Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:38 pm BST

PDB ID	:	6MEV
Title	:	Structure of JMJD6 bound to Mono-Methyl Arginine.
Authors	:	Lee, S.; Zhang, G.
Deposited on	:	2018-09-07
Resolution	:	2.60 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 following versions of software and data (see references ⓘ) were used in the production of this report:

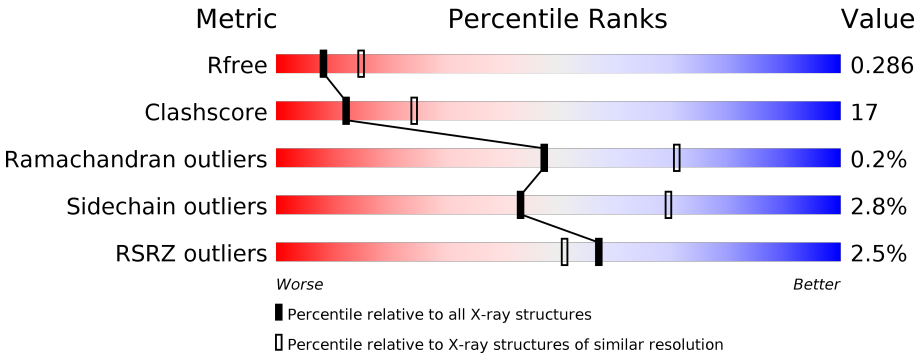
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	341	78% 21%
1	B	341	5% 62% 31%
1	C	341	3% 74% 22%
1	D	341	4% 62% 34%
1	E	341	% 74% 23%
1	F	341	2% 67% 28%

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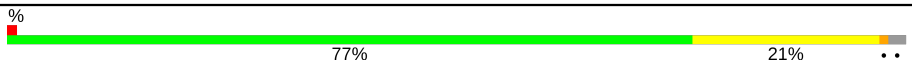
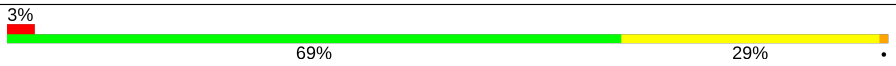
Mol	Chain	Length	Quality of chain
1	G	341	
1	H	341	

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
4	NMM	A	403	-	-	-	X
4	NMM	E	403	-	-	-	X

2 Entry composition (i)

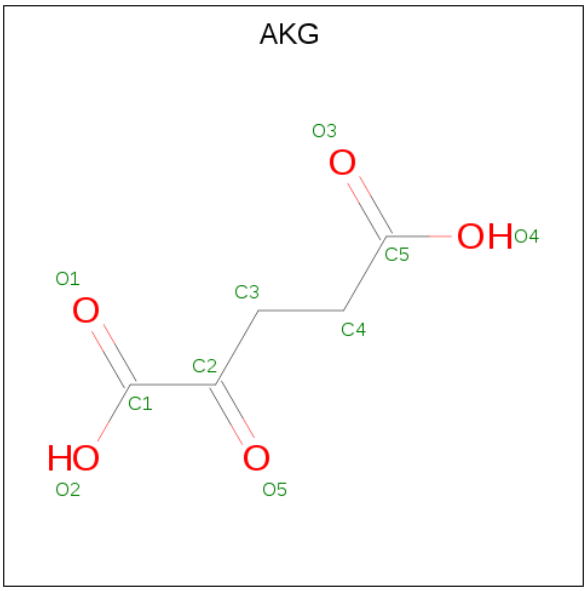
There are 5 unique types of molecules in this entry. The entry contains 23285 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	7	0	0
			2832	1813	499	513	7			
1	B	333	Total	C	N	O	S	5	0	0
			2779	1783	491	498	7			
1	C	335	Total	C	N	O	S	4	0	0
			2794	1791	493	503	7			
1	D	341	Total	C	N	O	S	2	0	0
			2832	1813	499	513	7			
1	E	341	Total	C	N	O	S	4	0	0
			2832	1813	499	513	7			
1	F	334	Total	C	N	O	S	5	0	0
			2788	1788	492	501	7			
1	G	335	Total	C	N	O	S	8	0	0
			2794	1791	493	503	7			
1	H	340	Total	C	N	O	S	4	0	0
			2824	1809	498	510	7			

- Molecule 2 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 5 5	10	0
2	B	1	Total C O 10 5 5	10	0
2	C	1	Total C O 10 5 5	10	0
2	D	1	Total C O 10 5 5	10	0
2	E	1	Total C O 10 5 5	10	0
2	F	1	Total C O 10 5 5	10	0
2	G	1	Total C O 10 5 5	10	0
2	H	1	Total C O 10 5 5	10	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Fe 1 1	1	0
3	D	1	Total Fe 1 1	1	0
3	E	1	Total Fe 1 1	1	0
3	H	1	Total Fe 1 1	1	0

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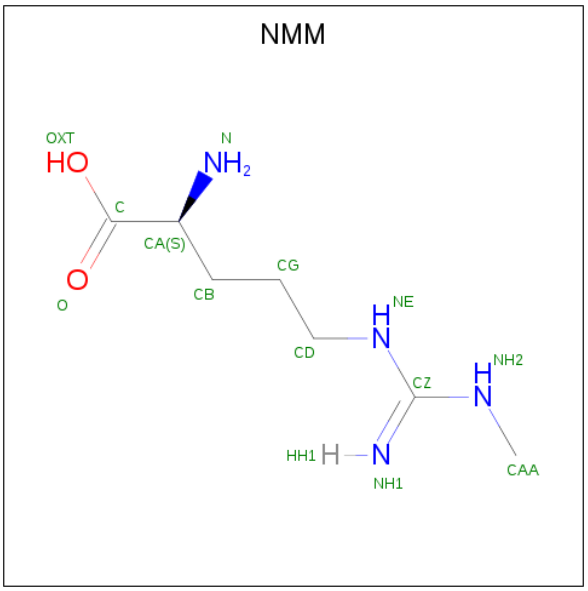
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Fe 1 1	1	0
3	C	1	Total Fe 1 1	1	0
3	A	1	Total Fe 1 1	1	0
3	F	1	Total Fe 1 1	1	0

- Molecule 4 is (2S)-2-amino-5-[(N-methylcarbamimidoyl)amino]pentanoic acid (three-letter code: NMM) (formula: $C_7H_{16}N_4O_2$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 13 7 4 2	0	0
4	E	1	Total C N O 13 7 4 2	0	0
4	G	1	Total C N O 13 7 4 2	0	0
4	H	1	Total C N O 13 7 4 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	115	Total O 115 115	0	0

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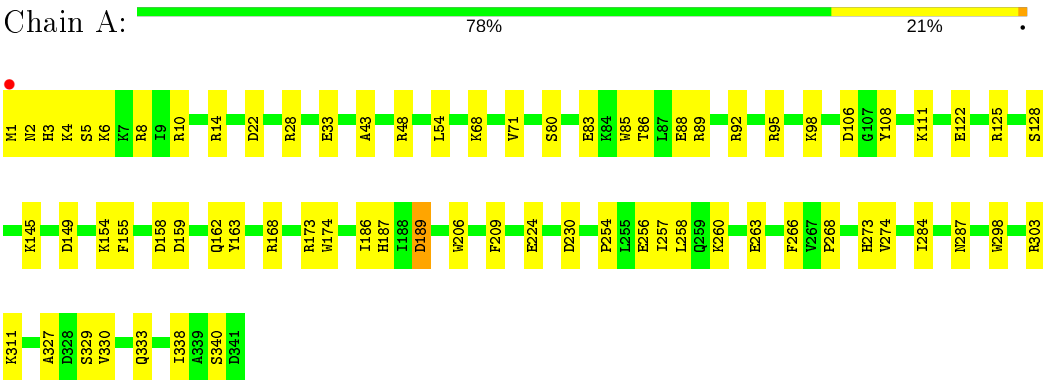
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	56	Total O 56 56	0	0
5	C	83	Total O 83 83	0	0
5	D	59	Total O 59 59	0	0
5	E	111	Total O 111 111	0	0
5	F	67	Total O 67 67	0	0
5	G	109	Total O 109 109	0	0
5	H	70	Total O 70 70	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

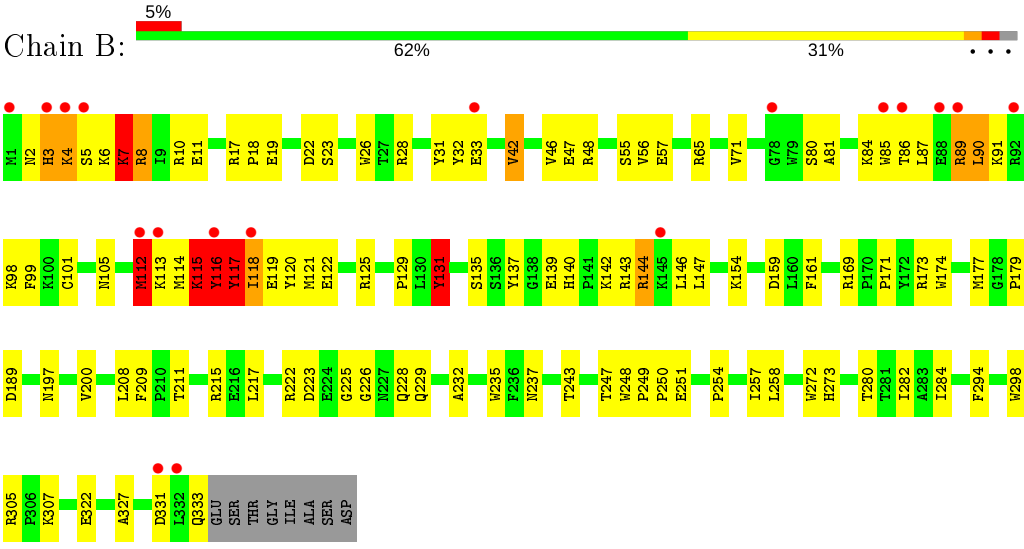
- Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6

Chain A:



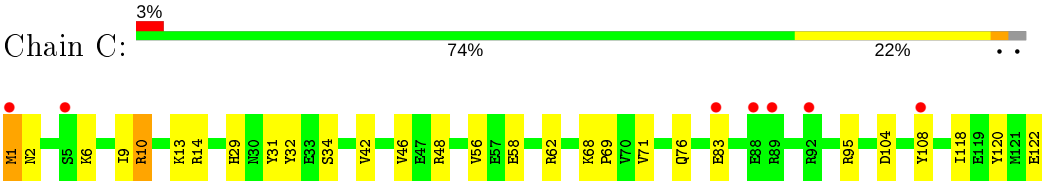
- Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6

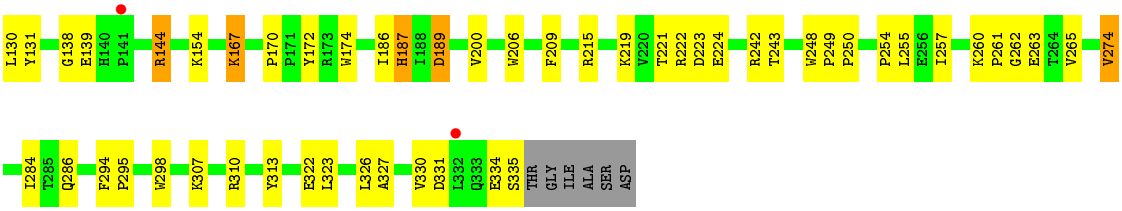
Chain B:



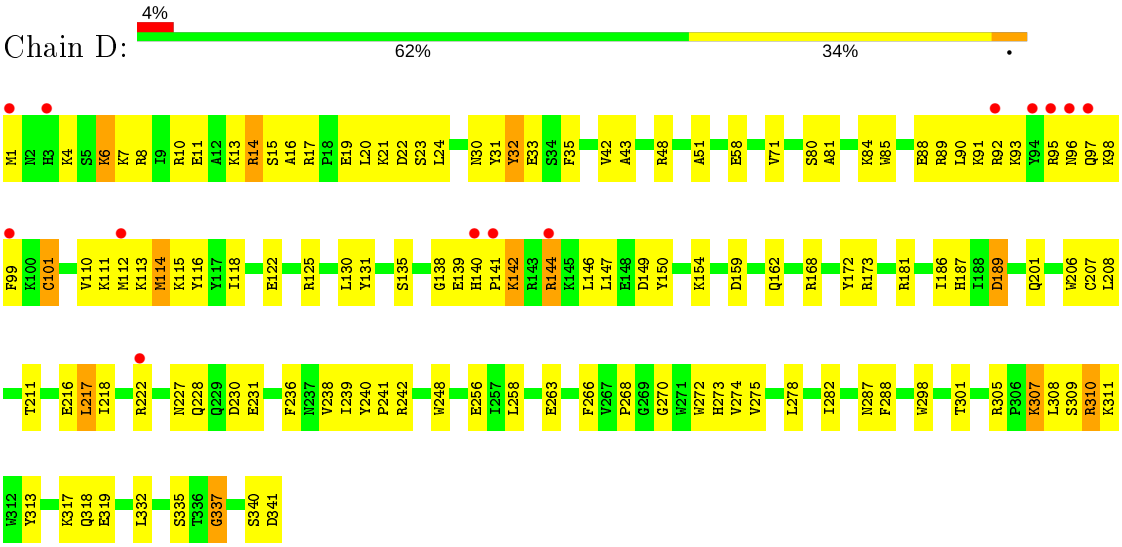
- Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6

Chain C:

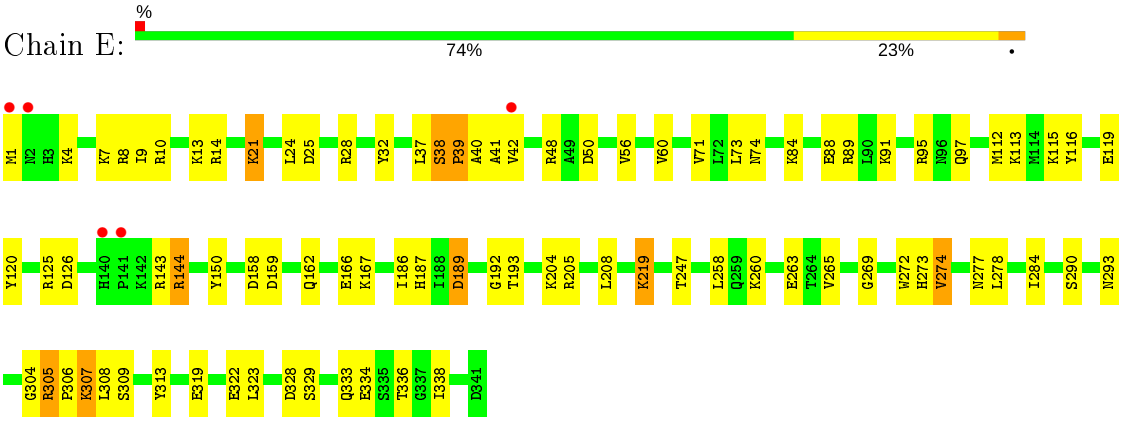




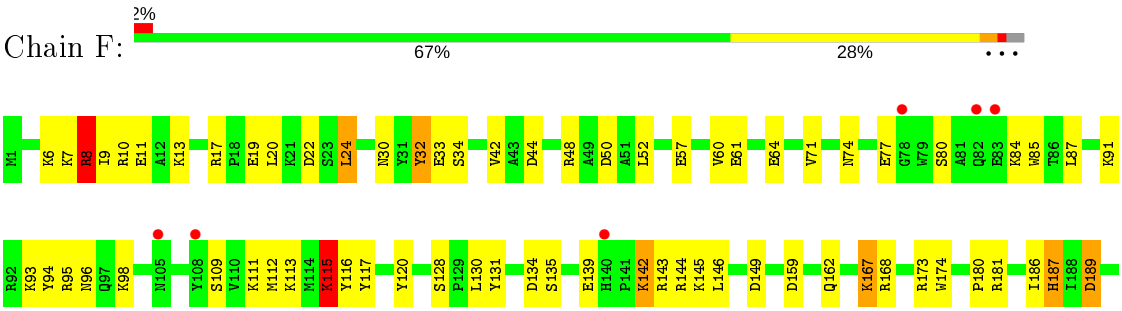
• Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6

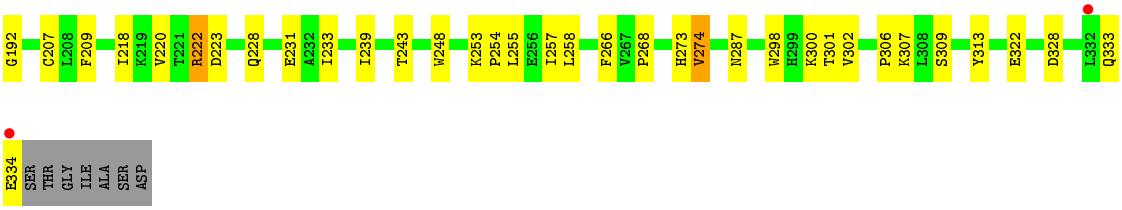


• Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6



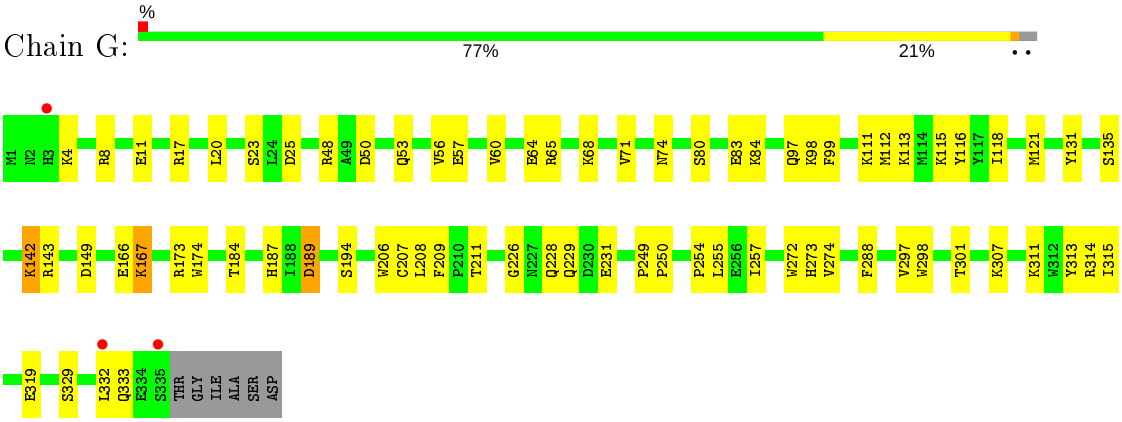
• Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6





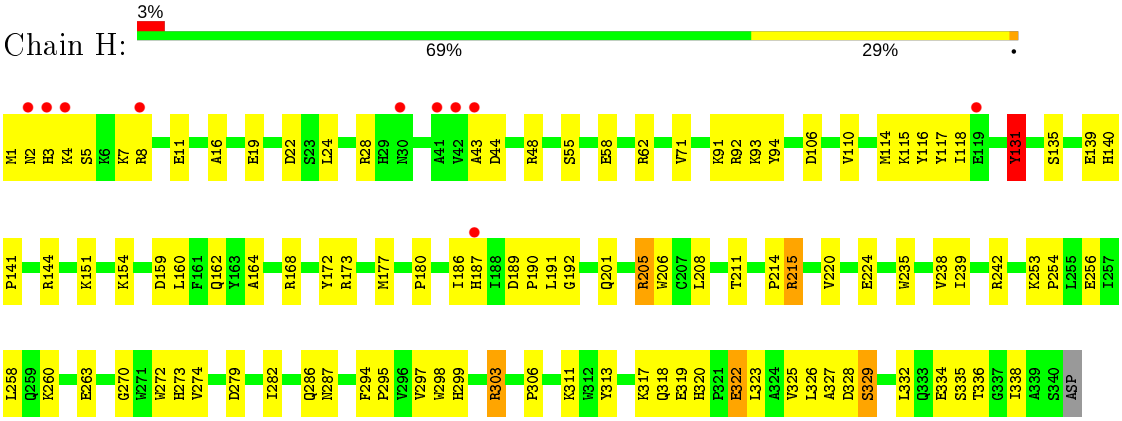
• Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6

Chain G:



• Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	100.55Å 141.91Å 149.26Å 90.00° 96.80° 90.00°	Depositor
Resolution (Å)	64.00 – 2.60 64.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (64.00-2.60) 99.1 (64.00-2.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.229 , 0.287 0.228 , 0.286	Depositor DCC
R_{free} test set	1999 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23285	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NMM, AKG, FE

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	0.53	0/2917	0.73	2/3956 (0.1%)
1	B	0.69	8/2864 (0.3%)	0.95	21/3884 (0.5%)
1	C	0.49	0/2879	0.70	2/3904 (0.1%)
1	D	0.65	7/2917 (0.2%)	0.80	9/3956 (0.2%)
1	E	0.50	0/2917	0.73	2/3956 (0.1%)
1	F	0.56	3/2873 (0.1%)	0.74	6/3896 (0.2%)
1	G	0.53	0/2879	0.74	2/3904 (0.1%)
1	H	0.49	0/2909	0.71	2/3945 (0.1%)
All	All	0.56	18/23155 (0.1%)	0.77	46/31401 (0.1%)

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	B	0	3
1	C	0	1
1	D	0	1
1	E	0	1
All	All	0	6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	116	TYR	CD1-CE1	-12.42	1.20	1.39
1	B	116	TYR	CE1-CZ	-11.72	1.23	1.38
1	D	32	TYR	CB-CG	-10.82	1.35	1.51
1	D	32	TYR	CD2-CE2	-9.84	1.24	1.39
1	F	115	LYS	CD-CE	-8.96	1.28	1.51
1	F	187	HIS	CA-CB	8.07	1.71	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	32	TYR	CE1-CZ	-7.72	1.28	1.38
1	D	144	ARG	CG-CD	-6.62	1.35	1.51
1	B	115	LYS	CD-CE	-6.60	1.34	1.51
1	B	117	TYR	CD2-CE2	-6.35	1.29	1.39
1	B	101	CYS	CB-SG	-6.01	1.72	1.82
1	D	101	CYS	CB-SG	-5.94	1.72	1.81
1	D	32	TYR	CD1-CE1	-5.61	1.30	1.39
1	B	117	TYR	CB-CG	-5.41	1.43	1.51
1	B	144	ARG	CB-CG	-5.39	1.38	1.52
1	F	115	LYS	CG-CD	-5.26	1.34	1.52
1	D	32	TYR	CG-CD2	-5.12	1.32	1.39
1	B	116	TYR	CG-CD1	-5.11	1.32	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	189	ASP	CB-CG-OD1	12.71	129.74	118.30
1	B	116	TYR	CB-CG-CD2	12.67	128.60	121.00
1	C	189	ASP	CB-CG-OD1	12.30	129.37	118.30
1	G	189	ASP	CB-CG-OD1	12.25	129.33	118.30
1	D	144	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	F	115	LYS	CD-CE-NZ	-10.40	87.78	111.70
1	A	189	ASP	CB-CG-OD1	10.28	127.55	118.30
1	B	116	TYR	CG-CD2-CE2	-8.83	114.24	121.30
1	C	189	ASP	CB-CG-OD2	-8.75	110.42	118.30
1	B	144	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	B	116	TYR	CB-CG-CD1	-8.59	115.85	121.00
1	B	89	ARG	CA-CB-CG	-8.55	94.59	113.40
1	B	112	MET	CG-SD-CE	8.33	113.53	100.20
1	B	189	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	H	303	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	D	310	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	B	89	ARG	CG-CD-NE	-7.61	95.81	111.80
1	D	32	TYR	CA-CB-CG	-7.52	99.12	113.40
1	B	116	TYR	CG-CD1-CE1	7.46	127.27	121.30
1	F	189	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	189	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	B	7	LYS	CD-CE-NZ	7.15	128.14	111.70
1	E	189	ASP	CB-CG-OD1	7.10	124.69	118.30
1	D	144	ARG	NH1-CZ-NH2	6.83	126.92	119.40
1	D	189	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	D	189	ASP	CB-CG-OD1	6.63	124.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	189	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	B	131	TYR	CA-CB-CG	6.26	125.30	113.40
1	F	8	ARG	CG-CD-NE	6.19	124.79	111.80
1	B	112	MET	CA-CB-CG	5.95	123.41	113.30
1	B	89	ARG	CB-CG-CD	5.87	126.87	111.60
1	D	144	ARG	CB-CA-C	-5.82	98.77	110.40
1	B	116	TYR	OH-CZ-CE2	5.79	135.72	120.10
1	B	8	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	B	114	MET	C-N-CA	5.59	135.68	121.70
1	B	112	MET	N-CA-CB	-5.51	100.68	110.60
1	H	131	TYR	CA-CB-CG	5.50	123.85	113.40
1	B	144	ARG	CG-CD-NE	-5.45	100.36	111.80
1	B	90	LEU	CA-CB-CG	5.36	127.63	115.30
1	E	305	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	F	144	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	D	125	ARG	CG-CD-NE	-5.22	100.83	111.80
1	F	24	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	116	TYR	CD1-CE1-CZ	5.21	124.49	119.80
1	D	217	LEU	CA-CB-CG	5.14	127.12	115.30
1	F	115	LYS	CB-CA-C	-5.11	100.19	110.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	117	TYR	Peptide
1	B	3	HIS	Peptide
1	B	4	LYS	Mainchain
1	C	187	HIS	Peptide
1	D	337	GLY	Peptide
1	E	41	ALA	Peptide

5.2 Too-close contacts (i)

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	2832	0	2781	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2779	0	2734	187	0
1	C	2794	0	2746	61	1
1	D	2832	0	2781	133	0
1	E	2832	0	2781	70	1
1	F	2788	0	2741	97	0
1	G	2794	0	2746	59	0
1	H	2824	0	2777	96	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
2	C	10	0	4	0	0
2	D	10	0	4	0	0
2	E	10	0	4	0	0
2	F	10	0	4	0	0
2	G	10	0	4	0	0
2	H	10	0	4	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	13	0	15	2	0
4	E	13	0	15	0	0
4	G	13	0	15	1	0
4	H	13	0	15	2	0
5	A	115	0	0	14	0
5	B	56	0	0	7	0
5	C	83	0	0	11	2
5	D	59	0	0	23	0
5	E	111	0	0	13	2
5	F	67	0	0	7	1
5	G	109	0	0	15	0
5	H	70	0	0	13	1
All	All	23285	0	22179	754	4

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 17.

All (754) 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:E:187:HIS:NE2	1:E:273:HIS:NE2	1.74	1.35
1:B:112:MET:SD	1:B:116:TYR:OH	1.92	1.27
1:B:112:MET:SD	1:B:116:TYR:CZ	2.31	1.23
1:B:112:MET:CE	1:B:116:TYR:CE2	2.30	1.15
1:G:315:ILE:HG23	1:G:319:GLU:OE1	1.51	1.10
1:E:187:HIS:CE1	1:E:273:HIS:CD2	2.39	1.09
1:E:187:HIS:CE1	1:E:273:HIS:NE2	2.19	1.09
1:H:189:ASP:OD1	5:H:501:HOH:O	1.70	1.08
1:B:112:MET:HG2	1:B:116:TYR:CE2	1.88	1.08
1:B:112:MET:CE	1:B:116:TYR:CZ	2.39	1.04
1:B:112:MET:HE2	1:B:116:TYR:CZ	1.96	1.01
1:A:95:ARG:NH2	5:A:503:HOH:O	1.94	0.99
1:B:115:LYS:HG2	1:B:116:TYR:H	1.27	0.98
1:H:299:HIS:CE1	1:H:303:ARG:HH22	1.81	0.98
1:G:315:ILE:CG2	1:G:319:GLU:OE1	2.13	0.96
1:A:287:ASN:O	5:A:501:HOH:O	1.81	0.96
1:F:115:LYS:H	1:F:115:LYS:HD2	1.29	0.96
1:B:116:TYR:O	1:B:120:TYR:N	1.99	0.95
1:F:57:GLU:O	1:F:61:GLU:OE1	1.82	0.94
1:B:112:MET:HG2	1:B:116:TYR:HE2	1.24	0.94
1:D:97:GLN:N	1:D:113:LYS:HZ3	1.66	0.93
1:B:4:LYS:O	1:B:7:LYS:HE3	1.69	0.92
1:B:7:LYS:HG2	1:B:8:ARG:H	1.32	0.92
1:B:5:SER:C	1:B:7:LYS:HD2	1.91	0.90
1:B:17:ARG:NH1	1:B:19:GLU:OE2	2.05	0.90
1:E:187:HIS:NE2	1:E:273:HIS:CE1	2.40	0.89
1:A:303:ARG:NH2	5:A:507:HOH:O	2.03	0.89
1:A:122:GLU:OE1	1:E:125:ARG:NH2	2.04	0.89
1:C:46:VAL:HG21	1:C:257:ILE:HG12	1.55	0.89
1:B:112:MET:HE3	1:B:116:TYR:CE2	2.05	0.88
1:B:7:LYS:CG	1:B:8:ARG:H	1.86	0.88
1:B:112:MET:CG	1:B:116:TYR:CE2	2.57	0.88
1:C:170:PRO:O	5:C:701:HOH:O	1.90	0.88
1:C:125:ARG:NH2	5:C:703:HOH:O	2.05	0.87
1:F:84:LYS:HD3	1:F:145:LYS:HZ1	1.37	0.87
1:B:98:LYS:HA	1:B:113:LYS:HA	1.55	0.87
1:G:17:ARG:NH2	1:G:228:GLN:OE1	2.08	0.86
1:F:187:HIS:CD2	1:F:189:ASP:OD1	2.07	0.86
1:D:96:ASN:C	1:D:113:LYS:HZ3	1.79	0.85
1:B:86:THR:HB	1:B:89:ARG:HD3	1.57	0.85
1:A:263:GLU:OE1	5:A:504:HOH:O	1.94	0.84
1:B:112:MET:SD	1:B:116:TYR:CE2	2.70	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:LYS:O	1:B:115:LYS:NZ	2.10	0.84
1:B:115:LYS:HE2	1:B:116:TYR:CE2	2.12	0.84
1:B:139:GLU:HA	1:B:144:ARG:HH22	1.43	0.83
1:D:238:VAL:O	5:D:701:HOH:O	1.95	0.83
1:C:224:GLU:OE2	1:C:242:ARG:NH2	2.11	0.83
1:F:17:ARG:NH2	1:F:228:GLN:OE1	2.12	0.83
1:H:4:LYS:NZ	5:H:505:HOH:O	2.10	0.83
1:E:247:THR:OG1	5:E:501:HOH:O	1.98	0.82
1:D:58:GLU:OE2	5:D:702:HOH:O	1.98	0.82
1:C:334:GLU:OE2	5:C:702:HOH:O	1.98	0.81
1:F:96:ASN:HA	1:F:115:LYS:HZ1	1.44	0.81
1:E:42:VAL:HB	5:E:521:HOH:O	1.79	0.81
1:B:112:MET:HE2	1:B:116:TYR:CE2	2.13	0.81
1:G:74:ASN:O	5:G:501:HOH:O	1.99	0.81
1:B:85:TRP:HA	1:B:89:ARG:NH2	1.95	0.81
1:E:144:ARG:NH2	5:E:506:HOH:O	2.12	0.81
1:F:17:ARG:O	5:F:701:HOH:O	2.00	0.80
1:B:115:LYS:CG	1:B:116:TYR:H	1.93	0.80
1:B:86:THR:HB	1:B:89:ARG:CD	2.12	0.79
1:H:224:GLU:OE2	1:H:242:ARG:NH2	2.15	0.79
1:A:187:HIS:NE2	4:A:403:NMM:OXT	2.15	0.79
1:B:140:HIS:H	1:B:144:ARG:HH12	1.27	0.79
1:A:307:LYS:H	1:A:307:LYS:HD3	1.47	0.79
1:D:131:TYR:O	5:D:703:HOH:O	2.01	0.79
1:B:112:MET:C	1:B:115:LYS:HZ1	1.86	0.79
1:B:116:TYR:C	1:B:116:TYR:CD1	2.56	0.78
1:D:97:GLN:HG2	1:D:142:LYS:HB2	1.65	0.78
1:F:17:ARG:NH1	1:F:19:GLU:OE1	2.17	0.78
1:B:65:ARG:NH1	5:B:704:HOH:O	2.13	0.78
1:B:115:LYS:HG2	1:B:116:TYR:N	2.00	0.77
1:D:1:MET:HG2	1:D:6:LYS:NZ	1.99	0.77
1:E:84:LYS:HA	1:E:89:ARG:HD3	1.65	0.77
1:B:112:MET:CG	1:B:116:TYR:HE2	1.95	0.77
1:E:193:THR:O	5:E:503:HOH:O	2.03	0.77
1:B:97:GLN:CD	1:B:142:LYS:HE3	2.06	0.76
1:A:128:SER:O	5:A:508:HOH:O	2.04	0.76
1:F:115:LYS:HD2	1:F:115:LYS:N	1.99	0.76
1:B:300:LYS:HZ2	1:B:303:ARG:HH12	1.32	0.76
1:D:97:GLN:N	1:D:113:LYS:NZ	2.34	0.75
1:C:222:ARG:NH1	5:C:705:HOH:O	2.18	0.75
1:B:112:MET:CG	1:B:116:TYR:CZ	2.70	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:O	1:C:6:LYS:NZ	2.19	0.75
1:D:230:ASP:OD2	5:D:704:HOH:O	2.04	0.74
1:B:3:HIS:O	1:B:3:HIS:ND1	2.19	0.74
1:H:235:TRP:NE1	1:H:239:ILE:HD11	2.01	0.74
1:G:64:GLU:OE1	5:G:502:HOH:O	2.06	0.74
1:D:20:LEU:O	5:D:705:HOH:O	2.05	0.73
1:B:116:TYR:CD1	1:B:117:TYR:N	2.57	0.73
1:E:37:LEU:O	5:E:505:HOH:O	2.07	0.73
1:H:135:SER:O	5:H:504:HOH:O	2.07	0.73
1:D:97:GLN:HG2	1:D:142:LYS:CB	2.19	0.73
1:D:99:PHE:HE1	1:D:114:MET:HG2	1.52	0.73
1:F:93:LYS:HZ1	1:F:145:LYS:HB3	1.54	0.73
1:F:116:TYR:O	1:F:120:TYR:N	2.22	0.72
1:G:65:ARG:NH2	5:G:511:HOH:O	2.22	0.72
1:D:33:GLU:OE2	5:D:706:HOH:O	2.06	0.72
1:D:51:ALA:O	5:D:708:HOH:O	2.08	0.72
1:A:4:LYS:NZ	5:A:510:HOH:O	2.17	0.72
1:F:8:ARG:NH2	1:F:11:GLU:HB3	2.04	0.72
1:B:2:ASN:OD1	1:B:4:LYS:N	2.23	0.72
1:E:40:ALA:O	5:E:504:HOH:O	2.07	0.72
1:D:31:TYR:OH	5:D:707:HOH:O	2.07	0.72
1:A:174:TRP:O	1:A:284:ILE:HD12	1.89	0.71
1:E:189:ASP:OD1	1:E:273:HIS:CE1	2.44	0.71
1:F:93:LYS:HE2	1:F:145:LYS:HE3	1.73	0.71
1:D:101:CYS:SG	1:D:112:MET:HG2	2.29	0.71
1:A:187:HIS:NE2	1:A:273:HIS:NE2	2.39	0.71
1:D:99:PHE:CE1	1:D:114:MET:HG2	2.25	0.71
1:F:6:LYS:O	5:F:703:HOH:O	2.08	0.70
1:H:205:ARG:NH1	5:H:509:HOH:O	2.25	0.70
1:G:48:ARG:O	5:G:503:HOH:O	2.09	0.70
1:B:81:ALA:O	1:B:85:TRP:N	2.24	0.70
1:H:22:ASP:N	1:H:22:ASP:OD1	2.23	0.70
1:B:140:HIS:N	1:B:144:ARG:HH12	1.89	0.70
1:D:139:GLU:C	1:D:144:ARG:HH12	1.94	0.70
1:H:187:HIS:NE2	4:H:403:NMM:O	2.25	0.70
1:C:187:HIS:CD2	1:C:189:ASP:OD1	2.24	0.69
1:G:187:HIS:NE2	1:G:273:HIS:NE2	2.27	0.69
1:D:140:HIS:HE1	5:D:746:HOH:O	1.74	0.69
1:F:42:VAL:HG11	1:F:258:LEU:HB2	1.75	0.69
1:D:144:ARG:HD3	1:D:144:ARG:N	2.08	0.69
1:B:137:TYR:O	1:B:144:ARG:NH1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:GLU:N	5:F:705:HOH:O	2.18	0.69
1:B:113:LYS:H	1:B:115:LYS:HE3	1.58	0.69
1:A:260:LYS:NZ	5:A:514:HOH:O	2.26	0.69
1:H:299:HIS:CE1	1:H:303:ARG:NH2	2.60	0.69
1:C:223:ASP:OD1	5:C:705:HOH:O	2.11	0.68
1:B:7:LYS:HE2	1:B:8:ARG:CZ	2.23	0.68
1:G:142:LYS:H	1:G:142:LYS:CD	2.07	0.68
1:G:167:LYS:HD3	1:G:167:LYS:H	1.58	0.68
1:B:113:LYS:N	1:B:115:LYS:HE3	2.09	0.68
1:B:112:MET:HE2	1:B:116:TYR:CE1	2.29	0.67
1:B:6:LYS:NZ	5:B:708:HOH:O	2.26	0.67
1:F:181:ARG:HB2	1:F:233:ILE:HD12	1.74	0.67
1:B:116:TYR:HD1	1:B:116:TYR:C	1.96	0.67
1:B:4:LYS:O	1:B:7:LYS:HG3	1.94	0.67
1:B:144:ARG:O	1:B:147:LEU:N	2.27	0.67
1:B:85:TRP:HB2	1:B:200:VAL:HG11	1.76	0.67
1:H:201:GLN:HG3	1:H:282:ILE:HD12	1.77	0.67
1:H:24:LEU:O	1:H:28:ARG:HG3	1.95	0.67
1:H:303:ARG:NH1	1:H:334:GLU:OE2	2.28	0.67
1:H:55:SER:OG	1:H:58:GLU:HG3	1.95	0.67
1:B:10:ARG:HH21	1:B:11:GLU:HG2	1.60	0.66
1:B:115:LYS:CD	1:B:115:LYS:N	2.59	0.66
1:D:242:ARG:NE	5:D:701:HOH:O	2.29	0.66
1:B:5:SER:CA	1:B:7:LYS:HD2	2.26	0.66
1:D:211:THR:OG1	1:D:270:GLY:O	2.10	0.66
1:D:313:TYR:HE1	1:D:317:LYS:HE3	1.60	0.66
1:G:166:GLU:OE2	5:G:504:HOH:O	2.13	0.66
1:B:139:GLU:CA	1:B:144:ARG:HH22	2.08	0.66
1:F:7:LYS:C	1:F:7:LYS:HZ2	1.99	0.65
1:A:2:ASN:OD1	1:A:3:HIS:N	2.28	0.65
1:B:2:ASN:HB3	1:B:5:SER:HB2	1.77	0.65
1:D:298:TRP:CH2	1:D:313:TYR:HB2	2.31	0.65
1:F:93:LYS:NZ	1:F:145:LYS:HB3	2.12	0.65
1:F:91:LYS:O	1:F:95:ARG:HG3	1.97	0.65
1:H:187:HIS:CE1	1:H:273:HIS:CD2	2.84	0.65
1:E:25:ASP:OD2	1:E:28:ARG:NH1	2.30	0.65
1:B:129:PRO:O	5:B:705:HOH:O	2.15	0.65
1:D:7:LYS:HG3	1:D:10:ARG:HD3	1.79	0.65
1:H:260:LYS:N	1:H:263:GLU:OE1	2.26	0.65
1:H:318:GLN:NE2	5:H:515:HOH:O	2.30	0.65
1:B:300:LYS:NZ	1:B:303:ARG:HH12	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LYS:HB3	1:D:118:ILE:HD12	1.79	0.65
1:B:116:TYR:HA	1:B:119:GLU:HB2	1.79	0.64
1:B:115:LYS:CG	1:B:116:TYR:N	2.60	0.64
1:G:187:HIS:HE2	1:G:273:HIS:HE2	1.43	0.64
1:H:238:VAL:HG23	1:H:239:ILE:HG23	1.80	0.64
1:B:84:LYS:O	1:B:85:TRP:CD1	2.50	0.64
1:D:97:GLN:O	1:D:113:LYS:NZ	2.31	0.64
1:B:117:TYR:OH	1:B:131:TYR:HA	1.98	0.64
1:B:118:ILE:O	1:B:122:GLU:HG3	1.98	0.64
1:B:115:LYS:HD2	1:B:115:LYS:H	1.62	0.64
1:E:167:LYS:NZ	5:E:516:HOH:O	2.28	0.63
1:F:61:GLU:N	1:F:61:GLU:OE1	2.32	0.63
1:B:17:ARG:NH2	1:B:228:GLN:OE1	2.32	0.63
1:D:287:ASN:O	5:D:710:HOH:O	2.15	0.63
1:H:253:LYS:HD2	1:H:254:PRO:HD2	1.79	0.63
1:B:84:LYS:O	1:B:85:TRP:HD1	1.80	0.63
1:D:310:ARG:CZ	1:H:306:PRO:HB2	2.28	0.63
1:G:48:ARG:HD3	1:G:71:VAL:HB	1.79	0.63
1:D:159:ASP:OD1	5:D:709:HOH:O	2.15	0.63
1:B:7:LYS:O	1:B:11:GLU:HG3	1.99	0.63
1:B:7:LYS:HG2	1:B:8:ARG:N	2.11	0.62
1:D:11:GLU:HA	1:D:14:ARG:HE	1.64	0.62
1:D:16:ALA:HB2	1:D:110:VAL:HG11	1.82	0.62
1:F:135:SER:HB3	1:F:174:TRP:NE1	2.15	0.62
1:D:114:MET:CE	1:D:118:ILE:HG13	2.29	0.61
1:B:7:LYS:HE2	1:B:8:ARG:NH1	2.16	0.61
1:D:1:MET:HG2	1:D:6:LYS:HZ1	1.66	0.61
1:C:221:THR:OG1	1:C:224:GLU:HG3	2.01	0.61
1:D:11:GLU:OE2	1:D:14:ARG:NH1	2.32	0.61
1:H:58:GLU:OE1	1:H:62:ARG:NH2	2.33	0.61
1:F:145:LYS:NZ	1:F:149:ASP:OD1	2.34	0.61
1:F:7:LYS:HZ1	1:F:8:ARG:HA	1.66	0.61
1:D:187:HIS:CE1	1:D:273:HIS:CD2	2.89	0.60
1:H:7:LYS:O	1:H:11:GLU:HG3	2.01	0.60
1:H:332:LEU:O	1:H:336:THR:HG23	2.01	0.60
1:D:16:ALA:HA	1:D:110:VAL:HG21	1.82	0.60
1:B:48:ARG:HD3	1:B:71:VAL:HB	1.83	0.60
1:F:222:ARG:HE	1:F:222:ARG:H	1.47	0.60
1:D:48:ARG:HD3	1:D:71:VAL:HB	1.84	0.60
1:F:80:SER:OG	1:F:149:ASP:HA	2.01	0.60
1:A:10:ARG:O	1:A:14:ARG:HG2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:MET:CG	1:B:116:TYR:OH	2.49	0.59
1:G:83:GLU:OE1	5:G:507:HOH:O	2.16	0.59
1:E:38:SER:O	1:E:40:ALA:N	2.36	0.59
1:B:86:THR:HB	1:B:89:ARG:NE	2.17	0.59
1:B:333:GLN:N	1:B:333:GLN:OE1	2.35	0.59
1:H:298:TRP:CH2	1:H:313:TYR:HB2	2.37	0.59
1:F:95:ARG:C	1:F:115:LYS:NZ	2.56	0.59
1:F:95:ARG:O	1:F:115:LYS:NZ	2.36	0.59
1:H:319:GLU:N	1:H:319:GLU:OE1	2.35	0.59
1:B:22:ASP:OD1	1:B:23:SER:N	2.36	0.58
1:A:307:LYS:HD3	1:A:307:LYS:N	2.17	0.58
1:C:295:PRO:HG3	1:C:326:LEU:HD21	1.85	0.58
1:D:168:ARG:HE	1:D:311:LYS:NZ	2.01	0.58
1:H:187:HIS:CE1	4:H:403:NMM:O	2.57	0.58
1:F:222:ARG:HD2	1:F:223:ASP:H	1.68	0.58
1:F:322:GLU:N	1:F:322:GLU:OE1	2.33	0.58
1:A:260:LYS:N	1:A:263:GLU:OE2	2.34	0.58
1:B:4:LYS:O	1:B:7:LYS:CE	2.47	0.58
1:H:44:ASP:CG	1:H:48:ARG:HH12	2.06	0.58
1:A:108:TYR:HE2	1:D:8:ARG:NH1	2.01	0.58
1:B:139:GLU:HA	1:B:144:ARG:NH2	2.15	0.58
1:D:32:TYR:CD2	1:D:33:GLU:N	2.72	0.58
1:H:117:TYR:OH	1:H:131:TYR:HA	2.03	0.58
1:C:42:VAL:O	5:C:706:HOH:O	2.17	0.58
1:C:48:ARG:HD3	1:C:71:VAL:HB	1.85	0.58
1:C:294:PHE:HD2	1:C:326:LEU:HD22	1.67	0.57
1:H:159:ASP:OD1	5:H:507:HOH:O	2.18	0.57
1:B:19:GLU:N	1:B:19:GLU:OE1	2.27	0.57
1:F:87:LEU:H	1:F:87:LEU:HD12	1.68	0.57
1:H:238:VAL:HG23	1:H:239:ILE:N	2.18	0.57
1:H:43:ALA:HB1	1:H:256:GLU:HB3	1.86	0.57
1:D:1:MET:HG2	1:D:6:LYS:HZ3	1.67	0.57
1:B:80:SER:O	1:B:84:LYS:N	2.34	0.57
1:G:112:MET:HE2	1:G:116:TYR:HB2	1.86	0.57
1:B:112:MET:HB3	1:B:116:TYR:OH	2.04	0.57
1:F:96:ASN:CA	1:F:115:LYS:HZ1	2.17	0.57
1:H:294:PHE:HD2	1:H:326:LEU:HD22	1.69	0.57
1:B:243:THR:HA	1:B:248:TRP:CD2	2.39	0.57
1:D:96:ASN:C	1:D:113:LYS:NZ	2.54	0.57
1:B:159:ASP:OD1	5:B:706:HOH:O	2.17	0.57
1:H:141:PRO:HA	1:H:144:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:GLU:HG3	1:F:34:SER:N	2.20	0.57
1:B:115:LYS:HD2	1:B:115:LYS:N	2.19	0.56
1:H:139:GLU:OE1	5:H:506:HOH:O	2.17	0.56
1:F:298:TRP:O	1:F:302:VAL:HG23	2.05	0.56
1:D:17:ARG:NH2	1:D:19:GLU:OE2	2.36	0.56
1:G:56:VAL:O	1:G:60:VAL:HG23	2.06	0.56
1:D:310:ARG:NH2	1:H:306:PRO:HB2	2.21	0.56
1:D:187:HIS:CE1	1:D:273:HIS:NE2	2.68	0.56
1:E:187:HIS:CD2	1:E:273:HIS:CE1	2.93	0.56
1:D:118:ILE:O	1:D:122:GLU:HG2	2.04	0.56
1:E:21:LYS:HD2	1:E:21:LYS:H	1.69	0.56
1:E:24:LEU:O	1:E:28:ARG:N	2.38	0.56
1:F:142:LYS:NZ	1:F:143:ARG:HH21	2.02	0.56
1:F:287:ASN:ND2	5:F:712:HOH:O	2.36	0.56
1:D:319:GLU:N	1:D:319:GLU:OE1	2.39	0.56
1:E:120:TYR:OH	1:E:126:ASP:OD2	2.16	0.56
1:F:80:SER:HB2	1:F:84:LYS:HD2	1.88	0.56
1:E:334:GLU:O	1:E:338:ILE:HG12	2.05	0.56
1:G:142:LYS:H	1:G:142:LYS:HD3	1.69	0.56
1:B:174:TRP:O	1:B:284:ILE:HD12	2.06	0.56
1:B:31:TYR:CE1	1:B:237:ASN:ND2	2.74	0.55
1:F:48:ARG:HD3	1:F:71:VAL:HB	1.88	0.55
1:A:125:ARG:NH1	1:E:1:MET:SD	2.73	0.55
1:B:97:GLN:HG3	1:B:143:ARG:HD3	1.89	0.55
1:G:297:VAL:O	1:G:301:THR:OG1	2.15	0.55
1:B:243:THR:HA	1:B:248:TRP:CG	2.41	0.55
1:H:235:TRP:CE2	1:H:239:ILE:HD11	2.41	0.55
1:H:92:ARG:NE	5:H:502:HOH:O	2.02	0.55
1:B:86:THR:O	1:B:90:LEU:HD12	2.07	0.55
1:E:48:ARG:HD2	1:E:73:LEU:HD21	1.89	0.55
1:B:86:THR:HG22	1:B:87:LEU:N	2.22	0.55
1:B:91:LYS:O	1:B:95:ARG:HB2	2.07	0.55
1:D:115:LYS:HG3	1:D:116:TYR:CD1	2.42	0.55
1:G:167:LYS:H	1:G:167:LYS:CD	2.19	0.55
1:A:224:GLU:OE1	5:A:511:HOH:O	2.18	0.54
1:G:57:GLU:H	1:G:57:GLU:CD	2.10	0.54
1:B:55:SER:OG	1:B:57:GLU:HG2	2.08	0.54
1:D:231:GLU:O	5:D:711:HOH:O	2.19	0.54
1:A:186:ILE:HB	1:A:274:VAL:HG22	1.89	0.54
1:H:235:TRP:HE1	1:H:239:ILE:HD11	1.72	0.54
1:B:209:PHE:CZ	1:B:254:PRO:HB3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:GLU:OE1	1:C:83:GLU:N	2.38	0.54
1:E:112:MET:HE2	1:E:116:TYR:HB3	1.90	0.54
1:F:180:PRO:O	1:F:181:ARG:HG2	2.07	0.54
1:B:97:GLN:NE2	1:B:142:LYS:HE3	2.23	0.54
1:F:8:ARG:O	1:F:8:ARG:HD3	2.08	0.54
1:D:23:SER:OG	5:D:712:HOH:O	2.19	0.54
1:H:19:GLU:OE2	1:H:19:GLU:N	2.35	0.54
1:H:335:SER:HA	1:H:338:ILE:HD12	1.90	0.54
1:D:335:SER:OG	1:H:328:ASP:OD2	2.18	0.54
1:C:14:ARG:NH2	5:C:713:HOH:O	2.34	0.53
1:F:93:LYS:HE3	1:F:94:TYR:CE1	2.42	0.53
1:B:89:ARG:HH21	1:B:90:LEU:HG	1.72	0.53
1:F:17:ARG:NH2	1:F:20:LEU:HD11	2.23	0.53
1:B:4:LYS:O	1:B:7:LYS:CD	2.56	0.53
1:C:206:TRP:HB2	1:C:257:ILE:HB	1.90	0.53
1:C:68:LYS:HE2	5:C:726:HOH:O	2.09	0.53
1:F:209:PHE:CZ	1:F:254:PRO:HB3	2.43	0.53
1:B:99:PHE:N	1:B:112:MET:O	2.30	0.53
1:B:118:ILE:HD12	1:B:118:ILE:H	1.73	0.53
1:B:117:TYR:HD2	1:B:177:MET:HE3	1.73	0.53
1:D:10:ARG:O	1:D:14:ARG:HG3	2.07	0.53
1:H:164:ALA:O	1:H:311:LYS:HE3	2.07	0.53
1:B:47:GLU:OE2	5:B:707:HOH:O	2.19	0.53
1:G:65:ARG:CZ	5:G:511:HOH:O	2.56	0.53
1:F:17:ARG:HH11	1:F:17:ARG:HG2	1.73	0.53
1:G:311:LYS:O	1:G:315:ILE:HD12	2.08	0.53
1:E:115:LYS:O	1:E:119:GLU:HG3	2.09	0.52
1:E:150:TYR:CZ	1:E:284:ILE:HD13	2.44	0.52
1:B:113:LYS:N	1:B:115:LYS:CE	2.70	0.52
1:C:215:ARG:HE	1:C:219:LYS:HD3	1.74	0.52
1:H:215:ARG:HD3	1:H:215:ARG:H	1.74	0.52
1:B:113:LYS:N	1:B:115:LYS:HZ1	2.06	0.52
1:H:286:GLN:NE2	5:H:510:HOH:O	2.25	0.52
1:B:4:LYS:O	1:B:7:LYS:CG	2.57	0.52
1:B:86:THR:CG2	1:B:87:LEU:N	2.72	0.52
1:H:295:PRO:HG3	1:H:326:LEU:HD21	1.91	0.52
1:B:116:TYR:O	1:B:119:GLU:N	2.43	0.52
1:B:46:VAL:HG11	1:B:257:ILE:HG12	1.92	0.52
1:C:219:LYS:HE3	5:C:761:HOH:O	2.09	0.52
1:E:189:ASP:CG	1:E:273:HIS:HE1	2.13	0.52
1:F:167:LYS:HG3	1:F:168:ARG:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:ILE:O	1:F:239:ILE:HD13	2.09	0.52
1:E:48:ARG:HD3	1:E:71:VAL:HB	1.91	0.52
1:C:307:LYS:HD3	1:C:310:ARG:HH21	1.75	0.52
1:E:189:ASP:OD1	1:E:273:HIS:HE1	1.92	0.52
1:F:94:TYR:OH	1:F:146:LEU:HG	2.10	0.52
1:D:140:HIS:CE1	5:D:746:HOH:O	2.53	0.52
1:D:144:ARG:O	1:D:147:LEU:N	2.28	0.52
1:E:204:LYS:NZ	1:E:277:ASN:OD1	2.36	0.52
1:E:32:TYR:CE2	1:E:125:ARG:HD3	2.45	0.52
1:F:17:ARG:HH21	1:F:20:LEU:HD11	1.75	0.52
1:A:298:TRP:CE2	1:A:327:ALA:HB1	2.44	0.51
1:B:117:TYR:CZ	1:B:131:TYR:HA	2.45	0.51
1:B:139:GLU:C	1:B:144:ARG:HH22	2.12	0.51
1:B:7:LYS:CG	1:B:8:ARG:N	2.65	0.51
1:B:116:TYR:HA	1:B:119:GLU:CB	2.40	0.51
1:D:88:GLU:O	1:D:92:ARG:HG2	2.09	0.51
1:E:208:LEU:HA	1:E:272:TRP:O	2.11	0.51
1:C:10:ARG:NH1	5:C:720:HOH:O	2.43	0.51
1:E:39:PRO:HB3	1:E:258:LEU:HD12	1.91	0.51
1:H:214:PRO:HA	1:H:215:ARG:HH21	1.76	0.51
1:B:113:LYS:C	1:B:115:LYS:HZ2	2.10	0.51
1:B:113:LYS:C	1:B:115:LYS:HD2	2.30	0.50
1:H:320:HIS:HB3	1:H:323:LEU:HD12	1.92	0.50
1:E:205:ARG:HB2	1:E:278:LEU:HD11	1.94	0.50
1:F:9:ILE:O	1:F:13:LYS:HG3	2.11	0.50
1:H:187:HIS:CD2	1:H:273:HIS:CE1	2.99	0.50
1:H:177:MET:HE2	1:H:282:ILE:HG12	1.92	0.50
1:B:56:VAL:HG23	1:B:154:LYS:HD2	1.94	0.50
1:B:86:THR:CG2	1:B:87:LEU:H	2.24	0.50
1:G:4:LYS:O	1:G:8:ARG:HG2	2.12	0.50
1:D:236:PHE:O	1:D:241:PRO:HD3	2.12	0.50
1:C:294:PHE:CD2	1:C:326:LEU:HD22	2.46	0.50
1:E:8:ARG:HG3	1:E:116:TYR:CE2	2.46	0.50
1:F:207:CYS:HA	1:F:255:LEU:O	2.11	0.50
1:H:151:LYS:HG3	1:H:151:LYS:O	2.11	0.50
1:H:220:VAL:HG13	1:H:238:VAL:HG21	1.93	0.50
1:F:333:GLN:O	1:F:334:GLU:HG3	2.10	0.50
1:A:206:TRP:HB2	1:A:257:ILE:HB	1.94	0.50
1:F:44:ASP:OD2	1:F:257:ILE:HA	2.11	0.50
1:H:211:THR:OG1	1:H:270:GLY:O	2.25	0.50
1:A:266:PHE:CE2	1:A:268:PRO:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:ASP:HB2	5:E:561:HOH:O	2.11	0.50
1:C:243:THR:HA	1:C:248:TRP:CD2	2.47	0.49
1:D:144:ARG:H	1:D:144:ARG:HD3	1.76	0.49
1:G:135:SER:HA	1:G:173:ARG:O	2.12	0.49
1:G:80:SER:OG	1:G:149:ASP:HA	2.12	0.49
4:G:403:NMM:HA	5:G:557:HOH:O	2.11	0.49
1:B:85:TRP:CE3	1:B:200:VAL:HG21	2.47	0.49
1:B:331:ASP:O	1:B:333:GLN:OE1	2.30	0.49
1:F:220:VAL:HG23	1:F:239:ILE:HD12	1.94	0.49
1:G:314:ARG:NH2	5:G:520:HOH:O	2.34	0.49
1:B:113:LYS:N	1:B:115:LYS:NZ	2.59	0.49
1:D:318:GLN:HB2	1:D:319:GLU:OE1	2.12	0.49
1:D:32:TYR:HA	1:D:181:ARG:HD3	1.94	0.49
1:A:86:THR:OG1	1:A:89:ARG:HG3	2.13	0.49
1:D:135:SER:HA	1:D:173:ARG:O	2.12	0.49
1:D:189:ASP:OD2	5:D:714:HOH:O	2.20	0.49
1:H:140:HIS:O	1:H:144:ARG:HG2	2.13	0.49
1:A:159:ASP:N	5:A:502:HOH:O	1.86	0.49
1:D:13:LYS:HG2	1:D:130:LEU:HD11	1.94	0.49
1:G:298:TRP:CH2	1:G:313:TYR:HB2	2.47	0.49
1:A:163:TYR:OH	5:A:512:HOH:O	2.19	0.49
1:H:287:ASN:ND2	5:H:513:HOH:O	2.44	0.49
1:C:209:PHE:CZ	1:C:254:PRO:HB3	2.47	0.49
1:B:118:ILE:HD12	1:B:118:ILE:N	2.27	0.49
1:B:89:ARG:NH2	1:B:90:LEU:HG	2.28	0.49
1:G:65:ARG:NE	5:G:511:HOH:O	2.46	0.49
1:H:159:ASP:O	1:H:162:GLN:HG2	2.12	0.49
1:A:154:LYS:HE3	1:A:155:PHE:CE1	2.47	0.49
1:D:144:ARG:O	1:D:146:LEU:N	2.46	0.49
1:D:337:GLY:O	1:D:341:ASP:HB2	2.13	0.49
1:G:115:LYS:HE3	1:G:116:TYR:CZ	2.47	0.49
1:B:2:ASN:C	1:B:5:SER:HB2	2.34	0.49
1:A:2:ASN:HB3	1:A:5:SER:OG	2.12	0.48
1:C:31:TYR:HA	1:C:34:SER:HB3	1.94	0.48
1:A:108:TYR:CE2	1:D:8:ARG:NH1	2.81	0.48
1:A:135:SER:HA	1:A:173:ARG:O	2.12	0.48
1:B:6:LYS:O	1:B:10:ARG:N	2.41	0.48
1:D:96:ASN:HA	1:D:113:LYS:HE2	1.95	0.48
1:F:93:LYS:HZ3	1:F:145:LYS:HD3	1.78	0.48
1:E:7:LYS:NZ	1:H:106:ASP:OD2	2.41	0.48
1:H:93:LYS:HE3	1:H:94:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:206:TRP:O	1:H:256:GLU:HA	2.12	0.48
1:A:209:PHE:CZ	1:A:254:PRO:HB3	2.49	0.48
1:B:113:LYS:HZ3	1:B:115:LYS:HG3	1.78	0.48
1:B:197:ASN:HB2	5:B:709:HOH:O	2.14	0.48
1:D:186:ILE:HD11	1:D:218:ILE:HD12	1.96	0.48
1:D:84:LYS:HA	1:D:89:ARG:HD2	1.95	0.48
1:E:219:LYS:NZ	5:E:528:HOH:O	2.43	0.48
1:B:228:GLN:HA	1:B:228:GLN:OE1	2.13	0.48
1:E:260:LYS:O	1:E:263:GLU:HG3	2.13	0.48
1:B:2:ASN:CB	1:B:5:SER:HB2	2.42	0.48
1:D:207:CYS:HB2	1:D:274:VAL:CG2	2.44	0.48
1:B:305:ARG:HE	1:B:307:LYS:NZ	2.11	0.48
1:B:298:TRP:CE2	1:B:327:ALA:HB1	2.48	0.48
1:D:21:LYS:HD3	1:D:21:LYS:HA	1.64	0.48
1:D:7:LYS:HA	1:D:10:ARG:HG3	1.95	0.48
1:E:97:GLN:O	1:E:113:LYS:HA	2.14	0.48
1:C:215:ARG:HE	1:C:219:LYS:CD	2.27	0.48
1:H:115:LYS:HE3	1:H:116:TYR:CE1	2.49	0.48
1:C:322:GLU:HG2	1:C:323:LEU:N	2.28	0.48
1:D:84:LYS:HG2	1:D:89:ARG:HH11	1.79	0.48
1:E:50:ASP:OD1	1:E:74:ASN:ND2	2.47	0.48
1:F:243:THR:HA	1:F:248:TRP:CG	2.49	0.48
1:B:121:MET:HG2	1:B:179:PRO:HB3	1.95	0.48
1:G:231:GLU:O	5:G:509:HOH:O	2.20	0.48
1:G:99:PHE:CZ	1:G:143:ARG:HD2	2.49	0.48
1:D:217:LEU:HG	1:D:248:TRP:CH2	2.49	0.47
1:D:85:TRP:HB3	1:D:282:ILE:HG21	1.96	0.47
1:F:52:LEU:HD11	1:F:77:GLU:HG3	1.96	0.47
1:G:20:LEU:HD22	1:G:25:ASP:HB3	1.95	0.47
1:D:239:ILE:HA	5:D:701:HOH:O	2.13	0.47
1:F:120:TYR:CE2	1:F:130:LEU:HB2	2.49	0.47
1:B:98:LYS:HA	1:B:113:LYS:CA	2.35	0.47
1:F:95:ARG:C	1:F:115:LYS:HZ2	2.16	0.47
1:B:84:LYS:O	1:B:89:ARG:NH2	2.48	0.47
1:C:120:TYR:CE2	1:C:130:LEU:HB2	2.49	0.47
1:D:31:TYR:O	1:D:35:PHE:N	2.42	0.47
1:G:4:LYS:NZ	5:G:505:HOH:O	2.14	0.47
1:H:215:ARG:HD3	1:H:215:ARG:N	2.29	0.47
1:A:186:ILE:CB	1:A:274:VAL:HG22	2.44	0.47
1:A:80:SER:O	1:A:83:GLU:HG2	2.15	0.47
1:C:174:TRP:O	1:C:284:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:LYS:O	1:D:10:ARG:HG3	2.14	0.47
1:D:154:LYS:NZ	5:D:708:HOH:O	2.47	0.47
1:E:187:HIS:HE1	1:E:273:HIS:CD2	2.19	0.47
1:F:266:PHE:CE2	1:F:268:PRO:HG3	2.49	0.47
1:H:154:LYS:NZ	5:H:519:HOH:O	2.44	0.47
1:C:71:VAL:HG22	1:C:265:VAL:HG22	1.95	0.47
1:G:206:TRP:HB2	1:G:257:ILE:HB	1.96	0.47
1:G:4:LYS:HE2	1:G:8:ARG:HE	1.79	0.47
1:C:76:GLN:OE1	1:C:262:GLY:HA2	2.15	0.47
1:F:52:LEU:HD13	1:F:74:ASN:CB	2.45	0.47
1:F:306:PRO:O	1:F:309:SER:OG	2.21	0.47
1:B:115:LYS:HE2	1:B:116:TYR:CZ	2.48	0.47
1:D:113:LYS:HD2	1:D:114:MET:N	2.30	0.47
1:D:6:LYS:N	1:D:6:LYS:HD2	2.29	0.47
1:D:88:GLU:OE2	1:D:92:ARG:NH2	2.47	0.47
1:A:128:SER:HB3	5:A:508:HOH:O	2.14	0.47
1:D:307:LYS:HD3	1:D:308:LEU:H	1.79	0.47
1:F:134:ASP:O	1:F:174:TRP:HA	2.15	0.47
1:F:222:ARG:H	1:F:222:ARG:NE	2.10	0.47
1:B:97:GLN:HG2	1:B:142:LYS:HG3	1.96	0.47
1:D:168:ARG:NH2	5:D:724:HOH:O	2.48	0.47
1:H:239:ILE:HG22	1:H:242:ARG:NH1	2.30	0.47
1:H:48:ARG:HD2	1:H:71:VAL:HB	1.97	0.47
1:A:159:ASP:O	1:A:162:GLN:HG2	2.15	0.46
1:A:168:ARG:NH2	5:A:519:HOH:O	2.36	0.46
1:A:187:HIS:NE2	1:A:189:ASP:OD1	2.48	0.46
1:A:28:ARG:NH1	1:G:20:LEU:O	2.49	0.46
1:B:144:ARG:HA	1:B:144:ARG:HD3	1.45	0.46
1:D:313:TYR:CE1	1:D:317:LYS:HE3	2.46	0.46
1:A:54:LEU:O	1:A:154:LYS:NZ	2.31	0.46
1:B:117:TYR:O	1:B:121:MET:HG3	2.14	0.46
1:B:331:ASP:C	1:B:333:GLN:OE1	2.53	0.46
1:F:8:ARG:HH21	1:F:11:GLU:HB3	1.80	0.46
1:H:173:ARG:CB	1:H:286:GLN:HG2	2.45	0.46
1:A:209:PHE:CE1	1:A:254:PRO:HB3	2.51	0.46
1:A:329:SER:O	1:A:333:GLN:HG3	2.16	0.46
1:B:135:SER:HA	1:B:173:ARG:O	2.16	0.46
1:A:158:ASP:HB2	5:A:502:HOH:O	2.15	0.46
1:B:249:PRO:HA	1:B:250:PRO:HD3	1.87	0.46
1:G:135:SER:HB3	1:G:174:TRP:NE1	2.30	0.46
1:D:168:ARG:HD2	1:D:311:LYS:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:LEU:HA	1:B:272:TRP:O	2.15	0.46
1:D:91:LYS:HB3	1:D:118:ILE:CD1	2.44	0.46
1:D:201:GLN:HG3	1:D:282:ILE:HD12	1.97	0.46
1:F:181:ARG:HB2	1:F:233:ILE:CD1	2.43	0.46
1:C:222:ARG:HD2	1:C:223:ASP:N	2.31	0.46
1:D:4:LYS:NZ	5:D:719:HOH:O	2.31	0.46
1:H:186:ILE:HA	1:H:273:HIS:O	2.16	0.46
1:H:43:ALA:O	1:H:258:LEU:HG	2.16	0.46
1:C:58:GLU:O	1:C:62:ARG:HG2	2.16	0.46
1:D:17:ARG:NH2	1:D:227:ASN:O	2.48	0.46
1:B:118:ILE:CD1	1:B:118:ILE:H	2.29	0.46
1:C:46:VAL:HG22	1:C:255:LEU:HG	1.98	0.46
1:F:95:ARG:C	1:F:115:LYS:HZ1	2.19	0.46
1:H:318:GLN:HB2	1:H:319:GLU:OE1	2.16	0.46
1:B:251:GLU:N	1:B:251:GLU:OE1	2.37	0.45
1:C:32:TYR:CD2	1:C:125:ARG:HD2	2.50	0.45
1:C:298:TRP:HD1	1:C:330:VAL:CG2	2.29	0.45
1:D:4:LYS:O	5:D:715:HOH:O	2.20	0.45
1:E:14:ARG:HA	1:E:14:ARG:HD3	1.78	0.45
1:E:159:ASP:O	1:E:162:GLN:HG2	2.15	0.45
1:D:1:MET:H3	1:D:6:LYS:HE2	1.82	0.45
1:E:71:VAL:HG22	1:E:265:VAL:HG22	1.98	0.45
1:E:260:LYS:NZ	5:E:530:HOH:O	2.43	0.45
1:E:32:TYR:CZ	1:E:125:ARG:HD3	2.51	0.45
1:F:42:VAL:CG1	1:F:258:LEU:HB2	2.44	0.45
1:H:94:TYR:O	1:H:114:MET:HB3	2.17	0.45
1:C:334:GLU:CD	5:C:702:HOH:O	2.51	0.45
1:D:310:ARG:NH1	1:H:306:PRO:HB2	2.31	0.45
1:D:97:GLN:C	1:D:113:LYS:NZ	2.69	0.45
1:E:307:LYS:HG2	1:E:308:LEU:N	2.31	0.45
1:E:313:TYR:OH	1:E:328:ASP:OD2	2.32	0.45
1:G:50:ASP:HB3	1:G:53:GLN:OE1	2.17	0.45
1:B:305:ARG:HE	1:B:307:LYS:HZ3	1.64	0.45
1:B:7:LYS:N	1:B:7:LYS:CD	2.80	0.45
1:D:298:TRP:HH2	1:D:313:TYR:HB2	1.77	0.45
1:F:22:ASP:OD1	1:F:24:LEU:HG	2.17	0.45
1:B:98:LYS:CA	1:B:113:LYS:HA	2.36	0.45
1:B:115:LYS:HE2	1:B:116:TYR:CD2	2.50	0.45
1:B:117:TYR:OH	1:B:179:PRO:HD3	2.17	0.45
1:C:172:TYR:O	1:C:286:GLN:HA	2.16	0.45
1:D:159:ASP:O	1:D:162:GLN:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:THR:O	1:D:305:ARG:N	2.44	0.45
1:H:16:ALA:HA	1:H:110:VAL:HG21	1.99	0.45
1:D:32:TYR:CD2	1:D:32:TYR:C	2.87	0.45
1:F:313:TYR:OH	1:F:328:ASP:OD2	2.33	0.45
1:F:7:LYS:NZ	1:F:8:ARG:HA	2.29	0.45
1:B:112:MET:HG2	1:B:116:TYR:CZ	2.35	0.45
1:C:260:LYS:O	1:C:263:GLU:HB2	2.17	0.45
1:C:322:GLU:N	1:C:322:GLU:OE2	2.42	0.45
1:D:208:LEU:HA	1:D:272:TRP:O	2.17	0.45
1:D:43:ALA:O	1:D:256:GLU:HB2	2.17	0.45
1:F:85:TRP:NE1	1:F:149:ASP:OD2	2.48	0.45
1:G:307:LYS:HG2	1:G:307:LYS:H	1.54	0.45
1:B:87:LEU:HD23	1:B:87:LEU:HA	1.68	0.45
1:D:301:THR:HG22	1:D:309:SER:HB3	1.99	0.45
1:F:186:ILE:HA	1:F:273:HIS:O	2.17	0.45
1:A:68:LYS:HE2	5:A:578:HOH:O	2.18	0.44
1:B:32:TYR:HD2	1:B:33:GLU:HG2	1.82	0.44
1:A:106:ASP:HB3	1:D:11:GLU:OE2	2.18	0.44
1:F:243:THR:HA	1:F:248:TRP:CD2	2.52	0.44
1:H:4:LYS:HE3	1:H:8:ARG:NH2	2.31	0.44
1:F:32:TYR:N	5:F:705:HOH:O	2.50	0.44
1:G:207:CYS:HA	1:G:255:LEU:O	2.17	0.44
1:B:112:MET:CB	1:B:116:TYR:OH	2.66	0.44
1:B:89:ARG:HG2	1:B:90:LEU:N	2.32	0.44
1:D:80:SER:OG	1:D:149:ASP:HA	2.17	0.44
1:C:1:MET:SD	1:C:1:MET:N	2.88	0.44
1:E:9:ILE:HG22	1:E:13:LYS:HE3	1.99	0.44
1:F:128:SER:OG	1:F:231:GLU:OE1	2.29	0.44
1:H:298:TRP:HH2	1:H:313:TYR:HB2	1.78	0.44
1:D:8:ARG:N	5:D:715:HOH:O	2.47	0.44
1:E:112:MET:HE2	1:E:116:TYR:CB	2.47	0.44
1:G:135:SER:HB3	1:G:174:TRP:CD1	2.52	0.44
1:H:208:LEU:HA	1:H:272:TRP:O	2.18	0.44
1:D:30:ASN:C	1:D:32:TYR:N	2.68	0.44
1:G:209:PHE:CZ	1:G:254:PRO:HB3	2.53	0.44
1:H:141:PRO:HA	1:H:144:ARG:CZ	2.48	0.44
1:C:200:VAL:O	1:C:261:PRO:HB3	2.17	0.44
1:F:186:ILE:N	1:F:274:VAL:HG13	2.33	0.44
1:B:222:ARG:O	1:B:226:GLY:N	2.33	0.44
1:D:7:LYS:HG3	1:D:10:ARG:HH11	1.83	0.44
1:F:98:LYS:HA	1:F:113:LYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:84:LYS:NZ	1:F:145:LYS:HE2	2.33	0.43
1:G:329:SER:O	1:G:333:GLN:HB3	2.18	0.43
1:B:161:PHE:HB2	1:B:169:ARG:HH21	1.83	0.43
1:B:80:SER:O	1:B:84:LYS:HB2	2.18	0.43
1:B:87:LEU:HD11	1:B:280:THR:HG21	1.99	0.43
1:D:95:ARG:O	1:D:113:LYS:HE3	2.18	0.43
1:B:18:PRO:HG2	1:B:105:ASN:OD1	2.19	0.43
1:B:17:ARG:HG3	1:B:26:TRP:CH2	2.52	0.43
1:B:5:SER:C	1:B:7:LYS:CD	2.75	0.43
1:A:230:ASP:HB3	4:A:403:NMM:HAA3	1.99	0.43
1:D:95:ARG:C	1:D:113:LYS:HZ1	2.22	0.43
1:E:306:PRO:O	1:E:309:SER:OG	2.25	0.43
1:E:91:LYS:O	1:E:95:ARG:HB2	2.19	0.43
1:E:97:GLN:HB3	1:E:143:ARG:HD2	2.00	0.43
1:F:135:SER:HA	1:F:173:ARG:O	2.18	0.43
1:C:9:ILE:O	1:C:13:LYS:HG3	2.18	0.43
1:D:16:ALA:CA	1:D:110:VAL:HG21	2.48	0.43
1:E:150:TYR:CZ	1:E:284:ILE:CD1	3.02	0.43
1:F:109:SER:CB	1:F:111:LYS:HE2	2.48	0.43
1:G:98:LYS:HB3	1:G:111:LYS:HB3	2.00	0.43
1:B:5:SER:HA	1:B:7:LYS:CE	2.49	0.43
1:H:180:PRO:HD3	1:H:279:ASP:C	2.39	0.43
1:B:2:ASN:OD1	1:B:3:HIS:N	2.51	0.43
1:D:138:GLY:O	1:D:144:ARG:CZ	2.66	0.43
1:D:17:ARG:HE	1:D:17:ARG:HB3	1.65	0.43
1:E:269:GLY:HA2	5:E:503:HOH:O	2.17	0.43
1:A:48:ARG:HD3	1:A:71:VAL:HB	2.01	0.43
1:B:115:LYS:HD3	1:B:115:LYS:N	2.34	0.43
1:C:104:ASP:OD2	1:C:108:TYR:HB2	2.17	0.43
1:C:298:TRP:CH2	1:C:313:TYR:HB2	2.54	0.43
1:E:189:ASP:CG	1:E:273:HIS:CE1	2.91	0.43
1:F:32:TYR:HB3	5:F:704:HOH:O	2.19	0.43
1:F:52:LEU:HD13	1:F:74:ASN:HB3	2.01	0.43
1:F:96:ASN:HA	1:F:115:LYS:NZ	2.25	0.43
1:G:118:ILE:HA	1:G:121:MET:HE2	2.01	0.43
1:H:2:ASN:OD1	1:H:3:HIS:N	2.52	0.43
1:A:98:LYS:HB3	1:A:111:LYS:HB3	2.00	0.43
1:B:113:LYS:HG3	1:B:115:LYS:CD	2.49	0.43
1:B:10:ARG:NH2	1:B:11:GLU:HG2	2.32	0.43
1:E:329:SER:O	1:E:333:GLN:HB2	2.19	0.43
1:F:93:LYS:HE3	1:F:94:TYR:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:OD1	1:A:273:HIS:NE2	2.52	0.43
1:B:217:LEU:HG	1:B:248:TRP:CH2	2.53	0.43
1:E:304:GLY:C	1:E:305:ARG:HG2	2.39	0.43
1:G:97:GLN:HG3	1:G:142:LYS:HG3	2.01	0.43
1:H:190:PRO:HD2	1:H:287:ASN:ND2	2.34	0.43
1:A:43:ALA:O	1:A:256:GLU:HB2	2.19	0.42
1:A:33:GLU:HG2	1:E:88:GLU:HG3	2.00	0.42
1:F:94:TYR:HE2	1:F:143:ARG:HA	1.84	0.42
1:H:91:LYS:HE3	1:H:118:ILE:HG21	2.01	0.42
1:H:334:GLU:O	1:H:338:ILE:HD12	2.19	0.42
1:A:142:LYS:O	1:A:145:LYS:HD2	2.18	0.42
1:A:22:ASP:OD2	1:G:23:SER:OG	2.36	0.42
1:H:238:VAL:HG23	1:H:239:ILE:H	1.81	0.42
1:B:8:ARG:HA	1:B:11:GLU:HG3	2.01	0.42
1:B:135:SER:HB2	1:B:171:PRO:HB3	2.01	0.42
1:D:4:LYS:HE3	1:D:116:TYR:OH	2.19	0.42
1:F:60:VAL:HA	1:F:64:GLU:HB3	2.01	0.42
1:G:187:HIS:CD2	1:G:189:ASP:OD1	2.66	0.42
1:B:225:GLY:HA3	1:B:229:GLN:HA	2.02	0.42
1:B:187:HIS:CD2	1:B:273:HIS:CE1	3.07	0.42
1:C:29:HIS:HB3	1:C:31:TYR:CE1	2.55	0.42
1:D:332:LEU:HA	1:D:332:LEU:HD12	1.80	0.42
1:G:166:GLU:HG3	5:G:589:HOH:O	2.19	0.42
1:G:226:GLY:O	1:G:229:GLN:HB2	2.19	0.42
1:C:13:LYS:NZ	1:C:126:ASP:OD2	2.46	0.42
1:C:46:VAL:CG2	1:C:257:ILE:HG12	2.39	0.42
1:C:298:TRP:HD1	1:C:330:VAL:HG21	1.85	0.42
1:F:159:ASP:O	1:F:162:GLN:HB2	2.20	0.42
1:A:4:LYS:HE3	1:A:8:ARG:NE	2.35	0.42
1:D:147:LEU:HA	1:D:150:TYR:CE1	2.55	0.42
1:D:172:TYR:N	1:D:172:TYR:CD1	2.88	0.42
1:G:209:PHE:CE2	1:G:254:PRO:HB3	2.55	0.42
1:H:7:LYS:HE2	1:H:11:GLU:OE1	2.19	0.42
1:B:177:MET:HG3	1:B:282:ILE:HG12	2.01	0.42
1:D:97:GLN:CA	1:D:113:LYS:HZ3	2.31	0.42
1:E:56:VAL:O	1:E:60:VAL:HG23	2.20	0.42
1:H:322:GLU:CD	1:H:322:GLU:H	2.22	0.42
1:H:298:TRP:CE2	1:H:327:ALA:HB1	2.55	0.42
1:B:96:ASN:HA	1:B:113:LYS:HD2	2.02	0.42
1:C:138:GLY:O	1:C:144:ARG:HG3	2.20	0.42
1:C:186:ILE:HB	1:C:274:VAL:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:MET:HE2	1:F:117:TYR:N	2.35	0.42
1:A:154:LYS:HE3	1:A:155:PHE:CZ	2.54	0.42
1:B:197:ASN:ND2	5:B:709:HOH:O	2.28	0.42
1:C:56:VAL:HG23	1:C:154:LYS:HD2	2.01	0.42
1:D:96:ASN:HA	1:D:113:LYS:CE	2.49	0.42
1:H:192:GLY:N	5:H:508:HOH:O	2.20	0.42
1:B:42:VAL:HG11	1:B:258:LEU:HD13	2.02	0.41
1:B:7:LYS:NZ	1:B:8:ARG:NH2	2.68	0.41
1:E:290:SER:N	1:E:293:ASN:OD1	2.30	0.41
1:H:191:LEU:O	1:H:297:VAL:HG22	2.20	0.41
1:H:44:ASP:OD1	1:H:48:ARG:NH1	2.51	0.41
1:B:179:PRO:HD2	1:B:182:SER:HB3	2.02	0.41
1:B:232:ALA:O	1:B:235:TRP:N	2.54	0.41
1:B:84:LYS:HA	1:B:89:ARG:NH1	2.35	0.41
1:C:249:PRO:HA	1:C:250:PRO:HD3	1.91	0.41
1:D:258:LEU:HD21	1:D:278:LEU:HD11	2.01	0.41
1:G:80:SER:HB2	1:G:84:LYS:HD2	2.02	0.41
1:B:294:PHE:HZ	1:B:327:ALA:HB2	1.84	0.41
1:B:97:GLN:C	1:B:113:LYS:HA	2.40	0.41
1:D:48:ARG:NE	1:D:263:GLU:OE1	2.39	0.41
1:D:90:LEU:HA	1:D:90:LEU:HD23	1.77	0.41
1:B:243:THR:HG22	1:B:248:TRP:CZ2	2.55	0.41
1:D:42:VAL:HG21	1:D:258:LEU:HD23	2.01	0.41
1:D:206:TRP:CD2	1:D:275:VAL:HG22	2.56	0.41
1:F:95:ARG:HG2	1:F:115:LYS:HE3	2.02	0.41
1:G:194:SER:HB2	1:G:288:PHE:CE1	2.55	0.41
1:G:97:GLN:O	1:G:113:LYS:HA	2.20	0.41
1:B:137:TYR:HA	1:B:143:ARG:HE	1.85	0.41
1:B:93:LYS:HD3	1:B:94:TYR:CE2	2.55	0.41
1:E:322:GLU:HG2	1:E:323:LEU:N	2.35	0.41
1:F:94:TYR:CE2	1:F:143:ARG:HA	2.56	0.41
1:G:208:LEU:HA	1:G:272:TRP:O	2.20	0.41
1:H:160:LEU:HA	1:H:160:LEU:HD23	1.91	0.41
1:H:1:MET:O	1:H:5:SER:HB2	2.20	0.41
1:D:15:SER:OG	1:D:110:VAL:HG22	2.20	0.41
1:D:313:TYR:C	1:D:313:TYR:CD1	2.93	0.41
1:E:189:ASP:OD1	1:E:273:HIS:NE2	2.54	0.41
1:F:301:THR:HG22	1:F:309:SER:HB3	2.02	0.41
1:A:338:ILE:HG21	1:A:338:ILE:HD13	1.80	0.41
1:B:2:ASN:O	1:B:5:SER:CB	2.69	0.41
1:B:2:ASN:CA	1:B:5:SER:HB2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ASP:O	1:C:335:SER:N	2.53	0.41
1:B:140:HIS:H	1:B:144:ARG:NH1	2.06	0.41
1:G:249:PRO:HA	1:G:250:PRO:HD3	1.93	0.41
1:H:168:ARG:HD2	1:H:168:ARG:HA	1.78	0.41
1:A:14:ARG:HD3	1:A:14:ARG:HA	1.92	0.41
1:A:1:MET:H3	1:A:6:LYS:HE3	1.86	0.41
1:B:8:ARG:HA	1:B:11:GLU:OE2	2.21	0.41
1:C:10:ARG:O	1:C:14:ARG:HG3	2.20	0.41
1:D:111:LYS:HB2	1:D:111:LYS:HE3	1.91	0.41
1:D:141:PRO:HA	1:D:144:ARG:CZ	2.51	0.41
1:D:216:GLU:H	1:D:216:GLU:CD	2.23	0.41
1:F:135:SER:HB3	1:F:174:TRP:CD1	2.56	0.41
1:G:65:ARG:HH11	1:G:65:ARG:HG2	1.84	0.41
1:G:68:LYS:HE2	5:G:535:HOH:O	2.20	0.41
1:B:140:HIS:N	1:B:144:ARG:NH1	2.61	0.41
1:B:144:ARG:C	1:B:146:LEU:N	2.71	0.41
1:C:118:ILE:O	1:C:122:GLU:HG3	2.21	0.41
1:C:206:TRP:HA	1:C:274:VAL:O	2.21	0.41
1:C:2:ASN:C	1:C:6:LYS:HZ2	2.23	0.41
1:E:192:GLY:HA2	5:E:582:HOH:O	2.20	0.41
1:E:186:ILE:N	1:E:274:VAL:HG13	2.36	0.41
1:A:260:LYS:O	1:A:263:GLU:HG3	2.21	0.41
1:A:2:ASN:O	1:A:6:LYS:HG2	2.21	0.41
1:D:95:ARG:O	1:D:113:LYS:CE	2.69	0.41
1:D:228:GLN:O	1:D:231:GLU:HB2	2.21	0.41
1:D:266:PHE:CE2	1:D:268:PRO:HG3	2.56	0.41
1:E:322:GLU:HG2	1:E:323:LEU:H	1.85	0.41
1:E:336:THR:N	5:E:519:HOH:O	2.30	0.41
1:H:135:SER:HA	1:H:173:ARG:O	2.21	0.41
1:H:325:VAL:O	1:H:329:SER:OG	2.38	0.41
1:B:57:GLU:CD	1:B:57:GLU:H	2.22	0.40
1:F:32:TYR:C	1:F:32:TYR:CD1	2.95	0.40
1:H:173:ARG:HB3	1:H:286:GLN:HG2	2.02	0.40
1:A:85:TRP:NE1	1:A:149:ASP:OD2	2.50	0.40
1:A:88:GLU:H	1:A:88:GLU:CD	2.25	0.40
1:B:135:SER:HB3	1:B:174:TRP:CD1	2.55	0.40
1:B:32:TYR:CE1	1:B:125:ARG:HD3	2.56	0.40
1:D:81:ALA:HB1	1:D:85:TRP:CD2	2.56	0.40
1:F:30:ASN:ND2	5:F:704:HOH:O	2.13	0.40
1:H:238:VAL:CG2	1:H:239:ILE:N	2.84	0.40
1:C:69:PRO:HG2	1:C:255:LEU:HD22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:ILE:O	1:D:240:TYR:C	2.59	0.40
1:E:4:LYS:O	1:E:7:LYS:HB3	2.21	0.40
1:F:149:ASP:OD1	1:F:149:ASP:N	2.54	0.40
1:F:192:GLY:N	1:F:300:LYS:HD2	2.36	0.40
1:H:317:LYS:NZ	5:H:521:HOH:O	2.50	0.40
1:C:327:ALA:O	1:C:330:VAL:HG22	2.21	0.40
1:D:93:LYS:HD2	5:D:738:HOH:O	2.21	0.40
1:G:189:ASP:O	5:G:510:HOH:O	2.22	0.40
1:H:172:TYR:O	1:H:286:GLN:HA	2.21	0.40
1:A:311:LYS:HE3	1:A:311:LYS:HB3	1.79	0.40
1:A:48:ARG:CD	1:A:71:VAL:HB	2.51	0.40
1:B:135:SER:HB3	1:B:174:TRP:NE1	2.37	0.40
1:E:166:GLU:H	1:E:166:GLU:HG2	1.51	0.40
1:F:50:ASP:OD1	1:F:52:LEU:HB2	2.21	0.40
1:H:43:ALA:HB1	1:H:256:GLU:CB	2.51	0.40

All (4) 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)
5:F:757:HOH:O	5:H:562:HOH:O[2_955]	1.85	0.35
5:C:783:HOH:O	5:E:611:HOH:O[2_946]	1.97	0.23
1:C:95:ARG:NH1	1:E:319:GLU:OE2[1_655]	2.14	0.06
5:C:754:HOH:O	5:E:544:HOH:O[1_655]	2.18	0.02

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	339/341 (99%)	333 (98%)	6 (2%)	0	100 100
1	B	331/341 (97%)	314 (95%)	14 (4%)	3 (1%)	17 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	333/341 (98%)	326 (98%)	6 (2%)	1 (0%)	41 64
1	D	339/341 (99%)	324 (96%)	15 (4%)	0	100 100
1	E	339/341 (99%)	321 (95%)	17 (5%)	1 (0%)	41 64
1	F	332/341 (97%)	319 (96%)	12 (4%)	1 (0%)	41 64
1	G	333/341 (98%)	330 (99%)	3 (1%)	0	100 100
1	H	338/341 (99%)	325 (96%)	13 (4%)	0	100 100
All	All	2684/2728 (98%)	2592 (97%)	86 (3%)	6 (0%)	47 71

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	LYS
1	B	115	LYS
1	C	167	LYS
1	B	118	ILE
1	F	167	LYS
1	E	39	PRO

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	306/306 (100%)	300 (98%)	6 (2%)	55 78
1	B	300/306 (98%)	288 (96%)	12 (4%)	31 57
1	C	302/306 (99%)	295 (98%)	7 (2%)	50 75
1	D	306/306 (100%)	295 (96%)	11 (4%)	35 61
1	E	306/306 (100%)	299 (98%)	7 (2%)	50 75
1	F	301/306 (98%)	290 (96%)	11 (4%)	34 60
1	G	302/306 (99%)	294 (97%)	8 (3%)	46 72
1	H	305/306 (100%)	299 (98%)	6 (2%)	55 78
All	All	2428/2448 (99%)	2360 (97%)	68 (3%)	43 69

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ARG
1	A	258	LEU
1	A	307	LYS
1	A	310	ARG
1	A	330	VAL
1	A	340	SER
1	B	7	LYS
1	B	28	ARG
1	B	42	VAL
1	B	112	MET
1	B	115	LYS
1	B	116	TYR
1	B	131	TYR
1	B	211	THR
1	B	215	ARG
1	B	223	ASP
1	B	247	THR
1	B	322	GLU
1	C	1	MET
1	C	10	ARG
1	C	131	TYR
1	C	139	GLU
1	C	144	ARG
1	C	167	LYS
1	C	274	VAL
1	D	6	LYS
1	D	14	ARG
1	D	22	ASP
1	D	24	LEU
1	D	98	LYS
1	D	114	MET
1	D	142	LYS
1	D	222	ARG
1	D	288	PHE
1	D	307	LYS
1	D	340	SER
1	E	10	ARG
1	E	21	LYS
1	E	38	SER
1	E	144	ARG
1	E	219	LYS
1	E	274	VAL

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Mol	Chain	Res	Type
1	E	307	LYS
1	F	8	ARG
1	F	10	ARG
1	F	32	TYR
1	F	115	LYS
1	F	131	TYR
1	F	139	GLU
1	F	142	LYS
1	F	222	ARG
1	F	253	LYS
1	F	274	VAL
1	F	307	LYS
1	G	11	GLU
1	G	131	TYR
1	G	142	LYS
1	G	167	LYS
1	G	184	THR
1	G	211	THR
1	G	274	VAL
1	G	332	LEU
1	H	131	TYR
1	H	205	ARG
1	H	215	ARG
1	H	274	VAL
1	H	322	GLU
1	H	329	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	97	GLN
1	D	237	ASN
1	F	30	ASN
1	F	201	GLN
1	H	201	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 20 ligands modelled in this entry, 8 are monoatomic - leaving 12 for Mogul analysis.

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	$\#\|Z\| > 2$
2	AKG	A	401	3	3,9,9	1.71	1 (33%)	4,11,11	2.33	2 (50%)
4	NMM	A	403	3	7,12,12	3.80	4 (57%)	7,14,14	4.16	6 (85%)
4	NMM	H	403	3	7,12,12	3.58	2 (28%)	7,14,14	4.18	4 (57%)
2	AKG	C	600	3	3,9,9	1.51	1 (33%)	4,11,11	1.28	1 (25%)
2	AKG	E	401	3	3,9,9	1.37	1 (33%)	4,11,11	1.94	2 (50%)
4	NMM	G	403	3	7,12,12	3.67	2 (28%)	7,14,14	4.82	4 (57%)
2	AKG	H	401	3	3,9,9	0.18	0	4,11,11	1.33	0
4	NMM	E	403	-	7,12,12	3.61	2 (28%)	7,14,14	4.48	4 (57%)
2	AKG	D	600	3	3,9,9	1.43	1 (33%)	4,11,11	1.51	1 (25%)
2	AKG	B	600	3	3,9,9	1.49	1 (33%)	4,11,11	1.38	1 (25%)
2	AKG	F	600	3	3,9,9	1.46	1 (33%)	4,11,11	1.30	1 (25%)
2	AKG	G	401	3	3,9,9	1.30	1 (33%)	4,11,11	1.93	2 (50%)

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
2	AKG	A	401	3	-	2/3/9/9	-
4	NMM	A	403	3	-	2/8/13/13	-
4	NMM	H	403	3	-	5/8/13/13	-
2	AKG	C	600	3	-	0/3/9/9	-
2	AKG	E	401	3	-	0/3/9/9	-
4	NMM	G	403	3	-	5/8/13/13	-
2	AKG	H	401	3	-	2/3/9/9	-
4	NMM	E	403	-	-	4/8/13/13	-
2	AKG	D	600	3	-	3/3/9/9	-
2	AKG	B	600	3	-	1/3/9/9	-
2	AKG	F	600	3	-	2/3/9/9	-
2	AKG	G	401	3	-	3/3/9/9	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	403	NMM	CZ-NH1	7.25	1.49	1.29
4	H	403	NMM	CZ-NH1	6.91	1.48	1.29
4	A	403	NMM	CZ-NH1	6.75	1.48	1.29
4	E	403	NMM	CZ-NH1	6.65	1.48	1.29
4	A	403	NMM	CZ-NH2	6.23	1.49	1.34
4	E	403	NMM	CZ-NH2	6.20	1.49	1.34
4	H	403	NMM	CZ-NH2	5.92	1.48	1.34
4	G	403	NMM	CZ-NH2	5.91	1.48	1.34
2	A	401	AKG	O5-C2	-2.52	1.18	1.22
4	A	403	NMM	CD-NE	2.47	1.51	1.46
2	B	600	AKG	O5-C2	-2.15	1.18	1.22
2	D	600	AKG	O5-C2	-2.14	1.18	1.22
2	C	600	AKG	O5-C2	-2.13	1.18	1.22
4	A	403	NMM	CA-N	2.11	1.51	1.47
2	E	401	AKG	O5-C2	-2.09	1.19	1.22
2	F	600	AKG	O5-C2	-2.08	1.19	1.22
2	G	401	AKG	O5-C2	-2.02	1.19	1.22

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	403	NMM	NE-CZ-NH2	-9.32	110.94	119.48
4	E	403	NMM	CD-NE-CZ	-7.50	109.81	123.50
4	A	403	NMM	NE-CZ-NH2	-6.88	113.17	119.48
4	H	403	NMM	CAA-NH2-CZ	-6.43	109.65	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	403	NMM	CAA-NH2-CZ	-6.40	109.71	123.86
4	E	403	NMM	NE-CZ-NH1	-5.79	109.41	120.26
4	H	403	NMM	NE-CZ-NH2	-5.53	114.41	119.48
4	A	403	NMM	CD-NE-CZ	-5.52	113.42	123.50
4	H	403	NMM	NE-CZ-NH1	-5.41	110.11	120.26
4	E	403	NMM	CAA-NH2-CZ	-5.04	112.73	123.86
4	G	403	NMM	CD-NE-CZ	-4.63	115.05	123.50
4	H	403	NMM	CD-NE-CZ	-4.52	115.24	123.50
4	E	403	NMM	NE-CZ-NH2	-4.40	115.44	119.48
4	A	403	NMM	NE-CZ-NH1	-4.14	112.50	120.26
2	A	401	AKG	C3-C4-C5	-3.66	106.53	112.67
4	A	403	NMM	CAA-NH2-CZ	-3.60	115.92	123.86
4	G	403	NMM	NE-CZ-NH1	-3.26	114.14	120.26
2	G	401	AKG	C4-C3-C2	-3.02	106.62	113.14
2	E	401	AKG	C4-C3-C2	-2.85	106.98	113.14
2	E	401	AKG	C3-C4-C5	-2.45	108.56	112.67
2	D	600	AKG	C4-C3-C2	-2.43	107.90	113.14
4	A	403	NMM	CG-CD-NE	2.42	119.12	112.21
2	A	401	AKG	O5-C2-C3	-2.34	116.38	120.38
4	A	403	NMM	CG-CB-CA	2.22	120.34	113.35
2	G	401	AKG	C3-C4-C5	-2.18	109.02	112.67
2	F	600	AKG	C4-C3-C2	-2.11	108.59	113.14
2	C	600	AKG	C3-C4-C5	-2.10	109.14	112.67
2	B	600	AKG	C4-C3-C2	-2.07	108.69	113.14

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	NMM	NH2-CZ-NE-CD
4	A	403	NMM	NH1-CZ-NE-CD
4	H	403	NMM	NH1-CZ-NE-CD
4	H	403	NMM	C-CA-CB-CG
4	E	403	NMM	NE-CZ-NH2-CAA
4	E	403	NMM	NH1-CZ-NE-CD
4	G	403	NMM	NE-CZ-NH2-CAA
4	G	403	NMM	NH1-CZ-NE-CD
4	G	403	NMM	C-CA-CB-CG
4	G	403	NMM	N-CA-CB-CG
4	G	403	NMM	NE-CD-CG-CB
4	E	403	NMM	NE-CD-CG-CB
4	H	403	NMM	NE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	D	600	AKG	C2-C3-C4-C5
2	D	600	AKG	C1-C2-C3-C4
4	H	403	NMM	CA-CB-CG-CD
4	E	403	NMM	CA-CB-CG-CD
2	H	401	AKG	C1-C2-C3-C4
2	H	401	AKG	O5-C2-C3-C4
2	G	401	AKG	O5-C2-C3-C4
2	D	600	AKG	O5-C2-C3-C4
2	G	401	AKG	C1-C2-C3-C4
2	F	600	AKG	C1-C2-C3-C4
4	H	403	NMM	NE-CZ-NH2-CAA
2	F	600	AKG	O5-C2-C3-C4
2	G	401	AKG	C2-C3-C4-C5
2	A	401	AKG	C1-C2-C3-C4
2	A	401	AKG	O5-C2-C3-C4
2	B	600	AKG	C1-C2-C3-C4

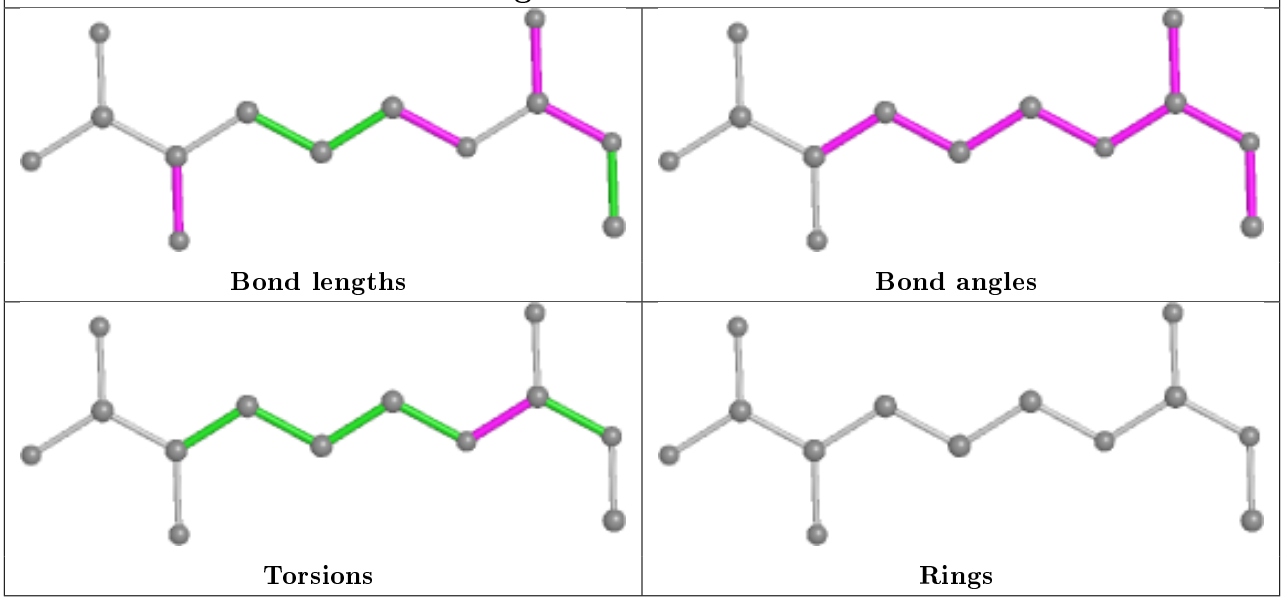
There are no ring outliers.

3 monomers are involved in 5 short contacts:

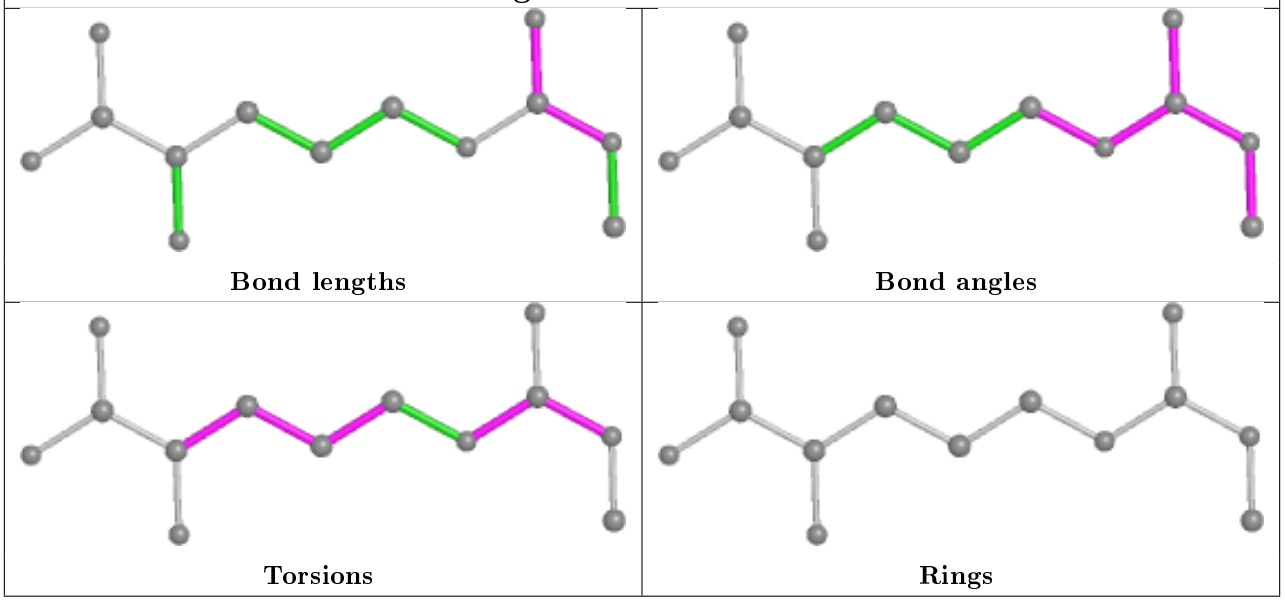
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	NMM	2	0
4	H	403	NMM	2	0
4	G	403	NMM	1	0

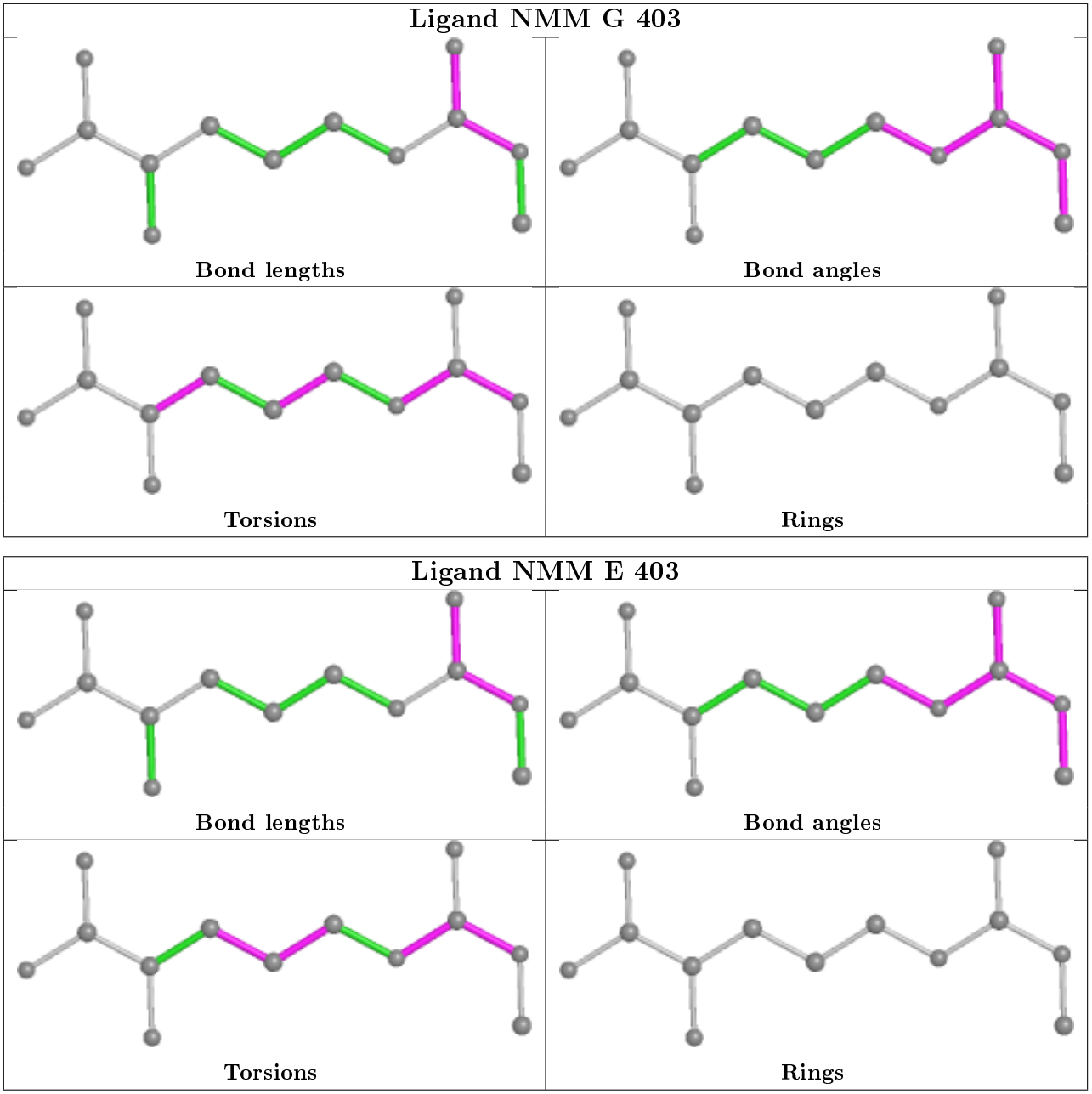
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand NMM A 403



Ligand NMM H 403





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	341/341 (100%)	-0.07	1 (0%)	94	93	20, 33, 55, 82	2 (0%)
1	B	333/341 (97%)	0.21	18 (5%)	25	20	31, 50, 77, 105	1 (0%)
1	C	335/341 (98%)	0.03	9 (2%)	54	48	22, 40, 64, 81	2 (0%)
1	D	341/341 (100%)	0.23	13 (3%)	40	33	32, 50, 72, 102	1 (0%)
1	E	341/341 (100%)	-0.08	5 (1%)	73	70	22, 36, 64, 89	2 (0%)
1	F	334/341 (97%)	0.14	8 (2%)	59	53	30, 48, 73, 92	2 (0%)
1	G	335/341 (98%)	-0.18	3 (0%)	84	82	20, 32, 52, 78	3 (0%)
1	H	340/341 (99%)	0.06	10 (2%)	51	45	24, 44, 70, 95	2 (0%)
All	All	2700/2728 (98%)	0.04	67 (2%)	57	51	20, 42, 69, 105	15 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	HIS	7.0
1	D	96	ASN	5.9
1	D	1	MET	5.8
1	F	332	LEU	5.7
1	H	41	ALA	5.5
1	E	2	ASN	5.0
1	B	5	SER	4.7
1	H	2	ASN	4.3
1	B	78	GLY	4.1
1	H	3	HIS	4.1
1	D	141	PRO	4.0
1	H	43	ALA	4.0
1	C	332	LEU	3.9
1	D	3	HIS	3.7
1	B	112	MET	3.5
1	D	92	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	1	MET	3.5
1	G	3	HIS	3.3
1	H	4	LYS	3.3
1	B	113	LYS	3.2
1	G	335	SER	3.2
1	F	140	HIS	3.2
1	A	1	MET	3.2
1	B	118	ILE	3.1
1	D	97	GLN	3.1
1	C	141	PRO	3.1
1	C	108	TYR	3.0
1	B	33	GLU	3.0
1	D	112	MET	3.0
1	E	42	VAL	3.0
1	B	92	ARG	3.0
1	C	1	MET	2.9
1	H	30	ASN	2.9
1	C	5	SER	2.9
1	F	105	ASN	2.9
1	G	332	LEU	2.8
1	B	89	ARG	2.8
1	F	83	GLU	2.8
1	C	83	GLU	2.8
1	B	86	THR	2.7
1	F	78	GLY	2.6
1	E	1	MET	2.6
1	B	4	LYS	2.6
1	D	95	ARG	2.6
1	H	42	VAL	2.6
1	C	92	ARG	2.5
1	B	331	ASP	2.5
1	H	8	ARG	2.5
1	D	94	TYR	2.5
1	B	88	GLU	2.4
1	D	222	ARG	2.4
1	B	332	LEU	2.3
1	C	89	ARG	2.3
1	B	116	TYR	2.3
1	E	140	HIS	2.3
1	B	145	LYS	2.3
1	F	108	TYR	2.2
1	D	140	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	99	PHE	2.2
1	C	88	GLU	2.2
1	B	85	TRP	2.1
1	H	187	HIS	2.1
1	H	119	GLU	2.1
1	D	144	ARG	2.1
1	E	141	PRO	2.1
1	F	334	GLU	2.0
1	F	82	GLN	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	FE	D	601	1/1	-	-	40,40,40,40	1
2	AKG	D	600	10/10	-	-	40,42,42,42	10
2	AKG	B	600	10/10	-	-	34,34,36,37	10
3	FE	G	402	1/1	-	-	30,30,30,30	1
2	AKG	F	600	10/10	-	-	31,32,33,33	10
2	AKG	G	401	10/10	-	-	24,28,29,30	10
4	NMM	G	403	13/13	0.70	0.34	30,43,52,55	0
3	FE	A	402	1/1	-	-	35,35,35,35	1
3	FE	F	601	1/1	-	-	31,31,31,31	1
3	FE	B	601	1/1	-	-	33,33,33,33	1
4	NMM	E	403	13/13	0.64	0.44	35,49,56,57	0
2	AKG	H	401	10/10	-	-	35,37,38,39	10
3	FE	H	402	1/1	-	-	36,36,36,36	1
2	AKG	E	401	10/10	-	-	25,30,31,31	10

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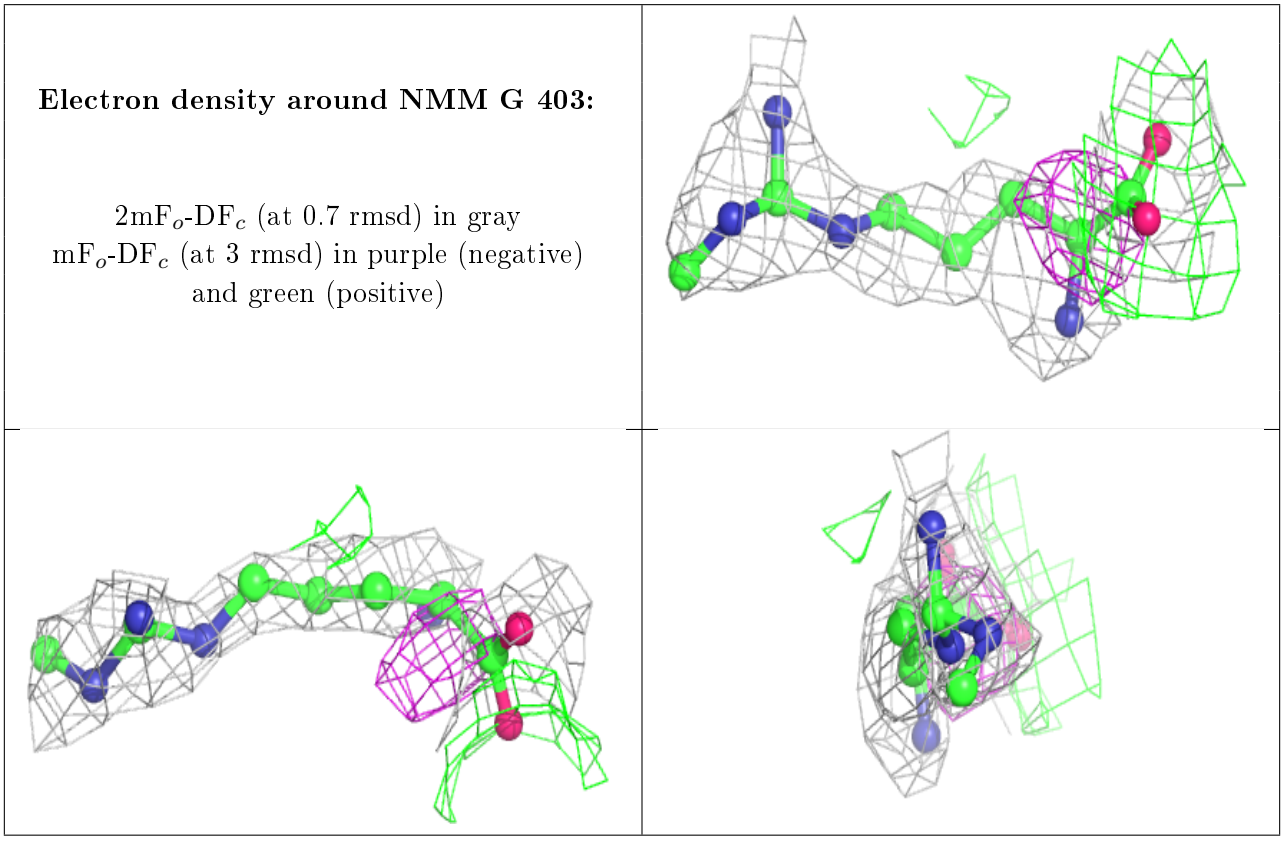
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AKG	C	600	10/10	-	-	29,30,33,33	10
3	FE	C	601	1/1	-	-	28,28,28,28	1
3	FE	E	402	1/1	-	-	32,32,32,32	1
4	NMM	A	403	13/13	0.57	0.40	36,42,48,53	0
4	NMM	H	403	13/13	0.61	0.33	45,47,60,61	0
2	AKG	A	401	10/10	-	-	26,31,34,36	10

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

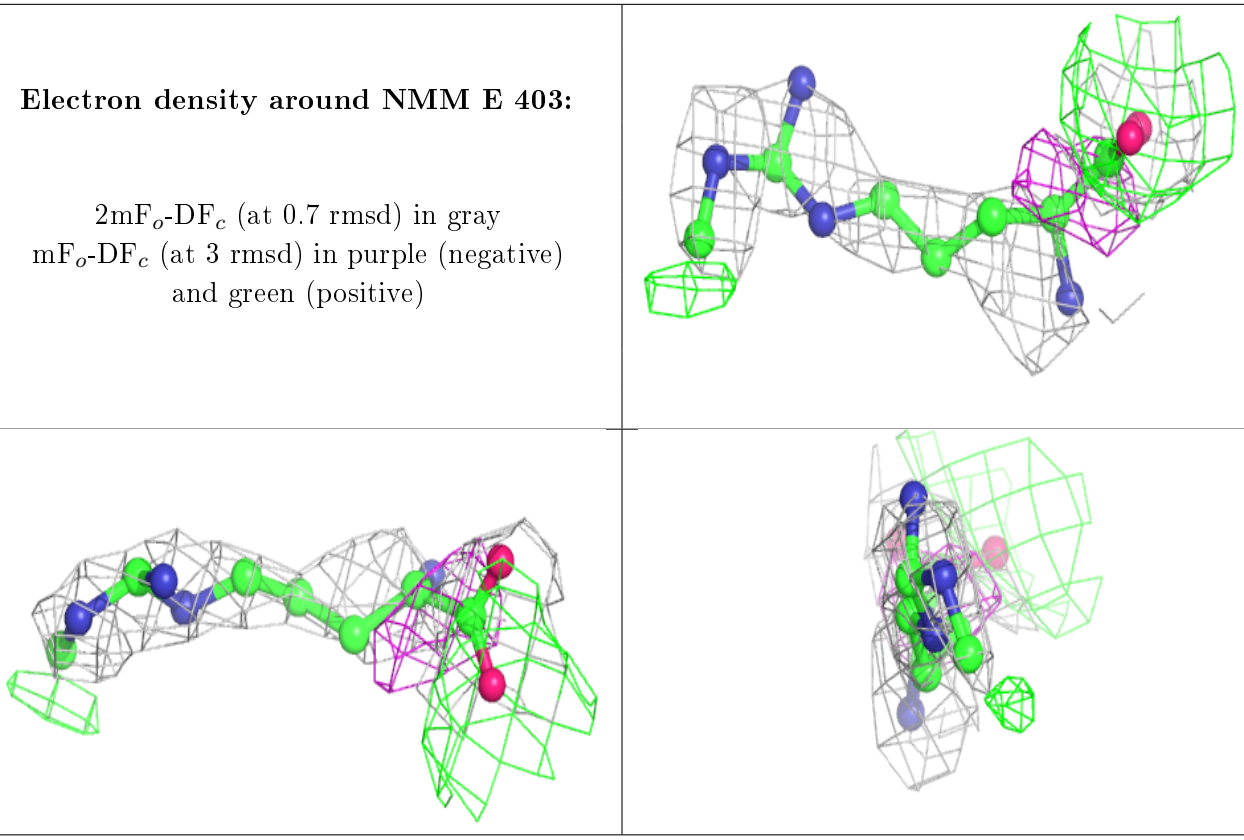
Electron density around NMM G 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



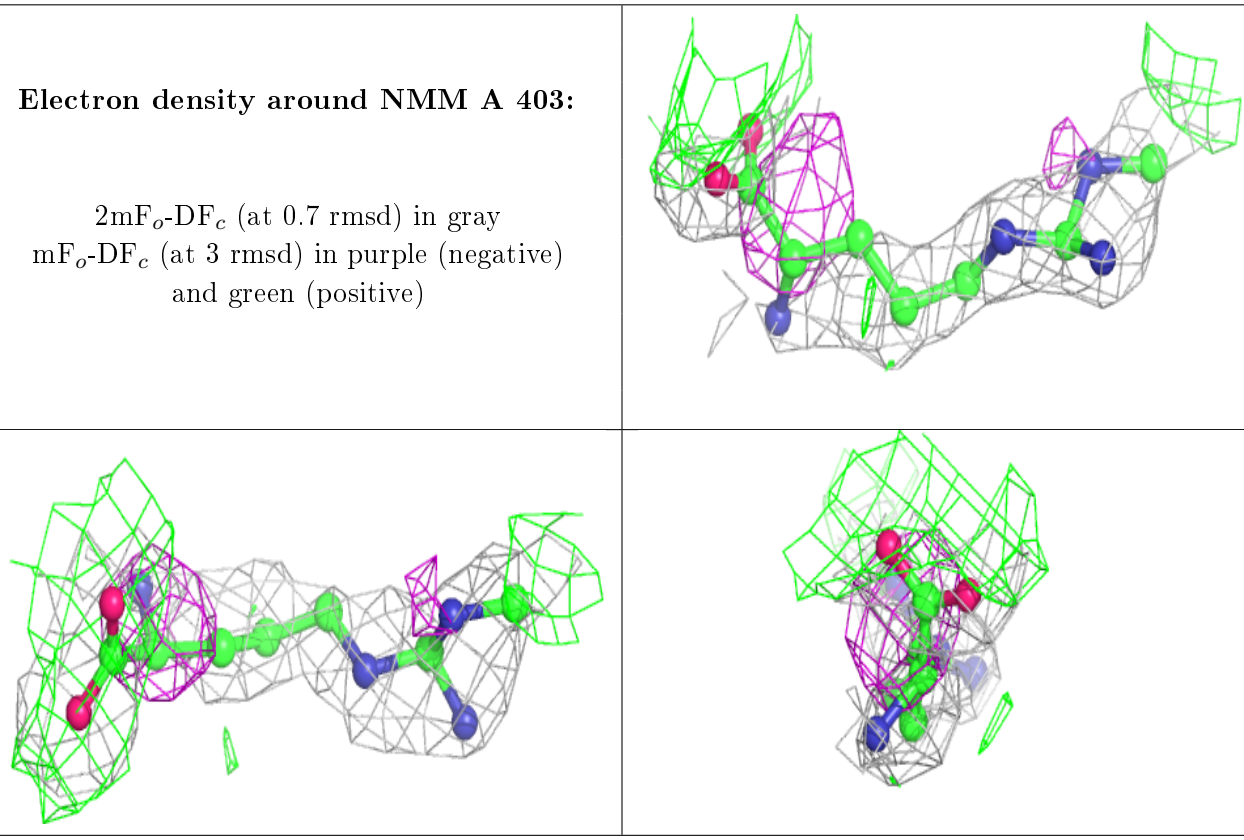
Electron density around NMM E 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



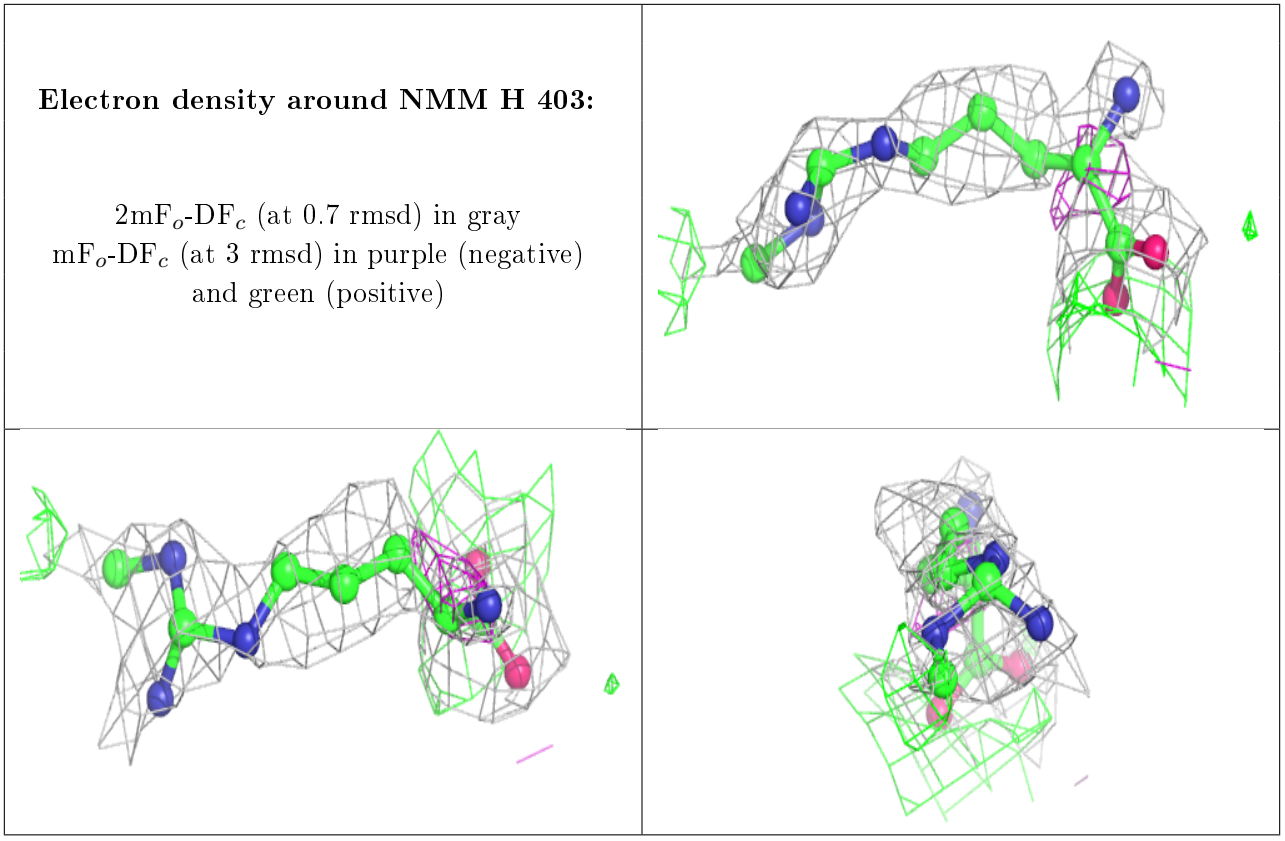
Electron density around NMM A 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around NMM H 403:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.