



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 05:29 am BST

PDB ID : 2XKA
Title : Crystal structure of a GTPyS-form protofilament of *Bacillus thuringiensis* serovar *israelensis* TubZ
Authors : Aylett, C.H.S.; Lowe, J.
Deposited on : 2010-07-07
Resolution : 3.00 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36.2
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) : 2.36.2

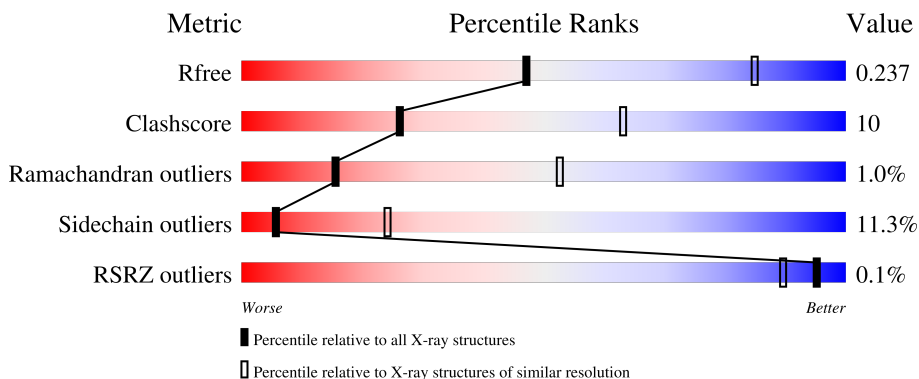
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	
1	C	421	
1	D	421	
1	E	421	

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Mol	Chain	Length	Quality of chain
1	F	421	 72% 23% . .
1	G	421	 71% 23% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22638 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.

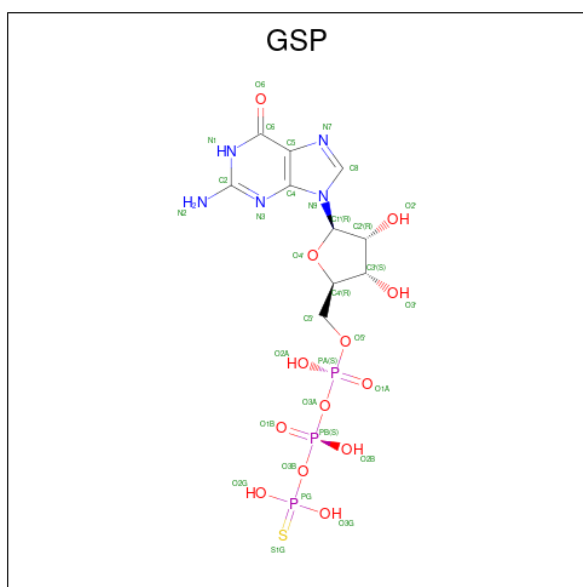
- Molecule 1 is a protein called FTSZ/TUBULIN-RELATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	3155	1987	540	616	12	0	0	0
1	B	400	3160	1991	542	615	12	0	0	0
1	C	410	3246	2044	556	634	12	0	0	0
1	D	402	3175	2000	544	619	12	0	0	0
1	E	395	3119	1967	534	606	12	0	0	0
1	F	414	3274	2060	561	640	13	0	0	0
1	G	414	3278	2062	563	641	12	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP Q8KNP3
B	2	VAL	LEU	engineered mutation	UNP Q8KNP3
C	2	VAL	LEU	engineered mutation	UNP Q8KNP3
D	2	VAL	LEU	engineered mutation	UNP Q8KNP3
E	2	VAL	LEU	engineered mutation	UNP Q8KNP3
F	2	VAL	LEU	engineered mutation	UNP Q8KNP3
G	2	VAL	LEU	engineered mutation	UNP Q8KNP3

- Molecule 2 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (three-letter code: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
2	B	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
2	C	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
2	D	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
2	E	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
2	F	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0
2	G	1	Total 32	C 10	N 5	O 13	P 3	S 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	Total 1	Mg 1	0	0
3	B	1	Total 1	Mg 1	0	0
3	C	1	Total 1	Mg 1	0	0
3	D	1	Total 1	Mg 1	0	0
3	E	1	Total 1	Mg 1	0	0

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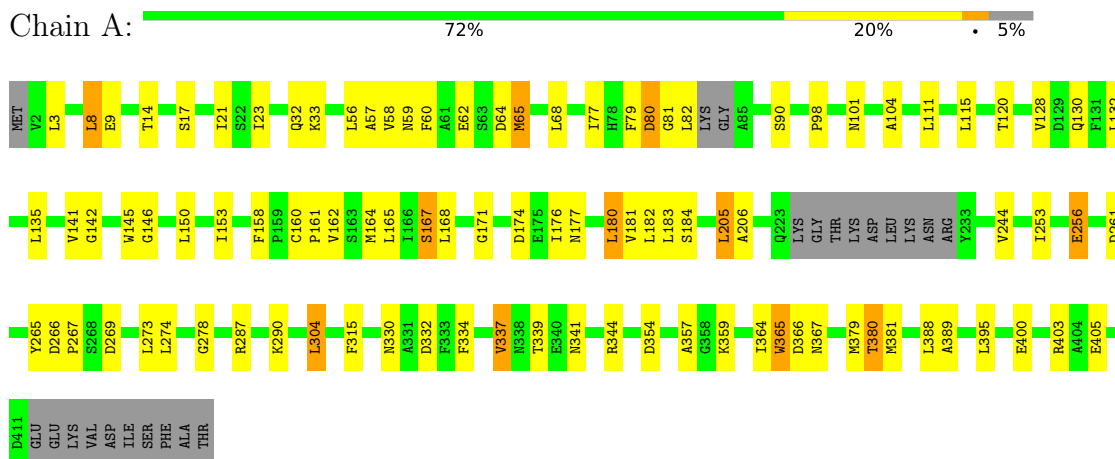
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total 1	Mg 1	0	0
3	G	1	Total 1	Mg 1	0	0

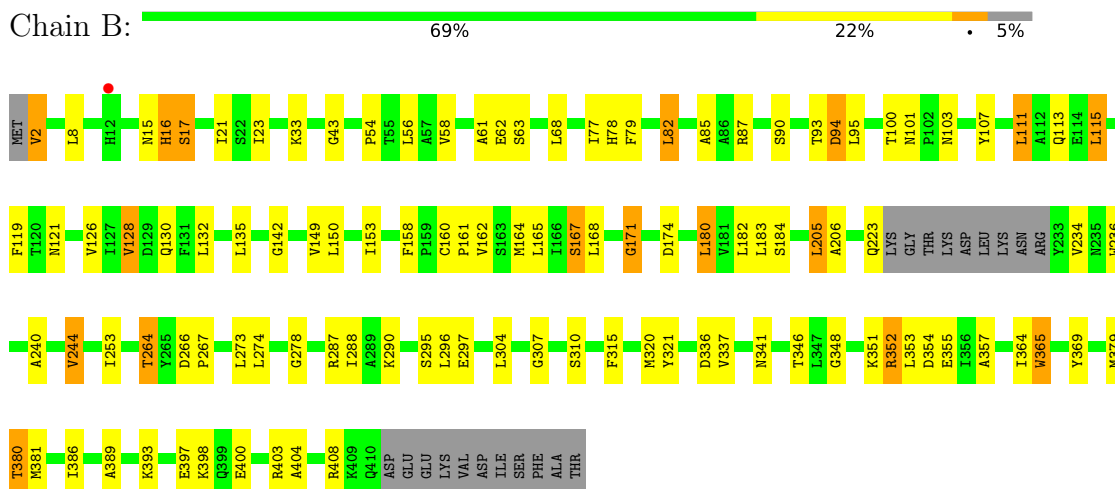
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

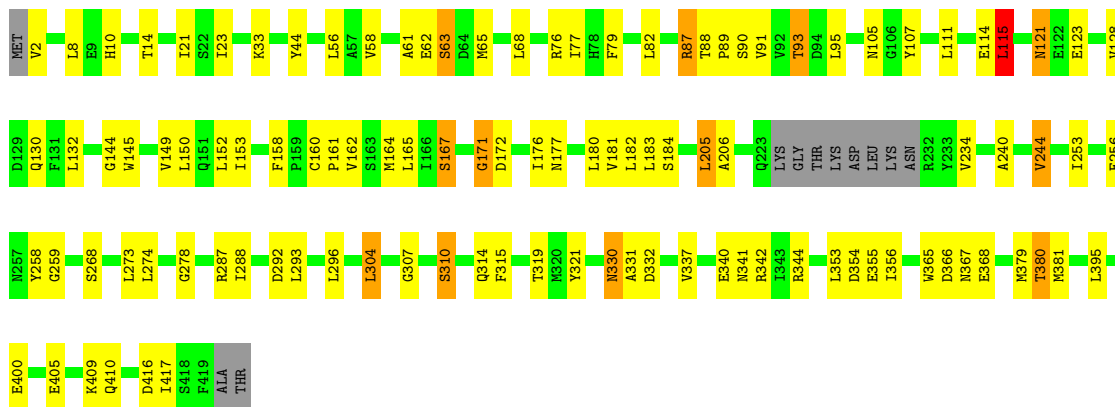


- Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN



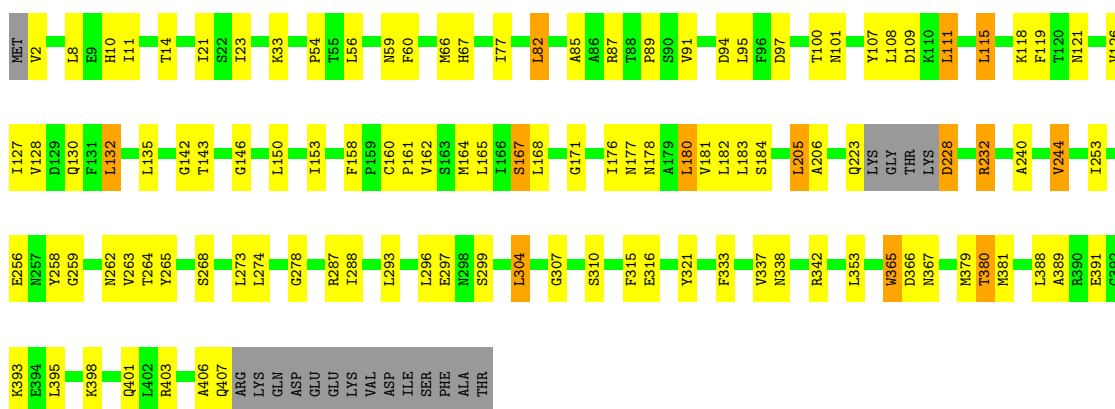
- Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN





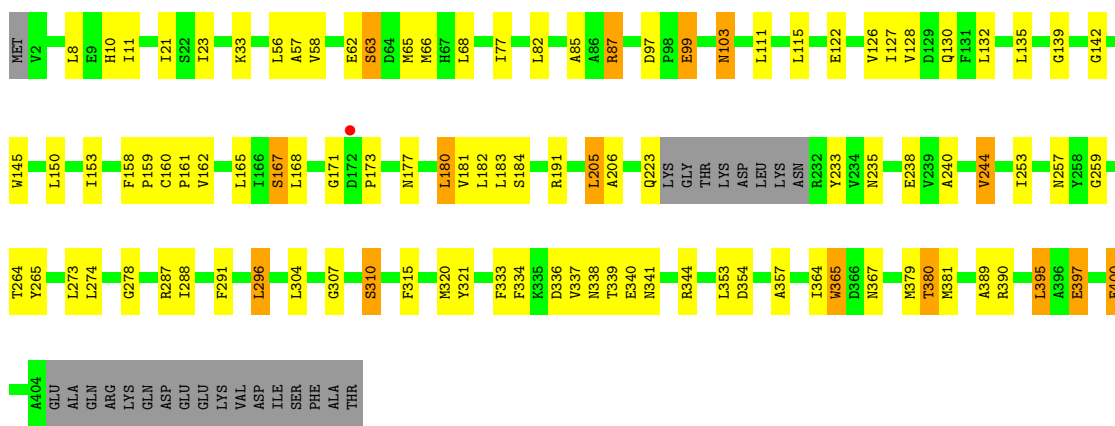
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain D: 69% 24% 5%



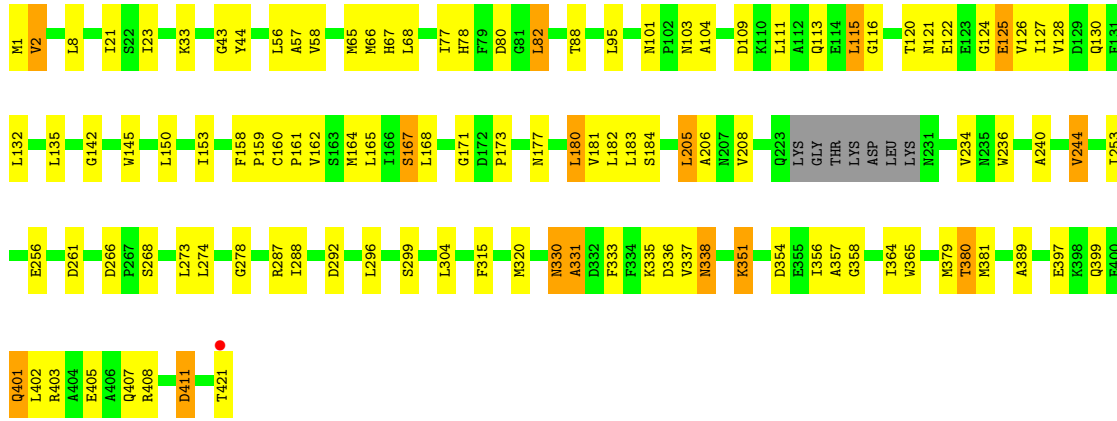
• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain E: 70% 20% 6%

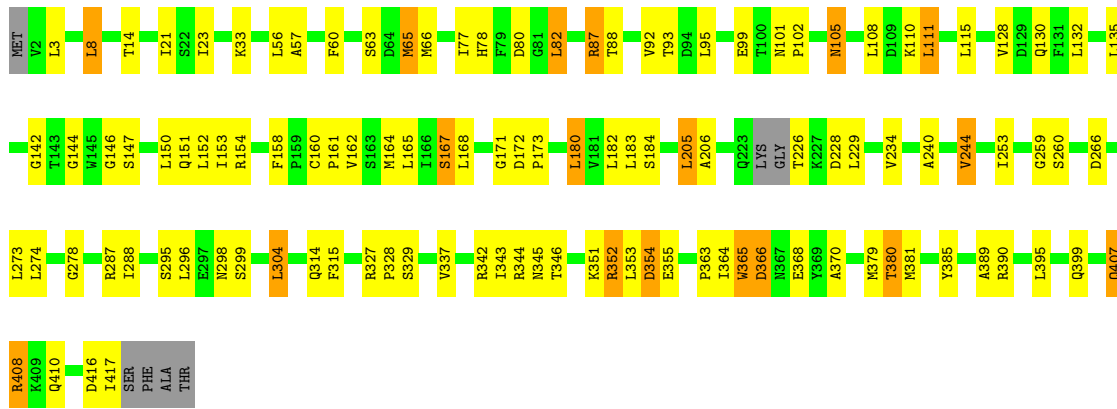


• Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN

Chain F: 72% 23% 5%



● Molecule 1: FTSZ/TUBULIN-RELATED PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.06Å 85.15Å 632.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 52.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.5 (50.00-3.00) 92.5 (52.69-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.232 , 0.284 0.235 , 0.237	Depositor DCC
R_{free} test set	2694 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtrriage
Anisotropy	0.968	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	22638	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GSP

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	0.56	0/3215	0.66	0/4348
1	B	0.57	0/3221	0.67	0/4356
1	C	0.57	0/3308	0.66	0/4472
1	D	0.58	1/3236 (0.0%)	0.67	1/4377 (0.0%)
1	E	0.59	0/3180	0.69	0/4302
1	F	0.60	1/3336 (0.0%)	0.68	0/4510
1	G	0.59	0/3339	0.69	2/4513 (0.0%)
All	All	0.58	2/22835 (0.0%)	0.67	3/30878 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	297	GLU	CG-CD	5.15	1.59	1.51
1	F	125	GLU	CG-CD	5.04	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	352	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	D	232	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	G	229	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3155	0	3064	61	0
1	B	3160	0	3077	81	0
1	C	3246	0	3157	73	0
1	D	3175	0	3090	71	0
1	E	3119	0	3037	71	0
1	F	3274	0	3187	59	0
1	G	3278	0	3197	82	0
2	A	32	0	12	1	0
2	B	32	0	12	2	0
2	C	32	0	12	0	0
2	D	32	0	12	0	0
2	E	32	0	12	1	0
2	F	32	0	12	0	0
2	G	32	0	12	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
All	All	22638	0	21893	465	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 10.

All (465) 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:G:63:SER:HB2	1:G:66:MET:CE	1.68	1.23
1:G:288:ILE:HD13	1:G:296:LEU:HD12	1.26	1.17
1:D:288:ILE:HD13	1:D:296:LEU:HD12	1.27	1.14
1:G:288:ILE:HD13	1:G:296:LEU:CD1	1.77	1.12
1:G:63:SER:HB2	1:G:66:MET:HE1	1.35	1.06
1:G:288:ILE:CD1	1:G:296:LEU:HD12	1.90	1.01
1:D:288:ILE:CD1	1:D:296:LEU:HD12	1.92	0.98
1:A:341:ASN:HA	1:A:344:ARG:HB3	1.46	0.96
1:G:288:ILE:CD1	1:G:296:LEU:CD1	2.44	0.93
1:G:63:SER:HB2	1:G:66:MET:HE2	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:183:LEU:HD22	1:D:381:MET:HE3	1.58	0.84
1:E:288:ILE:CD1	1:E:296:LEU:HD12	2.06	0.84
1:B:95:LEU:HD21	1:B:107:TYR:CG	2.11	0.84
1:B:288:ILE:CD1	1:B:296:LEU:HD12	2.08	0.84
1:C:355:GLU:O	1:C:356:ILE:HG23	1.77	0.83
1:F:357:ALA:HA	1:G:172:ASP:OD2	1.79	0.83
1:A:58:VAL:HG11	1:A:145:TRP:CZ2	2.13	0.83
1:G:23:ILE:HD12	1:G:274:LEU:HD12	1.60	0.82
1:F:23:ILE:HD12	1:F:274:LEU:HD12	1.60	0.82
1:B:288:ILE:HD13	1:B:296:LEU:HD12	1.61	0.81
1:E:23:ILE:HD12	1:E:274:LEU:HD12	1.62	0.81
1:C:82:LEU:HD11	1:C:91:VAL:HG12	1.63	0.81
1:B:82:LEU:HD12	1:B:82:LEU:H	1.44	0.80
1:A:23:ILE:HD12	1:A:274:LEU:HD12	1.64	0.80
1:D:268:SER:OG	1:E:85:ALA:O	2.01	0.79
1:B:400:GLU:O	1:B:404:ALA:HB2	1.83	0.79
1:D:23:ILE:HD12	1:D:274:LEU:HD12	1.64	0.79
1:B:15:ASN:OD1	1:B:17:SER:N	2.16	0.79
1:B:126:VAL:HG12	1:B:128:VAL:H	1.48	0.78
1:E:183:LEU:HD22	1:E:381:MET:HE3	1.65	0.78
1:B:2:VAL:HG21	1:B:43:GLY:C	2.02	0.78
1:G:63:SER:O	1:G:66:MET:HG2	1.84	0.77
1:A:59:ASN:HB2	1:A:65:MET:HE3	1.65	0.77
1:C:23:ILE:HD12	1:C:274:LEU:HD12	1.67	0.77
1:F:116:GLY:O	1:F:120:THR:OG1	2.03	0.76
1:A:81:GLY:O	1:A:82:LEU:HD23	1.87	0.75
1:A:3:LEU:HD13	1:A:9:GLU:HA	1.69	0.75
1:G:288:ILE:HB	1:G:370:ALA:HB3	1.69	0.74
1:B:23:ILE:HD12	1:B:274:LEU:HD12	1.69	0.74
1:F:288:ILE:HD13	1:F:296:LEU:HD12	1.70	0.74
1:B:95:LEU:HD11	1:B:107:TYR:CZ	2.22	0.73
1:C:258:TYR:C	1:D:66:MET:HE3	2.08	0.73
1:C:82:LEU:CD1	1:C:91:VAL:HG12	2.19	0.72
1:C:183:LEU:HD22	1:C:381:MET:HE3	1.71	0.72
1:D:288:ILE:HD13	1:D:296:LEU:CD1	2.16	0.72
1:A:357:ALA:HB2	1:B:174:ASP:OD1	1.92	0.69
1:C:77:ILE:HG22	1:C:79:PHE:CE2	2.27	0.69
1:B:183:LEU:HD22	1:B:381:MET:HE3	1.73	0.68
1:A:141:VAL:HG23	2:A:900:GSP:S1G	2.34	0.68
1:G:288:ILE:HD13	1:G:296:LEU:HD13	1.73	0.68
1:B:77:ILE:HG22	1:B:79:PHE:CE2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:288:ILE:HD13	1:E:296:LEU:HD12	1.74	0.67
1:D:391:GLU:O	1:D:395:LEU:HD23	1.95	0.66
1:D:288:ILE:CD1	1:D:296:LEU:CD1	2.70	0.66
1:F:288:ILE:CD1	1:F:296:LEU:HD12	2.26	0.66
1:G:56:LEU:HD22	1:G:77:ILE:CD1	2.25	0.66
1:B:393:LYS:HD3	1:C:417:ILE:HG23	1.78	0.66
1:G:60:PHE:O	1:G:78:HIS:CD2	2.48	0.66
1:A:58:VAL:HG11	1:A:145:TRP:CE2	2.31	0.65
1:C:341:ASN:HA	1:C:344:ARG:HB3	1.78	0.65
1:B:95:LEU:C	1:B:95:LEU:HD23	2.16	0.65
1:F:183:LEU:HD22	1:F:381:MET:HE3	1.78	0.65
1:A:183:LEU:HD22	1:A:381:MET:HE3	1.78	0.64
1:B:111:LEU:HD22	1:B:115:LEU:HD22	1.79	0.64
1:G:328:PRO:HA	1:G:365:TRP:O	1.98	0.64
1:G:351:LYS:NZ	1:G:355:GLU:OE2	2.27	0.64
1:G:65:MET:HE1	1:G:77:ILE:O	1.98	0.63
1:G:63:SER:O	1:G:66:MET:HE2	1.98	0.63
1:D:228:ASP:OD2	1:D:228:ASP:C	2.37	0.63
1:G:183:LEU:HD22	1:G:381:MET:HE3	1.80	0.63
1:C:288:ILE:HD13	1:C:296:LEU:HD12	1.80	0.63
1:E:58:VAL:HG11	1:E:145:TRP:CH2	2.33	0.62
1:F:177:ASN:O	1:F:181:VAL:HG13	1.99	0.62
1:G:56:LEU:HD22	1:G:77:ILE:HD11	1.81	0.62
1:C:288:ILE:CD1	1:C:296:LEU:HD12	2.30	0.62
1:D:56:LEU:HD22	1:D:77:ILE:CD1	2.29	0.62
1:F:358:GLY:N	1:G:172:ASP:OD2	2.30	0.62
1:D:21:ILE:HG22	1:D:253:ILE:HD13	1.82	0.62
1:D:2:VAL:HG23	1:D:2:VAL:O	1.99	0.61
1:D:23:ILE:CD1	1:D:274:LEU:HD12	2.31	0.61
1:C:56:LEU:HD22	1:C:77:ILE:CD1	2.31	0.61
1:F:23:ILE:CD1	1:F:274:LEU:HD12	2.30	0.60
1:D:262:ASN:ND2	1:D:263:VAL:HG23	2.15	0.60
1:F:122:GLU:OE2	1:F:122:GLU:HA	2.01	0.60
1:G:78:HIS:O	1:G:110:LYS:NZ	2.34	0.60
1:A:176:ILE:HG23	1:A:388:LEU:HD22	1.82	0.60
1:B:56:LEU:HD22	1:B:77:ILE:CD1	2.31	0.60
1:A:21:ILE:HG22	1:A:253:ILE:HD13	1.84	0.59
1:D:54:PRO:HB2	1:D:119:PHE:CE2	2.37	0.59
1:G:23:ILE:CD1	1:G:274:LEU:HD12	2.31	0.59
1:B:126:VAL:HG12	1:B:128:VAL:N	2.17	0.59
1:C:65:MET:HE1	1:C:77:ILE:N	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ILE:HG22	1:B:253:ILE:HD13	1.84	0.59
1:C:56:LEU:HD22	1:C:77:ILE:HD11	1.83	0.59
1:A:23:ILE:CD1	1:A:274:LEU:HD12	2.31	0.59
1:C:65:MET:HE1	1:C:76:ARG:C	2.22	0.59
1:E:23:ILE:CD1	1:E:274:LEU:HD12	2.32	0.59
1:E:321:TYR:CE1	1:E:353:LEU:HD13	2.37	0.59
1:F:56:LEU:HD22	1:F:77:ILE:CD1	2.32	0.59
1:G:63:SER:CB	1:G:66:MET:HE2	2.29	0.59
1:E:337:VAL:HG23	1:F:234:VAL:O	2.03	0.59
1:D:56:LEU:HD22	1:D:77:ILE:HD11	1.84	0.58
1:B:56:LEU:HD22	1:B:77:ILE:HD11	1.86	0.58
1:E:56:LEU:HD22	1:E:77:ILE:CD1	2.34	0.58
1:F:153:ILE:HG22	1:F:158:PHE:CD1	2.39	0.58
1:F:56:LEU:HD22	1:F:77:ILE:HD11	1.84	0.57
1:G:93:THR:HG22	1:G:144:GLY:O	2.04	0.57
1:E:153:ILE:HG22	1:E:158:PHE:CD1	2.39	0.57
1:B:23:ILE:CD1	1:B:274:LEU:HD12	2.35	0.57
1:C:153:ILE:HG22	1:C:158:PHE:CD1	2.39	0.57
1:G:206:ALA:O	1:G:278:GLY:HA2	2.05	0.57
1:A:56:LEU:HD22	1:A:77:ILE:CD1	2.35	0.56
1:C:23:ILE:CD1	1:C:274:LEU:HD12	2.35	0.56
1:D:153:ILE:HG22	1:D:158:PHE:CD1	2.41	0.56
1:F:401:GLN:HG2	1:F:402:LEU:N	2.20	0.56
1:A:176:ILE:CG2	1:A:388:LEU:HD22	2.36	0.56
1:B:381:MET:HB3	1:C:410:GLN:HE22	1.71	0.56
1:E:177:ASN:O	1:E:181:VAL:HG13	2.06	0.56
1:C:21:ILE:HG22	1:C:253:ILE:HD13	1.87	0.55
1:C:61:ALA:HB2	1:C:87:ARG:NH1	2.21	0.55
1:F:21:ILE:HG22	1:F:253:ILE:HD13	1.87	0.55
1:C:77:ILE:CG2	1:C:79:PHE:CE2	2.89	0.55
1:G:82:LEU:HD13	1:G:95:LEU:HD22	1.88	0.55
1:D:183:LEU:HD22	1:D:381:MET:CE	2.32	0.55
1:E:103:ASN:N	1:E:103:ASN:OD1	2.39	0.55
1:A:56:LEU:HD22	1:A:77:ILE:HD11	1.89	0.54
1:B:160:CYS:HB2	1:B:161:PRO:CD	2.37	0.54
1:B:320:MET:HG3	1:B:357:ALA:HB3	1.90	0.54
1:C:90:SER:HA	1:C:93:THR:HG23	1.89	0.54
1:E:183:LEU:HD22	1:E:381:MET:CE	2.36	0.54
1:G:173:PRO:HB3	1:G:395:LEU:HD12	1.89	0.54
1:G:329:SER:HA	1:G:364:ILE:HG21	1.90	0.54
1:A:160:CYS:HB2	1:A:161:PRO:CD	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ALA:O	1:C:278:GLY:HA2	2.08	0.54
1:D:91:VAL:HG12	1:D:91:VAL:O	2.07	0.54
1:A:153:ILE:HG22	1:A:158:PHE:CD1	2.43	0.53
1:D:380:THR:HG23	1:D:381:MET:N	2.23	0.53
1:B:95:LEU:HD11	1:B:107:TYR:CE2	2.43	0.53
1:D:11:ILE:HG22	1:D:365:TRP:HE3	1.73	0.53
1:E:56:LEU:HD22	1:E:77:ILE:HD11	1.89	0.53
1:A:359:LYS:NZ	2:B:900:GSP:O3G	2.41	0.53
1:E:87:ARG:NH2	2:E:900:GSP:O2G	2.42	0.53
1:D:160:CYS:HB2	1:D:161:PRO:CD	2.39	0.53
1:E:57:ALA:CB	1:E:65:MET:HE2	2.39	0.53
1:F:160:CYS:HB2	1:F:161:PRO:CD	2.39	0.53
1:G:228:ASP:OD2	1:G:228:ASP:C	2.47	0.53
1:D:111:LEU:HD22	1:D:115:LEU:HD22	1.91	0.53
1:D:177:ASN:O	1:D:181:VAL:HG13	2.09	0.53
1:D:14:THR:CG2	1:D:366:ASP:HB2	2.39	0.52
1:G:160:CYS:HB2	1:G:161:PRO:CD	2.39	0.52
1:G:353:LEU:HD23	1:G:353:LEU:N	2.22	0.52
1:E:57:ALA:C	1:E:65:MET:CE	2.78	0.52
1:A:57:ALA:HB1	1:A:65:MET:HE2	1.92	0.52
1:B:62:GLU:OE2	1:B:78:HIS:CB	2.58	0.52
1:F:357:ALA:CA	1:G:172:ASP:OD2	2.54	0.52
1:A:58:VAL:CA	1:A:65:MET:HE1	2.39	0.52
1:B:153:ILE:HG22	1:B:158:PHE:CD1	2.45	0.52
1:B:240:ALA:O	1:B:244:VAL:HG13	2.09	0.52
1:F:336:ASP:OD1	1:F:338:ASN:HB2	2.09	0.52
1:G:153:ILE:HG22	1:G:158:PHE:CD1	2.45	0.52
1:A:334:PHE:HA	1:A:339:THR:HG21	1.92	0.52
1:B:61:ALA:HB2	1:B:87:ARG:NH2	2.25	0.52
1:F:380:THR:HG23	1:F:381:MET:N	2.25	0.52
1:E:206:ALA:O	1:E:278:GLY:HA2	2.10	0.51
1:E:337:VAL:HG22	1:F:236:TRP:HB3	1.92	0.51
1:E:288:ILE:HD11	1:E:296:LEU:HD12	1.89	0.51
1:E:57:ALA:HB3	1:E:65:MET:HE2	1.92	0.51
1:E:364:ILE:HD12	1:F:67:HIS:CE1	2.45	0.51
1:C:2:VAL:HG23	1:C:44:TYR:CD1	2.45	0.51
1:C:183:LEU:HD22	1:C:381:MET:CE	2.41	0.51
1:D:264:THR:HG21	1:E:63:SER:HB2	1.92	0.51
1:E:126:VAL:HG21	1:E:159:PRO:CB	2.41	0.51
1:G:21:ILE:HG22	1:G:253:ILE:HD13	1.92	0.51
1:G:135:LEU:HD22	1:G:142:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:PRO:HG3	1:E:395:LEU:HD22	1.93	0.51
1:G:162:VAL:O	1:G:205:LEU:HD23	2.10	0.51
1:A:357:ALA:CB	1:B:174:ASP:OD1	2.58	0.51
1:C:160:CYS:HB2	1:C:161:PRO:CD	2.41	0.51
1:C:177:ASN:O	1:C:181:VAL:HG13	2.11	0.51
1:D:258:TYR:C	1:E:66:MET:HE3	2.31	0.51
1:A:98:PRO:HA	1:A:101:ASN:O	2.11	0.51
1:F:261:ASP:OD2	1:F:364:ILE:HD11	2.11	0.51
1:B:62:GLU:OE2	1:B:78:HIS:HB2	2.10	0.51
1:F:135:LEU:HD22	1:F:142:GLY:O	2.11	0.51
1:A:183:LEU:HD22	1:A:381:MET:CE	2.41	0.51
1:B:162:VAL:O	1:B:205:LEU:HD23	2.11	0.50
1:E:397:GLU:HA	1:E:400:GLU:HB2	1.93	0.50
1:G:206:ALA:HB1	1:G:274:LEU:O	2.11	0.50
1:C:206:ALA:HB1	1:C:274:LEU:O	2.11	0.50
1:C:315:PHE:CD2	1:C:379:MET:CE	2.94	0.50
1:E:240:ALA:O	1:E:244:VAL:HG13	2.11	0.50
1:E:11:ILE:CG2	1:E:365:TRP:HZ3	2.25	0.50
1:B:183:LEU:HD22	1:B:381:MET:CE	2.42	0.50
1:B:355:GLU:CB	1:C:395:LEU:HD22	2.41	0.50
1:B:380:THR:HG23	1:B:381:MET:N	2.26	0.50
1:D:259:GLY:N	1:E:66:MET:HE3	2.27	0.50
1:A:168:LEU:HD21	1:A:183:LEU:HD11	1.93	0.50
1:B:364:ILE:HG22	1:B:365:TRP:N	2.26	0.50
1:F:2:VAL:HG23	1:F:44:TYR:CD1	2.46	0.50
1:B:297:GLU:HG3	1:B:346:THR:OG1	2.11	0.50
1:F:330:ASN:CG	1:F:331:ALA:N	2.64	0.50
1:G:82:LEU:HD23	1:G:87:ARG:HG3	1.94	0.50
1:A:162:VAL:O	1:A:205:LEU:HD23	2.11	0.50
1:C:319:THR:HA	1:C:356:ILE:HG21	1.94	0.50
1:G:56:LEU:HD22	1:G:77:ILE:HD12	1.93	0.50
1:A:21:ILE:C	1:A:256:GLU:HG3	2.31	0.50
1:C:93:THR:HG22	1:C:144:GLY:CA	2.41	0.50
1:A:206:ALA:O	1:A:278:GLY:HA2	2.12	0.49
1:D:337:VAL:HG23	1:D:338:ASN:OD1	2.12	0.49
1:B:82:LEU:HD22	1:B:85:ALA:CB	2.42	0.49
1:B:364:ILE:CG2	1:B:365:TRP:N	2.75	0.49
1:E:21:ILE:HG22	1:E:253:ILE:HD13	1.94	0.49
1:E:11:ILE:CG2	1:E:365:TRP:CZ3	2.96	0.49
1:A:315:PHE:CD2	1:A:379:MET:CE	2.96	0.49
1:B:21:ILE:HD12	1:B:23:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:CYS:HB2	1:B:161:PRO:HD2	1.94	0.49
1:C:33:LYS:HE3	1:C:167:SER:HB3	1.95	0.49
1:D:206:ALA:O	1:D:278:GLY:HA2	2.13	0.49
1:E:160:CYS:HB2	1:E:161:PRO:CD	2.42	0.49
1:G:288:ILE:HD11	1:G:296:LEU:HD12	1.88	0.49
1:F:2:VAL:HG22	1:F:43:GLY:HA3	1.94	0.49
1:C:121:ASN:HB3	1:C:123:GLU:N	2.27	0.49
1:C:380:THR:HG23	1:C:381:MET:N	2.27	0.49
1:E:10:HIS:HB3	1:E:367:ASN:ND2	2.28	0.49
1:B:33:LYS:HE3	1:B:167:SER:HB3	1.95	0.49
1:A:98:PRO:HG3	1:A:104:ALA:HB3	1.94	0.48
1:E:320:MET:HG3	1:E:357:ALA:O	2.13	0.48
1:B:266:ASP:HB2	1:B:267:PRO:CD	2.43	0.48
1:C:162:VAL:O	1:C:205:LEU:HD23	2.13	0.48
1:B:100:THR:HG22	1:B:101:ASN:N	2.29	0.48
1:D:183:LEU:HD13	1:D:381:MET:HE1	1.95	0.48
1:D:293:LEU:HD13	1:D:342:ARG:HB2	1.96	0.48
1:G:168:LEU:HD21	1:G:183:LEU:HD11	1.95	0.48
1:G:343:ILE:O	1:G:346:THR:N	2.47	0.48
1:B:315:PHE:CD2	1:B:379:MET:CE	2.97	0.48
1:D:14:THR:HG21	1:D:366:ASP:HB2	1.96	0.48
1:E:334:PHE:HA	1:E:339:THR:HG21	1.96	0.48
1:C:58:VAL:HG11	1:C:145:TRP:CH2	2.49	0.48
1:A:354:ASP:HA	1:B:171:GLY:O	2.14	0.48
1:F:315:PHE:CD2	1:F:379:MET:CE	2.96	0.48
1:F:320:MET:HG3	1:F:357:ALA:O	2.13	0.48
1:B:397:GLU:O	1:B:398:LYS:C	2.52	0.48
1:C:149:VAL:HG11	1:C:164:MET:HE2	1.95	0.48
1:C:171:GLY:HA2	1:C:176:ILE:HD11	1.96	0.48
1:D:162:VAL:O	1:D:205:LEU:HD23	2.13	0.48
1:C:315:PHE:HA	1:C:379:MET:CE	2.44	0.47
1:D:95:LEU:HD11	1:D:107:TYR:CE1	2.49	0.47
1:G:101:ASN:OD1	1:G:101:ASN:C	2.52	0.47
1:C:330:ASN:O	1:C:332:ASP:N	2.45	0.47
1:D:264:THR:HG22	1:D:265:TYR:O	2.14	0.47
1:G:111:LEU:HD23	1:G:115:LEU:HD13	1.96	0.47
1:E:33:LYS:HE3	1:E:167:SER:HB3	1.96	0.47
1:F:33:LYS:HE3	1:F:167:SER:CB	2.44	0.47
1:F:402:LEU:HA	1:F:405:GLU:HB2	1.95	0.47
1:B:206:ALA:HB1	1:B:274:LEU:O	2.14	0.47
1:E:33:LYS:HE3	1:E:167:SER:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:LEU:HD21	1:E:183:LEU:HD11	1.95	0.47
1:F:121:ASN:HB2	1:F:125:GLU:O	2.13	0.47
1:G:3:LEU:HD22	1:G:8:LEU:HB3	1.95	0.47
1:A:33:LYS:HE3	1:A:167:SER:HB3	1.96	0.47
1:G:105:ASN:HA	1:G:108:LEU:HB2	1.97	0.47
1:B:206:ALA:O	1:B:278:GLY:HA2	2.14	0.47
1:F:315:PHE:HA	1:F:379:MET:CE	2.45	0.47
1:G:329:SER:HA	1:G:364:ILE:CG2	2.44	0.47
1:B:33:LYS:HE3	1:B:167:SER:CB	2.44	0.47
1:B:54:PRO:HB2	1:B:119:PHE:CE2	2.50	0.47
1:C:95:LEU:HD23	1:C:95:LEU:O	2.15	0.47
1:D:315:PHE:CD2	1:D:379:MET:CE	2.98	0.47
1:E:259:GLY:HA3	1:F:66:MET:HE2	1.97	0.47
1:G:57:ALA:O	1:G:65:MET:HE2	2.15	0.47
1:G:33:LYS:HE3	1:G:167:SER:HB3	1.97	0.47
1:E:183:LEU:HD13	1:E:381:MET:HE1	1.96	0.47
1:F:160:CYS:HB2	1:F:161:PRO:HD2	1.97	0.47
1:G:14:THR:HG21	1:G:366:ASP:OD2	2.14	0.47
1:A:33:LYS:HE3	1:A:167:SER:CB	2.45	0.47
1:F:183:LEU:HD13	1:F:381:MET:HE1	1.97	0.47
1:A:380:THR:HG23	1:A:381:MET:N	2.30	0.46
1:F:33:LYS:HE3	1:F:167:SER:HB3	1.97	0.46
1:G:183:LEU:HD22	1:G:381:MET:CE	2.45	0.46
1:C:183:LEU:HB3	1:C:381:MET:HE1	1.97	0.46
1:A:180:LEU:HD21	1:A:389:ALA:HA	1.97	0.46
1:F:168:LEU:HD21	1:F:183:LEU:HD11	1.98	0.46
1:B:307:GLY:O	1:B:310:SER:OG	2.34	0.46
1:E:87:ARG:HD2	1:E:139:GLY:HA2	1.97	0.46
1:E:291:PHE:HB3	1:E:333:PHE:CD2	2.51	0.46
1:B:95:LEU:HD21	1:B:107:TYR:CD1	2.50	0.46
1:D:54:PRO:HB2	1:D:119:PHE:HE2	1.80	0.46
1:B:321:TYR:CG	1:B:353:LEU:HD22	2.51	0.46
1:G:160:CYS:HB2	1:G:161:PRO:HD2	1.98	0.46
1:C:115:LEU:HD12	1:C:115:LEU:HA	1.65	0.46
1:C:160:CYS:HB2	1:C:161:PRO:HD2	1.98	0.46
1:D:259:GLY:HA3	1:E:66:MET:HE2	1.98	0.46
1:F:101:ASN:O	1:F:104:ALA:HB2	2.16	0.46
1:C:354:ASP:HB2	1:D:398:LYS:HZ1	1.80	0.46
1:D:2:VAL:O	1:D:2:VAL:CG2	2.63	0.46
1:D:160:CYS:HB2	1:D:161:PRO:HD2	1.97	0.46
1:C:88:THR:HB	1:C:89:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:HIS:HB3	1:D:367:ASN:CG	2.36	0.45
1:E:341:ASN:HA	1:E:344:ARG:HB3	1.98	0.45
1:F:162:VAL:O	1:F:205:LEU:HD23	2.15	0.45
1:G:63:SER:CB	1:G:66:MET:HE1	2.24	0.45
1:B:95:LEU:HD21	1:B:107:TYR:CD2	2.49	0.45
1:C:33:LYS:HE3	1:C:167:SER:CB	2.45	0.45
1:E:173:PRO:O	1:E:177:ASN:CG	2.55	0.45
1:B:62:GLU:HG2	1:B:78:HIS:CD2	2.51	0.45
1:D:240:ALA:O	1:D:244:VAL:HG13	2.17	0.45
1:C:82:LEU:CD1	1:C:91:VAL:CG1	2.91	0.45
1:D:85:ALA:HB1	1:D:91:VAL:HB	1.99	0.45
1:A:177:ASN:O	1:A:181:VAL:HG13	2.17	0.45
1:C:183:LEU:HD13	1:C:381:MET:HE1	1.99	0.45
1:C:321:TYR:CZ	1:C:353:LEU:HD23	2.52	0.45
1:E:315:PHE:CD2	1:E:379:MET:CE	3.00	0.45
1:F:126:VAL:HG21	1:F:159:PRO:CB	2.47	0.45
1:C:121:ASN:HB3	1:C:123:GLU:H	1.82	0.45
1:D:168:LEU:HD21	1:D:183:LEU:HD11	1.99	0.45
1:E:380:THR:HG23	1:E:381:MET:N	2.32	0.45
1:G:381:MET:HE2	1:G:385:TYR:HB2	1.99	0.45
1:E:354:ASP:O	1:F:173:PRO:HD3	2.17	0.45
1:A:79:PHE:O	1:A:80:ASP:C	2.55	0.45
1:A:160:CYS:HB2	1:A:161:PRO:HD2	1.98	0.45
1:C:82:LEU:HG	1:C:95:LEU:HD12	1.97	0.45
1:E:180:LEU:HD21	1:E:389:ALA:HA	1.99	0.45
1:B:56:LEU:HD22	1:B:77:ILE:HD12	2.00	0.45
1:B:149:VAL:HG11	1:B:164:MET:HE2	1.98	0.44
1:E:11:ILE:HG22	1:E:365:TRP:CE3	2.52	0.44
1:E:97:ASP:OD1	1:E:99:GLU:HB3	2.17	0.44
1:A:183:LEU:HB3	1:A:381:MET:HE1	2.00	0.44
1:B:386:ILE:HD11	1:C:409:LYS:NZ	2.32	0.44
1:D:33:LYS:HE3	1:D:167:SER:HB3	2.00	0.44
1:E:56:LEU:CD1	1:E:115:LEU:HD12	2.47	0.44
1:E:315:PHE:HA	1:E:379:MET:HE3	1.99	0.44
1:F:351:LYS:HD2	1:F:356:ILE:HD13	1.99	0.44
1:A:58:VAL:C	1:A:65:MET:HE1	2.37	0.44
1:A:315:PHE:HA	1:A:379:MET:CE	2.47	0.44
1:B:357:ALA:HA	1:C:172:ASP:OD2	2.17	0.44
1:G:110:LYS:O	1:G:111:LEU:C	2.54	0.44
1:A:60:PHE:CZ	1:A:81:GLY:HA3	2.52	0.44
1:B:168:LEU:HD21	1:B:183:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:THR:HG22	1:E:265:TYR:N	2.32	0.44
1:F:357:ALA:HA	1:G:172:ASP:CG	2.37	0.44
1:G:33:LYS:HE3	1:G:167:SER:CB	2.47	0.44
1:A:135:LEU:HD22	1:A:142:GLY:O	2.18	0.44
1:A:261:ASP:OD2	1:A:364:ILE:HD11	2.17	0.44
1:A:337:VAL:CG1	1:B:236:TRP:HB3	2.48	0.44
1:C:293:LEU:HD22	1:C:342:ARG:HG2	1.99	0.44
1:C:307:GLY:O	1:C:310:SER:OG	2.32	0.44
1:D:60:PHE:CD1	1:D:82:LEU:CD2	3.00	0.44
1:C:14:THR:CG2	1:C:366:ASP:HB2	2.47	0.44
1:C:314:GLN:OE1	1:C:380:THR:CG2	2.66	0.44
1:D:33:LYS:HE3	1:D:167:SER:CB	2.48	0.44
1:D:56:LEU:HD22	1:D:77:ILE:HD12	1.97	0.44
1:G:353:LEU:O	1:G:354:ASP:C	2.56	0.44
1:B:58:VAL:HG13	1:B:79:PHE:CE2	2.53	0.44
1:E:135:LEU:HD22	1:E:142:GLY:O	2.18	0.44
1:E:307:GLY:O	1:E:310:SER:OG	2.36	0.44
1:F:183:LEU:HB3	1:F:381:MET:HE1	2.00	0.44
1:A:57:ALA:C	1:A:65:MET:HE1	2.38	0.44
1:E:173:PRO:HB3	1:E:395:LEU:HD13	1.99	0.44
1:E:315:PHE:HA	1:E:379:MET:CE	2.48	0.44
1:F:315:PHE:HA	1:F:379:MET:HE3	2.00	0.44
1:D:180:LEU:HD21	1:D:389:ALA:HA	2.00	0.43
1:F:115:LEU:HD12	1:F:115:LEU:HA	1.85	0.43
1:G:180:LEU:HD21	1:G:389:ALA:HA	2.00	0.43
1:D:206:ALA:HB1	1:D:274:LEU:O	2.17	0.43
1:E:338:ASN:O	1:E:339:THR:C	2.56	0.43
1:F:121:ASN:HB3	1:F:124:GLY:H	1.84	0.43
1:D:11:ILE:HG22	1:D:365:TRP:CE3	2.52	0.43
1:G:314:GLN:OE1	1:G:380:THR:CG2	2.67	0.43
1:A:58:VAL:N	1:A:65:MET:HE1	2.33	0.43
1:A:14:THR:CG2	1:A:366:ASP:HB2	2.49	0.43
1:A:315:PHE:CD2	1:A:379:MET:HE1	2.54	0.43
1:C:82:LEU:HG	1:C:95:LEU:CD1	2.49	0.43
1:E:160:CYS:HB2	1:E:161:PRO:HD2	2.01	0.43
1:E:235:ASN:OD1	1:E:238:GLU:HB2	2.19	0.43
1:A:337:VAL:HG13	1:B:236:TRP:HB3	2.00	0.43
1:C:240:ALA:O	1:C:244:VAL:HG13	2.18	0.43
1:D:333:PHE:HB2	1:E:233:TYR:CZ	2.54	0.43
1:E:56:LEU:HD22	1:E:77:ILE:HD12	2.01	0.43
1:G:82:LEU:HD23	1:G:87:ARG:CD	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ALA:HB1	1:A:274:LEU:O	2.19	0.43
1:A:365:TRP:CE2	1:A:367:ASN:HB2	2.53	0.43
1:B:2:VAL:HG21	1:B:43:GLY:CA	2.47	0.43
1:B:400:GLU:O	1:B:404:ALA:CB	2.61	0.43
1:C:10:HIS:HB3	1:C:367:ASN:OD1	2.19	0.43
1:B:348:GLY:HA2	1:B:352:ARG:HA	2.00	0.43
1:F:109:ASP:O	1:F:113:GLN:HB2	2.18	0.43
1:F:153:ILE:HG22	1:F:158:PHE:HD1	1.82	0.43
1:F:240:ALA:O	1:F:244:VAL:HG13	2.19	0.43
1:G:327:ARG:O	1:G:364:ILE:HA	2.19	0.43
1:G:343:ILE:O	1:G:344:ARG:C	2.57	0.43
1:C:259:GLY:N	1:D:66:MET:HE3	2.33	0.42
1:D:176:ILE:HG12	1:D:388:LEU:HD22	2.01	0.42
1:F:82:LEU:HD21	1:F:95:LEU:CD1	2.49	0.42
1:F:180:LEU:HD21	1:F:389:ALA:HA	2.01	0.42
1:G:146:GLY:HA2	1:G:164:MET:HE1	2.01	0.42
1:G:315:PHE:CD2	1:G:379:MET:CE	3.01	0.42
1:B:321:TYR:CD1	1:B:353:LEU:HD22	2.54	0.42
1:G:260:SER:HB2	1:G:363:PRO:HA	2.01	0.42
1:G:93:THR:HG21	1:G:147:SER:HB2	2.00	0.42
1:G:380:THR:HG23	1:G:381:MET:N	2.35	0.42
1:B:82:LEU:HB2	1:B:85:ALA:HB3	2.02	0.42
1:G:183:LEU:HD13	1:G:381:MET:HE1	2.02	0.42
1:A:3:LEU:HD22	1:A:8:LEU:HB3	2.02	0.42
1:D:321:TYR:CE2	1:D:353:LEU:HD22	2.54	0.42
1:E:259:GLY:N	1:F:66:MET:HE3	2.35	0.42
1:G:315:PHE:HA	1:G:379:MET:CE	2.49	0.42
1:C:114:GLU:OE1	1:C:114:GLU:HA	2.19	0.42
1:D:307:GLY:O	1:D:310:SER:OG	2.37	0.42
1:G:240:ALA:O	1:G:244:VAL:HG13	2.20	0.42
1:G:304:LEU:HD12	1:G:304:LEU:HA	1.94	0.42
1:C:56:LEU:HD22	1:C:77:ILE:HD12	2.01	0.42
1:F:58:VAL:HG11	1:F:145:TRP:CH2	2.54	0.42
1:G:82:LEU:HD23	1:G:87:ARG:HD3	2.02	0.42
1:B:95:LEU:C	1:B:95:LEU:CD2	2.87	0.42
1:B:264:THR:O	1:B:264:THR:HG22	2.18	0.42
1:A:14:THR:HG21	1:A:366:ASP:HB2	2.01	0.42
1:D:304:LEU:HD12	1:D:304:LEU:HA	1.92	0.42
1:A:304:LEU:HD12	1:A:304:LEU:HA	1.91	0.41
1:B:58:VAL:HG13	1:B:79:PHE:HE2	1.85	0.41
1:D:89:PRO:HG3	1:D:143:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:VAL:HG11	1:E:145:TRP:CZ2	2.55	0.41
1:E:206:ALA:HB1	1:E:274:LEU:O	2.20	0.41
1:G:315:PHE:HA	1:G:379:MET:HE3	2.01	0.41
1:G:407:GLN:O	1:G:408:ARG:C	2.58	0.41
1:G:352:ARG:NH2	1:G:352:ARG:HB3	2.35	0.41
1:C:354:ASP:HB3	1:D:398:LYS:NZ	2.34	0.41
1:G:343:ILE:O	1:G:345:ASN:N	2.54	0.41
1:D:223:GLN:HE21	1:D:223:GLN:HB2	1.68	0.41
1:E:336:ASP:OD1	1:E:338:ASN:HB2	2.21	0.41
1:G:88:THR:O	1:G:92:VAL:HG23	2.20	0.41
1:D:135:LEU:HD22	1:D:142:GLY:O	2.20	0.41
1:B:180:LEU:HD21	1:B:389:ALA:HA	2.01	0.41
1:B:183:LEU:HB3	1:B:381:MET:HE1	2.03	0.41
1:B:183:LEU:HD13	1:B:381:MET:HE1	2.02	0.41
1:D:91:VAL:O	1:D:91:VAL:CG1	2.67	0.41
1:B:135:LEU:HD22	1:B:142:GLY:O	2.21	0.41
1:B:266:ASP:HB2	1:B:267:PRO:HD2	2.02	0.41
1:E:162:VAL:O	1:E:205:LEU:HD23	2.19	0.41
1:A:183:LEU:HD13	1:A:381:MET:HE1	2.02	0.41
1:A:265:TYR:CE1	1:A:269:ASP:HB3	2.55	0.41
1:A:315:PHE:HA	1:A:379:MET:HE2	2.03	0.41
1:B:15:ASN:OD1	1:B:16:HIS:N	2.54	0.41
1:D:132:LEU:HD23	1:D:132:LEU:HA	1.88	0.41
1:D:146:GLY:HA2	1:D:164:MET:HE1	2.02	0.41
1:F:206:ALA:O	1:F:278:GLY:HA2	2.21	0.41
1:G:151:GLN:O	1:G:154:ARG:HB3	2.21	0.41
1:B:142:GLY:N	2:B:900:GSP:O2B	2.52	0.41
1:C:259:GLY:O	1:D:67:HIS:NE2	2.54	0.41
1:C:354:ASP:CB	1:D:398:LYS:HZ1	2.34	0.41
1:C:61:ALA:HB2	1:C:87:ARG:HH11	1.86	0.40
1:C:95:LEU:CD2	1:C:107:TYR:CE1	3.04	0.40
1:F:164:MET:HB2	1:F:208:VAL:HG22	2.03	0.40
1:B:90:SER:O	1:B:94:ASP:HB2	2.21	0.40
1:C:82:LEU:HD11	1:C:91:VAL:CG1	2.42	0.40
1:D:10:HIS:HB3	1:D:367:ASN:OD1	2.21	0.40
1:E:191:ARG:NH1	1:F:411:ASP:HA	2.36	0.40
1:B:2:VAL:CG2	1:B:43:GLY:O	2.70	0.40
1:G:183:LEU:HB3	1:G:381:MET:HE1	2.04	0.40
1:A:146:GLY:HA2	1:A:164:MET:HE1	2.01	0.40
1:A:266:ASP:HB2	1:A:267:PRO:HD2	2.04	0.40
1:C:14:THR:HG21	1:C:366:ASP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:LEU:HD12	1:C:304:LEU:HA	1.91	0.40
1:D:178:ASN:O	1:D:181:VAL:HG22	2.21	0.40
1:F:57:ALA:O	1:F:65:MET:HE1	2.22	0.40
1:G:259:GLY:O	1:G:363:PRO:HA	2.21	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	393/421 (93%)	367 (93%)	24 (6%)	2 (0%)	29	68
1	B	396/421 (94%)	366 (92%)	27 (7%)	3 (1%)	19	57
1	C	406/421 (96%)	379 (93%)	22 (5%)	5 (1%)	13	48
1	D	398/421 (94%)	362 (91%)	31 (8%)	5 (1%)	12	45
1	E	391/421 (93%)	361 (92%)	26 (7%)	4 (1%)	15	53
1	F	410/421 (97%)	382 (93%)	23 (6%)	5 (1%)	13	48
1	G	410/421 (97%)	382 (93%)	25 (6%)	3 (1%)	22	60
All	All	2804/2947 (95%)	2599 (93%)	178 (6%)	27 (1%)	15	53

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	63	SER
1	E	99	GLU
1	E	340	GLU
1	F	338	ASN
1	A	62	GLU
1	D	121	ASN
1	D	406	ALA

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Mol	Chain	Res	Type
1	F	331	ALA
1	G	102	PRO
1	G	354	ASP
1	B	121	ASN
1	D	94	ASP
1	B	17	SER
1	C	115	LEU
1	C	331	ALA
1	D	127	ILE
1	F	333	PHE
1	C	340	GLU
1	A	171	GLY
1	B	171	GLY
1	C	171	GLY
1	D	171	GLY
1	E	127	ILE
1	E	171	GLY
1	F	127	ILE
1	F	171	GLY
1	G	171	GLY

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	344/363 (95%)	307 (89%)	37 (11%)	6	26
1	B	344/363 (95%)	302 (88%)	42 (12%)	5	21
1	C	354/363 (98%)	316 (89%)	38 (11%)	6	26
1	D	346/363 (95%)	308 (89%)	38 (11%)	6	25
1	E	340/363 (94%)	307 (90%)	33 (10%)	8	31
1	F	357/363 (98%)	312 (87%)	45 (13%)	4	20
1	G	358/363 (99%)	316 (88%)	42 (12%)	5	22
All	All	2443/2541 (96%)	2168 (89%)	275 (11%)	6	24

All (275) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	17	SER
1	A	32	GLN
1	A	64	ASP
1	A	65	MET
1	A	68	LEU
1	A	80	ASP
1	A	90	SER
1	A	111	LEU
1	A	115	LEU
1	A	120	THR
1	A	128	VAL
1	A	130	GLN
1	A	132	LEU
1	A	150	LEU
1	A	165	LEU
1	A	167	SER
1	A	174	ASP
1	A	180	LEU
1	A	182	LEU
1	A	184	SER
1	A	205	LEU
1	A	244	VAL
1	A	256	GLU
1	A	273	LEU
1	A	287	ARG
1	A	290	LYS
1	A	304	LEU
1	A	330	ASN
1	A	332	ASP
1	A	337	VAL
1	A	365	TRP
1	A	380	THR
1	A	395	LEU
1	A	400	GLU
1	A	403	ARG
1	A	405	GLU
1	B	2	VAL
1	B	8	LEU
1	B	16	HIS
1	B	63	SER
1	B	68	LEU

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Mol	Chain	Res	Type
1	B	82	LEU
1	B	93	THR
1	B	94	ASP
1	B	103	ASN
1	B	111	LEU
1	B	113	GLN
1	B	115	LEU
1	B	128	VAL
1	B	130	GLN
1	B	132	LEU
1	B	150	LEU
1	B	165	LEU
1	B	167	SER
1	B	180	LEU
1	B	182	LEU
1	B	184	SER
1	B	205	LEU
1	B	223	GLN
1	B	234	VAL
1	B	244	VAL
1	B	264	THR
1	B	273	LEU
1	B	287	ARG
1	B	290	LYS
1	B	295	SER
1	B	304	LEU
1	B	336	ASP
1	B	337	VAL
1	B	341	ASN
1	B	351	LYS
1	B	352	ARG
1	B	354	ASP
1	B	365	TRP
1	B	369	TYR
1	B	380	THR
1	B	403	ARG
1	B	408	ARG
1	C	8	LEU
1	C	62	GLU
1	C	63	SER
1	C	68	LEU
1	C	87	ARG

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Mol	Chain	Res	Type
1	C	93	THR
1	C	105	ASN
1	C	111	LEU
1	C	115	LEU
1	C	121	ASN
1	C	128	VAL
1	C	130	GLN
1	C	132	LEU
1	C	150	LEU
1	C	152	LEU
1	C	165	LEU
1	C	167	SER
1	C	180	LEU
1	C	182	LEU
1	C	184	SER
1	C	205	LEU
1	C	234	VAL
1	C	244	VAL
1	C	256	GLU
1	C	268	SER
1	C	273	LEU
1	C	287	ARG
1	C	292	ASP
1	C	304	LEU
1	C	310	SER
1	C	330	ASN
1	C	337	VAL
1	C	365	TRP
1	C	368	GLU
1	C	380	THR
1	C	400	GLU
1	C	405	GLU
1	C	416	ASP
1	D	8	LEU
1	D	59	ASN
1	D	82	LEU
1	D	87	ARG
1	D	97	ASP
1	D	100	THR
1	D	101	ASN
1	D	108	LEU
1	D	109	ASP

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Mol	Chain	Res	Type
1	D	111	LEU
1	D	115	LEU
1	D	118	LYS
1	D	126	VAL
1	D	128	VAL
1	D	130	GLN
1	D	132	LEU
1	D	150	LEU
1	D	165	LEU
1	D	167	SER
1	D	180	LEU
1	D	182	LEU
1	D	184	SER
1	D	205	LEU
1	D	228	ASP
1	D	232	ARG
1	D	244	VAL
1	D	256	GLU
1	D	273	LEU
1	D	287	ARG
1	D	299	SER
1	D	304	LEU
1	D	316	GLU
1	D	365	TRP
1	D	380	THR
1	D	393	LYS
1	D	401	GLN
1	D	403	ARG
1	D	407	GLN
1	E	8	LEU
1	E	62	GLU
1	E	63	SER
1	E	68	LEU
1	E	82	LEU
1	E	87	ARG
1	E	103	ASN
1	E	111	LEU
1	E	122	GLU
1	E	128	VAL
1	E	130	GLN
1	E	132	LEU
1	E	150	LEU

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Mol	Chain	Res	Type
1	E	165	LEU
1	E	167	SER
1	E	180	LEU
1	E	182	LEU
1	E	184	SER
1	E	205	LEU
1	E	223	GLN
1	E	244	VAL
1	E	257	ASN
1	E	273	LEU
1	E	287	ARG
1	E	296	LEU
1	E	304	LEU
1	E	310	SER
1	E	365	TRP
1	E	380	THR
1	E	390	ARG
1	E	395	LEU
1	E	397	GLU
1	E	400	GLU
1	F	1	MET
1	F	2	VAL
1	F	8	LEU
1	F	68	LEU
1	F	78	HIS
1	F	80	ASP
1	F	82	LEU
1	F	88	THR
1	F	103	ASN
1	F	111	LEU
1	F	115	LEU
1	F	128	VAL
1	F	130	GLN
1	F	132	LEU
1	F	150	LEU
1	F	165	LEU
1	F	167	SER
1	F	180	LEU
1	F	182	LEU
1	F	184	SER
1	F	205	LEU
1	F	244	VAL

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Mol	Chain	Res	Type
1	F	256	GLU
1	F	266	ASP
1	F	268	SER
1	F	273	LEU
1	F	287	ARG
1	F	292	ASP
1	F	299	SER
1	F	304	LEU
1	F	330	ASN
1	F	335	LYS
1	F	337	VAL
1	F	351	LYS
1	F	354	ASP
1	F	365	TRP
1	F	380	THR
1	F	397	GLU
1	F	399	GLN
1	F	401	GLN
1	F	403	ARG
1	F	407	GLN
1	F	408	ARG
1	F	411	ASP
1	F	421	THR
1	G	8	LEU
1	G	65	MET
1	G	80	ASP
1	G	82	LEU
1	G	87	ARG
1	G	99	GLU
1	G	105	ASN
1	G	111	LEU
1	G	128	VAL
1	G	130	GLN
1	G	132	LEU
1	G	150	LEU
1	G	152	LEU
1	G	165	LEU
1	G	167	SER
1	G	180	LEU
1	G	182	LEU
1	G	184	SER
1	G	205	LEU

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Mol	Chain	Res	Type
1	G	226	THR
1	G	234	VAL
1	G	244	VAL
1	G	266	ASP
1	G	273	LEU
1	G	287	ARG
1	G	295	SER
1	G	298	ASN
1	G	299	SER
1	G	304	LEU
1	G	337	VAL
1	G	342	ARG
1	G	365	TRP
1	G	366	ASP
1	G	368	GLU
1	G	380	THR
1	G	390	ARG
1	G	399	GLN
1	G	407	GLN
1	G	408	ARG
1	G	410	GLN
1	G	416	ASP
1	G	417	ILE

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

Mol	Chain	Res	Type
1	A	294	HIS
1	A	298	ASN
1	B	35	ASN
1	B	59	ASN
1	C	410	GLN
1	D	103	ASN
1	D	223	GLN
1	G	35	ASN
1	G	78	HIS
1	G	410	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	GSP	B	900	3	26,34,34	2.43	3 (11%)	27,54,54	1.79	7 (25%)
2	GSP	F	900	3	26,34,34	2.27	2 (7%)	27,54,54	1.63	8 (29%)
2	GSP	C	900	3	26,34,34	2.13	3 (11%)	27,54,54	1.54	5 (18%)
2	GSP	D	900	3	26,34,34	2.25	2 (7%)	27,54,54	1.44	4 (14%)
2	GSP	G	900	3	26,34,34	2.19	2 (7%)	27,54,54	1.69	6 (22%)
2	GSP	E	900	3	26,34,34	2.39	4 (15%)	27,54,54	1.80	7 (25%)
2	GSP	A	900	3	26,34,34	2.44	3 (11%)	27,54,54	1.68	7 (25%)

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	GSP	B	900	3	-	5/17/38/38	0/3/3/3
2	GSP	F	900	3	-	4/17/38/38	0/3/3/3
2	GSP	C	900	3	-	0/17/38/38	0/3/3/3
2	GSP	D	900	3	-	6/17/38/38	0/3/3/3
2	GSP	G	900	3	-	4/17/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GSP	E	900	3	-	5/17/38/38	0/3/3/3
2	GSP	A	900	3	-	5/17/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	GSP	PG-S1G	-10.82	1.67	1.90
2	B	900	GSP	PG-S1G	-10.13	1.68	1.90
2	F	900	GSP	PG-S1G	-9.91	1.69	1.90
2	G	900	GSP	PG-S1G	-9.72	1.69	1.90
2	E	900	GSP	PG-S1G	-9.66	1.69	1.90
2	D	900	GSP	PG-S1G	-9.51	1.70	1.90
2	C	900	GSP	PG-S1G	-8.51	1.72	1.90
2	E	900	GSP	C5-C6	-5.32	1.36	1.47
2	C	900	GSP	C5-C6	-5.16	1.36	1.47
2	B	900	GSP	C5-C6	-5.13	1.37	1.47
2	D	900	GSP	C5-C6	-4.15	1.39	1.47
2	G	900	GSP	C5-C6	-3.63	1.40	1.47
2	F	900	GSP	C5-C6	-3.63	1.40	1.47
2	A	900	GSP	C5-C6	-3.52	1.40	1.47
2	C	900	GSP	C2-N3	2.67	1.39	1.33
2	B	900	GSP	C5-C4	-2.52	1.36	1.43
2	E	900	GSP	C2-N3	2.38	1.38	1.33
2	A	900	GSP	C2'-C1'	-2.16	1.50	1.53
2	E	900	GSP	C2'-C1'	-2.06	1.50	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	900	GSP	PA-O3A-PB	-4.87	116.12	132.83
2	G	900	GSP	PA-O3A-PB	-4.75	116.54	132.83
2	A	900	GSP	C5-C6-N1	4.05	121.11	113.95
2	B	900	GSP	C5-C6-N1	3.98	120.97	113.95
2	C	900	GSP	PA-O3A-PB	-3.94	119.31	132.83
2	C	900	GSP	C5-C6-N1	3.54	120.20	113.95
2	D	900	GSP	C2-N1-C6	-3.41	118.82	125.10
2	E	900	GSP	C5-C6-N1	3.38	119.92	113.95
2	B	900	GSP	C8-N7-C5	3.36	109.38	102.99
2	F	900	GSP	PA-O3A-PB	-3.24	121.70	132.83
2	F	900	GSP	N2-C2-N1	3.18	123.49	116.71
2	B	900	GSP	O6-C6-C5	-3.18	118.16	124.37
2	E	900	GSP	O6-C6-C5	-3.13	118.26	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	900	GSP	C8-N7-C5	3.10	108.90	102.99
2	B	900	GSP	C2-N1-C6	-3.08	119.42	125.10
2	D	900	GSP	C5-C6-N1	3.05	119.33	113.95
2	A	900	GSP	C2-N1-C6	-3.03	119.52	125.10
2	C	900	GSP	O6-C6-C5	-2.96	118.60	124.37
2	E	900	GSP	C2-N1-C6	-2.90	119.75	125.10
2	A	900	GSP	N2-C2-N1	2.90	122.89	116.71
2	A	900	GSP	O3G-PG-O3B	2.90	114.31	104.64
2	G	900	GSP	C5-C6-N1	2.86	119.00	113.95
2	B	900	GSP	O3G-PG-O3B	2.85	114.15	104.64
2	A	900	GSP	C8-N7-C5	2.83	108.38	102.99
2	B	900	GSP	PA-O3A-PB	-2.81	123.20	132.83
2	G	900	GSP	C2-N1-C6	-2.79	119.97	125.10
2	F	900	GSP	C5-C6-N1	2.76	118.83	113.95
2	C	900	GSP	C8-N7-C5	2.70	108.13	102.99
2	F	900	GSP	C8-N7-C5	2.67	108.08	102.99
2	D	900	GSP	C8-N7-C5	2.66	108.05	102.99
2	C	900	GSP	C2-N1-C6	-2.64	120.23	125.10
2	D	900	GSP	O6-C6-C5	-2.64	119.22	124.37
2	G	900	GSP	N2-C2-N1	2.47	121.97	116.71
2	E	900	GSP	C8-N7-C5	2.38	107.53	102.99
2	F	900	GSP	N1-C2-N3	-2.33	118.97	123.32
2	F	900	GSP	C2'-C3'-C4'	2.24	107.00	102.64
2	E	900	GSP	O4'-C1'-C2'	-2.24	103.65	106.93
2	F	900	GSP	C2-N1-C6	-2.21	121.02	125.10
2	A	900	GSP	PA-O3A-PB	-2.17	125.39	132.83
2	B	900	GSP	N1-C2-N3	-2.15	119.31	123.32
2	F	900	GSP	O2A-PA-O5'	2.14	117.68	107.75
2	G	900	GSP	O4'-C1'-C2'	-2.11	103.84	106.93
2	A	900	GSP	O6-C6-N1	-2.11	118.16	120.65
2	E	900	GSP	O2G-PG-O3B	2.01	111.34	104.64

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	GSP	PB-O3B-PG-O2G
2	A	900	GSP	PB-O3B-PG-O3G
2	A	900	GSP	C5'-O5'-PA-O3A
2	B	900	GSP	PB-O3B-PG-O3G
2	B	900	GSP	O4'-C4'-C5'-O5'
2	D	900	GSP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	D	900	GSP	C5'-O5'-PA-O2A
2	E	900	GSP	C5'-O5'-PA-O1A
2	E	900	GSP	C5'-O5'-PA-O2A
2	E	900	GSP	C5'-O5'-PA-O3A
2	G	900	GSP	C5'-O5'-PA-O3A
2	B	900	GSP	C3'-C4'-C5'-O5'
2	E	900	GSP	O4'-C4'-C5'-O5'
2	B	900	GSP	PG-O3B-PB-O1B
2	D	900	GSP	C5'-O5'-PA-O3A
2	F	900	GSP	C5'-O5'-PA-O3A
2	D	900	GSP	PB-O3A-PA-O1A
2	F	900	GSP	PB-O3A-PA-O2A
2	A	900	GSP	C5'-O5'-PA-O2A
2	G	900	GSP	C5'-O5'-PA-O1A
2	G	900	GSP	C5'-O5'-PA-O2A
2	G	900	GSP	O4'-C4'-C5'-O5'
2	D	900	GSP	PA-O3A-PB-O2B
2	D	900	GSP	PB-O3B-PG-O3G
2	E	900	GSP	C3'-C4'-C5'-O5'
2	B	900	GSP	PA-O3A-PB-O2B
2	F	900	GSP	PB-O3A-PA-O1A
2	A	900	GSP	C5'-O5'-PA-O1A
2	F	900	GSP	C5'-O5'-PA-O1A

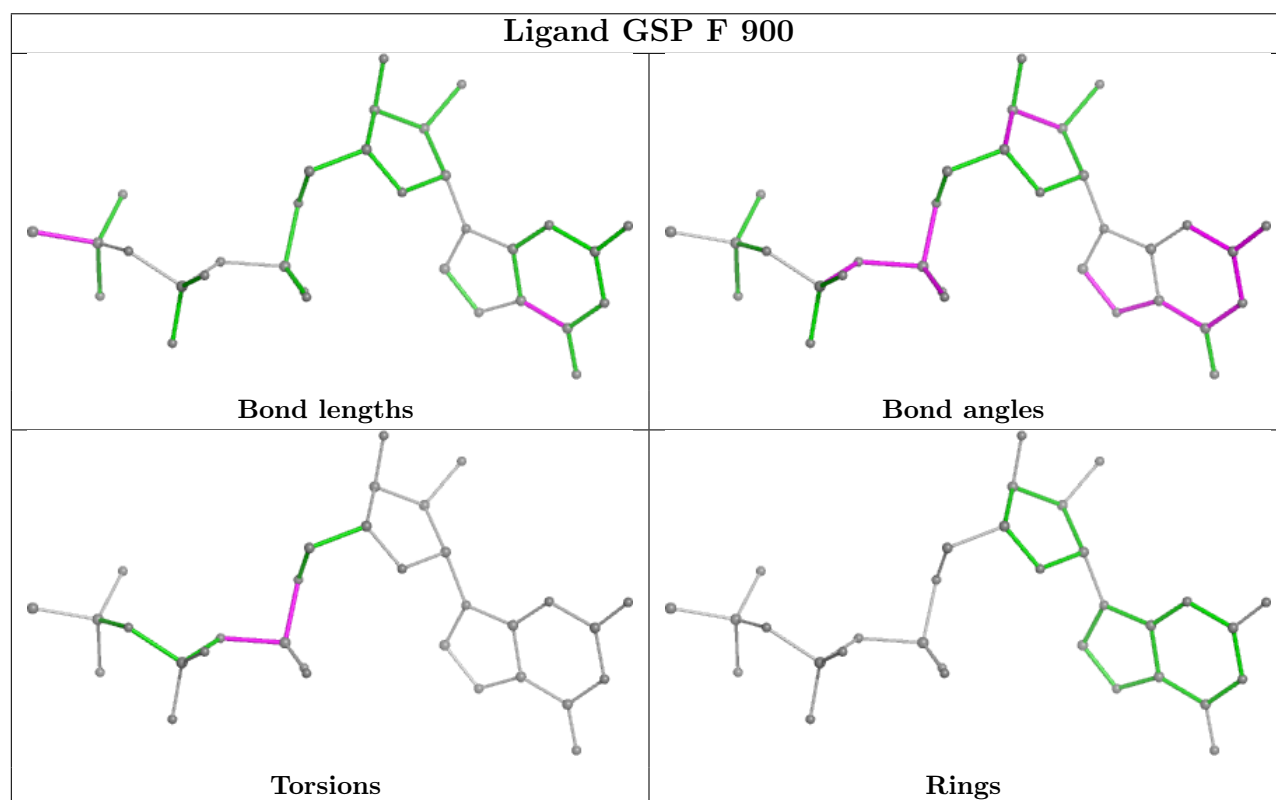
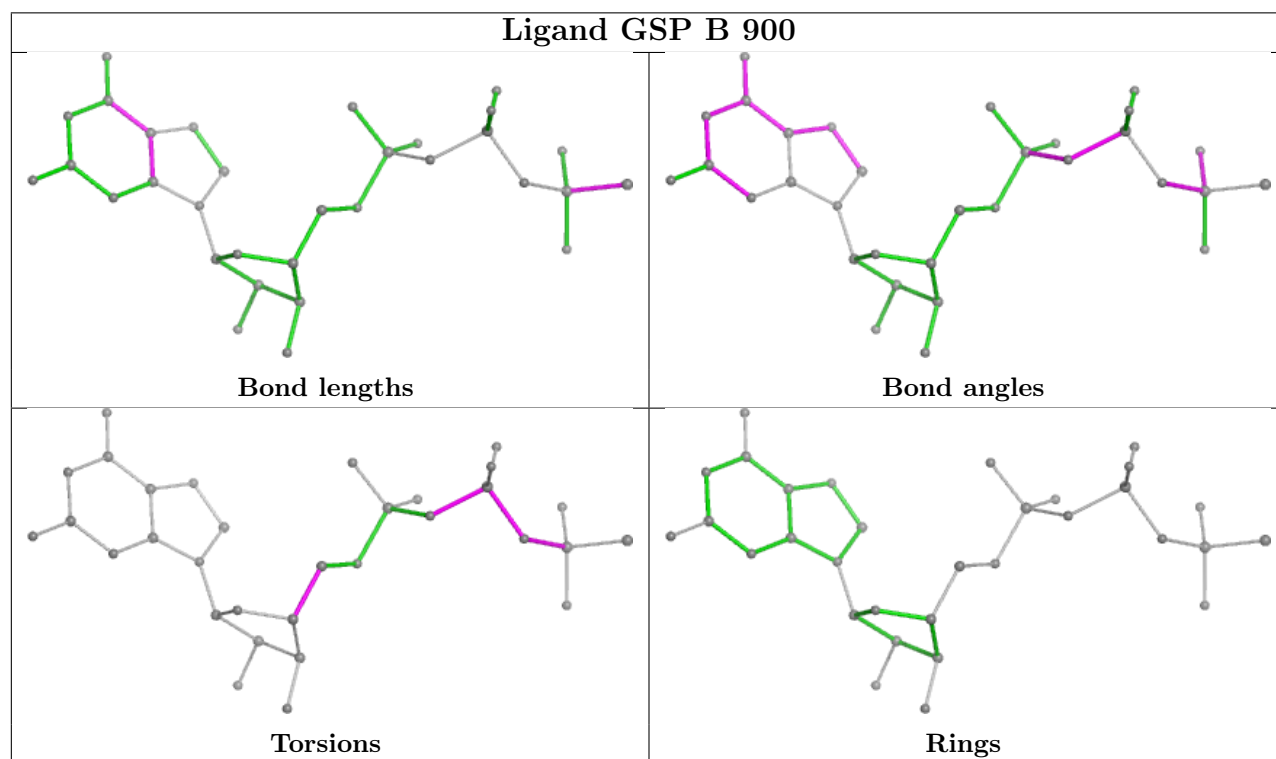
There are no ring outliers.

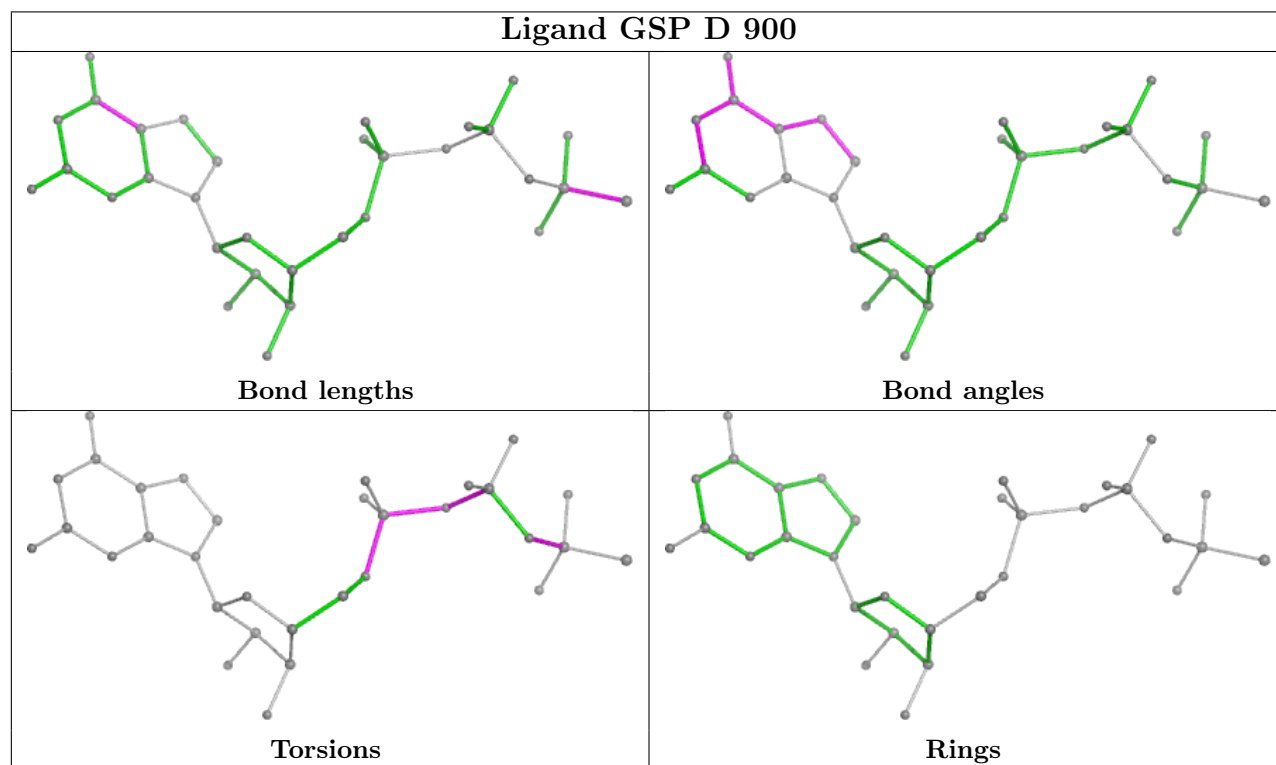
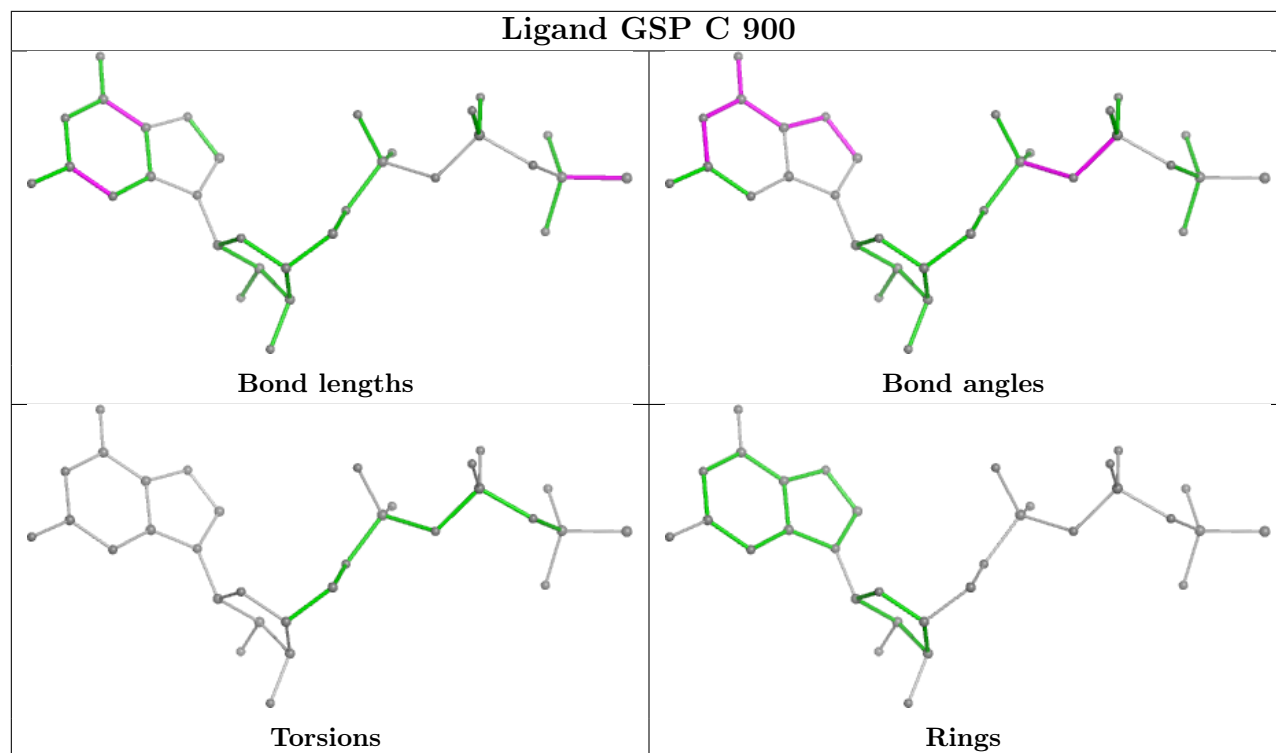
3 monomers are involved in 4 short contacts:

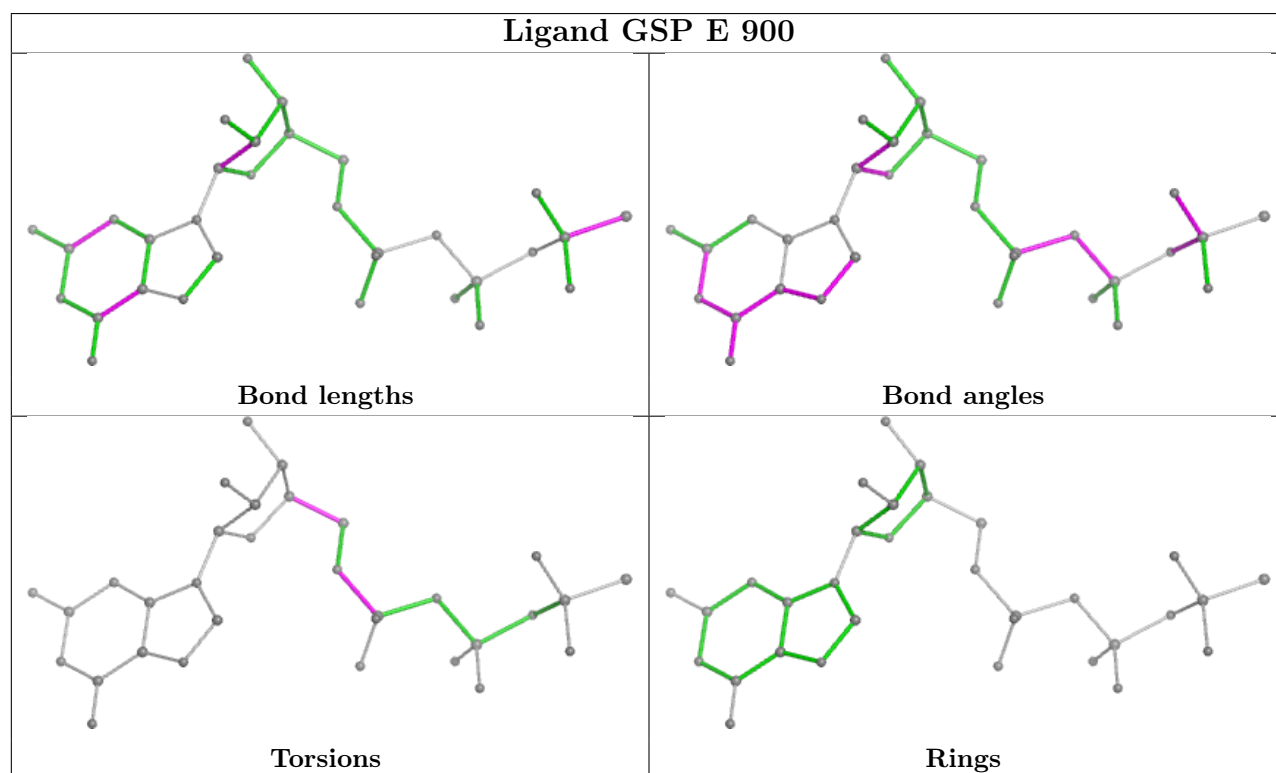
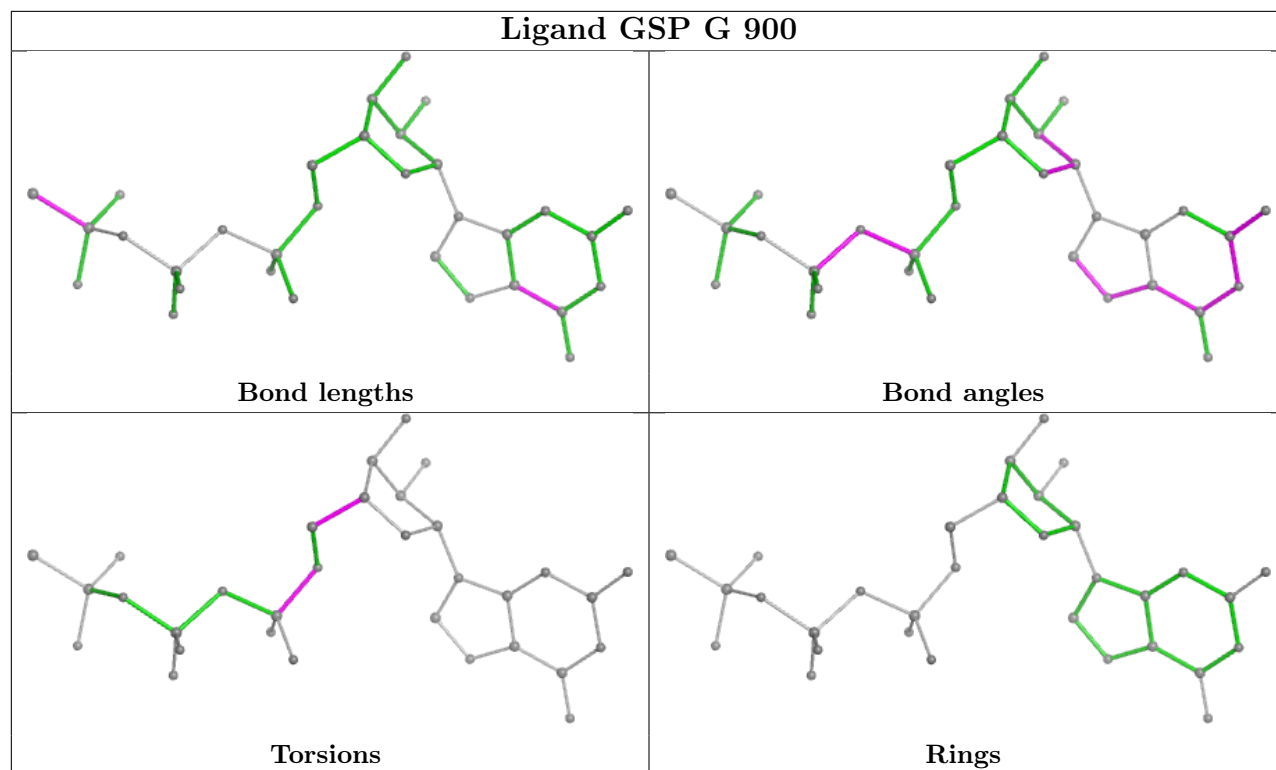
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	GSP	2	0
2	E	900	GSP	1	0
2	A	900	GSP	1	0

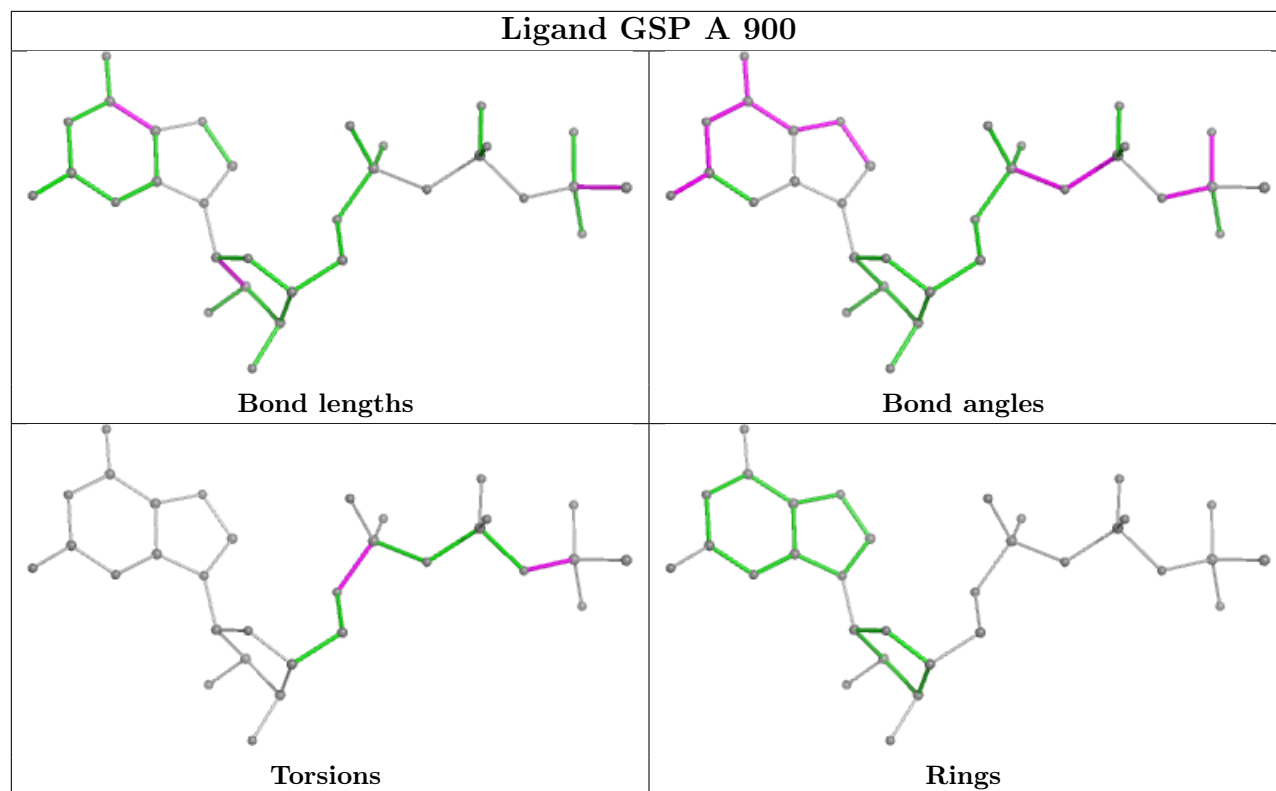
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	399/421 (94%)	-0.23	0 100 100	8, 29, 55, 66	0
1	B	400/421 (95%)	-0.23	1 (0%) 94 84	8, 29, 52, 78	0
1	C	410/421 (97%)	-0.23	0 100 100	8, 28, 46, 55	0
1	D	402/421 (95%)	-0.28	0 100 100	8, 27, 44, 64	0
1	E	395/421 (93%)	-0.34	1 (0%) 94 84	8, 24, 41, 57	0
1	F	414/421 (98%)	-0.32	1 (0%) 95 87	8, 26, 40, 48	0
1	G	414/421 (98%)	-0.25	0 100 100	8, 28, 42, 48	0
All	All	2834/2947 (96%)	-0.27	3 (0%) 95 89	8, 27, 45, 78	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	172	ASP	2.3
1	F	421	THR	2.2
1	B	12	HIS	2.1

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 monosaccharides in this entry.

6.4 Ligands

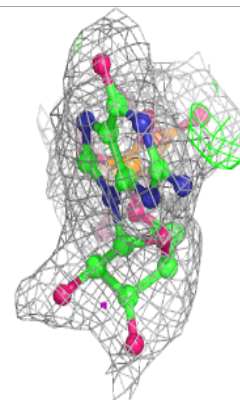
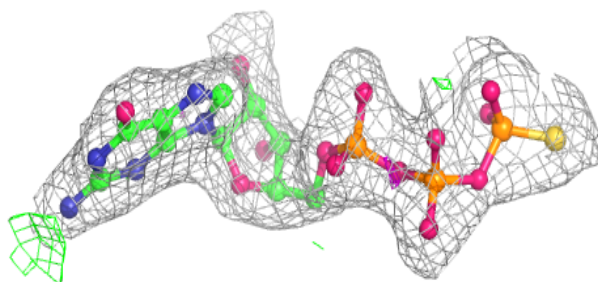
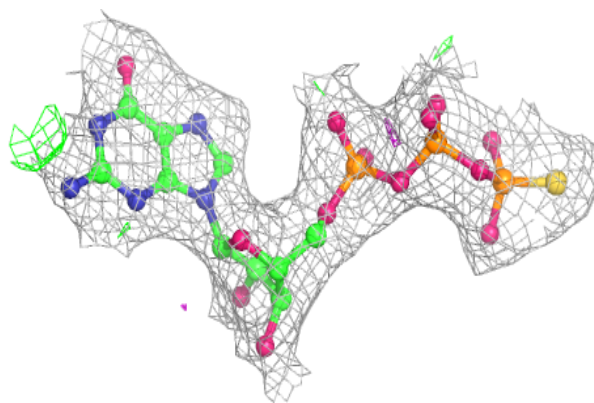
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	999	1/1	0.88	0.17	17,17,17,17	0
3	MG	E	999	1/1	0.92	0.15	2,2,2,2	0
3	MG	F	999	1/1	0.93	0.21	2,2,2,2	0
3	MG	C	999	1/1	0.96	0.17	2,2,2,2	0
2	GSP	C	900	32/32	0.96	0.12	11,13,16,18	0
2	GSP	A	900	32/32	0.96	0.13	13,19,23,23	0
3	MG	B	999	1/1	0.97	0.17	12,12,12,12	0
2	GSP	D	900	32/32	0.97	0.12	5,9,10,12	0
2	GSP	G	900	32/32	0.97	0.11	3,9,12,14	0
2	GSP	B	900	32/32	0.97	0.11	2,5,7,11	0
3	MG	G	999	1/1	0.97	0.14	17,17,17,17	0
2	GSP	E	900	32/32	0.98	0.12	2,3,6,8	0
2	GSP	F	900	32/32	0.98	0.12	2,4,6,7	0
3	MG	D	999	1/1	0.98	0.23	5,5,5,5	0

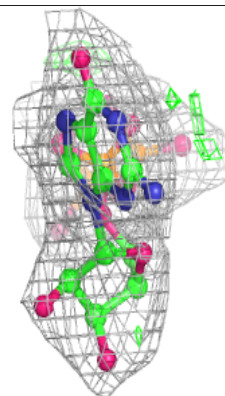
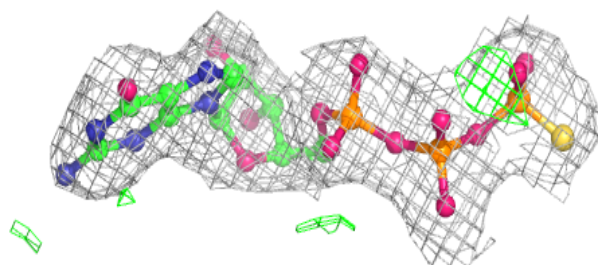
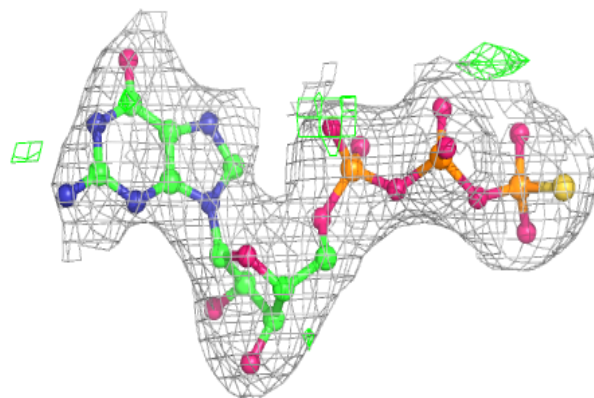
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GSP C 900:

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

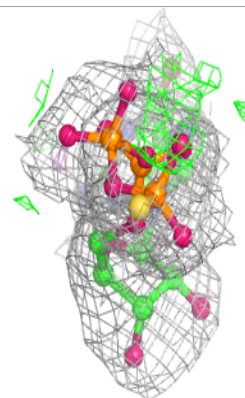
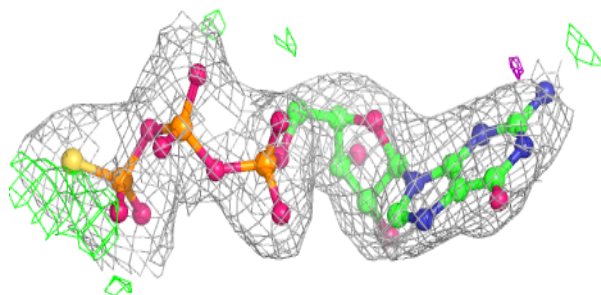
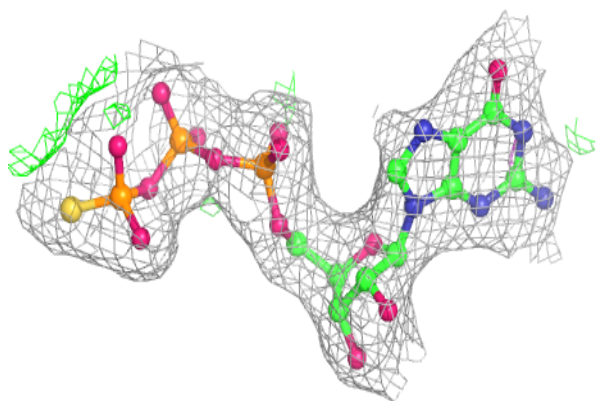
**Electron density around GSP A 900:**

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

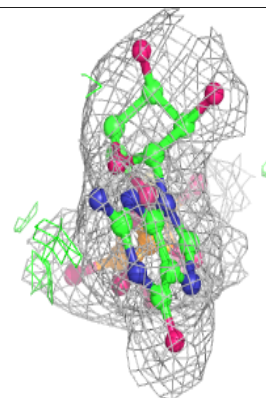
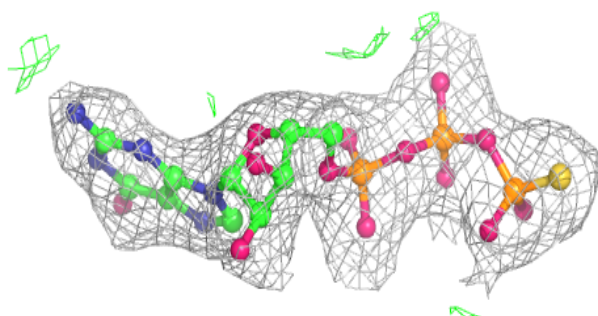
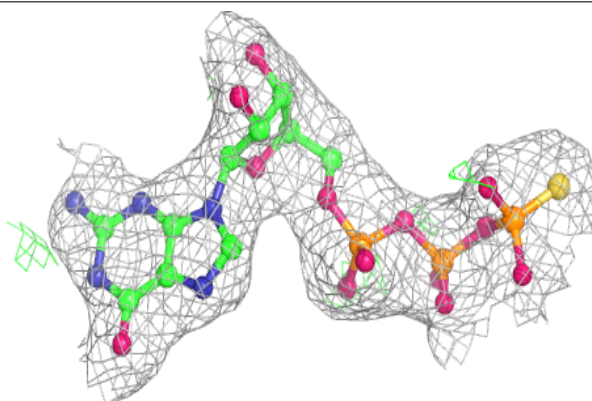


Electron density around GSP D 900:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

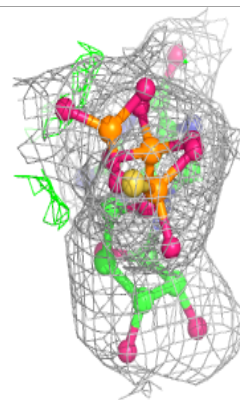
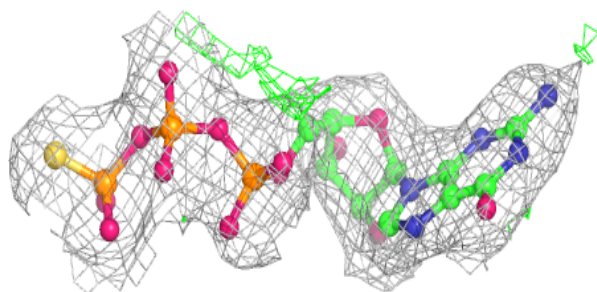
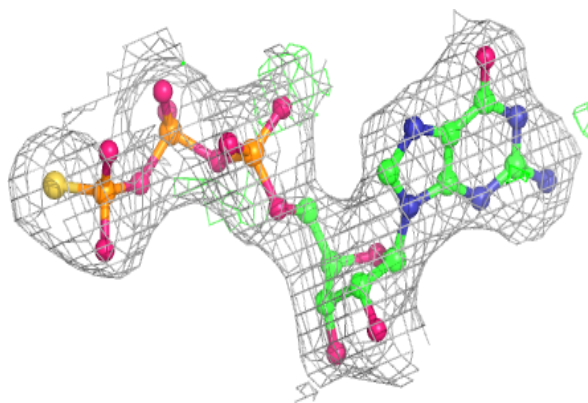
**Electron density around GSP G 900:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

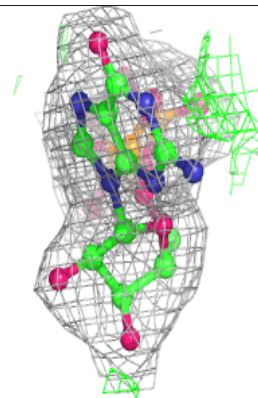
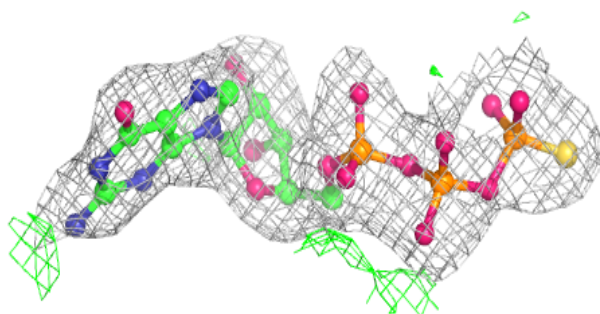
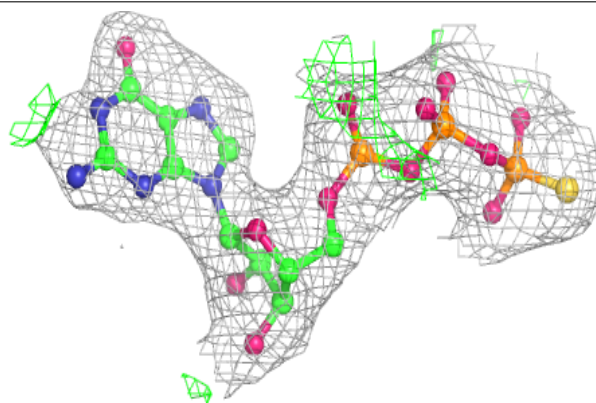


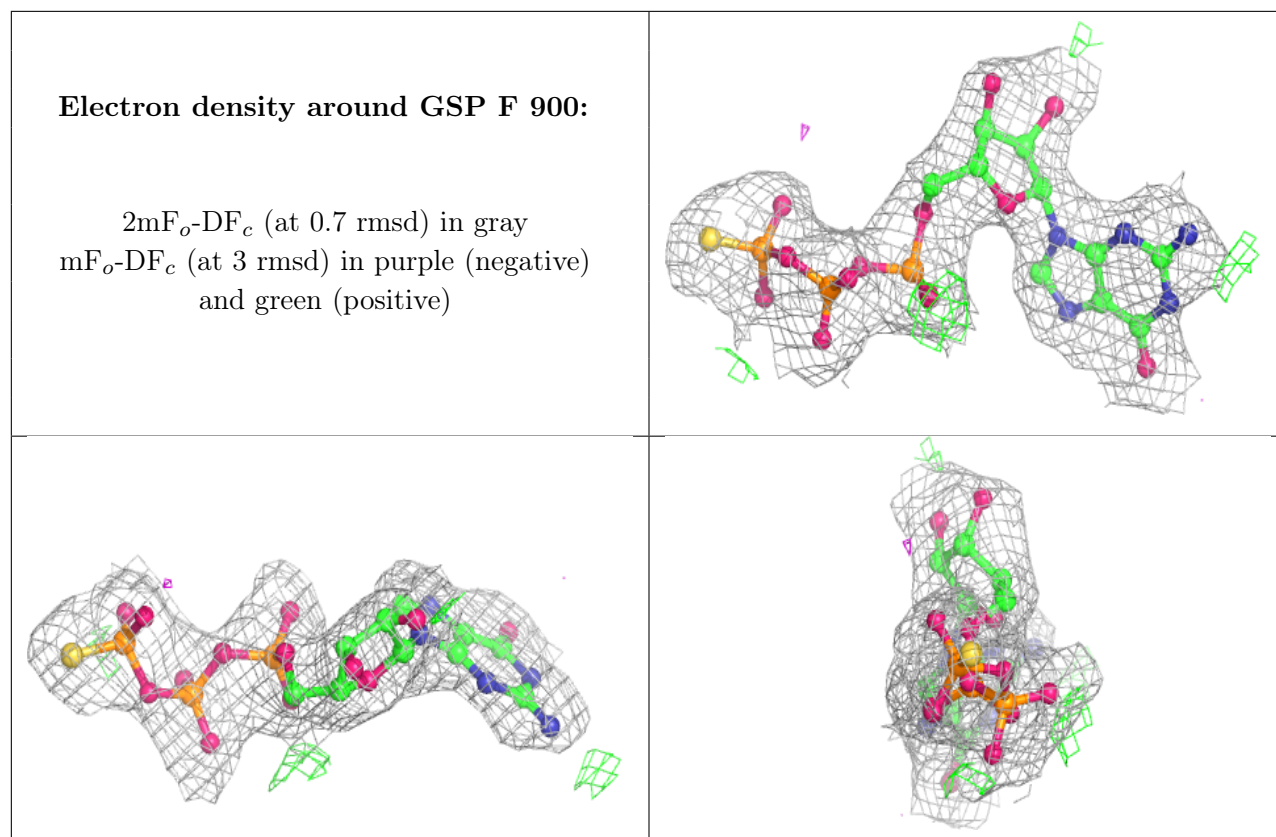
Electron density around GSP B 900:

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

**Electron density around GSP E 900:**

$2mF_o-DF_c$ (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.