



Full wwPDB X-ray Structure Validation Report i

May 23, 2023 – 02:08 PM JST

PDB ID : 8IN9
Title : The structure of the GfsA KSQ-AT didomain in complex with the GfsA ACP domain
Authors : Chisuga, T.; Murakami, S.; Miyanaga, A.; Kudo, F.; Eguchi, T.
Deposited on : 2023-03-09
Resolution : 3.40 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.33
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) : 2.33

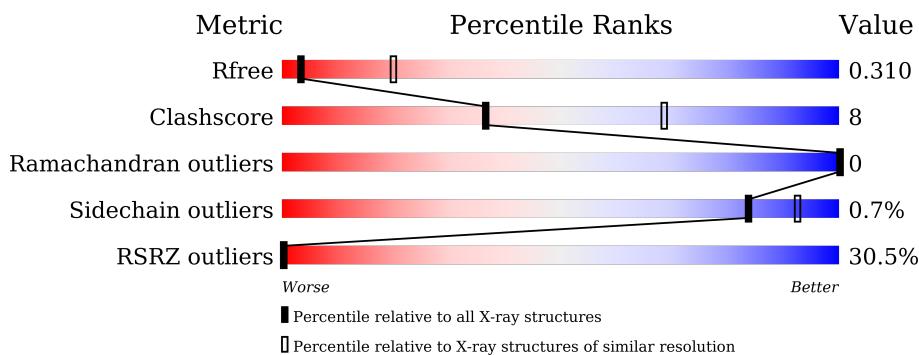
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

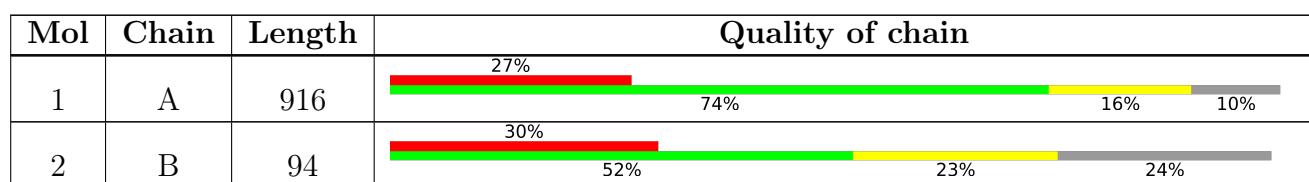
The reported resolution of this entry is 3.40 Å.

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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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.



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6597 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 Polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	820	Total	C 6026	N 3788	O 1083	S 1134	21	0	0

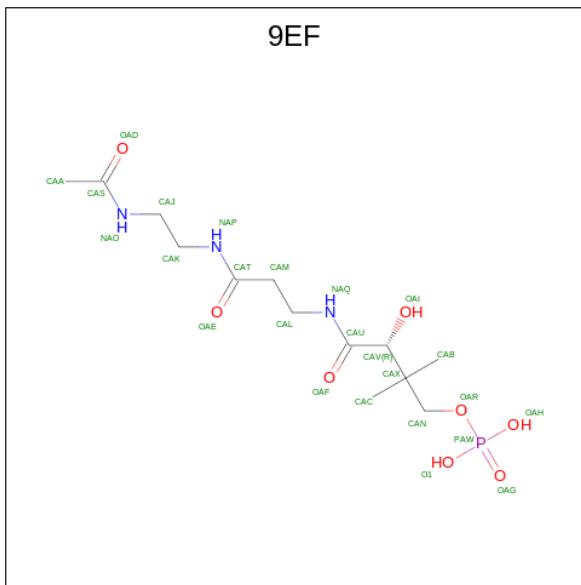
- Molecule 2 is a protein called Polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	71	Total	C 547	N 342	O 95	S 107	3	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	932	HIS	-	expression tag	UNP E0D202
B	933	MET	-	expression tag	UNP E0D202

- Molecule 3 is N-[2-(acetylamino)ethyl]-N 3 -[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alaninamide (three-letter code: 9EF) (formula: C₁₃H₂₆N₃O₈P) (labeled as "Ligand of Interest" by depositor).

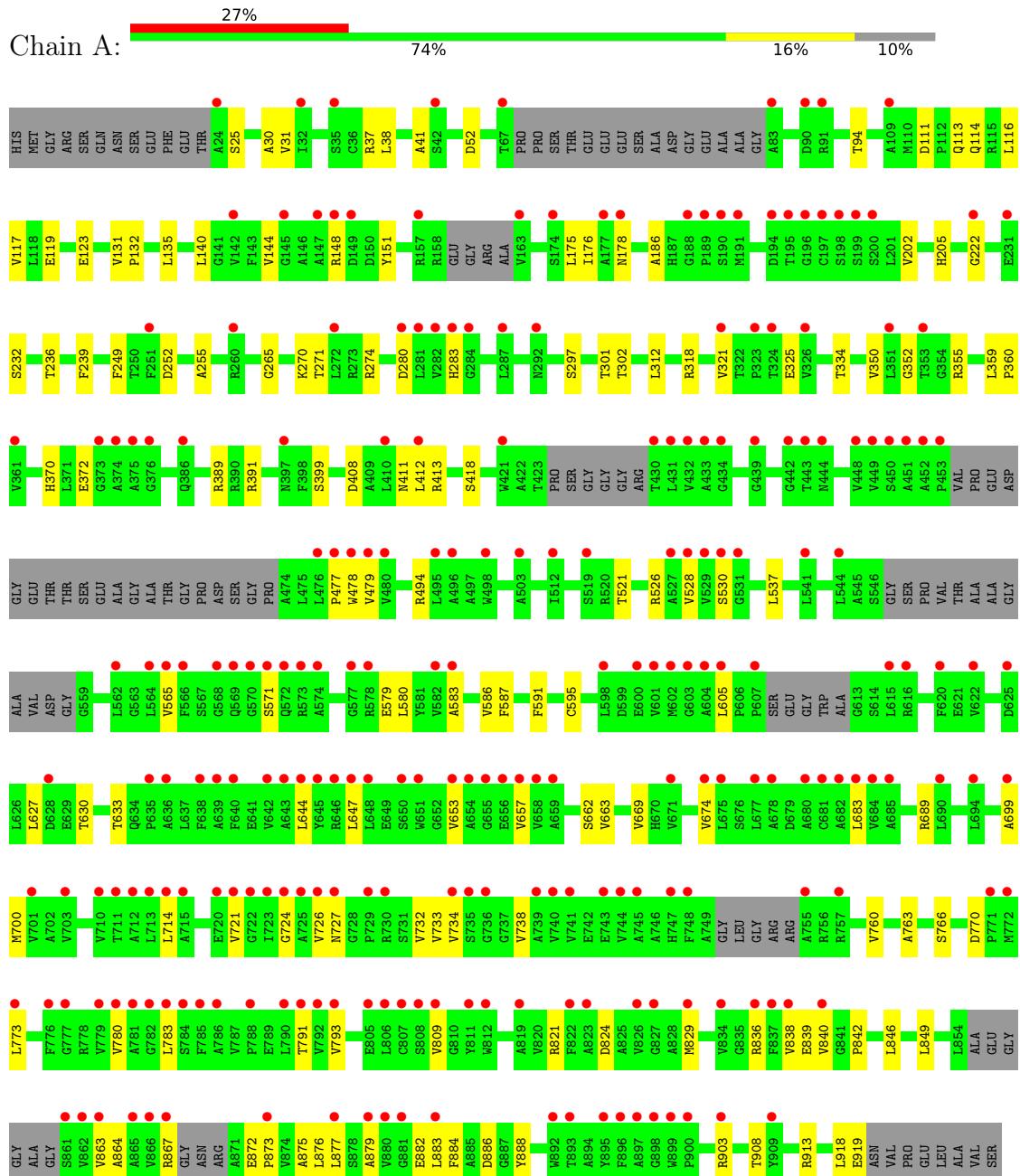


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			24	13	3	7	1		

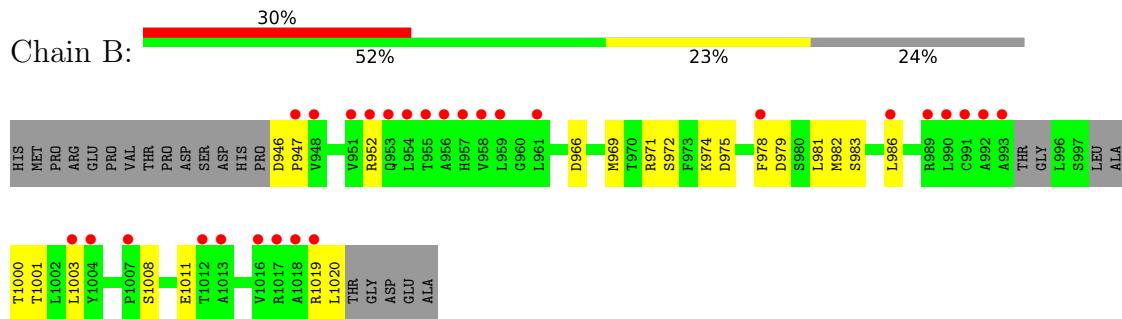
3 Residue-property plots

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: Polyketide synthase



- Molecule 2: Polyketide synthase



4 Data and refinement statistics i

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	102.21Å 102.21Å 408.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.33 – 3.40 43.33 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (43.33-3.40) 99.5 (43.33-3.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.53 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R , R_{free}	0.265 , 0.311 0.266 , 0.310	Depositor DCC
R_{free} test set	776 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	154.9	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 191.4	EDS
L-test for twinning ²	$< L > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6597	wwPDB-VP
Average B, all atoms (Å ²)	259.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 9EF

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	0.31	0/6137	0.49	0/8344
2	B	0.27	0/553	0.52	0/748
All	All	0.31	0/6690	0.50	0/9092

There are no bond length outliers.

There are no bond angle outliers.

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	6026	0	5975	93	0
2	B	547	0	543	11	0
3	A	24	0	0	1	0
All	All	6597	0	6518	104	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 8.

All (104) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:VAL:HG13	1:A:521:THR:HG22	1.62	0.80
1:A:280:ASP:HA	1:A:903:ARG:HH21	1.53	0.73
1:A:630:THR:HA	1:A:633:THR:HG22	1.71	0.72
1:A:111:ASP:HB3	1:A:114:GLN:HG3	1.74	0.70
1:A:763:ALA:O	1:A:766:SER:OG	2.09	0.70
1:A:280:ASP:OD1	1:A:903:ARG:NH2	2.26	0.68
1:A:872:GLU:HA	1:A:875:ALA:HB3	1.75	0.67
1:A:586:VAL:HB	1:A:647:LEU:HD13	1.77	0.66
1:A:37:ARG:HG3	1:A:116:LEU:HD11	1.76	0.66
1:A:727:ASN:HB3	1:A:849:LEU:HD22	1.81	0.62
1:A:352:GLY:O	1:A:411:ASN:ND2	2.28	0.61
1:A:479:VAL:HG12	1:A:528:VAL:HG22	1.84	0.60
1:A:683:LEU:HD21	1:A:780:VAL:HG12	1.85	0.59
1:A:52:ASP:OD1	1:A:418:SER:OG	2.18	0.59
1:A:700:MET:HG3	1:A:760:VAL:HG21	1.85	0.58
1:A:770:ASP:HA	1:A:773:LEU:HG	1.86	0.58
1:A:94:THR:HB	1:A:913:ARG:HB3	1.86	0.58
1:A:135:LEU:HD23	1:A:140:LEU:HD22	1.86	0.58
1:A:836:ARG:NH1	1:A:886:ASP:O	2.37	0.57
1:A:579:GLU:HB2	1:A:872:GLU:HB2	1.87	0.57
1:A:359:LEU:HB3	1:A:412:LEU:HD23	1.87	0.56
1:A:355:ARG:HB3	1:A:411:ASN:HD21	1.69	0.56
1:A:408:ASP:N	1:A:408:ASP:OD1	2.40	0.55
1:A:132:PRO:HD2	1:A:521:THR:CG2	2.37	0.54
1:A:726:VAL:HA	1:A:732:VAL:HG12	1.89	0.54
1:A:644:LEU:HD23	1:A:840:VAL:HG13	1.90	0.54
1:A:662:SER:OG	1:A:663:VAL:N	2.41	0.53
1:A:839:GLU:HB3	1:A:864:ALA:HA	1.90	0.53
1:A:821:ARG:NH2	1:A:824:ASP:OD2	2.41	0.53
1:A:271:THR:OG1	1:A:274:ARG:HB2	2.08	0.53
1:A:842:PRO:HA	1:A:867:ARG:HA	1.90	0.53
1:A:297:SER:OG	1:A:302:THR:O	2.10	0.52
1:A:494:ARG:NH2	1:A:908:THR:OG1	2.42	0.52
1:A:477:PRO:HB3	1:A:877:LEU:HD21	1.91	0.51
1:A:571:SER:HB3	1:A:842:PRO:O	2.09	0.51
1:A:232:SER:O	1:A:236:THR:HG23	2.11	0.51
1:A:113:GLN:O	1:A:117:VAL:HG23	2.11	0.50
2:B:952:ARG:HG2	2:B:969:MET:SD	2.51	0.50
1:A:919:GLU:N	1:A:919:GLU:OE1	2.44	0.50
1:A:355:ARG:HB3	1:A:411:ASN:ND2	2.27	0.50
1:A:321:VAL:HG13	1:A:325:GLU:HB2	1.94	0.49
1:A:653:VAL:HG11	1:A:883:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:LEU:HD11	1:A:734:VAL:HG13	1.95	0.49
1:A:863:VAL:HG23	1:A:882:GLU:OE1	2.12	0.49
1:A:780:VAL:HG23	1:A:809:VAL:HG12	1.96	0.48
1:A:583:ALA:HB2	1:A:873:PRO:HG3	1.95	0.48
1:A:391:ARG:NH2	1:A:418:SER:O	2.46	0.48
1:A:249:PHE:HB3	1:A:252:ASP:HB3	1.96	0.48
1:A:653:VAL:HA	1:A:888:TYR:CE2	2.49	0.48
1:A:478:TRP:CE2	1:A:537:LEU:HD13	2.49	0.48
2:B:1000:THR:OG1	2:B:1001:THR:N	2.46	0.47
1:A:587:PHE:HB2	1:A:647:LEU:HD22	1.96	0.47
1:A:360:PRO:HA	1:A:413:ARG:O	2.16	0.46
1:A:175:LEU:HA	1:A:178:ASN:HB2	1.97	0.45
1:A:669:VAL:HG22	1:A:674:VAL:HB	1.98	0.45
1:A:312:LEU:HB3	1:A:350:VAL:HG11	1.97	0.45
1:A:38:LEU:HB2	1:A:41:ALA:HB3	1.99	0.45
1:A:657:VAL:HG22	1:A:791:THR:HB	1.99	0.45
1:A:37:ARG:HG3	1:A:116:LEU:CD1	2.45	0.45
1:A:249:PHE:HB2	1:A:255:ALA:HA	1.99	0.44
1:A:312:LEU:HB2	1:A:350:VAL:HG21	2.00	0.44
1:A:239:PHE:HZ	1:A:301:THR:HG21	1.82	0.44
1:A:683:LEU:CD2	1:A:780:VAL:HG12	2.46	0.44
2:B:972:SER:HB3	2:B:975:ASP:CG	2.38	0.44
1:A:389:ARG:O	1:A:391:ARG:HG3	2.18	0.43
2:B:1019:ARG:O	2:B:1020:LEU:HD22	2.18	0.43
1:A:838:VAL:HG21	1:A:883:LEU:HD21	1.99	0.43
1:A:334:THR:HG21	3:A:1100:9EF:CAK	2.48	0.43
1:A:565:VAL:HB	1:A:846:LEU:HD23	2.00	0.43
1:A:627:LEU:O	1:A:633:THR:HB	2.17	0.43
1:A:793:VAL:HG21	1:A:829:MET:HG2	2.00	0.43
1:A:591:PHE:O	1:A:595:CYS:HB2	2.18	0.43
2:B:983:SER:O	2:B:1003:LEU:HD13	2.18	0.43
1:A:605:LEU:HD13	1:A:689:ARG:NH2	2.32	0.43
1:A:30:ALA:N	1:A:270:LYS:O	2.42	0.43
1:A:580:LEU:HG	1:A:872:GLU:HB3	2.01	0.43
2:B:971:ARG:HG2	2:B:975:ASP:HB2	2.01	0.43
1:A:144:VAL:HG11	1:A:176:ILE:HG22	2.01	0.42
1:A:683:LEU:HD23	1:A:783:LEU:HD12	2.01	0.42
2:B:1008:SER:HB3	2:B:1011:GLU:HB2	2.00	0.42
1:A:202:VAL:O	1:A:205:HIS:HB3	2.19	0.42
2:B:979:ASP:H	2:B:982:MET:HB2	1.84	0.42
2:B:946:ASP:N	2:B:947:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:TYR:OH	1:A:918:LEU:HG	2.19	0.42
1:A:222:GLY:HA3	1:A:265:GLY:O	2.20	0.42
2:B:969:MET:HE2	2:B:969:MET:HB3	1.96	0.42
1:A:25:SER:HB2	1:A:318:ARG:HG3	2.01	0.42
1:A:140:LEU:O	1:A:186:ALA:HB1	2.20	0.42
1:A:148:ARG:NH2	1:A:372:GLU:OE2	2.53	0.42
1:A:526:ARG:HD2	1:A:884:PHE:CZ	2.55	0.42
1:A:699:ALA:HB2	1:A:738:VAL:HG23	2.01	0.42
1:A:724:GLY:N	1:A:733:VAL:O	2.50	0.41
1:A:877:LEU:HD12	1:A:877:LEU:HA	1.95	0.41
1:A:148:ARG:HH11	1:A:232:SER:HB2	1.85	0.41
1:A:876:LEU:HD12	1:A:879:ALA:HB3	2.03	0.41
2:B:978:PHE:CE1	2:B:986:LEU:HD11	2.55	0.41
1:A:530:SER:HB2	1:A:877:LEU:HD23	2.01	0.41
1:A:714:LEU:HD22	1:A:721:VAL:HG11	2.02	0.41
1:A:31:VAL:O	1:A:283:HIS:N	2.45	0.41
1:A:587:PHE:HB2	1:A:647:LEU:CD2	2.52	0.40
1:A:653:VAL:HG21	1:A:883:LEU:HD13	2.03	0.40
1:A:579:GLU:O	1:A:873:PRO:HD3	2.20	0.40
1:A:119:GLU:O	1:A:123:GLU:HG3	2.22	0.40
1:A:700:MET:CG	1:A:760:VAL:HG21	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	800/916 (87%)	770 (96%)	30 (4%)	0	100 100
2	B	65/94 (69%)	57 (88%)	8 (12%)	0	100 100
All	All	865/1010 (86%)	827 (96%)	38 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	609/671 (91%)	607 (100%)	2 (0%)	92 97
2	B	60/79 (76%)	57 (95%)	3 (5%)	24 54
All	All	669/750 (89%)	664 (99%)	5 (1%)	84 92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	370	HIS
1	A	399	SER
2	B	966	ASP
2	B	974	LYS
2	B	981	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	569	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	9EF	A	1100	2,1	17,23,24	0.41	0	23,30,33	2.38	7 (30%)

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	9EF	A	1100	2,1	-	5/27/29/30	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1100	9EF	CAJ-NAO-CAS	7.89	134.69	122.56
3	A	1100	9EF	CAC-CAX-CAV	-3.69	102.42	108.82
3	A	1100	9EF	CAL-NAQ-CAU	3.56	128.94	122.59
3	A	1100	9EF	CAB-CAX-CAV	3.00	114.02	108.82
3	A	1100	9EF	CAJ-CAK-NAP	-2.77	102.23	111.44
3	A	1100	9EF	CAM-CAL-NAQ	-2.59	106.66	111.90
3	A	1100	9EF	CAK-NAP-CAT	2.17	126.86	122.84

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1100	9EF	OAR-CAN-CAX-CAC
3	A	1100	9EF	OAR-CAN-CAX-CAV
3	A	1100	9EF	CAK-CAJ-NAO-CAS

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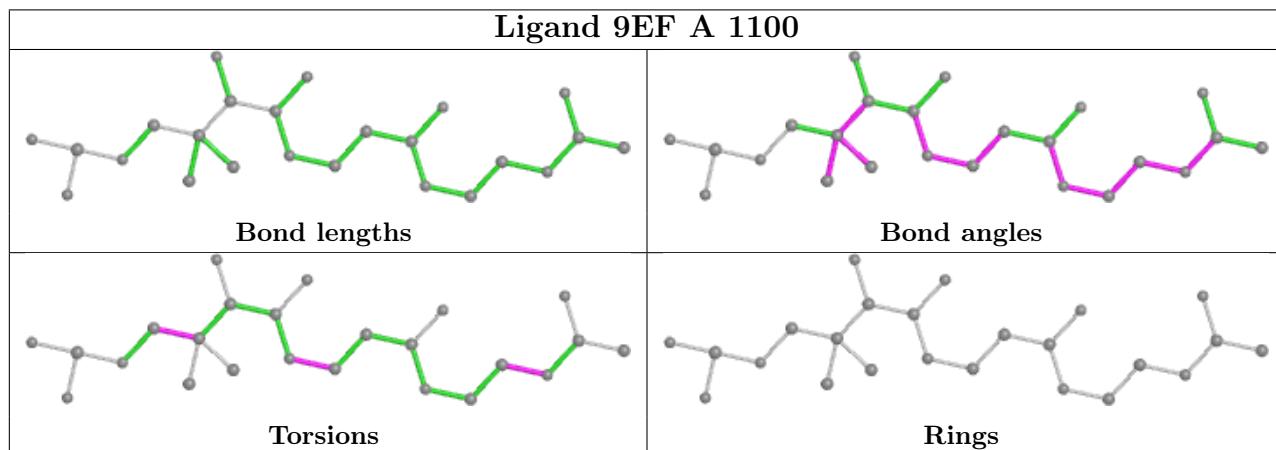
Mol	Chain	Res	Type	Atoms
3	A	1100	9EF	CAM-CAL-NAQ-CAU
3	A	1100	9EF	OAR-CAN-CAX-CAB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1100	9EF	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	820/916 (89%)	1.76	244 (29%) 0 0	133, 232, 467, 742	0
2	B	71/94 (75%)	1.73	28 (39%) 0 0	176, 241, 316, 492	0
All	All	891/1010 (88%)	1.76	272 (30%) 0 0	133, 234, 458, 742	0

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	785	PHE	16.2
1	A	643	ALA	15.6
1	A	896	PHE	14.4
1	A	647	LEU	13.4
1	A	725	ALA	12.9
1	A	681	CYS	11.6
1	A	748	PHE	11.4
1	A	433	ALA	11.3
1	A	724	GLY	10.2
1	A	603	GLY	10.1
1	A	780	VAL	9.6
1	A	602	MET	9.4
1	A	793	VAL	9.2
1	A	639	ALA	9.2
1	A	755	ALA	8.5
1	A	740	VAL	8.5
1	A	280	ASP	8.5
1	A	600	GLU	8.4
1	A	655	GLY	8.1
1	A	873	PRO	8.0
1	A	822	PHE	8.0
1	A	564	LEU	7.9
1	A	898	GLY	7.8
1	A	642	VAL	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	783	LEU	7.6
1	A	675	LEU	7.6
1	A	899	TRP	7.5
1	A	528	VAL	7.4
1	A	722	GLY	7.4
1	A	644	LEU	7.4
1	A	734	VAL	7.4
2	B	1003	LEU	7.3
1	A	744	VAL	7.2
1	A	782	GLY	7.2
1	A	653	VAL	7.1
1	A	680	ALA	7.1
1	A	880	VAL	7.0
1	A	723	ILE	7.0
1	A	812	TRP	6.9
1	A	430	THR	6.9
1	A	806	LEU	6.8
1	A	659	ALA	6.8
1	A	569	GLN	6.8
1	A	477	PRO	6.8
1	A	721	VAL	6.6
1	A	892	TRP	6.6
1	A	565	VAL	6.6
2	B	947	PRO	6.5
1	A	638	PHE	6.5
1	A	776	PHE	6.3
1	A	476	LEU	6.2
2	B	955	THR	6.2
1	A	321	VAL	6.1
1	A	529	VAL	6.1
1	A	648	LEU	6.0
1	A	861	SER	6.0
1	A	720	GLU	6.0
1	A	837	PHE	5.9
1	A	478	TRP	5.9
1	A	431	LEU	5.8
1	A	604	ALA	5.8
1	A	895	TYR	5.7
1	A	449	VAL	5.7
1	A	900	PRO	5.7
1	A	607	PRO	5.6
1	A	654	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	772	MET	5.4
1	A	739	ALA	5.4
1	A	671	VAL	5.4
1	A	877	LEU	5.4
1	A	197	CYS	5.3
1	A	811	TYR	5.3
1	A	677	LEU	5.3
1	A	893	THR	5.3
1	A	714	LEU	5.3
1	A	601	VAL	5.3
1	A	784	SER	5.1
1	A	527	ALA	5.0
1	A	879	ALA	5.0
1	A	866	VAL	5.0
1	A	747	HIS	5.0
1	A	682	ALA	5.0
1	A	786	ALA	5.0
1	A	574	ALA	4.9
1	A	735	SER	4.9
1	A	657	VAL	4.9
1	A	736	GLY	4.9
2	B	1019	ARG	4.8
1	A	651	TRP	4.8
1	A	622	VAL	4.8
1	A	829	MET	4.8
1	A	826	VAL	4.6
1	A	571	SER	4.6
1	A	412	LEU	4.6
2	B	948	VAL	4.6
1	A	190	SER	4.6
1	A	615	LEU	4.6
1	A	838	VAL	4.6
1	A	635	PRO	4.5
1	A	282	VAL	4.5
1	A	640	PHE	4.4
1	A	792	VAL	4.4
1	A	573	ARG	4.4
1	A	562	LEU	4.4
1	A	823	ALA	4.3
1	A	434	GLY	4.3
2	B	961	LEU	4.3
1	A	568	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	699	ALA	4.2
1	A	42	SER	4.2
1	A	432	VAL	4.2
1	A	351	LEU	4.2
1	A	862	VAL	4.1
1	A	283	HIS	4.1
1	A	658	VAL	4.1
1	A	196	GLY	4.0
1	A	645	TYR	4.0
1	A	678	ALA	4.0
1	A	373	GLY	3.9
1	A	713	LEU	3.9
1	A	636	ALA	3.9
1	A	779	VAL	3.8
1	A	453	PRO	3.8
2	B	954	LEU	3.8
1	A	791	THR	3.8
1	A	512	ILE	3.8
1	A	194	ASP	3.8
1	A	867	ARG	3.8
1	A	145	GLY	3.7
1	A	480	VAL	3.7
1	A	566	PHE	3.7
1	A	788	PRO	3.7
1	A	712	ALA	3.7
1	A	865	ALA	3.6
1	A	281	LEU	3.6
1	A	572	GLN	3.6
1	A	743	GLU	3.5
1	A	200	SER	3.5
1	A	646	ARG	3.5
1	A	625	ASP	3.5
1	A	450	SER	3.5
2	B	1017	ARG	3.5
2	B	953	GLN	3.5
1	A	24	ALA	3.5
1	A	883	LEU	3.4
1	A	177	ALA	3.4
1	A	703	VAL	3.4
1	A	324	THR	3.4
2	B	1007	PRO	3.4
2	B	959	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	B	989	ARG	3.3
1	A	198	SER	3.3
1	A	726	VAL	3.3
1	A	656	GLU	3.3
1	A	163	VAL	3.3
1	A	650	SER	3.3
1	A	251	PHE	3.2
1	A	479	VAL	3.2
1	A	757	ARG	3.2
1	A	448	VAL	3.2
1	A	443	THR	3.2
1	A	771	PRO	3.2
1	A	729	PRO	3.2
1	A	191	MET	3.1
1	A	178	ASN	3.1
1	A	90	ASP	3.1
2	B	978	PHE	3.1
1	A	583	ALA	3.1
1	A	840	VAL	3.1
1	A	897	ALA	3.1
1	A	694	LEU	3.0
1	A	730	ARG	3.0
1	A	790	LEU	3.0
1	A	715	ALA	3.0
1	A	272	LEU	2.9
1	A	451	ALA	2.9
1	A	544	LEU	2.9
2	B	990	LEU	2.9
1	A	174	SER	2.9
1	A	323	PRO	2.9
1	A	805	GLU	2.9
1	A	188	GLY	2.8
1	A	684	VAL	2.8
1	A	530	SER	2.8
1	A	690	LEU	2.8
1	A	541	LEU	2.8
1	A	32	ILE	2.8
1	A	83	ALA	2.8
1	A	361	VAL	2.8
1	A	582	VAL	2.8
1	A	374	ALA	2.7
2	B	1018	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	958	VAL	2.7
1	A	496	ALA	2.7
2	B	991	CYS	2.7
1	A	598	LEU	2.7
1	A	570	GLY	2.7
1	A	819	ALA	2.7
2	B	1004	TYR	2.7
1	A	578	ARG	2.7
2	B	992	ALA	2.6
1	A	683	LEU	2.6
2	B	993	ALA	2.6
1	A	452	ALA	2.6
2	B	952	ARG	2.6
1	A	199	SER	2.6
1	A	674	VAL	2.6
1	A	807	CYS	2.6
2	B	1012	THR	2.5
1	A	442	GLY	2.5
1	A	701	VAL	2.5
2	B	951	VAL	2.5
1	A	781	ALA	2.5
1	A	157	ARG	2.5
1	A	376	GLY	2.5
1	A	421	TRP	2.5
1	A	863	VAL	2.5
1	A	91	ARG	2.5
2	B	1016	VAL	2.4
2	B	957	HIS	2.4
1	A	628	ASP	2.4
1	A	35	SER	2.4
1	A	741	VAL	2.4
1	A	142	VAL	2.4
1	A	148	ARG	2.4
1	A	711	THR	2.4
1	A	498	TRP	2.4
1	A	827	GLY	2.3
1	A	147	ALA	2.3
1	A	67	THR	2.3
1	A	439	GLY	2.3
1	A	189	PRO	2.3
1	A	195	THR	2.3
1	A	685	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	710	VAL	2.3
1	A	605	LEU	2.3
1	A	903	ARG	2.3
1	A	326	VAL	2.3
1	A	809	VAL	2.2
1	A	386	GLN	2.2
1	A	808	SER	2.2
1	A	503	ALA	2.2
1	A	531	GLY	2.2
1	A	620	PHE	2.2
1	A	519	SER	2.2
1	A	353	THR	2.2
1	A	777	GLY	2.2
1	A	284	GLY	2.2
1	A	881	GLY	2.2
1	A	773	LEU	2.1
1	A	616	ARG	2.1
1	A	287	LEU	2.1
1	A	109	ALA	2.1
1	A	909	TYR	2.1
1	A	834	VAL	2.1
1	A	260	ARG	2.1
1	A	410	LEU	2.1
1	A	292	ASN	2.1
1	A	375	ALA	2.1
1	A	745	ALA	2.1
1	A	231	GLU	2.1
2	B	1013	ALA	2.1
1	A	149	ASP	2.1
1	A	836	ARG	2.0
1	A	444	ASN	2.0
1	A	495	LEU	2.0
1	A	577	GLY	2.0
2	B	956	ALA	2.0
1	A	397	ASN	2.0
1	A	222	GLY	2.0
1	A	727	ASN	2.0
2	B	986	LEU	2.0

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

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

6.3 Carbohydrates [\(i\)](#)

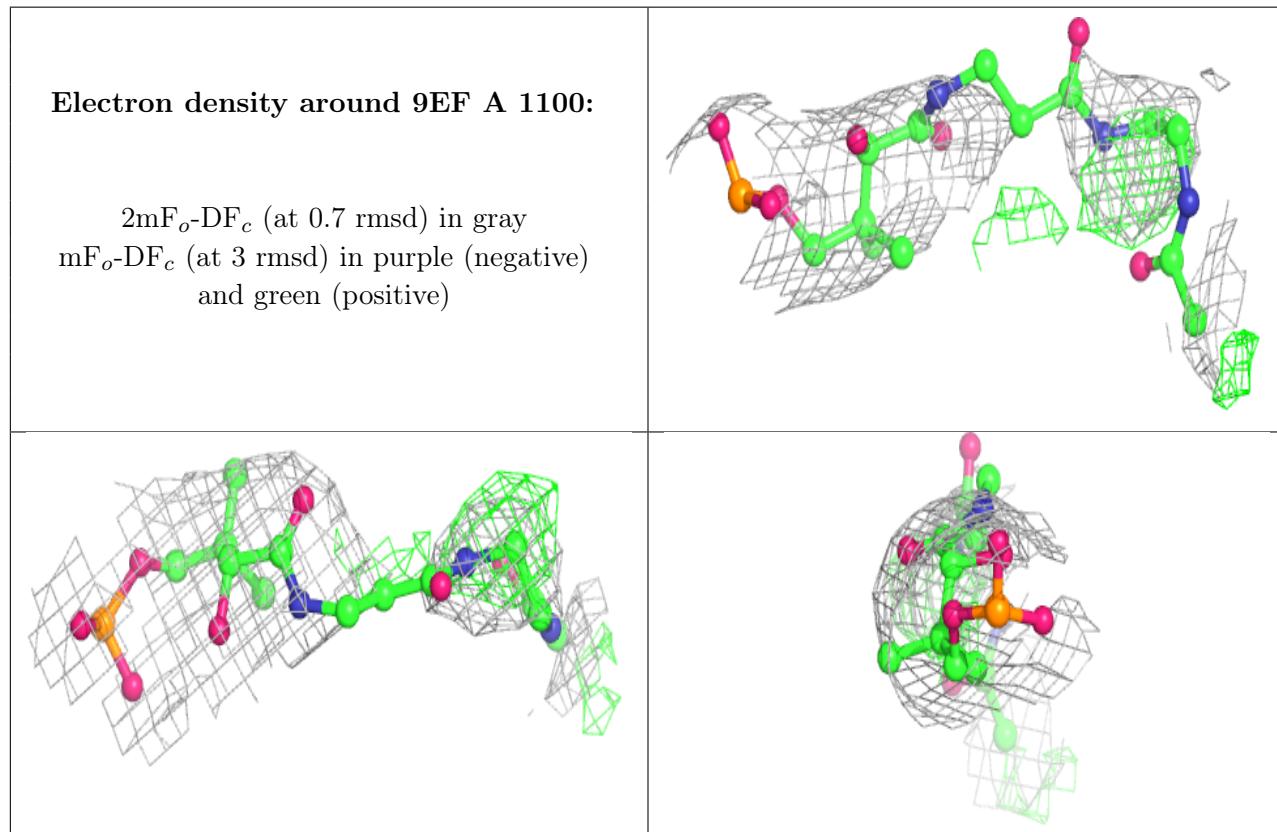
There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	9EF	A	1100	24/25	0.83	0.41	164,228,309,330	0

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



6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.