



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:55 PM UTC

PDB ID : 8FDV / pdb_00008fdv
Title : LSD1-CoREST in complex N-formyl FAD and SNAG peptide
Authors : Caroli, J.; Mattevi, A.
Deposited on : 2022-12-05
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

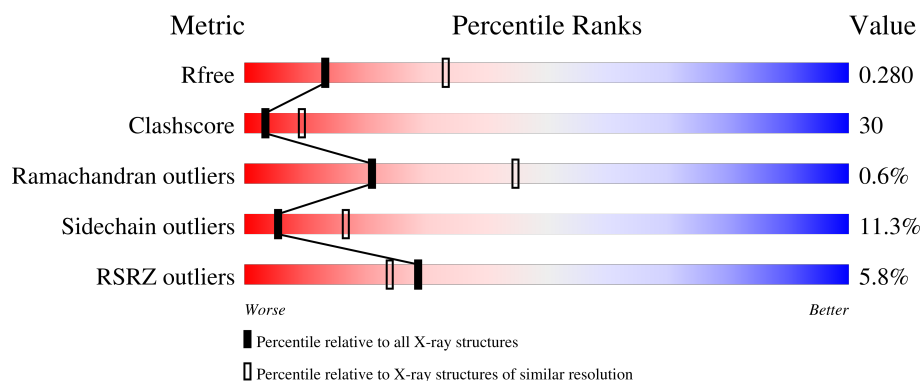
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	 4% 48% 24% 24%
2	B	144	 7% 38% 39% 15% 8%
3	C	9	 33% 56% 33% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6425 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

There are 19 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called REST corepressor 1.

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

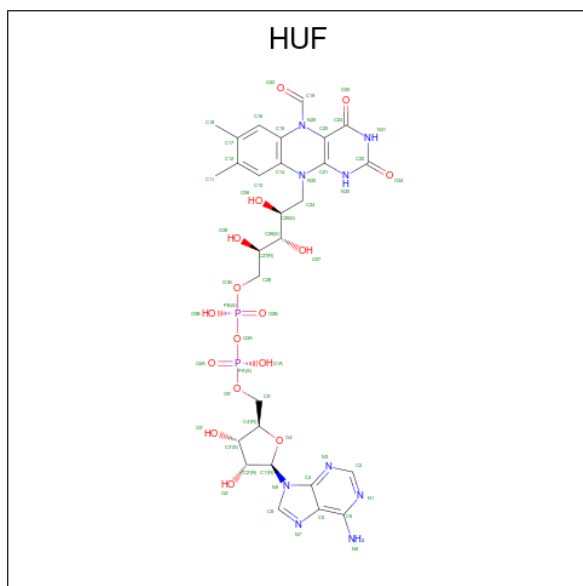
There are 8 discrepancies between the modelled and reference sequences:

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

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

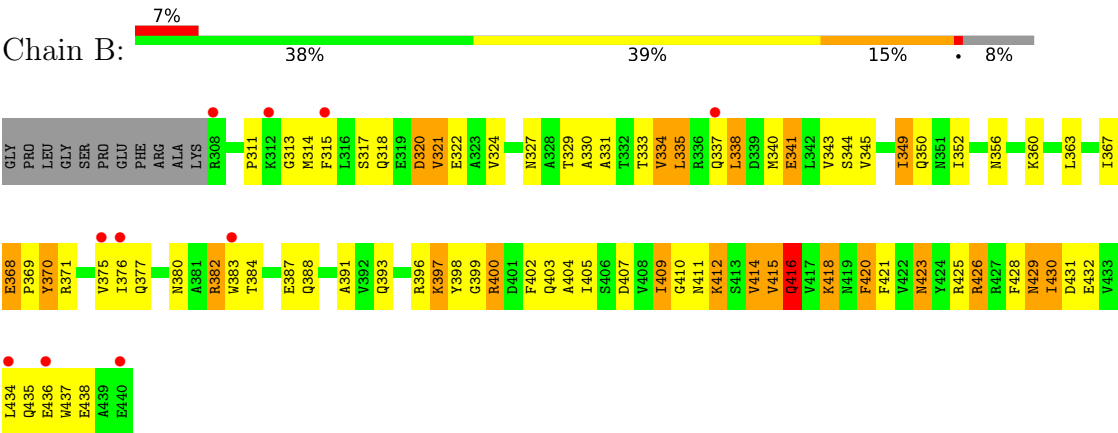
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	0	0	0
			77	51	16	10			

- 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).

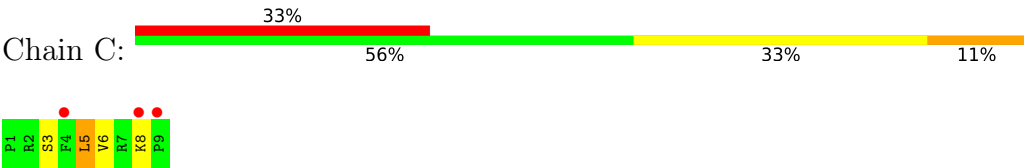


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O P	0	0
			55	28	9	16 2		

● Molecule 2: REST corepressor 1



● Molecule 3: Zinc finger protein SNAI1



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	119.30Å 180.39Å 232.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.95 48.92 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.92-2.95) 99.1 (48.92-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.18.2	Depositor
R, R_{free}	0.216 , 0.252 0.259 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å ²)	95.8	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 112.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6425	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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	0.88	2/5331 (0.0%)	1.13	14/7232 (0.2%)
2	B	0.80	0/1091	1.34	7/1471 (0.5%)
3	C	0.82	0/79	1.10	0/104
All	All	0.86	2/6501 (0.0%)	1.16	21/8807 (0.2%)

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
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	808	PRO	C-O	-7.77	1.15	1.23
1	A	590	VAL	C-O	-5.02	1.18	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	810	THR	CB-CA-C	-7.52	101.57	111.42
1	A	778	GLN	CB-CA-C	-7.13	98.42	109.62
1	A	654	MET	CA-C-N	-6.75	117.40	122.33
1	A	654	MET	C-N-CA	-6.75	117.40	122.33
1	A	591	ARG	CB-CG-CD	6.27	125.73	111.30
1	A	308	GLU	N-CA-CB	-6.01	100.97	110.77
1	A	270	ILE	N-CA-C	-5.97	105.31	110.74
1	A	800	GLY	CA-C-O	-5.80	118.27	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	VAL	N-CA-C	-5.79	105.09	110.53
2	B	430	ILE	CA-C-N	-5.75	112.96	120.44
2	B	430	ILE	C-N-CA	-5.75	112.96	120.44
1	A	381	GLU	CB-CG-CD	5.47	121.91	112.60
1	A	214	ARG	CA-C-O	-5.37	115.17	120.70
2	B	416	GLN	N-CA-C	-5.35	105.34	111.07
1	A	213	ILE	CA-C-O	-5.32	115.42	120.95
2	B	329	THR	CB-CA-C	-5.27	101.00	110.37
1	A	591	ARG	N-CA-C	-5.23	107.27	113.97
2	B	415	VAL	O-C-N	5.17	126.98	121.91
2	B	397	LYS	CA-C-N	-5.12	114.48	122.37
2	B	397	LYS	C-N-CA	-5.12	114.48	122.37
1	A	749	SER	O-C-N	5.02	129.26	122.59

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	214	ARG	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	A	5217	0	5252	277	1
2	B	1076	0	1091	133	0
3	C	77	0	89	15	0
4	A	55	0	0	4	0
All	All	6425	0	6432	384	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

All (384) 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:HB3	1.55	1.40
1:A:209:VAL:O	1:A:213:ILE:HD13	1.24	1.26
1:A:273:LEU:HD12	1:A:274:PRO:CD	1.65	1.25
1:A:209:VAL:O	1:A:213:ILE:CD1	1.85	1.24
2:B:412:LYS:HG3	2:B:416:GLN:CB	1.68	1.23
1:A:209:VAL:C	1:A:213:ILE:HD13	1.64	1.22
2:B:412:LYS:CG	2:B:416:GLN:HB3	1.68	1.21
1:A:463:LYS:O	1:A:467:GLU:HG2	1.43	1.15
1:A:435:VAL:HG12	2:B:349:ILE:HG12	1.14	1.12
2:B:430:ILE:O	2:B:434:LEU:HG	1.54	1.08
2:B:412:LYS:HD2	2:B:416:GLN:HG2	1.35	1.08
2:B:412:LYS:HG2	2:B:416:GLN:HB3	1.37	1.07
1:A:325:TYR:CE2	1:A:665:CYS:CB	2.43	1.01
1:A:273:LEU:HD12	1:A:274:PRO:HD2	1.03	1.01
1:A:325:TYR:HE2	1:A:665:CYS:HB3	1.23	0.98
1:A:435:VAL:CG1	2:B:349:ILE:HG12	1.94	0.97
1:A:325:TYR:CD2	1:A:665:CYS:HB3	2.01	0.96
2:B:412:LYS:CG	2:B:416:GLN:CB	2.36	0.95
1:A:273:LEU:CD1	1:A:274:PRO:HD2	1.97	0.94
1:A:535:ASN:OD1	3:C:6:VAL:HG12	1.66	0.94
2:B:383:TRP:CE2	2:B:420:PHE:HD1	1.86	0.93
2:B:412:LYS:HG3	2:B:416:GLN:HB3	1.35	0.93
1:A:273:LEU:CD1	1:A:274:PRO:CD	2.45	0.93
1:A:572:SER:O	1:A:575:PRO:HD2	1.69	0.92
2:B:324:VAL:HG13	2:B:331:ALA:HB2	1.48	0.92
1:A:435:VAL:HG12	2:B:349:ILE:CG1	1.98	0.92
1:A:801:GLU:HG3	1:A:809:ALA:HA	1.50	0.92
1:A:495:ASP:OD2	2:B:371:ARG:NH2	2.01	0.92
1:A:535:ASN:HD21	3:C:6:VAL:CG1	1.83	0.92
1:A:591:ARG:HH21	1:A:605:VAL:HG11	1.33	0.92
1:A:535:ASN:ND2	3:C:6:VAL:CG1	2.34	0.91
1:A:535:ASN:ND2	3:C:6:VAL:HG12	1.86	0.90
1:A:535:ASN:CG	3:C:6:VAL:HG12	1.97	0.90
2:B:412:LYS:HG3	2:B:416:GLN:HB2	1.54	0.90
1:A:654:MET:CE	1:A:776:MET:CG	2.50	0.89
2:B:400:ARG:HH11	2:B:400:ARG:HG2	1.36	0.88
2:B:320:ASP:OD1	2:B:320:ASP:N	2.07	0.87
1:A:372:LYS:CE	1:A:372:LYS:H	1.88	0.87
1:A:591:ARG:HD3	1:A:605:VAL:CG1	2.04	0.86
2:B:399:GLY:N	2:B:437:TRP:NE1	2.24	0.86
1:A:332:MET:HE2	1:A:661:LYS:NZ	1.92	0.85
1:A:479:LEU:HD12	1:A:479:LEU:O	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ASN:OD1	3:C:6:VAL:CG1	2.24	0.85
1:A:380:GLN:HE22	1:A:384:ARG:HH21	1.22	0.84
1:A:660:ASN:HD21	1:A:751:TRP:H	1.23	0.84
1:A:216:ARG:O	1:A:220:LEU:HD12	1.77	0.83
1:A:345:VAL:O	1:A:349:VAL:HG12	1.79	0.83
1:A:311:ASP:OD1	1:A:311:ASP:N	2.11	0.83
1:A:209:VAL:C	1:A:213:ILE:CD1	2.43	0.83
1:A:569:ASN:OD1	1:A:569:ASN:N	2.10	0.82
2:B:380:ASN:O	2:B:412:LYS:HD3	1.79	0.82
2:B:426:ARG:HG2	2:B:426:ARG:HH21	1.43	0.82
1:A:434:ILE:CG2	2:B:349:ILE:CD1	2.58	0.82
1:A:518:ASP:OD1	1:A:518:ASP:N	2.08	0.81
1:A:591:ARG:HD3	1:A:605:VAL:HG13	1.60	0.81
1:A:654:MET:HE1	1:A:776:MET:HG3	1.63	0.81
1:A:372:LYS:H	1:A:372:LYS:HE2	1.45	0.81
1:A:535:ASN:CG	3:C:6:VAL:CG1	2.54	0.81
2:B:382:ARG:HG2	2:B:382:ARG:HH11	1.46	0.81
1:A:325:TYR:HD2	1:A:665:CYS:SG	2.04	0.81
1:A:427:GLN:NE2	1:A:518:ASP:HA	1.95	0.81
2:B:384:THR:OG1	2:B:387:GLU:OE1	1.98	0.80
1:A:434:ILE:HG22	2:B:349:ILE:CD1	2.12	0.80
1:A:380:GLN:NE2	1:A:384:ARG:HH21	1.80	0.80
2:B:405:ILE:O	2:B:409:ILE:HG13	1.82	0.79
1:A:535:ASN:HD21	3:C:6:VAL:HG12	1.41	0.79
1:A:325:TYR:CD2	1:A:665:CYS:CB	2.65	0.79
2:B:324:VAL:HG13	2:B:331:ALA:CB	2.13	0.79
1:A:209:VAL:O	1:A:213:ILE:HD12	1.83	0.78
1:A:280:LYS:HD3	1:A:303:ASP:HB3	1.65	0.77
1:A:312:ARG:HH11	1:A:312:ARG:HG3	1.46	0.77
2:B:402:PHE:HB2	2:B:414:VAL:CG1	2.15	0.77
1:A:475:THR:HA	2:B:393:GLN:HE22	1.50	0.77
1:A:654:MET:CE	1:A:776:MET:HG2	2.14	0.77
2:B:399:GLY:H	2:B:437:TRP:CD1	2.02	0.77
1:A:325:TYR:CD2	1:A:665:CYS:SG	2.78	0.77
1:A:486:ASP:OD1	2:B:398:TYR:OH	2.02	0.77
2:B:412:LYS:HB2	2:B:412:LYS:NZ	1.97	0.76
2:B:430:ILE:HG22	2:B:434:LEU:HD11	1.65	0.76
1:A:441:LEU:HD23	2:B:356:ASN:HD22	1.49	0.76
1:A:456:LYS:HA	2:B:370:TYR:HE1	1.50	0.76
2:B:412:LYS:CD	2:B:416:GLN:HG2	2.16	0.76
1:A:209:VAL:HG12	1:A:213:ILE:HD11	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:THR:OG1	1:A:508:LEU:HD21	1.86	0.75
1:A:425:ASP:OD1	2:B:338:LEU:CD1	2.35	0.75
1:A:273:LEU:CD1	1:A:274:PRO:HD3	2.16	0.74
1:A:504:LEU:N	1:A:504:LEU:HD23	2.01	0.74
1:A:672:ASP:HB3	1:A:675:VAL:HG12	1.68	0.74
1:A:680:HIS:CE1	1:A:730:ILE:CD1	2.71	0.74
1:A:690:GLU:OE2	1:A:726:ARG:NH1	2.19	0.74
4:A:901:HUF:O38	4:A:901:HUF:O36	2.05	0.74
1:A:325:TYR:HD2	1:A:665:CYS:HG	1.36	0.74
1:A:308:GLU:HG2	1:A:586:LEU:HD23	1.69	0.73
2:B:396:ARG:NH1	2:B:436:GLU:HB3	2.02	0.73
2:B:425:ARG:HH11	2:B:425:ARG:HG2	1.52	0.73
1:A:691:LEU:CD2	1:A:727:CYS:SG	2.76	0.73
1:A:456:LYS:HA	2:B:370:TYR:CE1	2.23	0.73
1:A:654:MET:CE	1:A:776:MET:HG3	2.14	0.73
1:A:331:ALA:HA	4:A:901:HUF:N29	2.03	0.72
1:A:332:MET:HE2	1:A:661:LYS:HZ3	1.52	0.72
1:A:479:LEU:HD12	1:A:479:LEU:C	2.14	0.72
1:A:676:ASN:O	1:A:696:ASN:N	2.17	0.72
2:B:414:VAL:O	2:B:418:LYS:HB2	1.91	0.71
1:A:188:MET:HE1	1:A:199:ILE:HG22	1.72	0.71
1:A:535:ASN:ND2	3:C:6:VAL:HG13	2.04	0.71
1:A:650:ALA:O	1:A:654:MET:HG3	1.91	0.71
1:A:366:ASN:OD1	1:A:367:GLY:N	2.23	0.70
1:A:800:GLY:O	1:A:803:THR:OG1	2.09	0.70
2:B:425:ARG:HA	2:B:430:ILE:HD12	1.72	0.70
1:A:263:ASN:C	1:A:267:TYR:CE1	2.70	0.70
1:A:209:VAL:CG1	1:A:213:ILE:HD11	2.21	0.70
2:B:435:GLN:HA	2:B:438:GLU:HG3	1.74	0.70
2:B:377:GLN:CD	2:B:410:GLY:O	2.36	0.69
1:A:425:ASP:OD1	2:B:338:LEU:HD11	1.92	0.69
2:B:414:VAL:O	2:B:418:LYS:N	2.24	0.68
1:A:312:ARG:HG3	1:A:312:ARG:NH1	2.06	0.68
1:A:654:MET:HE1	1:A:776:MET:CG	2.21	0.68
1:A:755:PRO:HA	1:A:758:ARG:HD3	1.76	0.68
2:B:396:ARG:HH11	2:B:436:GLU:HB3	1.58	0.68
1:A:434:ILE:HG22	2:B:349:ILE:HD11	1.74	0.68
1:A:216:ARG:HG3	1:A:220:LEU:HD11	1.75	0.68
1:A:372:LYS:H	1:A:372:LYS:CD	2.07	0.68
1:A:198:ASP:OD2	1:A:251:ARG:NH2	2.27	0.67
1:A:332:MET:CE	1:A:661:LYS:NZ	2.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:PHE:HE1	1:A:249:VAL:HG12	1.59	0.67
1:A:591:ARG:HD3	1:A:605:VAL:HG11	1.76	0.67
1:A:385:LEU:HD13	2:B:314:MET:HE1	1.77	0.67
2:B:383:TRP:CE2	2:B:420:PHE:CD1	2.76	0.67
1:A:434:ILE:CG2	2:B:349:ILE:HD13	2.24	0.67
1:A:331:ALA:HA	4:A:901:HUF:C20	2.24	0.67
1:A:308:GLU:HG2	1:A:586:LEU:CD2	2.25	0.67
1:A:660:ASN:ND2	1:A:751:TRP:H	1.93	0.67
1:A:434:ILE:HG22	2:B:349:ILE:HD13	1.77	0.66
1:A:434:ILE:HG21	2:B:349:ILE:CD1	2.25	0.66
1:A:568:ARG:HB3	1:A:699:LYS:HE3	1.76	0.66
1:A:801:GLU:HG3	1:A:809:ALA:CA	2.24	0.66
2:B:376:ILE:O	2:B:376:ILE:HG13	1.95	0.66
2:B:425:ARG:HG2	2:B:425:ARG:NH1	2.09	0.66
2:B:399:GLY:H	2:B:437:TRP:NE1	1.92	0.66
1:A:434:ILE:CG2	2:B:349:ILE:HD11	2.25	0.65
1:A:440:GLU:OE2	1:A:440:GLU:HA	1.96	0.65
2:B:412:LYS:HD2	2:B:416:GLN:CG	2.21	0.65
1:A:533:PHE:O	1:A:537:GLU:HG3	1.96	0.65
1:A:325:TYR:HE2	1:A:665:CYS:CB	1.92	0.65
2:B:383:TRP:CZ2	2:B:420:PHE:HD1	2.14	0.65
1:A:660:ASN:HD21	1:A:751:TRP:N	1.93	0.64
1:A:213:ILE:HD12	1:A:213:ILE:N	2.13	0.64
1:A:501:GLN:O	1:A:501:GLN:HG2	1.97	0.64
1:A:509:GLN:O	1:A:513:ALA:HB2	1.98	0.64
2:B:400:ARG:HH11	2:B:400:ARG:CG	2.10	0.64
1:A:654:MET:HE2	1:A:776:MET:HG2	1.80	0.63
1:A:661:LYS:HD3	1:A:704:LEU:HD21	1.80	0.63
1:A:435:VAL:CG1	2:B:349:ILE:CG1	2.68	0.63
2:B:311:PRO:HG2	2:B:314:MET:HG3	1.81	0.62
1:A:321:ARG:NH2	1:A:569:ASN:O	2.30	0.62
2:B:403:GLN:OE1	2:B:403:GLN:HA	1.98	0.62
1:A:663:VAL:HG12	1:A:747:VAL:HB	1.81	0.61
1:A:345:VAL:O	1:A:349:VAL:CG1	2.49	0.61
1:A:364:GLU:HA	1:A:681:VAL:HB	1.81	0.61
1:A:536:LEU:HB3	1:A:544:LEU:HD21	1.82	0.61
1:A:521:LEU:HD22	1:A:525:ASP:HB3	1.83	0.61
1:A:216:ARG:O	1:A:220:LEU:CD1	2.48	0.61
2:B:380:ASN:O	2:B:412:LYS:CD	2.49	0.61
1:A:209:VAL:HG12	1:A:213:ILE:CD1	2.31	0.60
1:A:804:ILE:HG23	1:A:804:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:LYS:HA	1:A:565:LEU:HD13	1.84	0.60
2:B:382:ARG:HG2	2:B:382:ARG:NH1	2.17	0.59
2:B:418:LYS:HE3	2:B:418:LYS:O	2.01	0.59
2:B:399:GLY:N	2:B:437:TRP:CD1	2.66	0.59
2:B:412:LYS:HG3	2:B:416:GLN:CG	2.30	0.59
2:B:402:PHE:HB2	2:B:414:VAL:HG13	1.84	0.59
1:A:332:MET:CE	1:A:661:LYS:HZ3	2.15	0.59
1:A:427:GLN:HE21	1:A:518:ASP:HA	1.67	0.58
2:B:383:TRP:CZ2	2:B:420:PHE:CD1	2.91	0.58
2:B:412:LYS:HB2	2:B:412:LYS:HZ3	1.68	0.58
1:A:448:MET:HE3	2:B:363:LEU:HD13	1.83	0.58
1:A:468:VAL:HG12	1:A:468:VAL:O	2.04	0.58
1:A:591:ARG:CD	1:A:605:VAL:CG1	2.80	0.58
1:A:374:LYS:O	1:A:378:VAL:HG22	2.03	0.58
1:A:645:GLU:OE2	1:A:649:SER:OG	2.17	0.58
1:A:684:THR:HG22	1:A:686:ALA:H	1.69	0.57
1:A:691:LEU:HD21	1:A:727:CYS:SG	2.44	0.57
1:A:750:ARG:HB3	1:A:753:ALA:HB3	1.84	0.57
1:A:453:GLU:N	1:A:453:GLU:OE1	2.38	0.57
2:B:426:ARG:HH21	2:B:426:ARG:CG	2.12	0.57
1:A:366:ASN:OD1	1:A:368:GLN:N	2.37	0.57
2:B:338:LEU:N	2:B:338:LEU:HD23	2.19	0.57
1:A:591:ARG:NH2	1:A:605:VAL:HG11	2.14	0.57
1:A:609:SER:O	1:A:609:SER:OG	2.18	0.57
1:A:680:HIS:NE2	1:A:730:ILE:HD13	2.20	0.57
1:A:273:LEU:HD13	1:A:274:PRO:HD3	1.87	0.56
1:A:530:ASP:OD2	1:A:685:THR:HG22	2.04	0.56
2:B:402:PHE:CB	2:B:414:VAL:CG1	2.81	0.56
1:A:308:GLU:CG	1:A:586:LEU:HD23	2.34	0.56
2:B:370:TYR:N	2:B:370:TYR:CD2	2.72	0.56
1:A:283:ILE:HG12	1:A:622:LEU:HB3	1.86	0.56
1:A:372:LYS:HE2	1:A:372:LYS:N	2.19	0.56
2:B:405:ILE:O	2:B:409:ILE:CG1	2.53	0.56
2:B:430:ILE:HG22	2:B:434:LEU:CD1	2.36	0.56
2:B:402:PHE:CB	2:B:414:VAL:HG13	2.36	0.56
1:A:495:ASP:CG	2:B:371:ARG:NH2	2.63	0.56
1:A:306:LEU:HD11	1:A:582:LEU:HD23	1.88	0.55
2:B:420:PHE:CD2	2:B:420:PHE:C	2.83	0.55
1:A:320:PHE:CE1	1:A:747:VAL:HG21	2.41	0.55
2:B:412:LYS:CG	2:B:416:GLN:CG	2.84	0.55
1:A:588:THR:HG22	1:A:604:ALA:HB1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:ARG:HG3	1:A:218:LEU:HD11	1.88	0.55
1:A:213:ILE:CD1	1:A:213:ILE:H	2.20	0.54
2:B:418:LYS:CE	2:B:418:LYS:CA	2.85	0.54
2:B:387:GLU:HB2	2:B:409:ILE:HG23	1.89	0.54
2:B:399:GLY:N	2:B:437:TRP:CE2	2.76	0.54
1:A:233:ALA:O	1:A:237:GLN:HG3	2.08	0.54
2:B:382:ARG:HH11	2:B:382:ARG:CG	2.19	0.54
1:A:213:ILE:CD1	1:A:213:ILE:N	2.71	0.53
2:B:324:VAL:CG1	2:B:331:ALA:HB2	2.32	0.53
2:B:370:TYR:N	2:B:370:TYR:HD2	2.06	0.53
2:B:418:LYS:CE	2:B:418:LYS:HA	2.36	0.53
1:A:232:GLU:CD	1:A:232:GLU:H	2.17	0.53
2:B:400:ARG:HG2	2:B:400:ARG:NH1	2.14	0.53
2:B:430:ILE:O	2:B:434:LEU:CG	2.42	0.53
1:A:498:ALA:HA	1:A:501:GLN:HB3	1.91	0.52
2:B:335:LEU:N	2:B:335:LEU:HD23	2.24	0.52
1:A:216:ARG:HG3	1:A:220:LEU:CD1	2.40	0.52
1:A:535:ASN:HD21	3:C:6:VAL:HG13	1.62	0.52
1:A:663:VAL:CG1	1:A:747:VAL:HB	2.40	0.52
1:A:718:ILE:HG22	1:A:723:ILE:HD12	1.92	0.52
1:A:592:GLN:HB3	1:A:603:ILE:HD12	1.92	0.52
2:B:435:GLN:HA	2:B:438:GLU:CG	2.37	0.52
1:A:320:PHE:CZ	1:A:322:LYS:HG3	2.45	0.51
1:A:680:HIS:CE1	1:A:730:ILE:HD13	2.45	0.51
1:A:509:GLN:O	1:A:513:ALA:CB	2.59	0.51
1:A:654:MET:HE3	1:A:776:MET:CG	2.40	0.51
1:A:218:LEU:HD12	1:A:218:LEU:H	1.74	0.51
1:A:591:ARG:CD	1:A:605:VAL:HG11	2.39	0.51
1:A:263:ASN:C	1:A:267:TYR:HE1	2.18	0.51
1:A:572:SER:O	1:A:575:PRO:CD	2.53	0.51
2:B:375:VAL:HG23	2:B:375:VAL:O	2.11	0.51
2:B:402:PHE:HE1	2:B:421:PHE:CZ	2.28	0.51
2:B:412:LYS:CD	2:B:416:GLN:HE21	2.24	0.51
2:B:387:GLU:HB2	2:B:409:ILE:CG2	2.42	0.50
1:A:180:GLN:HA	1:A:339:GLY:HA2	1.92	0.50
1:A:282:ILE:HG21	1:A:602:VAL:HG21	1.93	0.50
1:A:280:LYS:HE2	1:A:303:ASP:OD2	2.11	0.50
2:B:334:VAL:HG12	2:B:335:LEU:HD23	1.94	0.50
1:A:331:ALA:HA	4:A:901:HUF:C15	2.41	0.49
1:A:667:ASP:OD1	1:A:667:ASP:N	2.42	0.49
1:A:280:LYS:HD3	1:A:303:ASP:CB	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:N	1:A:372:LYS:HD3	2.27	0.49
2:B:383:TRP:HE3	2:B:387:GLU:HG2	1.77	0.49
1:A:427:GLN:HE22	1:A:518:ASP:HA	1.74	0.49
2:B:412:LYS:CD	2:B:416:GLN:CG	2.86	0.49
2:B:429:ASN:OD1	2:B:432:GLU:OE2	2.30	0.49
2:B:377:GLN:OE1	2:B:410:GLY:O	2.30	0.49
2:B:397:LYS:C	2:B:437:TRP:HE1	2.20	0.49
1:A:343:ALA:O	1:A:346:SER:OG	2.26	0.49
1:A:391:TYR:HA	1:A:395:GLN:OE1	2.12	0.49
1:A:319:THR:HB	1:A:572:SER:HB3	1.95	0.49
1:A:214:ARG:HG2	1:A:214:ARG:HH11	1.78	0.49
1:A:449:VAL:HA	2:B:363:LEU:HD21	1.93	0.49
1:A:695:TRP:CE3	1:A:697:LEU:HD11	2.48	0.49
2:B:369:PRO:HB2	2:B:370:TYR:CD2	2.48	0.49
1:A:213:ILE:HD12	1:A:213:ILE:H	1.78	0.48
1:A:535:ASN:HD21	3:C:6:VAL:H	1.61	0.48
1:A:672:ASP:HB3	1:A:675:VAL:CG1	2.38	0.48
1:A:810:THR:O	1:A:810:THR:OG1	2.26	0.48
2:B:423:ASN:ND2	2:B:423:ASN:N	2.60	0.48
1:A:364:GLU:OE2	1:A:524:ARG:NH2	2.28	0.48
1:A:812:HIS:O	1:A:816:LEU:N	2.31	0.48
1:A:594:ARG:HG2	1:A:640:VAL:HB	1.95	0.48
1:A:748:VAL:O	1:A:748:VAL:HG13	2.14	0.48
2:B:400:ARG:CG	2:B:400:ARG:NH1	2.72	0.48
1:A:297:LEU:HB2	1:A:304:VAL:HG21	1.95	0.48
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.68	0.47
1:A:781:THR:HG23	1:A:793:ILE:O	2.14	0.47
1:A:351:MET:HE3	1:A:574:VAL:HG21	1.96	0.47
1:A:566:THR:HG21	1:A:697:LEU:HD13	1.95	0.47
1:A:773:TYR:CE2	1:A:808:PRO:HB3	2.50	0.47
2:B:426:ARG:CG	2:B:426:ARG:NH2	2.73	0.47
1:A:310:ARG:NH2	1:A:754:ASP:OD2	2.34	0.47
1:A:380:GLN:HE22	1:A:384:ARG:NH2	2.03	0.47
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.64	0.47
1:A:540:ASN:N	1:A:540:ASN:ND2	2.62	0.47
1:A:566:THR:HG21	1:A:697:LEU:HD22	1.96	0.47
2:B:425:ARG:CA	2:B:430:ILE:HD12	2.44	0.47
1:A:372:LYS:CD	1:A:372:LYS:N	2.72	0.47
1:A:463:LYS:O	1:A:467:GLU:CG	2.36	0.47
2:B:412:LYS:HD3	2:B:416:GLN:HE21	1.80	0.47
1:A:583:ASP:OD2	1:A:585:LYS:NZ	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:SER:N	1:A:801:GLU:OE1	2.45	0.47
2:B:431:ASP:HA	2:B:434:LEU:HD12	1.97	0.47
1:A:257:GLU:HG3	1:A:263:ASN:HD22	1.81	0.46
1:A:282:ILE:HD13	1:A:305:THR:HB	1.97	0.46
1:A:308:GLU:HB3	1:A:585:LYS:O	2.14	0.46
1:A:824:ARG:O	1:A:824:ARG:HG3	2.12	0.46
1:A:220:LEU:HD12	1:A:220:LEU:H	1.81	0.46
1:A:363:TYR:HB3	1:A:734:ILE:HD12	1.97	0.46
2:B:327:ASN:OD1	2:B:330:ALA:N	2.48	0.46
2:B:388:GLN:O	2:B:391:ALA:HB3	2.16	0.46
1:A:647:LYS:O	1:A:651:VAL:HG23	2.16	0.46
1:A:780:ILE:HB	1:A:796:LEU:HB3	1.98	0.46
1:A:659:LEU:HG	1:A:659:LEU:O	2.16	0.46
2:B:418:LYS:HE3	2:B:418:LYS:HA	1.98	0.46
1:A:658:ASN:ND2	1:A:752:ARG:HB2	2.30	0.46
2:B:412:LYS:HB2	2:B:412:LYS:HZ2	1.74	0.46
1:A:308:GLU:HB3	1:A:586:LEU:HA	1.98	0.46
1:A:810:THR:HB	1:A:812:HIS:CE1	2.50	0.46
1:A:231:PHE:CE1	1:A:249:VAL:HG12	2.45	0.45
1:A:320:PHE:CD1	1:A:747:VAL:HG21	2.51	0.45
1:A:601:GLU:HA	1:A:616:TYR:O	2.16	0.45
1:A:535:ASN:ND2	3:C:5:LEU:HD22	2.32	0.45
2:B:341:GLU:O	2:B:341:GLU:HG3	2.09	0.45
1:A:212:PHE:CE1	1:A:242:TYR:CD2	3.05	0.45
1:A:217:THR:HG23	1:A:234:THR:HG21	1.98	0.45
1:A:392:LEU:HD23	1:A:398:PHE:CD2	2.52	0.45
1:A:732:LYS:O	1:A:736:GLY:N	2.49	0.45
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.79	0.45
1:A:541:ALA:O	1:A:657:GLY:HA3	2.17	0.45
1:A:591:ARG:HD2	1:A:605:VAL:CG2	2.47	0.45
1:A:801:GLU:O	1:A:801:GLU:HG2	2.11	0.45
2:B:418:LYS:HA	2:B:418:LYS:HD2	1.77	0.45
1:A:319:THR:CB	1:A:572:SER:HB3	2.46	0.45
1:A:380:GLN:O	1:A:384:ARG:HG3	2.16	0.45
2:B:430:ILE:O	2:B:430:ILE:HG22	2.17	0.45
1:A:418:LEU:CD2	2:B:321:VAL:HG12	2.47	0.44
1:A:474:ILE:HA	1:A:474:ILE:HD12	1.71	0.44
1:A:508:LEU:HD13	1:A:508:LEU:HA	1.74	0.44
2:B:382:ARG:NH1	2:B:382:ARG:CG	2.76	0.44
2:B:404:ALA:O	2:B:407:ASP:N	2.50	0.44
1:A:522:SER:N	1:A:525:ASP:OD2	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:426:ARG:H	2:B:426:ARG:HG3	1.37	0.44
1:A:325:TYR:N	1:A:325:TYR:HD1	2.16	0.44
1:A:441:LEU:CD2	2:B:356:ASN:HD22	2.26	0.44
2:B:412:LYS:HG3	2:B:416:GLN:HE21	1.82	0.44
2:B:383:TRP:NE1	2:B:420:PHE:HD1	2.12	0.44
1:A:312:ARG:NH1	1:A:312:ARG:CG	2.72	0.43
2:B:356:ASN:O	2:B:360:LYS:HB2	2.18	0.43
1:A:471:PRO:O	1:A:471:PRO:HG2	2.17	0.43
1:A:325:TYR:N	1:A:325:TYR:CD1	2.86	0.43
1:A:659:LEU:HD12	1:A:659:LEU:C	2.44	0.43
1:A:351:MET:HE3	1:A:574:VAL:CG2	2.48	0.43
1:A:265:GLY:O	1:A:295:ARG:HD3	2.18	0.43
1:A:273:LEU:HD13	1:A:273:LEU:HA	1.60	0.43
1:A:319:THR:OG1	1:A:328:ASP:OD1	2.31	0.43
1:A:804:ILE:HD13	1:A:813:GLY:HA2	2.01	0.43
1:A:680:HIS:CD2	1:A:730:ILE:HD13	2.53	0.43
2:B:412:LYS:CG	2:B:416:GLN:HE21	2.32	0.43
1:A:248:LEU:HD12	1:A:248:LEU:HA	1.63	0.43
1:A:361:PRO:HB2	1:A:363:TYR:CE2	2.54	0.43
1:A:492:LYS:HD2	1:A:492:LYS:HA	1.84	0.43
2:B:368:GLU:N	2:B:369:PRO:CD	2.82	0.43
1:A:535:ASN:OD1	3:C:6:VAL:HG11	2.13	0.42
1:A:568:ARG:HE	1:A:699:LYS:CG	2.33	0.42
1:A:372:LYS:H	1:A:372:LYS:HD3	1.79	0.42
1:A:419:GLN:NE2	2:B:314:MET:HA	2.33	0.42
1:A:494:TYR:CD2	2:B:367:ILE:HD13	2.54	0.42
1:A:538:PHE:CD1	1:A:706:LEU:HD23	2.53	0.42
1:A:255:TYR:CE2	1:A:256:LEU:HD23	2.54	0.42
1:A:188:MET:SD	1:A:210:PHE:CD2	3.13	0.42
1:A:455:ILE:HG22	2:B:370:TYR:CD1	2.55	0.42
1:A:460:GLN:O	1:A:464:GLU:HG3	2.20	0.42
1:A:559:GLU:OE1	3:C:8:LYS:NZ	2.53	0.42
2:B:428:PHE:HD2	2:B:428:PHE:HA	1.65	0.42
1:A:568:ARG:HE	1:A:699:LYS:HG3	1.84	0.41
2:B:313:GLY:O	2:B:315:PHE:HD1	2.03	0.41
1:A:371:PRO:HA	1:A:372:LYS:NZ	2.35	0.41
1:A:775:LEU:HD23	1:A:775:LEU:HA	1.77	0.41
1:A:789:ALA:HB1	1:A:790:PRO:HD2	2.01	0.41
1:A:750:ARG:HH11	1:A:750:ARG:HD3	1.71	0.41
2:B:384:THR:O	2:B:388:GLN:HG3	2.21	0.41
1:A:209:VAL:HG13	1:A:213:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:VAL:HG21	1:A:528:ILE:HD13	2.02	0.41
1:A:395:GLN:OE1	1:A:395:GLN:N	2.54	0.41
1:A:469:LYS:HA	1:A:470:PRO:HD3	1.85	0.41
1:A:591:ARG:HD2	1:A:605:VAL:HG21	2.03	0.40
1:A:458:LEU:HD12	1:A:490:LEU:HD22	2.02	0.40
1:A:500:THR:C	1:A:502:GLY:N	2.79	0.40
1:A:537:GLU:OE2	1:A:544:LEU:HG	2.22	0.40
1:A:540:ASN:HB3	1:A:547:LEU:HD21	2.03	0.40
2:B:411:ASN:OD1	2:B:412:LYS:NZ	2.55	0.40
1:A:205:GLN:O	1:A:209:VAL:HG23	2.22	0.40
1:A:370:VAL:HA	1:A:371:PRO:HD3	1.92	0.40
1:A:810:THR:O	1:A:813:GLY:N	2.53	0.40
3:C:5:LEU:HA	3:C:5:LEU:HD23	1.62	0.40
1:A:320:PHE:O	1:A:321:ARG:HG3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ARG:NH1	1:A:610:THR:O[2_565]	2.06	0.14

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%)	622 (94%)	37 (6%)	5 (1%)	16	37
2	B	131/144 (91%)	127 (97%)	4 (3%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
All	All	802/1024 (78%)	756 (94%)	41 (5%)	5 (1%)	21	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	750	ARG
1	A	811	VAL
1	A	350	ASN
1	A	573	CYS
1	A	468	VAL

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%)	522 (92%)	44 (8%)	11	30
2	B	117/125 (94%)	85 (73%)	32 (27%)	0	0
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	2
All	All	692/849 (82%)	614 (89%)	78 (11%)	5	17

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ILE
1	A	213	ILE
1	A	214	ARG
1	A	216	ARG
1	A	269	ARG
1	A	273	LEU
1	A	281	VAL
1	A	311	ASP
1	A	326	VAL
1	A	349	VAL
1	A	351	MET
1	A	374	LYS
1	A	378	VAL
1	A	380	GLN
1	A	381	GLU
1	A	385	LEU
1	A	421	LYS
1	A	423	VAL

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Mol	Chain	Res	Type
1	A	425	ASP
1	A	429	GLU
1	A	434	ILE
1	A	471	PRO
1	A	474	ILE
1	A	479	LEU
1	A	480	VAL
1	A	482	SER
1	A	487	LEU
1	A	504	LEU
1	A	518	ASP
1	A	536	LEU
1	A	538	PHE
1	A	569	ASN
1	A	610	THR
1	A	654	MET
1	A	659	LEU
1	A	660	ASN
1	A	723	ILE
1	A	730	ILE
1	A	749	SER
1	A	750	ARG
1	A	786	ILE
1	A	791	GLN
1	A	801	GLU
1	A	824	ARG
2	B	317	SER
2	B	318	GLN
2	B	320	ASP
2	B	321	VAL
2	B	322	GLU
2	B	333	THR
2	B	334	VAL
2	B	335	LEU
2	B	337	GLN
2	B	338	LEU
2	B	340	MET
2	B	341	GLU
2	B	343	VAL
2	B	344	SER
2	B	345	VAL
2	B	349	ILE

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Mol	Chain	Res	Type
2	B	350	GLN
2	B	352	ILE
2	B	368	GLU
2	B	370	TYR
2	B	382	ARG
2	B	400	ARG
2	B	409	ILE
2	B	412	LYS
2	B	414	VAL
2	B	415	VAL
2	B	416	GLN
2	B	418	LYS
2	B	420	PHE
2	B	423	ASN
2	B	426	ARG
2	B	429	ASN
3	C	3	SER
3	C	5	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	236	GLN
1	A	324	ASN
1	A	380	GLN
1	A	383	ASN
1	A	402	ASN
1	A	427	GLN
1	A	540	ASN
2	B	337	GLN
2	B	393	GLN
2	B	416	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	HUF	A	901	-	59,60,60	1.32	7 (11%)	78,92,92	1.07	5 (6%)

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	-	-	13/36/52/52	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	-4.13	1.55	1.59
4	A	901	HUF	C20-C23	-3.41	1.34	1.43
4	A	901	HUF	PB-O3A	-3.14	1.56	1.59
4	A	901	HUF	O36-C25	-2.94	1.37	1.43
4	A	901	HUF	C16-C17	-2.66	1.36	1.39
4	A	901	HUF	C24-C25	-2.39	1.49	1.52
4	A	901	HUF	PA-O1A	-2.07	1.45	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	HUF	O33-C19-N29	-3.80	120.80	124.71
4	A	901	HUF	C20-C23-N31	3.62	117.30	110.94
4	A	901	HUF	C3'-C2'-C1'	-2.76	96.24	101.46
4	A	901	HUF	O1A-PA-O2A	2.62	124.64	112.44
4	A	901	HUF	O4'-C1'-C2'	-2.33	101.62	106.62

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	901	HUF	C28-O1B-PB-O3A
4	A	901	HUF	C28-O1B-PB-O3B
4	A	901	HUF	C28-O1B-PB-O2B
4	A	901	HUF	O33-C19-N29-C15
4	A	901	HUF	C25-C26-C27-O38
4	A	901	HUF	O37-C26-C27-O38
4	A	901	HUF	O37-C26-C27-C28
4	A	901	HUF	C25-C26-C27-C28
4	A	901	HUF	PA-O3A-PB-O1B
4	A	901	HUF	O33-C19-N29-C20
4	A	901	HUF	C24-C25-C26-O37
4	A	901	HUF	O36-C25-C26-C27
4	A	901	HUF	PA-O3A-PB-O3B

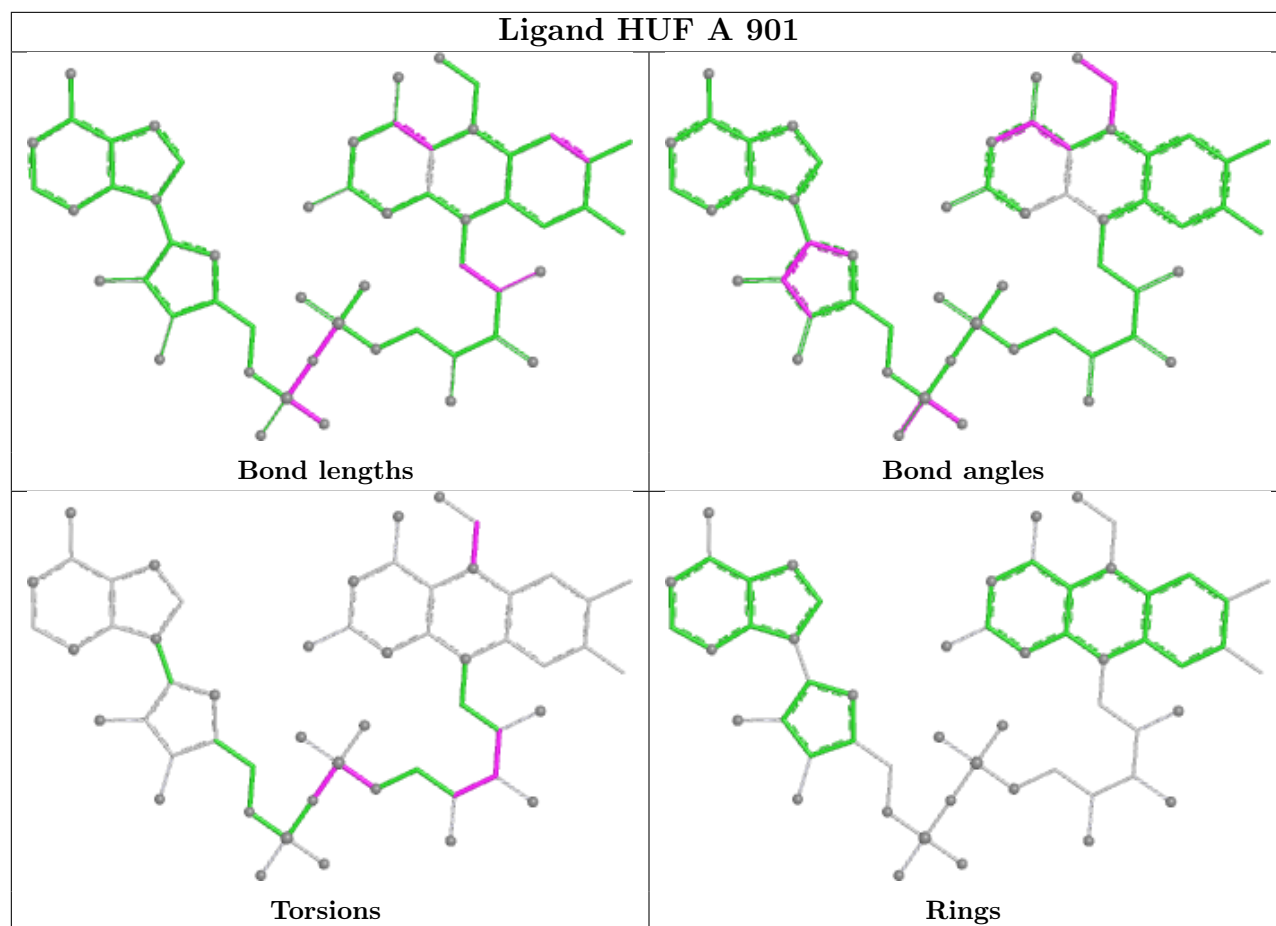
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	HUF	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	666/871 (76%)	0.57	34 (5%)	33 28	63, 97, 132, 147	0
2	B	133/144 (92%)	0.90	10 (7%)	20 18	94, 132, 149, 162	0
3	C	9/9 (100%)	2.45	3 (33%)	1 1	100, 111, 147, 154	0
All	All	808/1024 (78%)	0.64	47 (5%)	29 24	63, 104, 140, 162	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	9	PRO	7.8
1	A	836	LEU	6.7
1	A	749	SER	6.1
1	A	835	THR	5.6
3	C	8	LYS	4.3
2	B	375	VAL	4.2
1	A	331	ALA	4.2
2	B	376	ILE	4.0
1	A	287	GLY	3.5
1	A	171	PRO	3.4
1	A	810	THR	3.4
2	B	440	GLU	3.2
3	C	4	PHE	3.1
1	A	770	GLY	3.0
1	A	667	ASP	3.0
1	A	809	ALA	2.9
2	B	337	GLN	2.8
1	A	506	GLU	2.8
1	A	811	VAL	2.7
2	B	315	PHE	2.7
2	B	312	LYS	2.6
1	A	373	GLU	2.6
1	A	350	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	774	ASP	2.5
1	A	668	ARG	2.4
1	A	685	THR	2.4
1	A	316	ARG	2.3
2	B	383	TRP	2.3
2	B	436	GLU	2.2
1	A	431	TRP	2.2
1	A	695	TRP	2.2
1	A	363	TYR	2.2
1	A	761	TYR	2.2
1	A	384	ARG	2.2
1	A	591	ARG	2.2
2	B	308	ARG	2.2
1	A	315	GLY	2.2
2	B	434	LEU	2.2
1	A	684	THR	2.1
1	A	834	TYR	2.1
1	A	511	LEU	2.1
1	A	683	SER	2.1
1	A	720	ASP	2.1
1	A	462	TYR	2.1
1	A	499	GLU	2.1
1	A	698	TYR	2.1
1	A	440	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](#)

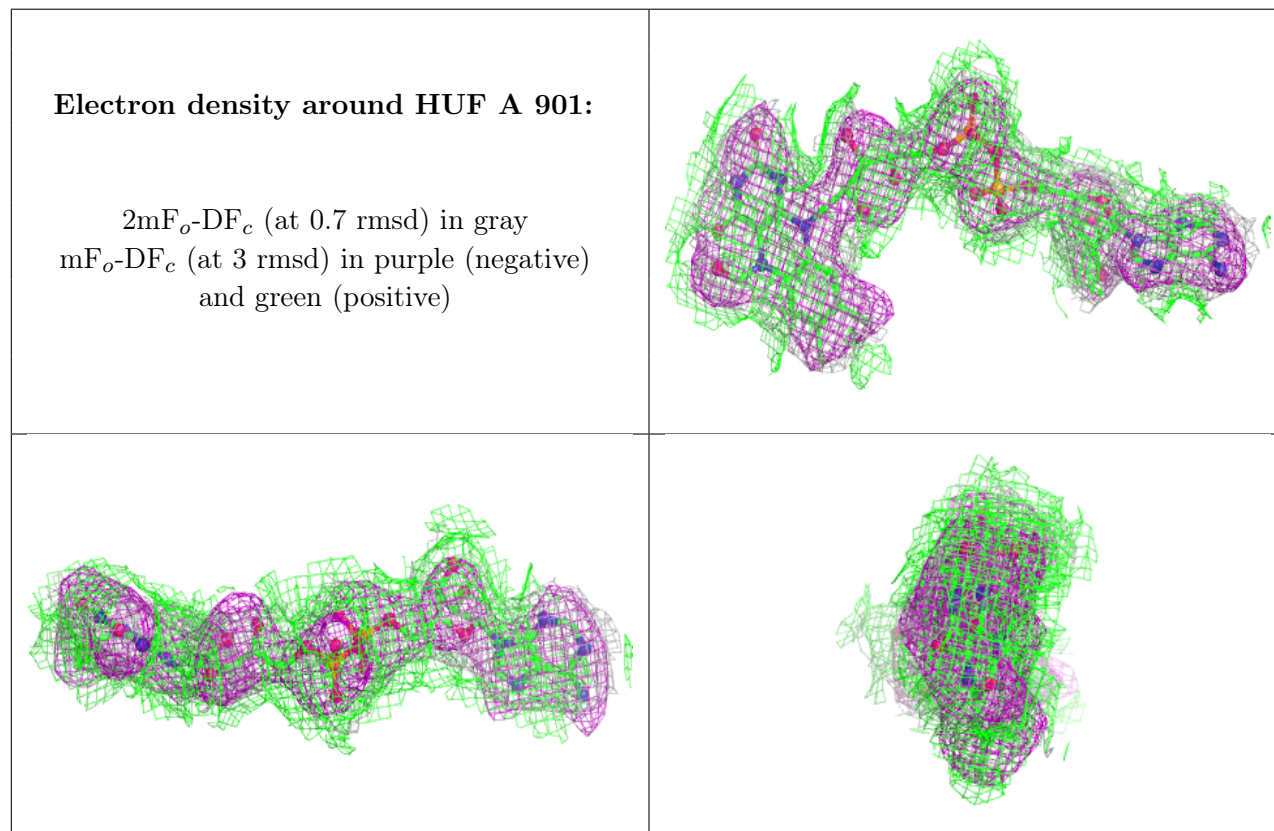
There are no oligosaccharides in this entry.

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, 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	0.90	0.12	0,0,0,0	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.