



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 04:01 PM UTC

PDB ID : 8UNI / pdb_00008uni
Title : LSD1-CoREST with N-formyl-FAD in complex with H3K4M histone tail
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2023-10-19
Resolution : 3.40 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

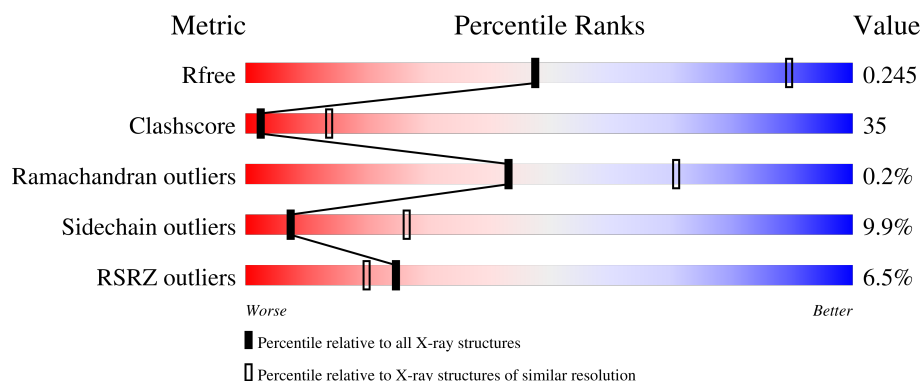
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	5% 43% 28% 5% 24%
2	B	144	4% 56% 30% 7% 8%
3	C	21	19% 24% 48% 5% 24%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6462 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

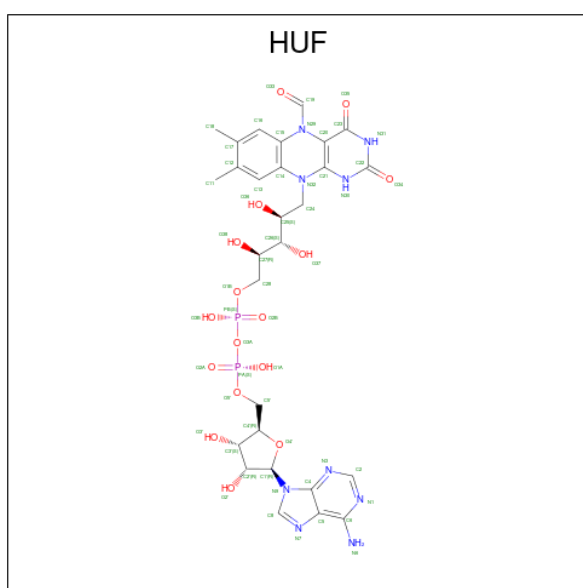
- Molecule 3 is a protein called Histone H3 (Fragment).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	S	0	0	0
			114	67	25	21	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	LYS	engineered mutation	UNP V9H1G0

- Molecule 4 is [[(2R,3S,4R,5R)-5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2R,3S,4S)-5-[5-methanoyl-7,8-dimethyl-2,4-bis(oxidanylidene)-1H-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).

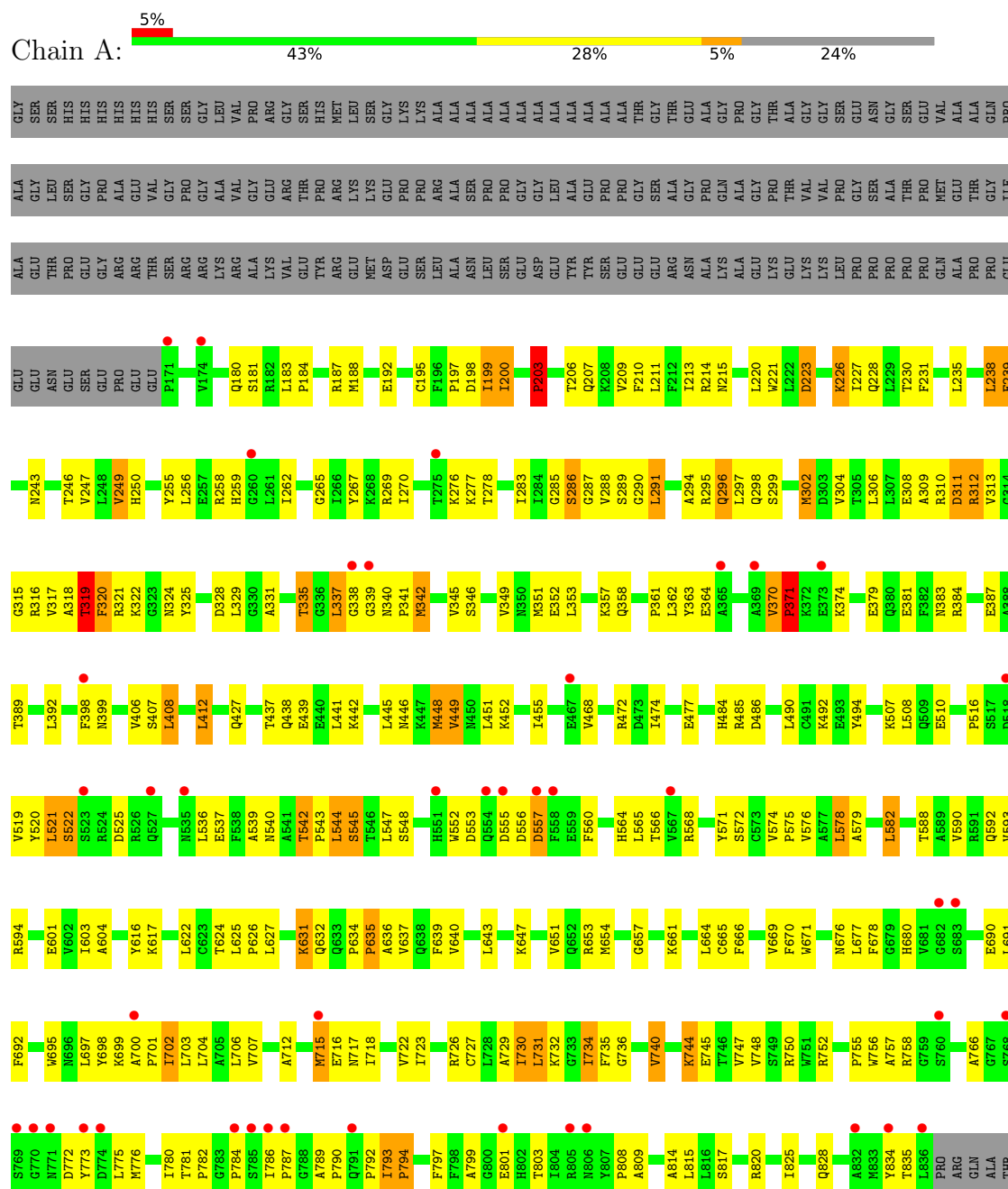


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			55	28	9	16	2		

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: Lysine-specific histone demethylase 1A

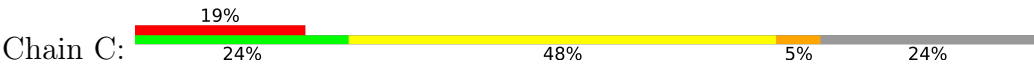


PRO
GLY
VAL
PRO
ALA
GLN
GLN
SER
PRO
SER
MET

● 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	117.78Å 178.17Å 234.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.13 – 3.40 49.13 – 3.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.13-3.40) 98.3 (49.13-3.40)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.222 , 0.252 0.244 , 0.245	Depositor DCC
R_{free} test set	2000 reflections (5.83%)	wwPDB-VP
Wilson B-factor (Å ²)	113.9	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 74.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6462	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: 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	0.74	2/5331 (0.0%)	1.11	18/7232 (0.2%)
2	B	0.57	0/1091	1.02	1/1471 (0.1%)
3	C	0.74	0/114	1.37	0/150
All	All	0.72	2/6536 (0.0%)	1.10	19/8853 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	635	PRO	C-O	-5.33	1.17	1.23
1	A	782	PRO	C-O	-5.01	1.17	1.23

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	ASP	CA-C-N	-8.25	113.09	122.00
1	A	223	ASP	C-N-CA	-8.25	113.09	122.00
1	A	319	THR	CA-C-N	-7.38	110.95	121.50
1	A	319	THR	C-N-CA	-7.38	110.95	121.50
1	A	740	VAL	N-CA-C	6.39	113.38	107.56
1	A	223	ASP	N-CA-CB	6.29	119.37	110.12
1	A	337	LEU	CA-C-N	-6.25	115.36	120.98
1	A	337	LEU	C-N-CA	-6.25	115.36	120.98
1	A	794	PRO	N-CA-C	-6.12	99.86	112.47
1	A	203	PRO	N-CA-CB	-6.03	96.92	103.25
1	A	698	TYR	CB-CA-C	5.96	120.50	109.54
1	A	636	ALA	N-CA-C	-5.40	105.55	111.82
1	A	286	SER	N-CA-C	-5.39	105.39	112.72
2	B	408	VAL	N-CA-C	-5.33	105.13	110.30
1	A	522	SER	CA-C-O	-5.33	115.34	121.47
1	A	223	ASP	CB-CA-C	-5.04	102.42	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	717	ASN	CB-CA-C	-5.04	100.53	110.11
1	A	371	PRO	N-CA-CB	-5.02	97.98	103.25
1	A	635	PRO	N-CA-C	5.00	118.74	111.03

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	373	0
2	B	1076	0	1091	91	0
3	C	114	0	125	21	0
4	A	55	0	0	17	0
All	All	6462	0	6468	450	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 35.

All (450) 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:325:TYR:CE2	1:A:665:CYS:CB	1.86	1.53
1:A:325:TYR:HE2	1:A:665:CYS:CB	1.16	1.46
1:A:325:TYR:CE2	1:A:665:CYS:HB3	0.90	1.42
2:B:400:ARG:O	2:B:402:PHE:CD2	1.82	1.31
1:A:664:LEU:HD11	1:A:727:CYS:SG	1.71	1.30
2:B:414:VAL:O	2:B:417:VAL:HG23	1.17	1.30
1:A:325:TYR:HD2	1:A:665:CYS:SG	1.58	1.25
2:B:400:ARG:O	2:B:402:PHE:HD2	1.16	1.25
1:A:325:TYR:CD2	1:A:665:CYS:HB3	1.72	1.24
1:A:670:PHE:O	1:A:735:PHE:CE1	1.93	1.22
1:A:671:TRP:HA	1:A:735:PHE:CE1	1.75	1.20
2:B:414:VAL:HA	2:B:417:VAL:CG2	1.70	1.19
2:B:414:VAL:C	2:B:417:VAL:CG2	2.17	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:VAL:C	2:B:417:VAL:HG23	1.67	1.18
1:A:325:TYR:CD2	1:A:665:CYS:SG	2.36	1.17
1:A:449:VAL:CG2	2:B:363:LEU:HD21	1.78	1.14
1:A:670:PHE:O	1:A:735:PHE:CD1	1.99	1.14
1:A:231:PHE:CE1	1:A:249:VAL:HG12	1.83	1.14
1:A:203:PRO:HD2	1:A:206:THR:HB	1.29	1.11
2:B:414:VAL:CA	2:B:417:VAL:CG2	2.28	1.11
1:A:231:PHE:HE1	1:A:249:VAL:HG12	0.95	1.10
1:A:537:GLU:HG3	1:A:544:LEU:HD21	1.22	1.10
1:A:339:GLY:O	1:A:560:PHE:CE1	2.05	1.10
1:A:265:GLY:O	1:A:295:ARG:NH1	1.86	1.09
2:B:414:VAL:O	2:B:417:VAL:CG2	2.02	1.06
2:B:414:VAL:HA	2:B:417:VAL:HG21	1.09	1.06
1:A:325:TYR:CD2	1:A:665:CYS:CB	2.33	1.06
1:A:322:LYS:NZ	1:A:745:GLU:CD	2.12	1.06
1:A:342:MET:HE3	1:A:342:MET:HA	1.38	1.05
1:A:716:GLU:OE2	1:A:750:ARG:CA	2.06	1.04
1:A:203:PRO:HG2	1:A:206:THR:OG1	1.56	1.04
1:A:566:THR:HG21	1:A:697:LEU:CD2	1.88	1.04
1:A:203:PRO:CG	1:A:206:THR:OG1	2.06	1.04
1:A:707:VAL:O	1:A:712:ALA:HB2	1.56	1.03
1:A:370:VAL:HG12	1:A:371:PRO:HD2	1.39	1.03
1:A:319:THR:HG21	1:A:321:ARG:NH2	1.72	1.03
1:A:389:THR:HG21	1:A:412:LEU:HD23	1.39	1.02
1:A:322:LYS:HZ3	1:A:745:GLU:CD	1.65	1.01
2:B:413:SER:O	2:B:417:VAL:HG22	1.60	1.00
2:B:414:VAL:CA	2:B:417:VAL:HG21	1.89	1.00
1:A:671:TRP:HA	1:A:735:PHE:HE1	1.06	0.99
1:A:449:VAL:HG23	2:B:363:LEU:HD21	1.42	0.99
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.01	0.98
1:A:316:ARG:NH1	4:A:901:HUF:O2A	1.96	0.98
1:A:521:LEU:HD12	1:A:525:ASP:CB	1.94	0.97
1:A:671:TRP:CA	1:A:735:PHE:HE1	1.81	0.94
1:A:716:GLU:OE2	1:A:750:ARG:HA	1.68	0.94
1:A:231:PHE:HE1	1:A:249:VAL:CG1	1.79	0.94
1:A:781:THR:HG23	1:A:793:ILE:O	1.66	0.93
1:A:556:ASP:OD2	3:C:2:ARG:NH1	2.01	0.93
2:B:400:ARG:O	2:B:402:PHE:CE2	2.21	0.93
1:A:339:GLY:O	1:A:560:PHE:HE1	1.44	0.92
1:A:537:GLU:CG	1:A:544:LEU:HD21	1.99	0.91
1:A:556:ASP:OD2	3:C:2:ARG:HD2	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HH22	1:A:299:SER:HB2	1.36	0.91
1:A:537:GLU:HG3	1:A:544:LEU:CD2	1.99	0.91
1:A:677:LEU:HD11	3:C:7:ALA:HB2	1.51	0.90
2:B:368:GLU:OE1	2:B:371:ARG:NH1	2.05	0.89
1:A:449:VAL:HG22	2:B:363:LEU:HD21	1.51	0.89
1:A:789:ALA:HB1	1:A:790:PRO:HD2	1.54	0.88
1:A:363:TYR:CB	1:A:734:ILE:CD1	2.53	0.87
1:A:238:LEU:HB3	1:A:243:ASN:HB3	1.57	0.87
1:A:328:ASP:OD2	1:A:571:TYR:HB2	1.73	0.87
1:A:203:PRO:CD	1:A:206:THR:HB	2.03	0.86
1:A:291:LEU:HD21	1:A:579:ALA:HB2	1.57	0.86
1:A:294:ALA:HB1	1:A:582:LEU:HD13	1.55	0.86
1:A:566:THR:CG2	1:A:697:LEU:HD22	1.97	0.85
1:A:363:TYR:CB	1:A:734:ILE:HD11	2.07	0.85
1:A:203:PRO:HD2	1:A:206:THR:CB	2.06	0.85
1:A:700:ALA:HB1	1:A:701:PRO:HD2	1.58	0.85
4:A:901:HUF:C20	3:C:4:MET:HE1	2.06	0.84
1:A:325:TYR:HD2	1:A:665:CYS:HG	0.87	0.84
1:A:363:TYR:CG	1:A:734:ILE:CD1	2.62	0.83
1:A:408:LEU:HD12	1:A:408:LEU:O	1.78	0.83
1:A:670:PHE:O	1:A:735:PHE:HD1	1.61	0.82
1:A:664:LEU:CD1	1:A:727:CYS:SG	2.65	0.81
1:A:362:LEU:HB2	1:A:370:VAL:HG21	1.62	0.81
1:A:449:VAL:CG2	2:B:363:LEU:CD2	2.57	0.81
2:B:368:GLU:CD	2:B:371:ARG:HH12	1.89	0.81
2:B:425:ARG:HG3	2:B:425:ARG:HH11	1.45	0.81
2:B:402:PHE:HD2	2:B:402:PHE:H	1.29	0.80
1:A:203:PRO:HG2	1:A:206:THR:CB	2.11	0.80
1:A:568:ARG:NH2	1:A:699:LYS:HG2	1.95	0.80
1:A:389:THR:CG2	1:A:412:LEU:HD23	2.12	0.80
1:A:389:THR:HG21	1:A:412:LEU:CD2	2.11	0.79
1:A:363:TYR:HB2	1:A:734:ILE:HD11	1.65	0.79
1:A:537:GLU:CG	1:A:544:LEU:CD2	2.56	0.79
2:B:425:ARG:HA	2:B:430:ILE:HD12	1.64	0.79
1:A:716:GLU:OE2	1:A:750:ARG:C	2.26	0.79
1:A:362:LEU:O	1:A:370:VAL:HG23	1.83	0.78
1:A:239:GLU:OE2	1:A:239:GLU:HA	1.83	0.78
1:A:329:LEU:HD21	1:A:747:VAL:HG11	1.64	0.78
1:A:318:ALA:O	1:A:328:ASP:OD1	2.01	0.78
2:B:403:GLN:NE2	2:B:403:GLN:O	2.16	0.78
1:A:449:VAL:HG22	2:B:363:LEU:CD2	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LEU:HD13	1:A:249:VAL:HG21	1.65	0.77
1:A:695:TRP:HE1	1:A:706:LEU:HD13	1.48	0.77
1:A:521:LEU:HD12	1:A:525:ASP:HB2	1.66	0.77
1:A:671:TRP:CA	1:A:735:PHE:CE1	2.60	0.77
1:A:200:ILE:HD12	1:A:200:ILE:O	1.86	0.76
1:A:291:LEU:CD2	1:A:579:ALA:HB2	2.14	0.76
1:A:544:LEU:HD23	1:A:544:LEU:N	2.00	0.76
1:A:325:TYR:OH	1:A:666:PHE:O	2.03	0.76
2:B:359:LEU:HD23	2:B:359:LEU:N	2.01	0.76
1:A:370:VAL:HG12	1:A:371:PRO:CD	2.15	0.75
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.04	0.75
1:A:407:SER:HB3	1:A:545:SER:O	1.86	0.74
1:A:445:LEU:HA	1:A:448:MET:HG3	1.67	0.74
1:A:328:ASP:OD2	1:A:571:TYR:CB	2.35	0.74
1:A:665:CYS:SG	1:A:702:ILE:HD13	2.28	0.74
1:A:331:ALA:HB3	1:A:571:TYR:CD2	2.23	0.74
1:A:352:GLU:OE2	1:A:699:LYS:HE2	1.88	0.74
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.51	0.74
1:A:680:HIS:ND1	1:A:730:ILE:CG2	2.51	0.74
1:A:716:GLU:OE2	1:A:750:ARG:CB	2.36	0.73
1:A:329:LEU:N	1:A:329:LEU:HD12	2.02	0.73
1:A:311:ASP:OD1	1:A:311:ASP:N	2.09	0.73
1:A:671:TRP:HA	1:A:735:PHE:CZ	2.21	0.73
1:A:294:ALA:HB1	1:A:582:LEU:CD1	2.19	0.73
1:A:381:GLU:OE2	1:A:520:TYR:OH	2.06	0.72
1:A:331:ALA:HB1	1:A:571:TYR:HE2	1.54	0.72
1:A:399:ASN:C	1:A:406:VAL:HG23	2.14	0.72
1:A:631:LYS:HE2	1:A:651:VAL:O	1.89	0.71
2:B:406:SER:OG	2:B:412:LYS:O	2.08	0.71
1:A:203:PRO:CD	1:A:206:THR:CB	2.66	0.71
1:A:744:LYS:HD2	1:A:744:LYS:N	2.02	0.70
1:A:331:ALA:CB	1:A:571:TYR:CE2	2.75	0.70
1:A:269:ARG:HH22	1:A:299:SER:CB	2.04	0.70
1:A:680:HIS:CE1	1:A:730:ILE:HG23	2.26	0.70
1:A:484:HIS:CD2	2:B:372:LEU:HD13	2.26	0.70
1:A:670:PHE:HZ	1:A:731:LEU:HD22	1.56	0.70
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.72	0.70
1:A:449:VAL:HG23	2:B:363:LEU:CD2	2.20	0.70
1:A:203:PRO:CG	1:A:206:THR:CB	2.69	0.69
1:A:408:LEU:HD12	1:A:408:LEU:C	2.16	0.69
1:A:320:PHE:CD1	1:A:747:VAL:HG21	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:SER:CB	1:A:545:SER:O	2.40	0.69
2:B:414:VAL:CA	2:B:417:VAL:HG22	2.20	0.69
2:B:425:ARG:HG3	2:B:425:ARG:NH1	2.03	0.69
1:A:568:ARG:HH21	1:A:699:LYS:HA	1.58	0.69
3:C:2:ARG:NH2	3:C:12:GLY:O	2.26	0.69
1:A:363:TYR:CD2	1:A:734:ILE:HD13	2.27	0.69
2:B:399:GLY:N	2:B:437:TRP:NE1	2.40	0.68
1:A:335:THR:O	1:A:335:THR:OG1	2.10	0.68
1:A:319:THR:HG21	1:A:321:ARG:CZ	2.23	0.67
1:A:680:HIS:CE1	1:A:730:ILE:CG2	2.77	0.67
1:A:199:ILE:HG23	1:A:206:THR:HG22	1.75	0.67
1:A:325:TYR:HE2	1:A:665:CYS:CA	2.03	0.67
1:A:446:ASN:OD1	2:B:359:LEU:CD1	2.42	0.67
1:A:437:THR:HB	1:A:508:LEU:HD21	1.77	0.67
1:A:521:LEU:HD12	1:A:525:ASP:HB3	1.76	0.66
1:A:626:PRO:HG3	4:A:901:HUF:C5'	2.25	0.66
1:A:331:ALA:HB3	1:A:571:TYR:CE2	2.30	0.66
1:A:296:GLN:HA	1:A:296:GLN:OE1	1.95	0.66
1:A:331:ALA:CB	1:A:571:TYR:HE2	2.09	0.66
1:A:338:GLY:O	1:A:560:PHE:HD1	1.79	0.66
1:A:342:MET:HE3	1:A:342:MET:CA	2.13	0.66
1:A:716:GLU:OE2	1:A:750:ARG:HB3	1.95	0.66
1:A:192:GLU:OE2	1:A:214:ARG:NE	2.29	0.66
1:A:793:ILE:HG22	1:A:794:PRO:CD	2.26	0.65
1:A:339:GLY:O	1:A:560:PHE:CD1	2.50	0.65
1:A:537:GLU:HG2	1:A:544:LEU:HD23	1.78	0.65
1:A:670:PHE:O	1:A:735:PHE:HE1	1.50	0.65
2:B:363:LEU:HD23	2:B:363:LEU:N	2.10	0.65
1:A:793:ILE:HG22	1:A:794:PRO:HD2	1.77	0.65
1:A:322:LYS:HZ2	1:A:745:GLU:CD	2.03	0.65
1:A:200:ILE:O	1:A:207:GLN:NE2	2.30	0.64
1:A:557:ASP:N	1:A:557:ASP:OD1	2.29	0.64
2:B:425:ARG:HH11	2:B:425:ARG:CG	2.10	0.64
1:A:294:ALA:CB	1:A:582:LEU:CD1	2.75	0.64
1:A:363:TYR:CG	1:A:734:ILE:HD13	2.32	0.64
2:B:399:GLY:CA	2:B:437:TRP:CE2	2.80	0.64
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.80	0.63
1:A:677:LEU:HD11	3:C:7:ALA:CB	2.27	0.63
1:A:695:TRP:NE1	1:A:706:LEU:HD13	2.12	0.63
1:A:362:LEU:CB	1:A:370:VAL:HG21	2.26	0.63
1:A:362:LEU:HB2	1:A:370:VAL:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:C	1:A:370:VAL:HG23	2.24	0.62
1:A:363:TYR:HB3	1:A:734:ILE:CD1	2.28	0.62
1:A:716:GLU:O	1:A:750:ARG:NE	2.32	0.62
1:A:670:PHE:C	1:A:735:PHE:HE1	2.08	0.62
1:A:695:TRP:HE1	1:A:706:LEU:CD1	2.12	0.62
1:A:338:GLY:O	1:A:560:PHE:CD1	2.53	0.62
1:A:340:ASN:OD1	1:A:341:PRO:HD2	2.00	0.62
1:A:781:THR:HG23	1:A:793:ILE:C	2.24	0.61
1:A:374:LYS:NZ	1:A:525:ASP:OD1	2.32	0.61
1:A:594:ARG:HG2	1:A:640:VAL:HB	1.82	0.61
2:B:399:GLY:N	2:B:437:TRP:CE2	2.68	0.61
1:A:319:THR:HG21	1:A:321:ARG:HH21	1.64	0.61
1:A:548:SER:HB2	1:A:766:ALA:HA	1.81	0.61
1:A:259:HIS:HE1	1:A:834:TYR:OH	1.83	0.61
1:A:540:ASN:CG	1:A:547:LEU:HD11	2.26	0.61
1:A:542:THR:OG1	1:A:543:PRO:HD2	2.00	0.61
2:B:317:SER:O	2:B:321:VAL:HG23	2.00	0.61
1:A:319:THR:HG22	1:A:319:THR:O	2.01	0.60
1:A:568:ARG:CZ	1:A:699:LYS:HG2	2.31	0.60
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.83	0.60
1:A:322:LYS:NZ	1:A:745:GLU:OE1	2.33	0.60
1:A:522:SER:OG	1:A:525:ASP:CG	2.43	0.60
1:A:438:GLN:OE1	1:A:508:LEU:HD13	2.02	0.60
1:A:230:THR:HG23	1:A:270:ILE:HD12	1.83	0.60
1:A:537:GLU:HG2	1:A:544:LEU:CD2	2.30	0.60
2:B:361:GLU:HA	2:B:361:GLU:OE1	2.02	0.60
1:A:231:PHE:CE1	1:A:249:VAL:CG1	2.67	0.60
2:B:402:PHE:HD2	2:B:402:PHE:N	2.00	0.59
2:B:375:VAL:HG12	2:B:375:VAL:O	2.01	0.59
1:A:740:VAL:HG12	1:A:740:VAL:O	2.02	0.59
1:A:317:VAL:HG12	1:A:317:VAL:O	2.01	0.59
1:A:269:ARG:NH2	1:A:299:SER:HB2	2.13	0.59
1:A:331:ALA:HB1	1:A:571:TYR:CE2	2.35	0.59
1:A:312:ARG:HH11	1:A:312:ARG:HG3	1.66	0.59
1:A:448:MET:HE3	2:B:363:LEU:HD12	1.86	0.58
1:A:451:LEU:HD23	1:A:494:TYR:HB2	1.85	0.58
1:A:670:PHE:CZ	1:A:731:LEU:HD22	2.37	0.58
1:A:542:THR:OG1	1:A:543:PRO:CD	2.52	0.58
1:A:627:LEU:O	1:A:631:LYS:HG3	2.04	0.58
1:A:319:THR:HB	1:A:572:SER:HB3	1.86	0.57
1:A:335:THR:HB	1:A:564:HIS:CE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:ASN:OD1	2:B:359:LEU:HD11	2.04	0.57
2:B:399:GLY:H	2:B:437:TRP:CD1	2.23	0.57
2:B:402:PHE:CD2	2:B:402:PHE:N	2.68	0.57
1:A:309:ALA:HB2	4:A:901:HUF:C2	2.35	0.56
1:A:203:PRO:HG3	1:A:206:THR:OG1	2.02	0.56
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.40	0.56
1:A:195:CYS:SG	1:A:834:TYR:HE2	2.28	0.56
1:A:203:PRO:O	1:A:206:THR:HB	2.05	0.56
1:A:691:LEU:HA	1:A:706:LEU:O	2.05	0.56
1:A:209:VAL:O	1:A:213:ILE:HG13	2.06	0.56
1:A:320:PHE:C	1:A:320:PHE:CD2	2.83	0.56
1:A:294:ALA:HA	1:A:304:VAL:HG11	1.88	0.56
1:A:556:ASP:CG	3:C:2:ARG:HD2	2.31	0.56
2:B:400:ARG:CB	2:B:402:PHE:HE2	2.19	0.56
1:A:670:PHE:HD1	1:A:735:PHE:CD1	2.24	0.55
1:A:337:LEU:HD23	1:A:337:LEU:N	2.19	0.55
1:A:258:ARG:HG2	1:A:834:TYR:HE1	1.71	0.55
2:B:414:VAL:HA	2:B:417:VAL:HG22	1.77	0.55
2:B:414:VAL:C	2:B:417:VAL:HG22	2.25	0.55
1:A:485:ARG:HG3	2:B:407:ASP:HB2	1.88	0.54
1:A:286:SER:O	1:A:286:SER:OG	2.16	0.54
1:A:379:GLU:O	1:A:383:ASN:ND2	2.40	0.54
1:A:357:LYS:HG3	1:A:676:ASN:OD1	2.07	0.54
1:A:657:GLY:HA2	1:A:752:ARG:HH22	1.72	0.54
2:B:399:GLY:HA3	2:B:437:TRP:CZ2	2.42	0.54
1:A:312:ARG:HH11	1:A:312:ARG:CG	2.21	0.54
2:B:406:SER:OG	2:B:406:SER:O	2.25	0.54
1:A:539:ALA:HB2	3:C:5:GLN:HG3	1.89	0.53
2:B:399:GLY:H	2:B:437:TRP:NE1	2.05	0.53
1:A:310:ARG:NH2	1:A:756:TRP:HB2	2.22	0.53
2:B:413:SER:C	2:B:417:VAL:HG22	2.33	0.53
1:A:732:LYS:O	1:A:736:GLY:N	2.34	0.53
1:A:214:ARG:NH1	1:A:215:ASN:OD1	2.42	0.53
1:A:363:TYR:CG	1:A:734:ILE:HD12	2.42	0.53
1:A:707:VAL:HG12	1:A:712:ALA:HA	1.89	0.53
2:B:381:ALA:HA	2:B:416:GLN:HE22	1.73	0.53
1:A:626:PRO:HD3	4:A:901:HUF:C5'	2.39	0.53
4:A:901:HUF:C23	3:C:4:MET:HE1	2.38	0.53
1:A:319:THR:HB	1:A:572:SER:CB	2.39	0.53
1:A:352:GLU:OE2	1:A:699:LYS:CE	2.56	0.53
1:A:297:LEU:HB2	1:A:304:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:ASN:O	1:A:542:THR:HG22	2.09	0.52
1:A:670:PHE:CE1	1:A:740:VAL:HG22	2.44	0.52
1:A:680:HIS:ND1	1:A:730:ILE:HG21	2.23	0.52
1:A:626:PRO:CG	4:A:901:HUF:C5'	2.87	0.52
1:A:665:CYS:SG	1:A:702:ILE:CD1	2.97	0.52
1:A:188:MET:HG2	1:A:210:PHE:HE2	1.74	0.52
1:A:312:ARG:CG	1:A:312:ARG:NH1	2.72	0.52
1:A:716:GLU:CD	1:A:750:ARG:HB3	2.34	0.52
1:A:363:TYR:CB	1:A:734:ILE:HD13	2.39	0.52
1:A:801:GLU:HB3	1:A:814:ALA:HB2	1.91	0.52
1:A:198:ASP:OD1	1:A:198:ASP:N	2.43	0.52
1:A:226:LYS:O	1:A:267:TYR:HA	2.09	0.52
1:A:521:LEU:CD1	1:A:525:ASP:HB3	2.39	0.52
1:A:669:VAL:HG13	1:A:671:TRP:CE2	2.44	0.52
1:A:325:TYR:CE2	1:A:665:CYS:CA	2.83	0.51
1:A:290:GLY:N	1:A:624:THR:HG21	2.26	0.51
1:A:363:TYR:HB3	1:A:734:ILE:HD11	1.87	0.51
2:B:399:GLY:HA3	2:B:437:TRP:CE2	2.45	0.51
1:A:631:LYS:CE	1:A:651:VAL:O	2.59	0.51
1:A:707:VAL:CG1	1:A:712:ALA:HA	2.41	0.51
1:A:790:PRO:O	1:A:790:PRO:HG2	2.09	0.51
1:A:707:VAL:HG12	1:A:712:ALA:CA	2.40	0.51
1:A:399:ASN:HA	1:A:406:VAL:CG2	2.40	0.51
2:B:381:ALA:HA	2:B:416:GLN:NE2	2.26	0.51
1:A:203:PRO:CG	1:A:206:THR:HB	2.36	0.50
1:A:781:THR:HA	1:A:794:PRO:HA	1.92	0.50
2:B:394:ALA:O	2:B:398:TYR:N	2.44	0.50
1:A:744:LYS:N	1:A:744:LYS:CD	2.73	0.50
1:A:537:GLU:HG2	1:A:542:THR:O	2.12	0.50
1:A:701:PRO:HG2	1:A:701:PRO:O	2.11	0.50
1:A:707:VAL:O	1:A:712:ALA:CB	2.44	0.50
1:A:231:PHE:CE2	1:A:250:HIS:ND1	2.80	0.50
1:A:442:LYS:HE3	2:B:355:THR:HG21	1.92	0.50
1:A:340:ASN:OD1	1:A:341:PRO:CD	2.58	0.50
1:A:695:TRP:HB3	1:A:697:LEU:CD1	2.42	0.50
1:A:283:ILE:HG12	1:A:622:LEU:HB3	1.94	0.49
2:B:363:LEU:CD2	2:B:363:LEU:N	2.74	0.49
1:A:322:LYS:NZ	1:A:745:GLU:CG	2.75	0.49
1:A:784:PRO:O	1:A:784:PRO:HG2	2.12	0.49
1:A:691:LEU:HD22	1:A:727:CYS:HA	1.95	0.49
1:A:331:ALA:CB	1:A:571:TYR:CD2	2.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:N	1:A:329:LEU:CD1	2.73	0.49
1:A:342:MET:HA	1:A:342:MET:CE	2.25	0.49
1:A:294:ALA:HB2	1:A:306:LEU:HD11	1.95	0.49
1:A:601:GLU:HB3	1:A:617:LYS:HD3	1.94	0.49
1:A:286:SER:HB3	1:A:308:GLU:HB2	1.95	0.48
1:A:363:TYR:HB3	1:A:734:ILE:HD13	1.94	0.48
1:A:384:ARG:NH1	2:B:312:LYS:O	2.45	0.48
1:A:351:MET:HE2	1:A:351:MET:HB3	1.65	0.48
4:A:901:HUF:O38	4:A:901:HUF:O36	2.32	0.48
1:A:548:SER:O	1:A:552:TRP:HB3	2.13	0.48
1:A:455:ILE:HD11	1:A:490:LEU:O	2.14	0.48
2:B:385:THR:O	2:B:389:LEU:HD12	2.13	0.48
1:A:228:GLN:OE1	1:A:270:ILE:N	2.44	0.48
4:A:901:HUF:O33	3:C:4:MET:HE1	2.13	0.48
1:A:474:ILE:HD12	1:A:477:GLU:HB3	1.96	0.47
1:A:601:GLU:HA	1:A:616:TYR:O	2.15	0.47
1:A:718:ILE:HG23	1:A:722:VAL:HB	1.95	0.47
1:A:329:LEU:HD21	1:A:747:VAL:CG1	2.39	0.47
2:B:403:GLN:NE2	2:B:403:GLN:C	2.72	0.47
1:A:594:ARG:HA	1:A:640:VAL:O	2.13	0.47
2:B:368:GLU:CD	2:B:371:ARG:NH1	2.62	0.47
1:A:362:LEU:C	1:A:370:VAL:CG2	2.88	0.47
2:B:402:PHE:CD1	2:B:418:LYS:HG2	2.50	0.47
1:A:310:ARG:CZ	1:A:756:TRP:HB2	2.45	0.46
2:B:429:ASN:HB3	2:B:432:GLU:CD	2.40	0.46
1:A:379:GLU:OE1	3:C:8:ARG:HD3	2.16	0.46
1:A:468:VAL:O	1:A:472:ARG:NH1	2.48	0.46
1:A:521:LEU:HD12	1:A:525:ASP:CG	2.40	0.46
1:A:794:PRO:HD2	1:A:828:GLN:HG2	1.98	0.46
1:A:452:LYS:NZ	2:B:366:GLY:O	2.37	0.46
2:B:402:PHE:CE1	2:B:418:LYS:HG2	2.50	0.46
1:A:723:ILE:HD12	1:A:748:VAL:HG11	1.96	0.46
1:A:448:MET:HB2	2:B:363:LEU:HD11	1.97	0.46
1:A:634:PRO:HA	1:A:635:PRO:HD3	1.80	0.46
2:B:400:ARG:HB3	2:B:402:PHE:HE2	1.80	0.46
1:A:203:PRO:O	1:A:206:THR:N	2.48	0.46
1:A:329:LEU:HD12	1:A:329:LEU:H	1.78	0.46
1:A:195:CYS:SG	1:A:834:TYR:CE2	3.05	0.46
1:A:670:PHE:CZ	1:A:731:LEU:CD2	2.99	0.46
1:A:389:THR:CG2	1:A:412:LEU:CD2	2.82	0.46
1:A:555:ASP:OD2	3:C:3:THR:HG21	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:SER:O	1:A:820:ARG:HB3	2.16	0.46
1:A:692:PHE:CD2	1:A:692:PHE:C	2.94	0.45
2:B:395:ILE:HG22	2:B:433:VAL:CG1	2.46	0.45
1:A:290:GLY:CA	1:A:624:THR:HG21	2.47	0.45
2:B:403:GLN:C	2:B:403:GLN:CD	2.85	0.45
1:A:801:GLU:OE1	1:A:809:ALA:HA	2.17	0.45
4:A:901:HUF:N29	3:C:4:MET:HE1	2.32	0.45
1:A:448:MET:HE3	1:A:448:MET:HB3	1.67	0.45
1:A:756:TRP:HB3	4:A:901:HUF:O2'	2.17	0.45
1:A:776:MET:HB3	1:A:803:THR:HG22	1.99	0.45
2:B:342:LEU:O	2:B:346:LYS:HB2	2.16	0.45
1:A:590:VAL:O	1:A:637:VAL:HG22	2.17	0.45
1:A:624:THR:HA	1:A:799:ALA:O	2.17	0.45
1:A:647:LYS:O	1:A:651:VAL:HG23	2.17	0.45
1:A:200:ILE:HD12	1:A:200:ILE:C	2.39	0.45
1:A:387:GLU:CG	3:C:12:GLY:HA2	2.47	0.45
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.52	0.45
1:A:695:TRP:NE1	1:A:706:LEU:CD1	2.77	0.45
2:B:395:ILE:HG22	2:B:433:VAL:HG11	1.98	0.45
1:A:346:SER:O	1:A:349:VAL:O	2.35	0.45
2:B:356:ASN:O	2:B:360:LYS:HG3	2.17	0.45
2:B:388:GLN:O	2:B:392:VAL:HG23	2.17	0.45
1:A:639:PHE:CD2	1:A:643:LEU:HD11	2.52	0.44
1:A:320:PHE:CE1	1:A:747:VAL:HG21	2.52	0.44
1:A:439:GLU:HG2	2:B:352:ILE:HD13	1.99	0.44
1:A:294:ALA:HB3	1:A:582:LEU:CD1	2.48	0.44
1:A:345:VAL:HG12	1:A:349:VAL:CG2	2.48	0.44
1:A:757:ALA:O	1:A:758:ARG:HB2	2.18	0.44
2:B:432:GLU:O	2:B:435:GLN:HG2	2.18	0.44
1:A:221:TRP:CD1	1:A:262:ILE:HA	2.53	0.44
1:A:320:PHE:CE1	1:A:747:VAL:CG2	3.01	0.44
1:A:319:THR:HB	1:A:572:SER:OG	2.18	0.43
1:A:399:ASN:C	1:A:406:VAL:CG2	2.88	0.43
1:A:593:VAL:HB	1:A:639:PHE:CD1	2.53	0.43
1:A:184:PRO:HG3	1:A:187:ARG:NH2	2.33	0.43
1:A:695:TRP:HB3	1:A:697:LEU:HD12	2.00	0.43
1:A:707:VAL:C	1:A:712:ALA:HB2	2.38	0.43
1:A:507:LYS:O	1:A:510:GLU:HB3	2.18	0.43
1:A:485:ARG:HG3	2:B:407:ASP:CB	2.47	0.43
1:A:625:LEU:HD22	4:A:901:HUF:N7	2.34	0.43
1:A:492:LYS:HE3	1:A:492:LYS:HB2	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:420:PHE:CD2	2:B:420:PHE:C	2.96	0.43
1:A:255:TYR:CD2	1:A:256:LEU:HD23	2.53	0.43
1:A:690:GLU:OE2	1:A:726:ARG:NH1	2.52	0.43
2:B:394:ALA:CB	2:B:405:ILE:HD13	2.48	0.43
1:A:289:SER:OG	1:A:624:THR:CG2	2.67	0.42
1:A:539:ALA:HB1	3:C:1:ALA:O	2.19	0.42
1:A:670:PHE:CD1	1:A:735:PHE:CD1	3.05	0.42
1:A:345:VAL:HG12	1:A:349:VAL:HG21	2.01	0.42
1:A:361:PRO:HG2	1:A:678:PHE:CB	2.49	0.42
1:A:729:ALA:O	1:A:732:LYS:N	2.51	0.42
1:A:801:GLU:N	4:A:901:HUF:O2B	2.46	0.42
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.57	0.42
1:A:308:GLU:HG3	1:A:310:ARG:H	1.85	0.42
1:A:316:ARG:NH1	1:A:626:PRO:HB3	2.34	0.42
1:A:654:MET:HE2	1:A:654:MET:HB3	1.90	0.42
1:A:744:LYS:HD2	1:A:744:LYS:HA	1.77	0.42
1:A:285:GLY:C	1:A:287:GLY:H	2.27	0.42
1:A:331:ALA:HB3	1:A:571:TYR:HD2	1.77	0.42
1:A:773:TYR:CE1	1:A:808:PRO:HB3	2.55	0.42
1:A:361:PRO:HG2	1:A:678:PHE:HB3	2.02	0.42
1:A:445:LEU:HD12	2:B:359:LEU:HB2	2.02	0.42
1:A:715:MET:HE3	1:A:715:MET:HB3	1.70	0.42
1:A:370:VAL:CG1	1:A:371:PRO:CD	2.94	0.42
1:A:815:LEU:C	1:A:815:LEU:HD23	2.45	0.42
1:A:319:THR:CB	1:A:572:SER:HB3	2.49	0.42
1:A:442:LYS:HD2	2:B:352:ILE:HG23	2.02	0.42
1:A:445:LEU:CD1	2:B:359:LEU:HB2	2.49	0.42
1:A:553:ASP:HB2	3:C:2:ARG:NH1	2.35	0.42
1:A:316:ARG:HH21	1:A:801:GLU:CG	2.32	0.41
2:B:399:GLY:CA	2:B:437:TRP:CD2	3.03	0.41
1:A:211:LEU:HD22	1:A:214:ARG:NH2	2.35	0.41
1:A:322:LYS:HZ2	1:A:745:GLU:CG	2.33	0.41
1:A:797:PHE:CE1	1:A:825:ILE:HG12	2.55	0.41
4:A:901:HUF:O33	3:C:4:MET:CE	2.68	0.41
1:A:278:THR:O	1:A:302:MET:HG3	2.19	0.41
1:A:295:ARG:HH11	1:A:295:ARG:HD3	1.71	0.41
1:A:353:LEU:HB3	1:A:565:LEU:HD23	2.01	0.41
1:A:536:LEU:HD12	3:C:5:GLN:HE22	1.85	0.41
1:A:197:PRO:HA	1:A:200:ILE:HG22	2.01	0.41
1:A:540:ASN:CB	1:A:547:LEU:HD11	2.50	0.41
1:A:588:THR:HG22	1:A:604:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:371:PRO:HG2	1:A:371:PRO:O	2.21	0.41
1:A:786:ILE:CG2	1:A:787:PRO:HD2	2.50	0.41
4:A:901:HUF:C19	3:C:4:MET:HE1	2.51	0.41
1:A:238:LEU:HD22	1:A:239:GLU:H	1.85	0.41
2:B:429:ASN:HD22	2:B:432:GLU:CD	2.29	0.41
3:C:14:LYS:O	3:C:16:PRO:HD3	2.21	0.41
1:A:316:ARG:HG3	4:A:901:HUF:O2A	2.20	0.41
1:A:427:GLN:HG2	1:A:516:PRO:HG2	2.02	0.41
1:A:358:GLN:OE1	3:C:9:LYS:NZ	2.54	0.41
1:A:671:TRP:N	1:A:735:PHE:HE1	2.19	0.41
1:A:578:LEU:HD22	1:A:578:LEU:HA	1.88	0.41
2:B:394:ALA:HB3	2:B:405:ILE:HD13	2.03	0.41
1:A:653:ARG:HH21	1:A:772:ASP:CG	2.29	0.40
1:A:320:PHE:CZ	1:A:322:LYS:HB2	2.56	0.40
2:B:333:THR:O	2:B:337:GLN:HG2	2.21	0.40
2:B:418:LYS:HE3	2:B:418:LYS:HB3	1.83	0.40
1:A:362:LEU:CB	1:A:370:VAL:CG2	2.97	0.40
1:A:474:ILE:HD12	1:A:474:ILE:HA	1.86	0.40
1:A:522:SER:O	1:A:525:ASP:N	2.54	0.40
1:A:755:PRO:HA	1:A:758:ARG:CZ	2.52	0.40
1:A:181:SER:O	1:A:183:LEU:HG	2.21	0.40
1:A:315:GLY:HA3	4:A:901:HUF:O1A	2.20	0.40
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.87	0.40
2:B:415:VAL:HG13	2:B:416:GLN:N	2.36	0.40
1:A:448:MET:CE	2:B:363:LEU:HD12	2.51	0.40
1:A:574:VAL:N	1:A:575:PRO:HD2	2.36	0.40
2:B:430:ILE:O	2:B:433:VAL:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	664/871 (76%)	616 (93%)	46 (7%)	2 (0%)	36	65
2	B	131/144 (91%)	118 (90%)	13 (10%)	0	100	100
3	C	14/21 (67%)	12 (86%)	2 (14%)	0	100	100
All	All	809/1036 (78%)	746 (92%)	61 (8%)	2 (0%)	43	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PRO
1	A	792	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	566/715 (79%)	511 (90%)	55 (10%)	8	28
2	B	117/125 (94%)	104 (89%)	13 (11%)	6	21
3	C	11/15 (73%)	10 (91%)	1 (9%)	9	30
All	All	694/855 (81%)	625 (90%)	69 (10%)	7	26

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ILE
1	A	200	ILE
1	A	203	PRO
1	A	220	LEU
1	A	223	ASP
1	A	226	LYS
1	A	227	ILE
1	A	238	LEU
1	A	239	GLU
1	A	246	THR
1	A	247	VAL

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Mol	Chain	Res	Type
1	A	249	VAL
1	A	276	LYS
1	A	277	LYS
1	A	288	VAL
1	A	291	LEU
1	A	296	GLN
1	A	298	GLN
1	A	302	MET
1	A	311	ASP
1	A	312	ARG
1	A	313	VAL
1	A	319	THR
1	A	320	PHE
1	A	324	ASN
1	A	335	THR
1	A	342	MET
1	A	364	GLU
1	A	370	VAL
1	A	371	PRO
1	A	408	LEU
1	A	412	LEU
1	A	448	MET
1	A	449	VAL
1	A	519	VAL
1	A	521	LEU
1	A	542	THR
1	A	544	LEU
1	A	545	SER
1	A	557	ASP
1	A	576	VAL
1	A	578	LEU
1	A	582	LEU
1	A	631	LYS
1	A	632	GLN
1	A	702	ILE
1	A	703	LEU
1	A	715	MET
1	A	730	ILE
1	A	731	LEU
1	A	734	ILE
1	A	744	LYS
1	A	780	ILE

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Mol	Chain	Res	Type
1	A	793	ILE
1	A	835	THR
2	B	359	LEU
2	B	361	GLU
2	B	363	LEU
2	B	364	ASP
2	B	372	LEU
2	B	374	GLU
2	B	376	ILE
2	B	400	ARG
2	B	402	PHE
2	B	403	GLN
2	B	405	ILE
2	B	417	VAL
2	B	425	ARG
3	C	8	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	259	HIS
1	A	410	GLN
1	A	450	ASN
1	A	540	ASN
1	A	587	ASN
1	A	742	GLN
2	B	318	GLN
2	B	327	ASN
2	B	403	GLN
2	B	419	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	0.62	0	78,92,92	0.64	1 (1%)

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	-	-	16/36/52/52	0/6/6/6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	HUF	C20-C23-N31	3.37	116.86	110.94

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	HUF	C5'-O5'-PA-O2A
4	A	901	HUF	C5'-O5'-PA-O1A
4	A	901	HUF	C5'-O5'-PA-O3A
4	A	901	HUF	C28-O1B-PB-O2B
4	A	901	HUF	O33-C19-N29-C15

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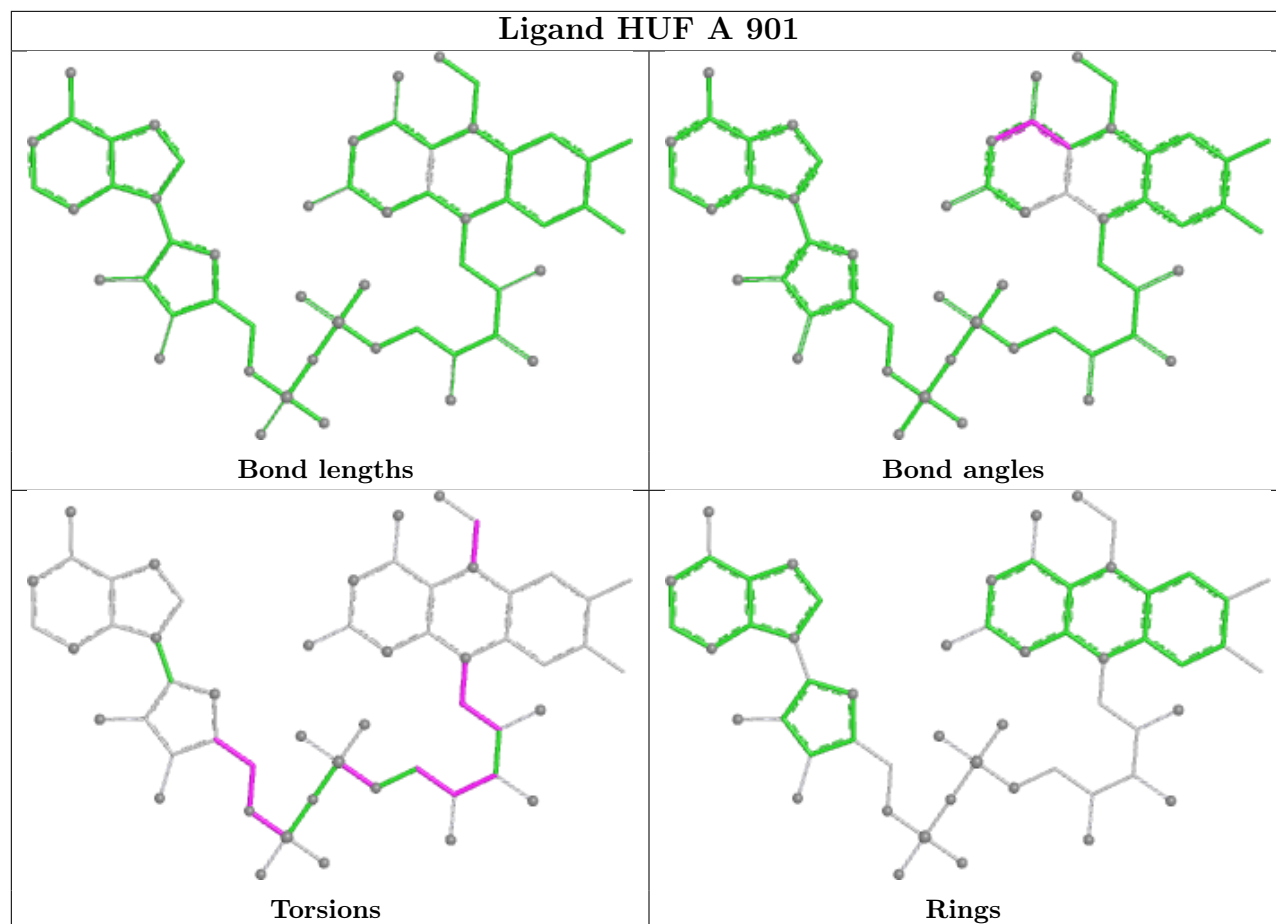
Mol	Chain	Res	Type	Atoms
4	A	901	HUF	O33-C19-N29-C20
4	A	901	HUF	N32-C24-C25-O36
4	A	901	HUF	C25-C24-N32-C21
4	A	901	HUF	O4'-C4'-C5'-O5'
4	A	901	HUF	C3'-C4'-C5'-O5'
4	A	901	HUF	O38-C27-C28-O1B
4	A	901	HUF	C26-C27-C28-O1B
4	A	901	HUF	C25-C26-C27-O38
4	A	901	HUF	C28-O1B-PB-O3A
4	A	901	HUF	C28-O1B-PB-O3B
4	A	901	HUF	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	HUF	17	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	43 (6%) 25 20	82, 112, 144, 167	0
2	B	133/144 (92%)	0.46	6 (4%) 38 28	102, 138, 163, 170	0
3	C	16/21 (76%)	1.30	4 (25%) 2 3	118, 127, 164, 169	0
All	All	815/1036 (78%)	0.53	53 (6%) 25 20	82, 118, 152, 170	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	557	ASP	7.0
1	A	836	LEU	4.8
1	A	770	GLY	4.8
1	A	806	ASN	4.7
1	A	774	ASP	4.2
1	A	171	PRO	4.2
1	A	339	GLY	4.0
1	A	558	PHE	4.0
1	A	771	ASN	3.8
1	A	786	ILE	3.7
3	C	6	THR	3.5
3	C	16	PRO	3.4
1	A	683	SER	3.3
1	A	773	TYR	3.2
2	B	405	ILE	3.1
1	A	834	TYR	3.1
2	B	324	VAL	3.0
1	A	554	GLN	3.0
1	A	275	THR	3.0
2	B	409	ILE	2.9
1	A	791	GLN	2.9
1	A	527	GLN	2.8
1	A	805	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	768	SER	2.8
1	A	787	PRO	2.7
1	A	760	SER	2.7
1	A	769	SER	2.5
2	B	375	VAL	2.5
1	A	373	GLU	2.5
1	A	801	GLU	2.4
1	A	715	MET	2.4
1	A	338	GLY	2.4
1	A	535	ASN	2.4
1	A	567	VAL	2.3
3	C	11	THR	2.3
1	A	518	ASP	2.3
1	A	784	PRO	2.3
1	A	832	ALA	2.3
1	A	785	SER	2.3
1	A	398	PHE	2.2
1	A	369	ALA	2.2
1	A	467	GLU	2.2
1	A	260	GLY	2.2
3	C	7	ALA	2.2
2	B	408	VAL	2.2
1	A	700	ALA	2.1
2	B	374	GLU	2.1
1	A	523	SER	2.1
1	A	174	VAL	2.1
1	A	682	GLY	2.1
1	A	365	ALA	2.1
1	A	551	HIS	2.0
1	A	555	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

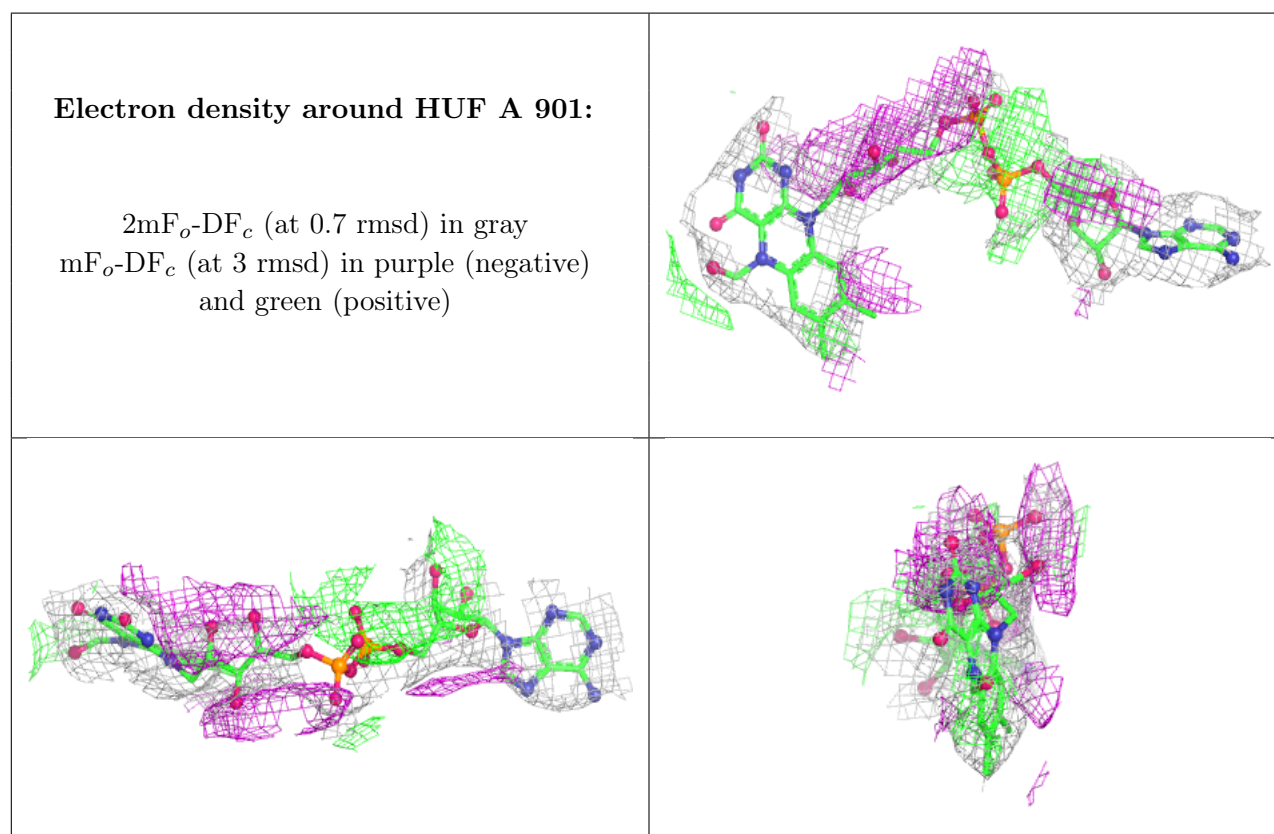
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HUF	A	901	55/55	0.90	0.15	85,98,108,119	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.