



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 12:45 AM BST

PDB ID : 3SEF
Title : 2.4 Angstrom resolution crystal structure of shikimate 5-dehydrogenase (aroE) from *Vibrio cholerae* O1 biovar eltor str. N16961 in complex with shikimate and NADPH
Authors : Halavaty, A.S.; Light, S.H.; Minasov, G.; Shuvalova, L.; Papazisi, L.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2011-06-10
Resolution : 2.40 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

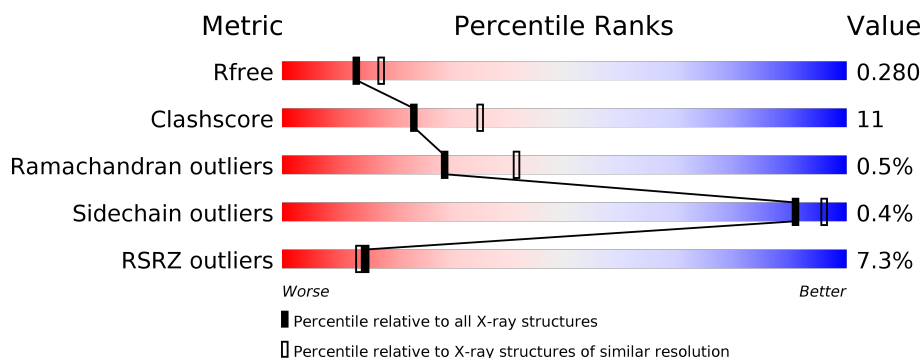
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	302	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>19%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	302	<div> <div>5%</div> <div> <div></div> <div>72%</div> <div>18%</div> <div>11%</div> </div> </div>
1	C	302	<div> <div>10%</div> <div> <div></div> <div>63%</div> <div>18%</div> <div>19%</div> </div> </div>
1	D	302	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>10%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8384 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 Shikimate 5-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	3	0
			2079	1313	363	393	10			
1	B	269	Total	C	N	O	S	0	1	0
			2069	1307	363	389	10			
1	C	244	Total	C	N	O	S	0	1	0
			1880	1189	328	354	9			
1	D	272	Total	C	N	O	S	0	2	0
			2101	1327	368	396	10			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	EXPRESSION TAG	UNP Q9KVT3
A	-22	HIS	-	EXPRESSION TAG	UNP Q9KVT3
A	-21	HIS	-	EXPRESSION TAG	UNP Q9KVT3
A	-20	HIS	-	EXPRESSION TAG	UNP Q9KVT3
A	-19	HIS	-	EXPRESSION TAG	UNP Q9KVT3
A	-18	HIS	-	EXPRESSION TAG	UNP Q9KVT3
A	-17	HIS	-	EXPRESSION TAG	UNP Q9KVT3
A	-16	SER	-	EXPRESSION TAG	UNP Q9KVT3
A	-15	SER	-	EXPRESSION TAG	UNP Q9KVT3
A	-14	GLY	-	EXPRESSION TAG	UNP Q9KVT3
A	-13	VAL	-	EXPRESSION TAG	UNP Q9KVT3
A	-12	ASP	-	EXPRESSION TAG	UNP Q9KVT3
A	-11	LEU	-	EXPRESSION TAG	UNP Q9KVT3
A	-10	GLY	-	EXPRESSION TAG	UNP Q9KVT3
A	-9	THR	-	EXPRESSION TAG	UNP Q9KVT3
A	-8	GLU	-	EXPRESSION TAG	UNP Q9KVT3
A	-7	ASN	-	EXPRESSION TAG	UNP Q9KVT3
A	-6	LEU	-	EXPRESSION TAG	UNP Q9KVT3
A	-5	TYR	-	EXPRESSION TAG	UNP Q9KVT3
A	-4	PHE	-	EXPRESSION TAG	UNP Q9KVT3
A	-3	GLN	-	EXPRESSION TAG	UNP Q9KVT3

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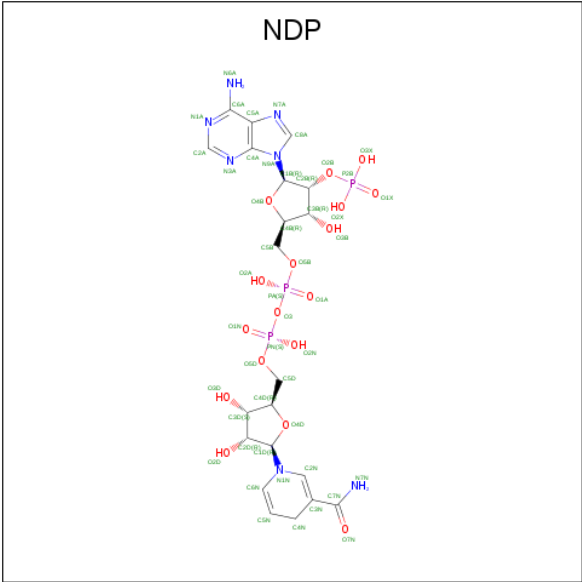
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q9KVT3
A	-1	ASN	-	EXPRESSION TAG	UNP Q9KVT3
A	0	ALA	-	EXPRESSION TAG	UNP Q9KVT3
B	-23	MET	-	EXPRESSION TAG	UNP Q9KVT3
B	-22	HIS	-	EXPRESSION TAG	UNP Q9KVT3
B	-21	HIS	-	EXPRESSION TAG	UNP Q9KVT3
B	-20	HIS	-	EXPRESSION TAG	UNP Q9KVT3
B	-19	HIS	-	EXPRESSION TAG	UNP Q9KVT3
B	-18	HIS	-	EXPRESSION TAG	UNP Q9KVT3
B	-17	HIS	-	EXPRESSION TAG	UNP Q9KVT3
B	-16	SER	-	EXPRESSION TAG	UNP Q9KVT3
B	-15	SER	-	EXPRESSION TAG	UNP Q9KVT3
B	-14	GLY	-	EXPRESSION TAG	UNP Q9KVT3
B	-13	VAL	-	EXPRESSION TAG	UNP Q9KVT3
B	-12	ASP	-	EXPRESSION TAG	UNP Q9KVT3
B	-11	LEU	-	EXPRESSION TAG	UNP Q9KVT3
B	-10	GLY	-	EXPRESSION TAG	UNP Q9KVT3
B	-9	THR	-	EXPRESSION TAG	UNP Q9KVT3
B	-8	GLU	-	EXPRESSION TAG	UNP Q9KVT3
B	-7	ASN	-	EXPRESSION TAG	UNP Q9KVT3
B	-6	LEU	-	EXPRESSION TAG	UNP Q9KVT3
B	-5	TYR	-	EXPRESSION TAG	UNP Q9KVT3
B	-4	PHE	-	EXPRESSION TAG	UNP Q9KVT3
B	-3	GLN	-	EXPRESSION TAG	UNP Q9KVT3
B	-2	SER	-	EXPRESSION TAG	UNP Q9KVT3
B	-1	ASN	-	EXPRESSION TAG	UNP Q9KVT3
B	0	ALA	-	EXPRESSION TAG	UNP Q9KVT3
C	-23	MET	-	EXPRESSION TAG	UNP Q9KVT3
C	-22	HIS	-	EXPRESSION TAG	UNP Q9KVT3
C	-21	HIS	-	EXPRESSION TAG	UNP Q9KVT3
C	-20	HIS	-	EXPRESSION TAG	UNP Q9KVT3
C	-19	HIS	-	EXPRESSION TAG	UNP Q9KVT3
C	-18	HIS	-	EXPRESSION TAG	UNP Q9KVT3
C	-17	HIS	-	EXPRESSION TAG	UNP Q9KVT3
C	-16	SER	-	EXPRESSION TAG	UNP Q9KVT3
C	-15	SER	-	EXPRESSION TAG	UNP Q9KVT3
C	-14	GLY	-	EXPRESSION TAG	UNP Q9KVT3
C	-13	VAL	-	EXPRESSION TAG	UNP Q9KVT3
C	-12	ASP	-	EXPRESSION TAG	UNP Q9KVT3
C	-11	LEU	-	EXPRESSION TAG	UNP Q9KVT3
C	-10	GLY	-	EXPRESSION TAG	UNP Q9KVT3
C	-9	THR	-	EXPRESSION TAG	UNP Q9KVT3

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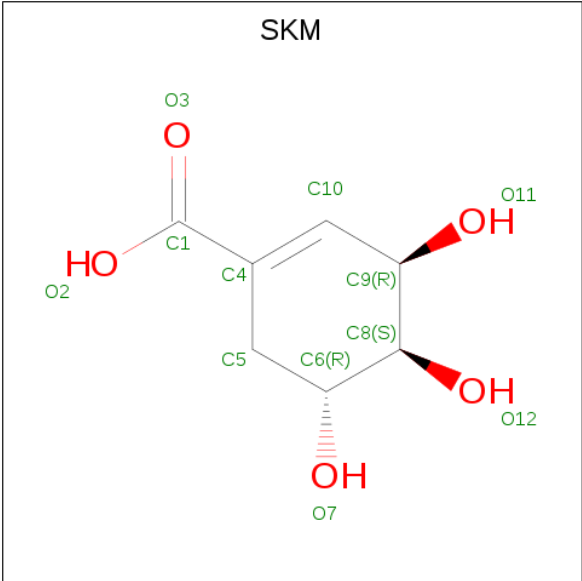
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	EXPRESSION TAG	UNP Q9KVT3
C	-7	ASN	-	EXPRESSION TAG	UNP Q9KVT3
C	-6	LEU	-	EXPRESSION TAG	UNP Q9KVT3
C	-5	TYR	-	EXPRESSION TAG	UNP Q9KVT3
C	-4	PHE	-	EXPRESSION TAG	UNP Q9KVT3
C	-3	GLN	-	EXPRESSION TAG	UNP Q9KVT3
C	-2	SER	-	EXPRESSION TAG	UNP Q9KVT3
C	-1	ASN	-	EXPRESSION TAG	UNP Q9KVT3
C	0	ALA	-	EXPRESSION TAG	UNP Q9KVT3
D	-23	MET	-	EXPRESSION TAG	UNP Q9KVT3
D	-22	HIS	-	EXPRESSION TAG	UNP Q9KVT3
D	-21	HIS	-	EXPRESSION TAG	UNP Q9KVT3
D	-20	HIS	-	EXPRESSION TAG	UNP Q9KVT3
D	-19	HIS	-	EXPRESSION TAG	UNP Q9KVT3
D	-18	HIS	-	EXPRESSION TAG	UNP Q9KVT3
D	-17	HIS	-	EXPRESSION TAG	UNP Q9KVT3
D	-16	SER	-	EXPRESSION TAG	UNP Q9KVT3
D	-15	SER	-	EXPRESSION TAG	UNP Q9KVT3
D	-14	GLY	-	EXPRESSION TAG	UNP Q9KVT3
D	-13	VAL	-	EXPRESSION TAG	UNP Q9KVT3
D	-12	ASP	-	EXPRESSION TAG	UNP Q9KVT3
D	-11	LEU	-	EXPRESSION TAG	UNP Q9KVT3
D	-10	GLY	-	EXPRESSION TAG	UNP Q9KVT3
D	-9	THR	-	EXPRESSION TAG	UNP Q9KVT3
D	-8	GLU	-	EXPRESSION TAG	UNP Q9KVT3
D	-7	ASN	-	EXPRESSION TAG	UNP Q9KVT3
D	-6	LEU	-	EXPRESSION TAG	UNP Q9KVT3
D	-5	TYR	-	EXPRESSION TAG	UNP Q9KVT3
D	-4	PHE	-	EXPRESSION TAG	UNP Q9KVT3
D	-3	GLN	-	EXPRESSION TAG	UNP Q9KVT3
D	-2	SER	-	EXPRESSION TAG	UNP Q9KVT3
D	-1	ASN	-	EXPRESSION TAG	UNP Q9KVT3
D	0	ALA	-	EXPRESSION TAG	UNP Q9KVT3

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is (3R,4S,5R)-3,4,5-TRIHydroxycyclohex-1-ene-1-carboxylic acid (three-letter code: SKM) (formula: C₇H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			12	7	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			12	7	5		

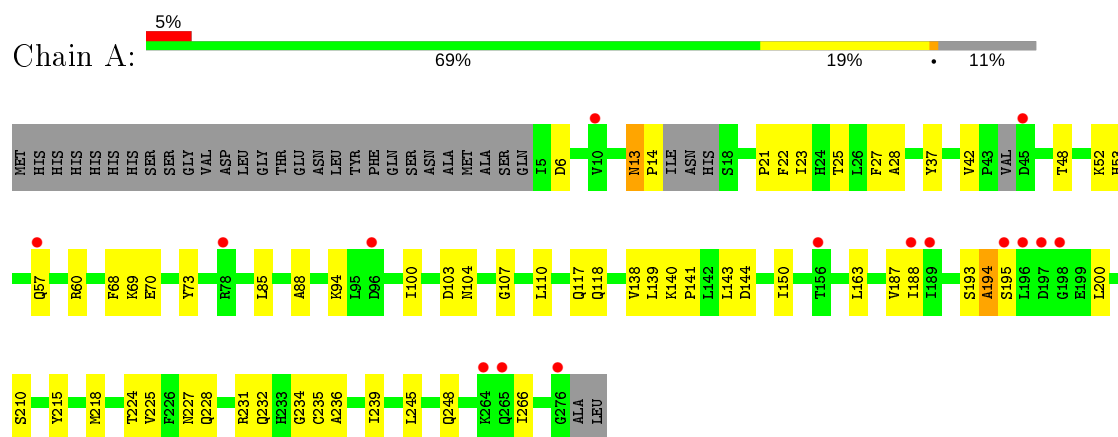
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	B	42	Total	O	0	0
			42	42		
4	C	19	Total	O	0	0
			19	19		
4	D	36	Total	O	0	1
			37	37		

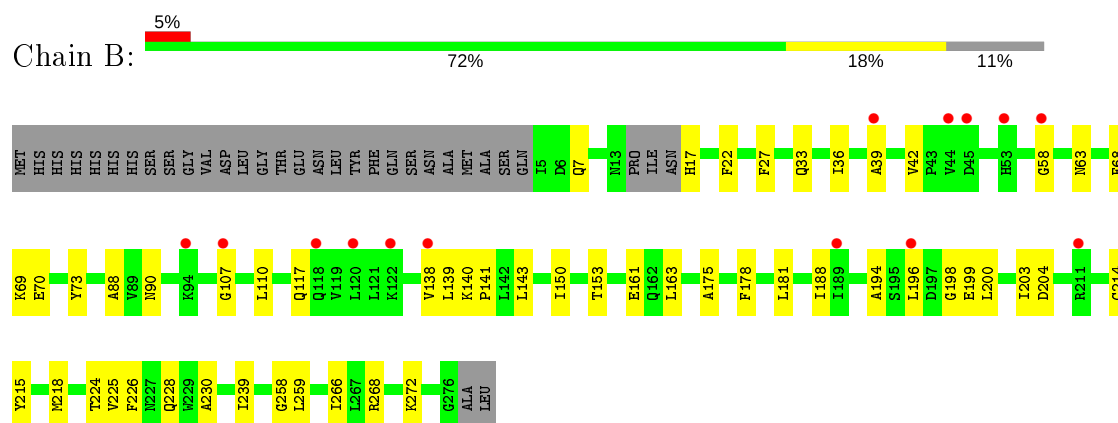
3 Residue-property plots [i](#)

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.

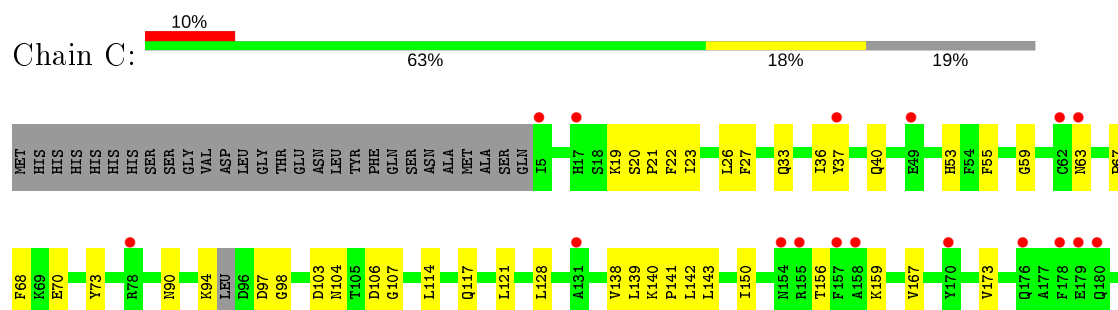
- Molecule 1: Shikimate 5-dehydrogenase

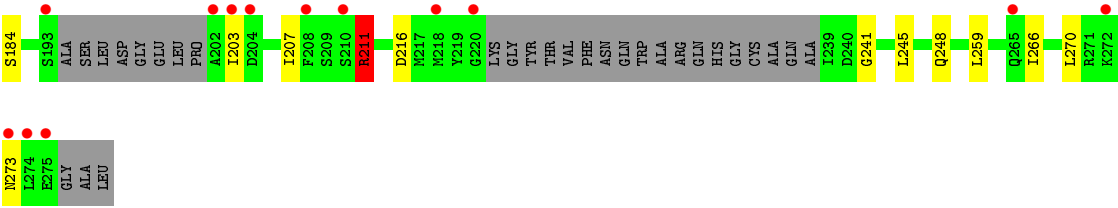


- Molecule 1: Shikimate 5-dehydrogenase

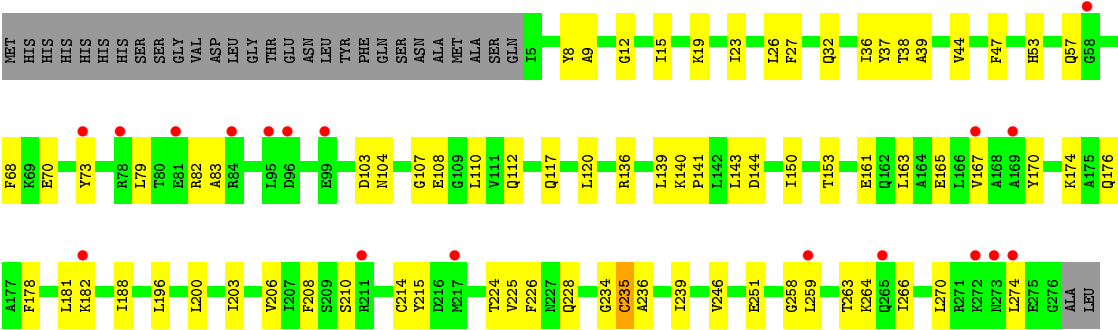


- Molecule 1: Shikimate 5-dehydrogenase





● Molecule 1: Shikimate 5-dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.03Å 86.08Å 81.02Å 90.00° 92.85° 90.00°	Depositor
Resolution (Å)	29.48 – 2.40 28.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.48-2.40) 99.7 (28.40-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.235 , 0.276 0.236 , 0.280	Depositor DCC
R_{free} test set	2059 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8384	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: SKM, NDP

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	0/2113	0.61	0/2851
1	B	0.30	0/2104	0.60	0/2841
1	C	0.28	0/1908	0.57	1/2573 (0.0%)
1	D	0.28	0/2138	0.57	0/2890
All	All	0.29	0/8263	0.59	1/11155 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	ARG	NE-CZ-NH1	5.14	122.87	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2079	0	2066	47	0
1	B	2069	0	2060	41	0
1	C	1880	0	1883	40	0
1	D	2101	0	2090	66	0
2	A	48	0	26	0	0
2	B	48	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	9	0	0
3	C	12	0	9	0	0
4	A	37	0	0	2	0
4	B	42	0	0	0	0
4	C	19	0	0	0	0
4	D	37	0	0	1	0
All	All	8384	0	8169	186	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 11.

All (186) 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:PHE:CE1	1:D:266:ILE:HD12	2.05	0.92
1:D:15:ILE:HG21	1:D:39:ALA:HB1	1.49	0.91
1:A:117:GLN:HG3	1:A:239:ILE:HD13	1.68	0.73
1:C:211:ARG:CG	1:C:211:ARG:HH11	2.04	0.69
1:C:140:LYS:HB3	1:C:141:PRO:HD3	1.75	0.68
1:D:47:PHE:HB2	1:D:68:PHE:CD1	2.28	0.67
1:A:27:PHE:CE1	1:A:266:ILE:HD12	2.29	0.67
1:B:194:ALA:HB1	1:B:199:GLU:O	1.96	0.66
1:D:140:LYS:NZ	1:D:144:ASP:OD2	2.28	0.66
1:C:27:PHE:CE1	1:C:266:ILE:HD12	2.31	0.66
1:A:210:SER:HA	1:A:234:GLY:O	1.97	0.64
1:C:143:LEU:CD2	1:C:150:ILE:HD12	2.28	0.64
1:C:107:GLY:HA3	1:C:141:PRO:HG2	1.78	0.64
1:B:181:LEU:HD12	1:B:203:ILE:HG23	1.79	0.63
1:D:210:SER:O	1:D:236:ALA:HB2	1.99	0.63
1:A:200:LEU:HD21	1:A:225:VAL:HG12	1.80	0.62
1:A:235:CYS:SG	4:A:294:HOH:O	2.49	0.62
1:D:27:PHE:CD1	1:D:266:ILE:HD12	2.34	0.62
1:B:140:LYS:HB3	1:B:141:PRO:HD3	1.82	0.61
1:B:139:LEU:HD11	1:B:163:LEU:HG	1.83	0.60
1:D:53:HIS:NE2	1:D:57:GLN:OE1	2.34	0.60
1:B:196:LEU:CD2	1:B:218:MET:HG2	2.31	0.60
1:A:140:LYS:HB3	1:A:141:PRO:HD3	1.83	0.60
1:D:107:GLY:HA3	1:D:141:PRO:HG2	1.83	0.60
1:A:94:LYS:NZ	4:A:288:HOH:O	2.34	0.60
1:C:203:ILE:HG21	1:C:207:ILE:HD13	1.84	0.59
1:B:196:LEU:HD23	1:B:218:MET:CG	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:GLY:CA	1:D:15:ILE:HD11	2.33	0.59
1:B:27:PHE:CE1	1:B:266:ILE:HD12	2.38	0.59
1:D:143:LEU:CD2	1:D:150:ILE:HD12	2.32	0.59
1:A:188:ILE:HD12	1:A:188:ILE:N	2.18	0.58
1:D:140:LYS:HB3	1:D:141:PRO:HD3	1.83	0.58
1:B:33:GLN:NE2	1:B:259:LEU:HD12	2.17	0.58
1:D:15:ILE:HG22	1:D:15:ILE:O	2.03	0.58
1:A:42:VAL:HG11	1:A:68:PHE:CZ	2.37	0.58
1:C:27:PHE:CD1	1:C:266:ILE:HD12	2.39	0.57
1:A:107:GLY:HA2	1:A:138:VAL:HG12	1.86	0.57
1:B:117:GLN:HG3	1:B:239:ILE:HD13	1.87	0.57
1:D:108[A]:GLU:OE2	1:D:112:GLN:NE2	2.32	0.57
1:A:42:VAL:HG11	1:A:68:PHE:CE2	2.40	0.57
1:B:22:PHE:HD1	1:C:36:ILE:HD11	1.70	0.56
1:B:188:ILE:HD12	1:B:188:ILE:N	2.20	0.56
1:D:117:GLN:HG3	1:D:239:ILE:HD13	1.88	0.56
1:B:70:GLU:OE2	1:B:70:GLU:N	2.38	0.56
1:B:198:GLY:HA2	1:B:225:VAL:HG21	1.87	0.56
1:C:143:LEU:HD23	1:C:150:ILE:HD12	1.87	0.55
1:D:110:LEU:CD1	1:D:215:TYR:CE1	2.90	0.55
1:D:182:LYS:O	1:D:182:LYS:HG2	2.07	0.55
1:B:200:LEU:HD21	1:B:225:VAL:HG12	1.87	0.55
1:C:103:ASP:OD1	1:C:104:ASN:N	2.40	0.54
1:C:26:LEU:HB2	1:C:266:ILE:HD13	1.89	0.54
1:A:195:SER:HB3	1:A:218[B]:MET:CE	2.37	0.54
1:C:97:ASP:OD2	1:C:98:GLY:N	2.40	0.54
1:D:188:ILE:N	1:D:188:ILE:HD12	2.24	0.53
1:D:174:LYS:NZ	1:D:174:LYS:HB3	2.25	0.52
1:A:23:ILE:HG22	1:A:27:PHE:CE2	2.44	0.52
1:D:196:LEU:N	1:D:196:LEU:HD12	2.24	0.52
1:B:107:GLY:HA2	1:B:138:VAL:HG12	1.90	0.52
1:A:48:THR:O	1:A:52:LYS:HG2	2.08	0.52
1:A:103:ASP:OD1	1:A:104:ASN:N	2.42	0.52
1:C:90:ASN:ND2	1:C:106:ASP:OD2	2.42	0.52
1:A:224:THR:O	1:A:228:GLN:HG3	2.08	0.52
1:B:200:LEU:CD2	1:B:225:VAL:HG12	2.40	0.52
1:B:107:GLY:HA3	1:B:141:PRO:HG2	1.92	0.51
1:B:22:PHE:CD1	1:C:36:ILE:HD11	2.45	0.51
1:D:139:LEU:HD11	1:D:163:LEU:HG	1.93	0.51
1:D:73:TYR:CE1	1:D:79:LEU:HD13	2.46	0.51
1:B:214[A]:CYS:SG	1:B:226:PHE:HE2	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLN:O	1:A:232:GLN:HG3	2.12	0.50
1:D:200:LEU:HD21	1:D:225:VAL:HG23	1.93	0.50
1:D:274:LEU:C	1:D:274:LEU:HD23	2.31	0.50
1:D:274:LEU:O	1:D:274:LEU:HD23	2.11	0.50
1:A:140:LYS:NZ	1:A:144:ASP:OD1	2.45	0.50
1:A:143:LEU:CD2	1:A:150:ILE:HD12	2.42	0.50
1:A:53:HIS:NE2	1:A:57:GLN:NE2	2.59	0.49
1:A:69:LYS:HB3	1:A:88:ALA:HB1	1.93	0.49
1:C:211:ARG:HH11	1:C:211:ARG:HG3	1.75	0.49
1:C:211:ARG:HG2	1:C:211:ARG:HH11	1.74	0.49
1:B:268:ARG:O	1:B:272:LYS:HG3	2.12	0.49
1:D:153:THR:HG23	1:D:178:PHE:HE1	1.77	0.49
1:C:143:LEU:HD21	1:C:150:ILE:HD12	1.95	0.49
1:D:120:LEU:HD12	1:D:120:LEU:N	2.28	0.49
1:D:234:GLY:O	1:D:235:CYS:C	2.51	0.49
1:B:39:ALA:HB3	1:C:40:GLN:HA	1.94	0.48
1:D:214[A]:CYS:SG	1:D:226:PHE:HE2	2.35	0.48
1:A:85:LEU:HD12	1:A:140:LYS:HG2	1.96	0.48
1:D:224:THR:O	1:D:228:GLN:HG3	2.14	0.48
1:A:195:SER:HB3	1:A:218[B]:MET:HE3	1.94	0.47
1:B:196:LEU:HD23	1:B:218:MET:HG2	1.94	0.47
1:B:224:THR:O	1:B:228:GLN:HG3	2.13	0.47
1:D:143:LEU:HD23	1:D:150:ILE:HD12	1.94	0.47
1:C:67:PRO:HD2	1:C:68:PHE:CE1	2.49	0.47
1:D:246:VAL:HG22	1:D:270:LEU:HD12	1.96	0.47
1:A:70:GLU:O	1:A:73:TYR:HB3	2.15	0.47
1:D:57:GLN:NE2	4:D:304:HOH:O	2.45	0.47
1:B:63:ASN:HA	1:B:90:ASN:O	2.15	0.47
1:A:13:ASN:ND2	1:A:13:ASN:O	2.44	0.47
1:B:69:LYS:HB3	1:B:88:ALA:HB1	1.97	0.46
1:A:210:SER:O	1:A:236:ALA:HB2	2.14	0.46
1:B:214[A]:CYS:SG	1:B:226:PHE:CE2	3.09	0.46
1:D:70:GLU:O	1:D:73:TYR:HB3	2.16	0.46
1:D:112:GLN:HG3	1:D:251:GLU:OE1	2.16	0.46
1:D:47:PHE:HB2	1:D:68:PHE:CE1	2.50	0.46
1:C:245:LEU:HD12	1:C:248:GLN:HE21	1.81	0.46
1:A:107:GLY:HA3	1:A:141:PRO:HG2	1.98	0.46
1:A:21:PRO:HA	1:A:37:TYR:CD1	2.51	0.46
1:C:184:SER:HA	1:C:207:ILE:HA	1.97	0.45
1:D:174:LYS:HZ1	1:D:176:GLN:HE21	1.63	0.45
1:D:12:GLY:N	1:D:15:ILE:HD11	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:HA	1:A:100:ILE:HD13	1.98	0.45
1:C:63:ASN:HA	1:C:90:ASN:O	2.17	0.45
1:A:22:PHE:CD1	1:D:36:ILE:HD13	2.51	0.45
1:D:82:ARG:NH1	1:D:108[B]:GLU:HG3	2.31	0.45
1:C:114:LEU:HD13	1:C:121:LEU:HD21	1.97	0.45
1:D:82:ARG:NH2	1:D:103:ASP:OD2	2.46	0.45
1:D:174:LYS:HB3	1:D:174:LYS:HZ3	1.81	0.45
1:D:214[A]:CYS:SG	1:D:226:PHE:CE2	3.10	0.45
1:B:143:LEU:CD2	1:B:150:ILE:HD12	2.46	0.45
1:C:22:PHE:CD2	1:C:270:LEU:HD21	2.52	0.45
1:D:9:ALA:HB1	1:D:38:THR:O	2.16	0.45
1:D:196:LEU:N	1:D:196:LEU:CD1	2.80	0.44
1:D:8:TYR:O	1:D:37:TYR:HA	2.17	0.44
1:A:118:GLN:N	1:A:118:GLN:OE1	2.51	0.44
1:C:19:LYS:O	1:C:23:ILE:HG13	2.16	0.44
1:C:70:GLU:O	1:C:73:TYR:HB3	2.17	0.44
1:D:47:PHE:CB	1:D:68:PHE:CD1	2.99	0.44
1:B:153:THR:OG1	1:B:178:PHE:HD1	2.00	0.44
1:B:196:LEU:HD21	1:B:218:MET:HG2	1.97	0.44
1:C:216:ASP:O	1:C:241:GLY:N	2.51	0.44
1:C:156:THR:HG22	1:C:159:LYS:H	1.83	0.44
1:A:227:ASN:O	1:A:231:ARG:HG3	2.18	0.44
1:B:17:HIS:HB3	1:C:53:HIS:HD2	1.82	0.44
1:B:153:THR:OG1	1:B:178:PHE:CD1	2.69	0.44
1:C:55:PHE:CD1	1:C:94:LYS:HG3	2.53	0.44
1:D:246:VAL:CG2	1:D:270:LEU:HD12	2.48	0.44
1:B:110:LEU:CD1	1:B:215:TYR:CE1	3.01	0.43
1:C:138:VAL:O	1:C:142:LEU:HG	2.18	0.43
1:C:33:GLN:NE2	1:C:259:LEU:HD12	2.32	0.43
1:D:181:LEU:HD12	1:D:203:ILE:HG23	2.00	0.43
1:A:6:ASP:OD2	1:A:60:ARG:NH2	2.51	0.43
1:C:23:ILE:HG22	1:C:27:PHE:CE2	2.53	0.43
1:A:25:THR:HB	1:D:36:ILE:HD11	2.00	0.43
1:B:258:GLY:O	1:B:259:LEU:HD23	2.19	0.43
1:D:103:ASP:OD1	1:D:104:ASN:N	2.50	0.43
1:B:139:LEU:CD1	1:B:163:LEU:HG	2.48	0.43
1:B:214[B]:CYS:SG	1:B:230:ALA:HB1	2.59	0.43
1:C:55:PHE:HB3	1:C:94:LYS:HD3	2.01	0.43
1:D:26:LEU:HB2	1:D:266:ILE:CD1	2.49	0.43
1:B:42:VAL:HG11	1:B:68:PHE:CE2	2.54	0.42
1:B:161:GLU:OE2	1:B:175:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:GLY:HA3	1:D:15:ILE:HD11	1.99	0.42
1:A:22:PHE:HA	1:D:36:ILE:HD11	1.99	0.42
1:B:196:LEU:CD2	1:B:218:MET:CG	2.95	0.42
1:A:245:LEU:HD12	1:A:248:GLN:HE21	1.84	0.42
1:B:70:GLU:O	1:B:73:TYR:HB3	2.20	0.42
1:C:117:GLN:OE1	1:C:117:GLN:HA	2.20	0.42
1:C:128:LEU:CD2	1:C:139:LEU:HD21	2.49	0.42
1:C:59:GLY:O	1:C:94:LYS:HE2	2.20	0.42
1:D:110:LEU:HD13	1:D:215:TYR:CE1	2.55	0.42
1:D:19:LYS:O	1:D:23:ILE:HG13	2.20	0.41
1:D:136:ARG:HA	1:D:163:LEU:HD11	2.01	0.41
1:A:193:SER:O	1:A:194:ALA:C	2.59	0.41
1:A:25:THR:O	1:A:28:ALA:HB3	2.20	0.41
1:D:140:LYS:HE2	1:D:170:TYR:CD1	2.55	0.41
1:D:182:LYS:HA	1:D:206:VAL:HG11	2.03	0.41
1:A:139:LEU:HD11	1:A:163:LEU:HG	2.03	0.41
1:A:70:GLU:OE1	1:A:70:GLU:N	2.45	0.41
1:A:110:LEU:CD1	1:A:215:TYR:CE1	3.04	0.41
1:D:258:GLY:O	1:D:259:LEU:HD23	2.20	0.41
1:C:21:PRO:HA	1:C:37:TYR:CD1	2.55	0.41
1:D:83:ALA:HB2	1:D:103:ASP:HA	2.03	0.41
1:D:208:PHE:HE1	1:D:214[B]:CYS:HG	1.68	0.41
1:B:203:ILE:CG2	1:B:204:ASP:N	2.84	0.41
1:A:13:ASN:N	1:A:14:PRO:CD	2.84	0.41
1:C:20:SER:N	1:C:21:PRO:CD	2.84	0.40
1:D:143:LEU:HD21	1:D:150:ILE:HD12	2.02	0.40
1:D:263:THR:O	1:D:264:LYS:C	2.60	0.40
1:B:7:GLN:OE1	1:B:36:ILE:CG2	2.69	0.40
1:A:143:LEU:HD21	1:A:150:ILE:HD12	2.04	0.40
1:A:187:VAL:C	1:A:188:ILE:HD12	2.41	0.40
1:A:188:ILE:N	1:A:188:ILE:CD1	2.84	0.40
1:C:167:VAL:HG23	1:C:173:VAL:HG21	2.02	0.40
1:D:139:LEU:HD13	1:D:167:VAL:HG21	2.03	0.40
1:A:140:LYS:NZ	1:A:144:ASP:OD2	2.54	0.40
1:D:161:GLU:O	1:D:165:GLU:HG3	2.22	0.40
1:A:22:PHE:HA	1:D:36:ILE:CD1	2.51	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	265/302 (88%)	256 (97%)	8 (3%)	1 (0%)	34	48
1	B	266/302 (88%)	257 (97%)	8 (3%)	1 (0%)	34	48
1	C	237/302 (78%)	228 (96%)	9 (4%)	0	100	100
1	D	272/302 (90%)	252 (93%)	17 (6%)	3 (1%)	14	20
All	All	1040/1208 (86%)	993 (96%)	42 (4%)	5 (0%)	29	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	44	VAL
1	A	194	ALA
1	D	32	GLN
1	D	235	CYS
1	B	58	GLY

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	214/240 (89%)	213 (100%)	1 (0%)	88	95
1	B	213/240 (89%)	213 (100%)	0	100	100
1	C	196/240 (82%)	194 (99%)	2 (1%)	76	88
1	D	217/240 (90%)	217 (100%)	0	100	100
All	All	840/960 (88%)	837 (100%)	3 (0%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	C	211	ARG
1	C	273	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	30	GLN
1	A	57	GLN
1	B	30	GLN
1	B	63	ASN
1	B	265	GLN
1	C	180	GLN
1	C	183	GLN
1	C	273	ASN
1	D	30	GLN
1	D	63	ASN
1	D	146	GLN
1	D	176	GLN
1	D	183	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	B	279	-	45,52,52	1.34	3 (6%)	53,80,80	1.81	6 (11%)
3	SKM	B	280	-	9,12,12	0.61	0	12,17,17	0.51	0
3	SKM	C	279	-	9,12,12	0.45	0	12,17,17	1.23	1 (8%)
2	NDP	A	279	-	45,52,52	1.31	3 (6%)	53,80,80	1.45	6 (11%)

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	NDP	B	279	-	-	10/30/77/77	0/5/5/5
3	SKM	B	280	-	-	0/0/20/20	0/1/1/1
3	SKM	C	279	-	-	0/0/20/20	0/1/1/1
2	NDP	A	279	-	-	10/30/77/77	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	279	NDP	C2N-C3N	6.69	1.53	1.34
2	A	279	NDP	C2N-C3N	6.37	1.52	1.34
2	A	279	NDP	C5A-C4A	2.53	1.47	1.40
2	A	279	NDP	C6N-N1N	2.43	1.43	1.37
2	B	279	NDP	C5A-C4A	2.42	1.47	1.40
2	B	279	NDP	C6N-N1N	2.22	1.42	1.37

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	279	NDP	C3N-C2N-N1N	-9.03	110.21	123.10
2	A	279	NDP	C3N-C2N-N1N	-5.55	115.17	123.10
2	B	279	NDP	C1D-N1N-C2N	-4.38	113.82	121.11
2	B	279	NDP	N3A-C2A-N1A	-4.36	121.86	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	279	NDP	N3A-C2A-N1A	-4.27	122.00	128.68
2	A	279	NDP	C4A-C5A-N7A	-3.15	106.12	109.40
2	B	279	NDP	PN-O3-PA	-3.02	122.45	132.83
2	B	279	NDP	C4A-C5A-N7A	-2.99	106.28	109.40
2	A	279	NDP	PN-O3-PA	-2.92	122.80	132.83
3	C	279	SKM	C5-C6-C8	2.82	113.69	110.30
2	A	279	NDP	C3D-C2D-C1D	2.73	106.61	101.43
2	B	279	NDP	O4D-C1D-N1N	2.04	112.05	108.06
2	A	279	NDP	C2A-N1A-C6A	2.04	122.24	118.75

There are no chirality outliers.

All (20) torsion outliers are listed below:

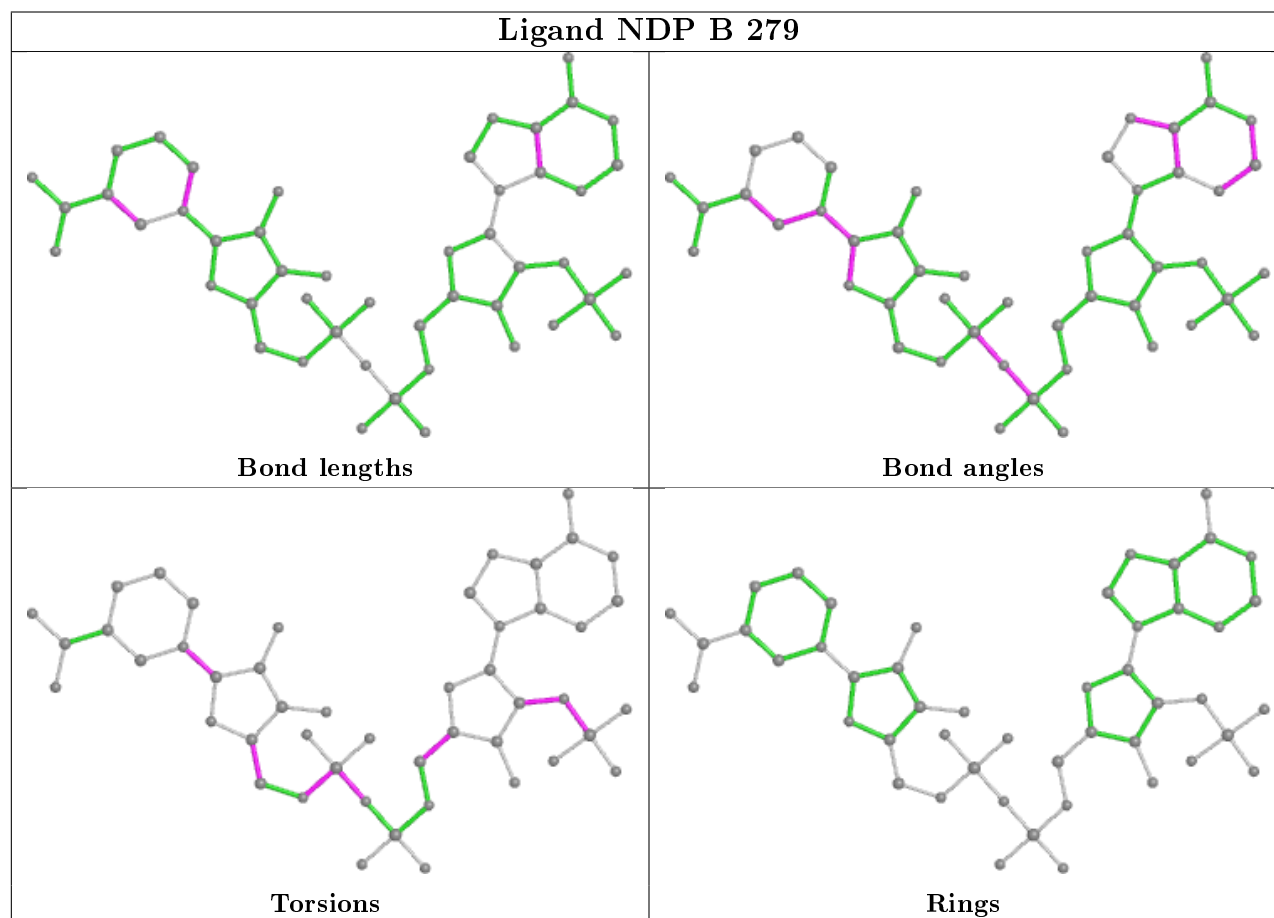
Mol	Chain	Res	Type	Atoms
2	B	279	NDP	C2B-O2B-P2B-O2X
2	B	279	NDP	C5D-O5D-PN-O1N
2	B	279	NDP	O4D-C1D-N1N-C2N
2	A	279	NDP	C5D-O5D-PN-O1N
2	A	279	NDP	C5D-O5D-PN-O2N
2	A	279	NDP	O4D-C1D-N1N-C2N
2	B	279	NDP	O4D-C4D-C5D-O5D
2	B	279	NDP	C3D-C4D-C5D-O5D
2	A	279	NDP	C3B-C2B-O2B-P2B
2	B	279	NDP	C5D-O5D-PN-O3
2	A	279	NDP	C2B-O2B-P2B-O2X
2	B	279	NDP	C5D-O5D-PN-O2N
2	A	279	NDP	C1B-C2B-O2B-P2B
2	B	279	NDP	C3B-C2B-O2B-P2B
2	A	279	NDP	C2B-O2B-P2B-O3X
2	A	279	NDP	C5D-O5D-PN-O3
2	A	279	NDP	O4B-C4B-C5B-O5B
2	B	279	NDP	PA-O3-PN-O2N
2	B	279	NDP	O4B-C4B-C5B-O5B
2	A	279	NDP	O4D-C4D-C5D-O5D

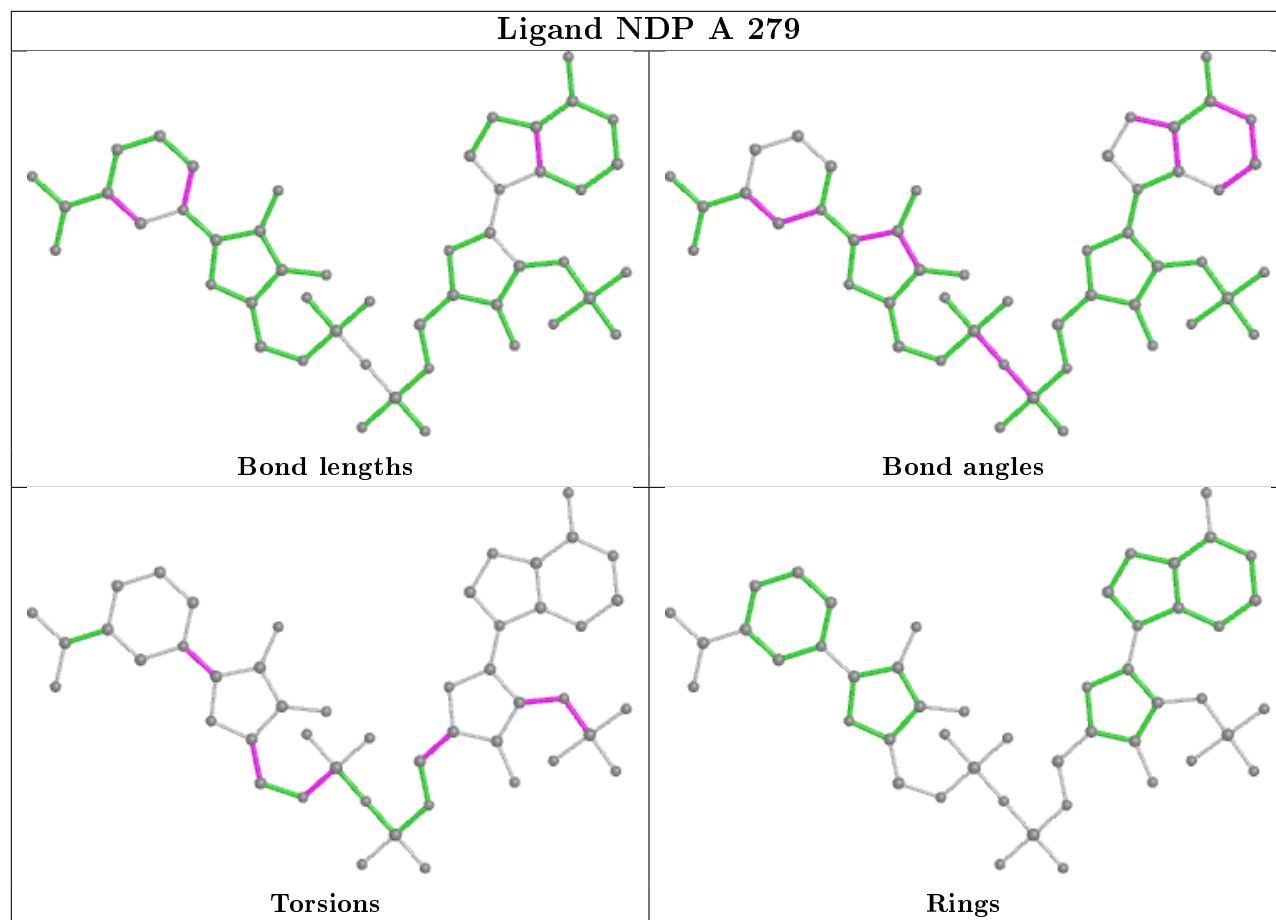
There are no ring outliers.

No monomer is involved in short contacts.

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	268/302 (88%)	0.33	15 (5%) 24 23	36, 50, 67, 80	0
1	B	269/302 (89%)	0.35	14 (5%) 27 26	35, 52, 70, 76	0
1	C	244/302 (80%)	0.81	30 (12%) 4 3	41, 63, 91, 103	0
1	D	272/302 (90%)	0.66	18 (6%) 18 17	39, 59, 83, 95	0
All	All	1053/1208 (87%)	0.53	77 (7%) 15 13	35, 55, 85, 103	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	196	LEU	6.8
1	D	273	ASN	5.4
1	C	220	GLY	5.1
1	C	179	GLU	4.7
1	D	274	LEU	4.5
1	A	198	GLY	4.2
1	C	203	ILE	4.0
1	C	154	ASN	4.0
1	A	196	LEU	4.0
1	C	210	SER	3.9
1	C	274	LEU	3.9
1	D	182	LYS	3.8
1	C	275	GLU	3.8
1	C	157	PHE	3.7
1	D	78	ARG	3.6
1	B	118	GLN	3.6
1	C	170	TYR	3.6
1	A	195	SER	3.5
1	C	204	ASP	3.4
1	A	189	ILE	3.4
1	D	272	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	180	GLN	3.3
1	C	17	HIS	3.2
1	C	208	PHE	3.2
1	C	218	MET	3.2
1	A	197	ASP	3.2
1	D	265	GLN	3.0
1	B	120	LEU	3.0
1	D	58	GLY	3.0
1	C	193	SER	2.9
1	D	99	GLU	2.7
1	D	96	ASP	2.7
1	B	44	VAL	2.7
1	B	45	ASP	2.7
1	C	158	ALA	2.7
1	D	84	ARG	2.6
1	C	176	GLN	2.6
1	C	49	GLU	2.6
1	C	178	PHE	2.6
1	A	156	THR	2.6
1	C	202	ALA	2.5
1	C	63	ASN	2.5
1	C	273	ASN	2.5
1	B	53	HIS	2.5
1	B	211	ARG	2.5
1	C	272	LYS	2.5
1	A	188	ILE	2.5
1	C	5	ILE	2.5
1	A	264	LYS	2.4
1	A	10	VAL	2.4
1	C	62	CYS	2.4
1	C	155	ARG	2.4
1	D	167	VAL	2.4
1	D	217	MET	2.3
1	B	58	GLY	2.3
1	D	259	LEU	2.3
1	C	78	ARG	2.3
1	D	73	TYR	2.3
1	B	94	LYS	2.2
1	A	265	GLN	2.2
1	C	265	GLN	2.2
1	A	45	ASP	2.2
1	D	211	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	57	GLN	2.2
1	B	138	VAL	2.2
1	D	169	ALA	2.2
1	D	95	LEU	2.2
1	C	37	TYR	2.1
1	D	81	GLU	2.1
1	A	96	ASP	2.1
1	B	122	LYS	2.1
1	B	189	ILE	2.1
1	B	39	ALA	2.1
1	B	107	GLY	2.1
1	A	78	ARG	2.0
1	C	131	ALA	2.0
1	A	276	GLY	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](#)

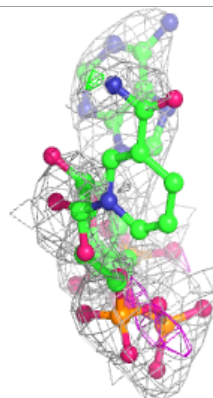
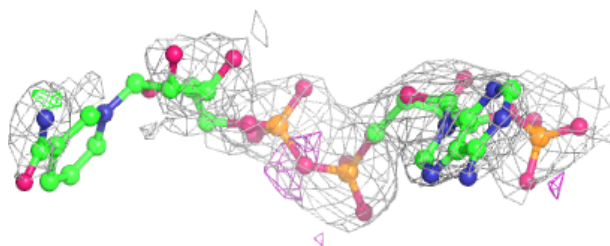
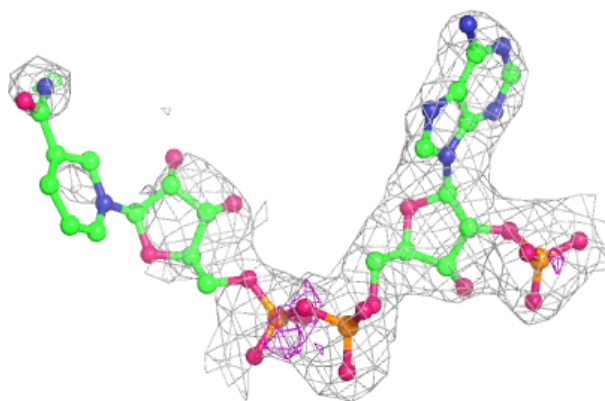
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SKM	B	280	12/12	0.74	0.34	77,80,86,86	0
2	NDP	A	279	48/48	0.86	0.23	80,93,121,123	0
3	SKM	C	279	12/12	0.87	0.36	71,78,85,91	0
2	NDP	B	279	48/48	0.88	0.20	54,76,107,112	0

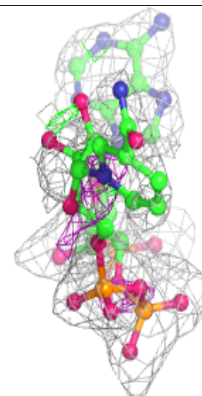
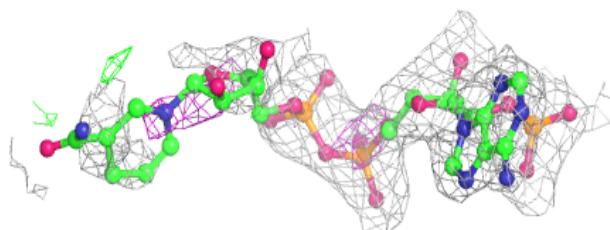
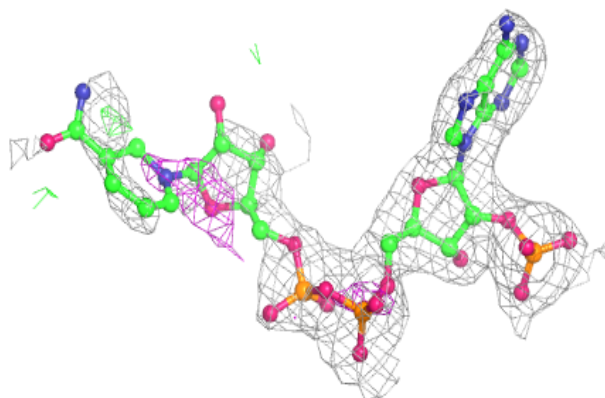
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP A 279:

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

**Electron density around NDP B 279:**

$2mF_o-DF_c$ (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.