



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:02 PM UTC

PDB ID : 3I5V / pdb_00003i5v
Title : Crystal structure of beta toxin 275-280 from Staphylococcus aureus
Authors : Huseby, M.; Shi, K.; Kruse, A.C.; Ohlendorf, D.H.
Deposited on : 2009-07-06
Resolution : 2.80 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

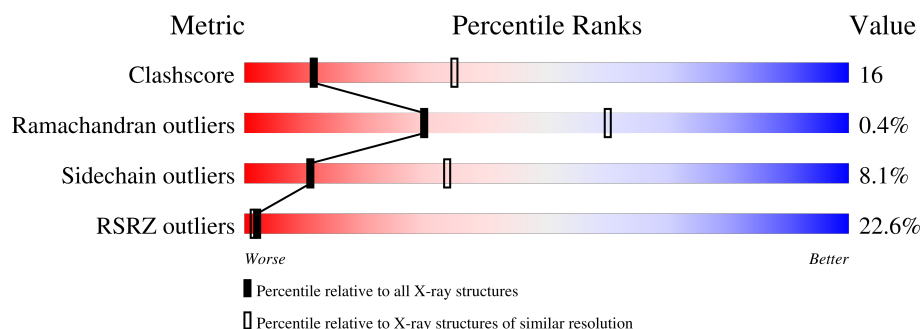
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	313	20% 62% 25% 5% 9%
1	B	313	21% 62% 24% 5% 9%
1	C	313	21% 63% 23% 5% 9%
1	D	313	21% 61% 25% 5% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DGA	D	401	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9255 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 Beta-hemolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2283	1443	388	447	5			
1	B	285	Total	C	N	O	S	0	0	0
			2283	1443	388	447	5			
1	C	284	Total	C	N	O	S	0	0	0
			2273	1437	386	445	5			
1	D	285	Total	C	N	O	S	0	0	0
			2283	1443	388	447	5			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP A7LAI8
A	-18	ARG	-	expression tag	UNP A7LAI8
A	-17	SER	-	expression tag	UNP A7LAI8
A	-16	SER	-	expression tag	UNP A7LAI8
A	-15	HIS	-	expression tag	UNP A7LAI8
A	-14	HIS	-	expression tag	UNP A7LAI8
A	-13	HIS	-	expression tag	UNP A7LAI8
A	-12	HIS	-	expression tag	UNP A7LAI8
A	-11	HIS	-	expression tag	UNP A7LAI8
A	-10	HIS	-	expression tag	UNP A7LAI8
A	-9	SER	-	expression tag	UNP A7LAI8
A	-8	SER	-	expression tag	UNP A7LAI8
A	-7	GLY	-	expression tag	UNP A7LAI8
A	-6	LEU	-	expression tag	UNP A7LAI8
A	-5	VAL	-	expression tag	UNP A7LAI8
A	-4	PRO	-	expression tag	UNP A7LAI8
A	-3	ARG	-	expression tag	UNP A7LAI8
A	-2	GLY	-	expression tag	UNP A7LAI8
A	-1	SER	-	expression tag	UNP A7LAI8
A	0	HIS	-	expression tag	UNP A7LAI8
A	1	MET	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	TYR	deletion	UNP A7LAI8
A	?	-	ALA	deletion	UNP A7LAI8
A	?	-	PHE	deletion	UNP A7LAI8
A	?	-	PRO	deletion	UNP A7LAI8
A	?	-	TYR	deletion	UNP A7LAI8
A	?	-	TYR	deletion	UNP A7LAI8
A	275	ASP	-	SEE REMARK 999	UNP A7LAI8
A	276	GLY	-	SEE REMARK 999	UNP A7LAI8
B	-19	MET	-	expression tag	UNP A7LAI8
B	-18	ARG	-	expression tag	UNP A7LAI8
B	-17	SER	-	expression tag	UNP A7LAI8
B	-16	SER	-	expression tag	UNP A7LAI8
B	-15	HIS	-	expression tag	UNP A7LAI8
B	-14	HIS	-	expression tag	UNP A7LAI8
B	-13	HIS	-	expression tag	UNP A7LAI8
B	-12	HIS	-	expression tag	UNP A7LAI8
B	-11	HIS	-	expression tag	UNP A7LAI8
B	-10	HIS	-	expression tag	UNP A7LAI8
B	-9	SER	-	expression tag	UNP A7LAI8
B	-8	SER	-	expression tag	UNP A7LAI8
B	-7	GLY	-	expression tag	UNP A7LAI8
B	-6	LEU	-	expression tag	UNP A7LAI8
B	-5	VAL	-	expression tag	UNP A7LAI8
B	-4	PRO	-	expression tag	UNP A7LAI8
B	-3	ARG	-	expression tag	UNP A7LAI8
B	-2	GLY	-	expression tag	UNP A7LAI8
B	-1	SER	-	expression tag	UNP A7LAI8
B	0	HIS	-	expression tag	UNP A7LAI8
B	1	MET	-	expression tag	UNP A7LAI8
B	?	-	TYR	deletion	UNP A7LAI8
B	?	-	ALA	deletion	UNP A7LAI8
B	?	-	PHE	deletion	UNP A7LAI8
B	?	-	PRO	deletion	UNP A7LAI8
B	?	-	TYR	deletion	UNP A7LAI8
B	?	-	TYR	deletion	UNP A7LAI8
B	275	ASP	-	SEE REMARK 999	UNP A7LAI8
B	276	GLY	-	SEE REMARK 999	UNP A7LAI8
C	-19	MET	-	expression tag	UNP A7LAI8
C	-18	ARG	-	expression tag	UNP A7LAI8
C	-17	SER	-	expression tag	UNP A7LAI8
C	-16	SER	-	expression tag	UNP A7LAI8
C	-15	HIS	-	expression tag	UNP A7LAI8

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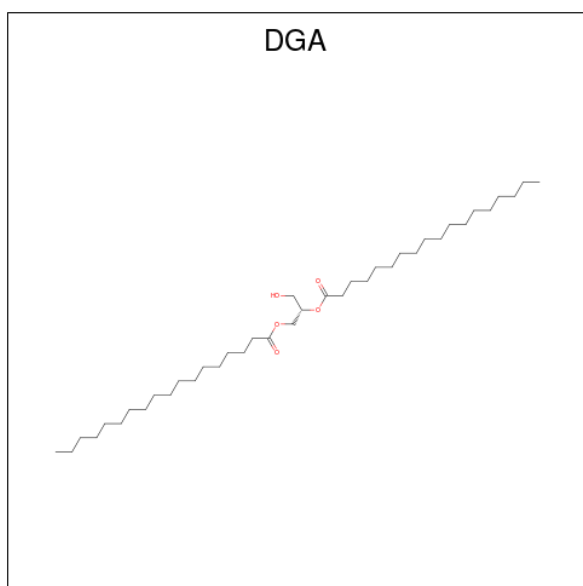
Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP A7LAI8
C	-13	HIS	-	expression tag	UNP A7LAI8
C	-12	HIS	-	expression tag	UNP A7LAI8
C	-11	HIS	-	expression tag	UNP A7LAI8
C	-10	HIS	-	expression tag	UNP A7LAI8
C	-9	SER	-	expression tag	UNP A7LAI8
C	-8	SER	-	expression tag	UNP A7LAI8
C	-7	GLY	-	expression tag	UNP A7LAI8
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C	-3	ARG	-	expression tag	UNP A7LAI8
C	-2	GLY	-	expression tag	UNP A7LAI8
C	-1	SER	-	expression tag	UNP A7LAI8
C	0	HIS	-	expression tag	UNP A7LAI8
C	1	MET	-	expression tag	UNP A7LAI8
C	?	-	TYR	deletion	UNP A7LAI8
C	?	-	ALA	deletion	UNP A7LAI8
C	?	-	PHE	deletion	UNP A7LAI8
C	?	-	PRO	deletion	UNP A7LAI8
C	?	-	TYR	deletion	UNP A7LAI8
C	?	-	TYR	deletion	UNP A7LAI8
C	275	ASP	-	SEE REMARK 999	UNP A7LAI8
C	276	GLY	-	SEE REMARK 999	UNP A7LAI8
D	-19	MET	-	expression tag	UNP A7LAI8
D	-18	ARG	-	expression tag	UNP A7LAI8
D	-17	SER	-	expression tag	UNP A7LAI8
D	-16	SER	-	expression tag	UNP A7LAI8
D	-15	HIS	-	expression tag	UNP A7LAI8
D	-14	HIS	-	expression tag	UNP A7LAI8
D	-13	HIS	-	expression tag	UNP A7LAI8
D	-12	HIS	-	expression tag	UNP A7LAI8
D	-11	HIS	-	expression tag	UNP A7LAI8
D	-10	HIS	-	expression tag	UNP A7LAI8
D	-9	SER	-	expression tag	UNP A7LAI8
D	-8	SER	-	expression tag	UNP A7LAI8
D	-7	GLY	-	expression tag	UNP A7LAI8
D	-6	LEU	-	expression tag	UNP A7LAI8
D	-5	VAL	-	expression tag	UNP A7LAI8
D	-4	PRO	-	expression tag	UNP A7LAI8
D	-3	ARG	-	expression tag	UNP A7LAI8
D	-2	GLY	-	expression tag	UNP A7LAI8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	SER	-	expression tag	UNP A7LAI8
D	0	HIS	-	expression tag	UNP A7LAI8
D	1	MET	-	expression tag	UNP A7LAI8
D	?	-	TYR	deletion	UNP A7LAI8
D	?	-	ALA	deletion	UNP A7LAI8
D	?	-	PHE	deletion	UNP A7LAI8
D	?	-	PRO	deletion	UNP A7LAI8
D	?	-	TYR	deletion	UNP A7LAI8
D	?	-	TYR	deletion	UNP A7LAI8
D	275	ASP	-	SEE REMARK 999	UNP A7LAI8
D	276	GLY	-	SEE REMARK 999	UNP A7LAI8

- Molecule 2 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			17	13	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	26	Total	O	0	0
			26	26		
3	C	31	Total	O	0	0
			31	31		

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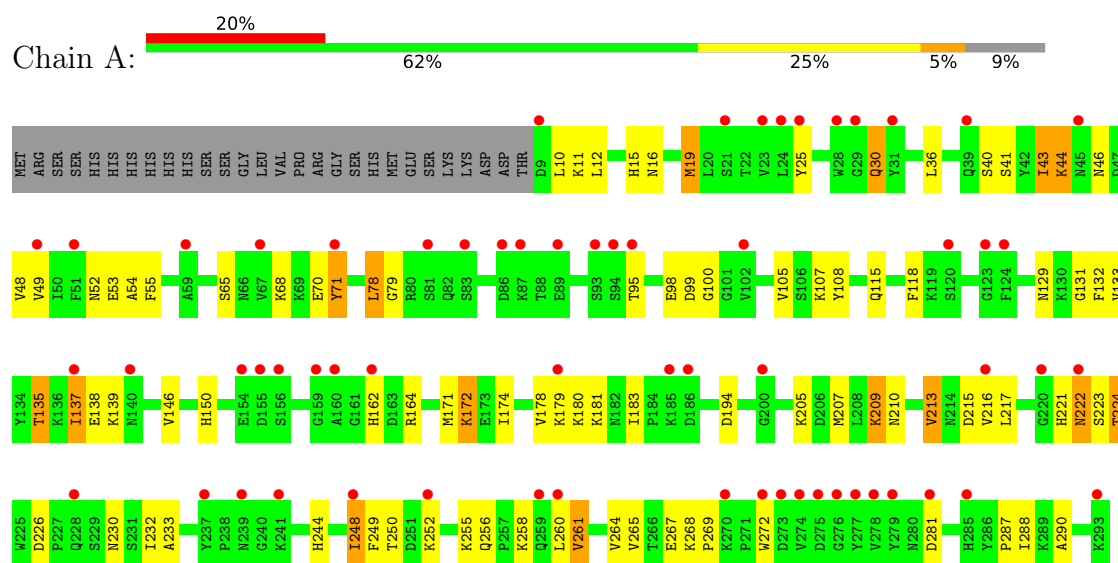
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	26	Total	O	0	0
			26	26		

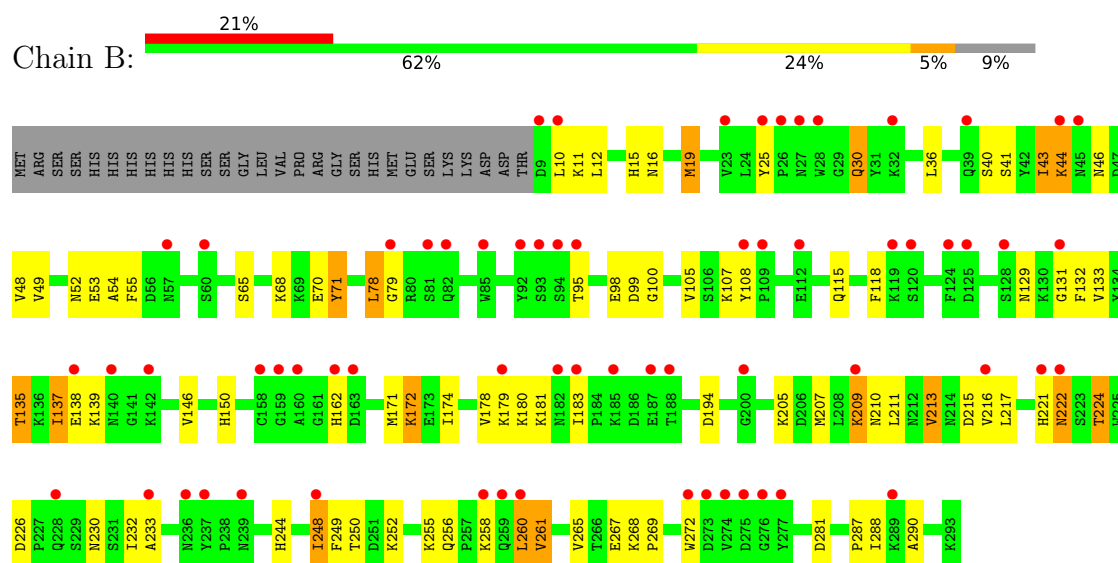
3 Residue-property plots [i](#)

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.

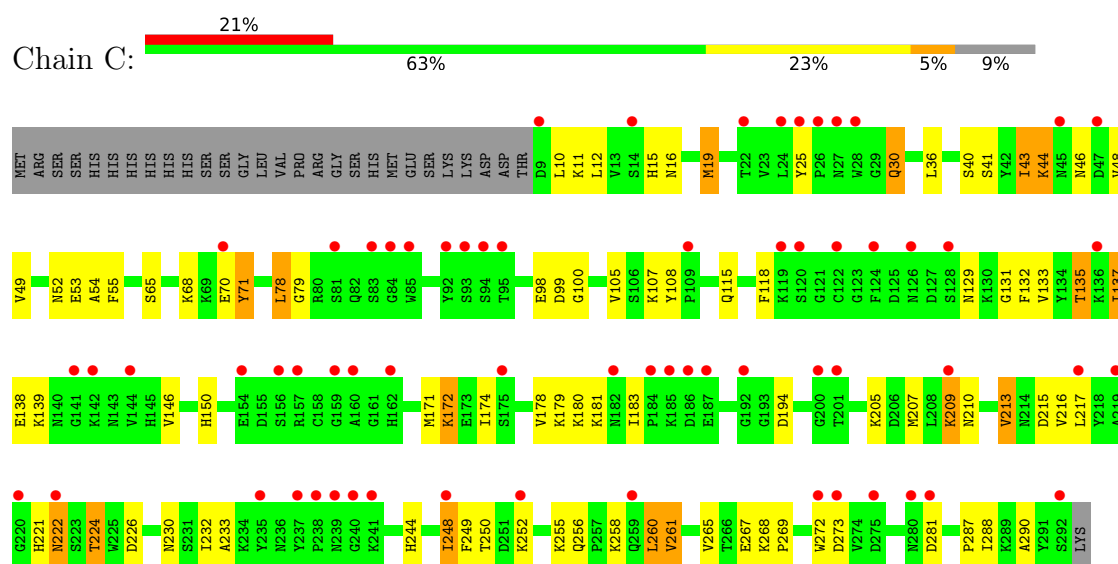
• Molecule 1: Beta-hemolysin



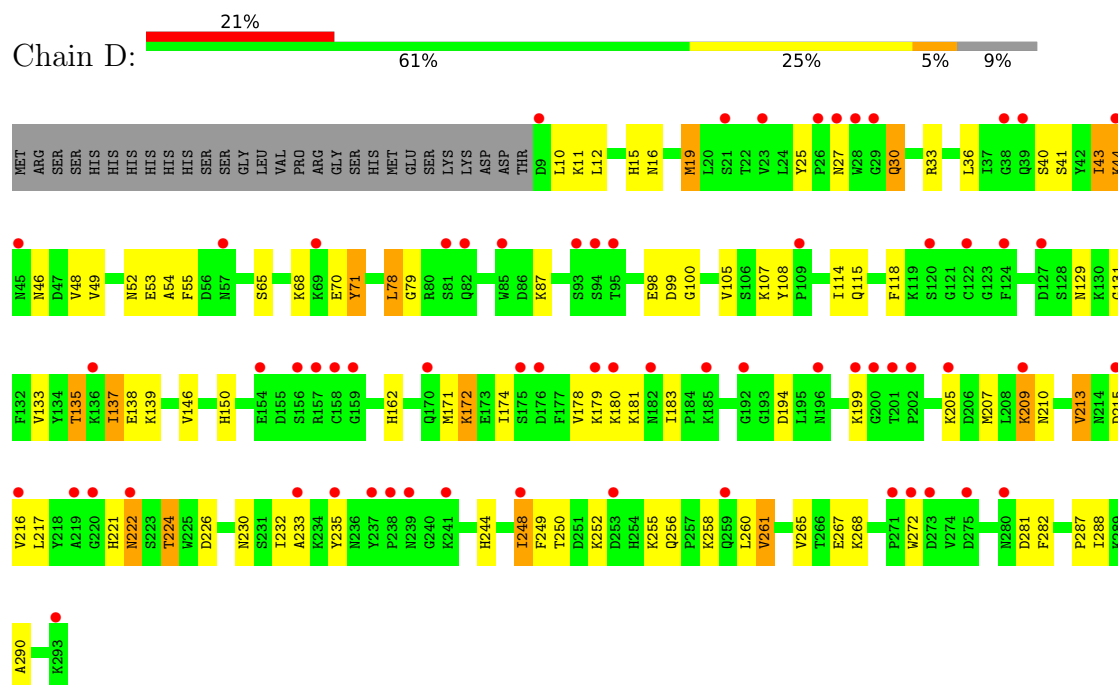
• Molecule 1: Beta-hemolysin



• Molecule 1: Beta-hemolysin



• Molecule 1: Beta-hemolysin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	55.18Å 69.05Å 75.65Å 93.06° 94.60° 92.13°	Depositor
Resolution (Å)	38.40 – 2.80 38.40 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.0 (38.40-2.80) 78.5 (38.40-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.48 (at 2.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.214 , 0.267 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	1.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9255	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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: DGA

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	0.29	0/2339	0.77	4/3162 (0.1%)
1	B	0.29	0/2339	0.77	4/3162 (0.1%)
1	C	0.29	0/2329	0.77	4/3151 (0.1%)
1	D	0.29	0/2339	0.77	4/3162 (0.1%)
All	All	0.29	0/9346	0.77	16/12637 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	TYR	CA-C-N	5.98	125.66	119.56
1	A	25	TYR	C-N-CA	5.98	125.66	119.56
1	B	25	TYR	CA-C-N	5.98	125.66	119.56
1	B	25	TYR	C-N-CA	5.98	125.66	119.56
1	D	25	TYR	CA-C-N	5.92	125.60	119.56
1	D	25	TYR	C-N-CA	5.92	125.60	119.56
1	C	25	TYR	CA-C-N	5.90	125.58	119.56
1	C	25	TYR	C-N-CA	5.90	125.58	119.56
1	A	71	TYR	CA-C-N	5.83	125.20	118.85
1	A	71	TYR	C-N-CA	5.83	125.20	118.85
1	C	71	TYR	CA-C-N	5.83	125.20	118.85
1	C	71	TYR	C-N-CA	5.83	125.20	118.85
1	B	71	TYR	CA-C-N	5.81	125.18	118.85
1	B	71	TYR	C-N-CA	5.81	125.18	118.85
1	D	71	TYR	CA-C-N	5.80	125.17	118.85
1	D	71	TYR	C-N-CA	5.80	125.17	118.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2283	0	2205	83	0
1	B	2283	0	2205	83	0
1	C	2273	0	2192	65	0
1	D	2283	0	2205	71	0
2	D	17	0	17	7	0
3	A	33	0	0	0	0
3	B	26	0	0	0	0
3	C	31	0	0	3	0
3	D	26	0	0	2	0
All	All	9255	0	8824	289	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 16.

All (289) 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:D:27:ASN:O	2:D:401:DGA:HG12	1.36	1.21
3:C:325:HOH:O	2:D:401:DGA:HB42	1.63	0.98
1:B:30:GLN:H	1:B:30:GLN:HE21	1.13	0.96
1:A:30:GLN:H	1:A:30:GLN:HE21	1.13	0.96
1:D:30:GLN:H	1:D:30:GLN:HE21	1.14	0.95
1:C:30:GLN:H	1:C:30:GLN:HE21	1.14	0.92
1:A:230:ASN:HD22	1:A:233:ALA:H	1.20	0.90
1:D:230:ASN:HD22	1:D:233:ALA:H	1.20	0.90
1:B:230:ASN:HD22	1:B:233:ALA:H	1.20	0.88
3:C:325:HOH:O	2:D:401:DGA:CB4	2.16	0.87
1:C:230:ASN:HD22	1:C:233:ALA:H	1.20	0.86
1:D:108:TYR:HB2	1:D:137:ILE:HD12	1.63	0.81
1:B:108:TYR:HB2	1:B:137:ILE:HD12	1.63	0.81
1:C:78:LEU:HD13	1:C:100:GLY:HA3	1.62	0.81
1:D:27:ASN:O	2:D:401:DGA:CG1	2.25	0.81
1:A:108:TYR:HB2	1:A:137:ILE:HD12	1.63	0.80
1:B:78:LEU:HD13	1:B:100:GLY:HA3	1.63	0.80
1:A:95:THR:HG21	1:B:162:HIS:CD2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:TYR:HB2	1:C:137:ILE:HD12	1.63	0.79
1:A:78:LEU:HD13	1:A:100:GLY:HA3	1.63	0.79
1:A:30:GLN:HE21	1:A:30:GLN:N	1.82	0.78
1:D:78:LEU:HD13	1:D:100:GLY:HA3	1.62	0.78
1:B:30:GLN:HE21	1:B:30:GLN:N	1.82	0.78
1:A:162:HIS:CD2	1:B:95:THR:HG21	2.18	0.77
1:D:30:GLN:HE21	1:D:30:GLN:N	1.83	0.77
1:C:30:GLN:HE21	1:C:30:GLN:N	1.82	0.76
1:A:162:HIS:CE1	1:B:95:THR:CG2	2.72	0.73
1:A:95:THR:CG2	1:B:162:HIS:CE1	2.73	0.71
1:A:164:ARG:HH12	1:C:273:ASP:HB3	1.55	0.69
1:A:162:HIS:CG	1:B:95:THR:HG21	2.28	0.67
1:A:230:ASN:ND2	1:A:233:ALA:H	1.93	0.66
1:D:230:ASN:ND2	1:D:233:ALA:H	1.94	0.66
1:C:30:GLN:H	1:C:30:GLN:NE2	1.92	0.65
1:C:230:ASN:ND2	1:C:233:ALA:H	1.93	0.65
1:D:235:TYR:OH	2:D:401:DGA:HB22	1.97	0.65
1:B:30:GLN:H	1:B:30:GLN:NE2	1.91	0.63
1:C:230:ASN:HB3	1:C:233:ALA:HB3	1.81	0.63
1:A:95:THR:CG2	1:B:162:HIS:NE2	2.62	0.62
1:D:162:HIS:HE1	3:D:316:HOH:O	1.83	0.62
1:B:213:VAL:HG11	1:B:249:PHE:CG	2.36	0.61
1:B:230:ASN:HB3	1:B:233:ALA:HB3	1.81	0.61
1:B:230:ASN:ND2	1:B:233:ALA:H	1.94	0.61
1:A:230:ASN:HB3	1:A:233:ALA:HB3	1.82	0.60
1:D:213:VAL:HG11	1:D:249:PHE:CG	2.36	0.60
1:C:213:VAL:HG11	1:C:249:PHE:CG	2.36	0.60
1:D:230:ASN:HB3	1:D:233:ALA:HB3	1.82	0.60
1:A:213:VAL:HG11	1:A:249:PHE:CG	2.36	0.60
1:B:209:LYS:HD2	1:B:209:LYS:N	2.17	0.60
1:D:30:GLN:H	1:D:30:GLN:NE2	1.92	0.59
1:D:209:LYS:HD2	1:D:209:LYS:N	2.17	0.59
1:A:95:THR:HG21	1:B:162:HIS:CG	2.36	0.59
1:A:30:GLN:H	1:A:30:GLN:NE2	1.91	0.59
1:C:172:LYS:HA	1:C:172:LYS:HE2	1.85	0.59
1:D:172:LYS:HE2	1:D:172:LYS:HA	1.85	0.59
1:A:209:LYS:N	1:A:209:LYS:HD2	2.17	0.59
1:A:172:LYS:HA	1:A:172:LYS:HE2	1.85	0.59
1:A:12:LEU:HD22	1:A:48:VAL:HB	1.85	0.58
1:D:10:LEU:HB3	1:D:12:LEU:HD21	1.86	0.58
1:A:162:HIS:NE2	1:B:95:THR:CG2	2.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:LEU:HD22	1:C:48:VAL:HB	1.85	0.58
1:C:209:LYS:HD2	1:C:209:LYS:N	2.17	0.58
1:D:12:LEU:HD22	1:D:48:VAL:HB	1.85	0.58
1:B:172:LYS:HE2	1:B:172:LYS:HA	1.85	0.58
1:A:78:LEU:HD23	1:A:115:GLN:HB2	1.86	0.57
1:B:10:LEU:HB3	1:B:12:LEU:HD21	1.86	0.57
1:A:10:LEU:HB3	1:A:12:LEU:HD21	1.87	0.57
1:A:40:SER:OG	1:A:43:ILE:HG13	2.04	0.57
1:A:171:MET:SD	1:A:207:MET:HG3	2.44	0.57
1:D:78:LEU:HD23	1:D:115:GLN:HB2	1.87	0.57
1:A:78:LEU:CD1	1:A:100:GLY:HA3	2.35	0.57
1:D:40:SER:OG	1:D:43:ILE:HG13	2.05	0.57
1:C:40:SER:OG	1:C:43:ILE:HG13	2.05	0.57
1:B:12:LEU:HD22	1:B:48:VAL:HB	1.86	0.57
1:C:10:LEU:HB3	1:C:12:LEU:HD21	1.86	0.57
1:C:171:MET:SD	1:C:207:MET:HG3	2.45	0.57
1:B:78:LEU:HD23	1:B:115:GLN:HB2	1.86	0.56
1:C:78:LEU:HD23	1:C:115:GLN:HB2	1.87	0.56
1:C:78:LEU:CD1	1:C:100:GLY:HA3	2.35	0.56
1:B:171:MET:SD	1:B:207:MET:HG3	2.45	0.56
1:D:171:MET:SD	1:D:207:MET:HG3	2.46	0.56
1:B:40:SER:OG	1:B:43:ILE:HG13	2.05	0.56
1:B:41:SER:HA	1:B:44:LYS:HE2	1.89	0.55
1:B:78:LEU:CD1	1:B:100:GLY:HA3	2.35	0.55
1:D:41:SER:HA	1:D:44:LYS:HE2	1.89	0.55
1:A:41:SER:HA	1:A:44:LYS:HE2	1.89	0.54
1:D:16:ASN:HA	1:D:52:ASN:HB2	1.90	0.54
1:C:41:SER:HA	1:C:44:LYS:HE2	1.89	0.54
1:A:16:ASN:HA	1:A:52:ASN:HB2	1.90	0.54
1:A:179:LYS:HD2	1:A:180:LYS:N	2.23	0.53
1:D:135:THR:HG22	1:D:146:VAL:HB	1.91	0.53
1:C:179:LYS:HD2	1:C:180:LYS:N	2.24	0.53
1:C:248:ILE:HG23	1:C:288:ILE:HD11	1.90	0.53
1:D:179:LYS:HD2	1:D:180:LYS:N	2.23	0.53
1:C:16:ASN:HA	1:C:52:ASN:HB2	1.90	0.53
1:A:135:THR:HG22	1:A:146:VAL:HB	1.91	0.53
1:A:49:VAL:HB	1:A:105:VAL:HG22	1.91	0.53
1:C:10:LEU:HD13	1:C:12:LEU:HD21	1.90	0.53
1:B:10:LEU:HD13	1:B:12:LEU:HD21	1.91	0.52
1:D:10:LEU:HD13	1:D:12:LEU:HD21	1.91	0.52
1:B:179:LYS:HD2	1:B:180:LYS:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:MET:HB2	1:C:54:ALA:HA	1.92	0.52
1:A:10:LEU:HD13	1:A:12:LEU:HD21	1.91	0.52
1:A:248:ILE:HG23	1:A:288:ILE:HD11	1.91	0.52
1:B:16:ASN:HA	1:B:52:ASN:HB2	1.90	0.52
1:B:248:ILE:HG23	1:B:288:ILE:HD11	1.91	0.52
1:D:248:ILE:HG23	1:D:288:ILE:HD11	1.91	0.52
1:B:118:PHE:CE2	1:B:131:GLY:HA2	2.45	0.52
1:C:135:THR:HG22	1:C:146:VAL:HB	1.91	0.52
1:A:118:PHE:CE2	1:A:131:GLY:HA2	2.45	0.52
1:D:49:VAL:HB	1:D:105:VAL:HG22	1.92	0.52
1:D:108:TYR:CZ	1:D:139:LYS:HD2	2.45	0.52
1:A:15:HIS:CE1	1:A:287:PRO:HG3	2.45	0.51
1:A:108:TYR:CZ	1:A:139:LYS:HD2	2.45	0.51
1:B:10:LEU:HB3	1:B:12:LEU:CD2	2.40	0.51
1:B:49:VAL:HB	1:B:105:VAL:HG22	1.91	0.51
1:D:15:HIS:CE1	1:D:287:PRO:HG3	2.46	0.51
1:C:118:PHE:CE2	1:C:131:GLY:HA2	2.46	0.51
1:D:19:MET:HB2	1:D:54:ALA:HA	1.92	0.51
1:A:19:MET:HB2	1:A:54:ALA:HA	1.92	0.51
1:C:78:LEU:HD22	1:C:79:GLY:N	2.26	0.51
1:D:10:LEU:HB3	1:D:12:LEU:CD2	2.40	0.51
1:A:78:LEU:HD22	1:A:79:GLY:N	2.25	0.51
1:A:10:LEU:HB3	1:A:12:LEU:CD2	2.40	0.51
1:C:10:LEU:HB3	1:C:12:LEU:CD2	2.40	0.51
1:D:78:LEU:CD1	1:D:100:GLY:HA3	2.34	0.51
1:D:118:PHE:CE2	1:D:131:GLY:HA2	2.46	0.51
1:A:162:HIS:CD2	1:B:95:THR:CG2	2.92	0.51
1:B:19:MET:HB2	1:B:54:ALA:HA	1.92	0.50
1:B:78:LEU:HD22	1:B:79:GLY:N	2.26	0.50
1:B:135:THR:HG22	1:B:146:VAL:HB	1.92	0.50
1:C:49:VAL:HB	1:C:105:VAL:HG22	1.92	0.50
1:C:108:TYR:CZ	1:C:139:LYS:HD2	2.45	0.50
1:D:78:LEU:HD22	1:D:79:GLY:N	2.26	0.50
1:B:15:HIS:CE1	1:B:287:PRO:HG3	2.45	0.50
1:C:15:HIS:CE1	1:C:287:PRO:HG3	2.46	0.50
1:B:108:TYR:CZ	1:B:139:LYS:HD2	2.46	0.50
1:A:95:THR:HG22	1:B:162:HIS:CE1	2.47	0.50
1:D:137:ILE:HG13	1:D:138:GLU:N	2.26	0.50
1:A:137:ILE:HG13	1:A:138:GLU:N	2.26	0.50
1:A:162:HIS:CE1	1:B:95:THR:HG22	2.47	0.49
1:C:150:HIS:CD2	1:C:194:ASP:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG21	1:B:162:HIS:NE2	2.27	0.49
1:A:150:HIS:CD2	1:A:194:ASP:HB3	2.47	0.49
1:B:137:ILE:HG13	1:B:138:GLU:N	2.27	0.49
1:B:118:PHE:CD2	1:B:131:GLY:HA2	2.48	0.49
1:B:150:HIS:CD2	1:B:194:ASP:HB3	2.47	0.49
1:C:118:PHE:CD2	1:C:131:GLY:HA2	2.48	0.49
1:C:232:ILE:HD11	1:C:272:TRP:HH2	1.78	0.48
1:A:118:PHE:CD2	1:A:131:GLY:HA2	2.47	0.48
1:D:118:PHE:CD2	1:D:131:GLY:HA2	2.48	0.48
1:D:150:HIS:CD2	1:D:194:ASP:HB3	2.48	0.48
1:B:268:LYS:HE2	1:B:281:ASP:OD2	2.14	0.48
1:C:43:ILE:HD12	1:C:44:LYS:N	2.28	0.48
1:D:162:HIS:CE1	3:D:316:HOH:O	2.61	0.48
1:D:268:LYS:HE2	1:D:281:ASP:OD2	2.14	0.48
1:A:43:ILE:HD12	1:A:44:LYS:N	2.29	0.48
1:B:43:ILE:HD12	1:B:44:LYS:N	2.29	0.48
1:B:65:SER:HA	1:B:68:LYS:HB2	1.96	0.48
1:C:137:ILE:HG13	1:C:138:GLU:N	2.27	0.48
1:A:268:LYS:HE2	1:A:281:ASP:OD2	2.14	0.47
1:B:49:VAL:HB	1:B:105:VAL:CG2	2.44	0.47
1:C:49:VAL:HB	1:C:105:VAL:CG2	2.44	0.47
1:D:49:VAL:HB	1:D:105:VAL:CG2	2.44	0.47
1:A:78:LEU:HB2	1:A:133:VAL:CG2	2.45	0.47
1:D:43:ILE:HD12	1:D:44:LYS:N	2.29	0.47
1:D:222:ASN:N	1:D:222:ASN:HD22	2.12	0.47
1:C:65:SER:HA	1:C:68:LYS:HB2	1.96	0.47
1:D:78:LEU:HB2	1:D:133:VAL:CG2	2.45	0.47
1:A:49:VAL:HB	1:A:105:VAL:CG2	2.44	0.47
1:B:232:ILE:HD11	1:B:272:TRP:HH2	1.79	0.47
1:B:78:LEU:HB2	1:B:133:VAL:CG2	2.44	0.47
1:C:268:LYS:HE2	1:C:281:ASP:OD2	2.14	0.47
1:D:248:ILE:HG12	1:D:290:ALA:HB2	1.97	0.47
1:A:248:ILE:HG12	1:A:290:ALA:HB2	1.97	0.47
1:B:41:SER:O	1:B:44:LYS:HG2	2.15	0.47
1:C:41:SER:O	1:C:44:LYS:HG2	2.15	0.47
1:B:265:VAL:HG12	1:B:267:GLU:H	1.80	0.47
1:D:41:SER:O	1:D:44:LYS:HG2	2.15	0.47
1:C:248:ILE:HG12	1:C:290:ALA:HB2	1.97	0.46
1:D:232:ILE:HD11	1:D:272:TRP:HH2	1.79	0.46
1:A:232:ILE:HD11	1:A:272:TRP:HH2	1.79	0.46
1:C:55:PHE:HB3	1:C:98:GLU:CD	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:THR:HG21	1:B:162:HIS:CE1	2.51	0.46
1:A:265:VAL:HG12	1:A:267:GLU:H	1.80	0.46
1:B:221:HIS:HE1	1:B:226:ASP:OD1	1.99	0.46
1:D:65:SER:HA	1:D:68:LYS:HB2	1.96	0.46
1:A:216:VAL:HG12	1:A:217:LEU:O	2.16	0.46
1:B:248:ILE:HG12	1:B:290:ALA:HB2	1.97	0.46
2:D:401:DGA:OB1	2:D:401:DGA:HG11	2.15	0.46
1:A:65:SER:HA	1:A:68:LYS:HB2	1.97	0.46
1:C:265:VAL:HG12	1:C:267:GLU:H	1.80	0.46
1:B:108:TYR:CE1	1:B:139:LYS:HD2	2.51	0.46
1:C:216:VAL:HG12	1:C:217:LEU:O	2.16	0.46
1:D:216:VAL:HG12	1:D:217:LEU:O	2.15	0.46
1:D:222:ASN:HD22	1:D:222:ASN:H	1.64	0.46
1:A:41:SER:O	1:A:44:LYS:HG2	2.16	0.46
1:A:222:ASN:HD22	1:A:222:ASN:N	2.13	0.46
1:A:108:TYR:CE1	1:A:139:LYS:HD2	2.51	0.45
1:C:78:LEU:HB2	1:C:133:VAL:CG2	2.45	0.45
1:C:108:TYR:CE1	1:C:139:LYS:HD2	2.51	0.45
1:C:261:VAL:O	1:C:290:ALA:HA	2.17	0.45
1:D:55:PHE:HB3	1:D:98:GLU:CD	2.41	0.45
1:C:222:ASN:N	1:C:222:ASN:HD22	2.13	0.45
1:A:222:ASN:HD22	1:A:222:ASN:H	1.65	0.45
1:B:216:VAL:HG12	1:B:217:LEU:O	2.16	0.45
1:C:53:GLU:HA	1:C:55:PHE:CE1	2.52	0.45
1:C:221:HIS:HE1	1:C:226:ASP:OD1	1.99	0.45
1:D:108:TYR:CE1	1:D:139:LYS:HD2	2.51	0.45
1:D:261:VAL:O	1:D:290:ALA:HA	2.17	0.45
1:D:265:VAL:HG12	1:D:267:GLU:H	1.80	0.45
1:B:55:PHE:HB3	1:B:98:GLU:CD	2.41	0.45
1:B:53:GLU:HA	1:B:55:PHE:CE1	2.52	0.45
1:B:222:ASN:N	1:B:222:ASN:HD22	2.14	0.45
1:A:55:PHE:HB3	1:A:98:GLU:CD	2.41	0.44
1:A:222:ASN:HB3	1:D:199:LYS:HD2	1.99	0.44
1:B:261:VAL:O	1:B:290:ALA:HA	2.17	0.44
1:A:53:GLU:HA	1:A:55:PHE:CE1	2.52	0.44
1:A:215:ASP:CG	1:A:216:VAL:H	2.26	0.44
1:B:215:ASP:CG	1:B:216:VAL:H	2.26	0.44
1:B:222:ASN:HD22	1:B:222:ASN:H	1.65	0.44
1:A:46:ASN:HB2	1:A:71:TYR:OH	2.18	0.44
1:A:261:VAL:O	1:A:290:ALA:HA	2.17	0.44
1:C:215:ASP:CG	1:C:216:VAL:H	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:ASN:HB2	1:D:71:TYR:OH	2.18	0.44
1:B:46:ASN:HB2	1:B:71:TYR:OH	2.18	0.44
1:C:46:ASN:HB2	1:C:71:TYR:OH	2.17	0.44
3:C:325:HOH:O	2:D:401:DGA:HB41	2.03	0.44
1:D:53:GLU:HA	1:D:55:PHE:CE1	2.52	0.44
1:A:221:HIS:HE1	1:A:226:ASP:OD1	2.00	0.43
1:D:215:ASP:CG	1:D:216:VAL:H	2.26	0.43
1:C:222:ASN:HD22	1:C:222:ASN:H	1.65	0.43
1:A:162:HIS:CE1	1:B:95:THR:HG21	2.54	0.43
1:D:135:THR:CG2	1:D:146:VAL:HB	2.49	0.43
1:D:221:HIS:HE1	1:D:226:ASP:OD1	2.00	0.43
1:B:70:GLU:O	1:B:107:LYS:HG2	2.19	0.43
1:A:98:GLU:HG3	1:A:99:ASP:N	2.33	0.43
1:A:174:ILE:O	1:A:178:VAL:HG23	2.19	0.43
1:B:98:GLU:HG3	1:B:99:ASP:N	2.33	0.43
1:B:172:LYS:HE3	1:B:210:ASN:HA	2.01	0.43
1:C:224:THR:HB	1:C:244:HIS:HA	2.01	0.43
1:D:216:VAL:HG13	1:D:260:LEU:O	2.19	0.43
1:C:70:GLU:O	1:C:107:LYS:HG2	2.19	0.42
1:D:11:LYS:C	1:D:12:LEU:HD23	2.44	0.42
1:D:174:ILE:O	1:D:178:VAL:HG23	2.19	0.42
1:A:216:VAL:HG13	1:A:260:LEU:O	2.19	0.42
1:C:11:LYS:C	1:C:12:LEU:HD23	2.44	0.42
1:A:70:GLU:O	1:A:107:LYS:HG2	2.19	0.42
1:B:224:THR:HB	1:B:244:HIS:HA	2.01	0.42
1:C:135:THR:CG2	1:C:146:VAL:HB	2.49	0.42
1:A:11:LYS:C	1:A:12:LEU:HD23	2.44	0.42
1:A:135:THR:CG2	1:A:146:VAL:HB	2.49	0.42
1:A:224:THR:HB	1:A:244:HIS:HA	2.00	0.42
1:B:11:LYS:C	1:B:12:LEU:HD23	2.44	0.42
1:B:174:ILE:O	1:B:178:VAL:HG23	2.20	0.42
1:B:181:LYS:HB3	1:B:183:ILE:HG13	2.02	0.42
1:B:216:VAL:HG13	1:B:260:LEU:O	2.20	0.42
1:C:98:GLU:HG3	1:C:99:ASP:N	2.34	0.42
1:C:174:ILE:O	1:C:178:VAL:HG23	2.19	0.42
1:D:70:GLU:O	1:D:107:LYS:HG2	2.19	0.42
1:D:172:LYS:HE3	1:D:210:ASN:HA	2.01	0.42
1:C:172:LYS:HE3	1:C:210:ASN:HA	2.01	0.42
1:D:181:LYS:HB3	1:D:183:ILE:HG13	2.02	0.42
1:A:181:LYS:HB3	1:A:183:ILE:HG13	2.02	0.42
1:C:181:LYS:HB3	1:C:183:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:LYS:HA	1:C:269:PRO:HD3	1.84	0.42
1:A:162:HIS:NE2	1:B:95:THR:HG23	2.33	0.41
1:B:135:THR:CG2	1:B:146:VAL:HB	2.49	0.41
1:B:213:VAL:HG22	1:B:250:THR:O	2.20	0.41
1:D:98:GLU:HG3	1:D:99:ASP:N	2.34	0.41
1:D:213:VAL:HG22	1:D:250:THR:O	2.20	0.41
1:A:172:LYS:HE3	1:A:210:ASN:HA	2.01	0.41
1:B:12:LEU:HD23	1:B:12:LEU:N	2.36	0.41
1:B:268:LYS:HA	1:B:269:PRO:HD3	1.84	0.41
1:C:213:VAL:HG22	1:C:250:THR:O	2.20	0.41
1:C:216:VAL:HG13	1:C:260:LEU:O	2.20	0.41
1:D:224:THR:HB	1:D:244:HIS:HA	2.01	0.41
1:A:15:HIS:ND1	1:A:287:PRO:HG3	2.36	0.41
1:A:268:LYS:HA	1:A:269:PRO:HD3	1.84	0.41
1:B:15:HIS:ND1	1:B:287:PRO:HG3	2.36	0.41
1:B:272:TRP:CD1	1:B:272:TRP:C	2.99	0.41
1:A:132:PHE:CD1	1:A:174:ILE:HG12	2.57	0.40
1:B:211:LEU:HD23	1:B:211:LEU:HA	1.96	0.40
1:D:87:LYS:HB3	1:D:114:ILE:HG13	2.03	0.40
1:B:132:PHE:CD1	1:B:174:ILE:HG12	2.57	0.40
1:D:33:ARG:HD2	1:D:282:PHE:O	2.22	0.40
1:A:223:SER:O	1:A:264:VAL:HG11	2.22	0.40
1:A:213:VAL:HG22	1:A:250:THR:O	2.20	0.40
1:C:132:PHE:CD1	1:C:174:ILE:HG12	2.57	0.40
1:D:12:LEU:HD23	1:D:12:LEU:N	2.36	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	283/313 (90%)	260 (92%)	22 (8%)	1 (0%)	30 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	283/313 (90%)	260 (92%)	22 (8%)	1 (0%)	30	60
1	C	282/313 (90%)	259 (92%)	22 (8%)	1 (0%)	30	60
1	D	283/313 (90%)	260 (92%)	22 (8%)	1 (0%)	30	60
All	All	1131/1252 (90%)	1039 (92%)	88 (8%)	4 (0%)	30	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	258	LYS
1	B	258	LYS
1	C	258	LYS
1	D	258	LYS

5.3.2 Protein sidechains ⓘ

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	254/280 (91%)	234 (92%)	20 (8%)	11	35
1	B	254/280 (91%)	233 (92%)	21 (8%)	10	32
1	C	253/280 (90%)	232 (92%)	21 (8%)	10	32
1	D	254/280 (91%)	234 (92%)	20 (8%)	11	35
All	All	1015/1120 (91%)	933 (92%)	82 (8%)	11	33

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	MET
1	A	30	GLN
1	A	36	LEU
1	A	43	ILE
1	A	44	LYS
1	A	78	LEU
1	A	129	ASN

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Mol	Chain	Res	Type
1	A	135	THR
1	A	137	ILE
1	A	172	LYS
1	A	205	LYS
1	A	209	LYS
1	A	213	VAL
1	A	222	ASN
1	A	224	THR
1	A	248	ILE
1	A	252	LYS
1	A	255	LYS
1	A	256	GLN
1	A	261	VAL
1	B	19	MET
1	B	30	GLN
1	B	36	LEU
1	B	43	ILE
1	B	44	LYS
1	B	78	LEU
1	B	129	ASN
1	B	135	THR
1	B	137	ILE
1	B	172	LYS
1	B	205	LYS
1	B	209	LYS
1	B	213	VAL
1	B	222	ASN
1	B	224	THR
1	B	248	ILE
1	B	252	LYS
1	B	255	LYS
1	B	256	GLN
1	B	260	LEU
1	B	261	VAL
1	C	19	MET
1	C	30	GLN
1	C	36	LEU
1	C	43	ILE
1	C	44	LYS
1	C	78	LEU
1	C	129	ASN
1	C	135	THR

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Mol	Chain	Res	Type
1	C	137	ILE
1	C	172	LYS
1	C	205	LYS
1	C	209	LYS
1	C	213	VAL
1	C	222	ASN
1	C	224	THR
1	C	248	ILE
1	C	252	LYS
1	C	255	LYS
1	C	256	GLN
1	C	260	LEU
1	C	261	VAL
1	D	19	MET
1	D	30	GLN
1	D	36	LEU
1	D	43	ILE
1	D	44	LYS
1	D	78	LEU
1	D	129	ASN
1	D	135	THR
1	D	137	ILE
1	D	172	LYS
1	D	205	LYS
1	D	209	LYS
1	D	213	VAL
1	D	222	ASN
1	D	224	THR
1	D	248	ILE
1	D	252	LYS
1	D	255	LYS
1	D	256	GLN
1	D	261	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	30	GLN
1	A	46	ASN
1	A	52	ASN
1	A	129	ASN

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Mol	Chain	Res	Type
1	A	140	ASN
1	A	150	HIS
1	A	210	ASN
1	A	212	ASN
1	A	214	ASN
1	A	221	HIS
1	A	222	ASN
1	A	230	ASN
1	A	236	ASN
1	A	256	GLN
1	A	259	GLN
1	B	27	ASN
1	B	30	GLN
1	B	46	ASN
1	B	52	ASN
1	B	129	ASN
1	B	140	ASN
1	B	150	HIS
1	B	162	HIS
1	B	210	ASN
1	B	212	ASN
1	B	214	ASN
1	B	221	HIS
1	B	222	ASN
1	B	230	ASN
1	B	236	ASN
1	B	256	GLN
1	B	259	GLN
1	C	27	ASN
1	C	30	GLN
1	C	46	ASN
1	C	52	ASN
1	C	129	ASN
1	C	140	ASN
1	C	150	HIS
1	C	162	HIS
1	C	210	ASN
1	C	212	ASN
1	C	214	ASN
1	C	221	HIS
1	C	222	ASN
1	C	230	ASN

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Mol	Chain	Res	Type
1	C	256	GLN
1	C	259	GLN
1	D	27	ASN
1	D	30	GLN
1	D	46	ASN
1	D	52	ASN
1	D	129	ASN
1	D	140	ASN
1	D	150	HIS
1	D	162	HIS
1	D	210	ASN
1	D	212	ASN
1	D	214	ASN
1	D	221	HIS
1	D	222	ASN
1	D	230	ASN
1	D	236	ASN
1	D	256	GLN
1	D	259	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 oligosaccharides 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	$\# Z > 2$
2	DGA	D	401	-	16,16,43	1.24	1 (6%)	17,17,45	1.94	5 (29%)

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	DGA	D	401	-	1/1/2/3	13/17/17/45	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	DGA	OG2-CB1	4.43	1.46	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	DGA	OG2-CB1-CB2	5.60	123.60	111.48
2	D	401	DGA	OB1-CB1-CB2	-2.43	114.27	123.78
2	D	401	DGA	OXT-CG3-CG2	2.24	117.54	111.77
2	D	401	DGA	CA3-CA2-CA1	-2.15	104.14	113.47
2	D	401	DGA	CA1-OG1-CG1	2.04	122.56	113.58

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	401	DGA	CG2

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	DGA	CB2-CB1-OG2-CG2
2	D	401	DGA	CG2-CG1-OG1-CA1
2	D	401	DGA	CG1-CG2-CG3-OXT
2	D	401	DGA	OG2-CG2-CG3-OXT
2	D	401	DGA	OB1-CB1-OG2-CG2
2	D	401	DGA	OG1-CA1-CA2-CA3

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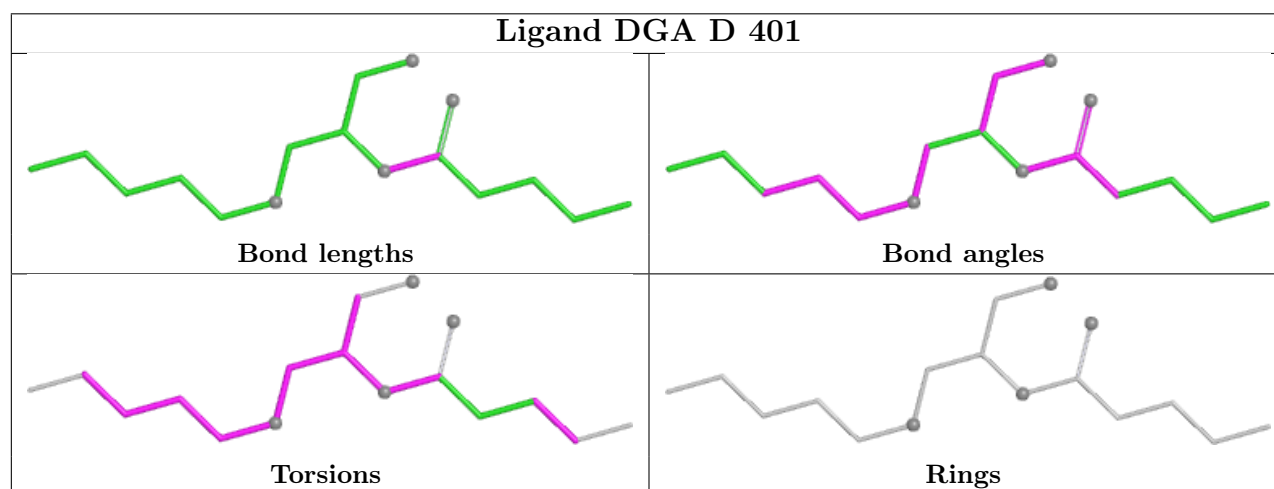
Mol	Chain	Res	Type	Atoms
2	D	401	DGA	CB2-CB3-CB4-CB5
2	D	401	DGA	OG1-CG1-CG2-CG3
2	D	401	DGA	CA2-CA3-CA4-CA5
2	D	401	DGA	CA2-CA1-OG1-CG1
2	D	401	DGA	OG1-CG1-CG2-OG2
2	D	401	DGA	CG1-CG2-OG2-CB1
2	D	401	DGA	CA1-CA2-CA3-CA4

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	DGA	7	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

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	285/313 (91%)	1.43	62 (21%)	2 2	51, 82, 141, 251	0
1	B	285/313 (91%)	1.44	65 (22%)	2 1	43, 80, 136, 268	0
1	C	284/313 (90%)	1.39	65 (22%)	2 1	44, 77, 132, 176	0
1	D	285/313 (91%)	1.38	65 (22%)	2 1	44, 78, 129, 186	0
All	All	1139/1252 (90%)	1.41	257 (22%)	2 1	43, 79, 136, 268	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	200	GLY	6.0
1	A	94	SER	6.0
1	B	160	ALA	5.8
1	B	94	SER	5.3
1	C	26	PRO	5.2
1	D	275	ASP	5.2
1	C	235	TYR	5.1
1	B	25	TYR	4.8
1	B	273	ASP	4.8
1	A	120	SER	4.7
1	D	222	ASN	4.7
1	A	23	VAL	4.7
1	A	93	SER	4.7
1	B	276	GLY	4.6
1	D	220	GLY	4.6
1	B	159	GLY	4.4
1	A	9	ASP	4.4
1	C	275	ASP	4.3
1	C	27	ASN	4.2
1	B	9	ASP	4.2
1	D	27	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	81	SER	4.0
1	A	272	TRP	4.0
1	D	235	TYR	3.9
1	C	28	TRP	3.9
1	A	25	TYR	3.8
1	A	275	ASP	3.8
1	D	9	ASP	3.8
1	B	182	ASN	3.7
1	B	216	VAL	3.7
1	C	273	ASP	3.7
1	B	259	GLN	3.6
1	A	276	GLY	3.6
1	A	28	TRP	3.6
1	B	93	SER	3.5
1	B	120	SER	3.5
1	C	238	PRO	3.4
1	A	216	VAL	3.4
1	C	292	SER	3.4
1	A	24	LEU	3.4
1	A	160	ALA	3.4
1	D	219	ALA	3.4
1	D	124	PHE	3.4
1	C	93	SER	3.4
1	B	209	LYS	3.3
1	B	109	PRO	3.3
1	D	248	ILE	3.3
1	C	81	SER	3.3
1	C	154	GLU	3.3
1	B	200	GLY	3.3
1	B	82	GLN	3.2
1	D	38	GLY	3.2
1	D	81	SER	3.2
1	D	237	TYR	3.2
1	A	228	GLN	3.2
1	C	182	ASN	3.2
1	D	29	GLY	3.2
1	A	140	ASN	3.2
1	C	9	ASP	3.1
1	A	185	LYS	3.1
1	C	241	LYS	3.1
1	A	278	VAL	3.1
1	D	127	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	239	ASN	3.1
1	A	259	GLN	3.1
1	A	260	LEU	3.1
1	A	186	ASP	3.1
1	C	237	TYR	3.0
1	C	200	GLY	3.0
1	C	25	TYR	3.0
1	D	57	ASN	3.0
1	C	119	LYS	3.0
1	D	45	ASN	3.0
1	D	182	ASN	3.0
1	A	154	GLU	3.0
1	C	95	THR	3.0
1	C	272	TRP	3.0
1	A	293	LYS	3.0
1	B	289	LYS	3.0
1	B	272	TRP	2.9
1	B	237	TYR	2.9
1	C	259	GLN	2.9
1	C	184	PRO	2.9
1	D	201	THR	2.9
1	C	128	SER	2.9
1	C	160	ALA	2.9
1	D	28	TRP	2.9
1	A	155	ASP	2.9
1	D	239	ASN	2.9
1	B	274	VAL	2.9
1	A	51	PHE	2.9
1	A	156	SER	2.9
1	A	273	ASP	2.8
1	A	274	VAL	2.8
1	D	273	ASP	2.8
1	A	124	PHE	2.8
1	C	124	PHE	2.8
1	A	39	GLN	2.8
1	B	260	LEU	2.8
1	C	141	GLY	2.8
1	B	28	TRP	2.7
1	A	31	TYR	2.7
1	C	92	TYR	2.7
1	B	236	ASN	2.7
1	D	271	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	39	GLN	2.7
1	D	93	SER	2.7
1	A	45	ASN	2.7
1	A	281	ASP	2.7
1	B	128	SER	2.7
1	D	179	LYS	2.7
1	B	162	HIS	2.7
1	C	45	ASN	2.7
1	B	125	ASP	2.7
1	C	94	SER	2.7
1	C	175	SER	2.7
1	B	32	LYS	2.6
1	B	185	LYS	2.6
1	A	200	GLY	2.6
1	B	187	GLU	2.6
1	C	187	GLU	2.6
1	D	180	LYS	2.6
1	A	29	GLY	2.6
1	A	159	GLY	2.6
1	A	241	LYS	2.6
1	B	10	LEU	2.6
1	B	27	ASN	2.6
1	D	293	LYS	2.6
1	B	275	ASP	2.6
1	D	120	SER	2.6
1	D	241	LYS	2.6
1	A	86	ASP	2.6
1	C	281	ASP	2.6
1	C	162	HIS	2.6
1	D	21	SER	2.6
1	B	112	GLU	2.6
1	B	45	ASN	2.6
1	B	124	PHE	2.6
1	A	162	HIS	2.5
1	D	175	SER	2.5
1	A	252	LYS	2.5
1	B	258	LYS	2.5
1	D	23	VAL	2.5
1	B	95	THR	2.5
1	A	59	ALA	2.5
1	B	163	ASP	2.5
1	D	157	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	83	SER	2.5
1	D	238	PRO	2.5
1	D	192	GLY	2.5
1	D	154	GLU	2.5
1	C	47	ASP	2.5
1	D	136	LYS	2.5
1	B	60	SER	2.5
1	B	26	PRO	2.5
1	A	248	ILE	2.5
1	A	279	TYR	2.5
1	A	239	ASN	2.5
1	D	109	PRO	2.5
1	D	39	GLN	2.5
1	C	280	ASN	2.5
1	B	158	CYS	2.4
1	B	183	ILE	2.4
1	D	216	VAL	2.4
1	B	81	SER	2.4
1	A	89	GLU	2.4
1	D	259	GLN	2.4
1	C	156	SER	2.4
1	D	82	GLN	2.4
1	B	221	HIS	2.4
1	C	24	LEU	2.4
1	D	202	PRO	2.4
1	A	270	LYS	2.4
1	D	176	ASP	2.4
1	B	228	GLN	2.4
1	A	87	LYS	2.3
1	C	222	ASN	2.3
1	C	185	LYS	2.3
1	D	199	LYS	2.3
1	A	123	GLY	2.3
1	C	84	GLY	2.3
1	C	159	GLY	2.3
1	C	239	ASN	2.3
1	C	120	SER	2.3
1	B	248	ILE	2.3
1	B	131	GLY	2.3
1	C	186	ASP	2.3
1	D	253	ASP	2.3
1	D	69	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	201	THR	2.3
1	D	280	ASN	2.3
1	D	44	LYS	2.3
1	C	240	GLY	2.3
1	C	142	LYS	2.2
1	D	205	LYS	2.2
1	D	158	CYS	2.2
1	D	85	TRP	2.2
1	B	23	VAL	2.2
1	A	237	TYR	2.2
1	B	277	TYR	2.2
1	C	14	SER	2.2
1	D	156	SER	2.2
1	B	140	ASN	2.2
1	C	85	TRP	2.2
1	A	21	SER	2.2
1	B	79	GLY	2.2
1	B	119	LYS	2.2
1	C	209	LYS	2.2
1	D	209	LYS	2.2
1	A	222	ASN	2.2
1	B	57	ASN	2.2
1	A	285	HIS	2.2
1	D	215	ASP	2.2
1	A	71	TYR	2.2
1	A	220	GLY	2.2
1	B	108	TYR	2.2
1	C	220	GLY	2.2
1	C	217	LEU	2.2
1	C	157	ARG	2.2
1	A	49	VAL	2.2
1	A	102	VAL	2.2
1	C	109	PRO	2.2
1	A	95	THR	2.2
1	D	159	GLY	2.2
1	D	122	CYS	2.2
1	B	233	ALA	2.2
1	D	185	LYS	2.1
1	C	192	GLY	2.1
1	B	222	ASN	2.1
1	C	126	ASN	2.1
1	B	85	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	272	TRP	2.1
1	D	233	ALA	2.1
1	B	138	GLU	2.1
1	B	142	LYS	2.1
1	D	26	PRO	2.1
1	D	196	ASN	2.1
1	B	92	TYR	2.1
1	C	70	GLU	2.1
1	B	188	THR	2.1
1	A	137	ILE	2.1
1	C	219	ALA	2.1
1	C	248	ILE	2.1
1	B	44	LYS	2.0
1	C	83	SER	2.0
1	C	122	CYS	2.0
1	C	252	LYS	2.0
1	D	94	SER	2.0
1	D	170	GLN	2.0
1	C	144	VAL	2.0
1	C	22	THR	2.0
1	D	95	THR	2.0
1	A	179	LYS	2.0
1	B	179	LYS	2.0
1	C	136	LYS	2.0
1	A	277	TYR	2.0
1	A	67	VAL	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 [i](#)

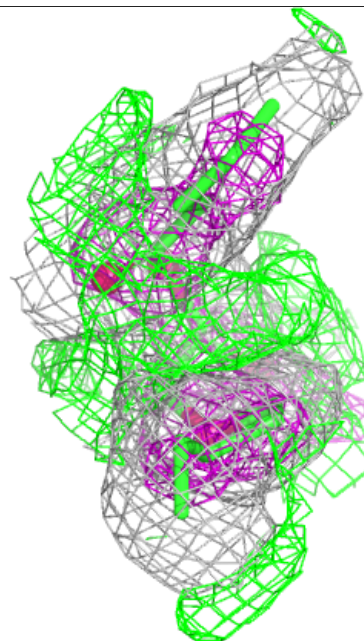
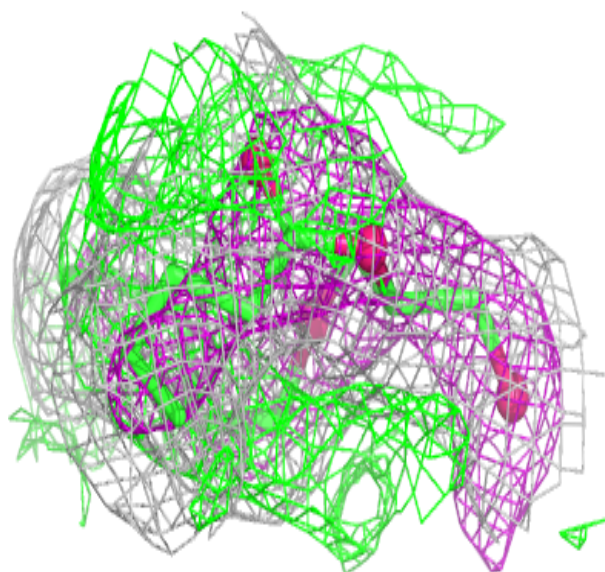
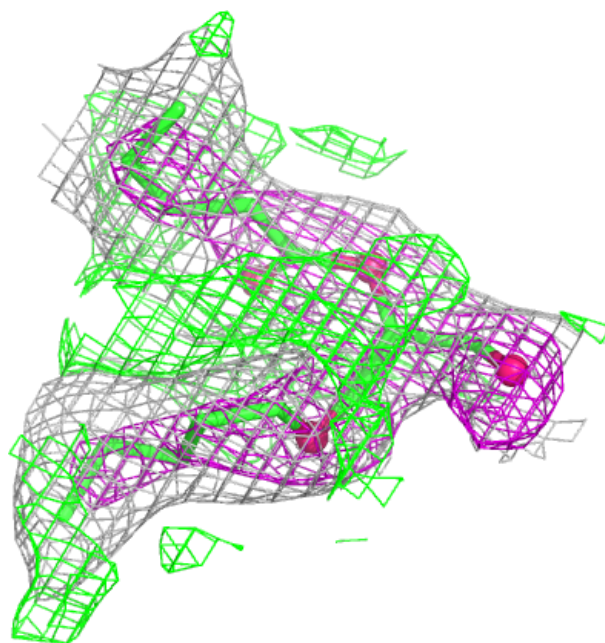
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DGA	D	401	17/44	0.80	0.23	20,20,20,20	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 DGA D 401:

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.