Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:13 pm BST

PDB ID	:	5X6E
Title	:	Crystal structure of PrfA-DNA binary complex
Authors	:	Wang, Y.; Feng, H.; Zhu, Y.L.; Gao, P.
Deposited on	:	2017-02-21
Resolution	:	2.99 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:

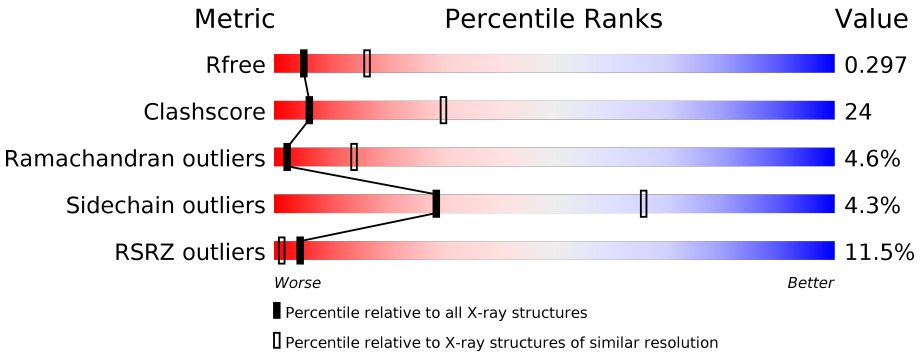
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	237	13% 54% 38% 5%
1	B	237	18% 53% 38% 7%
1	E	237	13% 59% 34% 5%
1	F	237	14% 55% 36% 5%
1	M	237	8% 59% 34%
1	N	237	12% 61% 30% 8%

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Mol	Chain	Length	Quality of chain
2	C	29	62% 38%
2	G	29	79% 17%
2	O	29	62% 38%
3	D	29	62% 38%
3	H	29	52% 48%
3	P	29	62% 34%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15154 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 Listeriolysin positive regulatory factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	236	Total	C	N	O	S	0	0	0
			1920	1253	301	359	7			
1	N	236	Total	C	N	O	S	0	0	0
			1920	1253	301	359	7			
1	A	236	Total	C	N	O	S	0	0	0
			1920	1253	301	359	7			
1	B	236	Total	C	N	O	S	0	0	0
			1920	1253	301	359	7			
1	E	236	Total	C	N	O	S	0	0	0
			1920	1253	301	359	7			
1	F	236	Total	C	N	O	S	0	0	0
			1920	1253	301	359	7			

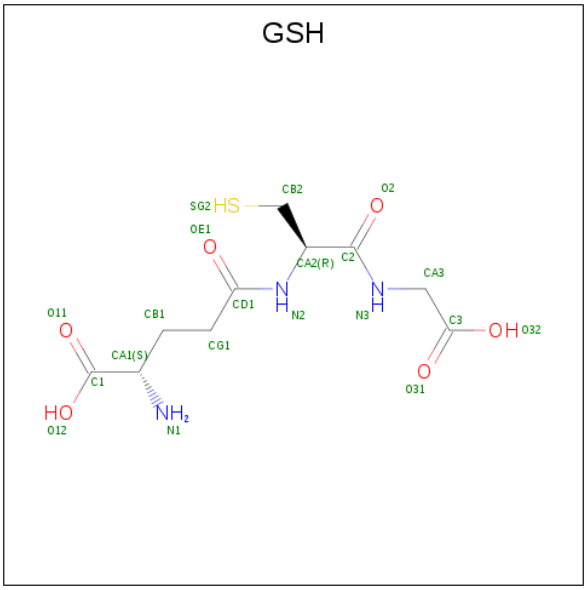
- Molecule 2 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	29	Total	C	N	O	P	0	0	0
			587	283	104	172	28			
2	C	29	Total	C	N	O	P	0	0	0
			587	283	104	172	28			
2	G	28	Total	C	N	O	P	0	0	0
			571	274	101	168	28			

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	28	Total	C	N	O	P	0	0	0
			577	276	105	168	28			
3	D	29	Total	C	N	O	P	0	0	0
			596	286	110	172	28			
3	H	29	Total	C	N	O	P	0	0	0
			596	286	110	172	28			

- Molecule 4 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



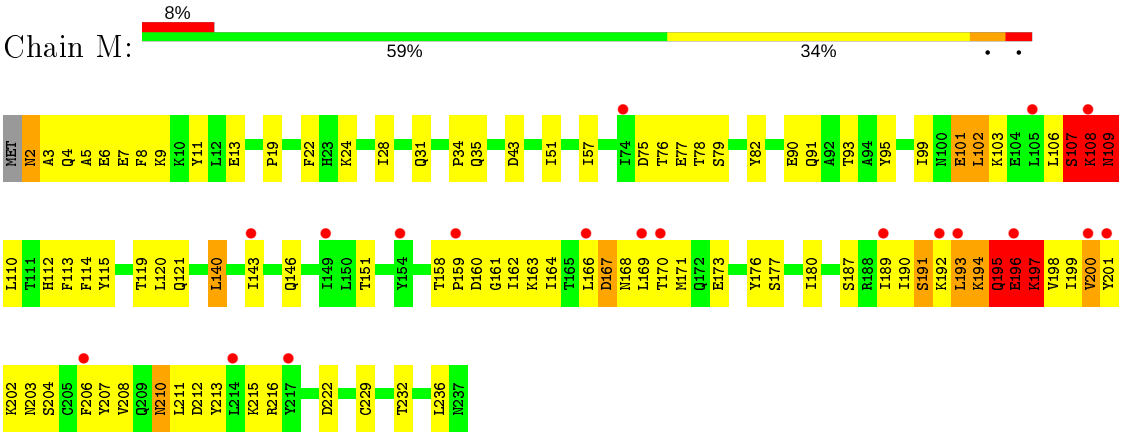
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	M	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	N	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	E	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
4	F	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

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.

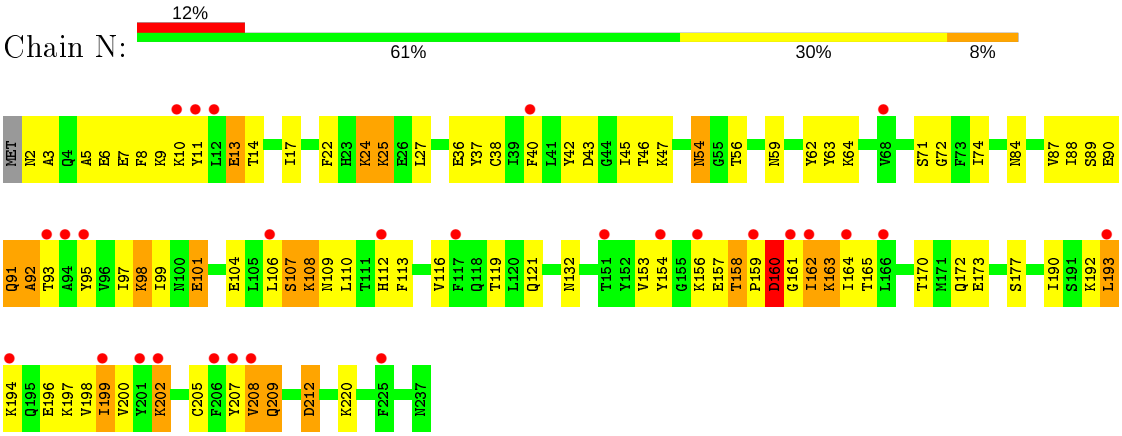
- Molecule 1: Listeriolysin positive regulatory factor A

Chain M:



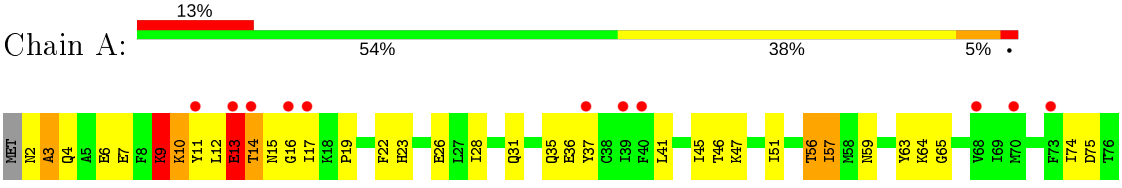
- Molecule 1: Listeriolysin positive regulatory factor A

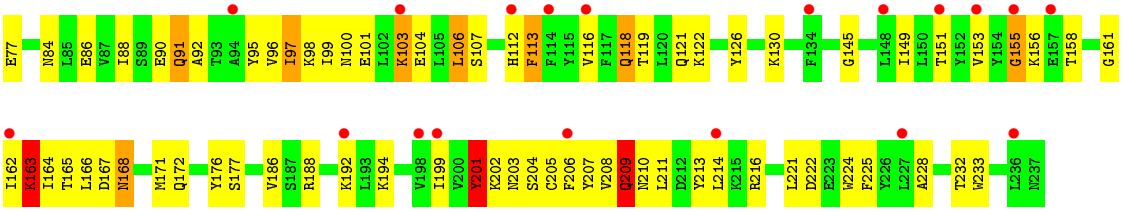
Chain N:



- Molecule 1: Listeriolysin positive regulatory factor A

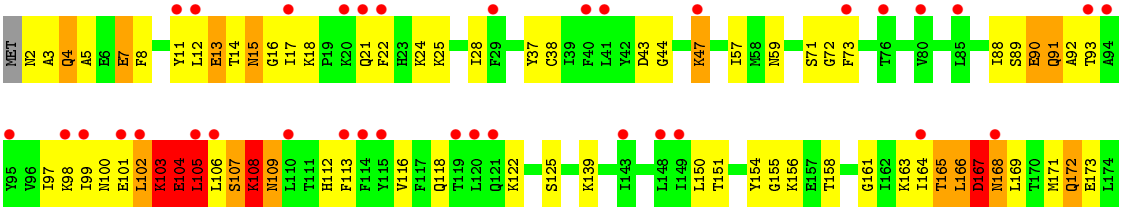
Chain A:

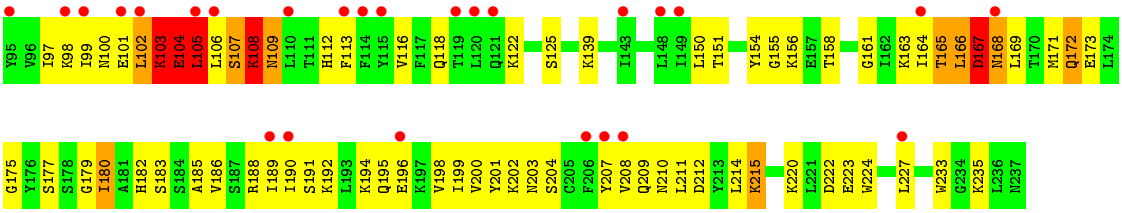




• Molecule 1: Listeriolysin positive regulatory factor A

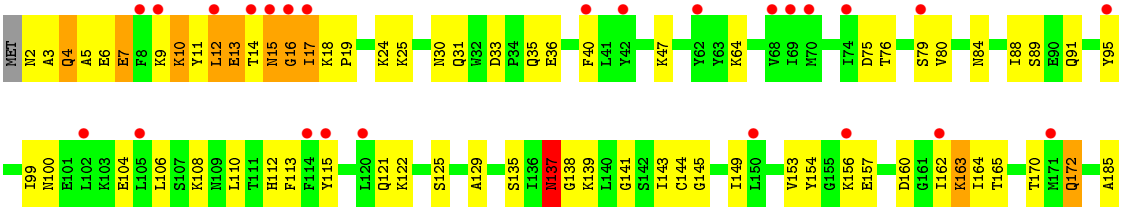
Chain B:

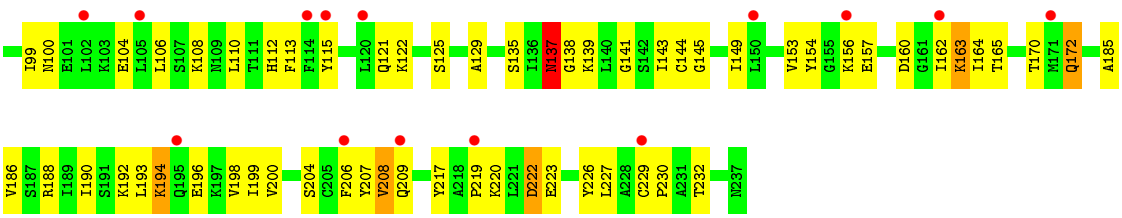




• Molecule 1: Listeriolysin positive regulatory factor A

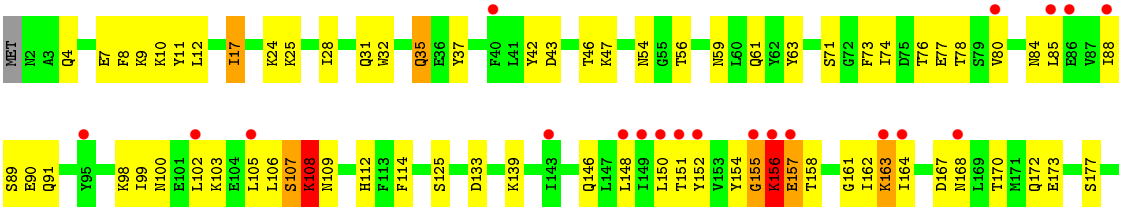
Chain E:

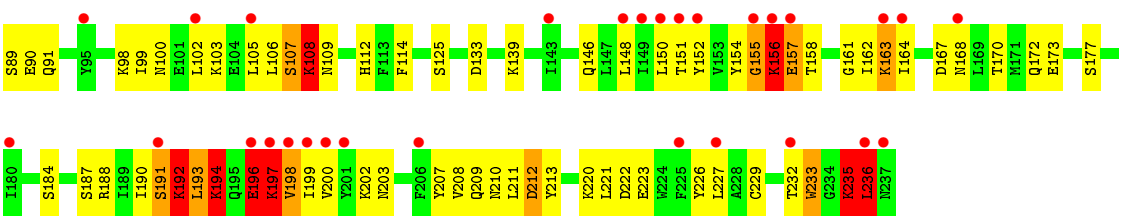




• Molecule 1: Listeriolysin positive regulatory factor A

Chain F:





- Molecule 2: DNA (29-MER)

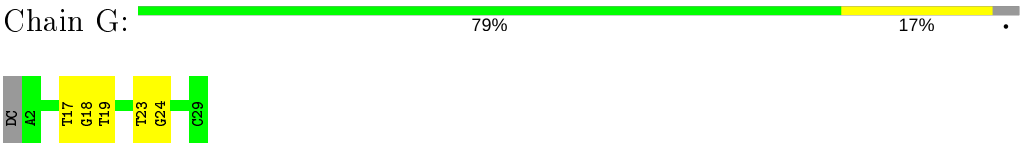
Chain O:

- Molecule 2: DNA (29-MER)

Chain C:

- Molecule 2: DNA (29-MER)

Chain G:



- Molecule 3: DNA (28-MER)

Chain P:

- Molecule 3: DNA (28-MER)

Chain D:

- Molecule 3: DNA (28-MER)

Chain H:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.02Å 96.59Å 370.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.47 – 2.99 96.59 – 2.99	Depositor EDS
% Data completeness (in resolution range)	96.0 (93.47-2.99) 96.6 (96.59-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.49 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.249 , 0.300 0.250 , 0.297	Depositor DCC
R_{free} test set	2358 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	92.7	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 78.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15154	wwPDB-VP
Average B, all atoms (Å^2)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: GSH

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	0.35	0/1964	0.65	4/2652 (0.2%)
1	B	0.35	0/1964	0.69	4/2652 (0.2%)
1	E	0.34	0/1964	0.62	0/2652
1	F	0.43	0/1964	0.79	8/2652 (0.3%)
1	M	0.39	0/1964	0.69	4/2652 (0.2%)
1	N	0.36	0/1964	0.63	0/2652
2	C	0.71	0/657	0.98	0/1011
2	G	0.65	0/639	0.97	0/983
2	O	0.69	0/657	1.00	0/1011
3	D	0.72	0/669	0.96	0/1032
3	H	0.69	0/669	0.98	0/1032
3	P	0.71	0/647	0.97	0/997
All	All	0.47	0/15722	0.77	20/21978 (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	A	0	6
1	B	0	8
1	E	0	4
1	F	0	10
1	M	0	7
1	N	0	4
All	All	0	39

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	195	GLN	N-CA-C	10.36	138.96	111.00
1	F	194	LYS	CB-CG-CD	-7.97	90.87	111.60
1	F	155	GLY	N-CA-C	7.76	132.49	113.10
1	F	194	LYS	N-CA-C	7.69	131.76	111.00
1	B	166	LEU	CB-CG-CD1	-6.84	99.37	111.00
1	M	195	GLN	CB-CA-C	-6.72	96.96	110.40
1	B	105	LEU	CA-CB-CG	6.67	130.63	115.30
1	A	163	LYS	N-CA-C	6.43	128.37	111.00
1	M	195	GLN	CA-C-N	-6.40	103.12	117.20
1	F	196	GLU	CB-CA-C	-6.32	97.75	110.40
1	F	196	GLU	CA-CB-CG	5.97	126.53	113.40
1	B	104	GLU	N-CA-C	5.88	126.89	111.00
1	A	201	TYR	CA-CB-CG	5.82	124.47	113.40
1	F	156	LYS	N-CA-C	5.68	126.35	111.00
1	F	108	LYS	N-CA-C	5.44	125.70	111.00
1	A	163	LYS	CB-CA-C	-5.31	99.79	110.40
1	B	104	GLU	CB-CA-C	-5.25	99.89	110.40
1	A	155	GLY	N-CA-C	5.06	125.75	113.10
1	M	140	LEU	CA-CB-CG	5.06	126.93	115.30
1	F	198	VAL	N-CA-C	5.02	124.54	111.00

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LYS	Peptide
1	A	101	GLU	Peptide
1	A	163	LYS	Peptide
1	A	201	TYR	Peptide
1	A	9	LYS	Peptide
1	A	90	GLU	Peptide
1	B	102	LEU	Peptide
1	B	103	LYS	Peptide
1	B	107	SER	Peptide
1	B	108	LYS	Peptide
1	B	13	GLU	Peptide
1	B	168	ASN	Peptide
1	B	195	GLN	Peptide
1	B	90	GLU	Peptide
1	E	10	LYS	Peptide
1	E	13	GLU	Peptide
1	E	194	LYS	Peptide
1	E	196	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	F	107	SER	Peptide
1	F	108	LYS	Peptide
1	F	154	TYR	Peptide
1	F	155	GLY	Peptide
1	F	156	LYS	Peptide
1	F	191	SER	Peptide
1	F	192	LYS	Peptide
1	F	194	LYS	Peptide
1	F	235	LYS	Peptide
1	F	236	LEU	Peptide
1	M	107	SER	Peptide
1	M	108	LYS	Peptide
1	M	191	SER	Peptide
1	M	193	LEU	Peptide
1	M	194	LYS	Peptide
1	M	195	GLN	Peptide
1	M	197	LYS	Peptide
1	N	107	SER	Peptide
1	N	13	GLU	Peptide
1	N	160	ASP	Peptide
1	N	209	GLN	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	1920	0	1920	103	0
1	B	1920	0	1920	119	0
1	E	1920	0	1920	95	0
1	F	1920	0	1920	135	0
1	M	1920	0	1920	88	0
1	N	1920	0	1920	105	0
2	C	587	0	330	8	0
2	G	571	0	318	6	0
2	O	587	0	330	10	0
3	D	596	0	330	7	0
3	H	596	0	330	11	0
3	P	577	0	318	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	15	2	0
4	B	20	0	15	0	0
4	E	20	0	15	1	0
4	F	20	0	15	1	0
4	M	20	0	15	0	0
4	N	20	0	15	1	0
All	All	15154	0	13566	671	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (671) 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:B:108:LYS:HG2	1:B:109:ASN:HB3	1.43	1.00
1:M:194:LYS:HG3	1:M:195:GLN:HB2	1.41	0.98
1:F:151:THR:HA	1:F:156:LYS:HE2	1.47	0.95
1:F:162:ILE:HG12	1:F:208:VAL:HB	1.57	0.87
1:F:198:VAL:O	1:F:209:GLN:N	2.06	0.87
1:B:91:GLN:HG3	1:B:92:ALA:H	1.39	0.86
1:N:162:ILE:HG12	1:N:208:VAL:HB	1.57	0.86
1:F:156:LYS:HD3	1:F:162:ILE:HD13	1.58	0.85
1:A:9:LYS:HE2	1:A:10:LYS:H	1.40	0.85
1:N:196:GLU:HB2	1:N:198:VAL:HG23	1.58	0.85
1:M:194:LYS:HA	1:M:195:GLN:HG2	1.59	0.84
1:A:75:ASP:HA	1:A:103:LYS:HE3	1.59	0.84
1:B:21:GLN:NE2	1:B:22:PHE:O	2.11	0.83
1:F:233:TRP:HB2	1:F:235:LYS:HD3	1.59	0.83
1:F:43:ASP:OD1	1:F:91:GLN:NE2	2.11	0.83
1:E:17:ILE:HG22	1:E:18:LYS:H	1.45	0.82
1:M:108:LYS:HG3	1:M:109:ASN:N	1.94	0.81
1:N:7:GLU:HG2	1:N:112:HIS:HE2	1.43	0.81
1:N:54:ASN:HD22	1:N:56:THR:H	1.26	0.81
1:M:192:LYS:NZ	1:M:196:GLU:OE2	2.14	0.80
1:N:194:LYS:HE2	1:N:199:ILE:HG23	1.64	0.80
1:E:162:ILE:HB	1:E:208:VAL:HG22	1.62	0.80
1:B:47:LYS:NZ	1:B:173:GLU:OE2	2.14	0.79
1:M:108:LYS:HZ1	1:M:112:HIS:HB2	1.48	0.79
1:F:196:GLU:O	1:F:198:VAL:N	2.16	0.79
1:M:166:LEU:HD23	1:M:169:LEU:HD13	1.65	0.78
1:A:10:LYS:HB2	1:A:13:GLU:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:LYS:HB2	1:E:13:GLU:H	1.49	0.78
1:A:12:LEU:O	1:A:14:THR:N	2.17	0.77
1:F:200:VAL:HG13	1:F:209:GLN:HE22	1.48	0.77
1:N:163:LYS:HG3	1:N:164:ILE:N	2.00	0.77
1:E:10:LYS:HD3	1:E:13:GLU:HB2	1.65	0.77
1:E:188:ARG:NH1	2:G:18:DG:N7	2.32	0.77
1:B:212:ASP:HA	1:B:215:LYS:HG3	1.68	0.76
1:B:202:LYS:O	1:B:204:SER:N	2.19	0.76
1:F:73:PHE:HB2	1:F:76:THR:HG22	1.66	0.76
1:F:190:ILE:HA	1:F:193:LEU:H	1.50	0.76
1:N:163:LYS:NZ	1:N:164:ILE:O	2.19	0.75
1:A:10:LYS:HG3	1:A:13:GLU:HG2	1.68	0.75
1:A:7:GLU:O	1:A:112:HIS:NE2	2.18	0.75
1:E:199:ILE:HA	1:E:208:VAL:HA	1.68	0.75
1:M:162:ILE:HB	1:M:208:VAL:HB	1.69	0.74
1:F:157:GLU:H	1:F:163:LYS:H	1.35	0.74
1:F:105:LEU:HD12	1:F:108:LYS:HZ3	1.52	0.73
1:A:59:ASN:HB2	1:A:177:SER:HA	1.70	0.72
1:E:5:ALA:O	1:E:9:LYS:N	2.21	0.72
1:F:151:THR:HG23	1:F:156:LYS:HD2	1.71	0.72
1:F:200:VAL:HG23	1:F:207:TYR:HB2	1.71	0.72
1:A:6:GLU:C	1:A:9:LYS:HG2	2.09	0.72
1:B:101:GLU:O	1:B:102:LEU:HD23	1.88	0.72
1:F:194:LYS:HB3	1:F:196:GLU:HB2	1.71	0.72
1:F:194:LYS:HZ2	1:F:199:ILE:H	1.38	0.72
1:B:98:LYS:HD2	1:B:99:ILE:H	1.54	0.71
1:N:208:VAL:HG12	1:N:209:GLN:H	1.54	0.71
1:F:47:LYS:HB3	1:F:88:ILE:HD11	1.72	0.71
1:M:199:ILE:HD12	1:M:208:VAL:HA	1.72	0.71
1:F:188:ARG:NH2	3:H:18:DG:N7	2.39	0.71
1:N:64:LYS:NZ	1:N:153:VAL:O	2.23	0.71
1:A:104:GLU:HA	1:A:107:SER:HB3	1.72	0.70
1:B:158:THR:HG21	1:B:163:LYS:HE2	1.73	0.70
1:N:11:TYR:CE1	1:N:108:LYS:HE3	2.26	0.70
1:B:167:ASP:OD1	1:B:167:ASP:N	2.25	0.70
1:B:97:ILE:HG21	1:B:102:LEU:HD21	1.73	0.70
1:E:160:ASP:O	1:E:209:GLN:NE2	2.24	0.70
1:F:76:THR:HG23	1:F:78:THR:H	1.55	0.70
1:A:47:LYS:HB2	1:A:88:ILE:HD11	1.75	0.69
1:M:194:LYS:HA	1:M:195:GLN:CG	2.21	0.69
1:B:108:LYS:HG2	1:B:109:ASN:CB	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:LYS:HB2	1:E:207:TYR:CD1	2.29	0.68
1:N:199:ILE:HG22	1:N:208:VAL:HG22	1.76	0.68
1:B:196:GLU:OE1	1:B:196:GLU:N	2.26	0.68
1:F:151:THR:HA	1:F:156:LYS:CE	2.24	0.68
1:N:90:GLU:HG2	1:N:91:GLN:HG2	1.75	0.68
1:A:202:LYS:HG3	1:A:203:ASN:HB2	1.75	0.68
1:E:186:VAL:HG12	1:E:190:ILE:HD11	1.76	0.68
1:F:24:LYS:HG2	1:F:25:LYS:HG3	1.75	0.68
1:F:151:THR:O	1:F:156:LYS:HG3	1.94	0.67
1:F:199:ILE:HD13	1:F:208:VAL:HG22	1.76	0.67
1:E:200:VAL:N	1:E:207:TYR:O	2.27	0.67
1:B:98:LYS:HD2	1:B:99:ILE:N	2.09	0.67
1:F:233:TRP:HA	1:F:235:LYS:HG2	1.77	0.67
1:A:164:ILE:CG1	1:A:206:PHE:HB2	2.25	0.67
1:A:163:LYS:HB3	1:A:164:ILE:HA	1.76	0.67
1:E:229:CYS:SG	1:E:232:THR:OG1	2.53	0.67
1:E:194:LYS:CD	1:E:199:ILE:HD12	2.25	0.66
1:N:13:GLU:HA	1:N:17:ILE:H	1.59	0.66
1:A:130:LYS:HA	1:A:221:LEU:HD11	1.76	0.66
1:F:35:GLN:NE2	1:F:37:TYR:OH	2.29	0.66
1:N:2:ASN:O	1:N:5:ALA:N	2.25	0.66
1:B:166:LEU:HD11	1:B:168:ASN:ND2	2.10	0.65
1:B:13:GLU:OE1	1:B:16:GLY:N	2.28	0.65
1:F:37:TYR:H	1:F:71:SER:HG	1.43	0.65
1:N:27:LEU:HD23	1:N:84:ASN:HB3	1.76	0.65
1:B:44:GLY:HA3	1:B:92:ALA:HB2	1.79	0.65
1:N:197:LYS:O	1:N:209:GLN:HG3	1.97	0.65
1:F:194:LYS:NZ	1:F:199:ILE:H	1.95	0.65
1:B:220:LYS:NZ	1:B:223:GLU:OE2	2.30	0.65
1:B:163:LYS:HD3	1:B:207:TYR:CE1	2.33	0.64
1:N:98:LYS:HB3	1:N:101:GLU:CD	2.17	0.64
1:F:193:LEU:O	1:F:196:GLU:HG3	1.97	0.64
1:F:190:ILE:HD12	1:F:193:LEU:HD12	1.78	0.64
1:B:24:LYS:HG2	1:B:25:LYS:HG3	1.78	0.64
1:E:163:LYS:HB2	1:E:207:TYR:CE1	2.33	0.64
1:F:47:LYS:NZ	1:F:173:GLU:OE2	2.23	0.64
1:N:54:ASN:ND2	1:N:56:THR:H	1.94	0.64
1:B:191:SER:HA	1:B:194:LYS:HB2	1.80	0.63
1:E:157:GLU:HG2	1:E:162:ILE:HG13	1.81	0.63
1:A:15:ASN:OD1	1:A:16:GLY:N	2.32	0.63
1:F:156:LYS:HA	1:F:163:LYS:N	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ASN:OD1	1:B:16:GLY:N	2.32	0.63
1:N:106:LEU:HB3	1:N:113:PHE:HD2	1.63	0.63
1:F:167:ASP:OD1	1:F:168:ASN:N	2.31	0.63
1:E:4:GLN:HA	1:E:7:GLU:HG2	1.81	0.63
1:F:192:LYS:NZ	1:F:194:LYS:O	2.27	0.63
1:A:11:TYR:HB2	1:A:112:HIS:ND1	2.14	0.63
1:E:188:ARG:HH11	2:G:17:DT:H2"	1.63	0.63
1:F:194:LYS:HZ2	1:F:199:ILE:HG12	1.62	0.63
2:O:5:DG:O6	3:P:25:DA:N6	2.32	0.62
1:N:158:THR:H	1:N:160:ASP:CG	2.02	0.62
1:F:161:GLY:HA3	1:F:207:TYR:HB3	1.81	0.62
1:A:118:GLN:O	1:A:122:LYS:N	2.32	0.62
1:E:199:ILE:HG22	1:E:208:VAL:HG12	1.81	0.62
1:F:156:LYS:CD	1:F:162:ILE:HD13	2.29	0.62
1:A:7:GLU:OE1	1:A:112:HIS:NE2	2.32	0.62
1:N:158:THR:HB	1:N:160:ASP:HB3	1.80	0.62
1:E:13:GLU:OE1	1:E:16:GLY:N	2.24	0.62
1:F:102:LEU:HA	1:F:105:LEU:HB3	1.82	0.62
1:M:108:LYS:NZ	1:M:112:HIS:HB2	2.15	0.62
1:E:15:ASN:N	1:E:15:ASN:HD22	1.96	0.62
1:F:109:ASN:OD1	1:F:112:HIS:ND1	2.31	0.62
1:B:103:LYS:C	1:B:104:GLU:HG3	2.19	0.61
1:E:200:VAL:HG22	1:E:207:TYR:HB2	1.80	0.61
1:F:194:LYS:HZ2	1:F:198:VAL:HB	1.66	0.61
1:B:108:LYS:CG	1:B:109:ASN:HB3	2.26	0.61
1:N:47:LYS:HD3	1:N:88:ILE:HD11	1.83	0.61
1:A:164:ILE:HG13	1:A:206:PHE:HB2	1.83	0.61
1:E:222:ASP:N	1:E:222:ASP:OD2	2.30	0.61
3:P:3:DT:H2'	3:P:4:DA:C8	2.36	0.61
1:B:199:ILE:HG22	1:B:208:VAL:HA	1.83	0.60
1:F:194:LYS:NZ	1:F:198:VAL:HB	2.17	0.60
1:M:75:ASP:OD1	1:M:76:THR:N	2.34	0.60
1:F:98:LYS:HD2	1:F:99:ILE:N	2.16	0.60
1:N:199:ILE:HA	1:N:208:VAL:HA	1.83	0.60
1:A:126:TYR:OH	4:A:301:GSH:O31	2.17	0.60
1:B:172:GLN:HE21	1:B:183:SER:HB3	1.67	0.60
1:M:121:GLN:NE2	1:N:72:GLY:O	2.34	0.60
1:E:156:LYS:O	1:E:163:LYS:N	2.30	0.60
1:M:191:SER:HA	1:M:194:LYS:H	1.67	0.60
1:E:24:LYS:HG2	1:E:25:LYS:HG2	1.83	0.60
1:M:35:GLN:N	1:M:35:GLN:OE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLN:HG3	1:B:92:ALA:N	2.15	0.59
1:E:17:ILE:CG2	1:E:18:LYS:H	2.12	0.59
1:B:104:GLU:C	1:B:106:LEU:H	2.05	0.59
1:A:201:TYR:HB2	1:A:205:CYS:O	2.02	0.59
1:B:8:PHE:CD1	1:B:112:HIS:HB3	2.37	0.59
1:E:194:LYS:HD2	1:E:200:VAL:HA	1.83	0.59
1:N:154:TYR:HB3	1:N:165:THR:HG22	1.83	0.59
1:M:101:GLU:O	1:M:103:LYS:N	2.34	0.59
1:N:160:ASP:OD1	1:N:161:GLY:N	2.36	0.59
1:N:194:LYS:HE2	1:N:199:ILE:CG2	2.32	0.59
1:B:4:GLN:HA	1:B:7:GLU:HG2	1.85	0.59
1:B:8:PHE:CE1	1:B:12:LEU:HD11	2.38	0.59
1:B:113:PHE:O	1:B:116:VAL:N	2.32	0.59
1:N:194:LYS:HG3	1:N:199:ILE:H	1.67	0.59
1:A:9:LYS:HG3	1:A:10:LYS:N	2.19	0.58
1:E:194:LYS:HG3	1:E:199:ILE:HD12	1.85	0.58
1:F:194:LYS:HD2	1:F:199:ILE:N	2.18	0.58
1:N:47:LYS:NZ	1:N:173:GLU:OE2	2.27	0.58
1:A:10:LYS:HA	1:A:12:LEU:H	1.69	0.58
1:A:151:THR:HG23	1:A:162:ILE:HD13	1.84	0.58
1:A:167:ASP:O	1:A:168:ASN:HB3	2.02	0.58
1:E:17:ILE:HG22	1:E:18:LYS:N	2.17	0.58
1:N:45:ILE:H	1:N:89:SER:CB	2.17	0.58
1:N:45:ILE:H	1:N:89:SER:HB2	1.69	0.58
1:B:105:LEU:O	1:B:108:LYS:HD2	2.04	0.57
1:B:11:TYR:OH	1:B:108:LYS:HG3	2.04	0.57
1:E:122:LYS:NZ	4:E:301:GSH:O11	2.37	0.57
1:B:164:ILE:O	1:B:166:LEU:N	2.35	0.57
1:M:193:LEU:HA	1:M:195:GLN:OE1	2.04	0.57
1:N:36:GLU:O	1:N:99:ILE:HG12	2.04	0.57
1:B:47:LYS:HE3	1:B:88:ILE:HD11	1.85	0.57
1:M:7:GLU:HG2	1:M:112:HIS:NE2	2.19	0.57
1:N:10:LYS:HZ2	1:N:14:THR:HG23	1.69	0.57
1:B:188:ARG:HA	1:B:192:LYS:HZ3	1.69	0.57
1:B:22:PHE:CZ	1:B:28:ILE:HG23	2.39	0.57
1:B:21:GLN:HE22	1:B:91:GLN:HG2	1.70	0.57
1:B:11:TYR:CE1	1:B:12:LEU:HG	2.39	0.57
1:A:22:PHE:HB2	1:A:91:GLN:NE2	2.20	0.57
1:M:146:GLN:OE1	1:M:177:SER:OG	2.20	0.57
1:E:14:THR:C	1:E:15:ASN:HD22	2.07	0.56
1:N:200:VAL:HG12	1:N:202:LYS:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:LYS:HD2	1:F:194:LYS:N	2.19	0.56
1:A:199:ILE:HA	1:A:208:VAL:HG22	1.86	0.56
1:F:156:LYS:HB3	1:F:162:ILE:HB	1.87	0.56
1:M:57:ILE:HD11	1:M:176:TYR:CG	2.40	0.56
1:B:156:LYS:O	1:B:163:LYS:N	2.35	0.56
1:F:194:LYS:HE3	1:F:199:ILE:HB	1.87	0.56
1:A:9:LYS:CG	1:A:10:LYS:H	2.19	0.56
1:B:158:THR:OG1	1:B:161:GLY:O	2.15	0.56
1:N:156:LYS:N	1:N:163:LYS:O	2.39	0.56
1:B:91:GLN:CG	1:B:92:ALA:H	2.16	0.56
1:F:152:TYR:OH	1:F:222:ASP:OD1	2.22	0.56
1:M:212:ASP:HA	1:M:215:LYS:HB2	1.86	0.56
1:A:164:ILE:HD12	1:A:164:ILE:O	2.06	0.56
1:A:162:ILE:HG13	1:A:208:VAL:O	2.06	0.56
1:B:108:LYS:HG2	1:B:109:ASN:N	2.20	0.56
1:F:212:ASP:OD1	1:F:213:TYR:N	2.39	0.56
1:M:106:LEU:HB3	1:M:113:PHE:CD1	2.41	0.56
1:F:152:TYR:HE1	1:F:211:LEU:HD21	1.70	0.56
1:F:200:VAL:CG2	1:F:207:TYR:HB2	2.35	0.56
1:M:195:GLN:HG3	1:M:198:VAL:HG12	1.88	0.56
1:N:156:LYS:HD2	1:N:157:GLU:H	1.71	0.56
1:A:222:ASP:OD1	1:A:233:TRP:NE1	2.36	0.56
1:A:77:GLU:HG2	1:A:99:ILE:HG22	1.87	0.56
1:E:193:LEU:HD12	1:E:198:VAL:HG11	1.87	0.55
1:M:51:ILE:HG12	1:M:57:ILE:HG22	1.88	0.55
1:F:107:SER:N	1:F:108:LYS:HG2	2.21	0.55
1:N:104:GLU:HB2	1:N:107:SER:HB3	1.88	0.55
1:M:107:SER:HA	1:N:110:LEU:HD13	1.87	0.55
1:A:156:LYS:HB3	1:A:163:LYS:CG	2.36	0.55
1:A:122:LYS:NZ	4:A:301:GSH:O11	2.34	0.55
1:F:188:ARG:HA	1:F:191:SER:HB3	1.88	0.55
1:A:201:TYR:HB3	1:A:206:PHE:HA	1.89	0.55
1:B:21:GLN:HB2	1:B:93:THR:HG22	1.87	0.55
1:N:194:LYS:HG2	1:N:199:ILE:HG12	1.88	0.55
1:N:37:TYR:N	1:N:71:SER:OG	2.31	0.55
1:F:152:TYR:CE1	1:F:211:LEU:HD21	2.41	0.55
1:B:37:TYR:H	1:B:71:SER:HG	1.53	0.55
1:F:157:GLU:H	1:F:163:LYS:HD3	1.71	0.55
1:B:108:LYS:NZ	1:B:112:HIS:HB2	2.22	0.55
1:E:13:GLU:OE2	1:E:17:ILE:N	2.39	0.55
1:B:125:SER:HB2	1:B:224:TRP:HE1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:LYS:HE2	1:F:207:TYR:CE2	2.42	0.54
1:F:164:ILE:O	1:F:164:ILE:HG13	2.07	0.54
1:N:194:LYS:CG	1:N:199:ILE:H	2.21	0.54
1:A:46:THR:HG22	1:A:63:TYR:HB2	1.88	0.54
2:C:7:DC:H2'	2:C:8:DG:C8	2.41	0.54
1:E:223:GLU:O	1:E:227:LEU:N	2.34	0.54
1:M:24:LYS:HB2	1:M:90:GLU:HA	1.90	0.54
1:B:194:LYS:HA	1:B:199:ILE:O	2.06	0.54
1:N:36:GLU:O	1:N:98:LYS:HD2	2.07	0.54
1:E:35:GLN:NE2	1:E:36:GLU:O	2.41	0.54
1:M:199:ILE:HG13	1:M:200:VAL:H	1.71	0.54
1:A:121:GLN:NE2	1:B:72:GLY:O	2.40	0.54
1:E:141:GLY:HA2	1:E:144:CYS:HB2	1.89	0.54
1:M:110:LEU:O	1:M:114:PHE:HD1	1.91	0.54
1:N:198:VAL:O	1:N:208:VAL:HG13	2.07	0.54
1:E:10:LYS:HB2	1:E:13:GLU:N	2.21	0.54
3:H:4:DA:H2"	3:H:5:DG:C8	2.43	0.54
1:N:132:ASN:HD22	1:N:220:LYS:HB2	1.71	0.54
1:E:10:LYS:HZ2	1:E:18:LYS:HD2	1.73	0.54
1:F:194:LYS:HZ2	1:F:199:ILE:N	2.06	0.54
3:H:17:DT:H2"	3:H:18:DG:H8	1.72	0.54
1:F:31:GLN:N	1:F:84:ASN:OD1	2.38	0.53
1:E:194:LYS:CG	1:E:199:ILE:HD12	2.38	0.53
1:F:194:LYS:CE	1:F:199:ILE:H	2.22	0.53
2:G:23:DT:H2"	2:G:24:DG:C8	2.42	0.53
1:M:120:LEU:HD21	1:N:121:GLN:HG2	1.89	0.53
1:B:163:LYS:HD3	1:B:207:TYR:HE1	1.73	0.53
1:A:201:TYR:CB	1:A:206:PHE:HA	2.38	0.53
1:M:193:LEU:O	1:M:199:ILE:HG22	2.08	0.53
1:M:2:ASN:CG	1:M:3:ALA:HB3	2.29	0.53
1:B:192:LYS:N	1:B:192:LYS:HD2	2.22	0.53
1:F:76:THR:HG23	1:F:78:THR:N	2.23	0.53
1:B:101:GLU:O	1:B:104:GLU:HG2	2.09	0.53
1:B:180:ILE:HG22	1:B:182:HIS:H	1.73	0.53
1:M:90:GLU:CD	1:M:90:GLU:H	2.11	0.53
1:B:24:LYS:NZ	1:B:89:SER:O	2.41	0.53
1:A:211:LEU:HD12	1:A:214:LEU:HB2	1.91	0.53
1:M:110:LEU:HA	1:M:113:PHE:HB3	1.89	0.53
1:E:4:GLN:HG2	1:E:115:TYR:HD2	1.72	0.53
1:A:162:ILE:O	1:A:207:TYR:HA	2.09	0.52
1:B:102:LEU:HA	1:B:104:GLU:CD	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:LYS:HD2	1:E:199:ILE:C	2.30	0.52
1:B:106:LEU:HG	1:B:113:PHE:CD2	2.44	0.52
1:B:21:GLN:NE2	1:B:91:GLN:HG2	2.24	0.52
1:B:211:LEU:HA	1:B:214:LEU:HD23	1.90	0.52
3:H:5:DG:H2"	3:H:6:DG:C8	2.45	0.52
1:M:102:LEU:O	1:M:106:LEU:N	2.42	0.52
1:A:9:LYS:HE2	1:A:10:LYS:N	2.18	0.52
1:B:185:ALA:O	1:B:189:ILE:HG13	2.09	0.52
1:B:194:LYS:HE3	1:B:201:TYR:H	1.74	0.52
1:E:220:LYS:HD3	1:E:223:GLU:OE2	2.09	0.52
1:F:170:THR:OG1	1:F:173:GLU:N	2.41	0.52
1:B:194:LYS:HE3	1:B:201:TYR:N	2.24	0.52
1:N:11:TYR:CD1	1:N:108:LYS:HE3	2.44	0.52
1:N:9:LYS:HE2	1:N:95:TYR:OH	2.10	0.52
1:F:24:LYS:HB2	1:F:90:GLU:HA	1.92	0.52
1:M:189:ILE:HA	1:M:192:LYS:HB3	1.92	0.52
1:F:187:SER:O	1:F:191:SER:N	2.43	0.51
3:D:27:DG:H2"	3:D:28:DA:C8	2.46	0.51
1:F:157:GLU:HA	1:F:162:ILE:HA	1.92	0.51
1:F:223:GLU:HG2	1:F:226:TYR:HB2	1.92	0.51
1:B:200:VAL:HG23	1:B:207:TYR:HB2	1.92	0.51
1:E:75:ASP:OD1	1:E:76:THR:OG1	2.25	0.51
1:N:194:LYS:HD2	1:N:194:LYS:N	2.26	0.51
1:N:106:LEU:HB3	1:N:113:PHE:CD2	2.45	0.51
1:E:10:LYS:HA	1:E:12:LEU:HB2	1.93	0.51
1:N:193:LEU:HB3	1:N:194:LYS:CE	2.40	0.51
1:E:4:GLN:HG2	1:E:115:TYR:CD2	2.46	0.51
1:E:80:VAL:O	1:F:125:SER:OG	2.25	0.51
1:E:31:GLN:HB2	1:E:84:ASN:ND2	2.26	0.51
1:M:195:GLN:HB3	1:M:196:GLU:C	2.31	0.51
1:N:38:CYS:N	1:N:97:ILE:O	2.31	0.51
1:E:198:VAL:O	1:E:209:GLN:N	2.23	0.51
1:M:197:LYS:HB3	1:M:210:ASN:ND2	2.26	0.51
1:N:200:VAL:N	1:N:207:TYR:O	2.37	0.51
1:N:212:ASP:N	1:N:212:ASP:OD1	2.44	0.51
1:F:194:LYS:CD	1:F:199:ILE:H	2.23	0.51
1:B:15:ASN:HD21	1:B:17:ILE:HG23	1.76	0.51
1:N:43:ASP:OD1	1:N:93:THR:OG1	2.17	0.51
1:B:186:VAL:O	1:B:190:ILE:HG12	2.11	0.50
1:E:200:VAL:CG2	1:E:207:TYR:HB2	2.41	0.50
1:E:3:ALA:O	1:E:5:ALA:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:9:LYS:HE3	1:M:13:GLU:OE2	2.11	0.50
1:A:167:ASP:OD1	1:A:167:ASP:N	2.44	0.50
1:A:116:VAL:O	1:A:119:THR:OG1	2.23	0.50
1:M:108:LYS:CD	1:M:109:ASN:HB3	2.41	0.50
1:M:11:TYR:CZ	1:M:108:LYS:HD3	2.47	0.50
1:M:11:TYR:OH	1:M:108:LYS:HD3	2.12	0.50
1:B:8:PHE:HD1	1:B:112:HIS:HB3	1.75	0.50
1:E:10:LYS:HA	1:E:12:LEU:N	2.26	0.50
1:E:10:LYS:HZ1	1:E:95:TYR:HE1	1.60	0.50
1:F:8:PHE:HA	1:F:112:HIS:CD2	2.47	0.50
1:F:89:SER:OG	1:F:91:GLN:O	2.26	0.50
2:O:4:DC:H42	3:P:27:DG:H1	1.60	0.50
1:A:10:LYS:HG3	1:A:13:GLU:CG	2.41	0.50
1:A:36:GLU:O	1:A:99:ILE:HG12	2.12	0.50
1:B:14:THR:O	1:B:15:ASN:HB3	2.11	0.50
1:B:192:LYS:H	1:B:192:LYS:HD2	1.74	0.50
1:E:137:ASN:HD21	1:E:141:GLY:H	1.60	0.50
1:F:4:GLN:H	1:F:4:GLN:CD	2.15	0.50
1:N:8:PHE:HD1	1:N:112:HIS:HB3	1.77	0.50
1:B:11:TYR:CZ	1:B:108:LYS:HG3	2.47	0.50
1:B:180:ILE:HG21	1:B:185:ALA:HB3	1.94	0.50
1:B:227:LEU:O	1:F:10:LYS:NZ	2.45	0.50
1:B:90:GLU:O	1:B:91:GLN:HB2	2.10	0.50
1:E:135:SER:O	1:F:139:LYS:NZ	2.45	0.50
1:F:194:LYS:HD2	1:F:199:ILE:H	1.77	0.50
1:N:22:PHE:O	1:N:92:ALA:HB3	2.11	0.50
1:N:163:LYS:HD3	1:N:207:TYR:CE1	2.47	0.49
1:A:11:TYR:HB2	1:A:112:HIS:CE1	2.47	0.49
1:M:163:LYS:HB2	1:M:207:TYR:CE2	2.47	0.49
1:N:156:LYS:NZ	1:N:158:THR:OG1	2.46	0.49
1:F:11:TYR:OH	1:F:108:LYS:NZ	2.36	0.49
1:F:235:LYS:O	1:F:236:LEU:HG	2.12	0.49
1:A:13:GLU:HG2	1:A:14:THR:N	2.27	0.49
1:M:106:LEU:HD22	1:M:113:PHE:HA	1.93	0.49
1:M:108:LYS:HD2	1:M:109:ASN:HB3	1.94	0.49
1:N:162:ILE:HD12	1:N:163:LYS:N	2.27	0.49
1:N:162:ILE:HD12	1:N:163:LYS:CA	2.42	0.49
1:B:43:ASP:O	1:B:92:ALA:HB1	2.12	0.49
1:E:99:ILE:HD12	1:E:100:ASN:H	1.78	0.49
1:M:151:THR:HG21	1:M:211:LEU:HD13	1.95	0.49
1:N:194:LYS:HG3	1:N:199:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:HD11	1:A:176:TYR:CE2	2.47	0.49
1:F:194:LYS:NZ	1:F:199:ILE:HG12	2.28	0.49
1:N:208:VAL:HG12	1:N:209:GLN:N	2.27	0.49
1:B:104:GLU:O	1:B:106:LEU:N	2.44	0.49
1:F:200:VAL:HG13	1:F:209:GLN:NE2	2.23	0.49
1:N:162:ILE:CG1	1:N:208:VAL:HB	2.37	0.49
1:F:197:LYS:HD3	1:F:197:LYS:N	2.27	0.48
3:H:2:DG:H4'	3:H:3:DT:OP1	2.12	0.48
2:O:17:DT:H1'	2:O:18:DG:C8	2.48	0.48
3:P:17:DT:H2"	3:P:18:DG:O5'	2.13	0.48
1:A:9:LYS:CG	1:A:10:LYS:N	2.75	0.48
1:E:7:GLU:HB2	1:E:112:HIS:NE2	2.27	0.48
1:A:9:LYS:HG3	1:A:10:LYS:H	1.77	0.48
2:O:27:DT:H2"	2:O:28:DA:C8	2.48	0.48
3:P:27:DG:H2"	3:P:28:DA:C8	2.48	0.48
1:A:209:GLN:HG2	1:A:209:GLN:H	1.17	0.48
1:A:35:GLN:HG3	1:A:37:TYR:CZ	2.48	0.48
1:F:194:LYS:HD2	1:F:199:ILE:O	2.12	0.48
1:F:197:LYS:HB2	1:F:198:VAL:HG23	1.95	0.48
2:O:7:DC:H2"	2:O:8:DG:C8	2.49	0.48
1:A:77:GLU:OE1	1:A:100:ASN:HA	2.13	0.48
2:G:17:DT:H1'	2:G:18:DG:C8	2.49	0.48
1:A:45:ILE:HG13	1:A:64:LYS:HB2	1.94	0.48
1:B:15:ASN:CB	1:B:105:LEU:HD21	2.43	0.48
1:N:172:GLN:N	1:N:172:GLN:OE1	2.31	0.48
1:F:156:LYS:CE	1:F:162:ILE:HD13	2.44	0.48
1:M:198:VAL:HG13	1:M:199:ILE:H	1.77	0.48
1:A:106:LEU:O	1:A:113:PHE:HD1	1.95	0.48
1:A:22:PHE:CZ	1:A:28:ILE:HG23	2.49	0.48
1:F:73:PHE:HD2	1:F:76:THR:HG21	1.79	0.48
1:A:51:ILE:HA	1:A:56:THR:O	2.13	0.48
1:B:191:SER:CA	1:B:194:LYS:HB2	2.44	0.48
1:F:223:GLU:HG2	1:F:226:TYR:CB	2.43	0.48
1:B:194:LYS:HE3	1:B:201:TYR:HB3	1.96	0.47
1:F:54:ASN:HB2	1:F:56:THR:HG22	1.96	0.47
1:M:189:ILE:HG22	1:M:193:LEU:HD12	1.96	0.47
1:F:194:LYS:HD3	1:F:196:GLU:O	2.15	0.47
1:M:106:LEU:HB3	1:M:113:PHE:HD1	1.79	0.47
1:A:57:ILE:HD11	1:A:176:TYR:CD2	2.49	0.47
1:B:104:GLU:O	1:B:107:SER:N	2.46	0.47
1:F:233:TRP:CE3	1:F:235:LYS:HE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LYS:HA	1:A:12:LEU:N	2.29	0.47
1:A:162:ILE:O	1:A:162:ILE:HD12	2.14	0.47
1:A:153:VAL:HA	1:A:232:THR:HG21	1.97	0.47
1:A:2:ASN:O	1:A:4:GLN:N	2.41	0.47
1:F:105:LEU:C	1:F:108:LYS:HD3	2.35	0.47
1:F:193:LEU:HD22	1:F:196:GLU:OE1	2.15	0.47
1:A:163:LYS:HE2	1:A:164:ILE:HA	1.95	0.47
1:E:121:GLN:OE1	1:F:73:PHE:HA	2.15	0.47
3:H:17:DT:H4'	3:H:18:DG:OP1	2.14	0.47
1:M:195:GLN:HB3	1:M:197:LYS:N	2.29	0.47
1:N:162:ILE:HD11	1:N:208:VAL:HG23	1.96	0.47
1:B:7:GLU:CD	1:B:7:GLU:H	2.17	0.47
1:M:162:ILE:N	1:M:208:VAL:O	2.47	0.47
1:N:158:THR:HB	1:N:160:ASP:CB	2.43	0.47
3:P:17:DT:H4'	3:P:18:DG:OP1	2.15	0.47
3:P:3:DT:H2"	3:P:4:DA:H5'	1.97	0.47
1:E:217:TYR:O	1:E:219:PRO:HD3	2.14	0.47
1:M:196:GLU:O	1:M:197:LYS:HB2	2.14	0.47
1:A:228:ALA:HB2	1:B:73:PHE:CE2	2.49	0.47
1:B:2:ASN:CG	1:B:3:ALA:N	2.68	0.47
1:F:156:LYS:CB	1:F:162:ILE:HB	2.44	0.47
1:N:104:GLU:HB2	1:N:107:SER:CB	2.44	0.47
1:N:90:GLU:HG2	1:N:91:GLN:N	2.29	0.47
1:M:162:ILE:HD13	1:M:236:LEU:HD13	1.97	0.47
1:N:199:ILE:HG13	1:N:200:VAL:N	2.30	0.47
1:N:9:LYS:HE2	1:N:95:TYR:CZ	2.49	0.47
1:E:156:LYS:HE3	1:E:165:THR:HG21	1.96	0.47
1:E:31:GLN:HB2	1:E:84:ASN:HD21	1.79	0.47
1:F:188:ARG:HH21	3:H:17:DT:H2'	1.79	0.47
1:B:172:GLN:O	1:B:175:GLY:N	2.48	0.47
1:E:106:LEU:HB3	1:E:113:PHE:CD1	2.50	0.46
1:E:30:ASN:OD1	1:E:33:ASP:N	2.48	0.46
1:M:194:LYS:HD3	1:M:199:ILE:O	2.15	0.46
1:M:171:MET:HE3	1:M:187:SER:N	2.31	0.46
1:M:215:LYS:NZ	1:M:222:ASP:OD2	2.48	0.46
1:M:140:LEU:HD11	2:O:16:DA:H3'	1.97	0.46
1:A:156:LYS:O	1:A:163:LYS:HG3	2.16	0.46
1:F:200:VAL:O	1:F:207:TYR:N	2.42	0.46
2:G:17:DT:H4'	2:G:18:DG:OP1	2.15	0.46
1:N:116:VAL:O	1:N:119:THR:OG1	2.32	0.46
1:A:172:GLN:HG3	1:A:176:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:O	1:A:23:HIS:ND1	2.48	0.46
1:E:194:LYS:HD3	1:E:199:ILE:HD12	1.98	0.46
1:M:2:ASN:N	1:M:5:ALA:H	2.13	0.46
2:O:3:DT:H2"	2:O:4:DC:C5	2.51	0.46
1:B:167:ASP:O	1:B:169:LEU:N	2.44	0.46
1:B:198:VAL:HG23	1:B:210:ASN:O	2.16	0.46
1:A:45:ILE:HD11	1:A:64:LYS:HD2	1.97	0.46
1:N:170:THR:OG1	1:N:172:GLN:NE2	2.49	0.46
1:N:90:GLU:OE1	1:N:90:GLU:N	2.36	0.46
1:F:12:LEU:HD22	1:F:17:ILE:HG21	1.98	0.46
1:M:2:ASN:OD1	1:M:2:ASN:N	2.47	0.46
1:A:15:ASN:ND2	1:A:17:ILE:HB	2.31	0.45
1:M:8:PHE:CD1	1:M:112:HIS:HB3	2.51	0.45
1:M:19:PRO:HB3	1:M:95:TYR:CZ	2.52	0.45
1:A:75:ASP:OD1	1:A:75:ASP:N	2.37	0.45
2:C:17:DT:H1'	2:C:18:DG:C8	2.51	0.45
1:E:19:PRO:HB3	1:E:95:TYR:CE1	2.51	0.45
1:M:229:CYS:HB3	1:M:232:THR:OG1	2.16	0.45
1:F:61:GLN:HE21	4:F:301:GSH:HB22	1.81	0.45
1:F:188:ARG:NH1	3:H:19:DT:O4	2.47	0.45
1:N:162:ILE:HD12	1:N:163:LYS:HA	1.99	0.45
1:A:158:THR:HB	1:A:161:GLY:O	2.16	0.45
1:A:113:PHE:CE2	1:B:113:PHE:CZ	3.04	0.45
1:E:36:GLU:HG3	1:E:79:SER:HA	1.97	0.45
1:M:3:ALA:O	1:M:6:GLU:N	2.50	0.45
1:A:74:ILE:HG23	1:A:103:LYS:HZ2	1.81	0.45
1:B:5:ALA:O	1:B:8:PHE:HB3	2.16	0.45
1:E:223:GLU:HA	1:E:226:TYR:HB3	1.99	0.45
1:M:22:PHE:CZ	1:M:28:ILE:HG23	2.51	0.45
1:M:198:VAL:HG13	1:M:199:ILE:N	2.32	0.45
1:B:103:LYS:HB3	1:B:104:GLU:H	1.32	0.45
1:E:137:ASN:CG	1:E:138:GLY:N	2.68	0.45
1:F:211:LEU:HD23	1:F:235:LYS:HZ1	1.81	0.45
1:B:38:CYS:HB3	1:B:102:LEU:HD12	1.99	0.45
1:F:198:VAL:HG13	1:F:210:ASN:O	2.17	0.45
1:E:125:SER:HB3	1:F:80:VAL:HB	1.98	0.45
1:N:198:VAL:HG12	1:N:198:VAL:O	2.17	0.45
1:E:13:GLU:OE1	1:E:15:ASN:HB2	2.17	0.45
3:H:11:DA:H2"	3:H:12:DA:C8	2.51	0.45
3:H:27:DG:H2'	3:H:28:DA:C8	2.52	0.45
1:M:195:GLN:CG	1:M:198:VAL:HG12	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:199:ILE:CG2	1:N:208:VAL:HG22	2.44	0.45
1:N:37:TYR:H	1:N:71:SER:HG	1.56	0.45
1:B:88:ILE:CG2	1:B:168:ASN:ND2	2.80	0.44
1:E:47:LYS:HD3	1:E:88:ILE:HD11	1.99	0.44
1:F:229:CYS:HB2	1:F:232:THR:HG23	1.98	0.44
1:M:199:ILE:HG23	1:M:200:VAL:N	2.32	0.44
1:A:31:GLN:N	1:A:84:ASN:OD1	2.50	0.44
1:A:41:LEU:HD11	1:A:92:ALA:HB1	1.99	0.44
1:B:38:CYS:N	1:B:97:ILE:O	2.27	0.44
1:E:64:LYS:HD3	1:E:153:VAL:HG22	1.98	0.44
1:F:198:VAL:HG13	1:F:208:VAL:HG13	1.99	0.44
1:F:162:ILE:HG13	1:F:208:VAL:H	1.83	0.44
1:F:233:TRP:CA	1:F:235:LYS:HG2	2.45	0.44
1:N:163:LYS:HE3	1:N:205:CYS:HB2	1.98	0.44
1:A:113:PHE:HE2	1:B:113:PHE:CZ	2.36	0.44
1:F:106:LEU:HD23	1:F:106:LEU:HA	1.84	0.44
1:A:163:LYS:HB3	1:A:164:ILE:CA	2.40	0.44
2:C:25:DC:H2'	2:C:26:DC:C6	2.52	0.44
2:C:6:DT:H2"	2:C:7:DC:O4'	2.17	0.44
1:F:157:GLU:N	1:F:163:LYS:H	2.11	0.44
1:F:235:LYS:HG3	1:F:236:LEU:N	2.33	0.44
1:A:213:TYR:O	1:A:216:ARG:HB3	2.18	0.44
1:F:198:VAL:HG22	1:F:210:ASN:OD1	2.17	0.44
1:F:7:GLU:HG2	1:F:112:HIS:NE2	2.32	0.44
1:A:145:GLY:O	1:A:149:ILE:HG13	2.17	0.44
1:A:64:LYS:HG3	1:A:65:GLY:N	2.32	0.44
1:E:164:ILE:HG12	1:E:206:PHE:HB2	2.00	0.44
3:P:13:DC:H2"	3:P:14:DA:C8	2.53	0.44
1:A:19:PRO:HB3	1:A:95:TYR:CZ	2.53	0.44
1:B:104:GLU:C	1:B:106:LEU:N	2.70	0.44
1:N:11:TYR:OH	1:N:108:LYS:HG3	2.18	0.44
1:F:74:ILE:HD11	1:F:102:LEU:HD23	2.00	0.44
1:N:194:LYS:HE2	1:N:199:ILE:HG12	1.99	0.44
1:E:170:THR:HG22	1:E:172:GLN:H	1.83	0.43
1:A:15:ASN:ND2	1:A:17:ILE:HD12	2.33	0.43
1:B:100:ASN:OD1	1:B:101:GLU:OE1	2.36	0.43
1:B:139:LYS:NZ	1:B:179:GLY:HA3	2.32	0.43
1:F:148:LEU:O	1:F:151:THR:HB	2.18	0.43
1:F:158:THR:N	1:F:161:GLY:O	2.44	0.43
1:N:46:THR:HA	1:N:87:VAL:HA	1.99	0.43
3:P:2:DG:H2"	3:P:3:DT:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:THR:O	1:B:155:GLY:HA3	2.18	0.43
1:E:149:ILE:O	1:E:153:VAL:HG12	2.17	0.43
1:N:101:GLU:N	1:N:101:GLU:OE1	2.32	0.43
1:A:47:LYS:N	1:A:86:GLU:O	2.52	0.43
1:B:201:TYR:CE1	1:B:204:SER:HA	2.53	0.43
1:M:43:ASP:H	1:M:93:THR:HG23	1.84	0.43
2:O:2:DA:H2"	2:O:3:DT:OP1	2.18	0.43
1:A:163:LYS:HD2	1:A:165:THR:HG23	2.00	0.43
1:E:193:LEU:O	1:E:198:VAL:HG12	2.18	0.43
1:F:146:GLN:O	1:F:150:LEU:HG	2.19	0.43
1:M:167:ASP:HA	1:M:168:ASN:HA	1.70	0.43
1:A:74:ILE:C	1:A:103:LYS:HZ1	2.16	0.43
1:A:46:THR:OG1	1:A:86:GLU:O	2.30	0.43
1:B:107:SER:O	1:B:109:ASN:N	2.48	0.43
1:B:38:CYS:CB	1:B:102:LEU:HD12	2.49	0.43
1:M:160:ASP:OD1	1:M:161:GLY:N	2.52	0.43
1:M:31:GLN:HB2	1:M:82:TYR:HB3	2.00	0.43
1:A:23:HIS:N	1:A:26:GLU:OE2	2.52	0.43
3:D:13:DC:H2"	3:D:14:DA:C8	2.53	0.43
3:D:2:DG:H2"	3:D:3:DT:O4'	2.19	0.43
1:F:198:VAL:CG1	1:F:208:VAL:HG13	2.48	0.43
1:N:74:ILE:H	1:N:74:ILE:HG13	1.55	0.43
1:A:209:GLN:HB2	1:A:210:ASN:H	1.59	0.43
1:A:46:THR:CG2	1:A:63:TYR:HB2	2.48	0.43
1:E:139:LYS:O	1:E:143:ILE:HG12	2.19	0.43
1:F:162:ILE:O	1:F:207:TYR:CD1	2.72	0.43
1:F:46:THR:O	1:F:63:TYR:N	2.48	0.43
1:B:2:ASN:CG	1:B:3:ALA:H	2.22	0.43
1:F:162:ILE:N	1:F:207:TYR:HD1	2.16	0.43
1:B:106:LEU:HD11	1:B:113:PHE:HA	1.99	0.43
1:E:64:LYS:HD2	1:E:154:TYR:CE1	2.54	0.43
1:N:59:ASN:HB2	1:N:177:SER:HA	2.01	0.43
1:F:156:LYS:NZ	1:F:163:LYS:O	2.52	0.42
1:F:162:ILE:CD1	1:F:207:TYR:HA	2.49	0.42
1:N:160:ASP:OD1	1:N:160:ASP:N	2.52	0.42
1:N:6:GLU:O	1:N:9:LYS:HB3	2.19	0.42
1:A:6:GLU:HA	1:A:9:LYS:HB3	2.02	0.42
1:B:215:LYS:HE2	1:B:215:LYS:HB3	1.90	0.42
1:E:110:LEU:HA	1:E:113:PHE:HB2	1.99	0.42
1:F:220:LYS:HA	1:F:220:LYS:HD3	1.70	0.42
1:N:193:LEU:HB3	1:N:194:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:192:LYS:O	1:N:196:GLU:HG2	2.19	0.42
1:B:97:ILE:CG2	1:B:102:LEU:HD21	2.47	0.42
1:B:106:LEU:HA	1:B:106:LEU:HD12	1.77	0.42
1:B:59:ASN:HB2	1:B:177:SER:HA	2.01	0.42
1:F:28:ILE:HD12	1:F:85:LEU:HD23	2.00	0.42
1:N:108:LYS:HD3	1:N:109:ASN:HB3	2.01	0.42
1:N:193:LEU:C	1:N:194:LYS:HD2	2.39	0.42
1:A:3:ALA:N	1:A:6:GLU:OE1	2.53	0.42
1:B:15:ASN:CG	1:B:16:GLY:N	2.73	0.42
2:C:3:DT:H2"	2:C:4:DC:C5	2.54	0.42
1:E:223:GLU:N	1:E:223:GLU:OE1	2.37	0.42
1:F:9:LYS:HD2	1:F:42:TYR:CE1	2.55	0.42
1:B:154:TYR:O	1:B:165:THR:HG22	2.19	0.42
1:B:73:PHE:O	1:B:99:ILE:HG21	2.20	0.42
1:E:31:GLN:N	1:E:84:ASN:OD1	2.52	0.42
1:F:98:LYS:HG3	1:F:100:ASN:HB2	2.02	0.42
1:N:158:THR:HG22	1:N:159:PRO:N	2.33	0.42
1:N:193:LEU:HD13	1:N:194:LYS:HZ1	1.85	0.42
2:O:27:DT:H2"	2:O:28:DA:H8	1.85	0.42
1:B:118:GLN:HE22	1:B:122:LYS:HE3	1.85	0.42
1:F:184:SER:O	1:F:188:ARG:N	2.41	0.42
1:M:115:TYR:O	1:M:119:THR:HG23	2.20	0.42
1:M:34:PRO:HG2	1:M:35:GLN:OE1	2.20	0.42
1:M:78:THR:OG1	1:M:79:SER:N	2.52	0.42
1:N:24:LYS:O	1:N:25:LYS:HB3	2.18	0.42
1:E:137:ASN:HD21	1:E:141:GLY:N	2.17	0.42
1:M:213:TYR:HA	1:M:216:ARG:HH21	1.85	0.42
1:N:194:LYS:CD	1:N:199:ILE:HG12	2.50	0.42
1:B:235:LYS:HE2	1:B:235:LYS:HB2	1.74	0.42
1:E:129:ALA:HB1	1:E:220:LYS:O	2.20	0.42
1:M:143:ILE:HD11	1:M:180:ILE:HD12	2.02	0.42
1:M:202:LYS:O	1:M:204:SER:N	2.53	0.42
1:A:149:ILE:O	1:A:153:VAL:HG12	2.20	0.41
1:E:194:LYS:HB3	1:E:194:LYS:NZ	2.34	0.41
1:F:162:ILE:O	1:F:162:ILE:HD12	2.20	0.41
1:M:170:THR:O	1:M:173:GLU:HB3	2.20	0.41
1:N:200:VAL:HG12	1:N:202:LYS:HB3	2.01	0.41
1:A:156:LYS:HB3	1:A:163:LYS:HG3	2.00	0.41
1:A:203:ASN:O	1:A:205:CYS:N	2.47	0.41
1:E:185:ALA:HB2	2:G:19:DT:C7	2.50	0.41
1:M:164:ILE:HG12	1:M:206:PHE:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:4:DC:H2"	2:O:5:DG:H8	1.86	0.41
1:B:108:LYS:HE2	1:B:109:ASN:HB3	2.02	0.41
1:B:150:LEU:HA	1:B:154:TYR:HD2	1.86	0.41
1:B:189:ILE:O	1:B:189:ILE:HG22	2.20	0.41
1:F:162:ILE:CG1	1:F:208:VAL:N	2.84	0.41
1:N:11:TYR:CG	1:N:11:TYR:O	2.73	0.41
1:A:171:MET:HG2	3:D:8:DA:P	2.60	0.41
2:C:27:DT:H2"	2:C:28:DA:C8	2.55	0.41
1:M:8:PHE:HD1	1:M:112:HIS:HB3	1.85	0.41
1:M:201:TYR:CZ	1:M:204:SER:HA	2.55	0.41
1:B:222:ASP:OD1	1:B:233:TRP:NE1	2.48	0.41
1:B:223:GLU:O	1:B:227:LEU:HG	2.20	0.41
1:F:74:ILE:HG23	1:F:103:LYS:HG2	2.01	0.41
1:N:36:GLU:N	1:N:36:GLU:OE1	2.52	0.41
2:C:27:DT:H2"	2:C:28:DA:N7	2.36	0.41
1:E:113:PHE:HZ	1:F:114:PHE:CE1	2.39	0.41
1:E:10:LYS:CD	1:E:13:GLU:HB2	2.43	0.41
1:F:192:LYS:HA	1:F:192:LYS:HD3	1.59	0.41
1:M:191:SER:C	1:M:193:LEU:N	2.74	0.41
1:M:77:GLU:HG2	1:M:99:ILE:HG22	2.03	0.41
1:B:192:LYS:O	1:B:196:GLU:OE1	2.39	0.41
1:F:133:ASP:OD2	1:F:221:LEU:N	2.51	0.41
1:F:210:ASN:ND2	1:F:212:ASP:OD2	2.54	0.41
3:H:21:DA:H2"	3:H:22:DA:C8	2.56	0.41
1:M:194:LYS:O	1:M:194:LYS:HG2	2.19	0.41
1:M:194:LYS:HE2	1:M:200:VAL:HB	2.01	0.41
1:A:23:HIS:O	1:A:26:GLU:HG2	2.21	0.41
1:A:46:THR:OG1	1:A:47:LYS:N	2.52	0.41
1:A:96:VAL:C	1:A:97:ILE:HG13	2.38	0.41
1:E:79:SER:O	1:F:227:LEU:HB3	2.20	0.41
1:F:59:ASN:O	1:F:177:SER:HA	2.20	0.41
1:M:3:ALA:O	1:M:5:ALA:N	2.54	0.41
1:A:188:ARG:O	1:A:192:LYS:HG3	2.20	0.41
3:D:4:DA:H2"	3:D:5:DG:C8	2.56	0.41
1:M:158:THR:OG1	1:M:159:PRO:HD2	2.20	0.41
1:B:171:MET:HB2	2:C:8:DG:OP2	2.21	0.41
1:E:229:CYS:N	1:E:230:PRO:HD3	2.36	0.41
1:E:3:ALA:C	1:E:5:ALA:H	2.24	0.41
1:E:89:SER:OG	1:E:91:GLN:O	2.33	0.41
1:F:156:LYS:HA	1:F:163:LYS:H	1.85	0.41
1:F:98:LYS:HE3	1:F:100:ASN:CG	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:194:LYS:HA	1:M:195:GLN:CB	2.50	0.41
3:D:24:DG:H2"	3:D:25:DA:C8	2.56	0.41
1:E:104:GLU:O	1:E:108:LYS:HG3	2.21	0.41
1:E:40:PHE:HD2	1:E:95:TYR:CD2	2.39	0.41
1:F:233:TRP:CG	1:F:233:TRP:O	2.74	0.41
1:M:166:LEU:HA	1:M:166:LEU:HD12	1.85	0.41
1:M:210:ASN:OD1	1:M:210:ASN:C	2.58	0.41
1:N:157:GLU:HA	1:N:160:ASP:OD2	2.21	0.41
1:N:62:TYR:HB2	4:N:301:GSH:O31	2.21	0.41
1:A:126:TYR:HB2	1:A:224:TRP:CE2	2.56	0.40
3:D:2:DG:H2"	3:D:3:DT:O5'	2.20	0.40
1:E:137:ASN:ND2	1:E:141:GLY:H	2.19	0.40
1:N:190:ILE:O	1:N:194:LYS:HD2	2.21	0.40
1:N:40:PHE:CE2	1:N:42:TYR:HB2	2.56	0.40
1:A:6:GLU:N	1:A:6:GLU:OE1	2.45	0.40
1:B:211:LEU:O	1:B:214:LEU:N	2.53	0.40
1:E:141:GLY:O	1:E:145:GLY:N	2.47	0.40
1:E:190:ILE:O	1:E:193:LEU:HB2	2.21	0.40
1:N:46:THR:O	1:N:63:TYR:N	2.53	0.40
1:A:225:PHE:O	1:A:233:TRP:HB2	2.22	0.40
1:N:101:GLU:H	1:N:101:GLU:CD	2.21	0.40
1:N:108:LYS:CD	1:N:109:ASN:HB3	2.51	0.40
1:N:194:LYS:HE2	1:N:199:ILE:CG1	2.51	0.40
1:B:106:LEU:HG	1:B:113:PHE:HD2	1.84	0.40
1:F:235:LYS:HG2	1:F:235:LYS:H	1.67	0.40
1:F:77:GLU:OE2	1:F:100:ASN:ND2	2.55	0.40
1:A:171:MET:O	1:A:186:VAL:HG11	2.22	0.40
1:B:15:ASN:HB3	1:B:105:LEU:HD21	2.02	0.40
1:E:6:GLU:HA	1:E:9:LYS:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	234/237 (99%)	195 (83%)	27 (12%)	12 (5%)	2 12
1	B	234/237 (99%)	197 (84%)	26 (11%)	11 (5%)	2 14
1	E	234/237 (99%)	204 (87%)	24 (10%)	6 (3%)	5 27
1	F	234/237 (99%)	202 (86%)	20 (8%)	12 (5%)	2 12
1	M	234/237 (99%)	207 (88%)	16 (7%)	11 (5%)	2 14
1	N	234/237 (99%)	206 (88%)	16 (7%)	12 (5%)	2 12
All	All	1404/1422 (99%)	1211 (86%)	129 (9%)	64 (5%)	2 14

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	M	4	GLN
1	M	102	LEU
1	M	107	SER
1	M	203	ASN
1	N	98	LYS
1	N	108	LYS
1	A	9	LYS
1	A	13	GLU
1	A	56	THR
1	A	155	GLY
1	A	163	LYS
1	A	209	GLN
1	B	4	GLN
1	B	103	LYS
1	B	105	LEU
1	B	108	LYS
1	B	109	ASN
1	B	167	ASP
1	B	203	ASN
1	E	12	LEU
1	F	157	GLU
1	F	196	GLU
1	F	197	LYS
1	F	235	LYS
1	F	236	LEU
1	M	101	GLU
1	M	109	ASN
1	M	167	ASP
1	M	197	LYS
1	N	202	LYS

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Mol	Chain	Res	Type
1	A	98	LYS
1	B	15	ASN
1	B	91	GLN
1	B	165	THR
1	E	4	GLN
1	F	17	ILE
1	F	156	LYS
1	F	163	LYS
1	F	193	LEU
1	F	203	ASN
1	N	193	LEU
1	A	91	GLN
1	A	103	LYS
1	A	166	LEU
1	E	16	GLY
1	F	212	ASP
1	M	108	LYS
1	M	195	GLN
1	N	3	ALA
1	N	24	LYS
1	N	92	ALA
1	N	101	GLU
1	N	160	ASP
1	B	172	GLN
1	E	137	ASN
1	E	204	SER
1	F	172	GLN
1	M	196	GLU
1	A	204	SER
1	N	158	THR
1	N	208	VAL
1	A	3	ALA
1	E	17	ILE
1	N	199	ILE

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	211/212 (100%)	199 (94%)	12 (6%)	20 56
1	B	211/212 (100%)	200 (95%)	11 (5%)	23 59
1	E	211/212 (100%)	201 (95%)	10 (5%)	26 63
1	F	211/212 (100%)	205 (97%)	6 (3%)	43 77
1	M	211/212 (100%)	202 (96%)	9 (4%)	29 66
1	N	211/212 (100%)	205 (97%)	6 (3%)	43 77
All	All	1266/1272 (100%)	1212 (96%)	54 (4%)	29 66

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	2	ASN
1	M	91	GLN
1	M	108	LYS
1	M	109	ASN
1	M	190	ILE
1	M	195	GLN
1	M	196	GLU
1	M	200	VAL
1	M	210	ASN
1	N	25	LYS
1	N	54	ASN
1	N	91	GLN
1	N	162	ILE
1	N	163	LYS
1	N	212	ASP
1	A	9	LYS
1	A	13	GLU
1	A	14	THR
1	A	57	ILE
1	A	97	ILE
1	A	106	LEU
1	A	113	PHE
1	A	118	GLN
1	A	168	ASN
1	A	194	LYS
1	A	201	TYR
1	A	209	GLN
1	B	7	GLU
1	B	18	LYS
1	B	47	LYS

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Mol	Chain	Res	Type
1	B	57	ILE
1	B	103	LYS
1	B	104	GLU
1	B	108	LYS
1	B	167	ASP
1	B	180	ILE
1	B	209	GLN
1	B	215	LYS
1	E	2	ASN
1	E	7	GLU
1	E	11	TYR
1	E	15	ASN
1	E	137	ASN
1	E	163	LYS
1	E	172	GLN
1	E	192	LYS
1	E	208	VAL
1	E	222	ASP
1	F	32	TRP
1	F	35	GLN
1	F	192	LYS
1	F	194	LYS
1	F	197	LYS
1	F	233	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	123	GLN
1	N	54	ASN
1	N	61	GLN
1	N	123	GLN
1	B	21	GLN
1	B	168	ASN
1	B	182	HIS
1	E	2	ASN
1	E	15	ASN
1	E	109	ASN
1	E	132	ASN
1	E	137	ASN
1	F	35	GLN
1	F	100	ASN

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Mol	Chain	Res	Type
1	F	209	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are 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	GSH	E	301	-	12,19,19	2.17	3 (25%)	15,24,24	1.55	2 (13%)
4	GSH	F	301	-	12,19,19	2.18	3 (25%)	15,24,24	1.44	2 (13%)
4	GSH	M	301	-	12,19,19	2.16	2 (16%)	15,24,24	1.49	2 (13%)
4	GSH	N	301	-	12,19,19	2.19	3 (25%)	15,24,24	1.46	3 (20%)
4	GSH	B	301	-	12,19,19	2.18	3 (25%)	15,24,24	1.85	5 (33%)
4	GSH	A	301	-	12,19,19	2.18	3 (25%)	15,24,24	1.47	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GSH	E	301	-	-	3/18/24/24	-
4	GSH	F	301	-	-	0/18/24/24	-
4	GSH	M	301	-	-	0/18/24/24	-
4	GSH	N	301	-	-	0/18/24/24	-
4	GSH	B	301	-	-	4/18/24/24	-
4	GSH	A	301	-	-	0/18/24/24	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	N	301	GSH	C2-N3	4.86	1.44	1.33
4	F	301	GSH	C2-N3	4.84	1.44	1.33
4	E	301	GSH	C2-N3	4.82	1.44	1.33
4	N	301	GSH	CD1-N2	4.82	1.44	1.34
4	A	301	GSH	C2-N3	4.78	1.44	1.33
4	B	301	GSH	C2-N3	4.76	1.44	1.33
4	A	301	GSH	CD1-N2	4.76	1.44	1.34
4	E	301	GSH	CD1-N2	4.73	1.44	1.34
4	M	301	GSH	C2-N3	4.72	1.43	1.33
4	M	301	GSH	CD1-N2	4.70	1.44	1.34
4	F	301	GSH	CD1-N2	4.67	1.44	1.34
4	B	301	GSH	CD1-N2	4.65	1.44	1.34
4	B	301	GSH	CA1-N1	-2.08	1.42	1.47
4	A	301	GSH	CA1-N1	-2.06	1.42	1.47
4	N	301	GSH	CA1-N1	-2.04	1.42	1.47
4	E	301	GSH	CA1-N1	-2.03	1.42	1.47
4	F	301	GSH	CA1-N1	-2.01	1.42	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	301	GSH	CA2-CB2-SG2	-3.62	110.12	114.19
4	E	301	GSH	CA2-CB2-SG2	-3.17	110.63	114.19
4	M	301	GSH	CA2-CB2-SG2	-3.14	110.66	114.19
4	F	301	GSH	CA2-CB2-SG2	-3.10	110.71	114.19
4	A	301	GSH	CA2-CB2-SG2	-2.66	111.21	114.19
4	B	301	GSH	CG1-CD1-N2	2.58	120.31	115.83
4	A	301	GSH	CG1-CD1-N2	2.58	120.31	115.83
4	B	301	GSH	CA3-N3-C2	-2.57	118.65	122.34
4	N	301	GSH	CG1-CD1-N2	2.51	120.18	115.83
4	M	301	GSH	CG1-CD1-N2	2.49	120.14	115.83
4	F	301	GSH	CG1-CD1-N2	2.48	120.13	115.83
4	E	301	GSH	CG1-CD1-N2	2.37	119.95	115.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	N	301	GSH	CA2-CB2-SG2	-2.35	111.55	114.19
4	B	301	GSH	CA2-C2-N3	2.34	121.26	116.54
4	N	301	GSH	CB1-CG1-CD1	-2.23	108.06	113.04
4	A	301	GSH	CB1-CG1-CD1	-2.09	108.36	113.04
4	B	301	GSH	CB1-CG1-CD1	-2.04	108.48	113.04

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	GSH	N2-CA2-CB2-SG2
4	B	301	GSH	C2-CA2-CB2-SG2
4	E	301	GSH	N1-CA1-CB1-CG1
4	E	301	GSH	OE1-CD1-CG1-CB1
4	E	301	GSH	N2-CD1-CG1-CB1
4	B	301	GSH	N1-CA1-CB1-CG1
4	B	301	GSH	OE1-CD1-CG1-CB1

There are no ring outliers.

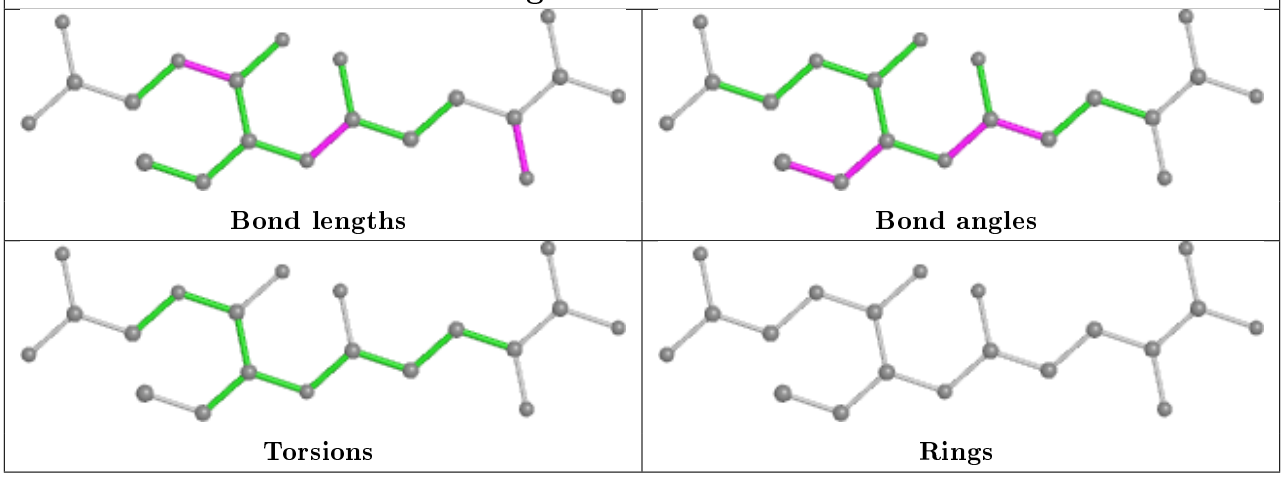
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	301	GSH	1	0
4	F	301	GSH	1	0
4	N	301	GSH	1	0
4	A	301	GSH	2	0

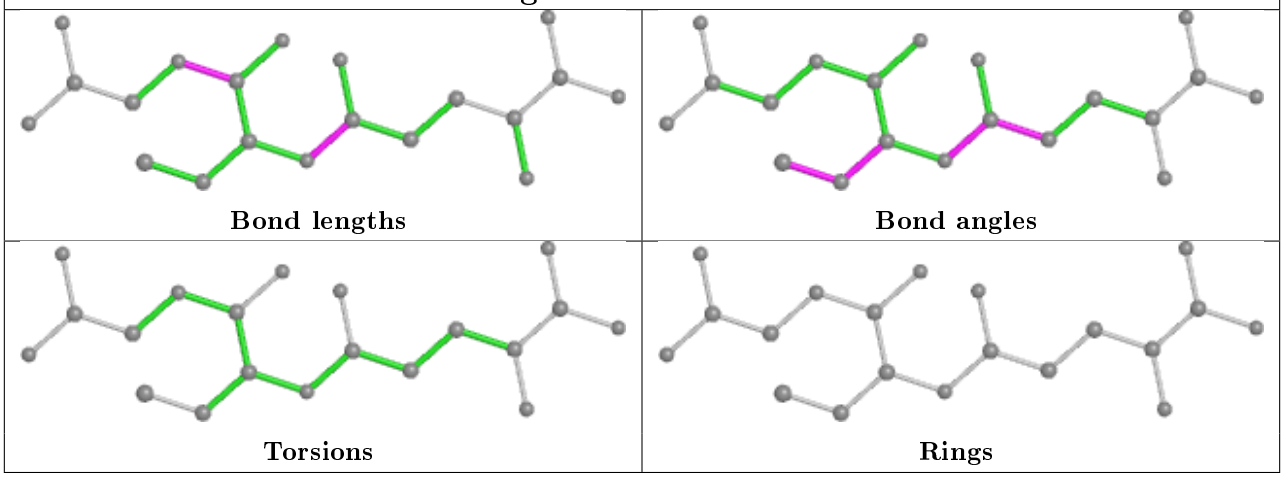
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

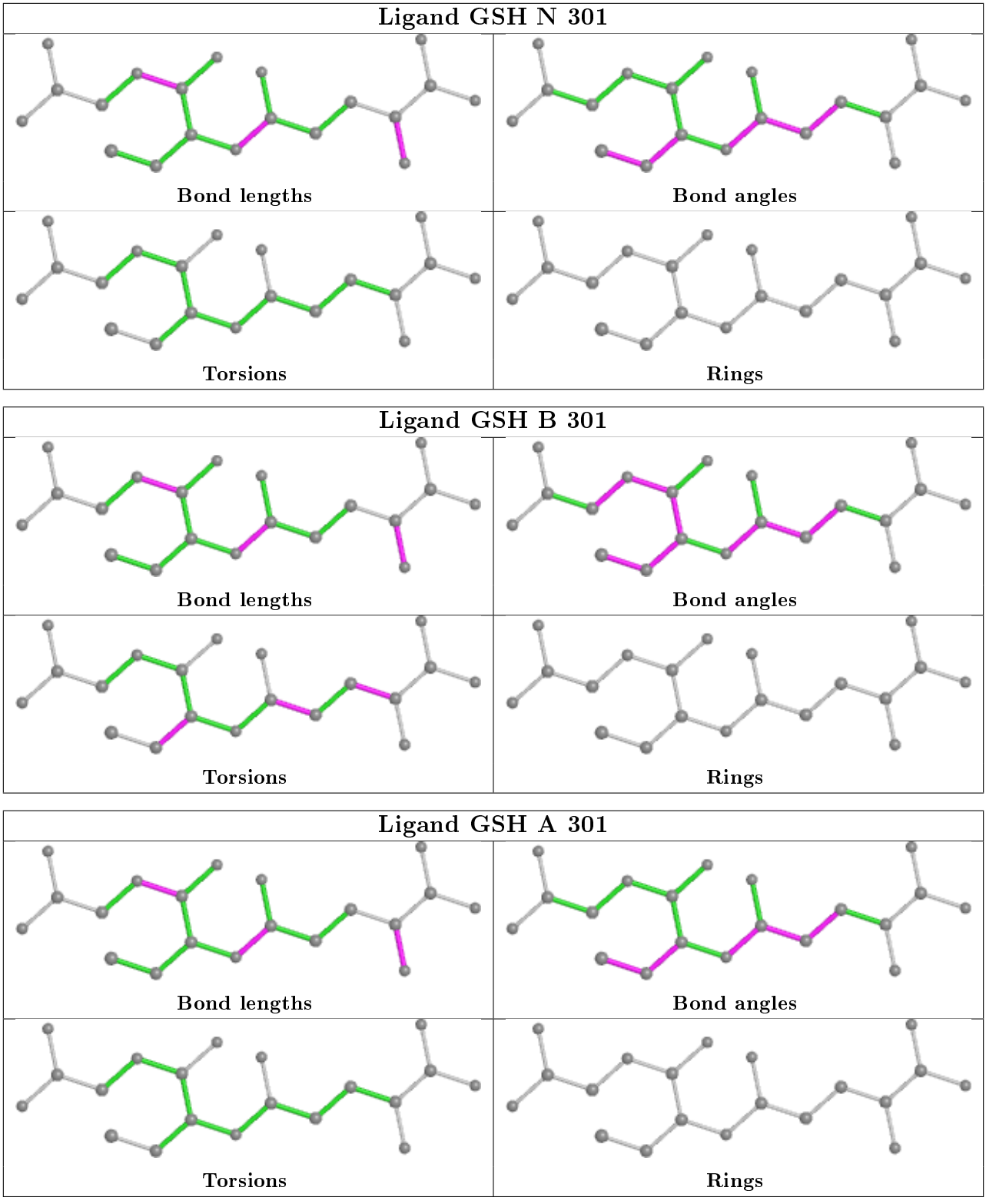
Ligand GSH E 301

Ligand GSH F 301



Ligand GSH M 301





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	236/237 (99%)	0.71	30 (12%) 3 1	63, 103, 162, 217	0
1	B	236/237 (99%)	0.93	42 (17%) 1 0	75, 109, 170, 217	0
1	E	236/237 (99%)	0.74	30 (12%) 3 1	71, 110, 175, 230	0
1	F	236/237 (99%)	0.91	34 (14%) 2 1	72, 111, 195, 268	0
1	M	236/237 (99%)	0.67	19 (8%) 12 3	64, 95, 143, 183	0
1	N	236/237 (99%)	0.73	28 (11%) 4 1	70, 101, 160, 202	0
2	C	29/29 (100%)	-0.47	0 100 100	84, 111, 130, 144	0
2	G	28/29 (96%)	-0.48	0 100 100	101, 135, 150, 157	0
2	O	29/29 (100%)	-0.57	0 100 100	87, 115, 146, 165	0
3	D	29/29 (100%)	-0.54	0 100 100	79, 106, 122, 141	0
3	H	29/29 (100%)	-0.52	0 100 100	105, 126, 149, 176	0
3	P	28/29 (96%)	-0.67	0 100 100	93, 114, 126, 132	0
All	All	1588/1596 (99%)	0.64	183 (11%) 4 1	63, 107, 168, 268	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	197	LYS	16.5
1	F	237	ASN	10.1
1	F	156	LYS	7.5
1	E	16	GLY	7.0
1	F	201	TYR	6.1
1	M	196	GLU	5.6
1	E	17	ILE	5.3
1	F	196	GLU	5.1
1	B	189	ILE	5.1
1	F	198	VAL	4.8
1	A	198	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	N	164	ILE	4.5
1	N	201	TYR	4.3
1	B	12	LEU	4.3
1	F	191	SER	4.3
1	B	99	ILE	4.2
1	M	200	VAL	4.2
1	F	155	GLY	4.2
1	A	40	PHE	4.1
1	A	199	ILE	4.0
1	M	201	TYR	4.0
1	B	105	LEU	3.9
1	B	110	LEU	3.9
1	N	156	LYS	3.7
1	M	166	LEU	3.7
1	F	152	TYR	3.7
1	A	16	GLY	3.6
1	B	106	LEU	3.6
1	F	164	ILE	3.6
1	B	95	TYR	3.5
1	B	196	GLU	3.5
1	M	192	LYS	3.4
1	N	193	LEU	3.3
1	A	236	LEU	3.3
1	F	157	GLU	3.3
1	N	40	PHE	3.3
1	M	193	LEU	3.3
1	B	164	ILE	3.3
1	A	112	HIS	3.3
1	F	180	ILE	3.3
1	B	119	THR	3.2
1	M	154	TYR	3.2
1	N	106	LEU	3.1
1	N	11	TYR	3.1
1	N	208	VAL	3.1
1	A	37	TYR	3.1
1	N	206	PHE	3.0
1	B	102	LEU	3.0
1	B	80	VAL	3.0
1	A	206	PHE	3.0
1	E	14	THR	3.0
1	M	206	PHE	2.9
1	A	153	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	148	LEU	2.9
1	B	206	PHE	2.9
1	N	154	TYR	2.9
1	N	207	TYR	2.9
1	B	21	GLN	2.9
1	N	161	GLY	2.9
1	B	101	GLU	2.9
1	E	102	LEU	2.9
1	B	148	LEU	2.8
1	M	159	PRO	2.8
1	E	115	TYR	2.8
1	B	143	ILE	2.7
1	F	232	THR	2.7
1	A	14	THR	2.7
1	B	76	THR	2.7
1	N	93	THR	2.7
1	A	116	VAL	2.6
1	B	47	LYS	2.6
1	N	95	TYR	2.6
1	F	227	LEU	2.6
1	F	199	ILE	2.6
1	E	40	PHE	2.6
1	B	85	LEU	2.5
1	B	115	TYR	2.5
1	A	11	TYR	2.5
1	B	94	ALA	2.5
1	F	200	VAL	2.5
1	E	8	PHE	2.5
1	A	94	ALA	2.5
1	B	121	GLN	2.5
1	A	227	LEU	2.5
1	M	108	LYS	2.5
1	B	227	LEU	2.5
1	A	73	PHE	2.5
1	A	114	PHE	2.5
1	A	103	LYS	2.5
1	B	93	THR	2.4
1	N	68	VAL	2.4
1	A	17	ILE	2.4
1	E	74	ILE	2.4
1	A	70	MET	2.4
1	N	162	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	148	LEU	2.4
1	F	105	LEU	2.4
1	B	120	LEU	2.4
1	B	20	LYS	2.4
1	B	168	ASN	2.4
1	F	88	ILE	2.4
1	N	199	ILE	2.4
1	B	41	LEU	2.4
1	B	114	PHE	2.4
1	B	11	TYR	2.4
1	M	169	LEU	2.4
1	A	157	GLU	2.4
1	B	98	LYS	2.4
1	F	149	ILE	2.4
1	A	155	GLY	2.3
1	M	189	ILE	2.3
1	E	209	GLN	2.3
1	F	102	LEU	2.3
1	N	202	LYS	2.3
1	F	85	LEU	2.3
1	A	13	GLU	2.3
1	F	236	LEU	2.3
1	E	79	SER	2.3
1	F	80	VAL	2.3
1	E	120	LEU	2.3
1	F	86	GLU	2.3
1	M	214	LEU	2.3
1	N	117	PHE	2.3
1	A	134	PHE	2.3
1	B	40	PHE	2.3
1	F	225	PHE	2.3
1	A	192	LYS	2.3
1	M	170	THR	2.2
1	N	159	PRO	2.2
1	F	151	THR	2.2
1	F	150	LEU	2.2
1	E	70	MET	2.2
1	E	195	GLN	2.2
1	E	156	LYS	2.2
1	E	114	PHE	2.2
1	N	194	LYS	2.2
1	E	15	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	151	THR	2.2
1	M	149	ILE	2.2
1	E	69	ILE	2.2
1	E	162	ILE	2.2
1	M	143	ILE	2.2
1	E	95	TYR	2.2
1	A	214	LEU	2.2
1	E	68	VAL	2.2
1	N	12	LEU	2.2
1	M	74	ILE	2.2
1	E	206	PHE	2.2
1	N	151	THR	2.2
1	N	94	ALA	2.2
1	E	229	CYS	2.2
1	B	208	VAL	2.1
1	E	62	TYR	2.1
1	B	190	ILE	2.1
1	F	168	ASN	2.1
1	B	29	PHE	2.1
1	B	73	PHE	2.1
1	A	39	ILE	2.1
1	E	219	PRO	2.1
1	M	217	TYR	2.1
1	F	40	PHE	2.1
1	A	162	ILE	2.1
1	A	68	VAL	2.1
1	N	112	HIS	2.1
1	N	225	PHE	2.1
1	B	22	PHE	2.1
1	F	95	TYR	2.1
1	F	163	LYS	2.1
1	B	149	ILE	2.1
1	B	207	TYR	2.1
1	E	9	LYS	2.1
1	N	166	LEU	2.0
1	N	10	LYS	2.0
1	E	105	LEU	2.0
1	B	17	ILE	2.0
1	F	143	ILE	2.0
1	E	42	TYR	2.0
1	E	171	MET	2.0
1	M	105	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	113	PHE	2.0
1	E	12	LEU	2.0
1	F	206	PHE	2.0
1	E	150	LEU	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)

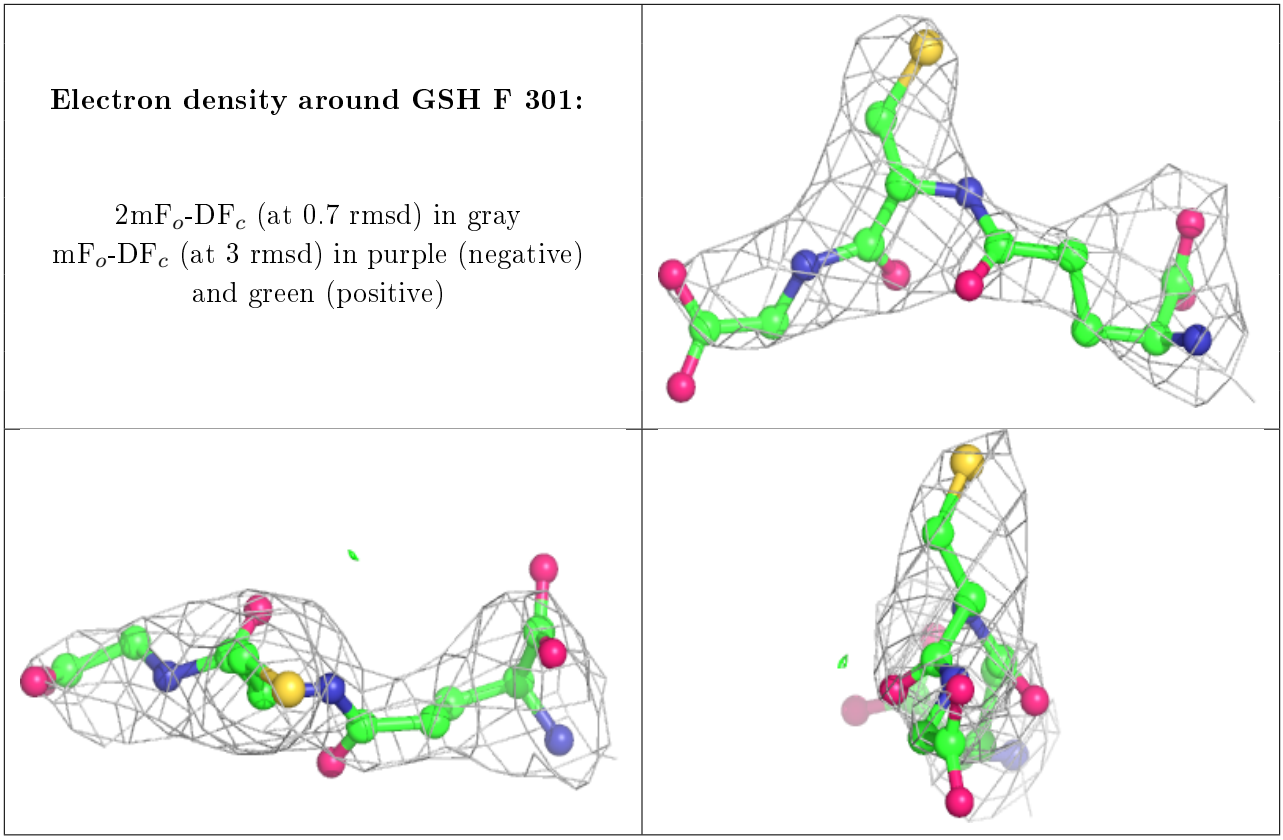
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GSH	F	301	20/20	0.82	0.41	83,110,146,176	0
4	GSH	N	301	20/20	0.85	0.32	93,111,142,144	0
4	GSH	A	301	20/20	0.85	0.27	83,101,136,150	0
4	GSH	B	301	20/20	0.86	0.35	95,120,137,176	0
4	GSH	E	301	20/20	0.87	0.32	98,113,157,230	0
4	GSH	M	301	20/20	0.91	0.25	72,96,124,149	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.

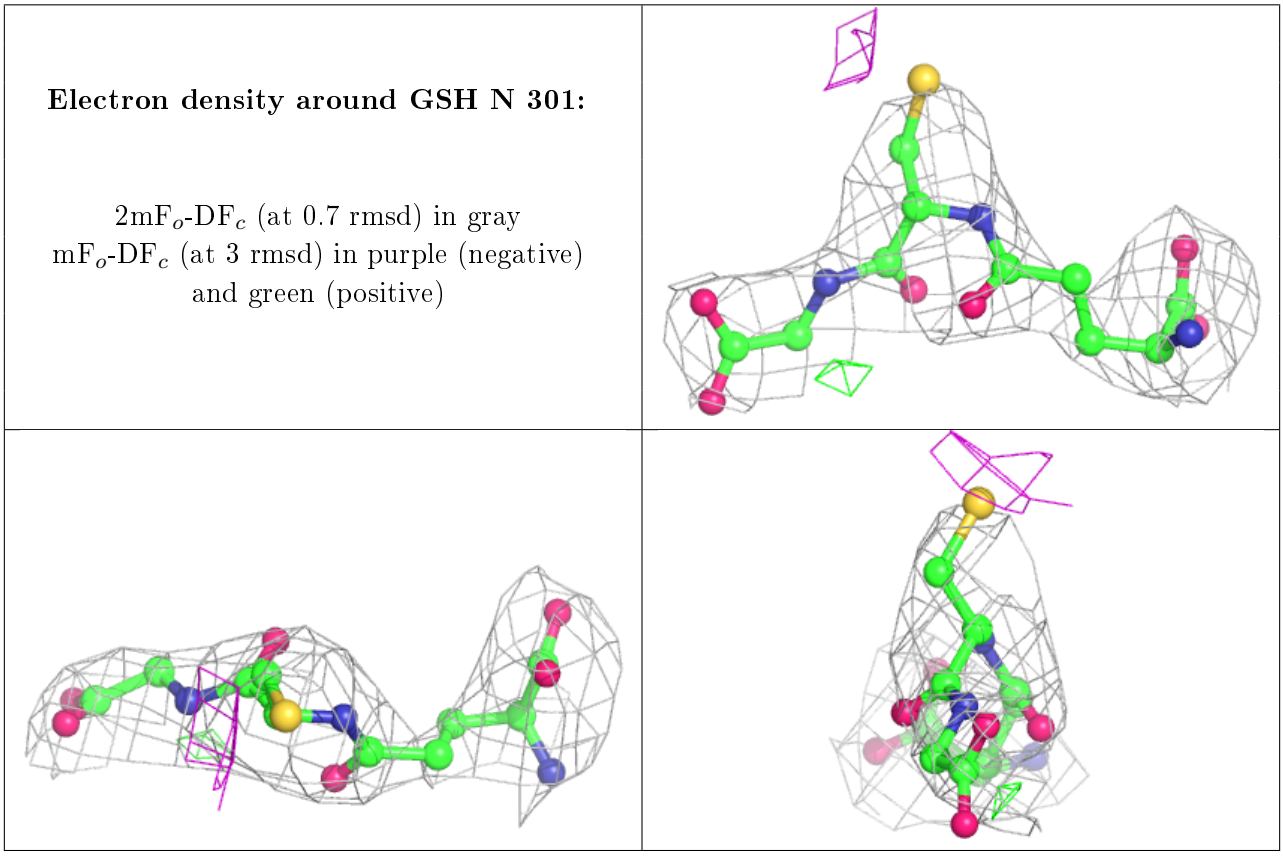
Electron density around GSH F 301:

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



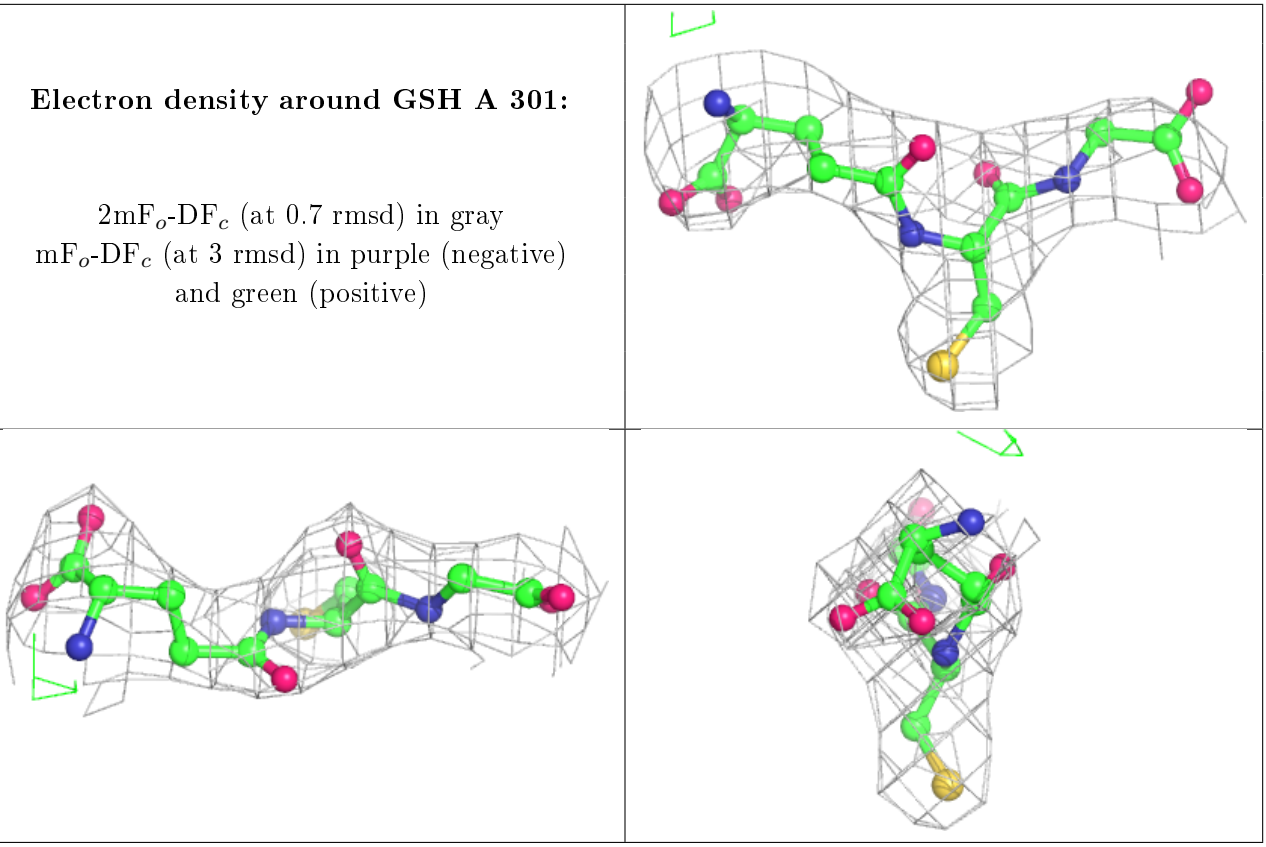
Electron density around GSH N 301:

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



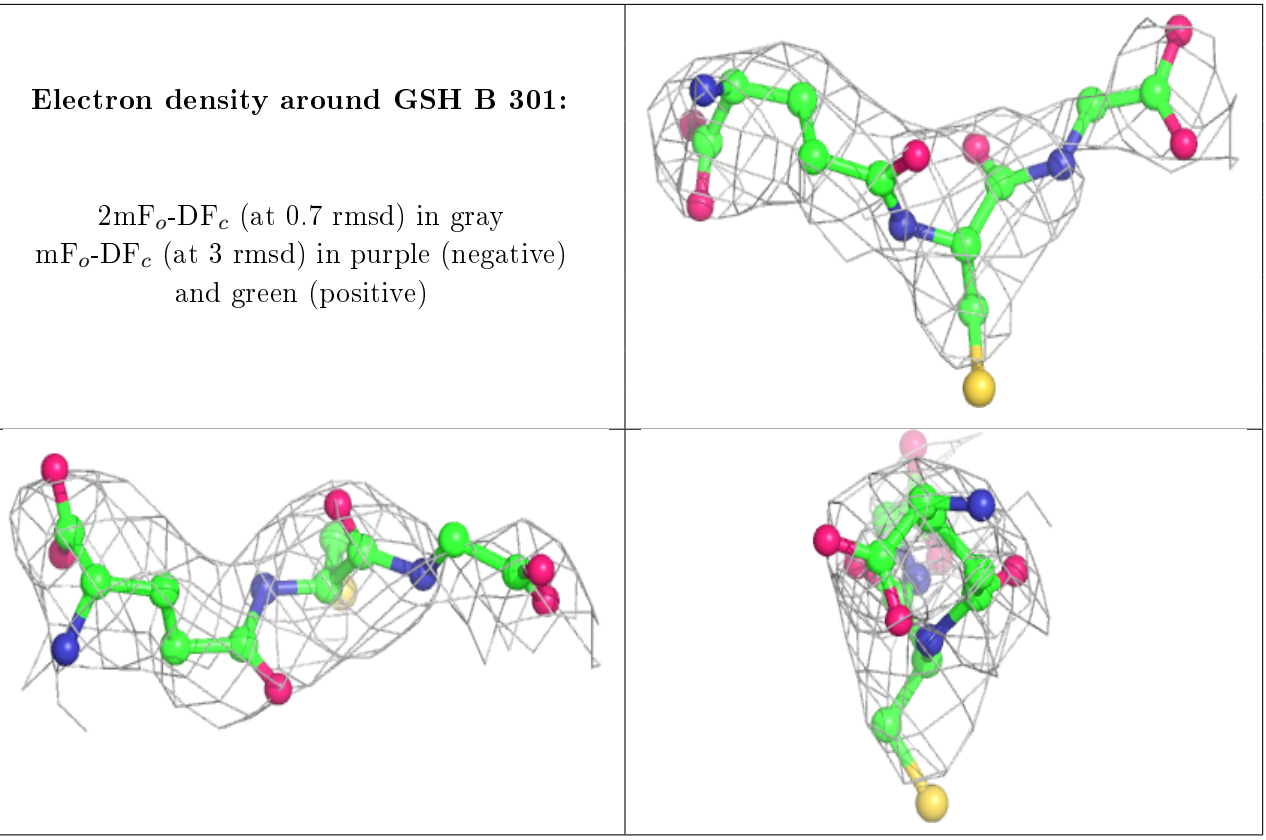
Electron density around GSH A 301:

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



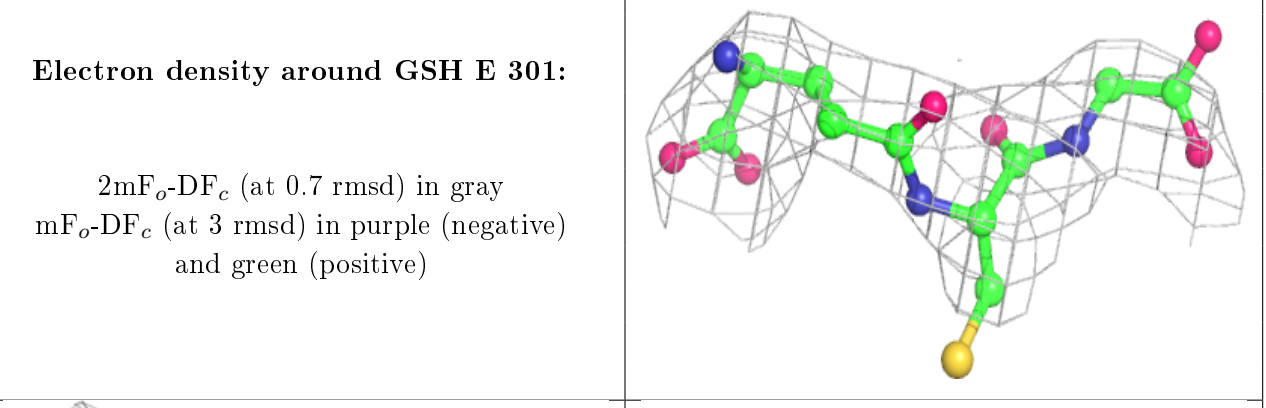
Electron density around GSH B 301:

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



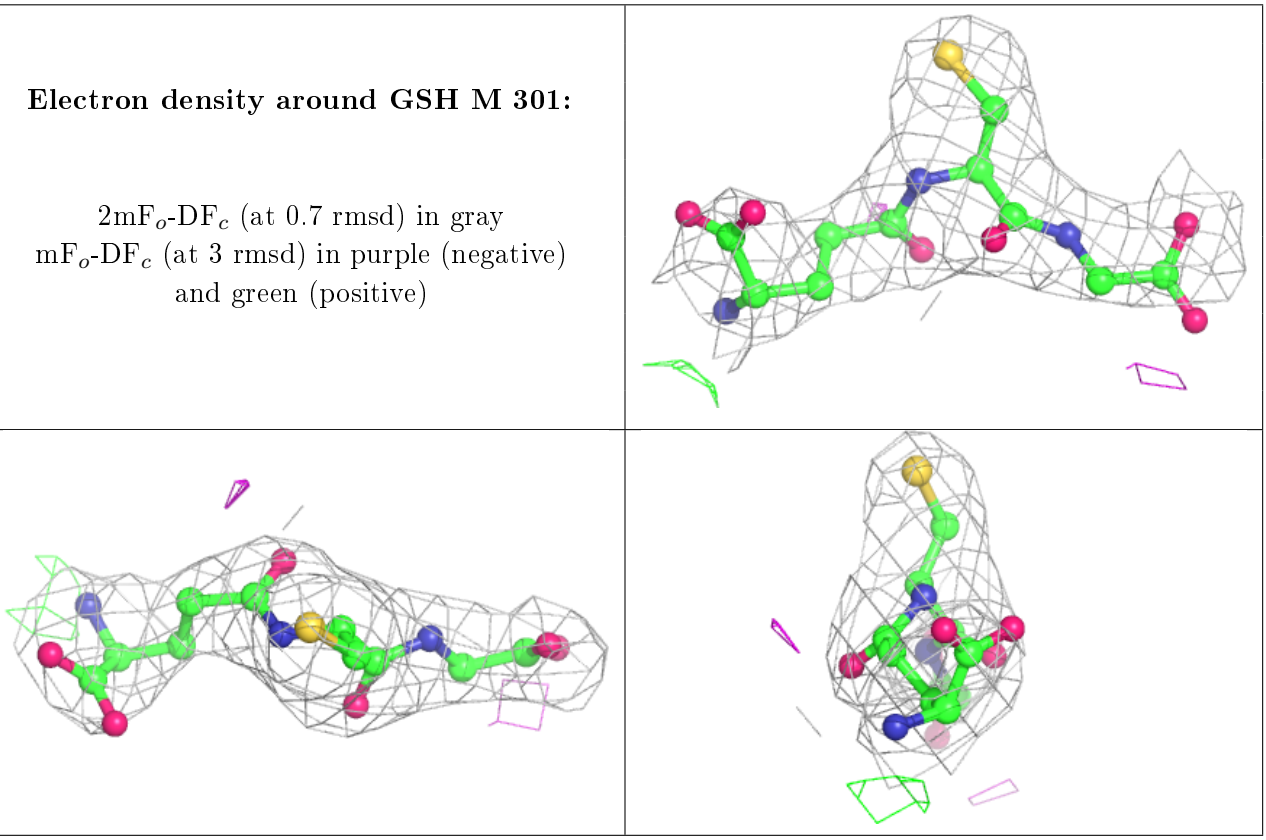
Electron density around GSH E 301:

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



Electron density around GSH M 301:

$2mF_o$-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 (i)

There are no such residues in this entry.