Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 10:43 AM EDT

PDB ID	:	8FJ6
Title	:	LSD1-CoREST in complex with T108, long soaking
Authors	:	Caroli, J.; Mattevi, A.
Deposited on	:	2022-12-19
Resolution	:	2.63 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:

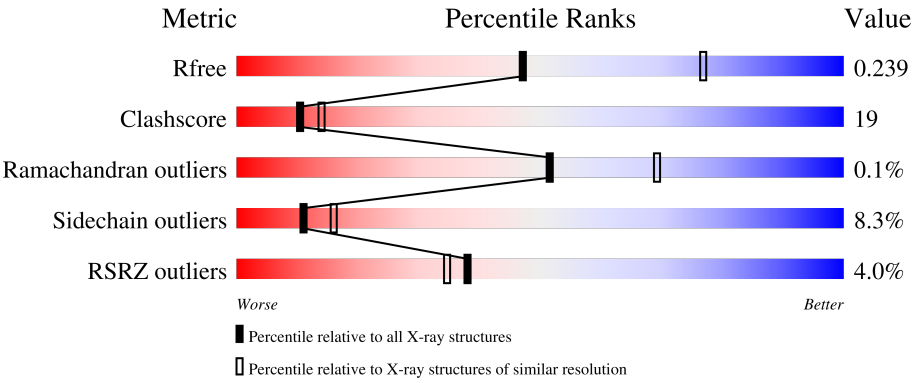
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.63 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1426 (2.66-2.62)
Clashscore	141614	1472 (2.66-2.62)
Ramachandran outliers	138981	1446 (2.66-2.62)
Sidechain outliers	138945	1446 (2.66-2.62)
RSRZ outliers	127900	1408 (2.66-2.62)

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 <=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	2% 52% 23% 24%
2	B	144	9% 49% 35% 8% 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6365 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

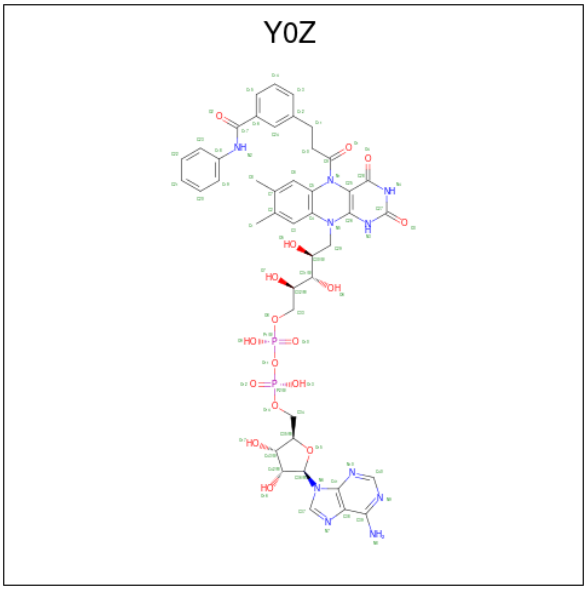
- Molecule 2 is a protein called REST corepressor 1.

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 [(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 (three-letter code: Y0Z) (formula: $C_{43}H_{48}N_{10}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).



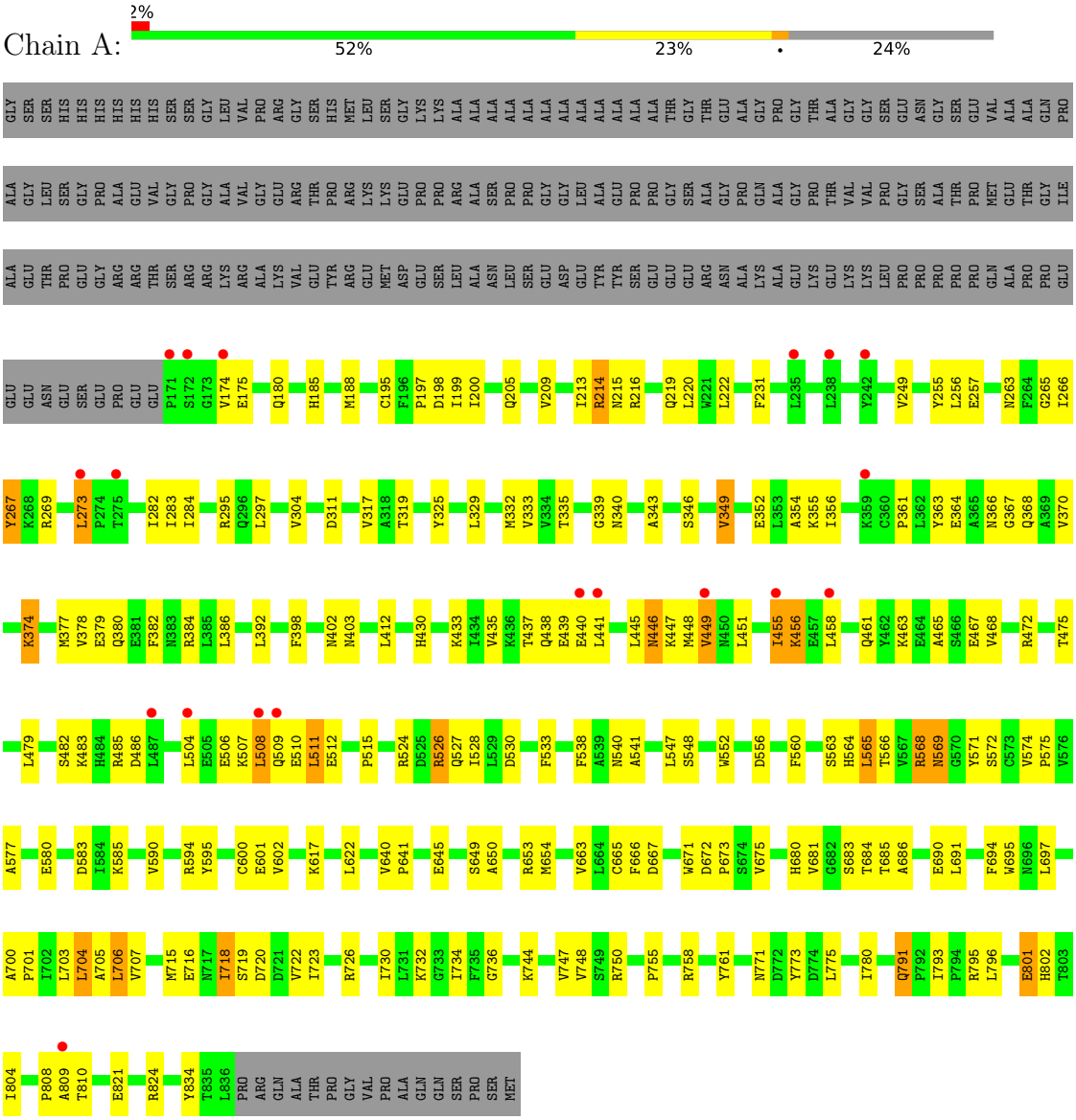
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	72	43	10	17	2	0	0

3 Residue-property plots (i)

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

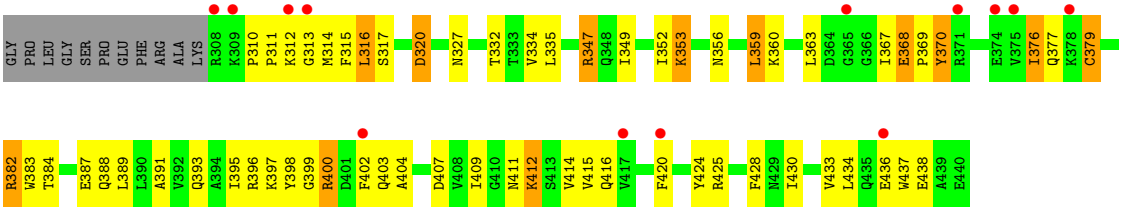
• Molecule 1: Lysine-specific histone demethylase 1A

Chain A:



• Molecule 2: REST corepressor 1

Chain B:


GLY PRO LEU GLY SER PRO GLU PHE ARG ALA LYS R308 K309 P310 P311 K312 G313 M314 F315 L316 S317 D320 N327 T332 T333 V334 L335 R347 Q348 I349 I352 K353 N356 L359 K360 L363 D364 G365 G366 I367 E368 P369 Y370 R371 E374 V375 I376 Q377 K378 C379
R382 W383 T384 E387 Q388 L389 L390 A391 V392 Q393 A394 I395 R396 K397 Y398 G399 R400 D401 F402 Q403 A404 D407 V408 I409 G410 N411 K412 S413 V414 V415 Q416 V417 F420 Y424 R425 F428 M429 I430 V433 L434 Q435 E436 W437 E438 A439 E440

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.04Å 179.36Å 233.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.57 – 2.63 48.57 – 2.63	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.57-2.63) 98.2 (48.57-2.63)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.219 , 0.240 0.220 , 0.239	Depositor DCC
R_{free} test set	1985 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å^2)	82.5	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6365	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.68	3/5331 (0.1%)	0.73	1/7232 (0.0%)
2	B	0.60	0/1091	0.78	1/1471 (0.1%)
All	All	0.67	3/6422 (0.0%)	0.74	2/8703 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	801	GLU	CD-OE2	-5.57	1.19	1.25
1	A	801	GLU	CD-OE1	-5.49	1.19	1.25
1	A	821	GLU	CD-OE2	-5.27	1.19	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	347	ARG	CB-CA-C	-5.59	99.22	110.40
1	A	214	ARG	CG-CD-NE	5.25	122.81	111.80

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	183	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1076	0	1091	79	1
3	A	72	0	0	2	0
All	All	6365	0	6343	236	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 19.

All (236) 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:793:ILE:HD12	1:A:793:ILE:H	1.23	1.00
1:A:384:ARG:NH2	2:B:312:LYS:O	2.02	0.91
1:A:456:LYS:HB2	2:B:370:TYR:HE1	1.36	0.90
1:A:195:CYS:HG	1:A:834:TYR:HE2	0.93	0.90
2:B:400:ARG:HH11	2:B:400:ARG:HG2	1.37	0.88
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.53	0.87
1:A:449:VAL:HG23	2:B:363:LEU:CD1	2.07	0.85
1:A:438:GLN:OE1	1:A:508:LEU:CD1	2.25	0.85
1:A:456:LYS:CB	2:B:370:TYR:HE1	1.88	0.85
1:A:463:LYS:O	1:A:467:GLU:HG2	1.76	0.84
1:A:343:ALA:O	1:A:346:SER:OG	1.95	0.84
1:A:526:ARG:HH11	1:A:526:ARG:HG3	1.43	0.83
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.60	0.82
1:A:273:LEU:O	1:A:273:LEU:HD23	1.78	0.82
2:B:376:ILE:HD12	2:B:376:ILE:H	1.44	0.82
1:A:438:GLN:OE1	1:A:508:LEU:HD12	1.78	0.82
1:A:380:GLN:O	1:A:384:ARG:HG3	1.79	0.82
1:A:449:VAL:HG23	2:B:363:LEU:HD11	1.60	0.82
1:A:439:GLU:HG2	2:B:352:ILE:CD1	2.10	0.82
1:A:486:ASP:OD1	2:B:398:TYR:OH	1.95	0.82
2:B:382:ARG:O	2:B:412:LYS:NZ	2.10	0.81
2:B:313:GLY:O	2:B:315:PHE:CD1	2.33	0.80
1:A:718:ILE:HG22	1:A:723:ILE:HG13	1.64	0.80
1:A:569:ASN:OD1	1:A:569:ASN:N	2.18	0.77
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.20	0.76
1:A:695:TRP:HE1	1:A:706:LEU:HD22	1.50	0.76
1:A:370:VAL:HG21	1:A:528:ILE:HD13	1.67	0.76
1:A:456:LYS:HA	2:B:370:TYR:CD1	2.21	0.75
2:B:382:ARG:C	2:B:412:LYS:HZ1	1.89	0.75
2:B:313:GLY:O	2:B:315:PHE:CE1	2.39	0.75
2:B:368:GLU:HA	2:B:368:GLU:OE1	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:O	1:A:213:ILE:HD12	1.88	0.74
2:B:359:LEU:HD23	2:B:359:LEU:N	2.00	0.73
1:A:355:LYS:HA	1:A:565:LEU:HD13	1.70	0.73
2:B:396:ARG:O	2:B:396:ARG:HD3	1.89	0.72
1:A:574:VAL:HB	1:A:575:PRO:HD3	1.71	0.72
1:A:440:GLU:OE2	1:A:504:LEU:HD21	1.89	0.71
2:B:320:ASP:OD1	2:B:320:ASP:N	2.20	0.71
1:A:755:PRO:HA	1:A:758:ARG:HE	1.57	0.70
2:B:376:ILE:HD12	2:B:376:ILE:N	2.06	0.69
1:A:195:CYS:SG	1:A:834:TYR:HE2	2.12	0.69
1:A:720:ASP:OD1	1:A:748:VAL:CG1	2.41	0.69
2:B:384:THR:OG1	2:B:387:GLU:HG3	1.94	0.67
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.75	0.67
1:A:666:PHE:O	1:A:701:PRO:HG2	1.94	0.67
1:A:601:GLU:HB3	1:A:617:LYS:HD3	1.76	0.67
1:A:361:PRO:HB2	1:A:363:TYR:HE2	1.59	0.67
1:A:511:LEU:N	1:A:511:LEU:HD23	2.11	0.66
2:B:368:GLU:N	2:B:369:PRO:CD	2.59	0.66
1:A:773:TYR:CE1	1:A:808:PRO:HB3	2.31	0.65
1:A:364:GLU:HA	1:A:681:VAL:HB	1.77	0.65
1:A:438:GLN:OE1	1:A:508:LEU:HD11	1.97	0.65
1:A:355:LYS:HA	1:A:565:LEU:CD1	2.27	0.65
1:A:583:ASP:OD1	1:A:585:LYS:NZ	2.30	0.64
1:A:456:LYS:HB2	2:B:370:TYR:CE1	2.27	0.64
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.79	0.64
1:A:716:GLU:O	1:A:750:ARG:NH1	2.33	0.62
1:A:446:ASN:ND2	2:B:359:LEU:HD11	2.14	0.62
2:B:388:GLN:HB3	2:B:428:PHE:HE1	1.65	0.62
1:A:437:THR:HG21	1:A:507:LYS:HE2	1.81	0.62
1:A:175:GLU:HG3	1:A:185:HIS:CD2	2.35	0.61
1:A:526:ARG:HH11	1:A:526:ARG:CG	2.13	0.61
1:A:366:ASN:OD1	1:A:367:GLY:N	2.34	0.61
2:B:310:PRO:HB3	2:B:316:LEU:HD12	1.82	0.60
2:B:400:ARG:HG2	2:B:400:ARG:NH1	2.11	0.60
1:A:666:PHE:O	1:A:701:PRO:CG	2.48	0.60
2:B:399:GLY:N	2:B:437:TRP:NE1	2.49	0.60
1:A:793:ILE:HD12	1:A:793:ILE:N	2.07	0.60
1:A:451:LEU:O	1:A:455:ILE:HG13	2.01	0.59
1:A:650:ALA:O	1:A:654:MET:HG3	2.02	0.59
1:A:461:GLN:OE1	1:A:483:LYS:HE3	2.01	0.59
1:A:445:LEU:N	1:A:445:LEU:HD23	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:LYS:CA	2:B:370:TYR:CE1	2.86	0.58
2:B:370:TYR:HD2	2:B:370:TYR:N	2.01	0.58
1:A:329:LEU:N	1:A:329:LEU:HD12	2.18	0.58
1:A:438:GLN:HG2	1:A:508:LEU:HD11	1.86	0.58
1:A:197:PRO:HA	1:A:200:ILE:HG22	1.85	0.58
1:A:690:GLU:OE2	1:A:726:ARG:NH1	2.36	0.58
2:B:403:GLN:OE1	2:B:403:GLN:HA	2.03	0.58
1:A:456:LYS:CB	2:B:370:TYR:CE1	2.79	0.57
1:A:363:TYR:CD1	1:A:734:ILE:HD12	2.39	0.57
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.69	0.57
1:A:366:ASN:OD1	1:A:368:GLN:N	2.38	0.57
1:A:468:VAL:HG12	1:A:468:VAL:O	2.04	0.56
1:A:439:GLU:HG2	2:B:352:ILE:HD12	1.86	0.56
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.41	0.56
2:B:370:TYR:N	2:B:370:TYR:CD2	2.72	0.56
1:A:667:ASP:OD1	1:A:667:ASP:N	2.39	0.56
2:B:379:CYS:SG	2:B:416:GLN:OE1	2.64	0.56
1:A:392:LEU:HD11	2:B:316:LEU:HD22	1.88	0.55
1:A:761:TYR:CD1	1:A:809:ALA:HB1	2.41	0.55
2:B:367:ILE:O	2:B:367:ILE:HG13	2.07	0.55
2:B:425:ARG:HA	2:B:430:ILE:HD12	1.88	0.55
1:A:446:ASN:ND2	2:B:359:LEU:CD1	2.70	0.54
2:B:399:GLY:N	2:B:437:TRP:CD1	2.75	0.54
1:A:446:ASN:HD22	2:B:359:LEU:CD1	2.20	0.54
1:A:198:ASP:OD1	1:A:198:ASP:N	2.40	0.54
1:A:319:THR:OG1	1:A:572:SER:HB3	2.07	0.54
2:B:402:PHE:HB2	2:B:414:VAL:CG1	2.38	0.54
1:A:793:ILE:H	1:A:793:ILE:CD1	1.95	0.54
1:A:475:THR:HA	2:B:393:GLN:HE22	1.73	0.53
1:A:356:ILE:HD11	1:A:566:THR:HG22	1.89	0.53
2:B:383:TRP:HB3	2:B:388:GLN:HG2	1.91	0.53
1:A:257:GLU:HG3	1:A:263:ASN:HD22	1.74	0.53
2:B:400:ARG:HH11	2:B:400:ARG:CG	2.13	0.53
1:A:530:ASP:OD2	1:A:685:THR:HA	2.09	0.53
2:B:388:GLN:HB3	2:B:428:PHE:CE1	2.43	0.53
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.91	0.53
1:A:231:PHE:HE2	1:A:249:VAL:HG12	1.74	0.53
1:A:511:LEU:N	1:A:511:LEU:CD2	2.72	0.53
2:B:387:GLU:OE2	2:B:412:LYS:HE3	2.09	0.52
1:A:265:GLY:O	1:A:295:ARG:HD3	2.10	0.52
1:A:329:LEU:N	1:A:329:LEU:CD1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HD22	1:A:273:LEU:H	1.73	0.52
1:A:273:LEU:N	1:A:273:LEU:CD2	2.72	0.52
1:A:548:SER:O	1:A:552:TRP:HB3	2.09	0.52
1:A:361:PRO:HB2	1:A:363:TYR:CE2	2.43	0.51
2:B:400:ARG:NH1	2:B:400:ARG:CG	2.73	0.51
1:A:438:GLN:HB3	2:B:352:ILE:HG21	1.93	0.51
1:A:804:ILE:HG23	1:A:804:ILE:O	2.09	0.51
1:A:508:LEU:N	1:A:508:LEU:HD23	2.26	0.51
1:A:649:SER:HB3	1:A:653:ARG:HH12	1.75	0.51
1:A:672:ASP:HB3	1:A:675:VAL:HG22	1.93	0.51
1:A:384:ARG:HH22	2:B:312:LYS:C	2.09	0.51
1:A:527:GLN:NE2	1:A:683:SER:O	2.44	0.51
1:A:465:ALA:CB	1:A:479:LEU:HD22	2.41	0.51
1:A:319:THR:CB	1:A:572:SER:HB3	2.41	0.50
1:A:780:ILE:HB	1:A:796:LEU:HB3	1.94	0.50
1:A:435:VAL:O	1:A:439:GLU:HG3	2.10	0.50
1:A:437:THR:HA	1:A:440:GLU:HG2	1.93	0.50
2:B:334:VAL:HG12	2:B:335:LEU:HD23	1.94	0.50
2:B:369:PRO:HB2	2:B:370:TYR:HD2	1.76	0.50
1:A:340:ASN:HA	1:A:560:PHE:CZ	2.47	0.49
1:A:430:HIS:HA	1:A:433:LYS:HE2	1.94	0.49
1:A:510:GLU:HG2	1:A:511:LEU:HD23	1.94	0.49
2:B:384:THR:O	2:B:388:GLN:HG3	2.12	0.49
1:A:205:GLN:O	1:A:209:VAL:HG23	2.13	0.49
1:A:701:PRO:HG2	1:A:701:PRO:O	2.13	0.49
1:A:335:THR:O	1:A:335:THR:OG1	2.23	0.49
2:B:402:PHE:HB2	2:B:414:VAL:HG13	1.95	0.49
2:B:404:ALA:O	2:B:407:ASP:N	2.44	0.48
1:A:456:LYS:CA	2:B:370:TYR:HE1	2.24	0.48
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.48	0.48
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.95	0.48
1:A:311:ASP:OD1	1:A:311:ASP:N	2.45	0.48
2:B:434:LEU:O	2:B:438:GLU:HG3	2.13	0.48
1:A:730:ILE:O	1:A:734:ILE:HG12	2.14	0.48
2:B:369:PRO:HB2	2:B:370:TYR:CD2	2.49	0.48
1:A:732:LYS:O	1:A:736:GLY:N	2.41	0.47
1:A:378:VAL:HG21	1:A:528:ILE:CG2	2.43	0.47
1:A:508:LEU:N	1:A:508:LEU:CD2	2.77	0.47
1:A:370:VAL:HG21	1:A:528:ILE:CD1	2.40	0.47
1:A:370:VAL:HG13	1:A:374:LYS:HB3	1.95	0.47
1:A:510:GLU:HG2	1:A:511:LEU:CD2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:684:THR:HG22	1:A:686:ALA:H	1.79	0.47
1:A:363:TYR:HD1	1:A:734:ILE:HD12	1.80	0.47
1:A:665:CYS:O	1:A:744:LYS:N	2.43	0.47
1:A:216:ARG:O	1:A:220:LEU:HD23	2.14	0.47
1:A:694:PHE:HA	1:A:704:LEU:O	2.15	0.47
1:A:363:TYR:CD1	1:A:734:ILE:HG23	2.50	0.46
1:A:267:TYR:CD1	1:A:267:TYR:N	2.83	0.46
2:B:368:GLU:N	2:B:369:PRO:HD3	2.30	0.46
1:A:273:LEU:HD23	1:A:273:LEU:C	2.36	0.46
1:A:802:HIS:ND1	1:A:802:HIS:N	2.63	0.46
2:B:415:VAL:HG13	2:B:416:GLN:H	1.81	0.46
1:A:773:TYR:HE1	1:A:808:PRO:HB3	1.78	0.46
1:A:352:GLU:HB2	1:A:568:ARG:HB2	1.97	0.46
1:A:214:ARG:NH1	1:A:215:ASN:OD1	2.49	0.46
1:A:526:ARG:CG	1:A:526:ARG:NH1	2.77	0.46
1:A:541:ALA:HB2	1:A:761:TYR:CZ	2.51	0.45
2:B:437:TRP:HE3	2:B:438:GLU:HG2	1.80	0.45
1:A:297:LEU:HB2	1:A:304:VAL:HG11	1.98	0.45
1:A:465:ALA:HB2	1:A:479:LEU:HD22	1.98	0.45
1:A:317:VAL:O	1:A:317:VAL:HG12	2.15	0.45
1:A:283:ILE:HG12	1:A:622:LEU:HB3	1.99	0.45
1:A:758:ARG:HA	1:A:758:ARG:HD3	1.72	0.45
1:A:354:ALA:C	1:A:565:LEU:HD12	2.37	0.45
1:A:574:VAL:CB	1:A:575:PRO:HD3	2.42	0.45
1:A:680:HIS:CG	1:A:730:ILE:HD12	2.52	0.45
1:A:808:PRO:O	1:A:810:THR:HG23	2.17	0.44
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.47	0.44
1:A:438:GLN:HB3	2:B:352:ILE:CG2	2.47	0.44
1:A:526:ARG:HG3	1:A:526:ARG:NH1	2.22	0.44
1:A:284:ILE:HD13	1:A:590:VAL:HG11	1.99	0.44
1:A:448:MET:HB3	2:B:363:LEU:HD21	2.00	0.44
1:A:791:GLN:HE21	1:A:791:GLN:HB2	1.57	0.44
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.72	0.43
1:A:382:PHE:CZ	1:A:386:LEU:HD11	2.53	0.43
1:A:594:ARG:HA	1:A:640:VAL:O	2.17	0.43
1:A:482:SER:OG	2:B:397:LYS:HE2	2.18	0.43
1:A:508:LEU:HD23	1:A:508:LEU:H	1.82	0.43
2:B:376:ILE:N	2:B:376:ILE:CD1	2.72	0.43
1:A:188:MET:CE	1:A:200:ILE:HA	2.49	0.43
1:A:325:TYR:CE1	1:A:665:CYS:HB3	2.53	0.43
1:A:720:ASP:OD1	1:A:748:VAL:HG12	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:810:THR:HG22	3:A:901:Y0Z:C14	2.48	0.43
2:B:415:VAL:HG13	2:B:416:GLN:N	2.33	0.43
1:A:188:MET:HE1	1:A:199:ILE:HG22	2.01	0.43
1:A:209:VAL:HG12	1:A:213:ILE:CD1	2.46	0.43
2:B:420:PHE:CE1	2:B:424:TYR:CD2	3.07	0.43
1:A:540:ASN:HB3	1:A:547:LEU:HD21	2.01	0.43
1:A:180:GLN:HA	1:A:339:GLY:HA2	2.01	0.42
1:A:595:TYR:CZ	1:A:641:PRO:HD2	2.54	0.42
1:A:600:CYS:SG	1:A:795:ARG:HB3	2.59	0.42
1:A:663:VAL:CG1	1:A:747:VAL:HB	2.50	0.42
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.76	0.42
1:A:231:PHE:CE2	1:A:249:VAL:HG12	2.53	0.42
1:A:374:LYS:HD3	1:A:374:LYS:HA	1.33	0.42
1:A:332:MET:HG3	1:A:333:VAL:HG23	2.00	0.42
1:A:412:LEU:HD13	1:A:533:PHE:CE2	2.54	0.42
2:B:368:GLU:H	2:B:369:PRO:HD3	1.85	0.42
1:A:719:SER:OG	1:A:722:VAL:HG23	2.20	0.42
1:A:485:ARG:HD3	1:A:485:ARG:C	2.40	0.42
1:A:691:LEU:HD22	1:A:705:ALA:HB1	2.02	0.42
2:B:397:LYS:HD3	2:B:398:TYR:CZ	2.54	0.42
2:B:420:PHE:CD1	2:B:424:TYR:CD2	3.08	0.42
1:A:649:SER:HB3	1:A:653:ARG:NH1	2.34	0.41
1:A:273:LEU:HD22	1:A:273:LEU:N	2.35	0.41
2:B:382:ARG:C	2:B:412:LYS:NZ	2.69	0.41
2:B:389:LEU:HD23	2:B:389:LEU:HA	1.91	0.41
2:B:391:ALA:HB1	2:B:420:PHE:HE2	1.86	0.41
1:A:255:TYR:CE2	1:A:256:LEU:HD23	2.56	0.41
1:A:340:ASN:HA	1:A:560:PHE:CE2	2.56	0.41
1:A:378:VAL:HG23	1:A:379:GLU:N	2.35	0.41
1:A:671:TRP:O	1:A:673:PRO:HD3	2.20	0.41
1:A:707:VAL:HG11	1:A:715:MET:HG3	2.02	0.41
1:A:174:VAL:HG12	1:A:219:GLN:OE1	2.21	0.40
1:A:349:VAL:HG21	1:A:577:ALA:CB	2.51	0.40
1:A:435:VAL:CG1	2:B:349:ILE:HG13	2.51	0.40
1:A:438:GLN:HE22	2:B:353:LYS:HG3	1.86	0.40
1:A:515:PRO:O	1:A:515:PRO:CG	2.70	0.40
1:A:695:TRP:HE3	1:A:697:LEU:HD21	1.87	0.40
3:A:901:Y0Z:O4	3:A:901:Y0Z:C9	2.69	0.40
1:A:402:ASN:O	1:A:403:ASN:HB2	2.20	0.40
1:A:319:THR:HB	1:A:572:SER:HB3	2.03	0.40
1:A:437:THR:OG1	1:A:508:LEU:HD21	2.22	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)
1:A:719:SER:OG	2:B:436:GLU:OE2[7_555]	2.18	0.02

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	664/871 (76%)	641 (96%)	23 (4%)	0	100 100
2	B	131/144 (91%)	126 (96%)	4 (3%)	1 (1%)	19 28
All	All	795/1015 (78%)	767 (96%)	27 (3%)	1 (0%)	51 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	379	CYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	566/715 (79%)	527 (93%)	39 (7%)	15 23
2	B	117/125 (94%)	99 (85%)	18 (15%)	2 2
All	All	683/840 (81%)	626 (92%)	57 (8%)	11 16

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	266	ILE
1	A	267	TYR
1	A	269	ARG
1	A	273	LEU
1	A	349	VAL
1	A	374	LYS
1	A	377	MET
1	A	446	ASN
1	A	447	LYS
1	A	449	VAL
1	A	455	ILE
1	A	456	LYS
1	A	458	LEU
1	A	472	ARG
1	A	506	GLU
1	A	508	LEU
1	A	509	GLN
1	A	511	LEU
1	A	512	GLU
1	A	524	ARG
1	A	526	ARG
1	A	538	PHE
1	A	556	ASP
1	A	563	SER
1	A	564	HIS
1	A	565	LEU
1	A	568	ARG
1	A	569	ASN
1	A	571	TYR
1	A	580	GLU
1	A	645	GLU
1	A	703	LEU
1	A	704	LEU
1	A	706	LEU
1	A	718	ILE
1	A	771	ASN
1	A	791	GLN
1	A	801	GLU
1	A	824	ARG
2	B	316	LEU
2	B	317	SER
2	B	320	ASP

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Mol	Chain	Res	Type
2	B	327	ASN
2	B	332	THR
2	B	347	ARG
2	B	353	LYS
2	B	359	LEU
2	B	360	LYS
2	B	368	GLU
2	B	370	TYR
2	B	376	ILE
2	B	377	GLN
2	B	382	ARG
2	B	400	ARG
2	B	409	ILE
2	B	411	ASN
2	B	412	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	259	HIS
1	A	422	HIS
1	A	446	ASN
1	A	791	GLN
1	A	812	HIS
2	B	393	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
3	Y0Z	A	901	-	73,79,79	1.48	10 (13%)	88,118,118	1.03	8 (9%)

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	Y0Z	A	901	-	-	13/47/67/67	0/8/8/8

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	Y0Z	C5-N1	-7.61	1.32	1.42
3	A	901	Y0Z	C25-C28	-4.13	1.32	1.43
3	A	901	Y0Z	O5-C30	-2.76	1.37	1.43
3	A	901	Y0Z	O6-C31	-2.59	1.36	1.43
3	A	901	Y0Z	C37-N7	-2.54	1.30	1.34
3	A	901	Y0Z	C5-C4	-2.45	1.36	1.40
3	A	901	Y0Z	C6-C7	-2.35	1.36	1.39
3	A	901	Y0Z	C29-C30	-2.26	1.49	1.52
3	A	901	Y0Z	P1-O9	-2.07	1.45	1.55
3	A	901	Y0Z	P2-O13	-2.03	1.45	1.55

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	Y0Z	C25-C28-N4	3.52	117.19	110.99
3	A	901	Y0Z	O15-C36-C42	-2.86	102.74	106.93
3	A	901	Y0Z	C38-C39-N8	2.62	124.33	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	901	Y0Z	C15-C16-C17	-2.48	112.60	120.62
3	A	901	Y0Z	C24-C16-C17	2.38	128.32	120.44
3	A	901	Y0Z	C11-C12-C24	2.26	124.25	120.54
3	A	901	Y0Z	C10-C11-C12	2.18	120.68	112.70
3	A	901	Y0Z	O13-P2-O12	2.06	122.42	112.24

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	901	Y0Z	C10-C9-N1-C5
3	A	901	Y0Z	C10-C9-N1-C25
3	A	901	Y0Z	O1-C9-N1-C5
3	A	901	Y0Z	O1-C9-N1-C25
3	A	901	Y0Z	C16-C17-N2-C18
3	A	901	Y0Z	P2-O11-P1-O8
3	A	901	Y0Z	O2-C17-N2-C18
3	A	901	Y0Z	C9-C10-C11-C12
3	A	901	Y0Z	C19-C18-N2-C17
3	A	901	Y0Z	C10-C11-C12-C24
3	A	901	Y0Z	C10-C11-C12-C13
3	A	901	Y0Z	O14-C34-C35-O15
3	A	901	Y0Z	C23-C18-N2-C17

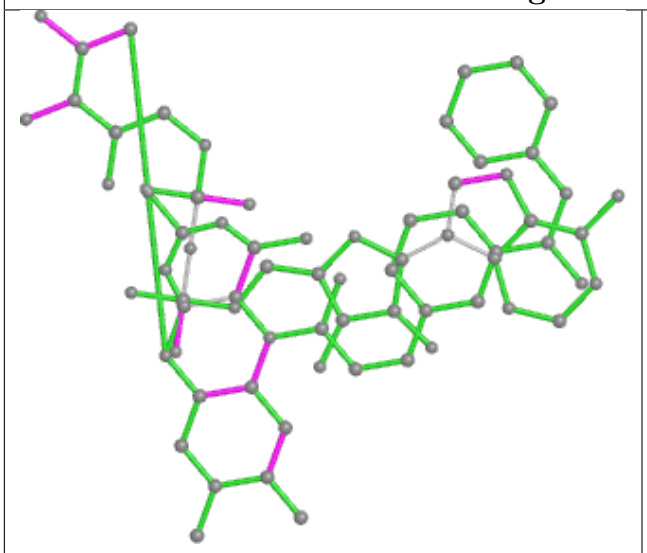
There are no ring outliers.

1 monomer is involved in 2 short contacts:

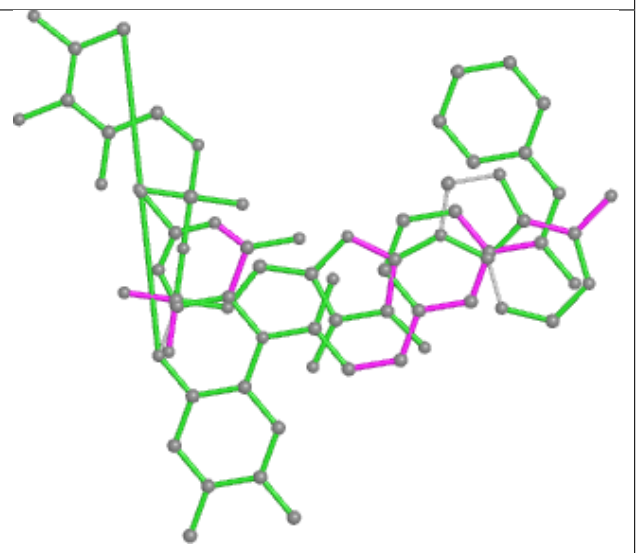
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	Y0Z	2	0

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 then 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.

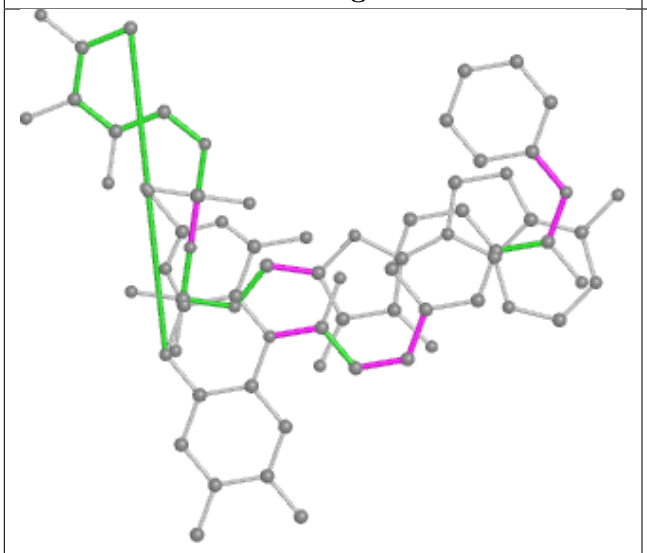
Ligand Y0Z A 901



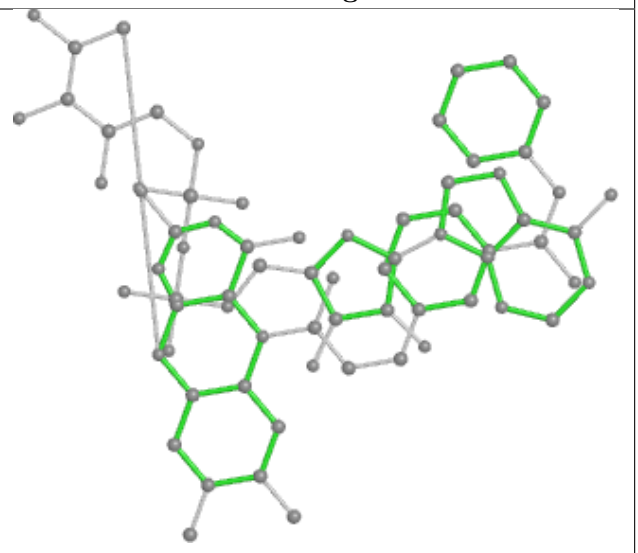
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.45	19 (2%) 51 48	55, 86, 118, 137	0
2	B	133/144 (92%)	0.66	13 (9%) 7 5	83, 116, 136, 158	0
All	All	799/1015 (78%)	0.49	32 (4%) 38 35	55, 92, 126, 158	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	171	PRO	6.1
2	B	308	ARG	4.0
2	B	312	LYS	3.8
1	A	242	TYR	3.5
1	A	273	LEU	3.0
2	B	309	LYS	2.8
1	A	275	THR	2.8
1	A	172	SER	2.8
2	B	374	GLU	2.7
1	A	458	LEU	2.7
2	B	313	GLY	2.6
1	A	487	LEU	2.6
1	A	508	LEU	2.6
1	A	238	LEU	2.5
1	A	455	ILE	2.5
2	B	371	ARG	2.5
1	A	504	LEU	2.5
2	B	375	VAL	2.5
2	B	365	GLY	2.4
2	B	417	VAL	2.4
1	A	235	LEU	2.4
1	A	809	ALA	2.3
2	B	378	LYS	2.2
1	A	359	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	436	GLU	2.1
1	A	441	LEU	2.1
1	A	440	GLU	2.1
1	A	449	VAL	2.1
2	B	420	PHE	2.1
1	A	509	GLN	2.0
2	B	402	PHE	2.0
1	A	174	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 monosaccharides in this entry.

6.4 Ligands (i)

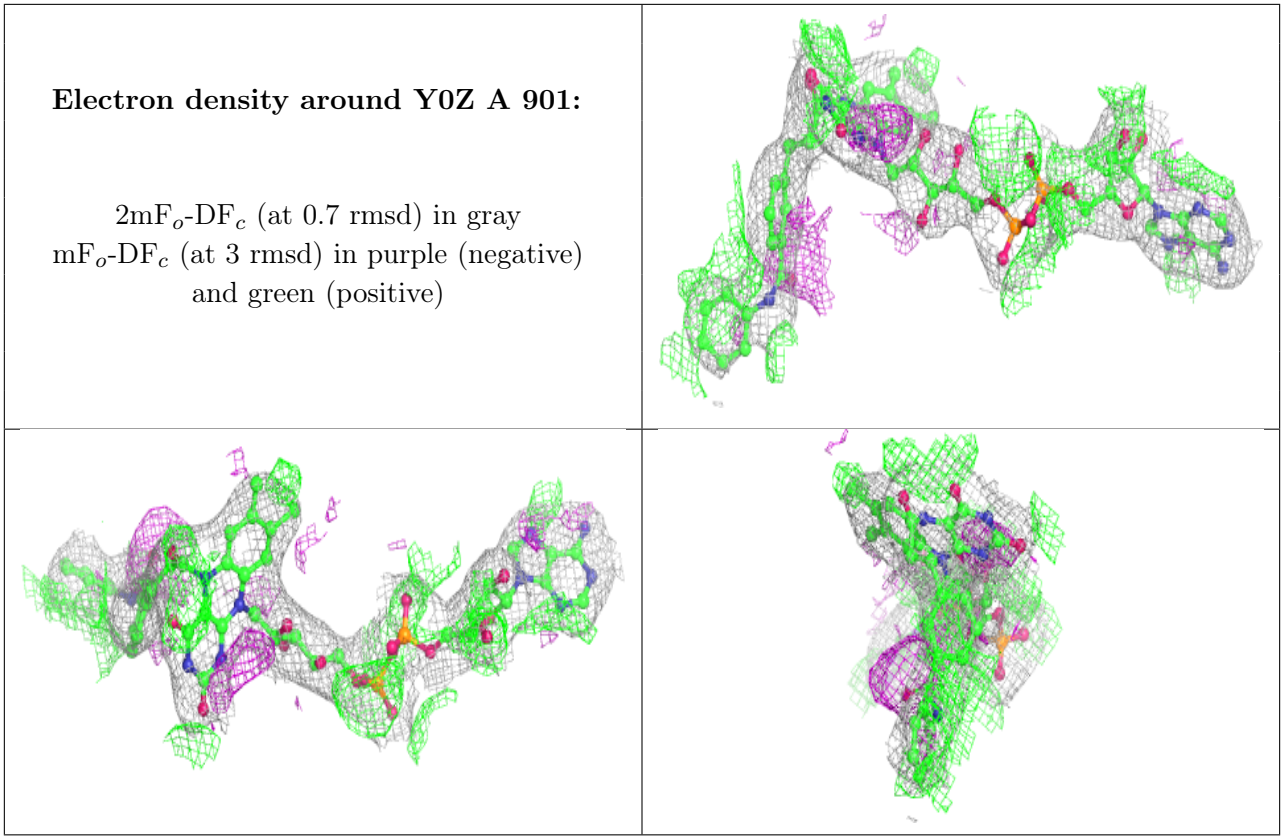
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	Y0Z	A	901	72/72	0.97	0.24	50,72,96,103	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.