



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:11 AM UTC

PDB ID : 3FSY / pdb_00003fsy
Title : Structure of tetrahydrodipicolinate N-succinyltransferase (Rv1201c;DapD) in complex with succinyl-CoA from Mycobacterium tuberculosis
Authors : Schuldt, L.; Weyand, S.; Kefala, G.; Weiss, M.S.
Deposited on : 2009-01-12
Resolution : 1.97 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

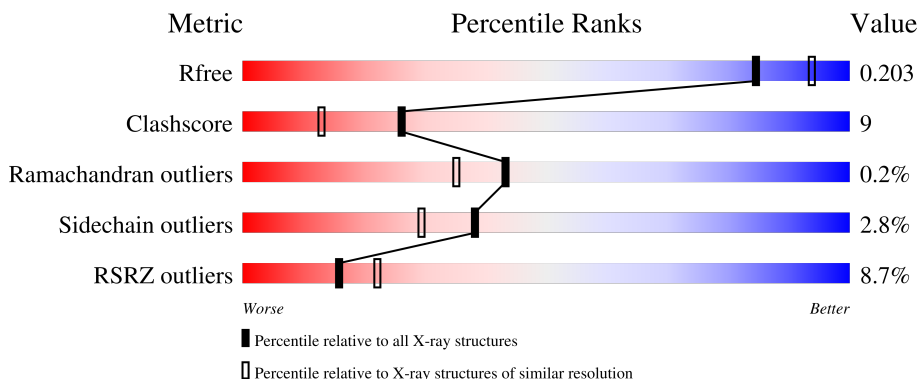
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	332	3% 82% 9% 8%
1	B	332	5% 80% 10% 8%
1	C	332	3% 80% 8% 11%
1	D	332	6% 81% 11% 7%
1	E	332	24% 71% 18% 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
6	ACY	B	332	-	-	X	-
6	ACY	C	331	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11992 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 Tetrahydrodipicolinate N-succinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	1	0
			2206	1370	402	426	8			
1	B	307	Total	C	N	O	S	0	3	0
			2229	1383	408	430	8			
1	C	297	Total	C	N	O	S	0	4	0
			2172	1351	397	416	8			
1	D	308	Total	C	N	O	S	0	6	0
			2247	1401	406	432	8			
1	E	301	Total	C	N	O	S	0	0	0
			2182	1355	399	420	8			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	expression tag	UNP O05302
A	0	ALA	-	expression tag	UNP O05302
A	1	VAL	-	expression tag	UNP O05302
A	318	GLY	-	expression tag	UNP O05302
A	319	VAL	-	expression tag	UNP O05302
A	320	PRO	-	expression tag	UNP O05302
A	321	ARG	-	expression tag	UNP O05302
A	322	GLY	-	expression tag	UNP O05302
A	323	LEU	-	expression tag	UNP O05302
A	324	GLU	-	expression tag	UNP O05302
A	325	HIS	-	expression tag	UNP O05302
A	326	HIS	-	expression tag	UNP O05302
A	327	HIS	-	expression tag	UNP O05302
A	328	HIS	-	expression tag	UNP O05302
A	329	HIS	-	expression tag	UNP O05302
A	330	HIS	-	expression tag	UNP O05302
B	-1	MET	-	expression tag	UNP O05302
B	0	ALA	-	expression tag	UNP O05302
B	1	VAL	-	expression tag	UNP O05302

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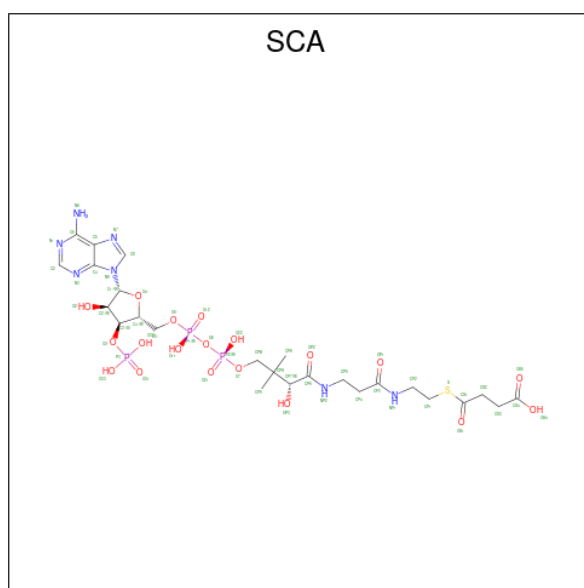
Chain	Residue	Modelled	Actual	Comment	Reference
B	318	GLY	-	expression tag	UNP O05302
B	319	VAL	-	expression tag	UNP O05302
B	320	PRO	-	expression tag	UNP O05302
B	321	ARG	-	expression tag	UNP O05302
B	322	GLY	-	expression tag	UNP O05302
B	323	LEU	-	expression tag	UNP O05302
B	324	GLU	-	expression tag	UNP O05302
B	325	HIS	-	expression tag	UNP O05302
B	326	HIS	-	expression tag	UNP O05302
B	327	HIS	-	expression tag	UNP O05302
B	328	HIS	-	expression tag	UNP O05302
B	329	HIS	-	expression tag	UNP O05302
B	330	HIS	-	expression tag	UNP O05302
C	-1	MET	-	expression tag	UNP O05302
C	0	ALA	-	expression tag	UNP O05302
C	1	VAL	-	expression tag	UNP O05302
C	318	GLY	-	expression tag	UNP O05302
C	319	VAL	-	expression tag	UNP O05302
C	320	PRO	-	expression tag	UNP O05302
C	321	ARG	-	expression tag	UNP O05302
C	322	GLY	-	expression tag	UNP O05302
C	323	LEU	-	expression tag	UNP O05302
C	324	GLU	-	expression tag	UNP O05302
C	325	HIS	-	expression tag	UNP O05302
C	326	HIS	-	expression tag	UNP O05302
C	327	HIS	-	expression tag	UNP O05302
C	328	HIS	-	expression tag	UNP O05302
C	329	HIS	-	expression tag	UNP O05302
C	330	HIS	-	expression tag	UNP O05302
D	-1	MET	-	expression tag	UNP O05302
D	0	ALA	-	expression tag	UNP O05302
D	1	VAL	-	expression tag	UNP O05302
D	318	GLY	-	expression tag	UNP O05302
D	319	VAL	-	expression tag	UNP O05302
D	320	PRO	-	expression tag	UNP O05302
D	321	ARG	-	expression tag	UNP O05302
D	322	GLY	-	expression tag	UNP O05302
D	323	LEU	-	expression tag	UNP O05302
D	324	GLU	-	expression tag	UNP O05302
D	325	HIS	-	expression tag	UNP O05302
D	326	HIS	-	expression tag	UNP O05302
D	327	HIS	-	expression tag	UNP O05302

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Chain	Residue	Modelled	Actual	Comment	Reference
D	328	HIS	-	expression tag	UNP O05302
D	329	HIS	-	expression tag	UNP O05302
D	330	HIS	-	expression tag	UNP O05302
E	-1	MET	-	expression tag	UNP O05302
E	0	ALA	-	expression tag	UNP O05302
E	1	VAL	-	expression tag	UNP O05302
E	318	GLY	-	expression tag	UNP O05302
E	319	VAL	-	expression tag	UNP O05302
E	320	PRO	-	expression tag	UNP O05302
E	321	ARG	-	expression tag	UNP O05302
E	322	GLY	-	expression tag	UNP O05302
E	323	LEU	-	expression tag	UNP O05302
E	324	GLU	-	expression tag	UNP O05302
E	325	HIS	-	expression tag	UNP O05302
E	326	HIS	-	expression tag	UNP O05302
E	327	HIS	-	expression tag	UNP O05302
E	328	HIS	-	expression tag	UNP O05302
E	329	HIS	-	expression tag	UNP O05302
E	330	HIS	-	expression tag	UNP O05302

- Molecule 2 is SUCCINYL-COENZYME A (CCD ID: SCA) (formula: $C_{25}H_{40}N_7O_{19}P_3S$).



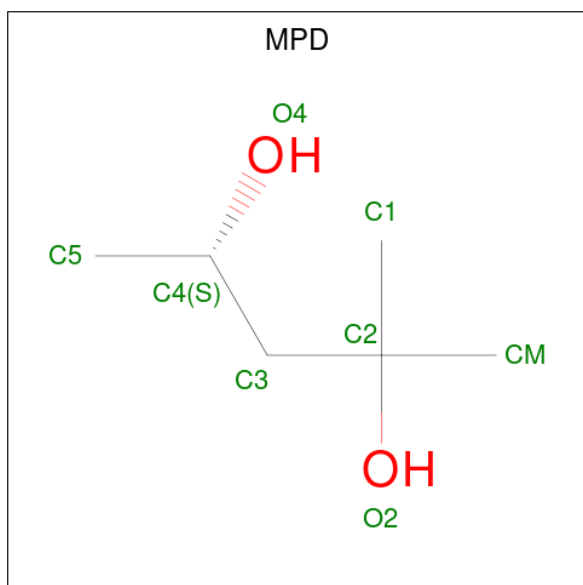
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	0	0	
			31	10	5	13	3			
2	A	1	Total	C	N	O	P	S	0	0
			55	25	7	19	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	B	1	Total	C	N	O	P	0	0	
			31	10	5	13	3			
2	E	1	Total	C	N	O	P	S	0	0
			52	23	7	18	3	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

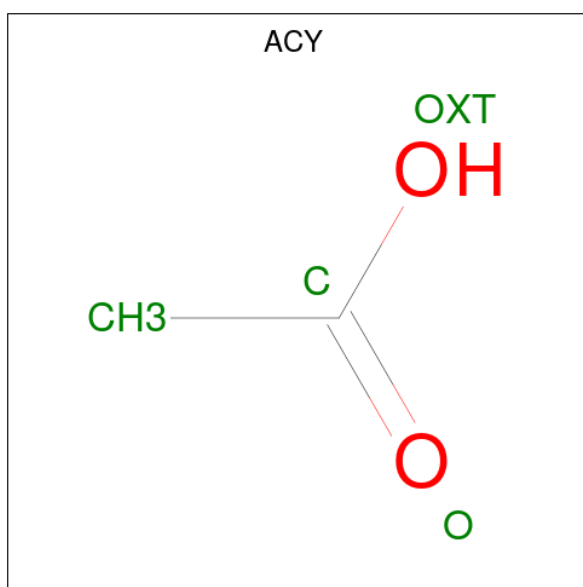
- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	Mg	0	0
			4	4		
4	B	1	Total	Mg	0	0
			1	1		
4	D	2	Total	Mg	0	0
			2	2		
4	E	3	Total	Mg	0	0
			3	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0
5	B	1	Total Na 1 1	0	0
5	D	1	Total Na 1 1	0	0
5	E	1	Total Na 1 1	0	0

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	C	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	176	Total O 176 176	0	0
7	B	174	Total O 174 174	0	0

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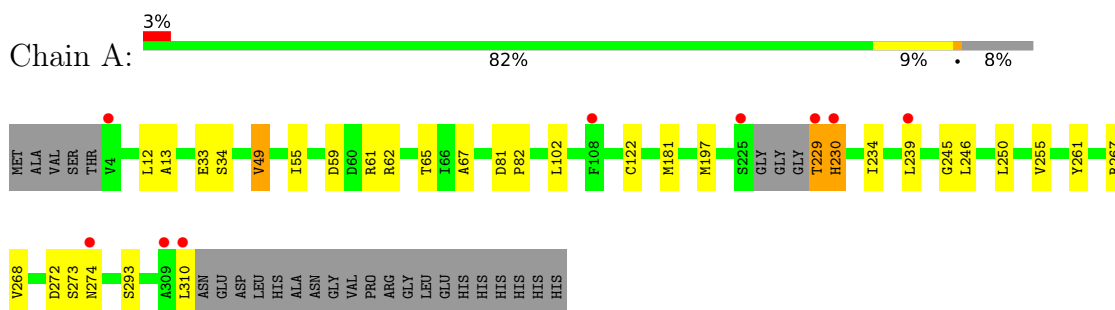
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	161	Total 161	O 161	0	0
7	D	203	Total 203	O 203	0	0
7	E	23	Total 23	O 23	0	0

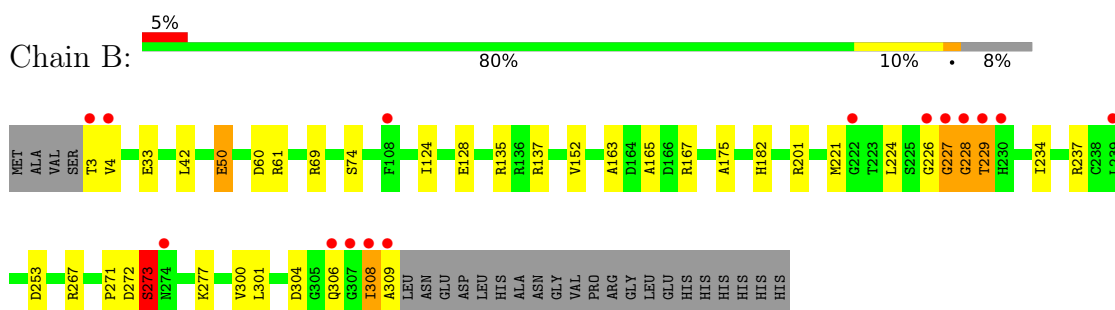
3 Residue-property plots [i](#)

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

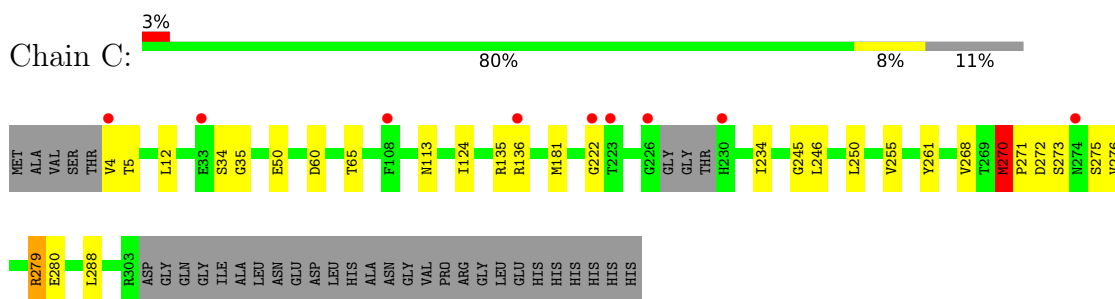
- Molecule 1: Tetrahydrodipicolinate N-succinyltransferase



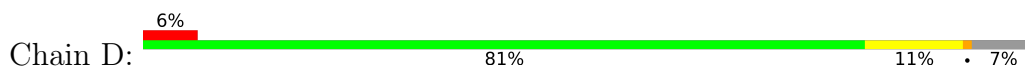
- Molecule 1: Tetrahydrodipicolinate N-succinyltransferase

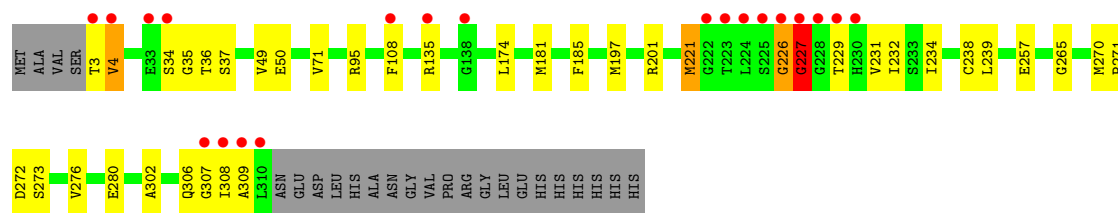


- Molecule 1: Tetrahydrodipicolinate N-succinyltransferase

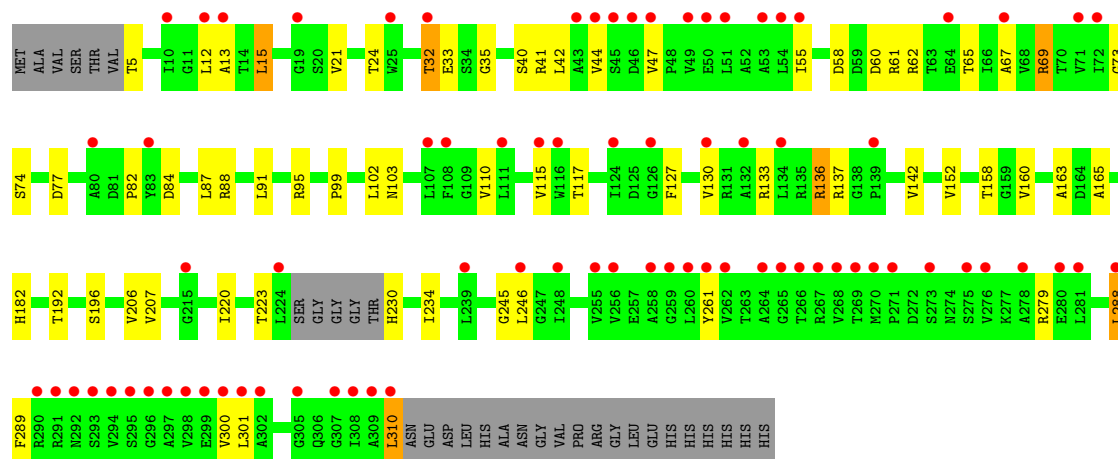


- Molecule 1: Tetrahydrodipicolinate N-succinyltransferase





● Molecule 1: Tetrahydrodipicolinate N-succinyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	216.96Å 216.96Å 216.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.97 30.00 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-1.97) 99.8 (30.00-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.161 , 0.200 0.163 , 0.203	Depositor DCC
R_{free} test set	1488 reflections (1.25%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11992	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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: MPD, SCA, NA, ACY, MG

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	1.06	0/2241	1.04	0/3049
1	B	1.09	1/2271 (0.0%)	1.14	6/3090 (0.2%)
1	C	0.99	0/2216	1.07	2/3014 (0.1%)
1	D	1.14	1/2301 (0.0%)	1.15	3/3131 (0.1%)
1	E	0.70	1/2214 (0.0%)	0.98	1/3011 (0.0%)
All	All	1.01	3/11243 (0.0%)	1.08	12/15295 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	115	VAL	CA-CB	6.03	1.60	1.53
1	B	175	ALA	CA-CB	5.39	1.61	1.53
1	D	265	GLY	C-O	-5.15	1.19	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	308	ILE	N-CA-C	8.36	122.32	109.12
1	B	124	ILE	CB-CA-C	-6.56	103.17	112.22
1	B	273	SER	N-CA-CB	-6.56	107.54	114.10
1	D	227	GLY	N-CA-C	-6.22	98.44	113.18
1	B	308	ILE	N-CA-C	5.93	116.71	110.72
1	B	61	ARG	NE-CZ-NH2	5.61	124.25	119.20
1	B	61	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	D	226	GLY	N-CA-C	5.50	126.21	113.18
1	B	167	ARG	CA-CB-CG	-5.50	103.11	114.10
1	C	270	MET	CA-C-N	5.23	125.29	119.32
1	C	270	MET	C-N-CA	5.23	125.29	119.32
1	E	127	PHE	N-CA-C	5.02	116.75	111.28

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	2206	0	2216	37	0
1	B	2229	0	2244	41	0
1	C	2172	0	2194	38	0
1	D	2247	0	2268	39	0
1	E	2182	0	2188	62	0
2	A	86	0	46	1	0
2	B	31	0	11	0	0
2	E	52	0	31	2	0
3	A	8	0	14	1	0
3	B	8	0	14	1	0
3	D	8	0	14	0	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	B	4	0	3	2	0
6	C	4	0	3	2	0
6	D	4	0	3	0	0
7	A	176	0	0	3	0
7	B	174	0	0	3	0
7	C	161	0	0	4	0
7	D	203	0	0	7	0
7	E	23	0	0	1	0
All	All	11992	0	11249	211	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 9.

All (211) 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:C:12:LEU:HD11	1:C:65[B]:THR:CG2	1.60	1.30
1:D:4:VAL:HG13	1:D:34:SER:CB	1.74	1.18
1:E:32:THR:HG22	1:E:33:GLU:O	1.42	1.16
1:C:12:LEU:CD1	1:C:65[B]:THR:CG2	2.25	1.14
1:D:4:VAL:CG1	1:D:34:SER:HB3	1.76	1.14
1:C:12:LEU:HD11	1:C:65[B]:THR:HG21	1.25	1.12
1:E:60:ASP:HB2	1:E:137:ARG:NH2	1.65	1.10
1:C:234:ILE:HD11	1:C:246:LEU:CD2	1.81	1.09
1:E:288:LEU:HD12	1:E:289:PHE:N	1.71	1.05
1:D:4:VAL:HG12	1:D:4:VAL:O	1.50	1.02
1:A:234:ILE:HD11	1:A:246:LEU:CD2	1.90	0.99
1:D:221:MET:HG3	1:D:232[B]:ILE:CD1	1.91	0.99
1:D:221:MET:HG3	1:D:232[B]:ILE:HD13	1.43	0.98
1:C:181:MET:HE3	7:C:549:HOH:O	1.62	0.98
1:C:135:ARG:HD2	7:C:415:HOH:O	1.66	0.95
1:D:4:VAL:CG1	1:D:4:VAL:O	2.14	0.95
1:E:288:LEU:HD12	1:E:288:LEU:C	1.90	0.94
1:D:4:VAL:HG13	1:D:34:SER:HB3	0.94	0.93
1:D:108[B]:PHE:CE1	7:D:489:HOH:O	2.21	0.92
1:E:234:ILE:HD11	1:E:246:LEU:CD2	2.00	0.92
1:E:32:THR:CG2	1:E:33:GLU:O	2.17	0.91
1:C:35:GLY:HA3	7:C:546:HOH:O	1.71	0.90
1:A:234:ILE:HD11	1:A:246:LEU:HD21	1.56	0.88
1:A:229:THR:O	1:A:229:THR:HG22	1.76	0.84
1:D:276:VAL:CG2	1:D:280:GLU:CD	2.50	0.84
1:C:272:ASP:O	1:C:273:SER:HB2	1.78	0.82
1:C:12:LEU:CD1	1:C:65[B]:THR:HG23	2.09	0.82
1:C:234:ILE:HD11	1:C:246:LEU:HD21	1.61	0.82
6:B:332:ACY:H1	7:B:493:HOH:O	1.79	0.81
1:B:308:ILE:O	1:B:309:ALA:CB	2.27	0.80
1:D:108[B]:PHE:CZ	7:D:489:HOH:O	2.32	0.80
1:E:300:VAL:C	1:E:301:LEU:HD12	2.06	0.80
1:B:267[B]:ARG:NH2	1:B:277:LYS:HE3	1.96	0.79
1:D:226:GLY:C	1:D:227:GLY:O	2.25	0.78
1:B:272:ASP:O	1:B:273:SER:CB	2.33	0.77
1:C:4:VAL:CG1	1:C:5:THR:H	1.99	0.76
1:C:276[A]:VAL:CG1	1:C:280:GLU:CD	2.59	0.76
1:C:12:LEU:HD11	1:C:65[B]:THR:HG22	1.64	0.75
1:C:12:LEU:HD13	1:C:65[B]:THR:HG23	1.69	0.75
1:D:276:VAL:HG23	1:D:280:GLU:OE2	1.88	0.74
1:C:12:LEU:HD13	1:C:65[B]:THR:CG2	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:310:LEU:N	1:E:310:LEU:HD12	2.03	0.74
1:E:55:ILE:HD11	1:E:67:ALA:HB2	1.69	0.72
1:E:301:LEU:HD12	1:E:301:LEU:N	2.05	0.72
1:E:60:ASP:CB	1:E:137:ARG:NH2	2.48	0.72
6:C:331:ACY:H1	7:C:493:HOH:O	1.90	0.71
1:D:238:CYS:O	1:D:239:LEU:HD23	1.91	0.71
1:B:301:LEU:HD12	1:B:301:LEU:N	2.05	0.70
1:D:181:MET:HE3	7:D:556:HOH:O	1.90	0.70
1:D:276:VAL:HG23	1:D:280:GLU:CD	2.17	0.70
1:E:288:LEU:C	1:E:288:LEU:CD1	2.65	0.70
1:D:108[B]:PHE:HE1	7:D:489:HOH:O	1.67	0.69
1:A:230:HIS:ND1	1:A:230:HIS:N	2.41	0.69
1:B:272:ASP:O	1:B:273:SER:HB2	1.92	0.69
1:C:12:LEU:CD1	1:C:65[B]:THR:HG22	2.19	0.68
1:A:49:VAL:HG13	7:A:508:HOH:O	1.92	0.68
1:A:181:MET:HE3	7:A:585:HOH:O	1.93	0.68
1:D:309:ALA:HB2	7:D:595:HOH:O	1.93	0.68
1:C:4:VAL:HG13	1:C:5:THR:H	1.59	0.68
1:B:267[B]:ARG:HH21	1:B:277:LYS:HE3	1.58	0.67
1:A:239:LEU:HD23	1:B:224:LEU:CG	2.25	0.67
1:D:276:VAL:CG2	1:D:280:GLU:OE2	2.44	0.65
1:A:229:THR:O	1:A:229:THR:CG2	2.45	0.65
1:D:221:MET:HG3	1:D:232[B]:ILE:HD12	1.79	0.65
1:A:239:LEU:CD2	1:B:224:LEU:HG	2.27	0.64
1:C:276[A]:VAL:HG13	1:C:280:GLU:CD	2.22	0.64
1:C:234:ILE:HD11	1:C:246:LEU:HD23	1.74	0.63
1:C:4:VAL:CG1	1:C:5:THR:N	2.59	0.63
1:B:271:PRO:HD2	1:B:308:ILE:CD1	2.29	0.63
1:A:272:ASP:O	1:A:273:SER:OG	2.16	0.63
1:E:60:ASP:OD2	1:E:137:ARG:NE	2.32	0.62
1:E:35:GLY:O	1:E:73:GLY:HA3	2.00	0.62
1:C:60:ASP:OD1	1:C:136[B]:ARG:NH2	2.32	0.62
1:E:310:LEU:HD12	1:E:310:LEU:H	1.64	0.62
1:E:32:THR:CG2	1:E:33:GLU:N	2.62	0.61
1:E:301:LEU:N	1:E:301:LEU:CD1	2.62	0.61
1:A:267:ARG:HD2	7:A:571:HOH:O	2.00	0.61
1:B:308:ILE:O	1:B:309:ALA:HB2	2.00	0.61
1:D:3:THR:HG22	1:D:3:THR:O	2.01	0.61
1:D:50:GLU:H	1:D:50:GLU:CD	2.09	0.60
1:B:50:GLU:H	1:B:50:GLU:CD	2.08	0.60
1:E:60:ASP:HB2	1:E:137:ARG:HH21	1.64	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:331:SCA:H4'	2:E:331:SCA:O31	2.02	0.60
1:B:308:ILE:O	1:B:309:ALA:HB3	2.01	0.59
1:D:272:ASP:O	1:D:273:SER:CB	2.50	0.59
1:B:271:PRO:CD	1:B:308:ILE:CD1	2.81	0.58
1:E:234:ILE:HD11	1:E:246:LEU:HD23	1.80	0.58
1:A:239:LEU:HD23	1:B:224:LEU:HG	1.83	0.58
1:E:152:VAL:HG21	1:E:165:ALA:HB1	1.85	0.58
1:B:227:GLY:HA2	7:B:525:HOH:O	2.03	0.58
1:C:4:VAL:O	1:C:34:SER:HB3	2.04	0.57
1:E:84:ASP:O	1:E:88:ARG:HG3	2.05	0.57
1:E:95:ARG:NH1	1:E:158:THR:O	2.23	0.56
1:A:12:LEU:HG	1:A:65[A]:THR:CG2	2.35	0.56
1:B:271:PRO:HD2	1:B:308:ILE:HD12	1.86	0.56
1:A:239:LEU:CD2	1:B:224:LEU:HD21	2.37	0.55
1:E:130:VAL:HG22	1:E:133:ARG:NH2	2.20	0.54
1:A:239:LEU:HD23	1:B:224:LEU:HD11	1.89	0.54
1:E:55:ILE:HD11	1:E:67:ALA:CB	2.35	0.54
1:E:62:ARG:NH1	1:E:62:ARG:HG2	2.22	0.54
1:E:87:LEU:O	1:E:91:LEU:HG	2.08	0.54
1:E:133:ARG:O	1:E:136:ARG:HD3	2.09	0.53
1:A:81:ASP:HB2	1:A:82:PRO:CD	2.38	0.53
1:E:234:ILE:HD11	1:E:246:LEU:HD21	1.87	0.53
1:E:223:THR:HB	1:E:230:HIS:O	2.08	0.53
1:B:300:VAL:C	1:B:301:LEU:HD12	2.34	0.53
1:C:4:VAL:HG12	1:C:5:THR:N	2.24	0.53
1:B:33:GLU:H	1:B:33:GLU:CD	2.16	0.52
1:C:234:ILE:HD12	1:C:250:LEU:HD12	1.91	0.52
1:B:42:LEU:HD21	1:B:69:ARG:HB2	1.92	0.52
1:E:58:ASP:OD2	1:E:61:ARG:HD3	2.09	0.52
1:A:255:VAL:HG13	1:B:224:LEU:HD11	1.92	0.52
1:B:271:PRO:CD	1:B:308:ILE:HD11	2.40	0.52
1:B:237:ARG:NH2	1:B:253:ASP:OD2	2.42	0.51
1:E:42:LEU:HD11	1:E:69:ARG:HB3	1.91	0.51
1:A:239:LEU:HD23	1:B:224:LEU:CD1	2.41	0.51
1:E:245:GLY:HA3	1:E:261:TYR:CD1	2.46	0.51
1:D:3:THR:O	1:D:4:VAL:HB	2.12	0.50
1:C:234:ILE:CD1	1:C:246:LEU:HD21	2.37	0.50
1:A:234:ILE:HD12	1:A:250:LEU:HD12	1.94	0.50
1:E:62:ARG:HG2	1:E:62:ARG:HH11	1.77	0.49
1:A:239:LEU:CD2	1:B:224:LEU:CG	2.88	0.49
1:E:117:THR:HG22	1:E:142:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HD11	1:A:246:LEU:HD22	1.86	0.49
1:E:35:GLY:O	1:E:73:GLY:CA	2.60	0.49
1:E:69:ARG:O	1:E:69:ARG:HG3	2.13	0.49
1:E:152:VAL:HG21	1:E:165:ALA:CB	2.43	0.49
1:B:227:GLY:O	1:B:229:THR:N	2.46	0.49
1:E:12:LEU:HG	1:E:65:THR:CG2	2.43	0.49
1:A:239:LEU:HD21	1:B:224:LEU:HG	1.94	0.49
1:B:304:ASP:OD1	1:B:306:GLN:N	2.36	0.49
1:A:33:GLU:HG2	1:A:34:SER:N	2.28	0.48
1:E:102:LEU:C	1:E:102:LEU:HD12	2.38	0.48
1:E:310:LEU:N	1:E:310:LEU:CD1	2.74	0.48
1:E:60:ASP:CG	1:E:137:ARG:HH21	2.22	0.47
1:C:234:ILE:CD1	1:C:246:LEU:CD2	2.74	0.47
1:D:95:ARG:HD3	1:D:174:LEU:O	2.15	0.47
1:E:32:THR:HG22	1:E:33:GLU:N	2.30	0.47
1:E:60:ASP:CB	1:E:137:ARG:HH21	2.25	0.47
1:D:221:MET:CG	1:D:232[B]:ILE:CD1	2.80	0.47
1:E:13:ALA:O	1:E:65:THR:HA	2.15	0.47
1:A:310:LEU:HD22	1:A:310:LEU:N	2.29	0.47
1:A:59:ASP:O	1:A:62:ARG:HD3	2.15	0.47
1:D:49:VAL:HG23	1:D:50:GLU:OE2	2.15	0.47
1:E:60:ASP:HB2	1:E:137:ARG:HH22	1.71	0.47
1:C:234:ILE:HD11	1:C:246:LEU:HD22	1.89	0.46
1:E:44:VAL:HA	1:E:47:VAL:HG23	1.97	0.46
1:A:272:ASP:OD1	1:A:272:ASP:C	2.58	0.46
1:B:152:VAL:HG21	1:B:165:ALA:HB1	1.97	0.46
1:B:226:GLY:HA2	1:D:306:GLN:HG3	1.97	0.46
1:C:222:GLY:HA2	6:C:331:ACY:H3	1.97	0.46
1:C:272:ASP:O	1:C:273:SER:CB	2.53	0.46
1:A:197:MET:HE2	1:A:197:MET:HB2	1.81	0.46
1:A:239:LEU:CD2	1:B:224:LEU:CD2	2.94	0.46
1:E:152:VAL:CG2	1:E:165:ALA:HB1	2.46	0.45
1:E:192:THR:HG21	1:E:196:SER:HB2	1.98	0.45
1:A:102:LEU:C	1:A:102:LEU:HD12	2.42	0.45
1:C:255:VAL:HB	1:C:288:LEU:HD12	1.99	0.45
1:C:270:MET:HB3	1:C:271:PRO:HD2	1.99	0.45
1:D:35:GLY:HA3	7:D:604:HOH:O	2.16	0.45
1:D:270:MET:HB3	1:D:271:PRO:CD	2.47	0.45
1:E:206:VAL:HG11	1:E:220:ILE:HG21	1.99	0.45
1:D:37:SER:HA	1:D:71:VAL:O	2.17	0.44
1:E:99:PRO:HG2	1:E:207:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276[A]:VAL:CG1	1:C:280:GLU:HB2	2.47	0.44
1:B:4:VAL:HG11	1:B:74:SER:HB2	1.98	0.44
1:D:272:ASP:O	1:D:273:SER:HB3	2.18	0.44
1:D:276:VAL:HG22	1:D:280:GLU:CD	2.40	0.44
3:A:340:MPD:HM3	1:B:128:GLU:HG3	1.99	0.44
1:E:152:VAL:HG22	7:E:402:HOH:O	2.18	0.44
1:A:61:ARG:HG2	1:A:122:CYS:SG	2.58	0.44
1:B:60:ASP:OD2	1:B:137:ARG:NH2	2.46	0.44
1:E:15:LEU:N	1:E:15:LEU:CD1	2.80	0.44
1:E:77:ASP:O	1:E:103:ASN:HB3	2.18	0.44
1:E:288:LEU:CD1	1:E:289:PHE:N	2.62	0.44
1:A:293:SER:N	2:A:331:SCA:N1	2.63	0.44
3:B:340:MPD:HM2	3:B:340:MPD:H4	1.86	0.44
1:A:12:LEU:HD11	1:A:65[A]:THR:HG22	2.00	0.43
1:E:69:ARG:HE	1:E:69:ARG:HB2	1.38	0.43
1:E:163:ALA:HB1	1:E:182:HIS:CE1	2.53	0.43
1:D:270:MET:HE3	1:D:270:MET:HB2	1.74	0.43
1:B:227:GLY:O	1:B:228:GLY:C	2.61	0.43
2:E:331:SCA:O31	2:E:331:SCA:C4'	2.63	0.43
1:A:12:LEU:CD1	1:A:65[A]:THR:HG22	2.49	0.43
1:C:113:ASN:ND2	1:C:124:ILE:HD11	2.33	0.43
1:E:21:VAL:HB	1:E:82:PRO:HB2	2.01	0.42
1:C:245:GLY:HA3	1:C:261:TYR:CD1	2.53	0.42
1:D:36:THR:N	7:D:604:HOH:O	2.15	0.42
1:D:185:PHE:HB3	1:D:201:ARG:HG2	2.01	0.42
1:D:197:MET:HB2	1:D:197:MET:HE2	1.60	0.42
1:D:221:MET:CG	1:D:232[B]:ILE:HD12	2.49	0.42
1:E:245:GLY:HA3	1:E:261:TYR:CE1	2.55	0.42
1:A:13:ALA:O	1:A:65[A]:THR:HA	2.20	0.42
1:D:226:GLY:O	1:D:227:GLY:C	2.59	0.42
1:A:245:GLY:HA3	1:A:261:TYR:CD1	2.55	0.41
1:B:163:ALA:HB1	1:B:182:HIS:CE1	2.54	0.41
1:C:268:VAL:O	1:C:275:SER:HA	2.20	0.41
1:C:270:MET:CB	1:C:271:PRO:CD	2.98	0.41
1:B:201:ARG:HE	6:B:332:ACY:C	2.32	0.41
1:E:12:LEU:O	1:E:24:THR:HA	2.20	0.41
1:E:61:ARG:O	1:E:62:ARG:HB2	2.19	0.41
1:B:301:LEU:N	1:B:301:LEU:CD1	2.78	0.41
1:E:95:ARG:NH1	1:E:160:VAL:HG23	2.35	0.41
1:C:276[A]:VAL:HG13	1:C:280:GLU:OE2	2.21	0.41
1:B:152:VAL:CG2	1:B:165:ALA:HB1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:MET:HE3	7:B:566:HOH:O	2.20	0.40
1:C:279:ARG:HH11	1:C:279:ARG:HD2	1.76	0.40
1:A:55:ILE:HD11	1:A:67:ALA:HB2	2.03	0.40
1:A:272:ASP:CG	1:A:274:ASN:HD22	2.30	0.40
1:E:99:PRO:HB2	1:E:207:VAL:CG2	2.51	0.40
1:D:302:ALA:CB	1:D:307:GLY:H	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	301/332 (91%)	295 (98%)	6 (2%)	0	100	100
1	B	308/332 (93%)	298 (97%)	8 (3%)	2 (1%)	21	12
1	C	297/332 (90%)	293 (99%)	4 (1%)	0	100	100
1	D	312/332 (94%)	303 (97%)	8 (3%)	1 (0%)	36	27
1	E	297/332 (90%)	292 (98%)	5 (2%)	0	100	100
All	All	1515/1660 (91%)	1481 (98%)	31 (2%)	3 (0%)	43	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	GLY
1	B	228	GLY
1	D	227	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	231/251 (92%)	227 (98%)	4 (2%)	53	48
1	B	233/251 (93%)	227 (97%)	6 (3%)	40	32
1	C	229/251 (91%)	226 (99%)	3 (1%)	61	57
1	D	237/251 (94%)	229 (97%)	8 (3%)	32	22
1	E	227/251 (90%)	215 (95%)	12 (5%)	20	9
All	All	1157/1255 (92%)	1124 (97%)	33 (3%)	38	28

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	229	THR
1	A	230	HIS
1	A	268	VAL
1	B	3	THR
1	B	50	GLU
1	B	135	ARG
1	B	229	THR
1	B	234	ILE
1	B	273	SER
1	C	50	GLU
1	C	270	MET
1	C	279	ARG
1	D	4	VAL
1	D	135	ARG
1	D	221	MET
1	D	229	THR
1	D	231	VAL
1	D	234[A]	ILE
1	D	234[B]	ILE
1	D	257	GLU
1	E	5	THR
1	E	15	LEU

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Mol	Chain	Res	Type
1	E	32	THR
1	E	40	SER
1	E	41	ARG
1	E	69	ARG
1	E	74	SER
1	E	110	VAL
1	E	136	ARG
1	E	279	ARG
1	E	288	LEU
1	E	310	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	B	230	HIS
1	C	286	ASN
1	D	230	HIS
1	D	286	ASN
1	E	182	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 14 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SCA	B	331	-	32,33,57	1.51	5 (15%)	50,52,84	1.72	10 (20%)
3	MPD	D	340	-	7,7,7	0.46	0	9,10,10	0.75	0
2	SCA	E	331	-	50,53,57	1.27	5 (10%)	72,78,84	1.63	10 (13%)
3	MPD	B	340	-	7,7,7	0.37	0	9,10,10	0.79	0
6	ACY	B	332	-	3,3,3	0.94	0	3,3,3	0.06	0
6	ACY	D	331	-	3,3,3	1.09	0	3,3,3	1.04	0
2	SCA	A	332	-	55,57,57	1.53	7 (12%)	78,84,84	1.95	20 (25%)
6	ACY	C	331	-	3,3,3	0.81	0	3,3,3	0.71	0
2	SCA	A	331	-	32,33,57	1.42	6 (18%)	50,52,84	1.81	12 (24%)
3	MPD	A	340	-	7,7,7	0.29	0	9,10,10	0.51	0

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	SCA	B	331	-	-	5/21/37/72	0/3/3/3
3	MPD	D	340	-	-	2/5/5/5	-
2	SCA	E	331	-	-	14/48/64/72	0/3/3/3
3	MPD	B	340	-	-	1/5/5/5	-
2	SCA	A	332	-	-	7/56/72/72	0/3/3/3
2	SCA	A	331	-	-	14/21/37/72	0/3/3/3
3	MPD	A	340	-	-	2/5/5/5	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	331	SCA	C5-C4	4.96	1.47	1.39
2	A	332	SCA	C5-C4	4.90	1.47	1.39
2	E	331	SCA	C5-C4	4.79	1.47	1.39
2	A	331	SCA	C5-C4	4.59	1.47	1.39
2	A	332	SCA	CS2-CS1	4.24	1.55	1.50
2	A	332	SCA	P3-O3'	4.22	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	332	SCA	CS1-S	-3.62	1.67	1.76
2	A	332	SCA	C4-N9	-2.96	1.31	1.37
2	E	331	SCA	C5-C6	2.90	1.49	1.41
2	A	332	SCA	C5-N7	-2.82	1.33	1.39
2	B	331	SCA	C5-C6	2.81	1.48	1.41
2	A	332	SCA	C8-N7	2.53	1.36	1.31
2	A	331	SCA	C5-N7	-2.42	1.34	1.39
2	E	331	SCA	C8-N7	2.42	1.36	1.31
2	A	331	SCA	C8-N7	2.42	1.36	1.31
2	B	331	SCA	C8-N7	2.35	1.36	1.31
2	A	331	SCA	P1-O6	2.34	1.62	1.59
2	B	331	SCA	P3-O3'	2.32	1.63	1.59
2	E	331	SCA	P3-O3'	2.26	1.63	1.59
2	A	331	SCA	C5-C6	2.17	1.47	1.41
2	B	331	SCA	C5-N7	-2.15	1.35	1.39
2	E	331	SCA	P2-O6	2.13	1.61	1.59
2	A	331	SCA	P3-O3'	2.09	1.63	1.59

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	332	SCA	OS1-CS1-S	-5.95	115.12	122.68
2	E	331	SCA	C5-C4-N3	-5.80	118.72	126.72
2	B	331	SCA	C5-C4-N3	-5.54	119.09	126.72
2	A	332	SCA	CS3-CS2-CS1	5.32	120.41	112.41
2	A	331	SCA	C5-C4-N3	-5.17	119.60	126.72
2	E	331	SCA	N3-C4-N9	5.09	135.82	127.17
2	A	331	SCA	N3-C4-N9	4.72	135.20	127.17
2	A	332	SCA	C4-N9-C8	4.63	110.60	105.74
2	A	332	SCA	N3-C4-N9	4.38	134.62	127.17
2	A	332	SCA	CS2-CS1-S	4.36	118.60	113.40
2	A	332	SCA	CP9-CPA-CP7	4.27	116.05	108.77
2	A	332	SCA	C5-C4-N3	-4.26	120.85	126.72
2	B	331	SCA	C4-C5-N7	-4.06	105.94	110.58
2	B	331	SCA	N3-C4-N9	4.02	134.00	127.17
2	A	331	SCA	N1-C2-N3	-3.73	122.94	128.58
2	E	331	SCA	N1-C2-N3	-3.70	122.99	128.58
2	E	331	SCA	C4-N9-C8	3.62	109.54	105.74
2	A	331	SCA	C4-N9-C8	3.61	109.53	105.74
2	E	331	SCA	C2-N3-C4	3.55	120.51	111.83
2	A	332	SCA	N1-C2-N3	-3.53	123.24	128.58
2	E	331	SCA	C4-C5-N7	-3.49	106.59	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	331	SCA	C2-N3-C4	3.39	120.11	111.83
2	A	331	SCA	C2-N3-C4	3.35	120.01	111.83
2	B	331	SCA	N1-C2-N3	-3.31	123.58	128.58
2	A	332	SCA	C2-N3-C4	3.07	119.32	111.83
2	E	331	SCA	C5-N7-C8	2.92	108.04	103.45
2	B	331	SCA	O22-P2-O21	2.75	121.56	110.83
2	A	332	SCA	N9-C8-N7	-2.74	110.05	113.94
2	A	332	SCA	N6-C6-N1	2.69	124.38	118.38
2	A	331	SCA	C4-C5-N7	-2.67	107.53	110.58
2	B	331	SCA	C5-N7-C8	2.67	107.64	103.45
2	A	332	SCA	O22-P2-O21	2.57	124.41	112.44
2	E	331	SCA	C2-N1-C6	2.56	122.94	118.73
2	A	331	SCA	C2-N1-C6	2.53	122.88	118.73
2	E	331	SCA	N9-C8-N7	-2.52	110.36	113.94
2	A	331	SCA	N9-C8-N7	-2.48	110.42	113.94
2	A	331	SCA	C5-N7-C8	2.46	107.31	103.45
2	A	331	SCA	N6-C6-N1	2.43	123.80	118.38
2	A	332	SCA	O6-P1-O12	-2.42	103.41	110.70
2	A	331	SCA	O22-P2-O21	2.37	120.06	110.83
2	A	332	SCA	CP1-S-CS1	2.33	108.73	101.84
2	B	331	SCA	O4'-C1'-N9	2.32	112.55	108.09
2	B	331	SCA	C6-C5-N7	2.30	136.52	132.09
2	A	332	SCA	C2-N1-C6	2.28	122.47	118.73
2	A	332	SCA	CP5-CP4-CP3	-2.26	108.64	112.39
2	A	331	SCA	O3'-P3-O31	-2.15	101.67	109.33
2	B	331	SCA	C2-N1-C6	2.15	122.26	118.73
2	A	332	SCA	C5-C6-N6	-2.10	118.09	123.29
2	A	332	SCA	CP5-NP2-CP6	-2.10	118.78	122.55
2	A	332	SCA	O33-P3-O32	2.09	115.64	107.80
2	E	331	SCA	CP9-CPA-CP7	2.05	112.27	108.77
2	A	332	SCA	C4-C5-N7	-2.04	108.25	110.58

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	331	SCA	C5'-O5'-P1-O11
2	A	331	SCA	C5'-O5'-P1-O12
2	A	331	SCA	C5'-O5'-P1-O6
2	A	331	SCA	P1-O6-P2-O22
2	A	332	SCA	C5'-O5'-P1-O11
2	A	332	SCA	C5'-O5'-P1-O6

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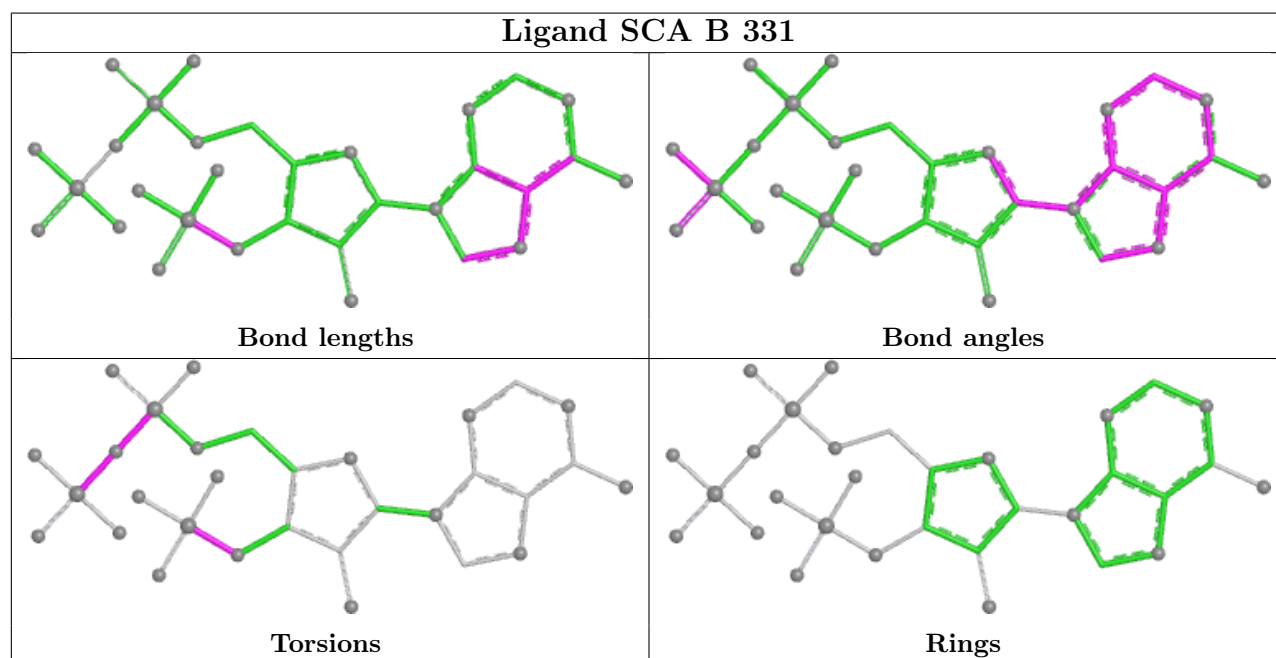
Mol	Chain	Res	Type	Atoms
2	B	331	SCA	P1-O6-P2-O22
2	E	331	SCA	C5'-O5'-P1-O11
2	E	331	SCA	C5'-O5'-P1-O6
2	E	331	SCA	CPB-O7-P2-O6
2	E	331	SCA	CP7-CPA-CPB-O7
2	E	331	SCA	CP9-CPA-CPB-O7
2	E	331	SCA	CP8-CPA-CPB-O7
2	E	331	SCA	CP7-CP6-NP2-CP5
2	E	331	SCA	CP3-CP4-CP5-NP2
2	E	331	SCA	OP2-CP6-NP2-CP5
2	A	331	SCA	C4'-C3'-O3'-P3
2	E	331	SCA	C2'-C3'-O3'-P3
2	E	331	SCA	C4'-C3'-O3'-P3
2	A	331	SCA	C2'-C3'-O3'-P3
2	A	331	SCA	C2'-C1'-N9-C8
2	A	331	SCA	C4'-C5'-O5'-P1
2	A	331	SCA	P1-O6-P2-O7
2	A	331	SCA	P2-O6-P1-O11
3	A	340	MPD	O2-C2-C3-C4
2	A	332	SCA	OP2-CP6-CP7-OP3
2	A	332	SCA	C5'-O5'-P1-O12
2	E	331	SCA	C5'-O5'-P1-O12
2	E	331	SCA	CPB-O7-P2-O21
2	B	331	SCA	P2-O6-P1-O11
2	A	331	SCA	C2'-C1'-N9-C4
2	B	331	SCA	C3'-O3'-P3-O33
2	B	331	SCA	C3'-O3'-P3-O31
2	A	331	SCA	P2-O6-P1-O12
2	A	332	SCA	P2-O6-P1-O5'
2	B	331	SCA	P1-O6-P2-O21
2	A	331	SCA	O4'-C1'-N9-C8
2	A	332	SCA	P1-O6-P2-O21
3	B	340	MPD	O2-C2-C3-C4
3	A	340	MPD	C2-C3-C4-O4
3	D	340	MPD	C2-C3-C4-O4
2	A	331	SCA	P1-O6-P2-O21
3	D	340	MPD	CM-C2-C3-C4
2	A	332	SCA	NP2-CP6-CP7-OP3
2	E	331	SCA	NP2-CP6-CP7-OP3

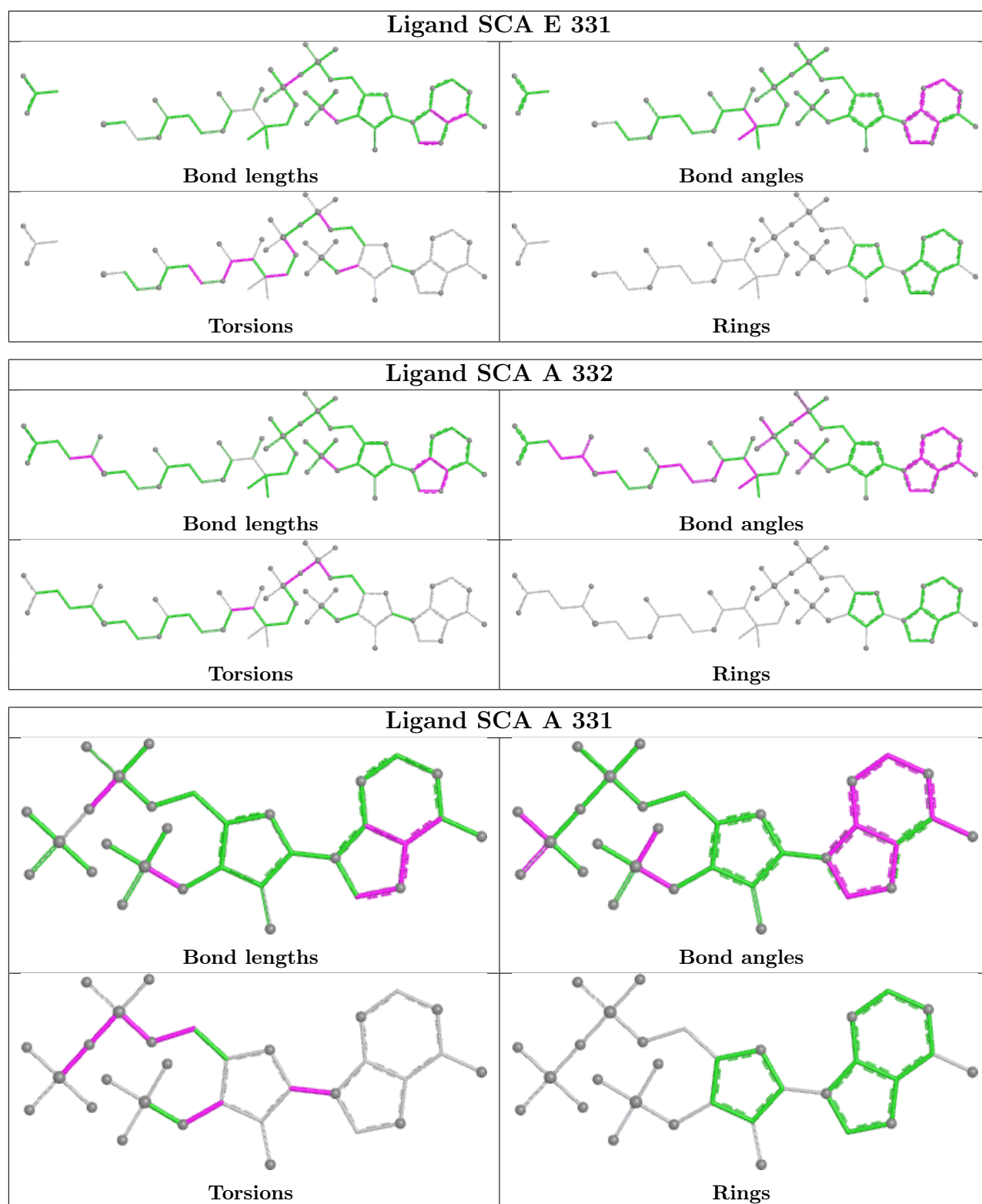
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	331	SCA	2	0
3	B	340	MPD	1	0
6	B	332	ACY	2	0
6	C	331	ACY	2	0
2	A	331	SCA	1	0
3	A	340	MPD	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	304/332 (91%)	0.25	9 (2%) 52 62	20, 32, 43, 59	1 (0%)
1	B	307/332 (92%)	0.25	15 (4%) 35 44	18, 32, 46, 69	3 (0%)
1	C	297/332 (89%)	0.44	9 (3%) 52 62	20, 32, 43, 60	4 (1%)
1	D	308/332 (92%)	0.40	20 (6%) 25 33	19, 32, 46, 75	6 (1%)
1	E	301/332 (90%)	1.55	79 (26%) 1 1	27, 33, 45, 69	0
All	All	1517/1660 (91%)	0.58	132 (8%) 16 22	18, 32, 45, 75	14 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	228	GLY	7.4
1	E	294	VAL	6.7
1	E	224	LEU	5.9
1	D	310	LEU	5.7
1	E	310	LEU	5.5
1	D	227	GLY	5.4
1	E	269	THR	5.4
1	E	297	ALA	5.0
1	E	296	GLY	5.0
1	D	309	ALA	4.7
1	B	228	GLY	4.6
1	B	309	ALA	4.6
1	A	309	ALA	4.6
1	E	55	ILE	4.5
1	D	226	GLY	4.4
1	E	305	GLY	4.4
1	E	268	VAL	4.4
1	B	227	GLY	4.3
1	E	260	LEU	4.3
1	E	276	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	108[A]	PHE	4.2
1	C	222	GLY	4.1
1	E	298	VAL	4.1
1	E	19	GLY	4.0
1	D	224	LEU	4.0
1	B	308	ILE	3.9
1	D	308	ILE	3.9
1	C	4	VAL	3.9
1	E	49	VAL	3.9
1	E	292	ASN	3.8
1	E	293	SER	3.8
1	E	300	VAL	3.8
1	D	229	THR	3.8
1	A	4	VAL	3.7
1	A	225	SER	3.6
1	D	3	THR	3.6
1	E	12	LEU	3.6
1	E	51	LEU	3.6
1	E	302	ALA	3.6
1	E	44	VAL	3.6
1	B	307	GLY	3.5
1	D	307	GLY	3.5
1	E	130	VAL	3.5
1	E	308	ILE	3.5
1	E	53	ALA	3.5
1	E	67	ALA	3.5
1	D	4	VAL	3.4
1	A	108	PHE	3.4
1	E	295	SER	3.4
1	E	271	PRO	3.4
1	E	259	GLY	3.3
1	E	266	THR	3.3
1	E	265	GLY	3.3
1	E	80	ALA	3.2
1	E	270	MET	3.1
1	E	307	GLY	3.1
1	E	46	ASP	3.1
1	B	306	GLN	3.0
1	E	54	LEU	3.0
1	B	229	THR	3.0
1	E	301	LEU	3.0
1	E	309	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	273	SER	2.9
1	E	83	TYR	2.9
1	E	248	ILE	2.9
1	E	291	ARG	2.8
1	E	132	ALA	2.8
1	E	10	ILE	2.8
1	B	3	THR	2.8
1	C	226	GLY	2.8
1	E	288	LEU	2.8
1	E	50	GLU	2.8
1	D	34	SER	2.7
1	E	261	TYR	2.7
1	C	230	HIS	2.7
1	A	310	LEU	2.7
1	E	239	LEU	2.7
1	E	116	TRP	2.6
1	E	290	ARG	2.6
1	E	107	LEU	2.6
1	E	115	VAL	2.6
1	D	230	HIS	2.5
1	E	108	PHE	2.5
1	E	256	VAL	2.5
1	E	134	LEU	2.5
1	C	274	ASN	2.5
1	E	278	ALA	2.5
1	D	222	GLY	2.5
1	E	264	ALA	2.5
1	E	258	ALA	2.4
1	E	299	GLU	2.4
1	D	223	THR	2.4
1	B	4	VAL	2.4
1	E	72	ILE	2.4
1	C	108	PHE	2.3
1	D	138	GLY	2.3
1	E	71	VAL	2.3
1	C	223	THR	2.3
1	E	246	LEU	2.3
1	B	108	PHE	2.2
1	B	222	GLY	2.2
1	E	13	ALA	2.2
1	E	215	GLY	2.2
1	E	255	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	239	LEU	2.2
1	D	33	GLU	2.2
1	B	230	HIS	2.2
1	E	47	VAL	2.2
1	A	239	LEU	2.2
1	D	135	ARG	2.2
1	E	111	LEU	2.2
1	E	126	GLY	2.2
1	E	280	GLU	2.1
1	E	124	ILE	2.1
1	E	25	TRP	2.1
1	A	230	HIS	2.1
1	B	226	GLY	2.1
1	A	274	ASN	2.1
1	B	274	ASN	2.1
1	C	136[A]	ARG	2.1
1	D	225	SER	2.1
1	E	32	THR	2.1
1	E	139	PRO	2.1
1	E	281	LEU	2.1
1	E	43	ALA	2.1
1	E	275	SER	2.0
1	A	229	THR	2.0
1	E	267	ARG	2.0
1	C	33	GLU	2.0
1	E	64	GLU	2.0
1	E	45	SER	2.0
1	E	262	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,

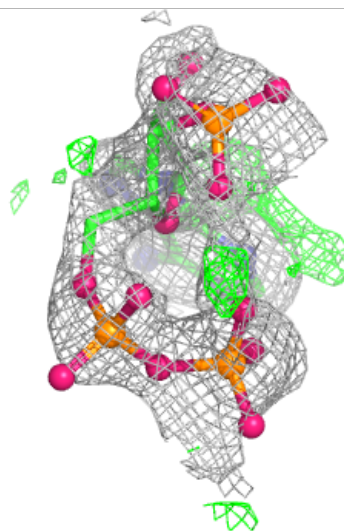
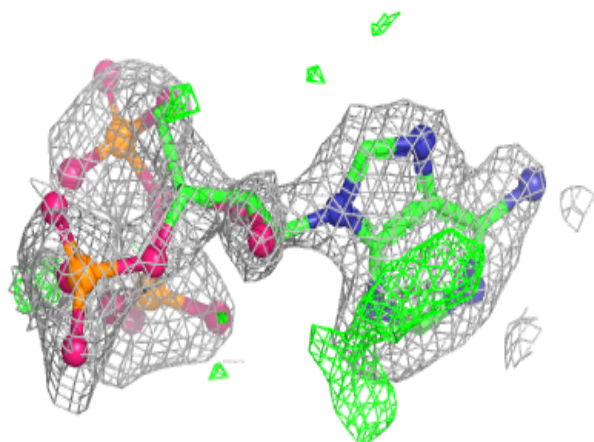
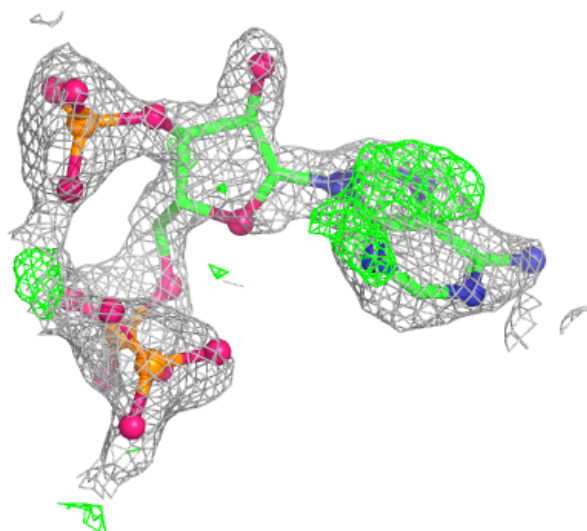
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SCA	A	331	31/55	0.79	0.17	26,41,53,55	31
2	SCA	B	331	31/55	0.82	0.15	23,38,50,55	31
2	SCA	E	331	52/55	0.86	0.12	38,57,68,73	0
3	MPD	B	340	8/8	0.88	0.15	28,43,51,52	0
4	MG	E	334	1/1	0.88	0.08	38,38,38,38	1
3	MPD	D	340	8/8	0.89	0.14	30,46,52,54	0
3	MPD	A	340	8/8	0.89	0.14	33,40,49,51	0
5	NA	E	335	1/1	0.89	0.26	29,29,29,29	1
5	NA	B	334	1/1	0.90	0.14	39,39,39,39	1
4	MG	A	335	1/1	0.90	0.10	50,50,50,50	0
6	ACY	D	331	4/4	0.91	0.15	31,34,36,36	0
5	NA	A	337	1/1	0.93	0.10	36,36,36,36	0
6	ACY	B	332	4/4	0.93	0.18	28,32,34,34	0
2	SCA	A	332	55/55	0.93	0.11	28,39,46,54	0
6	ACY	C	331	4/4	0.94	0.20	33,35,37,37	0
4	MG	A	336	1/1	0.94	0.11	45,45,45,45	0
4	MG	D	333	1/1	0.95	0.20	51,51,51,51	1
4	MG	E	333	1/1	0.96	0.10	45,45,45,45	1
4	MG	E	332	1/1	0.97	0.04	52,52,52,52	1
5	NA	D	334	1/1	0.97	0.09	39,39,39,39	1
4	MG	D	332	1/1	0.97	0.09	21,21,21,21	1
4	MG	A	334	1/1	0.98	0.16	29,29,29,29	0
4	MG	B	333	1/1	0.98	0.09	48,48,48,48	0
4	MG	A	333	1/1	0.99	0.13	23,23,23,23	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.

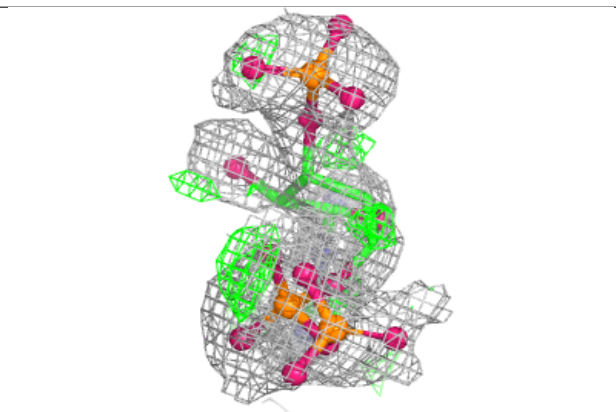
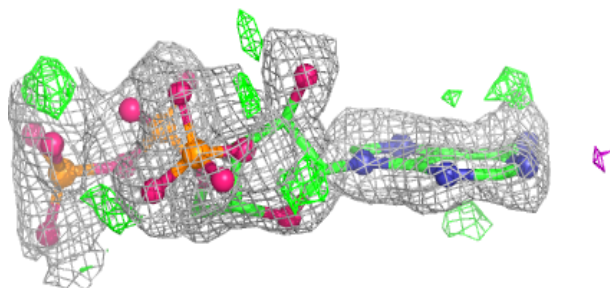
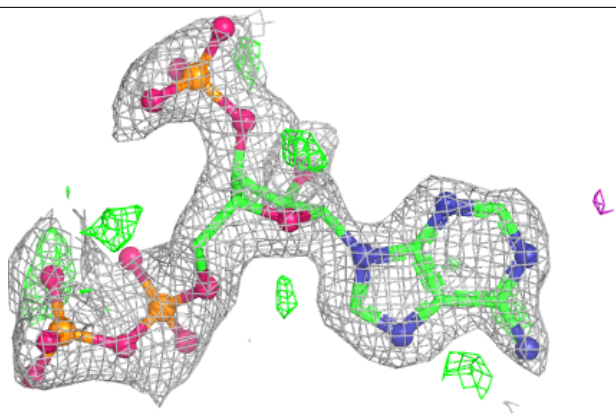
Electron density around SCA A 331:

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

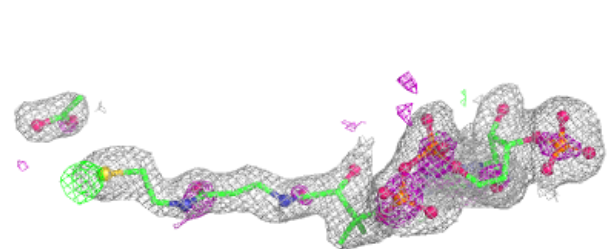
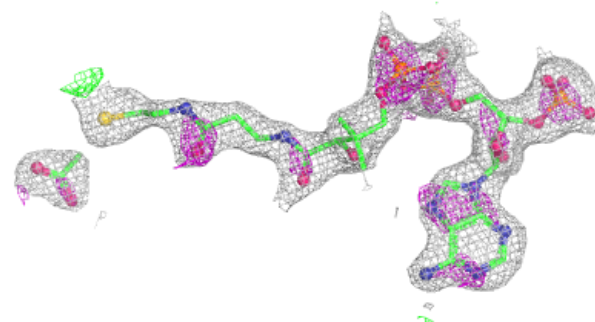


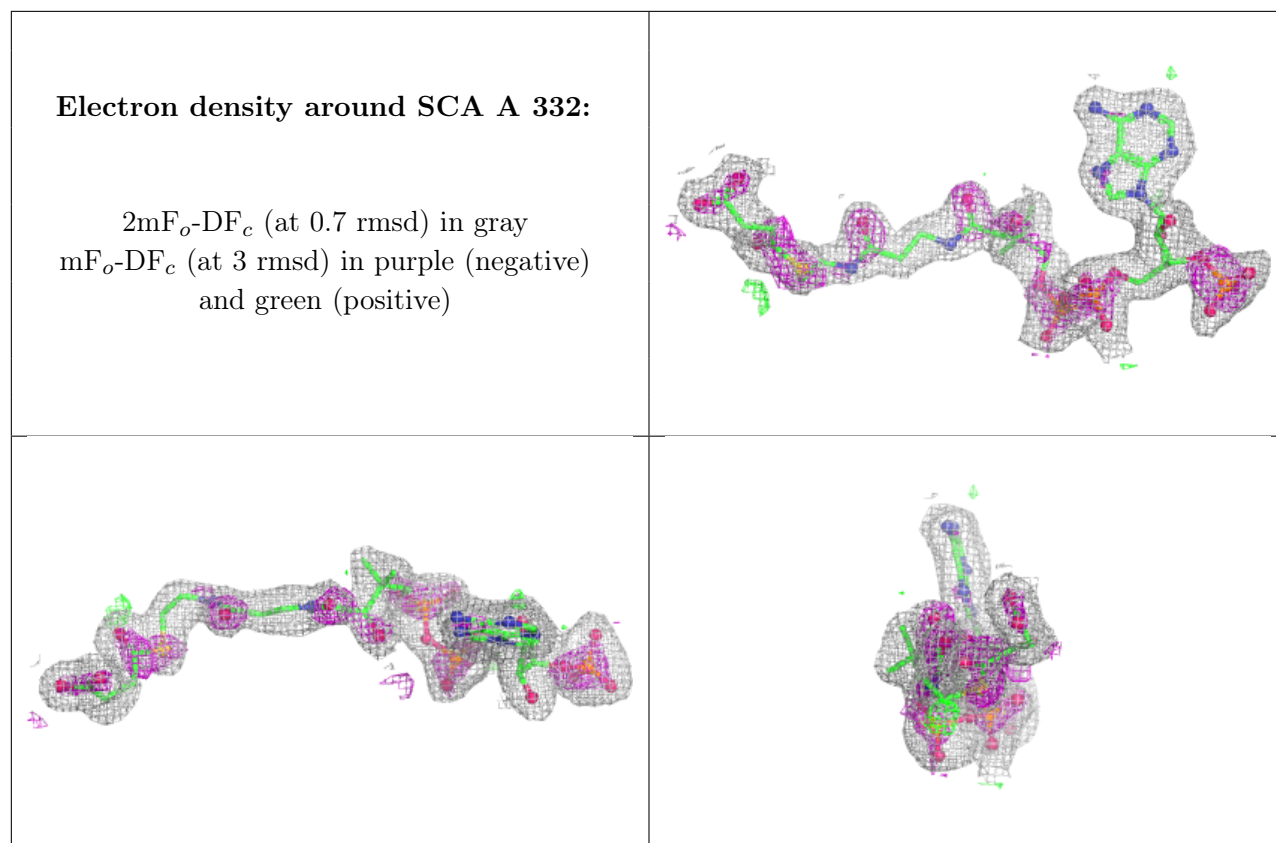
Electron density around SCA B 331:

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

**Electron density around SCA E 331:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.