



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2025 – 02:41 PM EDT

PDB ID : 8ULZ / pdb\_00008ulz  
Title : LSD1-CoREST in complex with T18 and SNAG peptide  
Authors : Caroli, J.; Mattevi, A.  
Deposited on : 2023-10-17  
Resolution : 3.32 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](mailto: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 Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.45.1

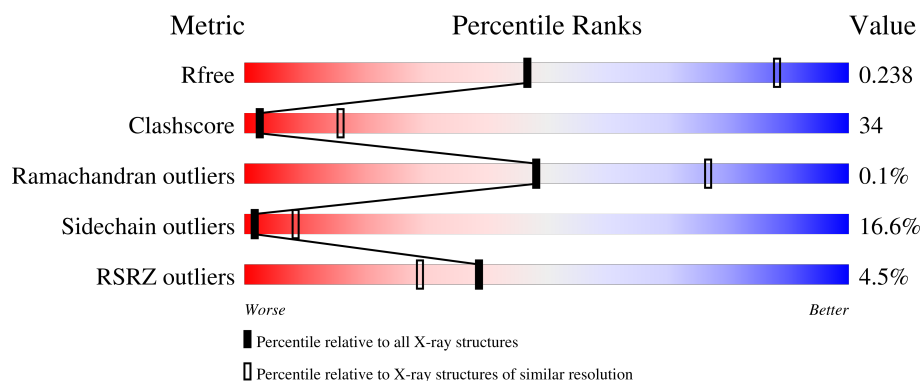
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.32 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))
$R_{free}$	164625	1066 (3.34-3.30)
Clashscore	180529	1111 (3.34-3.30)
Ramachandran outliers	177936	1109 (3.34-3.30)
Sidechain outliers	177891	1108 (3.34-3.30)
RSRZ outliers	164620	1066 (3.34-3.30)

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  $\geq 3$ , 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	C	9	<div> <div>33%</div> <div>11% 11% 11% 11%</div> <div>56%</div> </div>
2	A	871	<div> <div>2%</div> <div>43% 25% 7% 24%</div> </div>
3	B	144	<div> <div>12%</div> <div>56% 24% 12% 8%</div> </div>

## 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 Zinc finger protein SNAI1.

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

- Molecule 2 is a protein called Lysine-specific histone demethylase 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	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

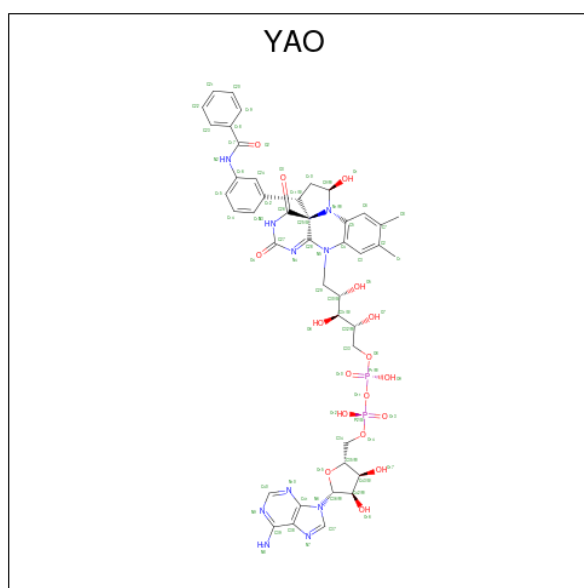
- Molecule 3 is a protein called REST corepressor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	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 4 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxyoxolan-2-yl]methyl (2R,3S,4S)-5-[(1R,3S,3aS,13R)-3-(3-benzamidophenyl)-1-hydroxy-10,11-dimethyl-4,6-dioxo-2,3,5,6-tetrahydro-1H-benzo[*g*]pyrrolo[2,1-*e*]pteridin-8(4H)-yl]-2,3,4-trihydroxypentyl dihydrogen diphosphate (non-preferred name) (CCD ID: YAO) (formula: C<sub>43</sub>H<sub>48</sub>N<sub>10</sub>O<sub>17</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).

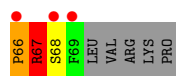
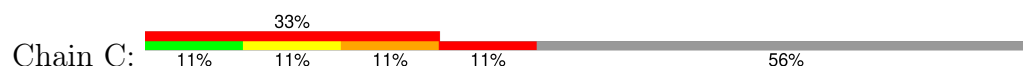


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			72	43	10	17	2		

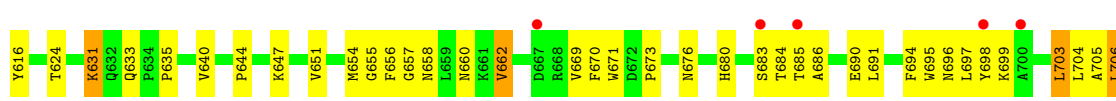
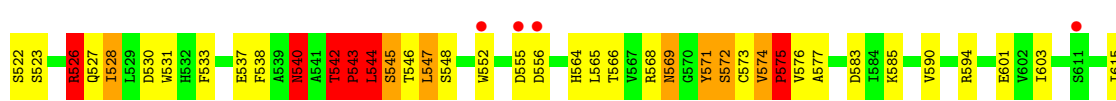
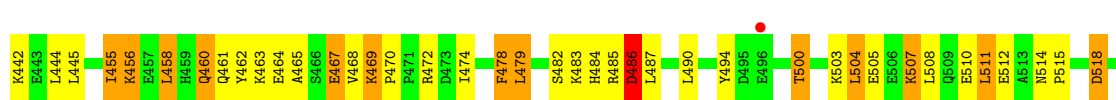
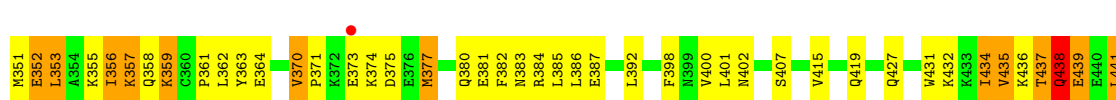
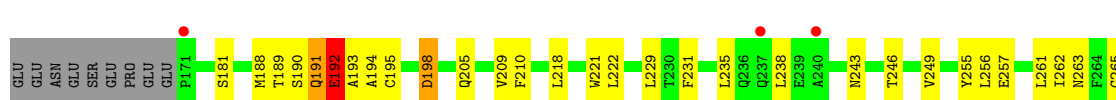
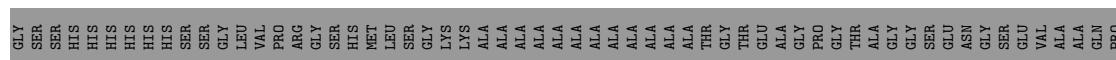
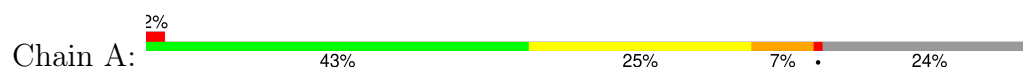
### 3 Residue-property plots

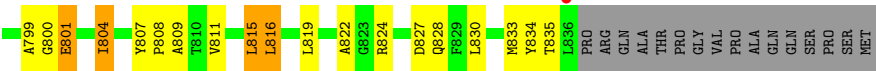
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Zinc finger protein SNAI1

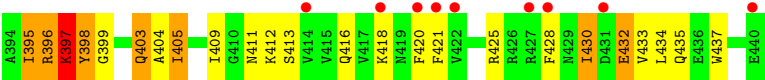


- Molecule 2: Lysine-specific histone demethylase 1A





● Molecule 3: REST corepressor 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.37Å 177.77Å 235.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.49 – 3.32 65.49 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.5 (65.49-3.32) 99.5 (65.49-3.32)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.47 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.199 , 0.231 0.233 , 0.238	Depositor DCC
$R_{free}$ test set	2000 reflections (5.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.9	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 98.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6400	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: YAO

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	C	1.19	0/36	2.13	2/46 (4.3%)
2	A	0.97	30/5331 (0.6%)	1.20	32/7232 (0.4%)
3	B	0.80	1/1091 (0.1%)	1.12	3/1471 (0.2%)
All	All	0.94	31/6458 (0.5%)	1.19	37/8749 (0.4%)

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
2	A	0	1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	575	PRO	C-O	-9.29	1.12	1.24
2	A	543	PRO	C-O	-8.55	1.14	1.23
2	A	574	VAL	C-O	-8.29	1.17	1.24
2	A	191	GLN	C-O	-8.09	1.14	1.24
2	A	655	GLY	CA-C	7.96	1.57	1.52
3	B	405	ILE	C-O	-7.55	1.15	1.24
2	A	577	ALA	C-O	-7.24	1.15	1.24
2	A	545	SER	CA-CB	-7.22	1.42	1.53
2	A	544	LEU	C-O	-7.20	1.14	1.24
2	A	576	VAL	C-O	-7.15	1.15	1.24
2	A	542	THR	C-O	-7.02	1.15	1.24
2	A	572	SER	C-O	-6.92	1.15	1.24
2	A	194	ALA	C-O	-6.81	1.16	1.24
2	A	192	GLU	C-O	-6.79	1.15	1.24
2	A	540	ASN	C-O	-6.75	1.15	1.24

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	547	LEU	C-O	-6.73	1.15	1.23
2	A	190	SER	CA-CB	-6.58	1.43	1.53
2	A	190	SER	C-O	-6.47	1.16	1.24
2	A	189	THR	C-O	-6.28	1.15	1.23
2	A	438	GLN	C-O	-6.13	1.16	1.24
2	A	660	ASN	C-O	-5.86	1.16	1.23
2	A	193	ALA	C-O	-5.82	1.17	1.24
2	A	662	VAL	C-O	-5.75	1.18	1.24
2	A	571	TYR	C-O	-5.73	1.16	1.24
2	A	470	PRO	C-O	-5.72	1.20	1.24
2	A	526	ARG	C-O	-5.60	1.17	1.24
2	A	573	CYS	C-O	-5.58	1.17	1.24
2	A	359	LYS	C-O	-5.30	1.17	1.24
2	A	635	PRO	C-O	-5.17	1.17	1.23
2	A	546	THR	C-O	-5.12	1.18	1.24
2	A	575	PRO	N-CD	-5.08	1.40	1.47

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	437	THR	CA-CB-OG1	-9.54	95.28	109.60
2	A	543	PRO	CB-CA-C	-7.99	100.51	110.98
2	A	486	ASP	CA-C-N	-7.93	107.20	120.68
2	A	486	ASP	C-N-CA	-7.93	107.20	120.68
2	A	189	THR	CB-CA-C	-7.85	94.15	110.40
2	A	575	PRO	CB-CA-C	-7.42	100.38	112.62
2	A	574	VAL	CB-CA-C	-7.26	104.49	114.00
2	A	486	ASP	N-CA-C	-6.78	104.11	112.38
2	A	191	GLN	CB-CA-C	-6.75	99.58	110.79
2	A	316	ARG	CG-CD-NE	6.28	125.81	112.00
2	A	546	THR	CB-CA-C	-6.20	100.31	110.85
2	A	731	LEU	O-C-N	5.96	128.43	122.12
2	A	486	ASP	CB-CA-C	-5.87	97.94	110.32
2	A	545	SER	CA-C-O	-5.85	114.35	120.55
3	B	398	TYR	CB-CA-C	5.83	120.24	110.44
2	A	192	GLU	CB-CA-C	-5.82	99.50	110.67
2	A	542	THR	CB-CA-C	-5.78	102.59	110.22
2	A	469	LYS	CA-C-N	5.77	123.82	119.66
2	A	469	LYS	C-N-CA	5.77	123.82	119.66
1	C	67	ARG	CA-C-N	-5.72	114.36	122.94
1	C	67	ARG	C-N-CA	-5.72	114.36	122.94
2	A	543	PRO	N-CA-CB	-5.67	98.06	103.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	GLY	CA-C-O	-5.64	118.25	122.37
3	B	397	LYS	CA-C-N	-5.50	113.34	122.08
3	B	397	LYS	C-N-CA	-5.50	113.34	122.08
2	A	573	CYS	CA-C-N	-5.49	115.94	120.33
2	A	573	CYS	C-N-CA	-5.49	115.94	120.33
2	A	355	LYS	CA-C-N	-5.41	115.88	123.13
2	A	355	LYS	C-N-CA	-5.41	115.88	123.13
2	A	660	ASN	CA-CB-CG	-5.32	107.28	112.60
2	A	348	GLN	CA-C-N	-5.26	116.25	123.14
2	A	348	GLN	C-N-CA	-5.26	116.25	123.14
2	A	545	SER	CA-C-N	5.25	127.74	120.29
2	A	545	SER	C-N-CA	5.25	127.74	120.29
2	A	735	PHE	CB-CA-C	-5.21	101.68	110.44
2	A	436	LYS	N-CA-C	-5.14	105.67	111.28
2	A	439	GLU	CA-C-O	-5.03	115.22	120.55

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	522	SER	Mainchain

## 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	C	35	0	34	7	0
2	A	5217	0	5249	360	0
3	B	1076	0	1091	116	0
4	A	72	0	0	12	0
All	All	6400	0	6374	430	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 34.

All (430) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:441:LEU:HG	3:B:356:ASN:ND2	1.34	1.40
1:C:66:PRO:HD3	4:A:901:YAO:C23	1.68	1.23
2:A:670:PHE:CE2	2:A:740:VAL:HG22	1.81	1.15
2:A:478:PHE:CE2	3:B:393:GLN:CB	2.31	1.14
2:A:478:PHE:CD2	3:B:393:GLN:HB2	1.84	1.12
2:A:456:LYS:HB2	3:B:370:TYR:CE2	1.84	1.11
2:A:478:PHE:HE2	3:B:393:GLN:C	1.58	1.10
2:A:695:TRP:HE1	2:A:706:LEU:HD13	1.16	1.10
2:A:456:LYS:HB2	3:B:370:TYR:HE2	0.97	1.10
2:A:478:PHE:CD2	3:B:393:GLN:CB	2.35	1.09
2:A:319:THR:HB	2:A:572:SER:HB3	1.26	1.08
2:A:537:GLU:HG2	2:A:544:LEU:CD2	1.85	1.06
2:A:316:ARG:NH2	2:A:801:GLU:OE1	1.89	1.05
2:A:456:LYS:CB	3:B:370:TYR:HE2	1.69	1.05
2:A:730:ILE:O	2:A:734:ILE:HD13	1.56	1.04
3:B:368:GLU:OE1	3:B:371:ARG:NH1	1.92	1.02
2:A:720:ASP:O	2:A:724:VAL:CG2	2.08	1.01
3:B:399:GLY:HA3	3:B:437:TRP:CZ2	1.95	1.00
3:B:432:GLU:O	3:B:435:GLN:HG2	1.58	1.00
2:A:568:ARG:NH1	2:A:699:LYS:N	2.09	1.00
2:A:631:LYS:HE2	2:A:651:VAL:O	1.62	1.00
2:A:695:TRP:HE1	2:A:706:LEU:CD1	1.75	1.00
2:A:319:THR:CB	2:A:572:SER:HB3	1.92	0.99
2:A:478:PHE:CE2	3:B:393:GLN:HB2	1.96	0.98
2:A:478:PHE:CE2	3:B:393:GLN:HB3	1.97	0.96
2:A:478:PHE:CE2	3:B:393:GLN:C	2.42	0.96
2:A:537:GLU:HG2	2:A:544:LEU:HD21	1.43	0.96
3:B:396:ARG:HG3	3:B:396:ARG:HH11	1.29	0.96
2:A:657:GLY:C	2:A:752:ARG:NH2	2.23	0.96
2:A:441:LEU:HG	3:B:356:ASN:HD21	1.26	0.96
2:A:341:PRO:HG3	2:A:816:LEU:HD11	1.47	0.96
2:A:407:SER:CB	2:A:545:SER:O	2.14	0.95
2:A:720:ASP:O	2:A:724:VAL:HG22	1.65	0.95
2:A:485:ARG:NH2	3:B:404:ALA:HB2	1.82	0.94
2:A:353:LEU:HD13	2:A:565:LEU:HD22	1.47	0.93
2:A:657:GLY:C	2:A:752:ARG:HH21	1.75	0.93
2:A:441:LEU:HG	3:B:356:ASN:HD22	1.15	0.93
2:A:538:PHE:CE1	2:A:706:LEU:HD21	2.04	0.93
2:A:460:GLN:O	2:A:464:GLU:HG3	1.68	0.93
2:A:441:LEU:CG	3:B:356:ASN:ND2	2.30	0.92
2:A:341:PRO:HG3	2:A:816:LEU:CD1	1.98	0.92
2:A:574:VAL:HB	2:A:575:PRO:HD3	1.52	0.92

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:399:GLY:CA	3:B:437:TRP:CE2	2.53	0.91
3:B:368:GLU:CD	3:B:371:ARG:NH1	2.30	0.90
2:A:456:LYS:HA	3:B:370:TYR:CD2	2.08	0.89
2:A:670:PHE:CE2	2:A:740:VAL:CG2	2.58	0.87
2:A:754:ASP:OD1	2:A:755:PRO:HD2	1.73	0.87
3:B:399:GLY:HA3	3:B:437:TRP:CE2	2.09	0.87
2:A:478:PHE:HE2	3:B:393:GLN:CB	1.78	0.87
1:C:66:PRO:CD	4:A:901:YAO:C23	2.52	0.86
2:A:407:SER:HB2	2:A:545:SER:O	1.76	0.86
2:A:441:LEU:HD12	2:A:441:LEU:O	1.76	0.86
2:A:384:ARG:NH1	3:B:312:LYS:O	2.09	0.85
2:A:478:PHE:CD2	3:B:393:GLN:HB3	2.06	0.85
2:A:537:GLU:HG2	2:A:544:LEU:HD23	1.59	0.84
2:A:478:PHE:HD2	3:B:393:GLN:CB	1.87	0.83
2:A:310:ARG:HD2	4:A:901:YAO:O16	1.79	0.83
2:A:456:LYS:HA	3:B:370:TYR:CE2	2.14	0.83
2:A:310:ARG:HG2	2:A:310:ARG:HH11	1.43	0.83
2:A:695:TRP:NE1	2:A:706:LEU:CD1	2.42	0.82
2:A:432:LYS:HA	2:A:435:VAL:CG2	2.10	0.82
3:B:368:GLU:CD	3:B:371:ARG:HH12	1.86	0.82
2:A:266:ILE:O	2:A:348:GLN:HG2	1.79	0.82
2:A:370:VAL:HG21	2:A:528:ILE:HD11	1.63	0.81
2:A:350:ASN:O	2:A:350:ASN:ND2	2.14	0.81
2:A:720:ASP:O	2:A:724:VAL:HG23	1.80	0.80
2:A:815:LEU:HD12	2:A:815:LEU:O	1.81	0.80
2:A:527:GLN:NE2	2:A:683:SER:O	2.15	0.79
2:A:657:GLY:CA	2:A:752:ARG:HH22	1.95	0.79
3:B:430:ILE:N	3:B:430:ILE:HD12	1.98	0.79
3:B:395:ILE:HD13	3:B:430:ILE:HG21	1.65	0.79
2:A:690:GLU:OE2	2:A:726:ARG:NH1	2.14	0.78
2:A:547:LEU:HD22	2:A:552:TRP:HB2	1.65	0.78
2:A:680:HIS:ND1	2:A:730:ILE:HG13	1.99	0.78
3:B:368:GLU:OE2	3:B:371:ARG:NH1	2.16	0.78
2:A:568:ARG:HH12	2:A:699:LYS:N	1.81	0.77
2:A:537:GLU:CG	2:A:544:LEU:HD21	2.14	0.77
2:A:319:THR:HB	2:A:572:SER:CB	2.12	0.77
2:A:478:PHE:HD2	3:B:393:GLN:HB2	1.46	0.77
2:A:568:ARG:HD3	2:A:699:LYS:HG3	1.67	0.77
2:A:730:ILE:C	2:A:730:ILE:HD13	2.11	0.76
2:A:441:LEU:CD1	2:A:445:LEU:HG	2.16	0.76
2:A:544:LEU:HD23	2:A:544:LEU:N	1.98	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:568:ARG:HH11	2:A:699:LYS:N	1.83	0.76
2:A:504:LEU:N	2:A:504:LEU:HD23	2.01	0.76
2:A:569:ASN:OD1	2:A:569:ASN:N	2.12	0.76
2:A:431:TRP:O	2:A:435:VAL:HG22	1.87	0.75
3:B:359:LEU:HD23	3:B:359:LEU:N	2.01	0.75
3:B:376:ILE:N	3:B:376:ILE:HD12	2.01	0.75
2:A:815:LEU:HD12	2:A:815:LEU:C	2.12	0.75
2:A:657:GLY:HA2	2:A:752:ARG:HH22	1.51	0.74
3:B:430:ILE:O	3:B:434:LEU:N	2.13	0.74
2:A:463:LYS:O	2:A:467:GLU:HG2	1.87	0.74
2:A:511:LEU:N	2:A:511:LEU:HD23	2.01	0.74
2:A:793:ILE:HD12	2:A:793:ILE:N	2.02	0.74
1:C:66:PRO:HD3	4:A:901:YAO:C18	2.17	0.74
2:A:370:VAL:HG21	2:A:528:ILE:CD1	2.18	0.74
2:A:695:TRP:NE1	2:A:706:LEU:HD13	1.99	0.73
2:A:266:ILE:O	2:A:348:GLN:CG	2.37	0.73
3:B:397:LYS:HG2	3:B:397:LYS:O	1.88	0.73
2:A:538:PHE:CD1	2:A:706:LEU:CD2	2.71	0.73
2:A:478:PHE:HE2	3:B:393:GLN:CA	2.02	0.72
2:A:441:LEU:HD12	2:A:441:LEU:C	2.12	0.72
2:A:441:LEU:HD11	2:A:445:LEU:HG	1.71	0.72
3:B:399:GLY:HA2	3:B:437:TRP:CD2	2.24	0.72
3:B:430:ILE:HD12	3:B:430:ILE:H	1.52	0.72
2:A:353:LEU:HD13	2:A:565:LEU:CD2	2.19	0.72
2:A:644:PRO:HD2	2:A:780:ILE:CD1	2.19	0.72
2:A:657:GLY:CA	2:A:752:ARG:NH2	2.53	0.71
3:B:396:ARG:HG3	3:B:396:ARG:NH1	2.04	0.71
2:A:657:GLY:O	2:A:752:ARG:NH2	2.24	0.70
2:A:462:TYR:CE2	2:A:484:HIS:HB2	2.26	0.70
2:A:568:ARG:NH1	2:A:699:LYS:CA	2.53	0.70
2:A:538:PHE:CE1	2:A:706:LEU:CD2	2.74	0.70
2:A:438:GLN:HG2	3:B:352:ILE:HG22	1.72	0.70
2:A:801:GLU:HG3	2:A:809:ALA:HA	1.73	0.70
3:B:396:ARG:HG3	3:B:396:ARG:O	1.89	0.70
2:A:755:PRO:HA	2:A:758:ARG:HD3	1.73	0.69
2:A:198:ASP:OD1	2:A:198:ASP:N	2.21	0.69
2:A:286:SER:OG	2:A:313:VAL:HG12	1.93	0.69
2:A:694:PHE:HA	2:A:704:LEU:O	1.93	0.68
2:A:273:LEU:HD12	2:A:273:LEU:N	2.09	0.68
2:A:456:LYS:CA	3:B:370:TYR:CE2	2.77	0.68
2:A:691:LEU:HD22	2:A:727:CYS:SG	2.34	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:425:ARG:HA	3:B:430:ILE:HD11	1.75	0.68
2:A:670:PHE:HE2	2:A:740:VAL:CG2	2.02	0.68
2:A:373:GLU:O	2:A:377:MET:HG3	1.93	0.68
2:A:460:GLN:OE1	2:A:464:GLU:OE2	2.10	0.68
2:A:465:ALA:HB1	2:A:479:LEU:HD23	1.74	0.67
2:A:441:LEU:CG	3:B:356:ASN:HD22	1.98	0.67
2:A:456:LYS:CB	3:B:370:TYR:CE2	2.60	0.67
2:A:670:PHE:HE2	2:A:740:VAL:HG22	1.47	0.67
3:B:399:GLY:CA	3:B:437:TRP:CD2	2.78	0.67
2:A:295:ARG:HG2	2:A:295:ARG:HH21	1.59	0.66
2:A:310:ARG:HG2	2:A:310:ARG:NH1	2.07	0.66
2:A:458:LEU:HB3	2:A:487:LEU:HD13	1.78	0.66
3:B:399:GLY:HA3	3:B:437:TRP:CH2	2.30	0.66
2:A:335:THR:HG21	4:A:901:YAO:C14	2.27	0.65
2:A:526:ARG:HG3	2:A:526:ARG:O	1.95	0.65
2:A:465:ALA:CB	2:A:479:LEU:HD23	2.26	0.65
2:A:644:PRO:HD2	2:A:780:ILE:HD12	1.77	0.65
2:A:297:LEU:HD21	2:A:822:ALA:HA	1.77	0.65
3:B:367:ILE:HD11	3:B:371:ARG:NH2	2.11	0.65
2:A:435:VAL:HG13	3:B:349:ILE:HG13	1.79	0.65
2:A:754:ASP:OD1	2:A:755:PRO:CD	2.44	0.64
2:A:328:ASP:OD2	2:A:571:TYR:N	2.20	0.64
2:A:341:PRO:HG3	2:A:816:LEU:HD12	1.79	0.63
3:B:403:GLN:NE2	3:B:403:GLN:O	2.30	0.63
2:A:362:LEU:HD23	2:A:531:TRP:CE2	2.34	0.62
2:A:231:PHE:HE1	2:A:249:VAL:HG12	1.64	0.62
2:A:478:PHE:CE2	3:B:393:GLN:O	2.52	0.62
2:A:793:ILE:HD12	2:A:793:ILE:H	1.63	0.62
3:B:430:ILE:HA	3:B:433:VAL:HB	1.81	0.62
2:A:724:VAL:HG11	2:A:746:THR:HG21	1.81	0.61
2:A:644:PRO:CD	2:A:780:ILE:CD1	2.77	0.61
2:A:312:ARG:HH11	2:A:312:ARG:HG3	1.65	0.61
2:A:370:VAL:CG2	2:A:528:ILE:HD11	2.29	0.61
2:A:494:TYR:CD2	3:B:367:ILE:HD12	2.36	0.61
2:A:740:VAL:HG12	2:A:740:VAL:O	1.99	0.61
2:A:266:ILE:H	2:A:348:GLN:CD	2.08	0.61
2:A:750:ARG:HB3	2:A:753:ALA:HB3	1.83	0.61
2:A:789:ALA:HB1	2:A:790:PRO:HD2	1.82	0.60
2:A:316:ARG:HD2	2:A:760:SER:O	2.01	0.60
2:A:657:GLY:HA2	2:A:752:ARG:NH2	2.16	0.60
2:A:384:ARG:NH2	3:B:312:LYS:O	2.34	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:662:VAL:HB	2:A:705:ALA:HB3	1.83	0.60
2:A:716:GLU:OE1	2:A:753:ALA:HB2	2.01	0.60
2:A:383:ASN:O	2:A:387:GLU:HG3	2.01	0.60
2:A:568:ARG:HH12	2:A:699:LYS:CA	2.14	0.60
2:A:333:VAL:HG12	2:A:565:LEU:O	2.02	0.60
2:A:188:MET:HE3	2:A:210:PHE:CE2	2.36	0.60
2:A:444:LEU:HD22	2:A:500:THR:HG22	1.82	0.60
2:A:266:ILE:N	2:A:348:GLN:OE1	2.22	0.60
2:A:721:ASP:HA	2:A:724:VAL:HG23	1.83	0.59
3:B:395:ILE:HG21	3:B:430:ILE:HG22	1.83	0.59
2:A:356:ILE:HG22	2:A:356:ILE:O	2.01	0.59
2:A:530:ASP:OD2	2:A:685:THR:HG22	2.02	0.59
2:A:478:PHE:HD1	2:A:478:PHE:O	1.85	0.59
2:A:538:PHE:CD1	2:A:706:LEU:HD23	2.36	0.59
3:B:327:ASN:ND2	3:B:330:ALA:HB2	2.17	0.59
2:A:644:PRO:CD	2:A:780:ILE:HD12	2.32	0.59
2:A:317:VAL:HG12	2:A:317:VAL:O	2.02	0.59
2:A:537:GLU:CG	2:A:544:LEU:CD2	2.72	0.59
2:A:684:THR:HG22	2:A:686:ALA:H	1.67	0.59
2:A:192:GLU:HG2	2:A:210:PHE:HZ	1.68	0.59
2:A:458:LEU:HB3	2:A:487:LEU:CD1	2.33	0.59
2:A:804:ILE:HG23	2:A:804:ILE:O	2.02	0.59
3:B:399:GLY:N	3:B:437:TRP:CE2	2.71	0.59
2:A:407:SER:OG	2:A:545:SER:O	2.21	0.58
2:A:566:THR:HG21	2:A:697:LEU:HD22	1.85	0.58
2:A:468:VAL:HG12	2:A:468:VAL:O	2.01	0.58
3:B:359:LEU:HD23	3:B:359:LEU:H	1.68	0.58
2:A:319:THR:HG22	2:A:319:THR:O	2.02	0.58
2:A:434:ILE:HG21	3:B:349:ILE:HD13	1.85	0.58
2:A:670:PHE:CZ	2:A:740:VAL:HG22	2.36	0.58
3:B:370:TYR:N	3:B:370:TYR:HD1	2.00	0.58
2:A:460:GLN:O	2:A:464:GLU:CG	2.49	0.58
2:A:750:ARG:NH1	2:A:750:ARG:HG3	2.17	0.58
2:A:316:ARG:CD	2:A:760:SER:O	2.52	0.58
2:A:352:GLU:HB3	2:A:568:ARG:HB2	1.84	0.58
2:A:455:ILE:HD11	2:A:490:LEU:O	2.04	0.58
2:A:742:GLN:HE21	2:A:742:GLN:CA	2.16	0.58
3:B:420:PHE:HZ	3:B:428:PHE:HE2	1.52	0.58
2:A:568:ARG:NH1	2:A:698:TYR:C	2.61	0.58
2:A:308:GLU:OE2	2:A:310:ARG:HD2	2.03	0.57
2:A:568:ARG:HH12	2:A:698:TYR:C	2.11	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:435:VAL:HG13	3:B:349:ILE:CG1	2.33	0.57
2:A:381:GLU:OE2	3:B:314:MET:HE1	2.04	0.57
2:A:441:LEU:HD11	2:A:445:LEU:CG	2.33	0.57
3:B:432:GLU:O	3:B:435:GLN:CG	2.44	0.57
2:A:310:ARG:CD	4:A:901:YAO:O16	2.51	0.57
2:A:332:MET:HG2	2:A:333:VAL:HG22	1.87	0.57
3:B:370:TYR:N	3:B:370:TYR:CD1	2.72	0.57
2:A:568:ARG:NH1	2:A:699:LYS:HA	2.20	0.56
2:A:542:THR:HG23	2:A:542:THR:O	2.05	0.56
2:A:363:TYR:HD2	2:A:734:ILE:HG13	1.70	0.55
2:A:478:PHE:CD1	2:A:478:PHE:C	2.84	0.55
2:A:568:ARG:HH12	2:A:699:LYS:HA	1.71	0.55
2:A:384:ARG:CZ	3:B:312:LYS:O	2.54	0.55
2:A:511:LEU:HD23	2:A:511:LEU:H	1.71	0.55
2:A:482:SER:O	2:A:486:ASP:OD1	2.25	0.55
2:A:342:MET:HE2	2:A:571:TYR:OH	2.07	0.55
2:A:478:PHE:HD1	2:A:478:PHE:C	2.14	0.55
2:A:485:ARG:HH21	3:B:404:ALA:HB2	1.66	0.55
3:B:363:LEU:HD23	3:B:363:LEU:N	2.22	0.55
3:B:399:GLY:N	3:B:437:TRP:NE1	2.54	0.55
2:A:257:GLU:HG3	2:A:263:ASN:HD22	1.71	0.54
2:A:484:HIS:C	2:A:484:HIS:CD2	2.85	0.54
2:A:427:GLN:NE2	2:A:518:ASP:HA	2.21	0.54
2:A:671:TRP:O	2:A:673:PRO:HD3	2.07	0.54
2:A:716:GLU:HG2	2:A:750:ARG:HG2	1.89	0.54
2:A:392:LEU:HD23	2:A:398:PHE:CD2	2.43	0.54
2:A:583:ASP:OD1	2:A:585:LYS:NZ	2.40	0.54
2:A:574:VAL:HB	2:A:575:PRO:CD	2.33	0.54
3:B:403:GLN:HE21	3:B:403:GLN:C	2.15	0.54
2:A:441:LEU:HD12	2:A:445:LEU:HG	1.89	0.53
2:A:297:LEU:HB2	2:A:304:VAL:HG21	1.90	0.53
2:A:432:LYS:HA	2:A:435:VAL:HG21	1.87	0.53
3:B:413:SER:OG	3:B:416:GLN:CG	2.57	0.53
3:B:432:GLU:C	3:B:435:GLN:HG2	2.30	0.53
2:A:533:PHE:O	2:A:537:GLU:HG3	2.08	0.53
2:A:456:LYS:CA	3:B:370:TYR:HE2	2.13	0.53
2:A:331:ALA:HA	4:A:901:YAO:N1	2.24	0.53
2:A:456:LYS:HA	3:B:370:TYR:HD2	1.64	0.53
2:A:514:ASN:N	2:A:515:PRO:CD	2.72	0.53
2:A:295:ARG:CG	2:A:295:ARG:NH2	2.72	0.53
3:B:397:LYS:HD3	3:B:398:TYR:CE2	2.44	0.53

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:442:LYS:HE3	3:B:355:THR:HG21	1.92	0.52
2:A:568:ARG:HH11	2:A:699:LYS:HG3	1.73	0.52
2:A:510:GLU:HG2	2:A:511:LEU:HD23	1.90	0.52
2:A:695:TRP:CE3	2:A:697:LEU:HD11	2.44	0.52
3:B:403:GLN:NE2	3:B:403:GLN:CA	2.73	0.52
2:A:485:ARG:CZ	3:B:404:ALA:HB2	2.39	0.52
2:A:507:LYS:O	2:A:510:GLU:HB3	2.10	0.52
3:B:369:PRO:HB2	3:B:370:TYR:HD1	1.74	0.52
2:A:333:VAL:HG23	4:A:901:YAO:O3	2.10	0.52
2:A:478:PHE:HD2	3:B:393:GLN:CD	2.17	0.52
2:A:540:ASN:N	2:A:540:ASN:ND2	2.57	0.52
2:A:718:ILE:HG22	2:A:723:ILE:HG13	1.92	0.52
2:A:205:GLN:O	2:A:209:VAL:HG23	2.10	0.51
2:A:734:ILE:CD1	2:A:734:ILE:N	2.73	0.51
2:A:750:ARG:HG3	2:A:750:ARG:HH11	1.74	0.51
2:A:427:GLN:HE21	2:A:518:ASP:HA	1.75	0.51
2:A:295:ARG:HH21	2:A:295:ARG:CG	2.21	0.51
2:A:486:ASP:OD1	2:A:486:ASP:N	2.32	0.51
3:B:413:SER:HG	3:B:416:GLN:H	1.57	0.51
2:A:568:ARG:HD3	2:A:699:LYS:CG	2.39	0.51
2:A:707:VAL:HG11	2:A:715:MET:HG3	1.91	0.51
2:A:631:LYS:HG3	2:A:651:VAL:HG12	1.92	0.51
2:A:441:LEU:CG	3:B:356:ASN:HD21	2.10	0.51
2:A:362:LEU:CD2	2:A:531:TRP:CE2	2.94	0.50
3:B:413:SER:HG	3:B:416:GLN:HG3	1.76	0.50
2:A:373:GLU:O	2:A:377:MET:CG	2.58	0.50
2:A:762:SER:OG	2:A:801:GLU:OE2	2.22	0.50
2:A:793:ILE:HG23	2:A:828:GLN:NE2	2.25	0.50
2:A:815:LEU:C	2:A:815:LEU:CD1	2.84	0.50
2:A:464:GLU:HA	2:A:467:GLU:HG3	1.93	0.50
2:A:656:PHE:CE2	2:A:759:GLY:HA3	2.47	0.50
2:A:335:THR:CG2	4:A:901:YAO:C14	2.89	0.50
2:A:461:GLN:OE1	2:A:483:LYS:HE3	2.12	0.50
2:A:346:SER:O	2:A:349:VAL:O	2.30	0.49
2:A:601:GLU:HA	2:A:616:TYR:O	2.12	0.49
2:A:321:ARG:HG2	2:A:326:VAL:HG22	1.93	0.49
2:A:485:ARG:NH2	3:B:404:ALA:CB	2.66	0.49
3:B:369:PRO:HB2	3:B:370:TYR:CD1	2.46	0.49
3:B:376:ILE:N	3:B:376:ILE:CD1	2.73	0.49
2:A:574:VAL:CB	2:A:575:PRO:HD3	2.32	0.49
2:A:511:LEU:N	2:A:511:LEU:CD2	2.72	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:413:SER:OG	3:B:416:GLN:CB	2.61	0.49
2:A:680:HIS:CG	2:A:730:ILE:HG13	2.47	0.49
2:A:357:LYS:HG3	2:A:676:ASN:OD1	2.13	0.49
2:A:542:THR:OG1	2:A:543:PRO:HD2	2.13	0.48
2:A:742:GLN:CA	2:A:742:GLN:NE2	2.73	0.48
2:A:801:GLU:HG3	2:A:809:ALA:CA	2.43	0.48
2:A:363:TYR:CD1	2:A:363:TYR:N	2.79	0.48
2:A:350:ASN:ND2	2:A:350:ASN:C	2.71	0.48
2:A:273:LEU:N	2:A:273:LEU:CD1	2.74	0.48
2:A:362:LEU:HD21	2:A:531:TRP:CH2	2.48	0.48
2:A:319:THR:HG21	2:A:321:ARG:NH2	2.29	0.48
2:A:458:LEU:HD11	2:A:486:ASP:HB2	1.95	0.48
2:A:255:TYR:CD2	2:A:256:LEU:HD23	2.49	0.48
2:A:750:ARG:O	2:A:753:ALA:HB3	2.13	0.48
2:A:319:THR:HA	2:A:328:ASP:HA	1.96	0.48
3:B:420:PHE:CZ	3:B:428:PHE:HE2	2.29	0.48
3:B:350:GLN:O	3:B:354:GLN:HB2	2.14	0.47
3:B:403:GLN:NE2	3:B:403:GLN:C	2.71	0.47
3:B:432:GLU:HA	3:B:435:GLN:HG2	1.95	0.47
2:A:742:GLN:HG3	2:A:743:PRO:HD2	1.97	0.47
2:A:786:ILE:H	2:A:786:ILE:HD12	1.80	0.47
2:A:793:ILE:HG22	2:A:794:PRO:HD2	1.96	0.47
2:A:363:TYR:CE2	2:A:734:ILE:HG23	2.50	0.47
2:A:568:ARG:HH11	2:A:699:LYS:H	1.58	0.47
2:A:742:GLN:NE2	2:A:742:GLN:HA	2.29	0.47
3:B:418:LYS:O	3:B:421:PHE:HB2	2.15	0.47
2:A:192:GLU:HG2	2:A:210:PHE:CZ	2.49	0.47
2:A:444:LEU:CD2	2:A:500:THR:HG22	2.45	0.47
2:A:624:THR:HG22	2:A:799:ALA:HB3	1.97	0.47
2:A:296:GLN:HG3	2:A:819:LEU:HD22	1.96	0.47
2:A:238:LEU:HB2	2:A:243:ASN:HB3	1.96	0.46
2:A:316:ARG:NE	2:A:760:SER:O	2.47	0.46
2:A:485:ARG:CZ	3:B:404:ALA:CB	2.92	0.46
2:A:730:ILE:O	2:A:734:ILE:CD1	2.46	0.46
3:B:432:GLU:HG3	3:B:435:GLN:NE2	2.30	0.46
2:A:540:ASN:N	2:A:540:ASN:HD22	2.12	0.46
2:A:680:HIS:ND1	2:A:730:ILE:CG1	2.76	0.46
2:A:283:ILE:HD12	2:A:294:ALA:HB2	1.98	0.46
2:A:320:PHE:CD1	2:A:747:VAL:HG21	2.51	0.46
2:A:331:ALA:HA	4:A:901:YAO:C5	2.46	0.46
2:A:474:ILE:HG23	3:B:393:GLN:NE2	2.30	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:456:LYS:CA	3:B:370:TYR:CD2	2.91	0.46
3:B:430:ILE:H	3:B:430:ILE:CD1	2.16	0.46
2:A:353:LEU:HD23	2:A:353:LEU:HA	1.71	0.46
2:A:386:LEU:HA	2:A:386:LEU:HD23	1.61	0.46
2:A:669:VAL:HG11	2:A:673:PRO:HG3	1.98	0.46
3:B:318:GLN:OE1	3:B:318:GLN:HA	2.16	0.45
2:A:485:ARG:C	2:A:487:LEU:N	2.71	0.45
2:A:316:ARG:O	2:A:330:GLY:HA3	2.16	0.45
2:A:514:ASN:N	2:A:515:PRO:HD3	2.32	0.45
2:A:566:THR:HG21	2:A:697:LEU:HD13	1.99	0.45
2:A:235:LEU:HD21	2:A:246:THR:HG22	1.97	0.45
2:A:330:GLY:O	4:A:901:YAO:C6	2.65	0.45
1:C:66:PRO:HB2	2:A:556:ASP:OD1	2.16	0.45
2:A:362:LEU:HD21	2:A:531:TRP:CZ3	2.52	0.45
2:A:691:LEU:CD2	2:A:727:CYS:SG	3.05	0.45
1:C:66:PRO:HG2	2:A:555:ASP:OD1	2.16	0.45
3:B:421:PHE:HE2	3:B:434:LEU:HD11	1.81	0.45
2:A:229:LEU:HA	2:A:229:LEU:HD12	1.84	0.44
2:A:729:ALA:O	2:A:732:LYS:HB2	2.17	0.44
2:A:295:ARG:HG2	2:A:295:ARG:NH2	2.28	0.44
2:A:458:LEU:HD23	2:A:458:LEU:HA	1.67	0.44
3:B:375:VAL:HG23	3:B:375:VAL:O	2.17	0.44
2:A:297:LEU:CB	2:A:304:VAL:HG21	2.46	0.44
2:A:695:TRP:NE1	2:A:706:LEU:HD11	2.28	0.44
3:B:403:GLN:NE2	3:B:403:GLN:HA	2.31	0.44
2:A:188:MET:HG2	2:A:210:PHE:HE2	1.82	0.44
2:A:431:TRP:CE3	2:A:434:ILE:HD12	2.53	0.44
2:A:494:TYR:CE2	3:B:367:ILE:HG23	2.52	0.44
2:A:504:LEU:HD23	2:A:504:LEU:H	1.81	0.44
2:A:542:THR:OG1	2:A:543:PRO:CD	2.65	0.44
2:A:744:LYS:HA	2:A:744:LYS:HD2	1.57	0.44
3:B:372:LEU:HD22	3:B:373:PRO:HD2	1.99	0.44
1:C:66:PRO:O	1:C:67:ARG:HB2	2.16	0.44
2:A:261:LEU:HD23	2:A:261:LEU:HA	1.72	0.44
2:A:494:TYR:CD2	3:B:367:ILE:CD1	3.00	0.44
2:A:603:ILE:HG12	2:A:615:ILE:CD1	2.47	0.44
2:A:721:ASP:CA	2:A:724:VAL:HG23	2.48	0.44
2:A:548:SER:O	2:A:552:TRP:HB3	2.18	0.44
2:A:695:TRP:HB3	2:A:697:LEU:HG	1.99	0.44
2:A:647:LYS:O	2:A:651:VAL:HG23	2.18	0.43
2:A:734:ILE:HG22	2:A:735:PHE:CG	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:362:LEU:CD2	2:A:531:TRP:CD2	3.02	0.43
1:C:66:PRO:CG	4:A:901:YAO:C22	2.96	0.43
2:A:671:TRP:HE1	2:A:696:ASN:ND2	2.16	0.43
2:A:715:MET:HE3	2:A:723:ILE:HG12	2.00	0.43
2:A:658:ASN:HB2	2:A:752:ARG:HH21	1.83	0.43
3:B:432:GLU:CA	3:B:435:GLN:HG2	2.48	0.43
2:A:564:HIS:C	2:A:565:LEU:HD12	2.44	0.43
2:A:684:THR:HG22	2:A:685:THR:N	2.34	0.43
2:A:312:ARG:NH1	2:A:312:ARG:CG	2.82	0.43
2:A:484:HIS:CD2	2:A:484:HIS:O	2.72	0.43
2:A:807:TYR:N	2:A:808:PRO:CD	2.82	0.42
2:A:221:TRP:CD1	2:A:262:ILE:HA	2.54	0.42
2:A:370:VAL:HG12	2:A:375:ASP:HB2	2.01	0.42
2:A:594:ARG:HA	2:A:640:VAL:O	2.19	0.42
3:B:413:SER:OG	3:B:416:GLN:HB2	2.19	0.42
2:A:188:MET:HG2	2:A:210:PHE:CE2	2.54	0.42
2:A:508:LEU:HA	2:A:508:LEU:HD23	1.80	0.42
3:B:413:SER:OG	3:B:416:GLN:N	2.39	0.42
2:A:370:VAL:HG21	2:A:528:ILE:HD13	1.99	0.42
2:A:752:ARG:HA	2:A:759:GLY:N	2.35	0.42
3:B:380:ASN:CG	3:B:381:ALA:H	2.28	0.42
3:B:413:SER:OG	3:B:416:GLN:HG3	2.17	0.42
2:A:255:TYR:CE2	2:A:256:LEU:HD23	2.54	0.42
2:A:181:SER:OG	2:A:218:LEU:HD22	2.20	0.42
2:A:419:GLN:NE2	3:B:314:MET:HA	2.35	0.42
2:A:793:ILE:HG23	2:A:828:GLN:CD	2.44	0.42
2:A:238:LEU:CB	2:A:243:ASN:HB3	2.50	0.42
2:A:441:LEU:HD11	2:A:445:LEU:CD1	2.48	0.42
2:A:322:LYS:NZ	2:A:745:GLU:OE2	2.47	0.42
2:A:353:LEU:HB3	2:A:565:LEU:HD23	2.02	0.42
2:A:463:LYS:O	2:A:467:GLU:CG	2.63	0.42
2:A:730:ILE:HD13	2:A:731:LEU:N	2.34	0.42
2:A:363:TYR:N	2:A:363:TYR:HD1	2.17	0.41
2:A:292:ALA:HB2	2:A:815:LEU:HD13	2.02	0.41
2:A:310:ARG:NH2	2:A:754:ASP:OD2	2.53	0.41
2:A:385:LEU:HD23	2:A:415:VAL:HG12	2.02	0.41
2:A:361:PRO:O	2:A:361:PRO:HG2	2.21	0.41
2:A:654:MET:HB3	2:A:654:MET:HE2	1.90	0.41
2:A:734:ILE:CD1	2:A:734:ILE:H	2.32	0.41
2:A:363:TYR:HE2	2:A:734:ILE:HG23	1.85	0.41
2:A:697:LEU:HD23	2:A:697:LEU:HA	1.96	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:703:LEU:HD22	2:A:703:LEU:HA	1.73	0.41
2:A:827:ASP:CG	2:A:834:TYR:HH	2.24	0.41
2:A:284:ILE:HD13	2:A:590:VAL:HG11	2.02	0.41
2:A:370:VAL:HA	2:A:371:PRO:HD3	1.91	0.41
2:A:363:TYR:CD2	2:A:734:ILE:HG13	2.53	0.41
2:A:434:ILE:CG2	3:B:349:ILE:HD13	2.50	0.41
2:A:462:TYR:CD2	2:A:484:HIS:HB2	2.56	0.41
3:B:363:LEU:N	3:B:363:LEU:CD2	2.83	0.41
2:A:195:CYS:SG	2:A:834:TYR:HE1	2.43	0.41
2:A:478:PHE:HE2	3:B:393:GLN:O	1.85	0.41
3:B:395:ILE:HD13	3:B:430:ILE:CG2	2.44	0.41
2:A:265:GLY:O	2:A:295:ARG:NH2	2.54	0.40
2:A:434:ILE:O	2:A:438:GLN:N	2.47	0.40
2:A:222:LEU:HD23	2:A:222:LEU:HA	1.88	0.40
2:A:382:PHE:C	2:A:384:ARG:N	2.79	0.40
2:A:793:ILE:N	2:A:793:ILE:CD1	2.73	0.40
2:A:333:VAL:CG1	2:A:565:LEU:O	2.68	0.40
2:A:763:TYR:CE1	2:A:765:ALA:HB2	2.56	0.40
2:A:286:SER:CB	2:A:313:VAL:HG12	2.51	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	C	2/9 (22%)	1 (50%)	0	1 (50%)	0	0
2	A	664/871 (76%)	633 (95%)	31 (5%)	0	100	100
3	B	131/144 (91%)	120 (92%)	11 (8%)	0	100	100
All	All	797/1024 (78%)	754 (95%)	42 (5%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	ARG

### 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	C	4/9 (44%)	1 (25%)	3 (75%)	0	0
2	A	566/715 (79%)	478 (84%)	88 (16%)	2	10
3	B	117/125 (94%)	94 (80%)	23 (20%)	1	5
All	All	687/849 (81%)	573 (83%)	114 (17%)	2	8

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	66	PRO
1	C	67	ARG
1	C	68	SER
2	A	191	GLN
2	A	192	GLU
2	A	198	ASP
2	A	268	LYS
2	A	269	ARG
2	A	270	ILE
2	A	273	LEU
2	A	276	LYS
2	A	295	ARG
2	A	298	GLN
2	A	310	ARG
2	A	313	VAL
2	A	319	THR
2	A	329	LEU
2	A	333	VAL
2	A	349	VAL
2	A	350	ASN
2	A	351	MET
2	A	352	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	353	LEU
2	A	356	ILE
2	A	357	LYS
2	A	358	GLN
2	A	359	LYS
2	A	364	GLU
2	A	370	VAL
2	A	374	LYS
2	A	377	MET
2	A	380	GLN
2	A	400	VAL
2	A	401	LEU
2	A	402	ASN
2	A	434	ILE
2	A	435	VAL
2	A	437	THR
2	A	438	GLN
2	A	439	GLU
2	A	441	LEU
2	A	455	ILE
2	A	456	LYS
2	A	458	LEU
2	A	460	GLN
2	A	467	GLU
2	A	469	LYS
2	A	472	ARG
2	A	478	PHE
2	A	479	LEU
2	A	486	ASP
2	A	500	THR
2	A	503	LYS
2	A	504	LEU
2	A	505	GLU
2	A	507	LYS
2	A	511	LEU
2	A	512	GLU
2	A	518	ASP
2	A	523	SER
2	A	526	ARG
2	A	528	ILE
2	A	540	ASN
2	A	542	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	A	543	PRO
2	A	544	LEU
2	A	569	ASN
2	A	575	PRO
2	A	631	LYS
2	A	633	GLN
2	A	703	LEU
2	A	706	LEU
2	A	724	VAL
2	A	730	ILE
2	A	734	ILE
2	A	742	GLN
2	A	744	LYS
2	A	752	ARG
2	A	780	ILE
2	A	785	SER
2	A	786	ILE
2	A	791	GLN
2	A	801	GLU
2	A	804	ILE
2	A	811	VAL
2	A	815	LEU
2	A	816	LEU
2	A	824	ARG
2	A	830	LEU
2	A	833	MET
2	A	835	THR
3	B	312	LYS
3	B	317	SER
3	B	318	GLN
3	B	359	LEU
3	B	360	LYS
3	B	363	LEU
3	B	364	ASP
3	B	367	ILE
3	B	368	GLU
3	B	370	TYR
3	B	371	ARG
3	B	372	LEU
3	B	376	ILE
3	B	395	ILE
3	B	396	ARG

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
3	B	397	LYS
3	B	403	GLN
3	B	405	ILE
3	B	409	ILE
3	B	411	ASN
3	B	412	LYS
3	B	430	ILE
3	B	432	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	296	GLN
2	A	350	ASN
2	A	368	GLN
2	A	380	GLN
2	A	395	GLN
2	A	399	ASN
2	A	402	ASN
2	A	417	GLN
2	A	427	GLN
2	A	484	HIS
2	A	527	GLN
2	A	532	HIS
2	A	540	ASN
2	A	696	ASN
2	A	742	GLN
2	A	791	GLN
3	B	327	ASN
3	B	403	GLN
3	B	435	GLN

### 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 [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	YAO	A	901	-	73,80,80	2.37	22 (30%)	91,123,123	1.84	19 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	YAO	A	901	-	-	9/42/114/114	0/8/9/9

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	YAO	P1-O11	-7.63	1.51	1.59
4	A	901	YAO	P2-O11	-7.09	1.51	1.59
4	A	901	YAO	O5-C30	-6.07	1.30	1.43
4	A	901	YAO	C36-N6	-5.82	1.35	1.49
4	A	901	YAO	C26-N3	-5.21	1.29	1.37
4	A	901	YAO	C5-N1	-4.07	1.34	1.41
4	A	901	YAO	C27-N4	-3.99	1.27	1.36
4	A	901	YAO	C9-N1	-3.78	1.41	1.46
4	A	901	YAO	O6-C31	-3.60	1.34	1.43
4	A	901	YAO	C5-C4	-3.44	1.34	1.41
4	A	901	YAO	C29-C30	-3.10	1.48	1.52
4	A	901	YAO	C6-C7	-2.82	1.35	1.39
4	A	901	YAO	O4-C27	-2.63	1.19	1.24

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	YAO	P2-O12	-2.56	1.43	1.55
4	A	901	YAO	C28-N5	-2.53	1.32	1.38
4	A	901	YAO	C27-N3	-2.51	1.33	1.39
4	A	901	YAO	P1-O9	-2.50	1.43	1.55
4	A	901	YAO	C3-C2	-2.48	1.36	1.39
4	A	901	YAO	C37-N7	-2.43	1.30	1.34
4	A	901	YAO	O1-C9	-2.39	1.36	1.41
4	A	901	YAO	C10-C11	-2.32	1.50	1.55
4	A	901	YAO	P1-O10	-2.27	1.42	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	YAO	C5-N1-C9	-7.39	106.98	123.92
4	A	901	YAO	C25-C11-C12	6.70	126.48	116.08
4	A	901	YAO	C11-C10-C9	-5.18	93.80	104.25
4	A	901	YAO	C26-N3-C27	-4.12	119.20	125.42
4	A	901	YAO	C25-N1-C9	-3.98	105.50	109.50
4	A	901	YAO	C26-C25-C28	-3.46	107.26	113.40
4	A	901	YAO	O6-C31-C32	-3.15	101.78	108.93
4	A	901	YAO	O6-C31-C30	-2.87	102.40	108.93
4	A	901	YAO	O8-C33-C32	2.85	116.96	109.36
4	A	901	YAO	O11-P1-O10	-2.83	102.18	110.70
4	A	901	YAO	C29-C30-C31	2.66	116.87	109.66
4	A	901	YAO	O11-P2-O13	-2.34	103.68	110.70
4	A	901	YAO	O17-C43-C35	-2.32	104.42	111.08
4	A	901	YAO	O15-C36-N6	-2.29	105.71	108.75
4	A	901	YAO	O5-C30-C31	-2.28	103.91	109.25
4	A	901	YAO	O5-C30-C29	-2.23	101.01	110.20
4	A	901	YAO	O7-C32-C31	-2.21	104.09	109.25
4	A	901	YAO	C15-C16-C24	2.15	122.26	119.66
4	A	901	YAO	N3-C27-N4	2.11	123.98	119.50

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	YAO	O6-C31-C32-C33
4	A	901	YAO	C34-O14-P2-O13
4	A	901	YAO	O6-C31-C32-O7
4	A	901	YAO	O14-C34-C35-C43
4	A	901	YAO	O14-C34-C35-O15

*Continued on next page...*

*Continued from previous page...*

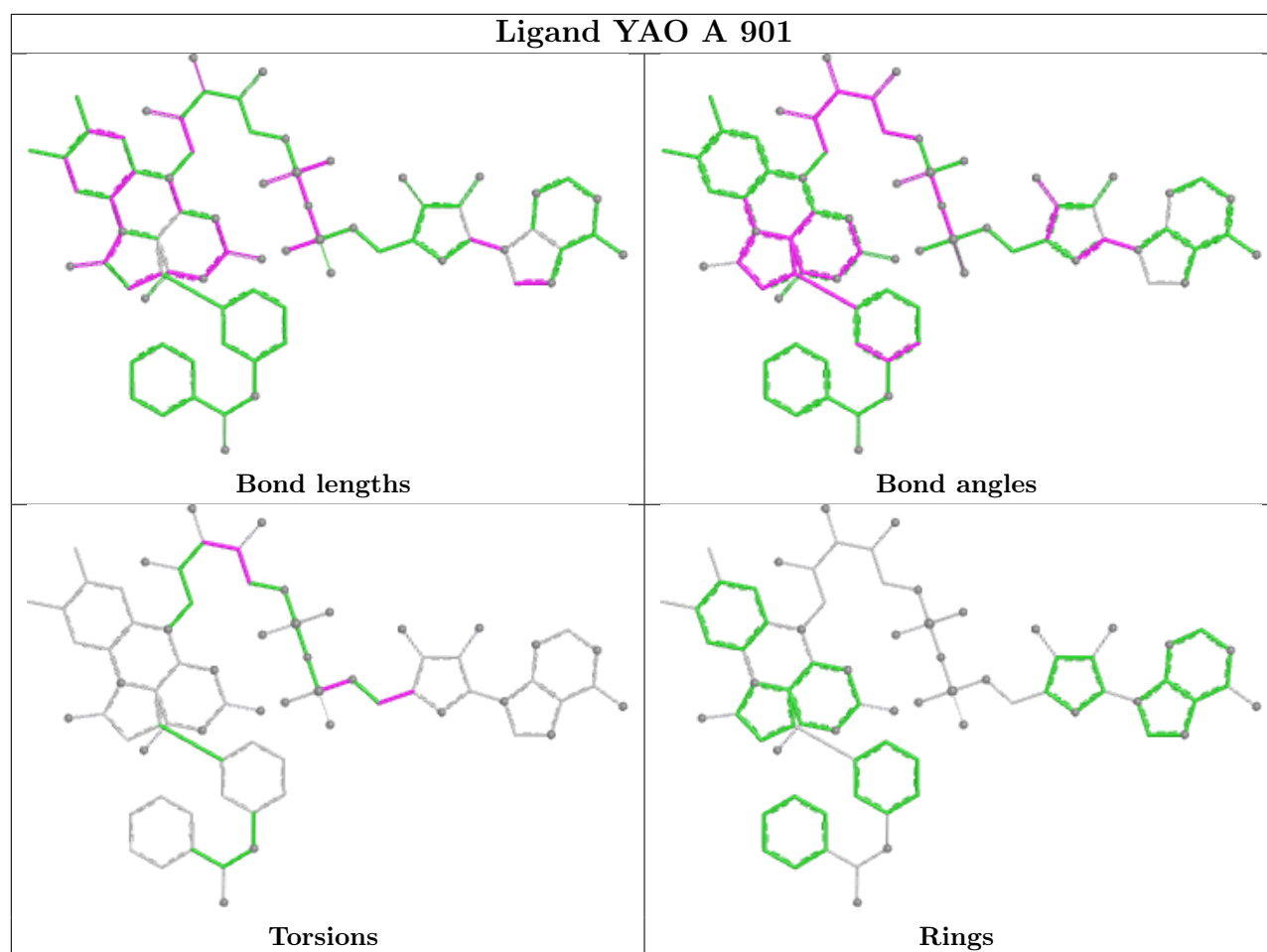
Mol	Chain	Res	Type	Atoms
4	A	901	YAO	C30-C31-C32-C33
4	A	901	YAO	O7-C32-C33-O8
4	A	901	YAO	C30-C31-C32-O7
4	A	901	YAO	C31-C32-C33-O8

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	YAO	12	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	C	4/9 (44%)	2.54	3 (75%) <b>0</b> <b>0</b>	121, 131, 131, 139	0
2	A	666/871 (76%)	0.35	16 (2%) 59 44	74, 112, 146, 170	0
3	B	133/144 (92%)	0.95	17 (12%) <b>9</b> <b>9</b>	107, 144, 167, 177	0
All	All	803/1024 (78%)	0.46	36 (4%) 39 29	74, 119, 157, 177	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	171	PRO	4.7
2	A	836	LEU	3.9
3	B	427	ARG	3.8
1	C	68	SER	3.4
3	B	375	VAL	3.4
2	A	555	ASP	3.3
2	A	611	SER	3.2
3	B	337	GLN	2.9
3	B	418	LYS	2.9
2	A	275	THR	2.9
1	C	66	PRO	2.9
1	C	69	PHE	2.9
3	B	414	VAL	2.8
3	B	376	ILE	2.8
2	A	556	ASP	2.7
3	B	368	GLU	2.7
2	A	683	SER	2.6
2	A	685	THR	2.6
2	A	552	TRP	2.4
3	B	440	GLU	2.3
3	B	431	ASP	2.3
3	B	421	PHE	2.3
3	B	422	VAL	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	A	373	GLU	2.2
3	B	420	PHE	2.2
3	B	348	GLN	2.2
3	B	393	GLN	2.2
3	B	428	PHE	2.2
3	B	382	ARG	2.1
2	A	700	ALA	2.1
2	A	667	ASP	2.1
2	A	496	GLU	2.1
2	A	240	ALA	2.1
2	A	698	TYR	2.1
2	A	237	GLN	2.0
3	B	387	GLU	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](#)

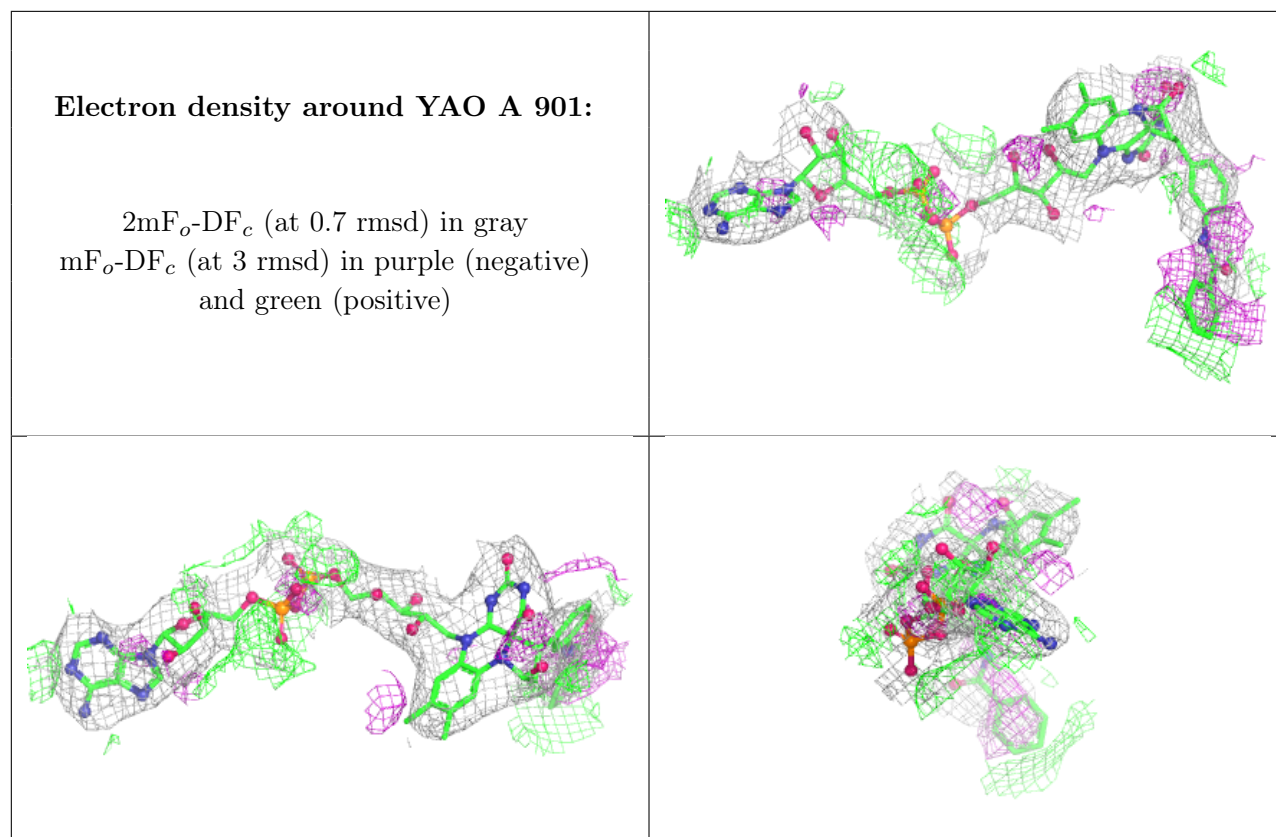
There are no oligosaccharides in this entry.

## 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, 95<sup>th</sup> 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	YAO	A	901	72/72	0.92	0.14	76,95,124,135	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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.