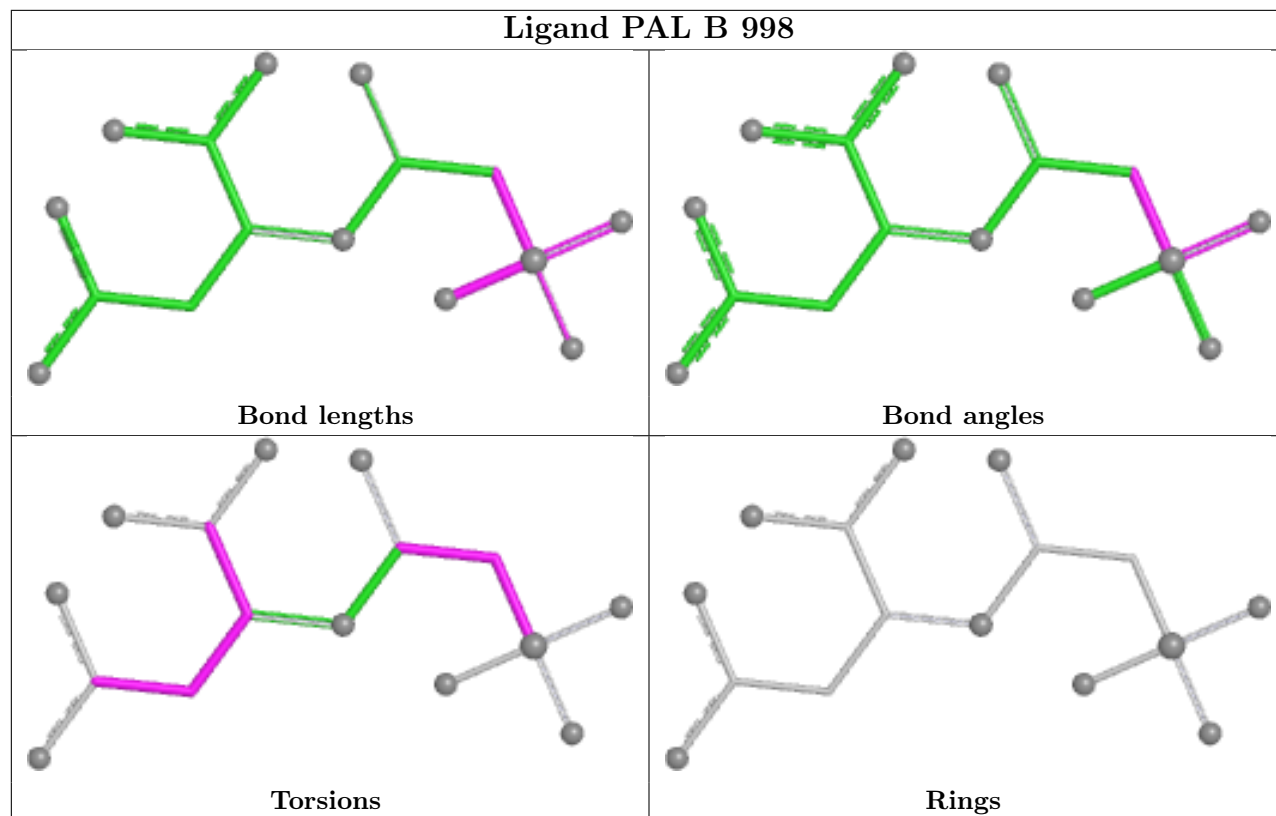
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	998	PAL	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 [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%)	-0.29	4 (1%) 75 66	2, 13, 85, 102	0
1	C	310/310 (100%)	-0.42	5 (1%) 70 61	2, 9, 75, 102	0
2	B	153/153 (100%)	0.31	10 (6%) 25 18	4, 41, 100, 103	0
2	D	153/153 (100%)	0.33	7 (4%) 37 29	4, 41, 100, 107	0
All	All	926/926 (100%)	-0.13	26 (2%) 55 45	2, 19, 94, 107	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	3	HIS	5.4
2	B	9	VAL	4.5
2	D	2	THR	4.1
2	B	8	GLN	4.0
2	D	5	ASN	3.7
2	B	50	SER	3.6
2	D	88	ASN	3.0
1	C	78	ASN	2.9
2	D	51	GLY	2.5
1	A	310	LEU	2.5
1	C	79	THR	2.5
2	D	87	ASP	2.5
1	C	242	ASN	2.5
2	B	4	ASP	2.4
2	D	50	SER	2.4
2	B	15	GLY	2.3
2	B	5	ASN	2.2
1	A	85	GLY	2.2
2	B	53	MET	2.2
1	A	77	ALA	2.2
2	B	63	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	87	ASP	2.1
1	C	243	VAL	2.1
1	C	236	ASP	2.1
2	B	54	GLY	2.1
1	A	243	VAL	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](#)

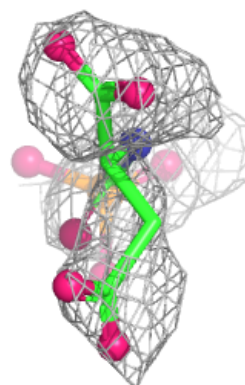
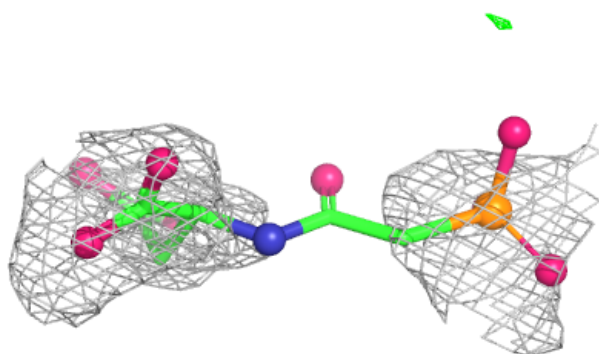
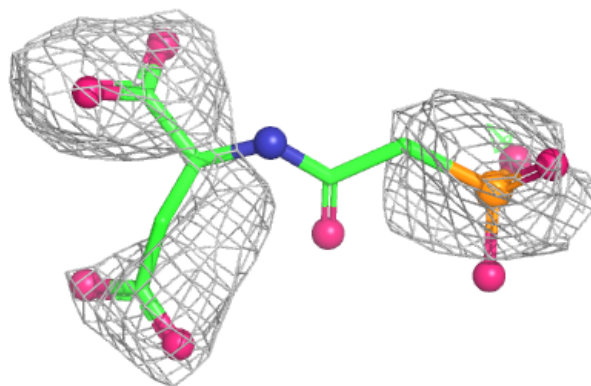
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PAL	B	998	16/16	0.57	0.14	67,77,94,95	16
3	ZN	D	409	1/1	0.98	0.04	2,2,2,2	0
3	ZN	B	309	1/1	0.98	0.05	2,2,2,2	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 B 998:

$2mF_o-DF_c$ (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.