



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:42 AM UTC

PDB ID : 8FJ7 / pdb_00008fj7
Title : LSD1-CoREST in complex with T108 and SNAG peptide
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2022-12-19
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

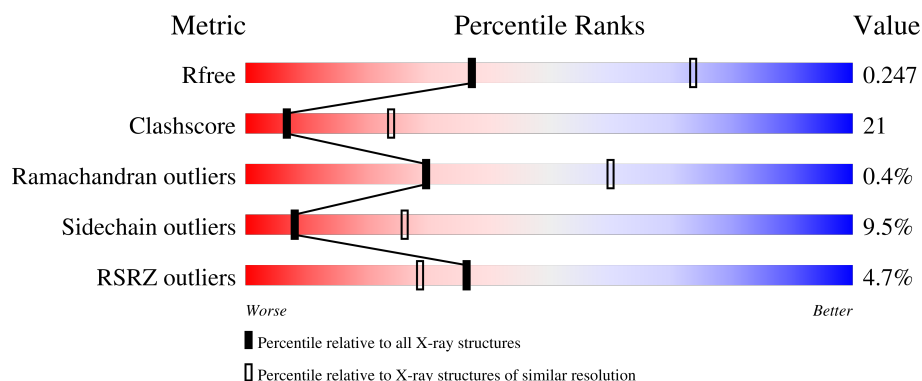
1 Overall quality at a glance

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))
R_{free}	180053	3866 (2.80-2.80)
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	871	3% 55% 19% • 24%
2	B	144	8% 53% 28% 10% • 8%
3	C	9	44% 11% 11% 22% 56%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6400 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 Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	666	Total	C	N	O	S	0	0	0
			5217	3324	906	967	20			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP O60341
A	-17	SER	-	expression tag	UNP O60341
A	-16	SER	-	expression tag	UNP O60341
A	-15	HIS	-	expression tag	UNP O60341
A	-14	HIS	-	expression tag	UNP O60341
A	-13	HIS	-	expression tag	UNP O60341
A	-12	HIS	-	expression tag	UNP O60341
A	-11	HIS	-	expression tag	UNP O60341
A	-10	HIS	-	expression tag	UNP O60341
A	-9	SER	-	expression tag	UNP O60341
A	-8	SER	-	expression tag	UNP O60341
A	-7	GLY	-	expression tag	UNP O60341
A	-6	LEU	-	expression tag	UNP O60341
A	-5	VAL	-	expression tag	UNP O60341
A	-4	PRO	-	expression tag	UNP O60341
A	-3	ARG	-	expression tag	UNP O60341
A	-2	GLY	-	expression tag	UNP O60341
A	-1	SER	-	expression tag	UNP O60341
A	0	HIS	-	expression tag	UNP O60341

- Molecule 2 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1076	676	194	203	3			

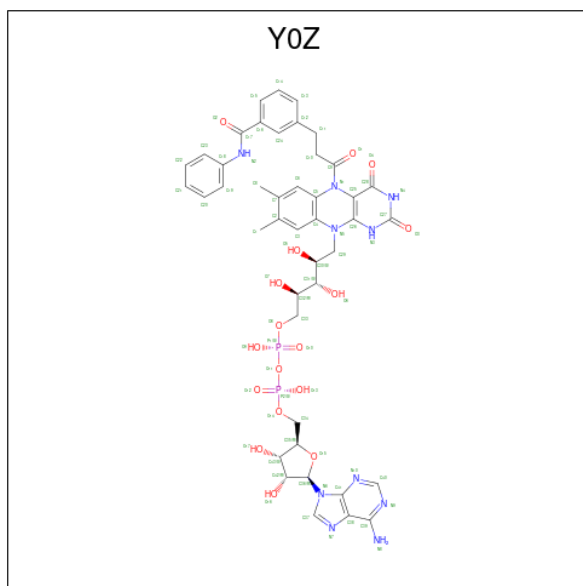
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	GLY	-	expression tag	UNP Q9UKL0
B	298	PRO	-	expression tag	UNP Q9UKL0
B	299	LEU	-	expression tag	UNP Q9UKL0
B	300	GLY	-	expression tag	UNP Q9UKL0
B	301	SER	-	expression tag	UNP Q9UKL0
B	302	PRO	-	expression tag	UNP Q9UKL0
B	303	GLU	-	expression tag	UNP Q9UKL0
B	304	PHE	-	expression tag	UNP Q9UKL0

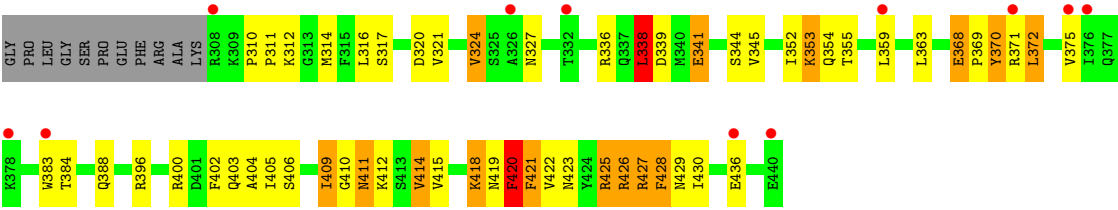
- Molecule 3 is a protein called Zinc finger protein SNAI1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total	C	N	O	0	0	0
			35	23	7	5			

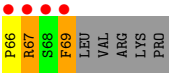
- Molecule 4 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl (2R,3S,4S)-5-[7,8-dimethyl-2,4-dioxo-5-{3-[3-(phenylcarbamoyl)phenyl]propanoyl}-1,3,4,5-tetrahydrobenzo[g]pteridin-10(2H)-yl]-2,3,4-trihydroxypentyl dihydrogen diphosphate (CCD ID: Y0Z) (formula: C₄₃H₄₈N₁₀O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	
			72	43	10	17	2	



● Molecule 3: Zinc finger protein SNAI1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.54Å 179.04Å 234.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.80 48.58 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.58-2.80) 99.3 (48.58-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.222 , 0.243 0.230 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (3.22%)	wwPDB-VP
Wilson B-factor (Å ²)	93.2	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 77.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6400	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: Y0Z

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	7/5331 (0.1%)	1.01	13/7232 (0.2%)
2	B	0.81	0/1091	1.24	4/1471 (0.3%)
3	C	0.86	0/36	1.85	0/46
All	All	0.83	7/6458 (0.1%)	1.05	17/8749 (0.2%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	PRO	C-O	-7.95	1.18	1.24
1	A	644	PRO	C-O	-5.92	1.16	1.23
1	A	515	PRO	C-O	-5.21	1.18	1.24
1	A	650	ALA	C-O	-5.20	1.18	1.24
1	A	642	PRO	C-O	-5.15	1.17	1.23
1	A	790	PRO	C-O	-5.11	1.18	1.23
1	A	801	GLU	C-O	-5.04	1.17	1.24

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	419	ASN	CB-CA-C	7.64	123.84	110.85
1	A	520	TYR	N-CA-C	-6.33	102.92	112.04
1	A	506	GLU	CB-CA-C	-6.11	101.30	110.88
1	A	750	ARG	CG-CD-NE	-5.86	99.11	112.00
1	A	521	LEU	CA-C-N	5.85	133.50	123.03
1	A	521	LEU	C-N-CA	5.85	133.50	123.03
1	A	654	MET	CA-C-N	-5.82	117.15	122.80
1	A	654	MET	C-N-CA	-5.82	117.15	122.80
1	A	206	THR	CA-CB-OG1	-5.77	100.95	109.60
1	A	308	GLU	CB-CG-CD	-5.74	102.84	112.60
1	A	566	THR	CA-C-N	-5.66	115.52	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	566	THR	C-N-CA	-5.66	115.52	122.93
1	A	525	ASP	CB-CA-C	-5.47	102.29	110.88
1	A	800	GLY	CA-C-O	-5.43	118.54	122.45
2	B	420	PHE	CA-CB-CG	5.31	119.11	113.80
2	B	338	LEU	N-CA-C	-5.21	106.61	113.12
2	B	421	PHE	CB-CA-C	-5.10	102.65	110.81

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	5217	0	5252	201	0
2	B	1076	0	1091	88	0
3	C	35	0	34	11	0
4	A	72	0	0	4	0
All	All	6400	0	6377	273	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 21.

All (273) 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:A:671:TRP:CE3	1:A:703:LEU:HD11	1.48	1.45
1:A:671:TRP:CZ3	1:A:703:LEU:HD12	1.57	1.40
1:A:671:TRP:CE3	1:A:703:LEU:CD1	2.12	1.30
1:A:671:TRP:CZ3	1:A:703:LEU:CD1	2.14	1.30
1:A:363:TYR:CD2	1:A:734:ILE:HD12	1.73	1.24
1:A:671:TRP:CD2	1:A:703:LEU:HD11	1.76	1.20
1:A:346:SER:HA	1:A:351:MET:CE	1.78	1.14
2:B:383:TRP:CD2	2:B:412:LYS:HE2	1.85	1.12
1:A:437:THR:OG1	1:A:508:LEU:HD21	1.56	1.06
2:B:383:TRP:CZ2	2:B:420:PHE:HD1	1.73	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:ARG:HG3	3:C:67:ARG:HH11	1.16	1.06
1:A:363:TYR:HD2	1:A:734:ILE:HD12	0.90	1.04
1:A:793:ILE:HD12	1:A:793:ILE:H	1.23	1.00
1:A:363:TYR:CE2	1:A:734:ILE:HG23	1.98	0.98
2:B:383:TRP:CH2	2:B:420:PHE:CD1	2.52	0.98
1:A:346:SER:HA	1:A:351:MET:HE2	1.47	0.96
2:B:383:TRP:CZ2	2:B:420:PHE:CD1	2.54	0.96
1:A:332:MET:HE2	1:A:661:LYS:NZ	1.81	0.95
1:A:427:GLN:NE2	1:A:518:ASP:HA	1.81	0.95
1:A:364:GLU:OE2	1:A:524:ARG:NH2	2.00	0.95
1:A:438:GLN:OE1	1:A:508:LEU:HD12	1.65	0.95
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.02	0.94
1:A:438:GLN:OE1	1:A:508:LEU:CD1	2.16	0.94
2:B:425:ARG:HA	2:B:430:ILE:HD12	1.54	0.89
2:B:383:TRP:CD2	2:B:412:LYS:CE	2.55	0.89
2:B:383:TRP:CE2	2:B:412:LYS:CE	2.56	0.88
2:B:383:TRP:CE2	2:B:420:PHE:HD1	1.91	0.88
1:A:332:MET:HE2	1:A:661:LYS:HZ1	1.37	0.88
2:B:383:TRP:CE3	2:B:412:LYS:HE2	2.08	0.87
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.55	0.86
1:A:671:TRP:CH2	1:A:703:LEU:HD12	2.09	0.86
1:A:346:SER:CA	1:A:351:MET:CE	2.53	0.85
1:A:427:GLN:HE21	1:A:518:ASP:HA	1.42	0.85
1:A:363:TYR:HE2	1:A:734:ILE:HG23	1.40	0.85
2:B:383:TRP:CZ3	2:B:420:PHE:CE1	2.66	0.84
1:A:438:GLN:HG2	1:A:508:LEU:HD11	1.58	0.84
1:A:660:ASN:OD1	1:A:749:SER:OG	1.95	0.83
1:A:518:ASP:OD2	1:A:518:ASP:N	2.07	0.83
1:A:380:GLN:O	1:A:384:ARG:HG3	1.79	0.82
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.64	0.80
2:B:383:TRP:CZ2	2:B:412:LYS:CD	2.65	0.80
2:B:383:TRP:CZ2	2:B:412:LYS:HD3	2.17	0.80
1:A:363:TYR:HD2	1:A:734:ILE:CD1	1.85	0.80
1:A:273:LEU:O	1:A:273:LEU:HD23	1.80	0.79
2:B:383:TRP:CH2	2:B:412:LYS:HD2	2.18	0.78
2:B:421:PHE:O	2:B:425:ARG:HB2	1.83	0.77
1:A:456:LYS:CB	2:B:370:TYR:HE2	1.97	0.77
2:B:383:TRP:CE2	2:B:412:LYS:HE3	2.21	0.75
3:C:67:ARG:HG3	3:C:67:ARG:NH1	1.93	0.74
1:A:497:LEU:N	1:A:497:LEU:HD23	2.01	0.73
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:CA	2:B:370:TYR:CE2	2.71	0.73
2:B:368:GLU:HA	2:B:368:GLU:OE1	1.88	0.72
1:A:195:CYS:HG	1:A:834:TYR:HE2	1.37	0.72
1:A:384:ARG:NH2	2:B:312:LYS:O	2.22	0.72
1:A:526:ARG:HH11	1:A:526:ARG:CG	2.02	0.72
2:B:383:TRP:CE3	2:B:420:PHE:HE1	2.09	0.71
1:A:344:VAL:O	1:A:348:GLN:HG3	1.88	0.71
1:A:363:TYR:CE2	1:A:734:ILE:CG2	2.72	0.71
1:A:569:ASN:OD1	1:A:569:ASN:N	2.26	0.69
1:A:437:THR:OG1	1:A:508:LEU:CD2	2.37	0.69
1:A:456:LYS:CA	2:B:370:TYR:HE2	2.06	0.68
1:A:341:PRO:HG3	1:A:816:LEU:CD1	2.23	0.68
1:A:346:SER:CA	1:A:351:MET:HE1	2.23	0.68
1:A:793:ILE:H	1:A:793:ILE:CD1	1.97	0.68
2:B:383:TRP:CE3	2:B:420:PHE:CE1	2.81	0.68
1:A:438:GLN:OE1	1:A:508:LEU:HD11	1.93	0.68
1:A:755:PRO:HA	1:A:758:ARG:HE	1.59	0.68
2:B:383:TRP:CZ3	2:B:420:PHE:CD1	2.82	0.68
1:A:750:ARG:HG2	1:A:750:ARG:NH2	2.07	0.67
2:B:426:ARG:HD3	2:B:427:ARG:HG2	1.76	0.67
1:A:418:LEU:CD1	2:B:321:VAL:HG12	2.25	0.66
1:A:418:LEU:HD11	2:B:321:VAL:HG12	1.76	0.66
1:A:671:TRP:O	1:A:673:PRO:HD3	1.96	0.66
2:B:427:ARG:C	2:B:429:ASN:H	2.04	0.65
1:A:356:ILE:HD11	1:A:566:THR:CG2	2.26	0.65
2:B:396:ARG:HH11	2:B:436:GLU:HB3	1.62	0.65
2:B:383:TRP:CE2	2:B:420:PHE:CD1	2.82	0.64
1:A:525:ASP:N	1:A:525:ASP:OD1	2.31	0.63
1:A:332:MET:CE	1:A:661:LYS:NZ	2.59	0.63
1:A:511:LEU:N	1:A:511:LEU:HD23	2.14	0.63
1:A:671:TRP:CH2	1:A:703:LEU:CD1	2.75	0.63
2:B:383:TRP:CH2	2:B:412:LYS:CD	2.80	0.62
1:A:671:TRP:CZ3	1:A:703:LEU:HD11	2.02	0.62
1:A:456:LYS:HA	2:B:370:TYR:CD2	2.34	0.62
1:A:793:ILE:HG22	1:A:794:PRO:CD	2.30	0.61
1:A:231:PHE:HE2	1:A:249:VAL:HG12	1.66	0.61
1:A:654:MET:HE1	1:A:776:MET:CG	2.31	0.61
2:B:427:ARG:C	2:B:429:ASN:N	2.58	0.61
2:B:396:ARG:NH1	2:B:436:GLU:HB3	2.15	0.61
1:A:438:GLN:CG	1:A:508:LEU:HD11	2.29	0.60
1:A:195:CYS:SG	1:A:834:TYR:HE2	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.66	0.60
1:A:346:SER:CB	1:A:351:MET:CE	2.80	0.60
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.83	0.60
1:A:793:ILE:HD12	1:A:793:ILE:N	2.05	0.59
1:A:456:LYS:HB2	2:B:370:TYR:HE2	1.65	0.59
1:A:325:TYR:CE2	1:A:665:CYS:HB3	2.37	0.59
2:B:370:TYR:N	2:B:370:TYR:HD1	2.01	0.59
1:A:363:TYR:HE2	1:A:734:ILE:CG2	2.12	0.59
1:A:495:ASP:OD2	2:B:371:ARG:NH1	2.36	0.59
1:A:332:MET:HE2	1:A:661:LYS:HZ3	1.67	0.59
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.84	0.59
2:B:402:PHE:HB2	2:B:414:VAL:CG1	2.34	0.58
1:A:750:ARG:HG2	1:A:750:ARG:HH21	1.68	0.58
1:A:793:ILE:HG22	1:A:794:PRO:HD2	1.85	0.58
1:A:456:LYS:HE2	2:B:370:TYR:OH	2.04	0.58
2:B:370:TYR:N	2:B:370:TYR:CD1	2.71	0.58
1:A:804:ILE:HG23	1:A:804:ILE:O	2.03	0.58
1:A:654:MET:HE1	1:A:776:MET:SD	2.44	0.58
1:A:468:VAL:HG12	1:A:468:VAL:O	2.02	0.58
1:A:198:ASP:OD1	1:A:198:ASP:N	2.37	0.57
2:B:341:GLU:HG3	2:B:341:GLU:O	2.02	0.57
1:A:510:GLU:O	1:A:513:ALA:N	2.38	0.57
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.85	0.57
2:B:403:GLN:OE1	2:B:403:GLN:HA	2.03	0.57
1:A:456:LYS:HG3	2:B:370:TYR:OH	2.04	0.56
3:C:69:PHE:C	3:C:69:PHE:CD2	2.83	0.56
3:C:69:PHE:C	3:C:69:PHE:HD2	2.13	0.56
3:C:67:ARG:HH11	3:C:67:ARG:CG	2.02	0.56
3:C:69:PHE:HD2	3:C:69:PHE:O	1.88	0.56
1:A:448:MET:HE2	2:B:363:LEU:HD23	1.88	0.56
1:A:487:LEU:HD23	2:B:372:LEU:HG	1.87	0.56
1:A:594:ARG:HG2	1:A:640:VAL:HB	1.89	0.55
2:B:427:ARG:O	2:B:429:ASN:N	2.40	0.55
2:B:420:PHE:CD2	2:B:420:PHE:C	2.85	0.55
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.32	0.55
1:A:485:ARG:HD3	1:A:485:ARG:C	2.31	0.55
1:A:663:VAL:CG1	1:A:747:VAL:HB	2.37	0.55
1:A:215:ASN:HA	1:A:218:LEU:HD12	1.89	0.54
1:A:346:SER:HB3	1:A:351:MET:HE1	1.88	0.54
2:B:426:ARG:H	2:B:426:ARG:HD2	1.72	0.54
3:C:67:ARG:CD	3:C:67:ARG:H	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:SER:CB	1:A:351:MET:HE1	2.38	0.54
1:A:209:VAL:O	1:A:213:ILE:HG13	2.07	0.53
1:A:230:THR:HG23	1:A:270:ILE:HD12	1.91	0.53
1:A:316:ARG:NH2	1:A:801:GLU:OE2	2.40	0.53
2:B:336:ARG:HA	2:B:339:ASP:HB2	1.91	0.53
1:A:273:LEU:N	1:A:273:LEU:CD2	2.71	0.53
2:B:324:VAL:HG23	2:B:324:VAL:O	2.09	0.53
1:A:231:PHE:CE2	1:A:249:VAL:HG12	2.43	0.53
1:A:440:GLU:HG3	1:A:504:LEU:CD1	2.38	0.53
1:A:449:VAL:HA	2:B:363:LEU:HD11	1.91	0.53
1:A:511:LEU:N	1:A:511:LEU:CD2	2.73	0.52
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.92	0.52
2:B:369:PRO:HB2	2:B:370:TYR:HD1	1.74	0.52
2:B:369:PRO:HB2	2:B:370:TYR:CD1	2.44	0.52
1:A:526:ARG:NH1	1:A:530:ASP:OD1	2.40	0.52
1:A:311:ASP:OD1	1:A:311:ASP:N	2.41	0.51
1:A:332:MET:CE	1:A:661:LYS:HZ3	2.22	0.51
1:A:755:PRO:HB3	1:A:758:ARG:HH21	1.75	0.51
1:A:341:PRO:HG3	1:A:816:LEU:HD13	1.90	0.51
1:A:266:ILE:N	1:A:348:GLN:OE1	2.28	0.51
1:A:308:GLU:HG2	1:A:586:LEU:CD2	2.40	0.51
1:A:320:PHE:HB2	1:A:329:LEU:HD11	1.93	0.51
1:A:755:PRO:HA	1:A:758:ARG:NE	2.23	0.51
1:A:439:GLU:HG2	2:B:352:ILE:HD13	1.93	0.51
1:A:693:LEU:HD12	1:A:694:PHE:H	1.75	0.51
1:A:701:PRO:HG2	1:A:701:PRO:O	2.11	0.51
2:B:425:ARG:HA	2:B:430:ILE:CD1	2.35	0.51
1:A:352:GLU:HB2	1:A:568:ARG:HB2	1.91	0.50
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.45	0.50
2:B:405:ILE:O	2:B:409:ILE:HG12	2.11	0.50
2:B:406:SER:O	2:B:410:GLY:N	2.44	0.50
1:A:456:LYS:CB	2:B:370:TYR:CE2	2.87	0.50
1:A:485:ARG:NH1	2:B:404:ALA:HB2	2.27	0.50
1:A:504:LEU:N	1:A:504:LEU:HD23	2.26	0.50
1:A:356:ILE:HG22	1:A:356:ILE:O	2.11	0.50
1:A:663:VAL:HG12	1:A:747:VAL:HB	1.93	0.50
1:A:793:ILE:CD1	1:A:793:ILE:N	2.72	0.50
1:A:801:GLU:HG2	1:A:809:ALA:H	1.77	0.50
1:A:265:GLY:O	1:A:295:ARG:HD3	2.11	0.50
2:B:384:THR:O	2:B:388:GLN:HG3	2.12	0.50
2:B:310:PRO:HB3	2:B:316:LEU:HD12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.95	0.49
1:A:690:GLU:OE2	1:A:726:ARG:NH1	2.41	0.49
2:B:405:ILE:O	2:B:409:ILE:CG1	2.61	0.49
1:A:331:ALA:HA	4:A:901:Y0Z:N1	2.27	0.49
1:A:763:TYR:HE1	1:A:765:ALA:HA	1.77	0.49
1:A:448:MET:HB3	2:B:363:LEU:HD21	1.95	0.49
1:A:541:ALA:O	1:A:657:GLY:HA3	2.13	0.49
2:B:410:GLY:C	2:B:412:LYS:H	2.20	0.49
1:A:802:HIS:ND1	1:A:802:HIS:N	2.60	0.48
2:B:383:TRP:CE2	2:B:412:LYS:CD	2.93	0.48
1:A:677:LEU:HD11	3:C:69:PHE:CE1	2.48	0.48
2:B:426:ARG:H	2:B:426:ARG:CD	2.25	0.48
3:C:67:ARG:CD	3:C:67:ARG:N	2.76	0.48
1:A:353:LEU:HD13	1:A:565:LEU:HG	1.96	0.48
1:A:521:LEU:HD22	1:A:525:ASP:CB	2.43	0.48
2:B:388:GLN:HB3	2:B:428:PHE:HE2	1.78	0.48
2:B:427:ARG:HG2	2:B:427:ARG:H	1.43	0.48
1:A:267:TYR:CD1	1:A:267:TYR:N	2.82	0.48
1:A:684:THR:HG22	1:A:686:ALA:H	1.78	0.47
1:A:205:GLN:OE1	1:A:205:GLN:HA	2.13	0.47
1:A:341:PRO:HG3	1:A:816:LEU:HD11	1.94	0.47
1:A:438:GLN:CD	1:A:508:LEU:HD11	2.39	0.47
1:A:763:TYR:CE1	1:A:765:ALA:HA	2.50	0.47
2:B:418:LYS:HD2	2:B:418:LYS:HA	1.51	0.47
1:A:273:LEU:HD22	1:A:273:LEU:H	1.80	0.47
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.97	0.47
1:A:308:GLU:HG2	1:A:586:LEU:HD23	1.96	0.47
1:A:331:ALA:HA	4:A:901:Y0Z:C5	2.44	0.47
1:A:334:VAL:HB	1:A:565:LEU:HB2	1.97	0.47
1:A:456:LYS:HG3	2:B:370:TYR:CE2	2.50	0.47
1:A:425:ASP:OD1	2:B:338:LEU:CD1	2.63	0.47
1:A:606:ASN:ND2	1:A:608:ARG:HB2	2.30	0.47
1:A:609:SER:O	1:A:609:SER:OG	2.22	0.47
1:A:511:LEU:HD23	1:A:511:LEU:H	1.80	0.47
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.50	0.47
1:A:512:GLU:CD	1:A:512:GLU:C	2.82	0.46
1:A:666:PHE:O	1:A:701:PRO:HG2	2.15	0.46
1:A:548:SER:O	1:A:552:TRP:HB3	2.15	0.46
1:A:331:ALA:CB	4:A:901:Y0Z:C25	2.94	0.46
1:A:658:ASN:ND2	1:A:752:ARG:HB2	2.31	0.46
1:A:456:LYS:HG3	2:B:370:TYR:CZ	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.77	0.45
2:B:423:ASN:O	2:B:426:ARG:NH1	2.50	0.45
1:A:346:SER:HB3	1:A:351:MET:CE	2.46	0.45
1:A:433:LYS:HE2	1:A:433:LYS:HB3	1.65	0.45
1:A:495:ASP:CG	2:B:371:ARG:HH12	2.24	0.45
2:B:383:TRP:CZ3	2:B:412:LYS:HD2	2.51	0.45
1:A:346:SER:CB	1:A:351:MET:HE3	2.46	0.45
1:A:654:MET:HE1	1:A:776:MET:HG2	1.99	0.45
1:A:471:PRO:HD2	1:A:471:PRO:O	2.16	0.45
1:A:572:SER:O	1:A:575:PRO:HD2	2.17	0.45
1:A:449:VAL:O	1:A:453:GLU:HG2	2.17	0.45
1:A:793:ILE:CG2	1:A:794:PRO:CD	2.95	0.44
1:A:439:GLU:HG2	2:B:352:ILE:CD1	2.47	0.44
1:A:547:LEU:HD22	1:A:552:TRP:HB2	1.99	0.44
3:C:69:PHE:CD2	3:C:69:PHE:O	2.70	0.44
1:A:526:ARG:HH11	1:A:526:ARG:HG2	1.81	0.44
2:B:410:GLY:C	2:B:412:LYS:N	2.76	0.43
1:A:438:GLN:HE22	2:B:353:LYS:HG3	1.82	0.43
3:C:67:ARG:H	3:C:67:ARG:HD3	1.83	0.43
2:B:368:GLU:N	2:B:369:PRO:CD	2.81	0.43
1:A:191:GLN:NE2	1:A:259:HIS:CD2	2.85	0.43
1:A:718:ILE:CG2	1:A:723:ILE:HG13	2.48	0.43
1:A:180:GLN:HA	1:A:339:GLY:HA2	2.00	0.43
1:A:647:LYS:O	1:A:651:VAL:HG23	2.18	0.43
1:A:669:VAL:HG13	1:A:671:TRP:CE2	2.53	0.43
2:B:383:TRP:NE1	2:B:412:LYS:HE3	2.33	0.43
1:A:362:LEU:N	1:A:362:LEU:CD1	2.81	0.43
2:B:320:ASP:O	2:B:324:VAL:HG13	2.19	0.43
1:A:325:TYR:CD2	1:A:665:CYS:HB3	2.54	0.43
1:A:566:THR:HG21	1:A:697:LEU:HD13	2.00	0.43
1:A:758:ARG:HD3	1:A:758:ARG:HA	1.87	0.43
1:A:286:SER:HB2	1:A:291:LEU:HD11	2.00	0.42
1:A:297:LEU:HB2	1:A:304:VAL:HG11	2.02	0.42
1:A:273:LEU:HA	1:A:274:PRO:HD3	1.90	0.42
1:A:386:LEU:O	1:A:389:THR:OG1	2.33	0.42
1:A:399:ASN:ND2	1:A:550:LYS:HE3	2.34	0.42
1:A:445:LEU:HD23	2:B:359:LEU:HB2	2.02	0.42
1:A:645:GLU:CD	1:A:645:GLU:C	2.88	0.42
2:B:402:PHE:HB2	2:B:414:VAL:HG12	2.00	0.42
1:A:276:LYS:HD3	1:A:276:LYS:HA	1.95	0.42
1:A:412:LEU:HD13	1:A:533:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:LEU:N	1:A:830:LEU:HD23	2.34	0.42
1:A:485:ARG:HD2	1:A:486:ASP:OD1	2.20	0.41
1:A:574:VAL:HB	1:A:575:PRO:HD3	2.02	0.41
2:B:426:ARG:CD	2:B:426:ARG:N	2.83	0.41
1:A:289:SER:OG	4:A:901:Y0Z:O9	2.26	0.41
1:A:381:GLU:HG3	1:A:385:LEU:CD2	2.50	0.41
1:A:362:LEU:N	1:A:362:LEU:HD12	2.35	0.41
2:B:336:ARG:C	2:B:338:LEU:N	2.76	0.41
2:B:420:PHE:C	2:B:420:PHE:HD2	2.28	0.41
1:A:672:ASP:O	1:A:675:VAL:HG22	2.21	0.41
2:B:338:LEU:N	2:B:338:LEU:HD23	2.36	0.41
1:A:232:GLU:OE2	1:A:232:GLU:N	2.50	0.41
1:A:781:THR:HA	1:A:794:PRO:HA	2.03	0.41
1:A:197:PRO:HA	1:A:200:ILE:HG22	2.02	0.40
1:A:469:LYS:HD2	1:A:469:LYS:HA	1.63	0.40
1:A:538:PHE:CD1	1:A:706:LEU:HD13	2.57	0.40
1:A:515:PRO:O	1:A:515:PRO:CG	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	664/871 (76%)	642 (97%)	21 (3%)	1 (0%)	43	72
2	B	131/144 (91%)	120 (92%)	9 (7%)	2 (2%)	8	28
3	C	2/9 (22%)	2 (100%)	0	0	100	100
All	All	797/1024 (78%)	764 (96%)	30 (4%)	3 (0%)	30	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	411	ASN
2	B	428	PHE
1	A	515	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	566/715 (79%)	529 (94%)	37 (6%)	15	43
2	B	117/125 (94%)	92 (79%)	25 (21%)	1	4
3	C	4/9 (44%)	1 (25%)	3 (75%)	0	0
All	All	687/849 (81%)	622 (90%)	65 (10%)	8	26

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	267	TYR
1	A	271	LYS
1	A	273	LEU
1	A	351	MET
1	A	353	LEU
1	A	356	ILE
1	A	370	VAL
1	A	463	LYS
1	A	469	LYS
1	A	472	ARG
1	A	497	LEU
1	A	500	THR
1	A	503	LYS
1	A	504	LEU
1	A	508	LEU
1	A	511	LEU
1	A	512	GLU
1	A	518	ASP
1	A	522	SER

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Mol	Chain	Res	Type
1	A	524	ARG
1	A	525	ASP
1	A	526	ARG
1	A	568	ARG
1	A	569	ASN
1	A	610	THR
1	A	611	SER
1	A	645	GLU
1	A	652	GLN
1	A	654	MET
1	A	703	LEU
1	A	704	LEU
1	A	718	ILE
1	A	719	SER
1	A	748	VAL
1	A	793	ILE
1	A	801	GLU
2	B	317	SER
2	B	324	VAL
2	B	327	ASN
2	B	338	LEU
2	B	341	GLU
2	B	344	SER
2	B	345	VAL
2	B	353	LYS
2	B	354	GLN
2	B	355	THR
2	B	368	GLU
2	B	370	TYR
2	B	372	LEU
2	B	375	VAL
2	B	400	ARG
2	B	409	ILE
2	B	411	ASN
2	B	414	VAL
2	B	415	VAL
2	B	418	LYS
2	B	420	PHE
2	B	422	VAL
2	B	425	ARG
2	B	426	ARG
2	B	427	ARG

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Mol	Chain	Res	Type
3	C	66	PRO
3	C	67	ARG
3	C	69	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	HIS
1	A	191	GLN
1	A	204	GLN
1	A	296	GLN
1	A	380	GLN
1	A	383	ASN
1	A	399	ASN
1	A	446	ASN
1	A	680	HIS
1	A	806	ASN
2	B	318	GLN
2	B	356	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](#)

1 ligand is 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	$\# Z > 2$
4	Y0Z	A	901	-	78,79,79	1.68	10 (12%)	104,118,118	1.01	8 (7%)

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	Y0Z	A	901	-	-	16/51/67/67	0/8/8/8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	Y0Z	C5-N1	-8.72	1.31	1.42
4	A	901	Y0Z	C25-C28	-4.63	1.31	1.43
4	A	901	Y0Z	P1-O11	-3.92	1.55	1.59
4	A	901	Y0Z	P2-O11	-3.83	1.55	1.59
4	A	901	Y0Z	O5-C30	-3.28	1.36	1.43
4	A	901	Y0Z	C5-C4	-2.77	1.36	1.41
4	A	901	Y0Z	C9-N1	-2.76	1.35	1.40
4	A	901	Y0Z	C6-C7	-2.74	1.35	1.39
4	A	901	Y0Z	C29-C30	-2.61	1.49	1.52
4	A	901	Y0Z	O6-C31	-2.40	1.37	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	Y0Z	C25-C28-N4	3.56	117.21	110.94
4	A	901	Y0Z	C5-N1-C9	-3.33	113.49	121.65
4	A	901	Y0Z	C6-C5-N1	-2.62	118.78	122.70
4	A	901	Y0Z	C43-C42-C36	-2.43	96.86	101.46
4	A	901	Y0Z	O1-C9-N1	2.35	122.96	120.33
4	A	901	Y0Z	O13-P2-O12	2.35	123.36	112.44
4	A	901	Y0Z	C28-N4-C27	-2.15	123.41	126.37
4	A	901	Y0Z	O4-C28-C25	-2.05	122.58	127.62

There are no chirality outliers.

All (16) torsion outliers are listed below:

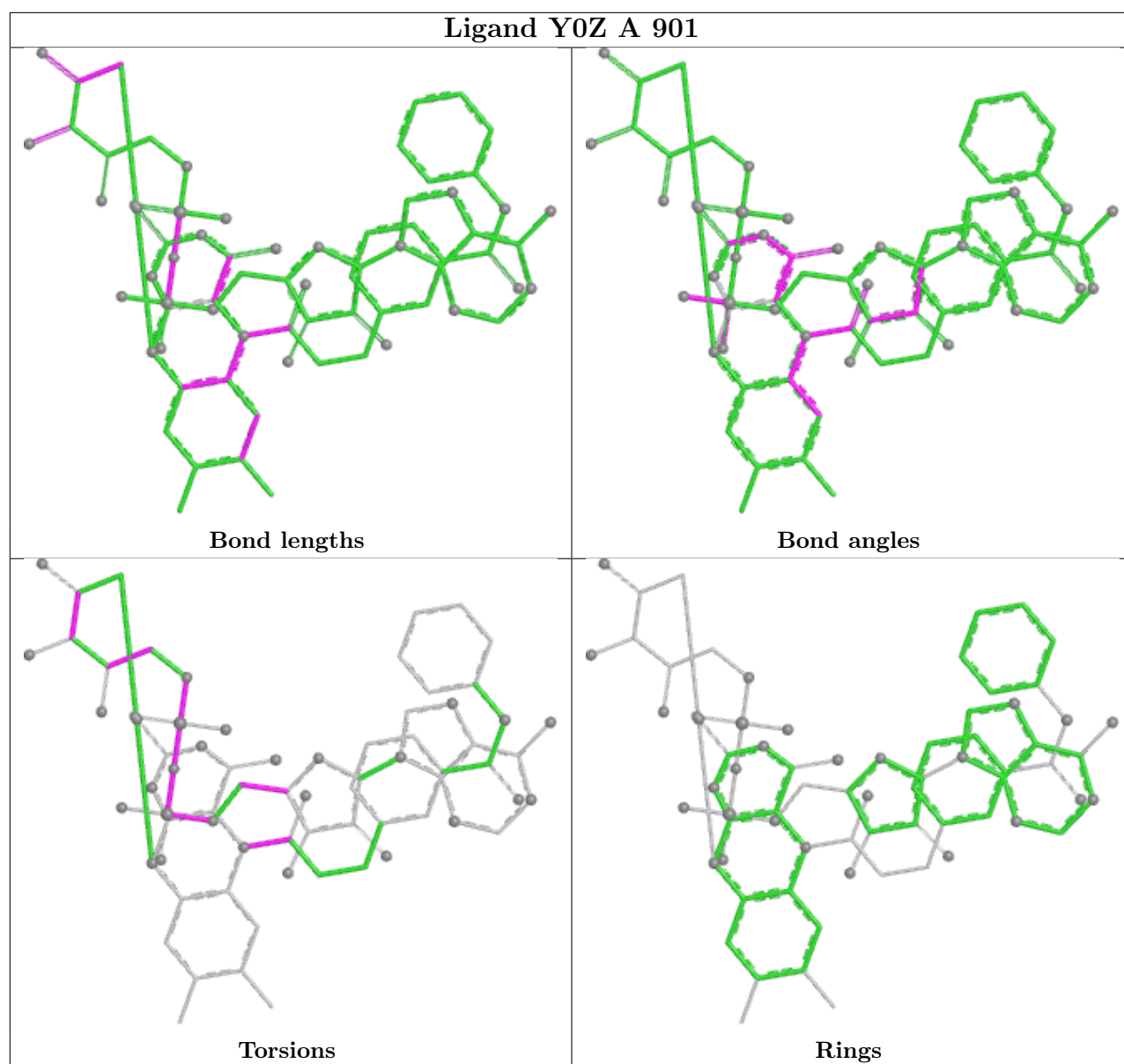
Mol	Chain	Res	Type	Atoms
4	A	901	Y0Z	C10-C9-N1-C5
4	A	901	Y0Z	C10-C9-N1-C25
4	A	901	Y0Z	O1-C9-N1-C5
4	A	901	Y0Z	O1-C9-N1-C25
4	A	901	Y0Z	O7-C32-C33-O8
4	A	901	Y0Z	C34-O14-P2-O12
4	A	901	Y0Z	C33-O8-P1-O10
4	A	901	Y0Z	C31-C32-C33-O8
4	A	901	Y0Z	P2-O11-P1-O8
4	A	901	Y0Z	C33-O8-P1-O11
4	A	901	Y0Z	C33-O8-P1-O9
4	A	901	Y0Z	O5-C30-C31-C32
4	A	901	Y0Z	P1-O11-P2-O12
4	A	901	Y0Z	O14-C34-C35-O15
4	A	901	Y0Z	P1-O11-P2-O13
4	A	901	Y0Z	O14-C34-C35-C43

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	Y0Z	4	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	666/871 (76%)	0.31	23 (3%) 47 38	65, 98, 129, 148	0
2	B	133/144 (92%)	0.85	11 (8%) 17 12	93, 127, 146, 166	0
3	C	4/9 (44%)	5.72	4 (100%) 0 0	129, 130, 134, 137	0
All	All	803/1024 (78%)	0.43	38 (4%) 36 29	65, 103, 137, 166	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	66	PRO	11.6
1	A	836	LEU	8.1
2	B	376	ILE	7.8
2	B	436	GLU	6.9
1	A	171	PRO	5.5
1	A	835	THR	5.3
3	C	68	SER	4.7
2	B	375	VAL	4.1
3	C	67	ARG	3.8
1	A	563	SER	3.4
1	A	834	TYR	3.3
1	A	239	GLU	3.1
1	A	374	LYS	2.8
1	A	611	SER	2.8
3	C	69	PHE	2.7
2	B	440	GLU	2.6
1	A	175	GLU	2.6
1	A	833	MET	2.6
1	A	172	SER	2.6
1	A	377	MET	2.5
2	B	383	TRP	2.4
2	B	378	LYS	2.4
2	B	332	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	785	SER	2.4
1	A	555	ASP	2.3
2	B	308	ARG	2.3
1	A	684	THR	2.3
1	A	324	ASN	2.2
1	A	269	ARG	2.2
1	A	556	ASP	2.2
2	B	371	ARG	2.2
1	A	667	ASP	2.2
2	B	326	ALA	2.1
1	A	325	TYR	2.1
1	A	273	LEU	2.1
1	A	786	ILE	2.1
1	A	770	GLY	2.1
2	B	359	LEU	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](#)

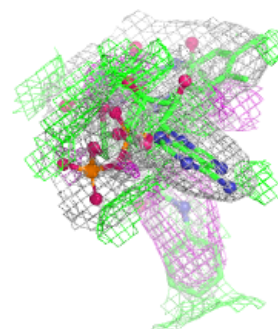
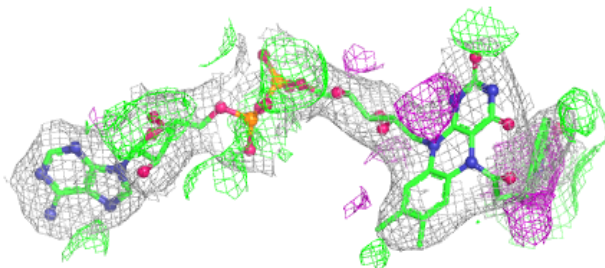
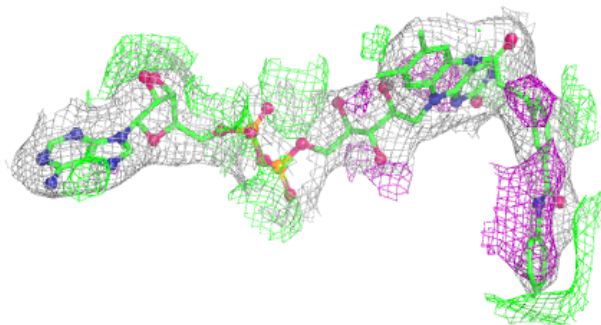
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	Y0Z	A	901	72/72	0.94	0.12	57,83,107,116	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 Y0Z A 901:

$2mF_o-DF_c$ (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.