



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:33 AM UTC

PDB ID : 8UOM / pdb_00008uom
Title : LSD1-CoREST with N-formyl-FAD in complex with H3dimeK4 histone tail
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2023-10-20
Resolution : 3.20 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

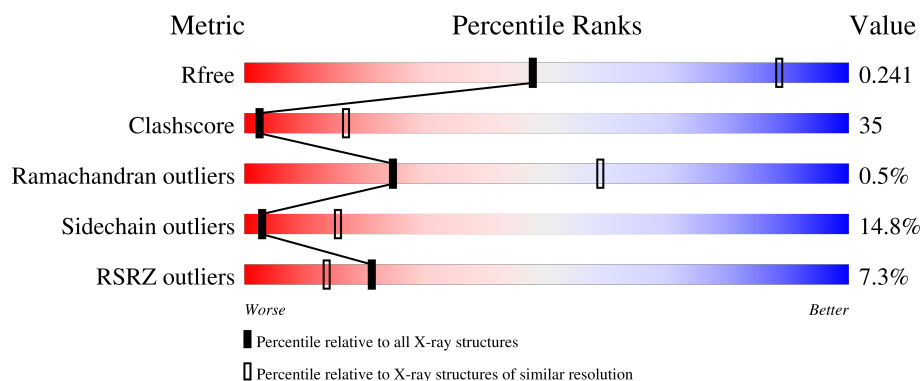
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	
2	B	144	
3	C	21	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MLY	C	4	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6414 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			

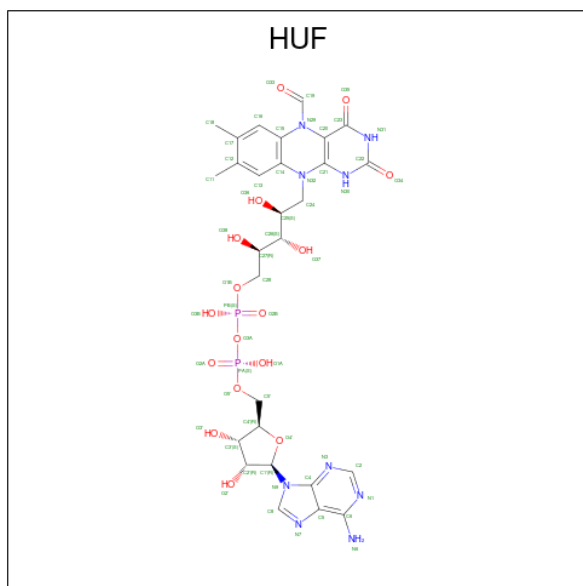
There are 8 discrepancies between the modelled and reference sequences:

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 Histone H3 (Fragment).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	8	Total	C	N	O	0	0	0
			66	39	16	11			

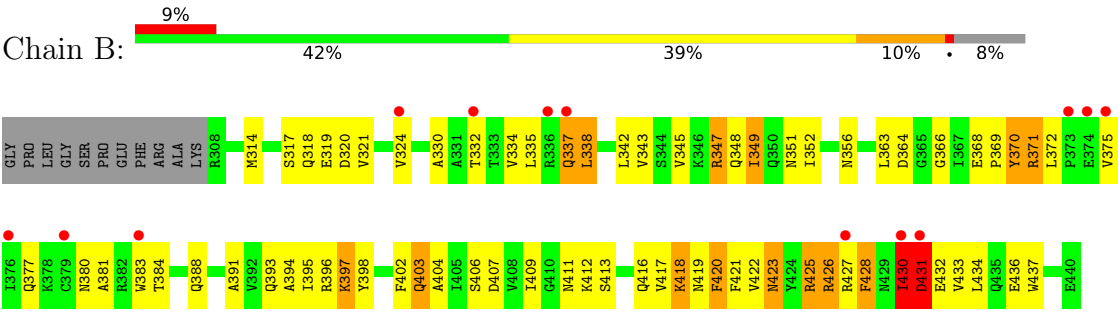
- Molecule 4 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy y-oxidanyl-phosphoryl] [(2R,3S,4S)-5-[5-methanoyl-7,8-dimethyl-2,4-bis(oxidanylidene)-1 H-benzo[g]pteridin-10-yl]-2,3,4-tris(oxidanyl)pentyl] hydrogen phosphate (CCD ID: HUF) (formula: C₂₈H₃₅N₉O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



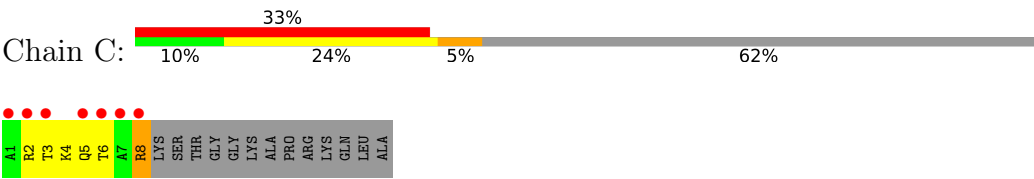
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			55	28	9	16	2		

VAL
PRO
ALA
GLN
SER
PRO
SER
MET

● Molecule 2: REST corepressor 1



● Molecule 3: Histone H3 (Fragment)



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	117.67Å 177.83Å 234.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.20 49.07 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.07-3.20) 99.7 (49.07-3.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.20 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.217 , 0.240 0.238 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	107.9	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6414	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: MLY, HUF

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	0.83	5/5331 (0.1%)	1.17	20/7232 (0.3%)
2	B	0.72	0/1091	1.27	10/1471 (0.7%)
3	C	0.87	0/54	1.44	0/71
All	All	0.82	5/6476 (0.1%)	1.19	30/8774 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	PRO	C-O	-6.58	1.19	1.24
1	A	755	PRO	C-O	-6.20	1.17	1.24
1	A	782	PRO	C-O	-5.96	1.16	1.23
1	A	197	PRO	C-O	-5.74	1.17	1.24
1	A	361	PRO	C-O	-5.19	1.17	1.24

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	430	ILE	CA-C-N	6.79	134.50	121.54
2	B	430	ILE	C-N-CA	6.79	134.50	121.54
1	A	727	CYS	CB-CA-C	-6.70	100.37	110.88
1	A	230	THR	CA-CB-OG1	-6.48	99.88	109.60
1	A	437	THR	CA-CB-OG1	-6.33	100.11	109.60
1	A	231	PHE	CB-CA-C	-6.04	101.40	110.88
1	A	639	PHE	CA-C-N	-5.84	117.77	122.85
1	A	639	PHE	C-N-CA	-5.84	117.77	122.85
2	B	432	GLU	N-CA-C	-5.78	105.06	111.36
2	B	421	PHE	CB-CA-C	-5.67	100.15	110.63
2	B	431	ASP	CB-CA-C	-5.62	99.23	110.42
1	A	278	THR	CB-CA-C	-5.50	99.74	109.70
2	B	330	ALA	CA-C-O	-5.44	115.08	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	470	PRO	CB-CA-C	-5.42	106.08	111.17
1	A	513	ALA	CA-C-N	-5.34	116.69	123.15
1	A	513	ALA	C-N-CA	-5.34	116.69	123.15
2	B	430	ILE	O-C-N	5.34	128.29	122.57
1	A	525	ASP	CB-CA-C	-5.31	102.78	110.96
1	A	266	ILE	CA-C-N	5.30	131.66	121.54
1	A	266	ILE	C-N-CA	5.30	131.66	121.54
1	A	347	LYS	N-CA-C	-5.28	105.61	111.36
1	A	266	ILE	CA-C-O	-5.25	114.22	120.78
2	B	428	PHE	CB-CA-C	-5.20	101.92	110.72
1	A	794	PRO	N-CA-C	-5.20	102.43	111.32
1	A	559	GLU	CB-CA-C	-5.16	101.16	109.72
2	B	431	ASP	N-CA-CB	5.13	119.17	110.49
1	A	786	ILE	CA-C-O	-5.13	116.33	119.51
1	A	213	ILE	CA-C-O	-5.11	115.64	120.95
1	A	510	GLU	N-CA-C	-5.05	105.68	111.14
2	B	430	ILE	CA-C-O	-5.00	116.44	121.59

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	363	3
2	B	1076	0	1091	109	2
3	C	66	0	76	4	0
4	A	55	0	0	11	0
All	All	6414	0	6419	447	3

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 35.

All (447) 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:188:MET:SD	1:A:210:PHE:CD2	2.22	1.33
1:A:206:THR:O	1:A:209:VAL:CG2	1.80	1.29
1:A:188:MET:SD	1:A:210:PHE:CE2	2.28	1.27
1:A:442:LYS:HB2	2:B:356:ASN:ND2	1.45	1.27
1:A:231:PHE:HE2	1:A:250:HIS:ND1	1.31	1.25
1:A:442:LYS:CB	2:B:356:ASN:HD21	1.50	1.23
1:A:280:LYS:CD	1:A:303:ASP:OD1	1.86	1.23
1:A:280:LYS:CE	1:A:303:ASP:OD1	1.92	1.17
1:A:206:THR:C	1:A:209:VAL:HG23	1.71	1.15
1:A:340:ASN:CG	1:A:560:PHE:HE2	1.53	1.15
1:A:206:THR:HA	1:A:209:VAL:CG2	1.77	1.14
1:A:568:ARG:HE	1:A:699:LYS:HG2	1.09	1.11
1:A:720:ASP:O	1:A:724:VAL:HG22	1.49	1.11
1:A:568:ARG:HE	1:A:699:LYS:CG	1.62	1.10
1:A:568:ARG:HD3	1:A:699:LYS:CE	1.82	1.09
1:A:206:THR:HA	1:A:209:VAL:HG21	1.28	1.09
1:A:658:ASN:ND2	1:A:752:ARG:HB2	1.68	1.08
1:A:206:THR:C	1:A:209:VAL:CG2	2.26	1.07
1:A:206:THR:O	1:A:209:VAL:HG23	0.87	1.05
1:A:188:MET:SD	1:A:210:PHE:HD2	1.72	1.04
1:A:568:ARG:HD3	1:A:699:LYS:HE2	1.05	1.04
1:A:485:ARG:HH11	1:A:485:ARG:HB3	1.21	1.04
2:B:396:ARG:O	2:B:437:TRP:HD1	1.38	1.04
2:B:426:ARG:HG2	2:B:426:ARG:HH11	1.19	1.03
1:A:526:ARG:NH1	1:A:530:ASP:OD1	1.91	1.03
1:A:231:PHE:CE2	1:A:250:HIS:ND1	2.14	1.02
1:A:340:ASN:CG	1:A:560:PHE:CE2	2.38	1.02
1:A:608:ARG:HH11	1:A:608:ARG:HB2	1.23	1.02
1:A:355:LYS:H	1:A:355:LYS:HD2	1.21	1.01
1:A:206:THR:CA	1:A:209:VAL:CG2	2.38	1.01
1:A:340:ASN:HA	1:A:560:PHE:CE2	1.95	1.00
1:A:779:PRO:HB3	1:A:797:PHE:CD2	1.97	0.99
1:A:231:PHE:HE2	1:A:250:HIS:CG	1.83	0.96
1:A:342:MET:HE3	1:A:811:VAL:HG12	1.45	0.96
1:A:720:ASP:O	1:A:724:VAL:CG2	2.13	0.96
1:A:188:MET:SD	1:A:210:PHE:HE2	1.84	0.94
1:A:374:LYS:O	1:A:378:VAL:HG23	1.65	0.94
1:A:331:ALA:HB1	4:A:901:HUF:C20	1.97	0.93
2:B:428:PHE:CB	2:B:430:ILE:HD11	1.98	0.93
1:A:568:ARG:CD	1:A:699:LYS:HE2	1.98	0.92
1:A:779:PRO:HB3	1:A:797:PHE:HD2	1.34	0.92
1:A:340:ASN:CB	1:A:560:PHE:CE2	2.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD12	1:A:218:LEU:H	1.34	0.90
1:A:690:GLU:OE2	1:A:726:ARG:NH1	2.05	0.89
1:A:556:ASP:C	1:A:559:GLU:OE1	2.15	0.88
1:A:331:ALA:CB	4:A:901:HUF:C20	2.50	0.88
1:A:485:ARG:HB3	1:A:485:ARG:NH1	1.87	0.88
2:B:419:ASN:O	2:B:423:ASN:OD1	1.92	0.88
1:A:568:ARG:NE	1:A:699:LYS:CG	2.37	0.87
1:A:205:GLN:O	1:A:209:VAL:HG22	1.74	0.87
1:A:331:ALA:HB2	4:A:901:HUF:C21	2.05	0.86
1:A:608:ARG:HH11	1:A:608:ARG:CB	1.88	0.86
1:A:331:ALA:CB	4:A:901:HUF:C21	2.52	0.86
1:A:568:ARG:NE	1:A:699:LYS:HG2	1.91	0.85
1:A:594:ARG:HG3	1:A:640:VAL:CG1	2.05	0.85
1:A:188:MET:CG	1:A:210:PHE:HE2	1.89	0.85
1:A:340:ASN:CA	1:A:560:PHE:CE2	2.59	0.85
2:B:396:ARG:O	2:B:437:TRP:CD1	2.29	0.84
2:B:428:PHE:HB2	2:B:430:ILE:HD11	1.58	0.84
1:A:524:ARG:O	1:A:528:ILE:HD12	1.77	0.84
1:A:421:LYS:NZ	2:B:320:ASP:OD1	2.09	0.83
1:A:280:LYS:HD3	1:A:303:ASP:OD1	1.79	0.83
1:A:332:MET:SD	1:A:661:LYS:NZ	2.52	0.82
1:A:754:ASP:OD1	1:A:755:PRO:HD2	1.78	0.82
1:A:280:LYS:HD2	1:A:303:ASP:OD1	1.77	0.81
2:B:317:SER:OG	2:B:320:ASP:OD2	1.98	0.81
1:A:485:ARG:NH1	2:B:398:TYR:OH	2.13	0.81
1:A:427:GLN:NE2	1:A:517:SER:O	2.14	0.80
1:A:444:LEU:HD12	1:A:444:LEU:O	1.80	0.80
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.12	0.80
1:A:319:THR:HB	1:A:572:SER:HB3	1.65	0.78
2:B:428:PHE:HB3	2:B:430:ILE:HD11	1.63	0.78
1:A:231:PHE:CE2	1:A:250:HIS:HA	2.19	0.77
1:A:232:GLU:N	1:A:232:GLU:OE1	2.14	0.77
2:B:403:GLN:OE1	2:B:407:ASP:OD1	2.03	0.77
1:A:667:ASP:OD1	1:A:668:ARG:HD2	1.84	0.77
1:A:568:ARG:CD	1:A:699:LYS:CE	2.59	0.77
1:A:245:ASP:OD1	1:A:247:VAL:HG22	1.85	0.76
1:A:340:ASN:HB2	1:A:560:PHE:CD2	2.19	0.76
1:A:671:TRP:HA	1:A:735:PHE:HE2	1.50	0.76
2:B:430:ILE:N	2:B:430:ILE:HD13	1.99	0.76
2:B:395:ILE:HG22	2:B:433:VAL:HG11	1.65	0.76
1:A:441:LEU:HD12	1:A:441:LEU:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:GLN:NE2	2:B:403:GLN:O	2.18	0.76
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.66	0.76
1:A:319:THR:CB	1:A:572:SER:HB3	2.16	0.76
1:A:651:VAL:HG22	1:A:776:MET:HE1	1.67	0.75
1:A:325:TYR:CE2	1:A:665:CYS:HB3	2.21	0.75
1:A:218:LEU:HD12	1:A:218:LEU:N	2.02	0.75
1:A:320:PHE:CE2	1:A:747:VAL:HG21	2.22	0.75
1:A:495:ASP:OD2	2:B:371:ARG:NH2	2.20	0.74
1:A:781:THR:HG23	1:A:793:ILE:O	1.86	0.74
1:A:779:PRO:CB	1:A:797:PHE:CD2	2.69	0.74
1:A:721:ASP:HA	1:A:724:VAL:HG23	1.68	0.74
1:A:485:ARG:HD2	2:B:404:ALA:HA	1.70	0.74
1:A:230:THR:HG23	1:A:233:ALA:H	1.53	0.74
1:A:511:LEU:N	1:A:511:LEU:HD23	2.02	0.74
1:A:331:ALA:HA	4:A:901:HUF:N29	2.03	0.73
1:A:336:GLY:O	1:A:560:PHE:HD2	1.72	0.73
1:A:342:MET:CE	1:A:811:VAL:HG12	2.19	0.73
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.71	0.72
2:B:338:LEU:N	2:B:338:LEU:HD23	2.04	0.72
1:A:331:ALA:HB1	4:A:901:HUF:C23	2.18	0.72
1:A:280:LYS:HE2	1:A:303:ASP:OD1	1.87	0.72
1:A:442:LYS:HB2	2:B:356:ASN:HD21	0.63	0.72
1:A:441:LEU:HD12	1:A:441:LEU:C	2.15	0.71
1:A:665:CYS:HB2	1:A:745:GLU:O	1.90	0.71
2:B:430:ILE:HG22	2:B:434:LEU:CD1	2.21	0.71
1:A:331:ALA:HB1	4:A:901:HUF:C21	2.19	0.71
1:A:442:LYS:HA	2:B:356:ASN:OD1	1.90	0.71
1:A:568:ARG:CD	1:A:699:LYS:NZ	2.53	0.71
1:A:340:ASN:CB	1:A:560:PHE:HE2	1.98	0.70
1:A:568:ARG:NE	1:A:699:LYS:HG3	2.06	0.70
1:A:231:PHE:CZ	1:A:250:HIS:HB2	2.26	0.70
1:A:755:PRO:HA	1:A:758:ARG:HH11	1.55	0.70
1:A:332:MET:CE	1:A:661:LYS:NZ	2.55	0.70
1:A:693:LEU:C	1:A:694:PHE:HD1	2.00	0.70
2:B:397:LYS:HG2	2:B:397:LYS:O	1.89	0.70
1:A:195:CYS:HG	1:A:834:TYR:HE1	1.38	0.70
1:A:218:LEU:H	1:A:218:LEU:CD1	2.05	0.70
2:B:426:ARG:HG2	2:B:426:ARG:NH1	1.94	0.70
2:B:428:PHE:HB3	2:B:430:ILE:CD1	2.22	0.70
1:A:217:THR:HG23	1:A:234:THR:CG2	2.22	0.69
1:A:173:GLY:C	1:A:219:GLN:NE2	2.50	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ASP:N	1:A:525:ASP:OD1	2.19	0.69
1:A:188:MET:HE3	1:A:200:ILE:HG12	1.75	0.69
1:A:608:ARG:HB2	1:A:608:ARG:NH1	2.05	0.69
1:A:781:THR:HG23	1:A:793:ILE:C	2.18	0.68
1:A:231:PHE:CE2	1:A:250:HIS:CB	2.75	0.68
1:A:721:ASP:HA	1:A:724:VAL:CG2	2.23	0.68
1:A:231:PHE:CZ	1:A:250:HIS:CA	2.77	0.68
1:A:815:LEU:HD12	1:A:815:LEU:O	1.93	0.68
1:A:472:ARG:NE	1:A:477:GLU:OE1	2.22	0.68
1:A:608:ARG:HH11	1:A:608:ARG:CG	2.06	0.68
2:B:337:GLN:HE21	2:B:337:GLN:CA	2.07	0.68
1:A:206:THR:CA	1:A:209:VAL:HG21	2.09	0.68
1:A:434:ILE:HD13	1:A:511:LEU:HD12	1.76	0.67
1:A:188:MET:CG	1:A:210:PHE:CE2	2.72	0.67
1:A:815:LEU:HD12	1:A:815:LEU:C	2.18	0.67
1:A:280:LYS:HE3	1:A:303:ASP:OD1	1.88	0.67
1:A:434:ILE:HD11	1:A:511:LEU:HB3	1.76	0.66
1:A:206:THR:CA	1:A:209:VAL:HG22	2.25	0.66
1:A:224:ASN:C	1:A:224:ASN:HD22	2.02	0.66
1:A:231:PHE:CZ	1:A:250:HIS:HA	2.30	0.66
2:B:352:ILE:O	2:B:356:ASN:HB2	1.94	0.66
1:A:379:GLU:HG3	1:A:532:HIS:NE2	2.10	0.66
1:A:594:ARG:HG3	1:A:640:VAL:HG13	1.76	0.66
1:A:430:HIS:CE1	1:A:515:PRO:HA	2.31	0.66
1:A:321:ARG:NH2	1:A:569:ASN:O	2.29	0.66
2:B:428:PHE:CB	2:B:430:ILE:CD1	2.73	0.66
1:A:340:ASN:CB	1:A:560:PHE:CD2	2.78	0.65
1:A:340:ASN:ND2	1:A:560:PHE:CE2	2.65	0.65
1:A:836:LEU:N	1:A:836:LEU:HD23	2.11	0.65
1:A:341:PRO:HG3	1:A:816:LEU:CD1	2.26	0.65
1:A:460:GLN:O	1:A:464:GLU:HG3	1.96	0.65
1:A:281:VAL:HG11	1:A:297:LEU:HD13	1.78	0.65
1:A:332:MET:CE	1:A:661:LYS:HZ3	2.10	0.65
2:B:380:ASN:OD1	2:B:381:ALA:N	2.29	0.65
1:A:568:ARG:HG3	1:A:568:ARG:HH11	1.62	0.64
1:A:331:ALA:HA	4:A:901:HUF:C15	2.27	0.64
1:A:568:ARG:NE	1:A:699:LYS:HZ3	1.95	0.64
1:A:594:ARG:HA	1:A:640:VAL:O	1.98	0.64
1:A:311:ASP:OD1	1:A:311:ASP:N	2.18	0.64
1:A:777:ALA:HB1	1:A:820:ARG:NH1	2.13	0.64
1:A:231:PHE:HZ	1:A:250:HIS:HB2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ALA:HB2	4:A:901:HUF:N32	2.12	0.64
1:A:342:MET:HE2	1:A:812:HIS:HA	1.80	0.64
2:B:423:ASN:OD1	2:B:423:ASN:N	2.21	0.64
1:A:355:LYS:H	1:A:355:LYS:CD	1.92	0.63
1:A:721:ASP:CA	1:A:724:VAL:HG23	2.28	0.63
2:B:426:ARG:HH11	2:B:426:ARG:CG	2.03	0.63
1:A:325:TYR:HD2	1:A:665:CYS:SG	2.22	0.63
2:B:395:ILE:CG2	2:B:433:VAL:HG11	2.28	0.62
1:A:217:THR:HG23	1:A:234:THR:HG23	1.80	0.62
1:A:325:TYR:HE2	1:A:665:CYS:HB3	1.64	0.62
1:A:231:PHE:CZ	1:A:250:HIS:CB	2.82	0.62
1:A:355:LYS:HD2	1:A:355:LYS:N	2.05	0.61
1:A:206:THR:HA	1:A:209:VAL:HG22	1.76	0.61
1:A:231:PHE:CE2	1:A:250:HIS:CG	2.73	0.61
2:B:337:GLN:HE21	2:B:337:GLN:HA	1.65	0.61
1:A:419:GLN:NE2	2:B:314:MET:HA	2.14	0.61
1:A:754:ASP:OD1	1:A:755:PRO:CD	2.48	0.61
2:B:426:ARG:HD3	2:B:427:ARG:H	1.66	0.61
1:A:379:GLU:CG	1:A:532:HIS:NE2	2.63	0.60
1:A:277:LYS:H	1:A:277:LYS:HD3	1.66	0.60
1:A:356:ILE:HG22	1:A:356:ILE:O	2.01	0.60
1:A:419:GLN:HE22	2:B:314:MET:HA	1.67	0.60
2:B:426:ARG:CD	2:B:426:ARG:H	2.13	0.60
1:A:231:PHE:CE2	1:A:250:HIS:CA	2.85	0.59
1:A:173:GLY:C	1:A:219:GLN:HE22	2.11	0.59
1:A:344:VAL:HG12	1:A:348:GLN:HE22	1.67	0.59
1:A:484:HIS:CD2	2:B:372:LEU:HD12	2.36	0.59
2:B:318:GLN:HG2	2:B:319:GLU:N	2.17	0.59
2:B:396:ARG:C	2:B:437:TRP:HD1	2.08	0.59
1:A:195:CYS:SG	1:A:834:TYR:HE1	2.26	0.59
1:A:207:GLN:O	1:A:210:PHE:HB3	2.03	0.58
2:B:403:GLN:HE21	2:B:403:GLN:HA	1.67	0.58
1:A:217:THR:HA	1:A:220:LEU:HD12	1.86	0.58
1:A:280:LYS:HD3	1:A:303:ASP:CG	2.28	0.58
1:A:569:ASN:OD1	1:A:569:ASN:N	2.36	0.58
1:A:556:ASP:CA	1:A:559:GLU:OE1	2.51	0.58
2:B:347:ARG:HH11	2:B:347:ARG:CG	2.17	0.58
2:B:403:GLN:OE1	2:B:407:ASP:CG	2.47	0.57
1:A:434:ILE:HD11	1:A:511:LEU:CB	2.34	0.57
1:A:280:LYS:CD	1:A:303:ASP:CG	2.76	0.57
1:A:287:GLY:O	1:A:291:LEU:HD12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:ARG:HH11	1:A:568:ARG:CG	2.16	0.57
1:A:203:PRO:O	1:A:206:THR:HG22	2.05	0.57
2:B:317:SER:O	2:B:321:VAL:HG23	2.05	0.57
1:A:188:MET:HG3	1:A:210:PHE:CE2	2.40	0.57
1:A:340:ASN:HA	1:A:560:PHE:CZ	2.40	0.56
2:B:370:TYR:N	2:B:370:TYR:CD1	2.72	0.56
1:A:320:PHE:CD1	1:A:320:PHE:C	2.83	0.56
2:B:420:PHE:CD1	2:B:420:PHE:C	2.84	0.56
1:A:595:TYR:OH	1:A:641:PRO:O	2.21	0.56
1:A:364:GLU:CD	1:A:365:ALA:H	2.13	0.56
1:A:331:ALA:HB2	4:A:901:HUF:C14	2.36	0.56
1:A:520:TYR:CD1	1:A:520:TYR:C	2.82	0.56
2:B:370:TYR:N	2:B:370:TYR:HD1	2.03	0.56
1:A:444:LEU:HD12	1:A:444:LEU:C	2.28	0.56
1:A:357:LYS:HD3	1:A:676:ASN:OD1	2.05	0.55
1:A:495:ASP:CG	2:B:371:ARG:HH22	2.14	0.55
1:A:206:THR:C	1:A:209:VAL:HG22	2.27	0.55
1:A:198:ASP:OD2	1:A:251:ARG:NH2	2.39	0.55
1:A:341:PRO:HG3	1:A:816:LEU:HD11	1.87	0.55
2:B:430:ILE:HG22	2:B:434:LEU:HD11	1.88	0.55
1:A:264:PHE:CD1	1:A:264:PHE:C	2.85	0.55
1:A:690:GLU:CD	1:A:715:MET:HE3	2.32	0.55
1:A:654:MET:HE1	1:A:776:MET:CG	2.37	0.54
1:A:320:PHE:CD2	1:A:747:VAL:HG21	2.41	0.54
1:A:188:MET:HG3	1:A:210:PHE:HE2	1.72	0.54
1:A:312:ARG:HH21	1:A:312:ARG:HG3	1.73	0.54
1:A:217:THR:HG23	1:A:234:THR:HG21	1.90	0.54
1:A:667:ASP:OD2	1:A:744:LYS:HE3	2.08	0.54
1:A:215:ASN:HA	1:A:218:LEU:HD13	1.89	0.54
1:A:658:ASN:HD21	1:A:752:ARG:HB2	1.66	0.54
1:A:520:TYR:CD1	1:A:521:LEU:HG	2.43	0.54
1:A:606:ASN:O	1:A:609:SER:O	2.25	0.54
2:B:337:GLN:CA	2:B:337:GLN:NE2	2.71	0.54
1:A:173:GLY:O	1:A:219:GLN:NE2	2.42	0.53
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.90	0.53
2:B:403:GLN:NE2	2:B:403:GLN:HA	2.22	0.53
1:A:351:MET:HA	1:A:569:ASN:HD21	1.72	0.53
1:A:801:GLU:HG2	1:A:809:ALA:H	1.72	0.53
2:B:430:ILE:N	2:B:430:ILE:CD1	2.71	0.53
1:A:325:TYR:HD2	1:A:665:CYS:HG	1.54	0.53
1:A:693:LEU:HD12	1:A:694:PHE:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:LEU:HD12	1:A:694:PHE:N	2.22	0.53
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.44	0.53
1:A:485:ARG:CD	2:B:404:ALA:HB1	2.39	0.53
2:B:337:GLN:HE21	2:B:337:GLN:N	2.07	0.53
2:B:430:ILE:HG22	2:B:434:LEU:HD12	1.89	0.53
1:A:606:ASN:HB3	1:A:609:SER:O	2.09	0.52
1:A:695:TRP:HE1	1:A:706:LEU:HD13	1.75	0.52
1:A:484:HIS:CD2	2:B:372:LEU:CD1	2.92	0.52
2:B:403:GLN:NE2	2:B:403:GLN:CA	2.72	0.52
1:A:319:THR:OG1	1:A:572:SER:HB3	2.09	0.52
1:A:332:MET:CE	1:A:661:LYS:HZ1	2.21	0.52
1:A:434:ILE:O	1:A:437:THR:OG1	2.26	0.52
1:A:537:GLU:HG2	1:A:542:THR:O	2.10	0.52
1:A:720:ASP:C	1:A:724:VAL:CG2	2.82	0.52
1:A:340:ASN:HB2	1:A:560:PHE:HD2	1.70	0.52
1:A:724:VAL:HG11	1:A:746:THR:HG21	1.91	0.52
1:A:664:LEU:HD11	1:A:727:CYS:SG	2.50	0.52
1:A:258:ARG:NH1	1:A:827:ASP:OD1	2.43	0.51
1:A:595:TYR:N	1:A:595:TYR:CD1	2.78	0.51
2:B:413:SER:H	2:B:416:GLN:NE2	2.08	0.51
1:A:781:THR:HA	1:A:794:PRO:HA	1.93	0.51
2:B:425:ARG:HA	2:B:430:ILE:HG12	1.91	0.51
1:A:435:VAL:HG12	2:B:349:ILE:HG12	1.92	0.51
1:A:445:LEU:O	1:A:448:MET:N	2.42	0.51
2:B:397:LYS:HD3	2:B:398:TYR:CE1	2.45	0.51
1:A:174:VAL:HA	1:A:219:GLN:NE2	2.26	0.51
1:A:485:ARG:HH12	2:B:398:TYR:HH	1.55	0.51
1:A:568:ARG:NE	1:A:699:LYS:NZ	2.59	0.51
1:A:721:ASP:C	1:A:724:VAL:HG23	2.36	0.51
1:A:479:LEU:HD11	1:A:483:LYS:HE3	1.92	0.50
2:B:347:ARG:CG	2:B:347:ARG:NH1	2.73	0.50
2:B:428:PHE:O	2:B:430:ILE:HD13	2.11	0.50
1:A:478:PHE:CE1	1:A:482:SER:HB2	2.45	0.50
1:A:520:TYR:HD1	1:A:520:TYR:O	1.95	0.50
1:A:568:ARG:CG	1:A:568:ARG:NH1	2.73	0.50
1:A:817:SER:HB2	1:A:820:ARG:NH2	2.26	0.50
2:B:337:GLN:NE2	2:B:337:GLN:N	2.60	0.50
1:A:445:LEU:N	1:A:445:LEU:HD23	2.26	0.50
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.94	0.50
1:A:332:MET:HE2	1:A:661:LYS:HZ1	1.76	0.50
1:A:362:LEU:HD23	1:A:362:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:ASP:OD2	2:B:397:LYS:NZ	2.44	0.50
1:A:720:ASP:O	1:A:724:VAL:HG23	2.05	0.50
1:A:595:TYR:CZ	1:A:641:PRO:HG2	2.46	0.50
2:B:391:ALA:HB2	2:B:409:ILE:HD11	1.93	0.50
1:A:291:LEU:HD22	1:A:578:LEU:HB2	1.93	0.49
1:A:338:GLY:HA3	1:A:561:THR:OG1	2.12	0.49
1:A:353:LEU:HB3	1:A:565:LEU:HD23	1.93	0.49
1:A:366:ASN:OD1	1:A:367:GLY:N	2.45	0.49
1:A:459:HIS:HB2	1:A:487:LEU:HD11	1.94	0.49
2:B:395:ILE:HG22	2:B:433:VAL:HG12	1.93	0.49
1:A:418:LEU:HD21	2:B:321:VAL:HG22	1.93	0.49
1:A:720:ASP:C	1:A:724:VAL:HG22	2.31	0.49
1:A:485:ARG:HD3	2:B:404:ALA:HB1	1.94	0.49
2:B:416:GLN:HA	2:B:419:ASN:HB2	1.94	0.49
1:A:695:TRP:HE3	1:A:697:LEU:HD21	1.76	0.49
1:A:364:GLU:CD	1:A:365:ALA:N	2.71	0.49
1:A:618:CYS:SG	1:A:621:VAL:HG22	2.53	0.49
1:A:804:ILE:HG23	1:A:804:ILE:O	2.12	0.48
2:B:369:PRO:HB2	2:B:370:TYR:CD1	2.49	0.48
2:B:413:SER:O	2:B:417:VAL:HG23	2.12	0.48
1:A:353:LEU:HB3	1:A:565:LEU:CD2	2.43	0.48
1:A:481:LYS:HB3	1:A:481:LYS:HE3	1.38	0.48
2:B:320:ASP:O	2:B:324:VAL:HG23	2.12	0.48
1:A:419:GLN:HB2	1:A:520:TYR:CE2	2.48	0.48
1:A:667:ASP:OD1	1:A:667:ASP:C	2.55	0.48
1:A:336:GLY:O	1:A:560:PHE:CD2	2.60	0.48
1:A:442:LYS:CA	2:B:356:ASN:HD21	2.19	0.48
1:A:448:MET:HE2	2:B:363:LEU:HD13	1.95	0.48
1:A:346:SER:HB3	1:A:351:MET:HE3	1.96	0.48
2:B:338:LEU:N	2:B:338:LEU:CD2	2.72	0.48
1:A:321:ARG:NH1	1:A:572:SER:OG	2.35	0.47
1:A:193:ALA:CB	1:A:200:ILE:HG13	2.45	0.47
1:A:344:VAL:HG12	1:A:348:GLN:NE2	2.29	0.47
1:A:716:GLU:O	1:A:750:ARG:NH2	2.46	0.47
1:A:601:GLU:HA	1:A:616:TYR:O	2.15	0.47
1:A:693:LEU:O	1:A:694:PHE:HD1	1.96	0.47
1:A:758:ARG:HA	1:A:758:ARG:HD2	1.67	0.47
1:A:210:PHE:C	1:A:210:PHE:CD1	2.92	0.47
1:A:485:ARG:CD	2:B:404:ALA:CB	2.93	0.47
1:A:485:ARG:HG3	2:B:407:ASP:CB	2.45	0.47
1:A:647:LYS:O	1:A:651:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:ILE:HG23	2:B:356:ASN:HD22	1.79	0.47
1:A:556:ASP:HA	1:A:559:GLU:OE1	2.15	0.47
2:B:419:ASN:O	2:B:422:VAL:HB	2.15	0.47
1:A:574:VAL:HB	1:A:575:PRO:CD	2.44	0.47
1:A:805:ARG:O	1:A:808:PRO:HD3	2.15	0.47
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.63	0.46
1:A:608:ARG:NH1	1:A:608:ARG:CG	2.70	0.46
1:A:671:TRP:HA	1:A:735:PHE:CE2	2.41	0.46
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.51	0.46
2:B:403:GLN:NE2	2:B:403:GLN:C	2.73	0.46
2:B:398:TYR:O	2:B:437:TRP:CZ2	2.69	0.46
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.97	0.46
1:A:836:LEU:N	1:A:836:LEU:CD2	2.79	0.46
1:A:340:ASN:ND2	1:A:560:PHE:CD2	2.84	0.46
2:B:397:LYS:HD3	2:B:398:TYR:CZ	2.51	0.46
1:A:218:LEU:N	1:A:218:LEU:CD1	2.72	0.46
1:A:270:ILE:O	1:A:272:PRO:HD3	2.16	0.46
1:A:345:VAL:O	1:A:349:VAL:N	2.45	0.46
1:A:434:ILE:CD1	1:A:511:LEU:HD12	2.43	0.46
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.98	0.46
1:A:332:MET:HE1	1:A:661:LYS:HZ3	1.81	0.46
1:A:343:ALA:O	1:A:346:SER:OG	2.34	0.46
1:A:658:ASN:HD22	1:A:752:ARG:HB2	1.70	0.46
2:B:352:ILE:CG2	2:B:356:ASN:HD22	2.28	0.46
2:B:428:PHE:C	2:B:430:ILE:HD13	2.41	0.46
1:A:224:ASN:C	1:A:224:ASN:ND2	2.73	0.46
1:A:456:LYS:HA	2:B:370:TYR:CE2	2.51	0.45
1:A:658:ASN:ND2	1:A:752:ARG:CB	2.60	0.45
2:B:426:ARG:CD	2:B:426:ARG:N	2.80	0.45
2:B:402:PHE:N	2:B:402:PHE:CD1	2.83	0.45
1:A:379:GLU:HG2	1:A:532:HIS:NE2	2.31	0.45
1:A:521:LEU:HD22	1:A:525:ASP:CB	2.45	0.45
1:A:325:TYR:CD2	1:A:665:CYS:HB3	2.51	0.45
2:B:388:GLN:O	2:B:391:ALA:HB3	2.17	0.45
1:A:271:LYS:HE3	1:A:271:LYS:HB2	1.66	0.45
1:A:310:ARG:NH1	1:A:754:ASP:OD2	2.42	0.45
1:A:322:LYS:HE2	1:A:745:GLU:CD	2.42	0.45
1:A:755:PRO:HA	1:A:758:ARG:HD3	1.98	0.45
2:B:431:ASP:H	2:B:434:LEU:HD12	1.81	0.45
1:A:267:TYR:O	1:A:267:TYR:CD2	2.70	0.44
1:A:277:LYS:HD3	1:A:277:LYS:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ASP:CG	2:B:371:ARG:NH2	2.73	0.44
2:B:391:ALA:O	2:B:394:ALA:HB3	2.18	0.44
1:A:469:LYS:HA	1:A:470:PRO:HD3	1.81	0.44
1:A:548:SER:HB2	1:A:766:ALA:HA	1.98	0.44
2:B:403:GLN:C	2:B:403:GLN:CD	2.85	0.44
1:A:478:PHE:O	1:A:482:SER:HB3	2.17	0.44
2:B:384:THR:O	2:B:388:GLN:HG3	2.18	0.44
2:B:402:PHE:CE2	2:B:418:LYS:HG3	2.53	0.44
3:C:6:THR:HB	3:C:8:ARG:NE	2.33	0.44
1:A:264:PHE:CD1	1:A:264:PHE:O	2.71	0.44
1:A:363:TYR:CD2	1:A:734:ILE:HG23	2.52	0.44
1:A:625:LEU:HA	1:A:625:LEU:HD23	1.75	0.44
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.70	0.44
1:A:366:ASN:HD21	1:A:368:GLN:HB2	1.83	0.44
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.43	0.44
1:A:568:ARG:HE	1:A:699:LYS:HZ3	1.65	0.43
1:A:385:LEU:O	1:A:388:ALA:HB3	2.18	0.43
1:A:395:GLN:C	1:A:396:LEU:HD23	2.43	0.43
1:A:410:GLN:O	1:A:414:VAL:HG23	2.17	0.43
1:A:478:PHE:O	1:A:482:SER:N	2.34	0.43
2:B:426:ARG:H	2:B:426:ARG:HD2	1.82	0.43
1:A:485:ARG:CD	2:B:404:ALA:HA	2.45	0.43
1:A:817:SER:HB2	1:A:820:ARG:HH21	1.84	0.43
1:A:540:ASN:HB3	1:A:547:LEU:HD21	2.00	0.43
1:A:594:ARG:HG3	1:A:640:VAL:HG12	1.91	0.43
1:A:797:PHE:CD1	1:A:825:ILE:CD1	3.02	0.43
1:A:718:ILE:HG22	1:A:722:VAL:HB	2.01	0.43
2:B:364:ASP:C	2:B:366:GLY:H	2.27	0.43
2:B:377:GLN:NE2	2:B:411:ASN:HB3	2.33	0.43
1:A:282:ILE:HA	1:A:282:ILE:HD13	1.80	0.42
2:B:406:SER:OG	2:B:412:LYS:O	2.33	0.42
1:A:174:VAL:N	1:A:219:GLN:HE22	2.17	0.42
1:A:357:LYS:CD	1:A:357:LYS:H	2.32	0.42
1:A:662:VAL:HG13	1:A:748:VAL:HG22	2.00	0.42
2:B:426:ARG:HD3	2:B:427:ARG:N	2.32	0.42
1:A:380:GLN:HG2	1:A:384:ARG:CD	2.49	0.42
2:B:347:ARG:NH1	2:B:347:ARG:HG2	2.34	0.42
1:A:294:ALA:HB1	1:A:582:LEU:HD23	2.00	0.42
1:A:308:GLU:HB3	1:A:586:LEU:HD23	2.00	0.42
1:A:349:VAL:O	1:A:349:VAL:HG12	2.19	0.42
1:A:695:TRP:NE1	1:A:706:LEU:HD13	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:383:TRP:CD2	2:B:412:LYS:NZ	2.88	0.42
1:A:335:THR:O	1:A:560:PHE:HB2	2.19	0.42
1:A:574:VAL:HB	1:A:575:PRO:HD3	2.02	0.42
1:A:266:ILE:HB	1:A:348:GLN:HG2	2.00	0.42
1:A:499:GLU:HA	1:A:499:GLU:OE1	2.19	0.42
1:A:295:ARG:HG2	1:A:582:LEU:HD11	2.02	0.42
1:A:520:TYR:C	1:A:520:TYR:HD1	2.25	0.41
1:A:695:TRP:HE1	1:A:706:LEU:CD1	2.32	0.41
1:A:541:ALA:O	1:A:657:GLY:HA3	2.20	0.41
1:A:653:ARG:NH1	1:A:772:ASP:CG	2.78	0.41
1:A:235:LEU:HD11	1:A:243:ASN:HB2	2.02	0.41
1:A:530:ASP:OD2	1:A:685:THR:HA	2.21	0.41
1:A:793:ILE:HG22	1:A:794:PRO:CD	2.51	0.41
2:B:375:VAL:HG23	2:B:375:VAL:O	2.19	0.41
1:A:357:LYS:H	1:A:357:LYS:HD2	1.85	0.41
1:A:484:HIS:HD2	2:B:372:LEU:HD13	1.85	0.41
1:A:280:LYS:N	1:A:619:ASP:OD2	2.51	0.41
1:A:361:PRO:O	1:A:361:PRO:HG2	2.20	0.41
1:A:458:LEU:HD23	1:A:461:GLN:OE1	2.20	0.41
1:A:734:ILE:HG22	1:A:735:PHE:CD1	2.56	0.41
1:A:793:ILE:HG22	1:A:794:PRO:HD2	2.02	0.41
1:A:325:TYR:CD2	1:A:665:CYS:SG	3.10	0.41
1:A:595:TYR:CE1	1:A:641:PRO:HD2	2.56	0.41
1:A:275:THR:H	1:A:275:THR:HG22	1.61	0.40
1:A:564:HIS:CE1	3:C:6:THR:O	2.74	0.40
1:A:228:GLN:HA	1:A:263:ASN:OD1	2.21	0.40
3:C:4:MLY:H	3:C:4:MLY:HG3	1.50	0.40
1:A:215:ASN:CA	1:A:218:LEU:HD13	2.50	0.40
1:A:255:TYR:CE2	1:A:256:LEU:HD23	2.55	0.40
1:A:485:ARG:HH11	1:A:485:ARG:CB	2.09	0.40
2:B:395:ILE:CG2	2:B:433:VAL:CG1	2.88	0.40
1:A:539:ALA:O	3:C:4:MLY:HE3	2.21	0.40
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.99	0.40
1:A:564:HIS:C	1:A:565:LEU:HD12	2.46	0.40
1:A:626:PRO:HD3	4:A:901:HUF:C5'	2.51	0.40
2:B:369:PRO:HB2	2:B:370:TYR:HD1	1.84	0.40

All (3) 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:744:LYS:NZ	2:B:348:GLN:NE2[8_455]	1.54	0.66
1:A:324:ASN:OD1	2:B:351:ASN:ND2[8_455]	1.90	0.30
1:A:591:ARG:NH2	1:A:610:THR:O[2_565]	1.97	0.23

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%)	620 (93%)	41 (6%)	3 (0%)	24	59
2	B	131/144 (91%)	122 (93%)	8 (6%)	1 (1%)	16	50
3	C	5/21 (24%)	4 (80%)	1 (20%)	0	100	100
All	All	800/1036 (77%)	746 (93%)	50 (6%)	4 (0%)	24	59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	214	ARG
1	A	267	TYR
1	A	215	ASN
2	B	431	ASP

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%)	492 (87%)	74 (13%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	117/125 (94%)	93 (80%)	24 (20%)	1	7
3	C	5/14 (36%)	1 (20%)	4 (80%)	0	0
All	All	688/854 (81%)	586 (85%)	102 (15%)	3	15

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	199	ILE
1	A	200	ILE
1	A	209	VAL
1	A	211	LEU
1	A	213	ILE
1	A	216	ARG
1	A	217	THR
1	A	226	LYS
1	A	235	LEU
1	A	238	LEU
1	A	239	GLU
1	A	268	LYS
1	A	269	ARG
1	A	275	THR
1	A	277	LYS
1	A	311	ASP
1	A	324	ASN
1	A	326	VAL
1	A	332	MET
1	A	348	GLN
1	A	355	LYS
1	A	356	ILE
1	A	358	GLN
1	A	359	LYS
1	A	362	LEU
1	A	372	LYS
1	A	374	LYS
1	A	377	MET
1	A	378	VAL
1	A	379	GLU
1	A	432	LYS
1	A	441	LEU
1	A	442	LYS

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Mol	Chain	Res	Type
1	A	443	GLU
1	A	444	LEU
1	A	445	LEU
1	A	472	ARG
1	A	481	LYS
1	A	482	SER
1	A	485	ARG
1	A	487	LEU
1	A	511	LEU
1	A	512	GLU
1	A	520	TYR
1	A	522	SER
1	A	523	SER
1	A	525	ASP
1	A	557	ASP
1	A	559	GLU
1	A	568	ARG
1	A	569	ASN
1	A	571	TYR
1	A	576	VAL
1	A	595	TYR
1	A	608	ARG
1	A	610	THR
1	A	611	SER
1	A	659	LEU
1	A	723	ILE
1	A	724	VAL
1	A	727	CYS
1	A	730	ILE
1	A	758	ARG
1	A	778	GLN
1	A	780	ILE
1	A	786	ILE
1	A	793	ILE
1	A	801	GLU
1	A	811	VAL
1	A	815	LEU
1	A	816	LEU
1	A	833	MET
1	A	836	LEU
2	B	332	THR
2	B	334	VAL

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Mol	Chain	Res	Type
2	B	335	LEU
2	B	337	GLN
2	B	338	LEU
2	B	342	LEU
2	B	343	VAL
2	B	345	VAL
2	B	347	ARG
2	B	349	ILE
2	B	368	GLU
2	B	370	TYR
2	B	371	ARG
2	B	393	GLN
2	B	397	LYS
2	B	403	GLN
2	B	418	LYS
2	B	420	PHE
2	B	423	ASN
2	B	425	ARG
2	B	426	ARG
2	B	430	ILE
2	B	431	ASP
2	B	436	GLU
3	C	2	ARG
3	C	3	THR
3	C	5	GLN
3	C	8	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	GLN
1	A	224	ASN
1	A	383	ASN
1	A	399	ASN
1	A	410	GLN
1	A	430	HIS
1	A	438	GLN
1	A	450	ASN
1	A	484	HIS
1	A	535	ASN
1	A	592	GLN
1	A	742	GLN

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Mol	Chain	Res	Type
1	A	828	GLN
2	B	337	GLN
2	B	351	ASN
2	B	356	ASN
2	B	403	GLN
2	B	429	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	MLY	C	4	3	9,10,11	0.46	0	6,11,13	0.14	0

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	MLY	C	4	3	-	5/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	4	MLY	N-CA-CB-CG
3	C	4	MLY	C-CA-CB-CG
3	C	4	MLY	CD-CE-NZ-CH1
3	C	4	MLY	CD-CE-NZ-CH2
3	C	4	MLY	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4	MLY	2	0

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	HUF	A	901	-	59,60,60	1.25	7 (11%)	78,92,92	0.93	3 (3%)

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	HUF	A	901	-	-	9/36/52/52	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	HUF	PA-O3A	-3.74	1.55	1.59
4	A	901	HUF	C20-C23	-3.13	1.35	1.43
4	A	901	HUF	PB-O3A	-3.06	1.56	1.59
4	A	901	HUF	C16-C17	-2.59	1.36	1.39
4	A	901	HUF	O36-C25	-2.42	1.38	1.43
4	A	901	HUF	O37-C26	-2.10	1.37	1.43
4	A	901	HUF	C13-C12	-2.08	1.36	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	HUF	C20-C23-N31	3.64	117.34	110.94
4	A	901	HUF	O33-C19-N29	-3.03	121.59	124.71
4	A	901	HUF	O4'-C1'-C2'	-2.05	102.23	106.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	HUF	C5'-O5'-PA-O2A
4	A	901	HUF	O33-C19-N29-C15
4	A	901	HUF	O33-C19-N29-C20
4	A	901	HUF	O38-C27-C28-O1B
4	A	901	HUF	C26-C27-C28-O1B
4	A	901	HUF	C3'-C4'-C5'-O5'
4	A	901	HUF	O4'-C4'-C5'-O5'
4	A	901	HUF	C5'-O5'-PA-O3A
4	A	901	HUF	O36-C25-C26-C27

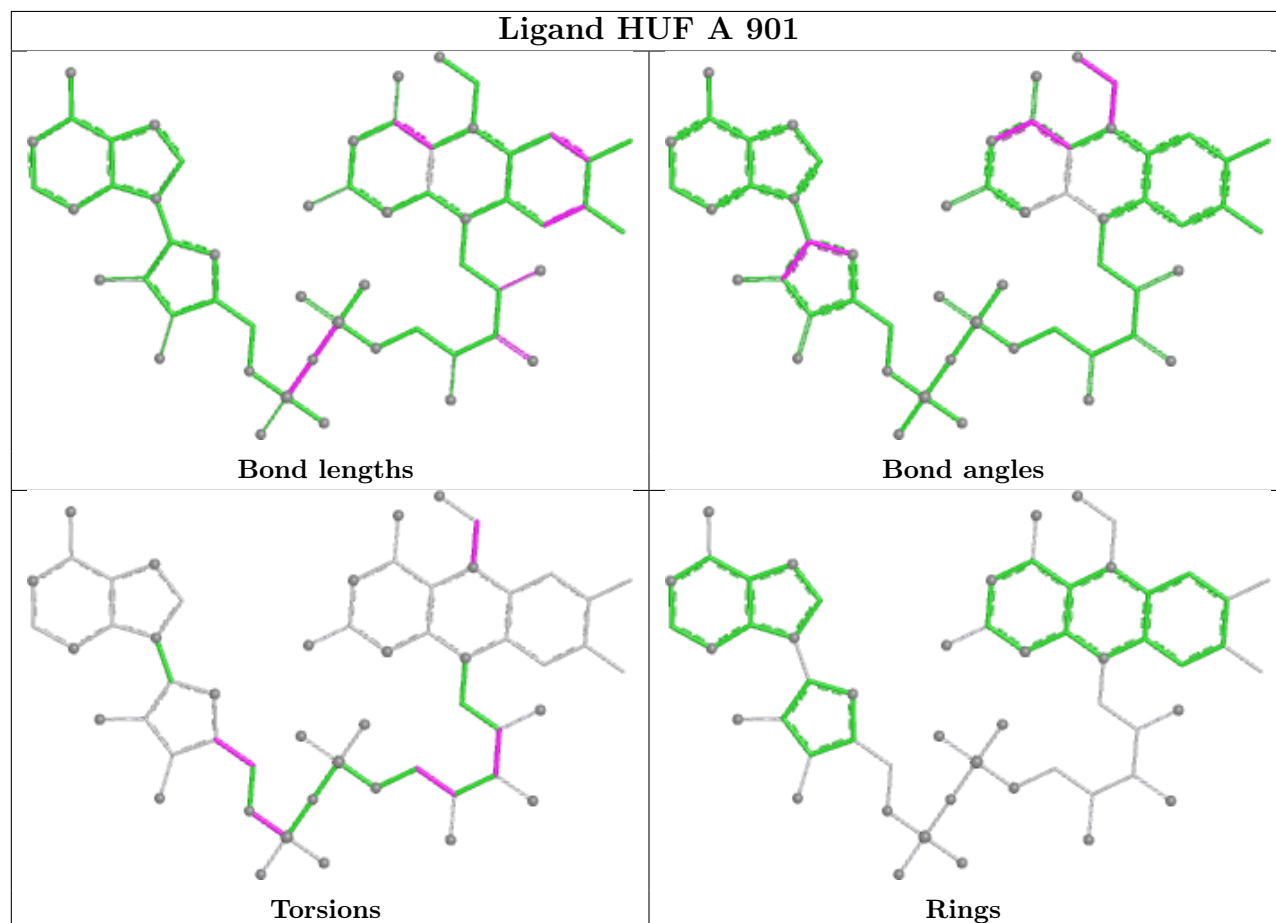
There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	HUF	11	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%)	0.53	39 (5%)	28 18	70, 100, 132, 151	0
2	B	133/144 (92%)	0.75	13 (9%)	13 9	99, 128, 149, 161	0
3	C	7/21 (33%)	3.77	7 (100%)	0 0	112, 131, 137, 142	0
All	All	806/1036 (77%)	0.59	59 (7%)	21 13	70, 107, 138, 161	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	836	LEU	7.2
3	C	1	ALA	6.0
3	C	5	GLN	5.7
2	B	375	VAL	5.3
1	A	171	PRO	5.0
3	C	3	THR	4.7
1	A	770	GLY	4.6
1	A	791	GLN	4.6
1	A	683	SER	4.4
1	A	806	ASN	4.4
1	A	557	ASP	4.3
1	A	558	PHE	4.3
1	A	769	SER	4.2
1	A	555	ASP	4.0
1	A	771	ASN	4.0
1	A	773	TYR	3.7
1	A	556	ASP	3.6
1	A	559	GLU	3.5
2	B	376	ILE	3.5
1	A	760	SER	3.5
1	A	275	THR	3.5
1	A	785	SER	3.5
3	C	2	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	774	ASP	3.3
1	A	373	GLU	3.3
1	A	805	ARG	3.2
1	A	834	TYR	3.0
2	B	427	ARG	3.0
1	A	554	GLN	3.0
1	A	447	LYS	2.8
1	A	338	GLY	2.7
1	A	667	ASP	2.7
1	A	369	ALA	2.7
1	A	768	SER	2.7
2	B	383	TRP	2.7
2	B	430	ILE	2.6
1	A	567	VAL	2.5
1	A	523	SER	2.4
2	B	431	ASP	2.4
2	B	379	CYS	2.4
1	A	273	LEU	2.4
1	A	514	ASN	2.4
2	B	336	ARG	2.4
3	C	7	ALA	2.3
1	A	739	ALA	2.3
1	A	563	SER	2.3
3	C	8	ARG	2.2
2	B	332	THR	2.2
2	B	324	VAL	2.2
2	B	337	GLN	2.1
1	A	787	PRO	2.1
1	A	833	MET	2.1
1	A	269	ARG	2.1
3	C	6	THR	2.1
2	B	373	PRO	2.1
2	B	374	GLU	2.1
1	A	527	GLN	2.1
1	A	232	GLU	2.0
1	A	758	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MLY	C	4	11/12	0.76	0.42	109,120,141,143	0

6.3 Carbohydrates [i](#)

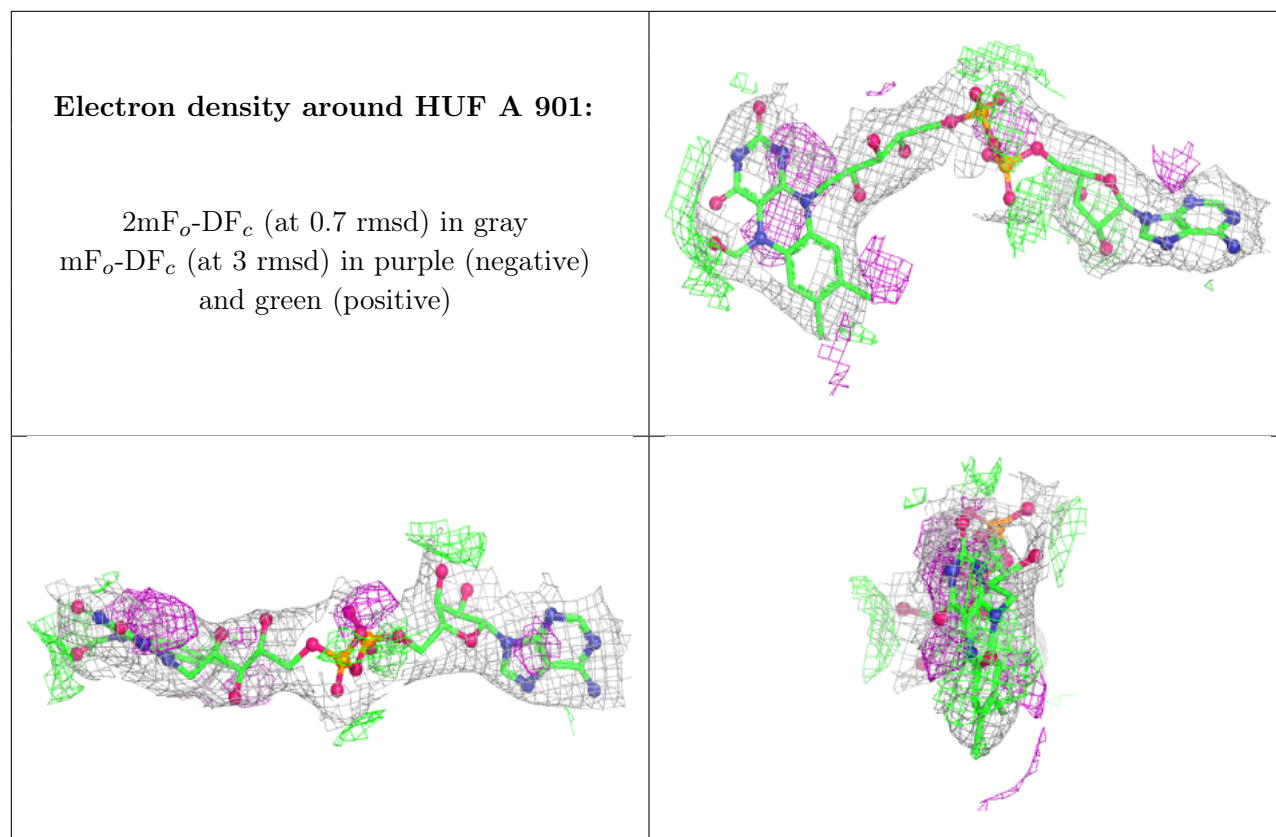
There are no oligosaccharides in this entry.

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	HUF	A	901	55/55	0.93	0.12	69,82,98,107	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.