



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:24 AM UTC

PDB ID : 5CCV / pdb_00005ccv
Title : Crystal structure of full-length NS5 from dengue virus type 3
Authors : Klema, V.J.; Choi, K.H.
Deposited on : 2015-07-02
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

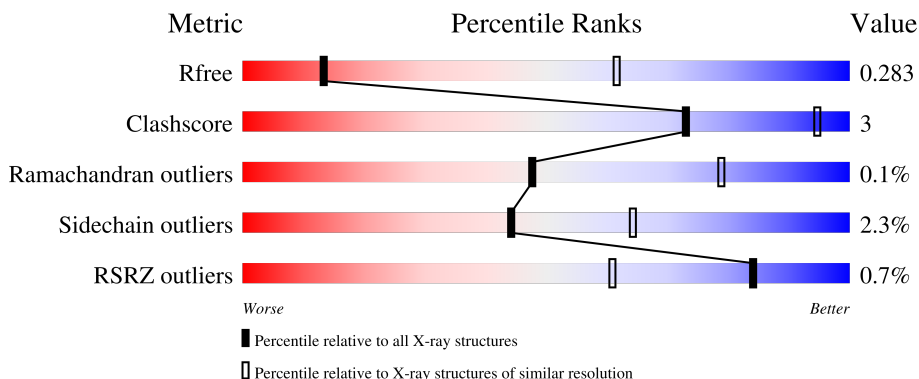
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	905	
1	B	905	
1	C	905	
1	D	905	
1	E	905	

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Mol	Chain	Length	Quality of chain
1	F	905	 85% 8% • 6%
1	G	905	 85% 9% 6%
1	H	905	 2% 81% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 52681 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 RNA-directed RNA polymerase NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	849	Total 6831	C 4301	N 1229	O 1255	S 46	0	0	0
1	B	851	Total 6892	C 4346	N 1236	O 1263	S 47	0	0	0
1	C	852	Total 6879	C 4339	N 1229	O 1263	S 48	0	0	0
1	D	848	Total 6827	C 4302	N 1226	O 1252	S 47	0	0	0
1	E	852	Total 6885	C 4341	N 1231	O 1266	S 47	0	0	0
1	F	850	Total 6846	C 4311	N 1231	O 1257	S 47	0	0	0
1	G	847	Total 6813	C 4292	N 1222	O 1252	S 47	0	0	0
1	H	767	Total 4484	C 2739	N 870	O 866	S 9	0	0	0

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	763	ALA	THR	conflict	UNP P27915
A	?	-	TRP	deletion	UNP P27915
A	?	-	SER	deletion	UNP P27915
A	?	-	ILE	deletion	UNP P27915
A	?	-	HIS	deletion	UNP P27915
A	?	-	ALA	deletion	UNP P27915
A	?	-	HIS	deletion	UNP P27915
A	901	ALA	-	expression tag	UNP P27915
A	902	ALA	-	expression tag	UNP P27915
A	903	ALA	-	expression tag	UNP P27915
A	904	LEU	-	expression tag	UNP P27915
A	905	GLU	-	expression tag	UNP P27915
A	906	HIS	-	expression tag	UNP P27915

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Chain	Residue	Modelled	Actual	Comment	Reference
A	907	HIS	-	expression tag	UNP P27915
A	908	HIS	-	expression tag	UNP P27915
A	909	HIS	-	expression tag	UNP P27915
A	910	HIS	-	expression tag	UNP P27915
A	911	HIS	-	expression tag	UNP P27915
B	763	ALA	THR	conflict	UNP P27915
B	?	-	TRP	deletion	UNP P27915
B	?	-	SER	deletion	UNP P27915
B	?	-	ILE	deletion	UNP P27915
B	?	-	HIS	deletion	UNP P27915
B	?	-	ALA	deletion	UNP P27915
B	?	-	HIS	deletion	UNP P27915
B	901	ALA	-	expression tag	UNP P27915
B	902	ALA	-	expression tag	UNP P27915
B	903	ALA	-	expression tag	UNP P27915
B	904	LEU	-	expression tag	UNP P27915
B	905	GLU	-	expression tag	UNP P27915
B	906	HIS	-	expression tag	UNP P27915
B	907	HIS	-	expression tag	UNP P27915
B	908	HIS	-	expression tag	UNP P27915
B	909	HIS	-	expression tag	UNP P27915
B	910	HIS	-	expression tag	UNP P27915
B	911	HIS	-	expression tag	UNP P27915
C	763	ALA	THR	conflict	UNP P27915
C	?	-	TRP	deletion	UNP P27915
C	?	-	SER	deletion	UNP P27915
C	?	-	ILE	deletion	UNP P27915
C	?	-	HIS	deletion	UNP P27915
C	?	-	ALA	deletion	UNP P27915
C	?	-	HIS	deletion	UNP P27915
C	901	ALA	-	expression tag	UNP P27915
C	902	ALA	-	expression tag	UNP P27915
C	903	ALA	-	expression tag	UNP P27915
C	904	LEU	-	expression tag	UNP P27915
C	905	GLU	-	expression tag	UNP P27915
C	906	HIS	-	expression tag	UNP P27915
C	907	HIS	-	expression tag	UNP P27915
C	908	HIS	-	expression tag	UNP P27915
C	909	HIS	-	expression tag	UNP P27915
C	910	HIS	-	expression tag	UNP P27915
C	911	HIS	-	expression tag	UNP P27915
D	763	ALA	THR	conflict	UNP P27915

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	TRP	deletion	UNP P27915
D	?	-	SER	deletion	UNP P27915
D	?	-	ILE	deletion	UNP P27915
D	?	-	HIS	deletion	UNP P27915
D	?	-	ALA	deletion	UNP P27915
D	?	-	HIS	deletion	UNP P27915
D	901	ALA	-	expression tag	UNP P27915
D	902	ALA	-	expression tag	UNP P27915
D	903	ALA	-	expression tag	UNP P27915
D	904	LEU	-	expression tag	UNP P27915
D	905	GLU	-	expression tag	UNP P27915
D	906	HIS	-	expression tag	UNP P27915
D	907	HIS	-	expression tag	UNP P27915
D	908	HIS	-	expression tag	UNP P27915
D	909	HIS	-	expression tag	UNP P27915
D	910	HIS	-	expression tag	UNP P27915
D	911	HIS	-	expression tag	UNP P27915
E	763	ALA	THR	conflict	UNP P27915
E	?	-	TRP	deletion	UNP P27915
E	?	-	SER	deletion	UNP P27915
E	?	-	ILE	deletion	UNP P27915
E	?	-	HIS	deletion	UNP P27915
E	?	-	ALA	deletion	UNP P27915
E	?	-	HIS	deletion	UNP P27915
E	901	ALA	-	expression tag	UNP P27915
E	902	ALA	-	expression tag	UNP P27915
E	903	ALA	-	expression tag	UNP P27915
E	904	LEU	-	expression tag	UNP P27915
E	905	GLU	-	expression tag	UNP P27915
E	906	HIS	-	expression tag	UNP P27915
E	907	HIS	-	expression tag	UNP P27915
E	908	HIS	-	expression tag	UNP P27915
E	909	HIS	-	expression tag	UNP P27915
E	910	HIS	-	expression tag	UNP P27915
E	911	HIS	-	expression tag	UNP P27915
F	763	ALA	THR	conflict	UNP P27915
F	?	-	TRP	deletion	UNP P27915
F	?	-	SER	deletion	UNP P27915
F	?	-	ILE	deletion	UNP P27915
F	?	-	HIS	deletion	UNP P27915
F	?	-	ALA	deletion	UNP P27915
F	?	-	HIS	deletion	UNP P27915

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Chain	Residue	Modelled	Actual	Comment	Reference
F	901	ALA	-	expression tag	UNP P27915
F	902	ALA	-	expression tag	UNP P27915
F	903	ALA	-	expression tag	UNP P27915
F	904	LEU	-	expression tag	UNP P27915
F	905	GLU	-	expression tag	UNP P27915
F	906	HIS	-	expression tag	UNP P27915
F	907	HIS	-	expression tag	UNP P27915
F	908	HIS	-	expression tag	UNP P27915
F	909	HIS	-	expression tag	UNP P27915
F	910	HIS	-	expression tag	UNP P27915
F	911	HIS	-	expression tag	UNP P27915
G	763	ALA	THR	conflict	UNP P27915
G	?	-	TRP	deletion	UNP P27915
G	?	-	SER	deletion	UNP P27915
G	?	-	ILE	deletion	UNP P27915
G	?	-	HIS	deletion	UNP P27915
G	?	-	ALA	deletion	UNP P27915
G	?	-	HIS	deletion	UNP P27915
G	901	ALA	-	expression tag	UNP P27915
G	902	ALA	-	expression tag	UNP P27915
G	903	ALA	-	expression tag	UNP P27915
G	904	LEU	-	expression tag	UNP P27915
G	905	GLU	-	expression tag	UNP P27915
G	906	HIS	-	expression tag	UNP P27915
G	907	HIS	-	expression tag	UNP P27915
G	908	HIS	-	expression tag	UNP P27915
G	909	HIS	-	expression tag	UNP P27915
G	910	HIS	-	expression tag	UNP P27915
G	911	HIS	-	expression tag	UNP P27915
H	763	ALA	THR	conflict	UNP P27915
H	?	-	TRP	deletion	UNP P27915
H	?	-	SER	deletion	UNP P27915
H	?	-	ILE	deletion	UNP P27915
H	?	-	HIS	deletion	UNP P27915
H	?	-	ALA	deletion	UNP P27915
H	?	-	HIS	deletion	UNP P27915
H	901	ALA	-	expression tag	UNP P27915
H	902	ALA	-	expression tag	UNP P27915
H	903	ALA	-	expression tag	UNP P27915
H	904	LEU	-	expression tag	UNP P27915
H	905	GLU	-	expression tag	UNP P27915
H	906	HIS	-	expression tag	UNP P27915

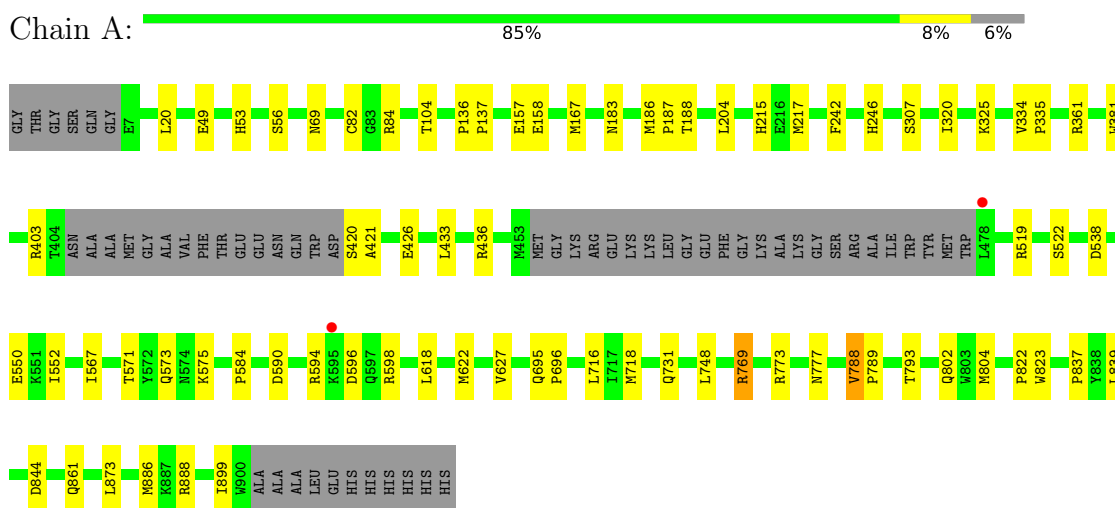
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	G	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	H	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

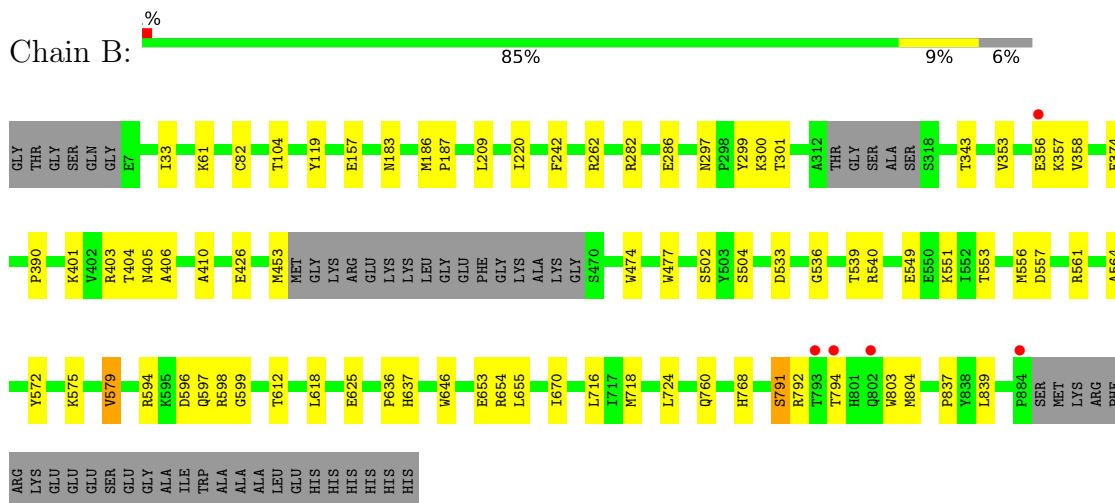
3 Residue-property plots [i](#)

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.

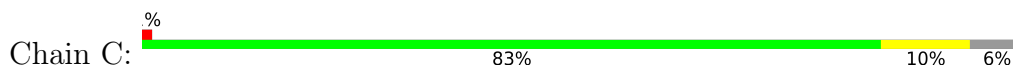
- Molecule 1: RNA-directed RNA polymerase NS5

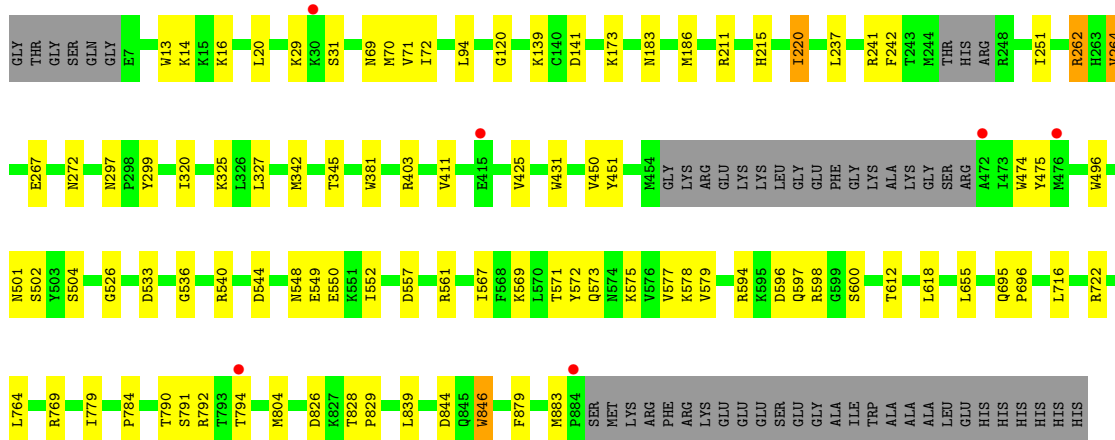


- Molecule 1: RNA-directed RNA polymerase NS5



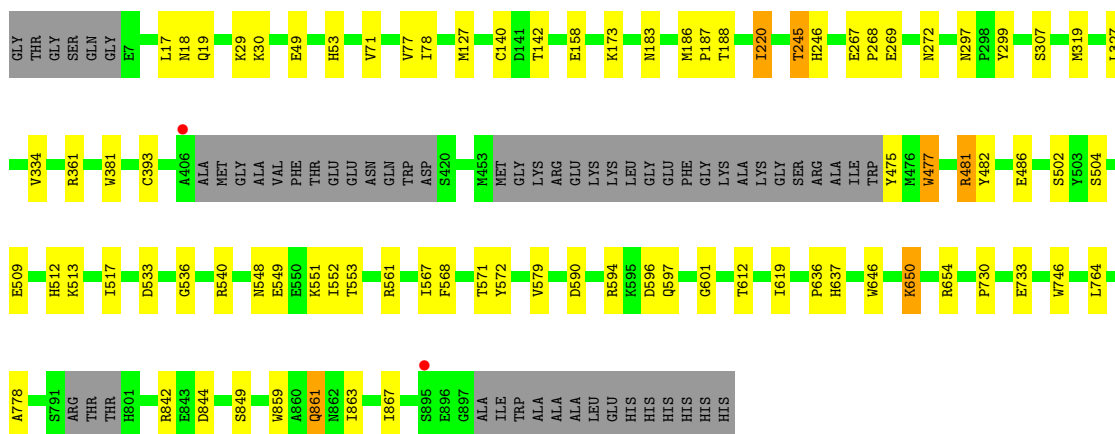
- Molecule 1: RNA-directed RNA polymerase NS5





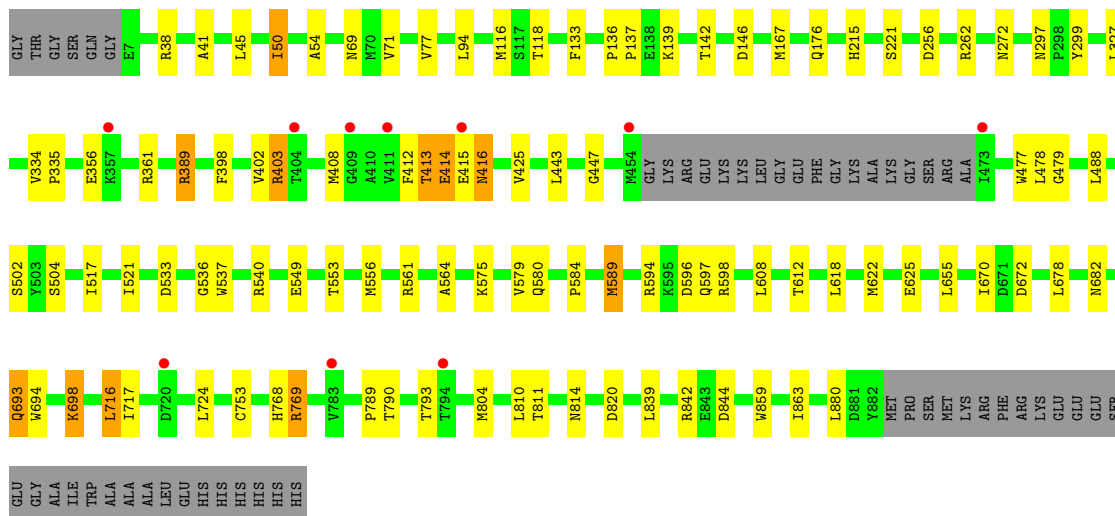
• Molecule 1: RNA-directed RNA polymerase NS5

Chain D: 84% 9% • 6%



• Molecule 1: RNA-directed RNA polymerase NS5

Chain E: 83% 10% • 6%



LYS
GLU
GLU
GLU
SER
GLU
GLY
ALA
ILE
TRP
ALA
ALA
ALA
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.31Å 215.31Å 480.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.22 – 3.60 49.22 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.22-3.60) 94.2 (49.22-3.60)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 3.57Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.238 , 0.274 0.258 , 0.283	Depositor DCC
R_{free} test set	2004 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.054 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	52681	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% 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: SAH, ZN

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	0.27	0/6992	0.68	0/9454
1	B	0.27	0/7060	0.69	3/9551 (0.0%)
1	C	0.27	0/7046	0.69	2/9533 (0.0%)
1	D	0.28	0/6990	0.68	2/9452 (0.0%)
1	E	0.26	0/7053	0.68	0/9544
1	F	0.27	0/7009	0.68	2/9477 (0.0%)
1	G	0.27	0/6976	0.68	0/9434
1	H	0.28	0/4563	0.77	2/6318 (0.0%)
All	All	0.27	0/53689	0.69	11/72763 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	135	LEU	CA-C-N	7.31	124.92	119.66
1	F	135	LEU	C-N-CA	7.31	124.92	119.66
1	H	329	LYS	CA-C-N	-6.17	113.33	119.56
1	H	329	LYS	C-N-CA	-6.17	113.33	119.56
1	B	791	SER	CB-CA-C	-5.57	110.14	116.54
1	B	242	PHE	N-CA-C	-5.36	107.76	114.56
1	D	334	VAL	CA-C-N	5.14	124.32	118.97
1	D	334	VAL	C-N-CA	5.14	124.32	118.97
1	B	406	ALA	CB-CA-C	-5.14	110.63	116.54
1	C	186	MET	CA-C-N	5.03	124.47	119.24
1	C	186	MET	C-N-CA	5.03	124.47	119.24

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	6831	0	6746	40	0
1	B	6892	0	6803	41	0
1	C	6879	0	6788	47	0
1	D	6827	0	6724	51	0
1	E	6885	0	6788	60	0
1	F	6846	0	6757	40	0
1	G	6813	0	6712	46	0
1	H	4484	0	2810	18	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
3	C	26	0	19	0	0
3	D	26	0	19	0	0
3	E	26	0	19	1	0
3	F	26	0	19	0	0
3	G	26	0	19	0	0
3	H	26	0	19	0	0
All	All	52681	0	50280	327	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 3.

All (327) 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:420:SER:O	1:G:422:ARG:N	1.97	0.97
1:A:82:CYS:HG	1:A:104:THR:HG1	1.37	0.70
1:D:475:TYR:C	1:D:477:TRP:H	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:ARG:HA	1:D:594:ARG:HH22	1.58	0.68
1:D:245:THR:O	1:G:861:GLN:NE2	2.27	0.68
1:G:13:TRP:HZ2	1:G:215:HIS:HB2	1.58	0.67
1:A:899:ILE:HG13	1:F:237:LEU:HD12	1.78	0.66
1:G:422:ARG:O	1:G:425:VAL:N	2.30	0.64
1:E:553:THR:HA	1:E:556:MET:HE2	1.78	0.64
1:B:716:LEU:HD21	1:B:839:LEU:HD23	1.80	0.63
1:C:544:ASP:O	1:C:548:ASN:ND2	2.31	0.63
1:B:358:VAL:HG13	1:B:597:GLN:HE22	1.62	0.63
1:E:556:MET:HE1	1:E:564:ALA:HB3	1.78	0.63
1:B:82:CYS:SG	1:B:104:THR:OG1	2.57	0.63
1:B:556:MET:HE1	1:B:564:ALA:HB3	1.81	0.63
1:G:716:LEU:HD21	1:G:839:LEU:HD23	1.82	0.61
1:B:553:THR:HA	1:B:556:MET:HE2	1.85	0.58
1:G:145:CYS:HB3	1:G:179:ILE:HG23	1.85	0.58
1:D:49:GLU:OE1	1:D:53:HIS:NE2	2.33	0.57
1:B:549:GLU:OE2	1:B:612:THR:OG1	2.22	0.57
1:B:556:MET:HE3	1:B:561:ARG:HA	1.86	0.57
1:E:769:ARG:NH1	1:E:844:ASP:OD1	2.38	0.57
1:A:567:ILE:O	1:A:571:THR:OG1	2.21	0.57
1:D:844:ASP:OD1	1:D:849:SER:OG	2.24	0.56
1:G:127:MET:HG2	1:H:526:GLY:HA2	1.88	0.55
1:H:424:ALA:O	1:H:431:TRP:NE1	2.39	0.55
1:B:82:CYS:HG	1:B:104:THR:HG1	1.52	0.55
1:F:244:MET:HE3	1:F:247:ARG:HE	1.70	0.54
1:A:718:MET:HG2	1:A:837:PRO:HG3	1.89	0.54
1:C:550:GLU:OE1	1:C:573:GLN:NE2	2.41	0.54
1:B:453:MET:HG3	1:B:579:VAL:HB	1.89	0.54
1:H:580:GLN:HA	1:H:589:MET:HA	1.89	0.54
1:D:861:GLN:HG2	1:G:244:MET:HG3	1.90	0.54
1:A:594:ARG:NE	1:A:596:ASP:OD1	2.33	0.53
1:E:327:LEU:O	1:E:859:TRP:NE1	2.39	0.53
1:E:678:LEU:O	1:E:682:ASN:ND2	2.39	0.53
1:E:556:MET:HE3	1:E:561:ARG:HA	1.89	0.53
1:F:92:ALA:O	1:F:262:ARG:NH1	2.41	0.53
1:C:425:VAL:HG13	1:C:431:TRP:HZ2	1.74	0.52
1:G:176:GLN:OE1	1:G:221:SER:OG	2.25	0.52
1:B:539:THR:HA	1:B:597:GLN:HG3	1.91	0.52
1:A:769:ARG:NH2	1:A:844:ASP:OD1	2.43	0.52
1:A:49:GLU:OE1	1:A:53:HIS:NE2	2.34	0.51
1:D:482:TYR:O	1:D:486:GLU:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLU:HB2	1:A:183:ASN:HD22	1.76	0.51
1:B:594:ARG:NE	1:B:596:ASP:OD1	2.44	0.51
1:F:94:LEU:O	1:F:262:ARG:NH2	2.44	0.50
1:G:328:THR:OG1	1:G:739:ARG:NH2	2.43	0.50
1:A:575:LYS:NZ	1:A:596:ASP:O	2.33	0.50
1:D:327:LEU:O	1:D:859:TRP:NE1	2.43	0.50
1:G:80:LEU:HD13	1:G:167:MET:HE1	1.93	0.50
1:B:718:MET:HG2	1:B:837:PRO:HG3	1.94	0.50
1:E:537:TRP:HZ2	1:E:612:THR:HG23	1.75	0.50
1:G:420:SER:C	1:G:422:ARG:N	2.68	0.49
1:C:716:LEU:HD21	1:C:839:LEU:HD23	1.93	0.49
1:D:319:MET:HE1	1:D:746:TRP:H	1.77	0.49
1:F:484:GLU:OE1	1:F:572:TYR:OH	2.24	0.49
1:E:810:LEU:O	1:E:814:ASN:ND2	2.45	0.49
1:C:251:ILE:HB	1:C:342:MET:HE1	1.94	0.49
1:F:791:SER:O	1:F:792:ARG:NE	2.33	0.49
1:G:133:PHE:HD1	1:G:167:MET:HG3	1.78	0.49
1:G:568:PHE:HA	1:G:572:TYR:HB2	1.94	0.49
1:B:401:LYS:O	1:B:403:ARG:NE	2.44	0.49
1:C:791:SER:OG	1:C:792:ARG:N	2.46	0.49
1:G:94:LEU:O	1:G:262:ARG:NH2	2.46	0.49
1:A:773:ARG:O	1:A:777:ASN:ND2	2.42	0.48
1:B:572:TYR:O	1:B:575:LYS:NZ	2.36	0.48
1:A:861:GLN:NE2	1:F:245:THR:O	2.47	0.48
1:C:567:ILE:O	1:C:571:THR:OG1	2.31	0.48
1:D:549:GLU:OE2	1:D:612:THR:OG1	2.31	0.48
1:G:241:ARG:HG2	1:G:244:MET:HE2	1.95	0.48
1:G:652:VAL:HA	1:G:655:LEU:HD12	1.95	0.48
1:C:425:VAL:O	1:C:431:TRP:NE1	2.37	0.48
1:C:496:TRP:O	1:C:501:ASN:ND2	2.46	0.48
1:D:594:ARG:NE	1:D:596:ASP:OD1	2.46	0.48
1:C:297:ASN:HB2	1:C:299:TYR:HD2	1.79	0.48
1:B:374:GLU:HG2	1:B:551:LYS:HE2	1.96	0.48
1:D:567:ILE:O	1:D:571:THR:OG1	2.24	0.48
1:E:693:GLN:HB3	1:E:694:TRP:HD1	1.78	0.48
1:F:263:HIS:O	1:F:265:ASN:N	2.45	0.48
1:A:69:ASN:HD22	1:A:584:PRO:HD3	1.79	0.48
1:A:420:SER:OG	1:A:421:ALA:N	2.45	0.48
1:B:301:THR:HB	1:B:594:ARG:HH12	1.79	0.48
1:C:474:TRP:CD1	1:C:600:SER:H	2.31	0.48
1:D:475:TYR:C	1:D:477:TRP:N	2.65	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:581:ARG:N	1:H:588:VAL:O	2.43	0.48
1:C:94:LEU:O	1:C:262:ARG:NH2	2.48	0.47
1:D:78:ILE:HD13	1:D:140:CYS:HB3	1.96	0.47
1:E:693:GLN:C	1:E:694:TRP:HD1	2.22	0.47
1:B:653:GLU:OE2	1:B:654:ARG:NH1	2.46	0.47
1:H:621:GLN:O	1:H:625:GLU:N	2.45	0.47
1:E:389:ARG:HG2	1:H:842:ARG:HH12	1.79	0.47
1:A:215:HIS:O	1:A:215:HIS:ND1	2.47	0.47
1:C:320:ILE:HG21	1:C:325:LYS:HD2	1.95	0.47
1:E:361:ARG:HA	1:E:594:ARG:HH22	1.78	0.47
1:E:753:CYS:HB2	1:E:789:PRO:HA	1.96	0.47
1:G:302:TRP:NE1	1:G:594:ARG:HH21	2.13	0.47
1:E:215:HIS:ND1	1:E:215:HIS:O	2.46	0.47
1:E:753:CYS:SG	1:E:790:THR:HG22	2.55	0.47
1:G:168:VAL:HG21	1:G:179:ILE:HD13	1.97	0.47
1:B:410:ALA:HB2	1:B:477:TRP:HB3	1.97	0.46
1:E:69:ASN:HD22	1:E:584:PRO:HD3	1.80	0.46
1:G:722:ARG:NH1	1:G:828:THR:O	2.41	0.46
1:C:794:THR:HA	1:C:804:MET:HG3	1.98	0.46
1:F:502:SER:O	1:F:504:SER:N	2.44	0.46
1:F:550:GLU:OE2	1:F:569:LYS:NZ	2.46	0.46
1:A:361:ARG:HA	1:A:594:ARG:HH22	1.80	0.46
1:E:549:GLU:CD	1:E:598:ARG:HH22	2.24	0.46
1:G:718:MET:HG2	1:G:837:PRO:HG3	1.97	0.46
1:A:433:LEU:HD23	1:A:436:ARG:HH21	1.79	0.46
1:C:549:GLU:OE2	1:C:612:THR:OG1	2.34	0.46
1:F:550:GLU:OE1	1:F:573:GLN:NE2	2.49	0.46
1:B:536:GLY:O	1:B:540:ARG:HG2	2.16	0.46
1:B:557:ASP:O	1:B:561:ARG:N	2.44	0.45
1:C:549:GLU:OE2	1:C:598:ARG:NH2	2.42	0.45
1:D:475:TYR:HE1	1:D:477:TRP:HD1	1.65	0.45
1:F:132:VAL:HA	1:F:135:LEU:HD23	1.98	0.45
1:G:502:SER:O	1:G:504:SER:N	2.44	0.45
1:B:618:LEU:HD11	1:B:655:LEU:HD21	1.97	0.45
1:C:70:MET:HB3	1:C:220:ILE:HG21	1.97	0.45
1:D:778:ALA:HB1	1:D:867:ILE:HD11	1.97	0.45
1:G:69:ASN:HD22	1:G:72:ILE:HD11	1.80	0.45
1:D:548:ASN:HA	1:D:551:LYS:HE2	1.99	0.45
1:D:650:LYS:HD3	1:D:654:ARG:HH22	1.81	0.45
1:E:502:SER:C	1:E:504:SER:H	2.25	0.45
1:F:536:GLY:O	1:F:540:ARG:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ILE:H	1:C:220:ILE:HG13	1.63	0.45
1:D:77:VAL:HG22	1:D:142:THR:HB	1.98	0.45
1:E:536:GLY:O	1:E:540:ARG:HG2	2.16	0.45
1:F:435:ASP:OD1	1:F:438:ARG:NH1	2.49	0.45
1:D:475:TYR:HE1	1:D:477:TRP:CD1	2.35	0.45
1:A:204:LEU:HG	1:A:217:MET:HE2	1.99	0.45
1:B:768:HIS:HB2	1:B:839:LEU:HG	1.99	0.45
1:A:873:LEU:HD11	1:F:322:GLY:HA3	1.98	0.45
1:E:608:LEU:O	1:E:612:THR:HG22	2.17	0.45
1:B:502:SER:C	1:B:504:SER:H	2.24	0.44
1:C:769:ARG:NE	1:C:844:ASP:OD1	2.46	0.44
1:D:29:LYS:HG3	1:D:30:LYS:HG3	1.99	0.44
1:D:475:TYR:CD1	1:D:475:TYR:O	2.70	0.44
1:A:381:TRP:CE3	1:A:552:ILE:HD13	2.52	0.44
1:B:297:ASN:HB2	1:B:299:TYR:HD2	1.83	0.44
1:E:94:LEU:O	1:E:262:ARG:NH2	2.50	0.44
1:E:133:PHE:HD1	1:E:167:MET:HG3	1.83	0.44
1:F:652:VAL:HA	1:F:655:LEU:HD12	2.00	0.44
1:F:870:VAL:O	1:F:874:ILE:HG12	2.17	0.44
1:C:536:GLY:O	1:C:540:ARG:HG2	2.18	0.44
1:F:716:LEU:HD21	1:F:839:LEU:HD23	1.98	0.44
1:A:307:SER:OG	1:A:590:ASP:OD1	2.35	0.44
1:A:748:LEU:HD22	1:F:748:LEU:HD22	1.98	0.44
1:E:136:PRO:HA	1:E:137:PRO:HD3	1.88	0.44
1:E:412:PHE:O	1:E:414:GLU:N	2.50	0.44
1:E:693:GLN:HB3	1:E:694:TRP:CD1	2.52	0.44
1:G:297:ASN:HB2	1:G:299:TYR:HD2	1.82	0.44
1:C:784:PRO:HG3	1:C:879:PHE:HE1	1.81	0.44
1:E:594:ARG:NE	1:E:596:ASP:OD1	2.50	0.44
1:F:549:GLU:OE2	1:F:612:THR:OG1	2.35	0.44
1:A:82:CYS:SG	1:A:104:THR:OG1	2.58	0.44
1:C:502:SER:C	1:C:504:SER:H	2.26	0.44
1:D:269:GLU:OE1	1:D:361:ARG:NH2	2.40	0.44
1:D:646:TRP:CH2	1:D:654:ARG:HG3	2.52	0.44
1:G:876:ASN:OD1	1:G:876:ASN:N	2.50	0.44
1:C:13:TRP:HD1	1:C:242:PHE:HE2	1.66	0.44
1:C:183:ASN:OD1	1:C:183:ASN:N	2.50	0.44
1:D:536:GLY:O	1:D:540:ARG:HG2	2.18	0.44
1:F:319:MET:HE1	1:F:746:TRP:HB2	2.00	0.44
1:G:423:ALA:O	1:G:427:ASP:N	2.50	0.44
1:H:253:LYS:HD3	1:H:254:ASP:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:256:ASP:HB3	1:E:356:GLU:HB3	1.99	0.44
1:E:402:VAL:HG21	1:E:425:VAL:HG11	1.99	0.44
1:E:716:LEU:O	1:E:724:LEU:N	2.47	0.44
1:E:716:LEU:HD21	1:E:839:LEU:HD23	1.99	0.44
1:G:810:LEU:O	1:G:814:ASN:ND2	2.48	0.44
1:B:404:THR:HB	1:B:405:ASN:H	1.67	0.43
1:C:618:LEU:HD11	1:C:655:LEU:HD21	2.00	0.43
1:D:17:LEU:O	1:D:19:GLN:N	2.46	0.43
1:F:263:HIS:C	1:F:265:ASN:H	2.26	0.43
1:D:267:GLU:H	1:D:268:PRO:HD2	1.82	0.43
1:E:416:ASN:O	1:E:416:ASN:ND2	2.44	0.43
1:E:167:MET:HE3	1:E:167:MET:HB3	1.93	0.43
1:E:297:ASN:HB2	1:E:299:TYR:HD2	1.84	0.43
1:B:157:GLU:HB2	1:B:183:ASN:HD22	1.83	0.43
1:B:474:TRP:CE3	1:B:599:GLY:HA2	2.54	0.43
1:E:38:ARG:HD3	1:E:41:ALA:HB3	2.00	0.43
1:F:361:ARG:HA	1:F:594:ARG:NH2	2.34	0.43
1:C:141:ASP:OD1	1:C:141:ASP:N	2.51	0.43
1:E:412:PHE:C	1:E:413:THR:HG1	2.27	0.43
1:C:451:TYR:HB2	1:C:577:VAL:HG22	2.01	0.43
1:F:77:VAL:HG22	1:F:142:THR:HB	2.00	0.43
1:B:390:PRO:HB2	1:B:556:MET:HG2	2.00	0.43
1:B:636:PRO:HG2	1:B:637:HIS:CD2	2.53	0.43
1:D:481:ARG:NH2	1:D:601:GLY:O	2.52	0.43
1:E:618:LEU:HD11	1:E:655:LEU:HD21	1.99	0.43
1:A:136:PRO:HA	1:A:137:PRO:HD3	1.88	0.43
1:C:120:GLY:HA2	1:C:262:ARG:HB2	2.01	0.43
1:D:596:ASP:OD1	1:D:597:GLN:N	2.52	0.43
1:H:425:VAL:HA	1:H:431:TRP:CZ2	2.53	0.43
1:B:282:ARG:O	1:B:286:GLU:HG2	2.19	0.43
1:B:625:GLU:OE1	1:B:646:TRP:NE1	2.37	0.43
1:C:557:ASP:O	1:C:561:ARG:N	2.42	0.43
1:D:512:HIS:CD2	1:D:513:LYS:HG3	2.54	0.43
1:E:768:HIS:H	1:E:768:HIS:CD2	2.36	0.43
1:A:167:MET:HE3	1:A:167:MET:HB3	1.88	0.43
1:B:760:GLN:NE2	1:B:803:TRP:O	2.52	0.43
1:C:596:ASP:OD1	1:C:597:GLN:N	2.52	0.43
1:F:828:THR:HA	1:F:829:PRO:HD3	1.89	0.43
1:G:136:PRO:HA	1:G:137:PRO:HD3	1.89	0.43
1:D:863:ILE:O	1:D:867:ILE:HG12	2.18	0.42
1:E:116:MET:HB3	1:E:118:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:636:PRO:HG2	1:G:637:HIS:CD2	2.54	0.42
1:C:381:TRP:CE3	1:C:552:ILE:HD13	2.54	0.42
1:D:220:ILE:H	1:D:220:ILE:HG13	1.63	0.42
1:F:512:HIS:CD2	1:F:802:GLN:HE22	2.36	0.42
1:G:220:ILE:H	1:G:220:ILE:HG13	1.67	0.42
1:H:136:PRO:HA	1:H:137:PRO:HD3	1.89	0.42
1:A:550:GLU:OE2	1:A:573:GLN:NE2	2.51	0.42
1:D:636:PRO:HG2	1:D:637:HIS:CD2	2.53	0.42
1:E:77:VAL:HG22	1:E:142:THR:HB	2.01	0.42
1:E:334:VAL:HA	1:E:335:PRO:HD3	1.91	0.42
1:H:151:SER:HA	1:H:152:PRO:HD3	1.91	0.42
1:A:822:PRO:HG2	1:A:823:TRP:CE3	2.55	0.42
1:E:50:ILE:H	1:E:50:ILE:HD13	1.85	0.42
1:E:517:ILE:O	1:E:521:ILE:HG13	2.19	0.42
1:F:451:TYR:HA	1:F:476:MET:HB3	2.00	0.42
1:G:100:VAL:HB	1:G:124:VAL:HA	2.01	0.42
1:A:695:GLN:HA	1:A:696:PRO:HD3	1.94	0.42
1:C:594:ARG:NE	1:C:596:ASP:OD1	2.52	0.42
1:E:580:GLN:HG3	1:E:589:MET:HE2	2.01	0.42
1:F:196:LEU:HB3	1:F:219:TRP:CH2	2.54	0.42
1:G:61:LYS:NZ	1:G:216:GLU:OE1	2.52	0.42
1:D:842:ARG:HE	1:E:880:LEU:HD11	1.85	0.42
1:H:177:PHE:H	1:H:221:SER:HB3	1.83	0.42
1:A:519:ARG:O	1:A:522:SER:OG	2.37	0.42
1:E:625:GLU:HG2	1:E:670:ILE:HD11	2.02	0.42
1:C:572:TYR:O	1:C:575:LYS:NZ	2.51	0.42
1:E:398:PHE:O	1:E:402:VAL:HG23	2.20	0.42
1:E:504:SER:OG	1:E:655:LEU:O	2.31	0.42
1:A:622:MET:HB3	1:A:627:VAL:HB	2.01	0.42
1:C:262:ARG:NH1	1:C:267:GLU:OE1	2.53	0.42
1:D:17:LEU:HG	1:D:18:ASN:H	1.84	0.42
1:A:20:LEU:HD11	1:A:242:PHE:HE1	1.85	0.42
1:A:731:GLN:HB2	1:A:769:ARG:HH12	1.84	0.42
1:D:183:ASN:OD1	1:D:186:MET:HG2	2.20	0.42
1:D:297:ASN:HB2	1:D:299:TYR:HD2	1.84	0.42
1:D:568:PHE:HA	1:D:572:TYR:HB2	2.02	0.42
1:D:475:TYR:O	1:D:475:TYR:CG	2.72	0.41
1:D:553:THR:HB	1:D:561:ARG:HG3	2.02	0.41
1:G:215:HIS:O	1:G:215:HIS:ND1	2.51	0.41
1:B:353:VAL:O	1:B:357:LYS:HB2	2.19	0.41
1:B:625:GLU:HG2	1:B:670:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:MET:HE2	1:B:724:LEU:HG	2.01	0.41
1:C:29:LYS:HE2	1:C:211:ARG:HD2	2.02	0.41
1:C:411:VAL:HG21	1:C:578:LYS:HD2	2.01	0.41
1:C:790:THR:OG1	1:C:791:SER:N	2.54	0.41
1:D:246:HIS:HB2	1:G:861:GLN:HE22	1.85	0.41
1:D:393:CYS:HB2	1:D:486:GLU:HA	2.02	0.41
1:E:176:GLN:OE1	1:E:221:SER:OG	2.33	0.41
1:E:403:ARG:H	1:E:403:ARG:HD2	1.85	0.41
1:D:502:SER:O	1:D:504:SER:N	2.42	0.41
1:D:730:PRO:HB2	1:D:733:GLU:HG3	2.02	0.41
1:C:722:ARG:HD3	1:C:826:ASP:HB3	2.02	0.41
1:F:186:MET:HA	1:F:187:PRO:HD3	1.92	0.41
1:F:484:GLU:CD	1:F:603:VAL:H	2.29	0.41
1:F:716:LEU:N	1:F:724:LEU:O	2.44	0.41
1:G:711:HIS:NE2	1:G:729:ARG:HD2	2.35	0.41
1:C:526:GLY:HA2	1:D:127:MET:HG3	2.02	0.41
1:C:828:THR:HA	1:C:829:PRO:HD3	1.85	0.41
1:F:61:LYS:HA	1:F:209:LEU:HD13	2.03	0.41
1:A:56:SER:HB3	1:A:84:ARG:HD3	2.02	0.41
1:B:61:LYS:HA	1:B:209:LEU:HD12	2.02	0.41
1:D:307:SER:OG	1:D:590:ASP:OD1	2.27	0.41
1:B:186:MET:HA	1:B:187:PRO:HD3	1.90	0.41
1:C:237:LEU:O	1:C:241:ARG:HG2	2.20	0.41
1:D:186:MET:HA	1:D:187:PRO:HD3	1.91	0.41
1:G:484:GLU:OE2	1:G:572:TYR:OH	2.34	0.41
1:G:655:LEU:HA	1:G:658:MET:HE2	2.02	0.41
1:A:158:GLU:OE2	1:A:188:THR:OG1	2.28	0.41
1:C:550:GLU:OE2	1:C:569:LYS:HE3	2.21	0.41
1:D:158:GLU:OE2	1:D:188:THR:OG1	2.24	0.41
1:D:381:TRP:CE3	1:D:552:ILE:HD13	2.56	0.41
1:G:512:HIS:CD2	1:G:513:LYS:HG3	2.56	0.41
1:G:652:VAL:HG12	1:G:656:LYS:HE3	2.02	0.41
1:H:186:MET:HA	1:H:187:PRO:HD3	1.87	0.41
1:H:557:ASP:HA	1:H:558:PRO:HD3	1.93	0.41
1:A:334:VAL:HA	1:A:335:PRO:HD3	1.90	0.41
1:E:38:ARG:HH22	1:E:54:ALA:HB3	1.86	0.41
1:E:477:TRP:CZ2	1:E:479:GLY:HA3	2.55	0.41
1:E:698:LYS:H	1:E:698:LYS:HD3	1.85	0.41
1:F:143:LEU:HD22	1:F:171:TRP:HB2	2.03	0.41
1:F:477:TRP:CZ2	1:F:479:GLY:HA3	2.56	0.41
1:G:731:GLN:HB2	1:G:769:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:HIS:N	1:F:861:GLN:OE1	2.54	0.40
1:A:320:ILE:HG21	1:A:325:LYS:HD2	2.03	0.40
1:B:549:GLU:CD	1:B:598:ARG:HH22	2.29	0.40
1:D:17:LEU:C	1:D:19:GLN:H	2.28	0.40
1:E:820:ASP:OD2	1:G:23:LYS:NZ	2.53	0.40
1:F:66:VAL:HG21	1:F:90:TYR:HE2	1.86	0.40
1:F:793:THR:HB	1:F:801:HIS:CE1	2.56	0.40
1:G:112:GLU:HB3	1:H:701:HIS:CE1	2.56	0.40
1:G:362:THR:HA	1:G:363:PRO:HD3	1.96	0.40
1:H:598:ARG:CZ	1:H:608:LEU:HG	2.52	0.40
1:A:788:VAL:HA	1:A:789:PRO:HD3	1.87	0.40
1:C:215:HIS:O	1:C:215:HIS:ND1	2.53	0.40
1:E:146:ASP:HB3	3:E:1003:SAH:HG1	2.02	0.40
1:E:575:LYS:NZ	1:E:596:ASP:O	2.52	0.40
1:G:13:TRP:HE1	1:G:215:HIS:HD2	1.69	0.40
1:H:307:SER:HA	1:H:590:ASP:HA	2.03	0.40
1:H:348:PHE:HD1	1:H:348:PHE:HA	1.68	0.40
1:H:728:CYS:SG	1:H:729:ARG:N	2.94	0.40
1:A:538:ASP:HB3	1:A:598:ARG:HB3	2.03	0.40
1:B:119:TYR:CE2	1:B:262:ARG:HD2	2.57	0.40
1:C:695:GLN:HA	1:C:696:PRO:HD3	1.93	0.40
1:C:846:TRP:CD1	1:E:842:ARG:HD3	2.57	0.40
1:E:672:ASP:HB3	1:F:115:PRO:HB3	2.04	0.40
1:A:403:ARG:NH2	1:A:426:GLU:OE2	2.53	0.40
1:B:791:SER:OG	1:B:792:ARG:N	2.52	0.40
1:C:327:LEU:HD12	1:C:779:ILE:HG12	2.03	0.40
1:E:45:LEU:HD22	1:E:116:MET:HE1	2.03	0.40
1:E:596:ASP:HB2	1:E:597:GLN:H	1.69	0.40
1:E:618:LEU:O	1:E:622:MET:HG3	2.21	0.40
1:F:718:MET:HG2	1:F:837:PRO:HG3	2.02	0.40
1:G:618:LEU:O	1:G:622:MET:HG3	2.21	0.40
1:A:186:MET:HA	1:A:187:PRO:HD3	1.91	0.40
1:B:596:ASP:OD1	1:B:597:GLN:N	2.54	0.40
1:C:69:ASN:HD22	1:C:72:ILE:HD11	1.86	0.40
1:D:509:GLU:HG2	1:D:517:ILE:HD11	2.03	0.40
1:F:362:THR:HA	1:F:363:PRO:HD3	1.92	0.40
1:G:374:GLU:HG3	1:G:551:LYS:HE3	2.03	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	843/905 (93%)	811 (96%)	32 (4%)	0	100	100
1	B	845/905 (93%)	806 (95%)	38 (4%)	1 (0%)	48	79
1	C	846/905 (94%)	808 (96%)	37 (4%)	1 (0%)	48	79
1	D	840/905 (93%)	808 (96%)	32 (4%)	0	100	100
1	E	848/905 (94%)	812 (96%)	34 (4%)	2 (0%)	43	72
1	F	844/905 (93%)	804 (95%)	38 (4%)	2 (0%)	43	72
1	G	841/905 (93%)	796 (95%)	42 (5%)	3 (0%)	30	61
1	H	747/905 (82%)	706 (94%)	41 (6%)	0	100	100
All	All	6654/7240 (92%)	6351 (95%)	294 (4%)	9 (0%)	48	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	264	VAL
1	F	264	VAL
1	G	421	ALA
1	G	11	GLU
1	E	413	THR
1	F	791	SER
1	G	791	SER
1	B	33	ILE
1	E	447	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	259/786 (33%)	249 (96%)	10 (4%)	28	54
1	B	747/786 (95%)	738 (99%)	9 (1%)	63	73
1	C	745/786 (95%)	725 (97%)	20 (3%)	39	61
1	D	737/786 (94%)	724 (98%)	13 (2%)	51	68
1	E	746/786 (95%)	721 (97%)	25 (3%)	32	57
1	F	741/786 (94%)	723 (98%)	18 (2%)	43	63
1	G	736/786 (94%)	728 (99%)	8 (1%)	65	74
1	H	193/786 (25%)	185 (96%)	8 (4%)	27	53
All	All	4904/6288 (78%)	4793 (98%)	111 (2%)	44	64

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	618	LEU
1	A	716	LEU
1	A	769	ARG
1	A	788	VAL
1	A	793	THR
1	A	802	GLN
1	A	804	MET
1	A	839	LEU
1	A	886	MET
1	A	888	ARG
1	B	220	ILE
1	B	300	LYS
1	B	343	THR
1	B	356	GLU
1	B	426	GLU
1	B	533	ASP
1	B	579	VAL
1	B	794	THR
1	B	804	MET
1	C	14	LYS
1	C	16	LYS
1	C	20	LEU
1	C	31	SER
1	C	71	VAL
1	C	139	LYS

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Mol	Chain	Res	Type
1	C	173	LYS
1	C	220	ILE
1	C	262	ARG
1	C	264	VAL
1	C	272	ASN
1	C	345	THR
1	C	403	ARG
1	C	450	VAL
1	C	475	TYR
1	C	533	ASP
1	C	579	VAL
1	C	764	LEU
1	C	846	TRP
1	C	883	MET
1	D	71	VAL
1	D	173	LYS
1	D	220	ILE
1	D	245	THR
1	D	272	ASN
1	D	477	TRP
1	D	481	ARG
1	D	533	ASP
1	D	579	VAL
1	D	619	ILE
1	D	650	LYS
1	D	764	LEU
1	D	861	GLN
1	E	50	ILE
1	E	71	VAL
1	E	139	LYS
1	E	272	ASN
1	E	389	ARG
1	E	403	ARG
1	E	408	MET
1	E	414	GLU
1	E	415	GLU
1	E	416	ASN
1	E	443	LEU
1	E	478	LEU
1	E	488	LEU
1	E	533	ASP
1	E	579	VAL

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Mol	Chain	Res	Type
1	E	589	MET
1	E	693	GLN
1	E	698	LYS
1	E	716	LEU
1	E	717	ILE
1	E	769	ARG
1	E	793	THR
1	E	804	MET
1	E	811	THR
1	E	863	ILE
1	F	71	VAL
1	F	135	LEU
1	F	139	LYS
1	F	220	ILE
1	F	233	MET
1	F	237	LEU
1	F	245	THR
1	F	264	VAL
1	F	333	VAL
1	F	389	ARG
1	F	453	MET
1	F	477	TRP
1	F	506	VAL
1	F	533	ASP
1	F	645	GLN
1	F	742	GLN
1	F	788	VAL
1	F	804	MET
1	G	15	LYS
1	G	71	VAL
1	G	333	VAL
1	G	420	SER
1	G	533	ASP
1	G	579	VAL
1	G	804	MET
1	G	881	ASP
1	H	9	LEU
1	H	198	ARG
1	H	253	LYS
1	H	323	VAL
1	H	348	PHE
1	H	608	LEU

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Mol	Chain	Res	Type
1	H	671	ASP
1	H	688	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	760	GLN
1	A	861	GLN
1	B	297	ASN
1	B	574	ASN
1	B	597	GLN
1	B	602	GLN
1	B	637	HIS
1	B	704	GLN
1	C	272	ASN
1	C	704	GLN
1	C	802	GLN
1	D	297	ASN
1	D	351	GLN
1	D	512	HIS
1	D	565	ASN
1	D	580	GLN
1	D	760	GLN
1	D	861	GLN
1	E	69	ASN
1	E	240	ASN
1	E	339	GLN
1	E	405	ASN
1	E	501	ASN
1	E	547	HIS
1	E	554	GLN
1	E	760	GLN
1	E	802	GLN
1	F	175	ASN
1	F	240	ASN
1	F	339	GLN
1	F	512	HIS
1	F	617	GLN
1	F	742	GLN
1	G	554	GLN
1	G	613	ASN
1	G	617	GLN

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Mol	Chain	Res	Type
1	G	637	HIS
1	G	693	GLN
1	G	760	GLN
1	G	861	GLN
1	H	565	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\# Z > 2$
3	SAH	E	1003	-	27,28,28	1.26	2 (7%)	36,40,40	0.99	1 (2%)
3	SAH	F	1003	-	27,28,28	1.26	1 (3%)	36,40,40	0.98	1 (2%)
3	SAH	G	1003	-	27,28,28	1.27	1 (3%)	36,40,40	0.98	1 (2%)
3	SAH	A	1003	-	27,28,28	1.27	1 (3%)	36,40,40	0.99	1 (2%)
3	SAH	H	1003	-	27,28,28	1.29	2 (7%)	36,40,40	0.98	1 (2%)
3	SAH	B	1003	-	27,28,28	1.27	1 (3%)	36,40,40	1.01	1 (2%)
3	SAH	C	1003	-	27,28,28	1.30	2 (7%)	36,40,40	1.00	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SAH	D	1003	-	27,28,28	1.23	1 (3%)	36,40,40	0.98	1 (2%)

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
3	SAH	E	1003	-	-	1/15/31/31	0/3/3/3
3	SAH	F	1003	-	-	2/15/31/31	0/3/3/3
3	SAH	G	1003	-	-	0/15/31/31	0/3/3/3
3	SAH	A	1003	-	-	1/15/31/31	0/3/3/3
3	SAH	H	1003	-	-	2/15/31/31	0/3/3/3
3	SAH	B	1003	-	-	2/15/31/31	0/3/3/3
3	SAH	C	1003	-	-	1/15/31/31	0/3/3/3
3	SAH	D	1003	-	-	1/15/31/31	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	SAH	C8-N9	2.98	1.42	1.37
3	E	1003	SAH	C8-N9	2.96	1.42	1.37
3	B	1003	SAH	C8-N9	2.95	1.42	1.37
3	H	1003	SAH	C8-N9	2.94	1.42	1.37
3	F	1003	SAH	C8-N9	2.92	1.42	1.37
3	G	1003	SAH	C8-N9	2.89	1.42	1.37
3	D	1003	SAH	C8-N9	2.81	1.42	1.37
3	A	1003	SAH	C8-N9	2.77	1.42	1.37
3	H	1003	SAH	C5-C4	2.08	1.42	1.39
3	C	1003	SAH	C5-C4	2.05	1.42	1.39
3	E	1003	SAH	C5-C4	2.03	1.42	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1003	SAH	C5'-C4'-C3'	-2.24	109.46	115.06
3	F	1003	SAH	C5'-C4'-C3'	-2.11	109.79	115.06
3	C	1003	SAH	C5'-C4'-C3'	-2.09	109.83	115.06
3	B	1003	SAH	C5'-C4'-C3'	-2.08	109.84	115.06
3	H	1003	SAH	C5'-C4'-C3'	-2.06	109.90	115.06
3	A	1003	SAH	C5'-C4'-C3'	-2.05	109.93	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1003	SAH	C5'-C4'-C3'	-2.03	109.97	115.06
3	D	1003	SAH	C5'-C4'-C3'	-2.03	109.97	115.06

There are no chirality outliers.

All (10) torsion outliers are listed below:

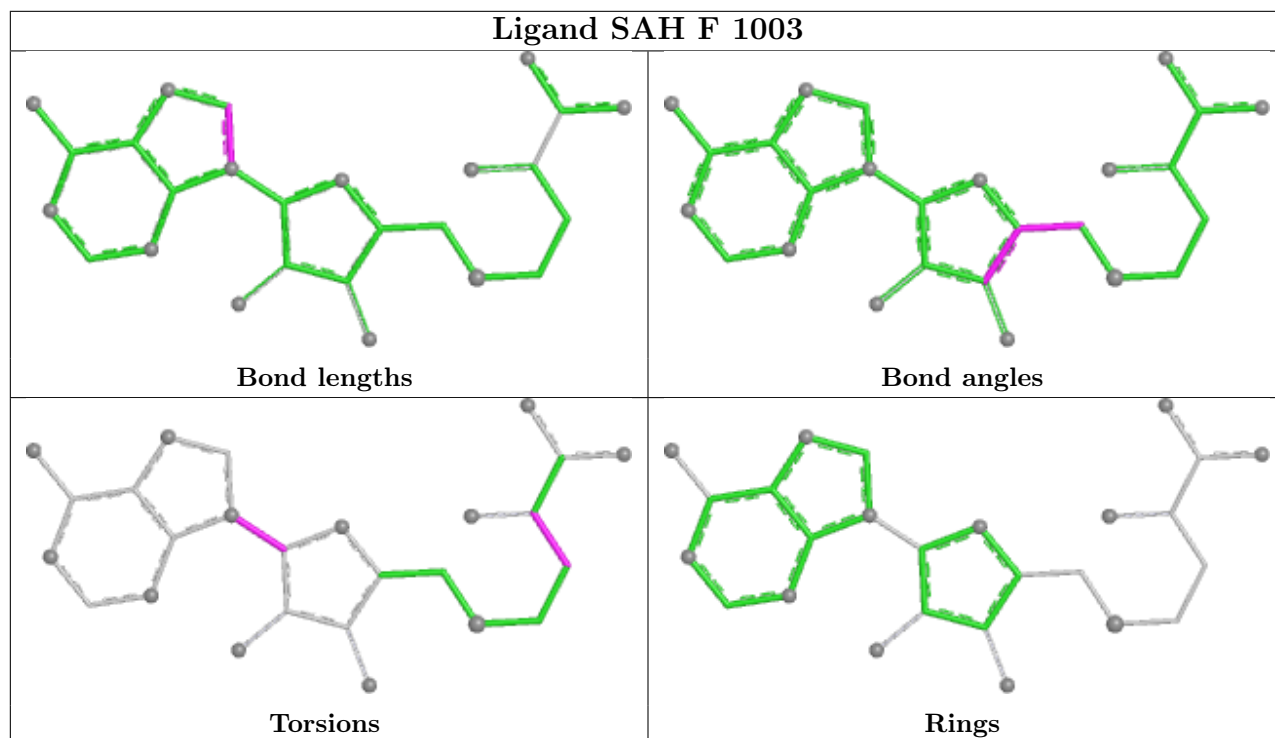
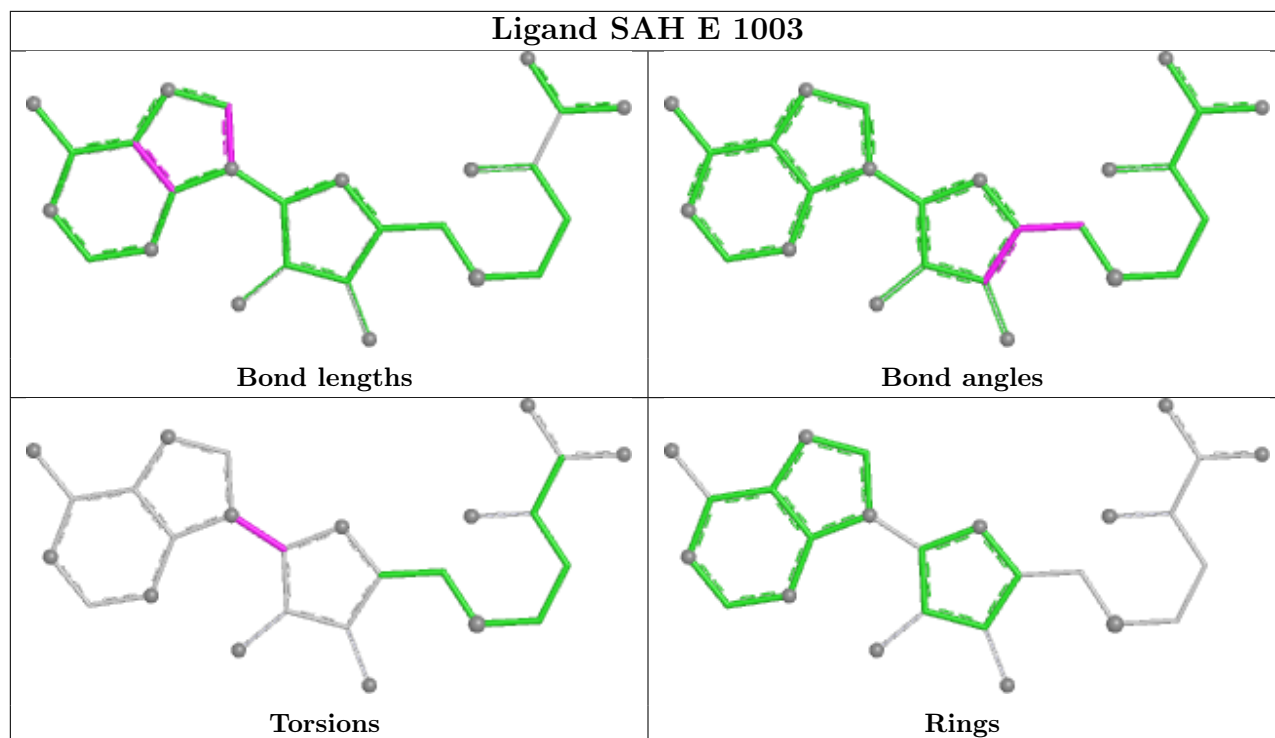
Mol	Chain	Res	Type	Atoms
3	H	1003	SAH	OXT-C-CA-CB
3	B	1003	SAH	C-CA-CB-CG
3	E	1003	SAH	C2'-C1'-N9-C8
3	H	1003	SAH	O-C-CA-CB
3	A	1003	SAH	C-CA-CB-CG
3	C	1003	SAH	C-CA-CB-CG
3	F	1003	SAH	C-CA-CB-CG
3	B	1003	SAH	C2'-C1'-N9-C8
3	F	1003	SAH	C2'-C1'-N9-C8
3	D	1003	SAH	C2'-C1'-N9-C8

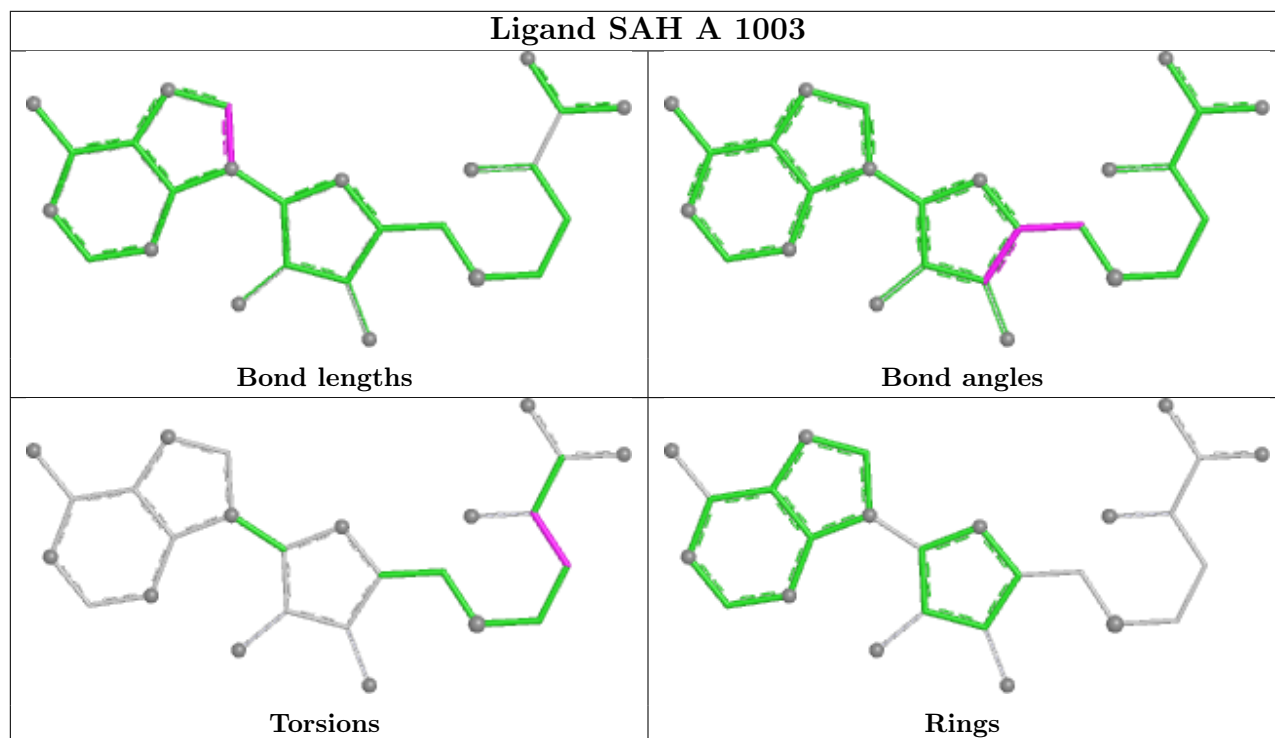
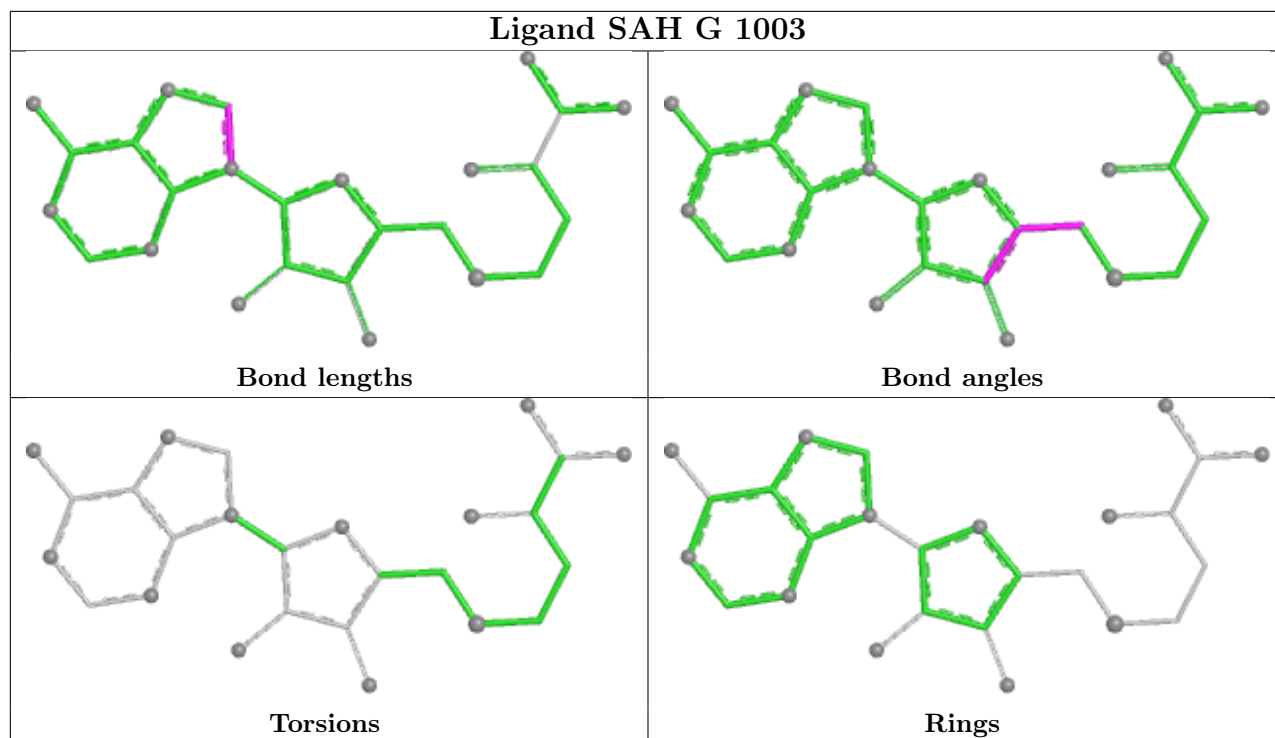
There are no ring outliers.

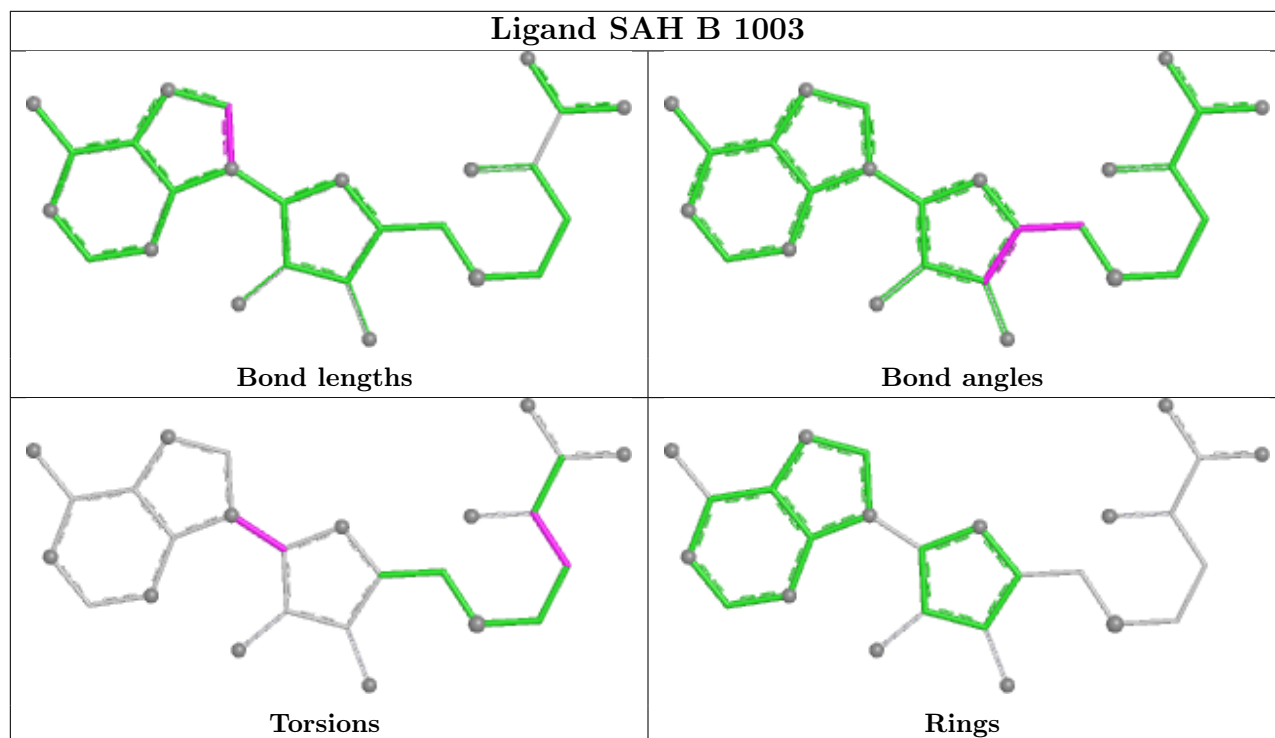
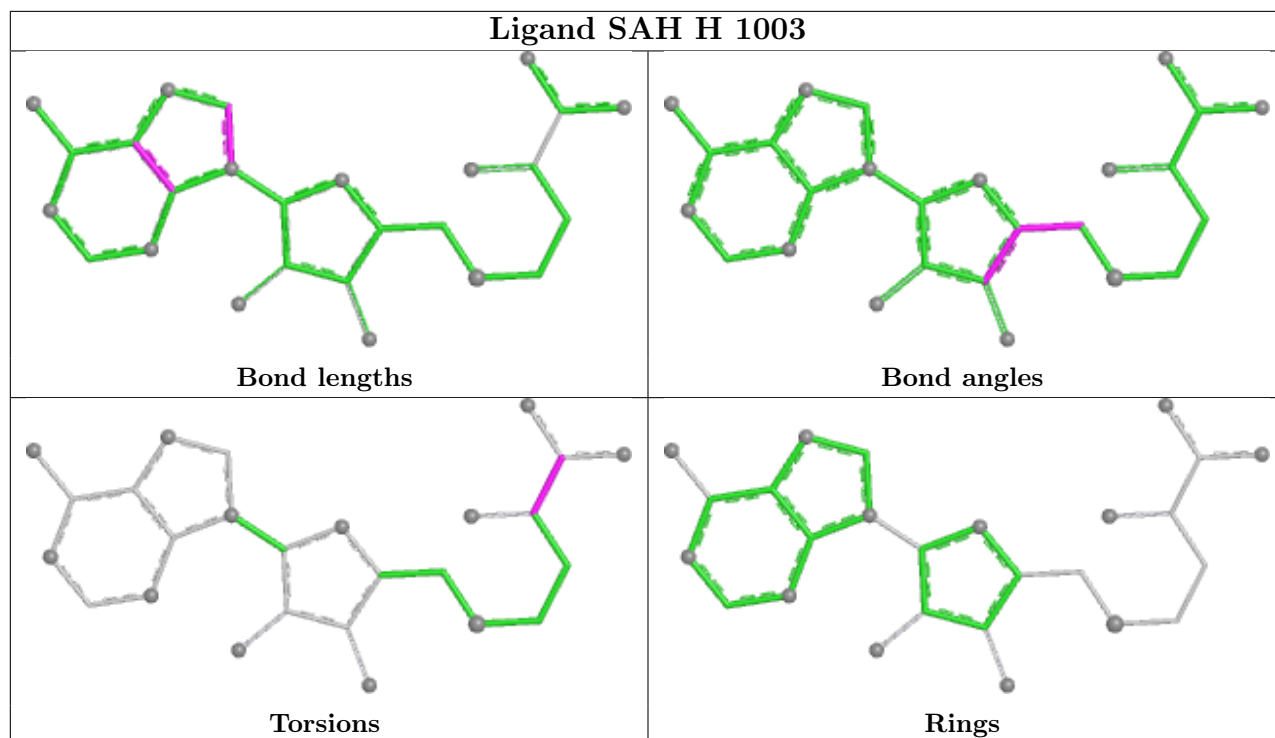
1 monomer is involved in 1 short contact:

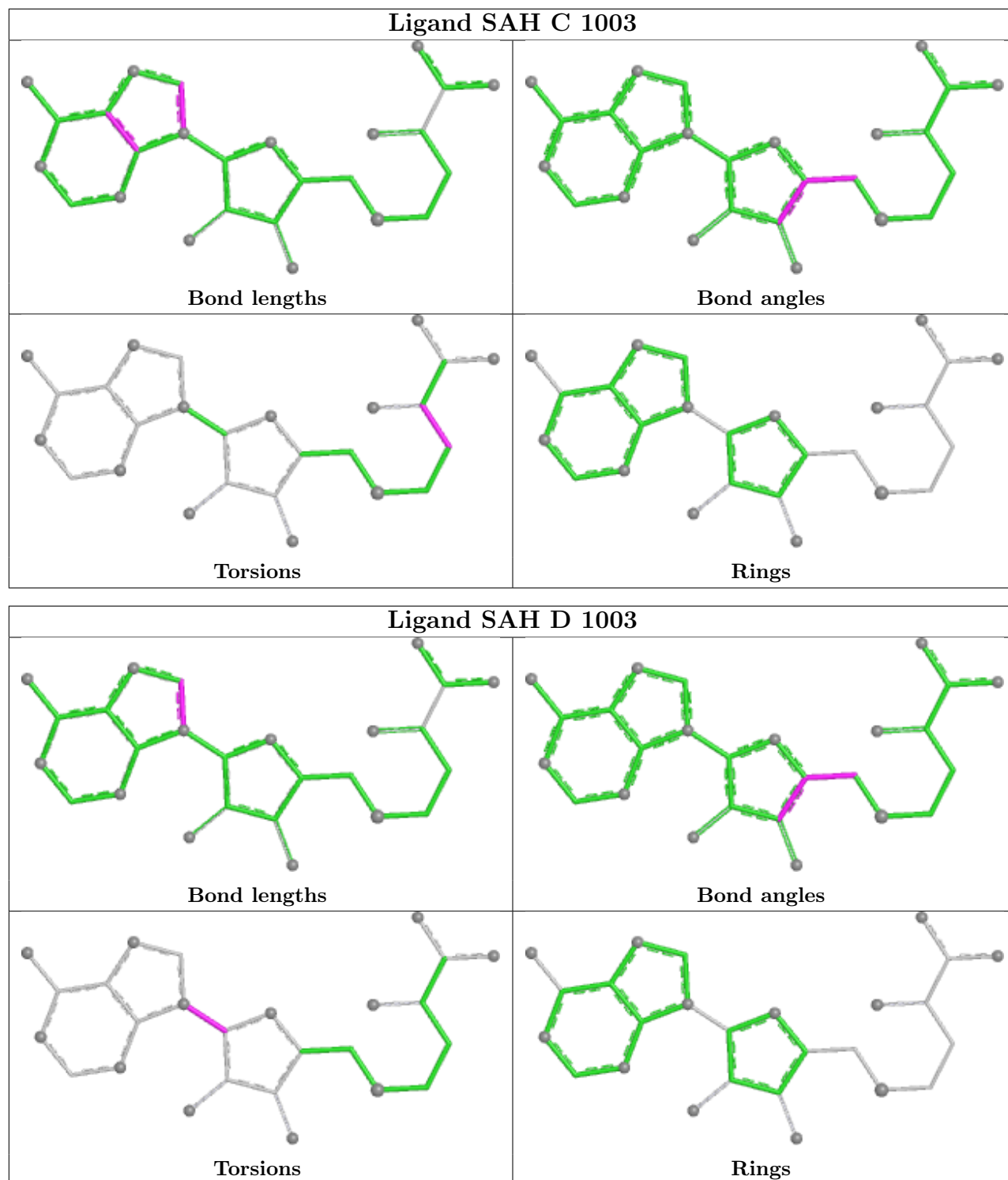
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1003	SAH	1	0

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

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	849/905 (93%)	-0.05	2 (0%) 91 80	72, 85, 130, 207	0
1	B	851/905 (94%)	0.05	5 (0%) 85 64	75, 86, 123, 201	0
1	C	852/905 (94%)	0.01	6 (0%) 84 61	72, 87, 142, 187	0
1	D	848/905 (93%)	-0.03	2 (0%) 91 80	72, 83, 114, 232	0
1	E	852/905 (94%)	0.11	10 (1%) 76 50	78, 101, 142, 188	0
1	F	850/905 (93%)	0.11	0 100 100	74, 93, 116, 173	0
1	G	847/905 (93%)	0.08	1 (0%) 92 85	77, 97, 116, 189	0
1	H	767/905 (84%)	0.48	22 (2%) 53 30	93, 122, 171, 211	0
All	All	6716/7240 (92%)	0.09	48 (0%) 84 61	72, 93, 140, 232	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	545	ASP	3.3
1	C	472	ALA	3.3
1	H	254	ASP	3.0
1	C	794	THR	3.0
1	E	473	ILE	2.9
1	C	884	PRO	2.9
1	H	82	CYS	2.9
1	H	393	CYS	2.8
1	H	597	GLN	2.7
1	H	755	GLY	2.7
1	H	766	TYR	2.6
1	H	79	ASP	2.6
1	E	411	VAL	2.6
1	H	183	ASN	2.5
1	B	802	GLN	2.5
1	H	758	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	454	MET	2.5
1	B	793	THR	2.5
1	C	415	GLU	2.5
1	H	732	ASP	2.5
1	E	409	GLY	2.4
1	H	762	TRP	2.4
1	A	478	LEU	2.3
1	D	406	ALA	2.3
1	B	884	PRO	2.3
1	E	783	VAL	2.3
1	H	805	THR	2.3
1	H	184	PRO	2.3
1	H	595	LYS	2.3
1	G	802	GLN	2.2
1	B	356	GLU	2.2
1	E	415	GLU	2.2
1	A	595	LYS	2.2
1	C	30	LYS	2.2
1	E	794	THR	2.2
1	H	664	ASP	2.2
1	C	476	MET	2.2
1	E	720	ASP	2.1
1	D	895	SER	2.1
1	H	763	ALA	2.1
1	H	593	SER	2.1
1	B	794	THR	2.1
1	E	404	THR	2.1
1	H	228	VAL	2.1
1	E	357	LYS	2.0
1	H	590	ASP	2.0
1	H	88	SER	2.0
1	H	128	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

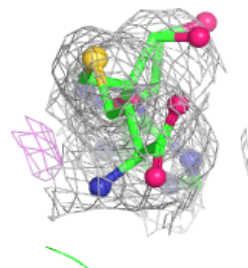
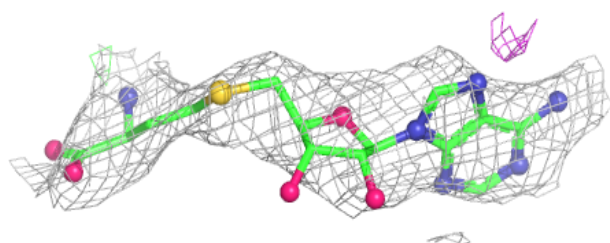
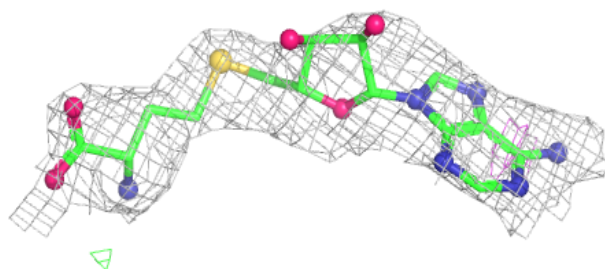
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SAH	H	1003	26/26	0.76	0.12	96,106,159,164	0
3	SAH	E	1003	26/26	0.85	0.12	93,96,103,171	0
3	SAH	C	1003	26/26	0.85	0.11	88,110,137,210	0
3	SAH	G	1003	26/26	0.86	0.11	94,98,143,184	0
3	SAH	F	1003	26/26	0.87	0.11	76,83,114,118	0
3	SAH	B	1003	26/26	0.90	0.11	77,79,94,100	0
3	SAH	D	1003	26/26	0.91	0.10	71,72,124,177	0
3	SAH	A	1003	26/26	0.92	0.10	78,79,92,153	0
2	ZN	H	1002	1/1	0.95	0.11	146,146,146,146	0
2	ZN	A	1001	1/1	0.99	0.04	75,75,75,75	0
2	ZN	A	1002	1/1	0.99	0.04	101,101,101,101	0
2	ZN	C	1001	1/1	0.99	0.05	82,82,82,82	0
2	ZN	D	1001	1/1	0.99	0.02	83,83,83,83	0
2	ZN	E	1001	1/1	0.99	0.02	100,100,100,100	0
2	ZN	E	1002	1/1	0.99	0.02	79,79,79,79	0
2	ZN	F	1001	1/1	0.99	0.06	84,84,84,84	0
2	ZN	F	1002	1/1	0.99	0.07	99,99,99,99	0
2	ZN	H	1001	1/1	0.99	0.06	99,99,99,99	0
2	ZN	G	1001	1/1	1.00	0.07	98,98,98,98	0
2	ZN	G	1002	1/1	1.00	0.03	84,84,84,84	0
2	ZN	B	1001	1/1	1.00	0.07	90,90,90,90	0
2	ZN	C	1002	1/1	1.00	0.03	76,76,76,76	0
2	ZN	B	1002	1/1	1.00	0.02	77,77,77,77	0
2	ZN	D	1002	1/1	1.00	0.02	82,82,82,82	0

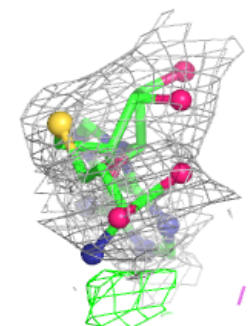
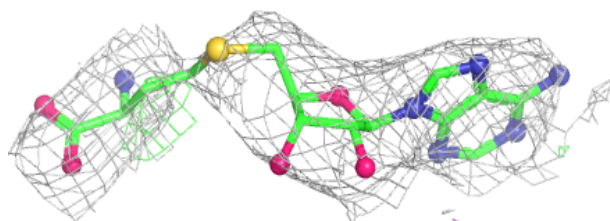
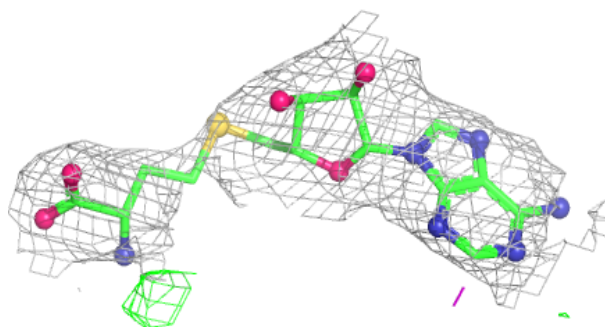
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH H 1003:

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

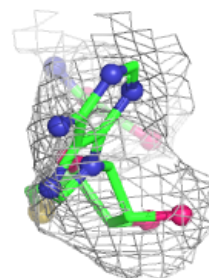
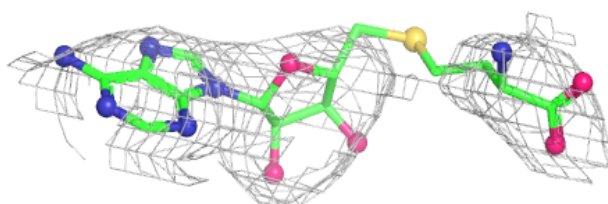
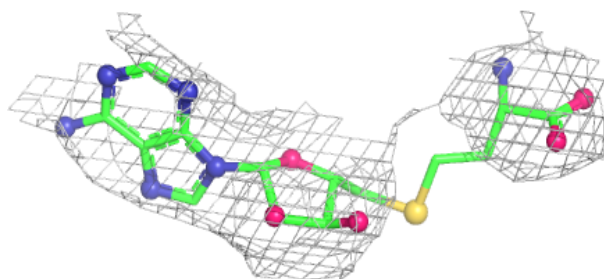
**Electron density around SAH E 1003:**

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

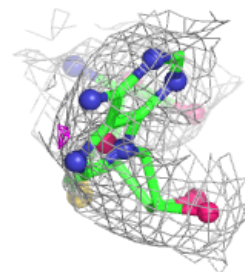
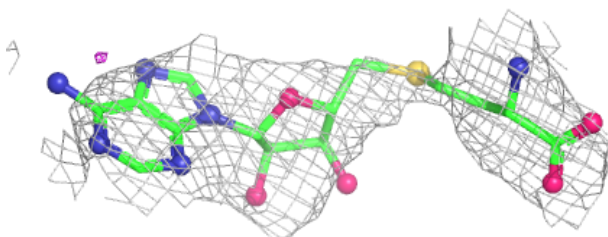
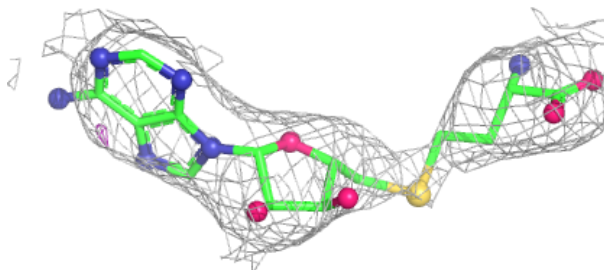


Electron density around SAH C 1003:

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

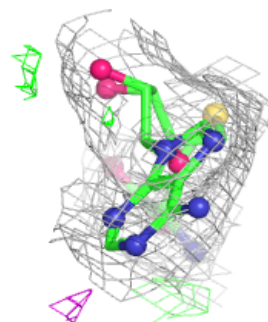
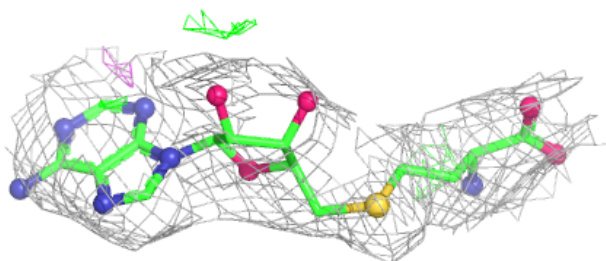
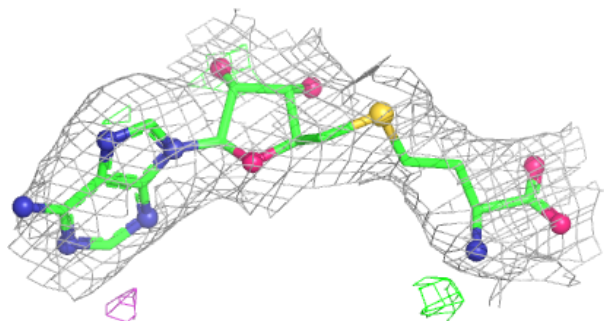
**Electron density around SAH G 1003:**

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

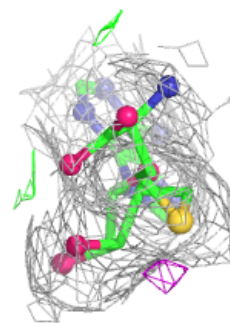
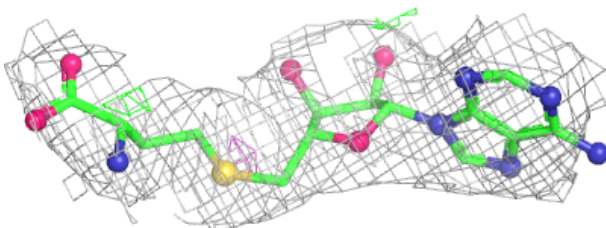
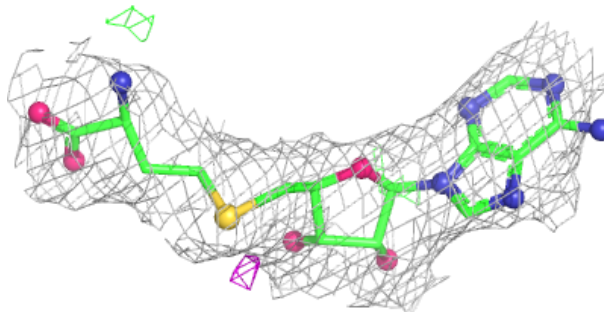


Electron density around SAH F 1003:

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

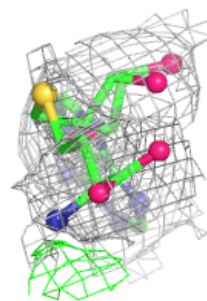
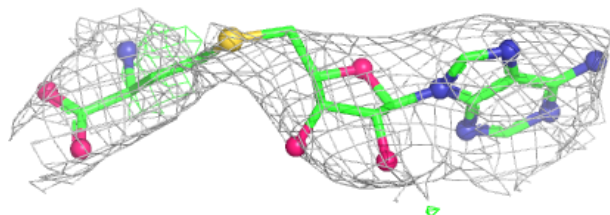
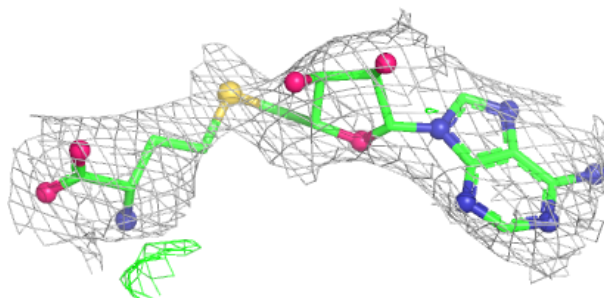
**Electron density around SAH B 1003:**

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

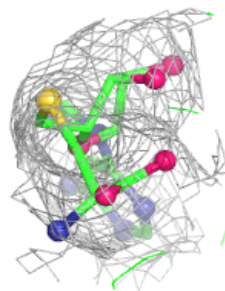
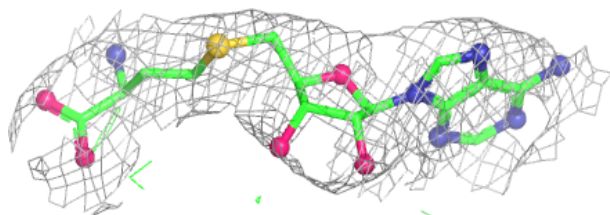
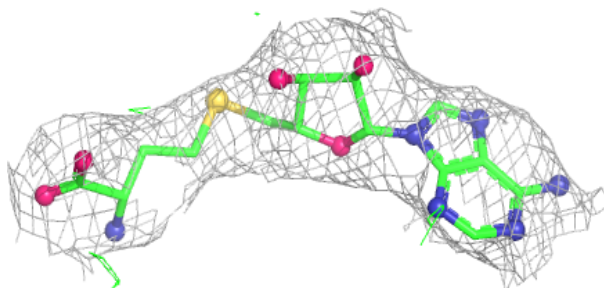


Electron density around SAH D 1003:

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

**Electron density around SAH A 1003:**

$2mF_o-DF_c$ (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.