



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 22, 2024 – 06:54 PM JST

PDB ID : 8I3Y
Title : Crystal structure of ASCT from Trypanosoma brucei in complex with Succinyl-CoA.
Authors : Mochizuki, K.; Inaoka, D.K.; Fukuda, K.; Kurasawa, H.; Iyoda, K.; Nakai, U.; Harada, S.; Balogun, E.O.; Mazet, M.; Millerioux, Y.; Bringaud, F.; Boshart, M.; Hirayama, K.; Kita, K.; Shiba, T.
Deposited on : 2023-01-18
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 types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

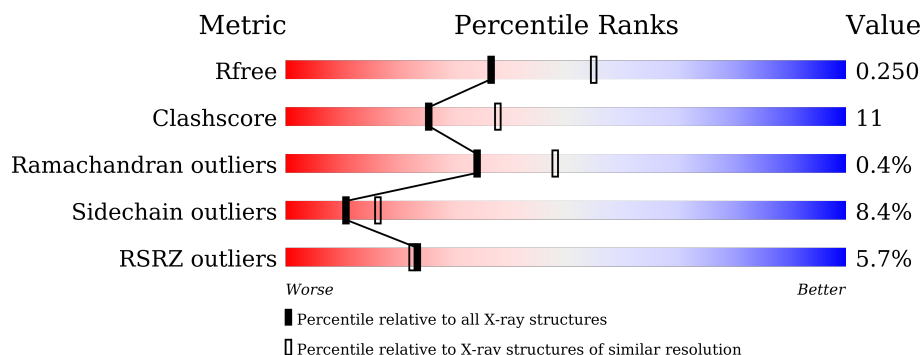
1 Overall quality at a glance

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 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	483	 13% 67% 22% 5% • 5%
1	B	483	 86% 9% • •
1	C	483	 8% 80% 13% • •
1	D	483	 85% 11% • •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14225 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.

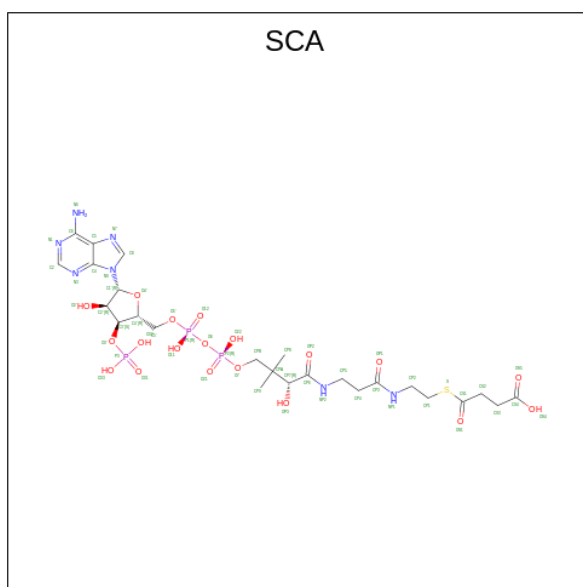
- Molecule 1 is a protein called Succinyl-CoA:3-ketoacid-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	459	3454	2173	603	655	23	0	0	0
1	B	470	3539	2222	621	673	23	0	0	0
1	C	464	3493	2197	612	661	23	0	0	0
1	D	471	3544	2225	622	674	23	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	ASN	SER	conflict	UNP Q386P1
B	419	ASN	SER	conflict	UNP Q386P1
C	419	ASN	SER	conflict	UNP Q386P1
D	419	ASN	SER	conflict	UNP Q386P1

- Molecule 2 is SUCCINYL-COENZYME A (three-letter code: SCA) (formula: C₂₅H₄₀N₇O₁₉P₃S) (labeled as "Ligand of Interest" by depositor).

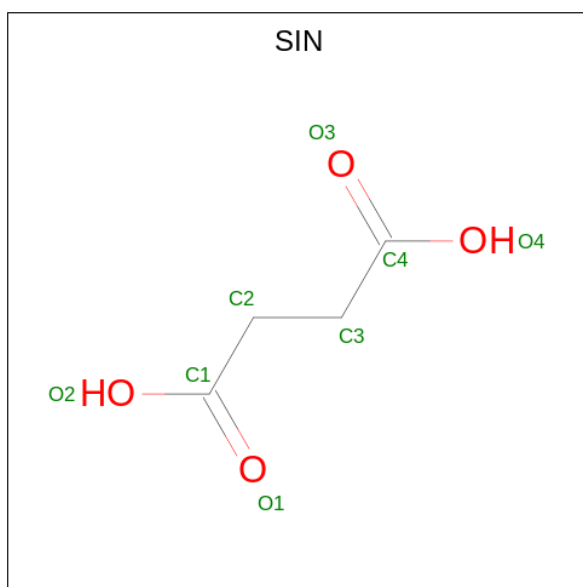


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	P			S
2	A	1	55	25	7	19	3	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SUCCINIC ACID (three-letter code: SIN) (formula: C₄H₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 8 4 4	0	0
4	D	1	Total C O 8 4 4	0	0

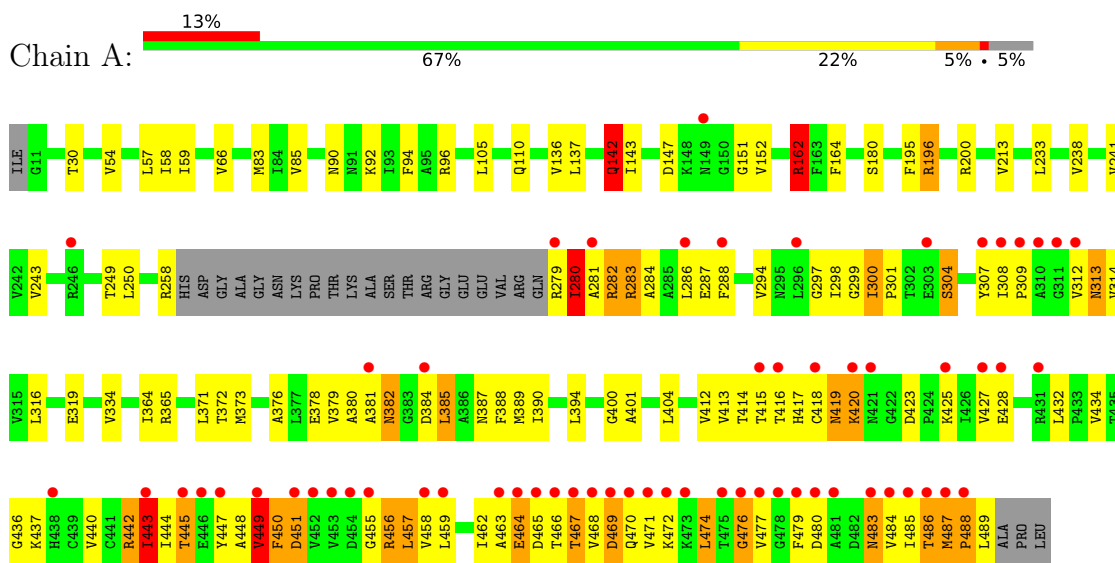
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	28	Total O 28 28	0	0
5	B	28	Total O 28 28	0	0
5	C	24	Total O 24 24	0	0
5	D	40	Total O 40 40	0	0

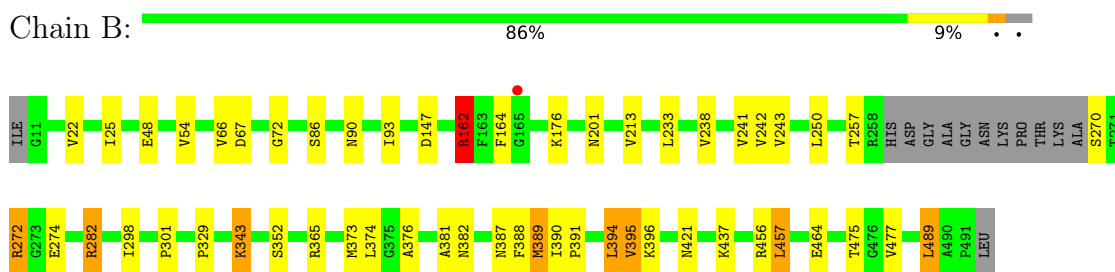
3 Residue-property plots i

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.

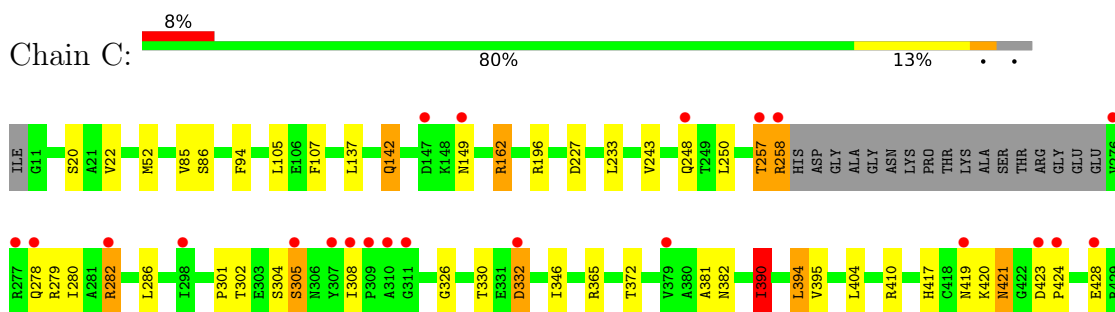
- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase

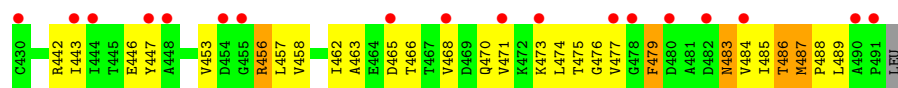


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase

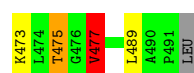
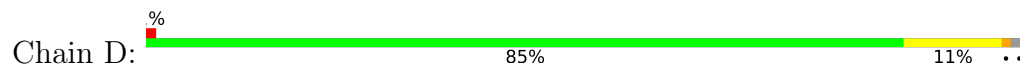


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase





- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.80Å 163.65Å 186.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.98-2.40) 99.9 (19.98-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.41Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.192 , 0.248 0.199 , 0.250	Depositor DCC
R_{free} test set	3585 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtrriage
Anisotropy	0.075	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14225	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.24% 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: SIN, CA, SCA

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	0.72	0/3510	0.97	12/4749 (0.3%)
1	B	0.67	0/3596	0.90	6/4865 (0.1%)
1	C	0.71	0/3550	0.90	8/4804 (0.2%)
1	D	0.63	0/3601	0.87	6/4872 (0.1%)
All	All	0.68	0/14257	0.91	32/19290 (0.2%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	162	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	D	365	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	B	162	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	A	365	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	C	162	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	142	GLN	N-CA-C	-7.30	91.30	111.00
1	A	365	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	365	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	365	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	C	162	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	A	162	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	365	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	476	GLY	N-CA-C	6.89	130.34	113.10
1	B	162	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	D	365	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	467	THR	N-CA-C	6.64	128.93	111.00
1	A	442	ARG	C-N-CA	6.18	137.15	121.70
1	C	365	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	B	282	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	C	390	ILE	N-CA-C	-5.61	95.86	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	227	ASP	CB-CG-OD1	5.48	123.24	118.30
1	A	96	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	449	VAL	N-CA-C	5.35	125.44	111.00
1	B	147	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	196	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	D	390	ILE	C-N-CD	5.20	139.32	128.40
1	D	162	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	442	ARG	CA-C-N	-5.19	105.78	117.20
1	D	477	VAL	CB-CA-C	-5.18	101.55	111.40
1	A	313	ASN	N-CA-C	5.17	124.96	111.00
1	C	326	GLY	C-N-CD	5.08	139.06	128.40

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	3454	0	3470	182	0
1	B	3539	0	3552	29	0
1	C	3493	0	3512	58	0
1	D	3544	0	3557	22	0
2	A	55	0	35	14	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	B	8	0	4	2	0
4	D	8	0	4	1	0
5	A	28	0	0	0	0
5	B	28	0	0	0	0
5	C	24	0	0	0	0
5	D	40	0	0	0	0
All	All	14225	0	14134	298	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 (298) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:ARG:HG2	1:A:443:ILE:CD1	1.64	1.26
1:A:443:ILE:CG1	1:A:449:VAL:H	1.49	1.25
1:A:442:ARG:CG	1:A:443:ILE:HD12	1.70	1.22
1:A:471:VAL:O	1:A:474:LEU:HD12	1.45	1.14
1:A:443:ILE:HG13	1:A:449:VAL:HA	1.14	1.13
1:A:280:ILE:N	1:A:304:SER:HB3	1.65	1.11
1:A:443:ILE:HG12	1:A:449:VAL:N	1.66	1.10
1:A:281:ALA:HB3	1:A:284:ALA:HB3	1.25	1.09
1:A:309:PRO:HB2	1:A:312:VAL:HG21	1.33	1.07
1:B:390:ILE:HD12	1:B:391:PRO:CD	1.91	1.00
1:A:443:ILE:CG1	1:A:449:VAL:N	2.22	1.00
1:A:281:ALA:CB	1:A:284:ALA:HB3	1.91	0.99
1:A:443:ILE:HG12	1:A:449:VAL:H	0.87	0.98
1:A:282:ARG:HG2	1:A:489:LEU:HG	1.42	0.97
1:A:309:PRO:HB2	1:A:312:VAL:CG2	1.94	0.97
1:A:280:ILE:H	1:A:304:SER:HB3	1.16	0.96
1:A:280:ILE:H	1:A:304:SER:CB	1.82	0.92
1:C:419:ASN:ND2	1:C:423:ASP:HB2	1.85	0.91
1:A:456:ARG:HG3	1:A:456:ARG:HH11	1.35	0.91
1:A:443:ILE:HD12	1:A:443:ILE:H	1.37	0.90
1:A:443:ILE:CG1	1:A:449:VAL:HA	2.03	0.88
1:A:443:ILE:HG13	1:A:449:VAL:CA	2.00	0.87
1:D:340:ASN:HD21	1:D:344:GLN:HE21	1.18	0.86
1:A:420:LYS:HD3	1:A:420:LYS:N	1.90	0.86
1:A:280:ILE:HG22	1:A:304:SER:O	1.78	0.83
1:B:389:MET:HG2	1:B:390:ILE:N	1.92	0.83
1:C:419:ASN:HB2	1:C:423:ASP:H	1.44	0.83
1:A:471:VAL:O	1:A:474:LEU:CD1	2.27	0.82
1:C:468:VAL:O	1:C:471:VAL:HG12	1.81	0.80
1:A:282:ARG:CG	1:A:489:LEU:HG	2.11	0.80
1:A:419:ASN:ND2	1:A:423:ASP:H	1.79	0.79
1:B:390:ILE:HD12	1:B:391:PRO:HD2	1.65	0.78
1:C:278:GLN:O	1:C:282:ARG:HG3	1.83	0.78
1:A:376:ALA:HB3	1:A:415:THR:HG21	1.66	0.77
1:A:443:ILE:CD1	1:A:443:ILE:H	1.92	0.77
1:A:442:ARG:HG2	1:A:443:ILE:HD12	0.81	0.76
1:D:407:CYS:SG	1:D:409:THR:HG22	2.25	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:VAL:O	1:C:475:THR:HG23	1.86	0.73
1:C:302:THR:O	1:C:305:SER:HB2	1.90	0.72
1:C:420:LYS:HD3	1:C:420:LYS:N	2.05	0.72
1:C:421:ASN:O	1:C:421:ASN:ND2	2.23	0.71
1:A:428:GLU:HG3	1:A:476:GLY:O	1.89	0.71
1:A:281:ALA:HB3	1:A:284:ALA:CB	2.14	0.71
1:A:462:ILE:CG2	1:A:462:ILE:O	2.38	0.71
1:A:280:ILE:CA	1:A:304:SER:HB3	2.20	0.70
1:A:468:VAL:O	1:A:472:LYS:N	2.24	0.70
1:A:456:ARG:HG3	1:A:456:ARG:NH1	2.04	0.70
1:A:442:ARG:CG	1:A:443:ILE:CD1	2.48	0.69
1:A:457:LEU:HD21	1:A:477:VAL:CG2	2.22	0.69
1:A:443:ILE:CD1	1:A:443:ILE:N	2.54	0.69
1:A:400:GLY:N	2:A:601:SCA:OS1	2.21	0.68
1:C:394:LEU:HD23	1:C:394:LEU:O	1.94	0.68
1:A:300:ILE:HG23	1:A:414:THR:OG1	1.94	0.68
1:A:458:VAL:HG13	1:A:480:ASP:HB3	1.76	0.67
1:A:286:LEU:CD1	1:A:488:PRO:O	2.41	0.67
1:A:457:LEU:HD12	1:A:457:LEU:H	1.60	0.67
1:C:453:VAL:HG21	1:C:458:VAL:HG21	1.77	0.66
1:A:443:ILE:HG13	1:A:449:VAL:N	1.99	0.66
1:B:381:ALA:HA	1:B:457:LEU:HD13	1.77	0.66
1:A:281:ALA:CB	1:A:284:ALA:CB	2.73	0.66
1:A:443:ILE:HG21	1:A:450:PHE:N	2.11	0.66
1:A:457:LEU:HD11	1:A:477:VAL:HG21	1.78	0.65
1:C:473:LYS:HG3	1:C:473:LYS:O	1.96	0.65
1:A:468:VAL:HG12	1:A:472:LYS:HG2	1.77	0.65
1:D:385:LEU:HD23	1:D:405:VAL:HG11	1.77	0.65
1:A:416:THR:O	1:A:425:LYS:HD3	1.97	0.65
1:A:381:ALA:HB1	1:A:477:VAL:HG22	1.78	0.64
1:A:489:LEU:O	1:A:489:LEU:HD23	1.98	0.64
1:A:443:ILE:HD12	1:A:443:ILE:N	2.11	0.63
1:C:488:PRO:C	1:C:489:LEU:HD12	2.19	0.62
1:A:451:ASP:O	1:A:457:LEU:HA	2.00	0.62
1:C:419:ASN:HB2	1:C:423:ASP:N	2.15	0.62
1:A:110:GLN:HE22	2:A:601:SCA:HS31	1.64	0.62
1:A:379:VAL:HG22	1:A:385:LEU:CD1	2.30	0.61
1:A:279:ARG:C	1:A:281:ALA:H	2.02	0.61
1:A:282:ARG:HD3	1:A:489:LEU:O	2.00	0.61
1:A:280:ILE:HG23	1:A:307:TYR:HB2	1.83	0.61
1:A:280:ILE:CG2	1:A:304:SER:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:SCA:H91	2:A:601:SCA:OP2	2.00	0.60
1:A:464:GLU:N	1:A:487:MET:SD	2.69	0.60
1:A:469:ASP:HA	1:A:472:LYS:HB2	1.84	0.60
1:A:147:ASP:OD2	1:A:151:GLY:N	2.24	0.60
2:A:601:SCA:HN1	2:A:601:SCA:CS1	2.07	0.60
1:C:424:PRO:HB3	1:C:474:LEU:O	2.01	0.60
1:C:485:ILE:HG22	1:C:486:THR:N	2.17	0.60
1:A:443:ILE:HG12	1:A:448:ALA:HB1	1.84	0.59
1:A:463:ALA:HA	1:A:487:MET:SD	2.42	0.59
1:A:376:ALA:HB3	1:A:415:THR:CG2	2.31	0.59
1:A:162:ARG:HD2	1:A:164:PHE:CE2	2.37	0.59
1:C:332:ASP:N	1:C:332:ASP:OD2	2.29	0.59
1:D:287:GLU:OE1	1:D:410:ARG:NH2	2.35	0.59
1:C:419:ASN:CG	1:C:423:ASP:HB2	2.24	0.59
1:A:462:ILE:O	1:A:462:ILE:HG23	2.02	0.58
1:B:25:ILE:O	1:B:54:VAL:HG21	2.03	0.58
1:A:451:ASP:O	1:A:458:VAL:N	2.35	0.57
1:A:450:PHE:CE2	1:A:459:LEU:HB2	2.40	0.57
1:A:447:TYR:CG	1:A:448:ALA:N	2.72	0.57
1:D:343:LYS:NZ	4:D:501:SIN:O4	2.37	0.57
1:B:394:LEU:HD23	1:B:395:VAL:H	1.70	0.57
1:A:382:ASN:HD21	1:A:384:ASP:CG	2.09	0.56
1:A:287:GLU:HG2	1:A:442:ARG:NH1	2.20	0.56
1:B:343:LYS:CE	4:B:501:SIN:O3	2.53	0.56
1:A:484:VAL:HG12	1:A:485:ILE:N	2.21	0.56
1:A:412:VAL:HG13	1:A:442:ARG:HB3	1.87	0.56
1:A:442:ARG:CD	1:A:443:ILE:CD1	2.85	0.55
1:D:376:ALA:HB2	1:D:385:LEU:HD11	1.89	0.55
1:A:287:GLU:OE2	1:A:287:GLU:HA	2.06	0.55
1:A:457:LEU:HD21	1:A:477:VAL:HG23	1.88	0.55
1:A:143:ILE:HD12	1:A:152:VAL:HG22	1.87	0.55
1:A:457:LEU:HD11	1:A:477:VAL:CG2	2.35	0.55
1:C:447:TYR:CE2	1:C:474:LEU:CD1	2.89	0.55
1:B:394:LEU:HD13	1:B:396:LYS:NZ	2.22	0.55
1:B:343:LYS:NZ	4:B:501:SIN:O3	2.39	0.54
1:A:419:ASN:HD21	1:A:423:ASP:H	1.55	0.54
1:C:453:VAL:CG2	1:C:458:VAL:CG2	2.85	0.54
1:C:447:TYR:CE2	1:C:474:LEU:HD13	2.43	0.54
1:A:282:ARG:HG2	1:A:489:LEU:CG	2.29	0.54
1:A:309:PRO:CB	1:A:312:VAL:HG21	2.23	0.54
1:D:18:LEU:HD13	1:D:242:VAL:HG11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:ARG:HD2	1:D:164:PHE:CE2	2.43	0.54
1:A:280:ILE:O	1:A:281:ALA:HB3	2.08	0.53
1:A:418:CYS:HA	1:A:425:LYS:HG3	1.91	0.53
1:A:142:GLN:O	1:A:142:GLN:HG3	2.08	0.53
1:C:286:LEU:CD1	1:C:488:PRO:HG2	2.39	0.53
1:A:414:THR:HG22	1:A:444:ILE:CG2	2.38	0.53
1:C:453:VAL:CG2	1:C:458:VAL:HG21	2.38	0.53
1:A:66:VAL:HG23	1:A:90:ASN:O	2.09	0.53
1:A:427:VAL:HG22	1:A:428:GLU:N	2.22	0.53
1:C:381:ALA:HA	1:C:457:LEU:HD13	1.90	0.53
1:A:94:PHE:CZ	1:A:105:LEU:HD13	2.44	0.53
1:C:394:LEU:HD23	1:C:394:LEU:C	2.29	0.53
1:D:213:VAL:HG22	1:D:238:VAL:HA	1.90	0.53
1:A:379:VAL:HG22	1:A:385:LEU:HD13	1.91	0.53
1:A:464:GLU:CG	1:A:465:ASP:H	2.22	0.53
2:A:601:SCA:CS1	2:A:601:SCA:NP1	2.72	0.53
1:A:427:VAL:CG2	1:A:428:GLU:N	2.71	0.52
1:C:447:TYR:CD2	1:C:474:LEU:HD13	2.44	0.52
1:A:300:ILE:HD12	1:A:414:THR:CB	2.40	0.52
1:A:379:VAL:HG22	1:A:385:LEU:HD12	1.91	0.52
1:B:162:ARG:HD2	1:B:164:PHE:CE2	2.44	0.52
1:A:300:ILE:N	1:A:301:PRO:CD	2.73	0.52
1:C:390:ILE:HG13	1:C:394:LEU:HB3	1.92	0.52
1:A:417:HIS:HA	1:A:445:THR:HG21	1.91	0.52
1:B:394:LEU:CD2	1:B:395:VAL:N	2.73	0.52
1:C:419:ASN:N	1:C:423:ASP:O	2.40	0.52
1:A:300:ILE:HD12	1:A:414:THR:HB	1.91	0.52
1:B:389:MET:HE2	1:B:391:PRO:HG3	1.92	0.52
1:A:309:PRO:HB2	1:A:312:VAL:HG23	1.87	0.51
1:B:390:ILE:HD12	1:B:391:PRO:N	2.25	0.51
1:C:485:ILE:CG2	1:C:486:THR:N	2.72	0.51
1:A:476:GLY:O	1:A:477:VAL:HG13	2.11	0.51
1:B:389:MET:CE	1:B:391:PRO:HG3	2.40	0.51
1:B:394:LEU:HD13	1:B:396:LYS:HZ3	1.76	0.51
1:A:283:ARG:HG3	1:A:283:ARG:O	2.11	0.51
1:A:447:TYR:CD1	1:A:448:ALA:N	2.72	0.51
1:C:419:ASN:HD22	1:C:423:ASP:HB2	1.72	0.51
2:A:601:SCA:OP2	2:A:601:SCA:H81	2.11	0.50
1:A:455:GLY:C	1:A:456:ARG:HG2	2.31	0.50
1:A:412:VAL:HG22	1:A:442:ARG:HB2	1.93	0.50
1:B:66:VAL:O	1:B:72:GLY:HA3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:VAL:O	1:A:485:ILE:HG23	2.11	0.50
1:A:287:GLU:HG2	1:A:442:ARG:HH11	1.77	0.50
1:D:196:ARG:NH1	1:D:337:ASP:OD2	2.45	0.50
1:A:300:ILE:CG2	1:A:414:THR:OG1	2.59	0.49
1:A:319:GLU:OE2	2:A:601:SCA:CS3	2.60	0.49
1:D:428:GLU:HA	1:D:477:VAL:HG11	1.93	0.49
1:A:457:LEU:HD12	1:A:457:LEU:N	2.27	0.49
1:B:301:PRO:HB3	1:B:373:MET:HB3	1.94	0.49
1:A:442:ARG:CD	1:A:443:ILE:HD11	2.42	0.49
1:A:286:LEU:HD11	1:A:488:PRO:HB2	1.94	0.49
1:A:474:LEU:HD23	1:A:477:VAL:H	1.78	0.49
1:A:474:LEU:HD22	1:A:477:VAL:O	2.11	0.49
1:D:15:VAL:HG22	1:D:241:VAL:HG22	1.94	0.49
2:A:601:SCA:P3	2:A:601:SCA:HO2'	2.36	0.49
1:B:390:ILE:HD12	1:B:391:PRO:HD3	1.87	0.49
1:A:419:ASN:N	1:A:419:ASN:HD22	2.11	0.49
1:A:450:PHE:HZ	1:A:479:PHE:CD1	2.31	0.49
1:C:94:PHE:CZ	1:C:105:LEU:HD13	2.48	0.49
1:A:280:ILE:N	1:A:304:SER:CB	2.50	0.48
1:D:471:VAL:O	1:D:475:THR:HG22	2.12	0.48
1:A:300:ILE:HD12	1:A:414:THR:OG1	2.14	0.48
1:A:180:SER:HB2	1:A:213:VAL:HB	1.94	0.48
1:A:443:ILE:HG21	1:A:450:PHE:HB2	1.95	0.48
2:A:601:SCA:O2'	2:A:601:SCA:O32	2.30	0.48
1:A:319:GLU:OE2	2:A:601:SCA:HS32	2.14	0.48
2:A:601:SCA:H5'2	2:A:601:SCA:HPB2	1.96	0.47
1:A:279:ARG:HG3	1:A:279:ARG:O	2.14	0.47
1:A:280:ILE:HA	1:A:304:SER:HB3	1.96	0.47
1:C:257:THR:O	1:C:257:THR:HG22	2.14	0.47
1:A:213:VAL:HG22	1:A:238:VAL:HA	1.95	0.47
1:C:485:ILE:HG22	1:C:486:THR:O	2.15	0.47
1:A:379:VAL:HG12	1:A:380:ALA:N	2.29	0.47
1:A:294:VAL:HG13	1:A:316:LEU:HD13	1.96	0.47
1:B:376:ALA:HA	1:B:387:ASN:HB3	1.95	0.47
1:A:472:LYS:C	1:A:474:LEU:H	2.18	0.47
1:A:364:ILE:CG2	1:A:404:LEU:HD23	2.45	0.46
1:A:59:ILE:HB	1:A:83:MET:SD	2.56	0.46
1:A:381:ALA:HB1	1:A:477:VAL:CG2	2.45	0.46
1:A:462:ILE:O	1:A:462:ILE:HG22	2.15	0.46
1:A:297:GLY:O	1:A:301:PRO:HB2	2.15	0.46
1:B:270:SER:HB3	1:B:274:GLU:CD	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLU:O	1:A:486:THR:HG23	2.15	0.46
1:A:484:VAL:CG1	1:A:485:ILE:N	2.77	0.46
1:C:107:PHE:HD2	1:C:142:GLN:HE22	1.63	0.46
1:A:413:VAL:HG23	1:A:440:VAL:HG13	1.98	0.46
1:A:414:THR:HG22	1:A:444:ILE:HG23	1.98	0.46
1:B:22:VAL:HG21	1:B:48:GLU:HG3	1.97	0.46
1:C:443:ILE:HD12	1:C:457:LEU:HD11	1.97	0.46
1:A:376:ALA:HA	1:A:387:ASN:CB	2.45	0.46
1:C:453:VAL:O	1:C:456:ARG:HD3	2.16	0.46
1:A:378:GLU:OE1	1:A:432:LEU:N	2.40	0.45
1:B:213:VAL:HG22	1:B:238:VAL:HA	1.98	0.45
1:C:476:GLY:O	1:C:477:VAL:HG13	2.16	0.45
1:A:419:ASN:HD22	1:A:423:ASP:H	1.60	0.45
1:C:417:HIS:CD2	1:C:474:LEU:HB3	2.52	0.45
1:C:94:PHE:HZ	1:C:105:LEU:HD13	1.81	0.45
1:A:288:PHE:HD1	1:A:314:VAL:HG11	1.82	0.45
1:A:474:LEU:HD13	1:A:479:PHE:HE1	1.82	0.45
1:B:257:THR:HG22	1:B:329:PRO:O	2.18	0.44
1:B:394:LEU:HD23	1:B:395:VAL:N	2.32	0.44
1:C:420:LYS:N	1:C:420:LYS:CD	2.74	0.44
1:A:94:PHE:HZ	1:A:105:LEU:HD13	1.83	0.44
1:A:162:ARG:HD2	1:A:164:PHE:CZ	2.51	0.44
1:C:453:VAL:HG23	1:C:458:VAL:CG2	2.47	0.44
1:A:385:LEU:HB2	1:A:440:VAL:HG21	1.98	0.44
1:A:373:MET:HA	1:A:412:VAL:O	2.18	0.44
1:A:456:ARG:HD3	1:D:152:VAL:O	2.17	0.44
1:A:472:LYS:C	1:A:474:LEU:N	2.70	0.44
1:D:255:THR:O	1:D:329:PRO:HD2	2.18	0.44
1:A:279:ARG:C	1:A:281:ALA:N	2.70	0.44
1:D:180:SER:HB2	1:D:213:VAL:HB	2.00	0.44
1:C:330:THR:HB	1:C:332:ASP:OD2	2.18	0.44
1:C:483:ASN:C	1:C:484:VAL:HG23	2.38	0.44
1:D:109:PRO:HD3	1:D:137:LEU:HD23	2.00	0.44
1:C:489:LEU:HD12	1:C:489:LEU:N	2.33	0.44
1:D:66:VAL:HG23	1:D:90:ASN:HB3	1.99	0.44
1:A:442:ARG:HD3	1:A:443:ILE:CD1	2.47	0.44
1:A:476:GLY:C	1:A:477:VAL:HG13	2.39	0.44
1:C:479:PHE:CD1	1:C:479:PHE:N	2.86	0.44
1:A:401:ALA:HB2	2:A:601:SCA:CP3	2.48	0.43
1:C:258:ARG:O	1:C:258:ARG:HG3	2.17	0.43
1:B:282:ARG:NH2	1:B:489:LEU:HD23	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:THR:HG23	1:B:257:THR:O	2.18	0.43
1:C:428:GLU:HA	1:C:477:VAL:HG11	2.00	0.43
1:B:272:ARG:HD3	1:B:272:ARG:HA	1.66	0.43
1:A:428:GLU:HB2	1:A:476:GLY:HA2	2.01	0.43
1:A:487:MET:O	1:A:487:MET:HG2	2.18	0.43
1:D:25:ILE:O	1:D:54:VAL:HG21	2.18	0.43
1:C:417:HIS:NE2	1:C:475:THR:HG22	2.33	0.43
1:C:468:VAL:HA	1:C:471:VAL:HG12	2.01	0.43
1:D:162:ARG:HD2	1:D:164:PHE:CZ	2.53	0.43
1:A:284:ALA:O	1:A:287:GLU:HB2	2.19	0.43
1:A:371:LEU:HD21	1:A:373:MET:HE3	1.99	0.43
1:A:384:ASP:HB2	1:A:437:LYS:HA	2.01	0.43
1:D:466:THR:HG22	1:D:470:GLN:HE21	1.83	0.43
1:A:380:ALA:HA	1:A:427:VAL:O	2.19	0.42
1:A:434:VAL:HG12	1:A:436:GLY:N	2.32	0.42
1:C:410:ARG:HH22	1:C:442:ARG:HE	1.67	0.42
1:A:30:THR:HG22	1:A:58:ILE:HB	2.01	0.42
1:A:54:VAL:CG1	1:A:57:LEU:HD21	2.49	0.42
1:A:381:ALA:CB	1:A:477:VAL:HG22	2.46	0.42
1:A:418:CYS:CA	1:A:425:LYS:HG3	2.48	0.42
1:A:443:ILE:HG12	1:A:448:ALA:CB	2.49	0.42
1:A:443:ILE:HG12	1:A:448:ALA:CA	2.49	0.42
1:B:67:ASP:OD2	1:B:93:ILE:HG12	2.20	0.42
1:C:280:ILE:HG12	1:C:446:GLU:N	2.34	0.42
1:C:301:PRO:O	1:C:304:SER:OG	2.34	0.42
1:C:421:ASN:ND2	1:C:421:ASN:C	2.73	0.42
1:C:453:VAL:HG21	1:C:458:VAL:CG2	2.46	0.42
1:B:394:LEU:CD2	1:B:396:LYS:HG3	2.50	0.42
1:A:376:ALA:HA	1:A:387:ASN:HB2	2.02	0.41
1:A:286:LEU:CD1	1:A:488:PRO:HB2	2.49	0.41
1:C:372:THR:HG21	1:C:404:LEU:HB3	2.02	0.41
1:A:299:GLY:C	1:A:301:PRO:CD	2.89	0.41
1:C:305:SER:O	1:C:308:ILE:HG13	2.20	0.41
1:A:419:ASN:ND2	1:A:419:ASN:C	2.72	0.41
1:A:483:ASN:C	1:A:483:ASN:HD22	2.23	0.41
1:A:286:LEU:HD12	1:A:488:PRO:O	2.21	0.41
1:A:417:HIS:HA	1:A:445:THR:CG2	2.49	0.41
1:A:450:PHE:CD2	1:A:459:LEU:HA	2.55	0.41
1:D:294:VAL:CG2	1:D:316:LEU:HD22	2.50	0.41
1:A:443:ILE:CG2	1:A:450:PHE:HB2	2.50	0.41
1:A:195:PHE:CD2	1:A:200:ARG:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ILE:O	2:A:601:SCA:CP9	2.69	0.41
1:A:373:MET:HG2	1:A:412:VAL:HB	2.03	0.41
1:A:471:VAL:HG12	1:A:474:LEU:CD1	2.51	0.41
2:A:601:SCA:P3	2:A:601:SCA:O2'	2.79	0.41
1:C:463:ALA:HB2	1:C:487:MET:HB3	2.02	0.41
1:C:466:THR:HG23	1:C:470:GLN:NE2	2.36	0.41
1:A:378:GLU:OE1	1:A:432:LEU:HG	2.21	0.41
1:A:420:LYS:N	1:A:420:LYS:CD	2.72	0.41
1:A:485:ILE:HG21	1:A:485:ILE:HD13	1.86	0.41
1:A:372:THR:HG21	1:A:404:LEU:HB3	2.03	0.40
1:A:280:ILE:O	1:A:281:ALA:CB	2.70	0.40
1:A:483:ASN:C	1:A:483:ASN:ND2	2.75	0.40
1:C:22:VAL:HG23	1:C:52:MET:CE	2.51	0.40
1:A:54:VAL:HG11	1:A:57:LEU:HD21	2.04	0.40
1:A:476:GLY:O	1:A:477:VAL:CG1	2.70	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	455/483 (94%)	432 (95%)	18 (4%)	5 (1%)	14	20
1	B	466/483 (96%)	457 (98%)	8 (2%)	1 (0%)	47	62
1	C	460/483 (95%)	448 (97%)	11 (2%)	1 (0%)	47	62
1	D	467/483 (97%)	456 (98%)	11 (2%)	0	100	100
All	All	1848/1932 (96%)	1793 (97%)	48 (3%)	7 (0%)	34	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	280	ILE
1	C	465	ASP
1	A	488	PRO
1	A	445	THR
1	A	449	VAL
1	B	201	ASN
1	A	443	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	369/387 (95%)	326 (88%)	43 (12%)	5 7
1	B	378/387 (98%)	351 (93%)	27 (7%)	14 23
1	C	373/387 (96%)	344 (92%)	29 (8%)	12 19
1	D	378/387 (98%)	351 (93%)	27 (7%)	14 23
All	All	1498/1548 (97%)	1372 (92%)	126 (8%)	11 16

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	VAL
1	A	92	LYS
1	A	136	VAL
1	A	137	LEU
1	A	142	GLN
1	A	162	ARG
1	A	196	ARG
1	A	233	LEU
1	A	241	VAL
1	A	243	VAL
1	A	249	THR
1	A	250	LEU
1	A	258	ARG
1	A	280	ILE
1	A	282	ARG

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Mol	Chain	Res	Type
1	A	283	ARG
1	A	300	ILE
1	A	304	SER
1	A	308	ILE
1	A	313	ASN
1	A	334	VAL
1	A	382	ASN
1	A	385	LEU
1	A	388	PHE
1	A	389	MET
1	A	390	ILE
1	A	394	LEU
1	A	419	ASN
1	A	420	LYS
1	A	443	ILE
1	A	450	PHE
1	A	451	ASP
1	A	456	ARG
1	A	457	LEU
1	A	464	GLU
1	A	466	THR
1	A	467	THR
1	A	469	ASP
1	A	470	GLN
1	A	474	LEU
1	A	483	ASN
1	A	486	THR
1	A	487	MET
1	B	86	SER
1	B	90	ASN
1	B	162	ARG
1	B	176	LYS
1	B	233	LEU
1	B	241	VAL
1	B	242	VAL
1	B	243	VAL
1	B	250	LEU
1	B	272	ARG
1	B	298	ILE
1	B	343	LYS
1	B	352	SER
1	B	374	LEU

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Mol	Chain	Res	Type
1	B	382	ASN
1	B	388	PHE
1	B	389	MET
1	B	394	LEU
1	B	395	VAL
1	B	421	ASN
1	B	437	LYS
1	B	456	ARG
1	B	457	LEU
1	B	464	GLU
1	B	475	THR
1	B	477	VAL
1	B	489	LEU
1	C	20	SER
1	C	85	VAL
1	C	86	SER
1	C	137	LEU
1	C	142	GLN
1	C	149	ASN
1	C	162	ARG
1	C	233	LEU
1	C	243	VAL
1	C	248	GLN
1	C	250	LEU
1	C	257	THR
1	C	258	ARG
1	C	279	ARG
1	C	282	ARG
1	C	305	SER
1	C	332	ASP
1	C	346	ILE
1	C	382	ASN
1	C	390	ILE
1	C	394	LEU
1	C	395	VAL
1	C	421	ASN
1	C	456	ARG
1	C	462	ILE
1	C	479	PHE
1	C	483	ASN
1	C	486	THR
1	C	487	MET

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Mol	Chain	Res	Type
1	D	19	SER
1	D	52	MET
1	D	82	LYS
1	D	85	VAL
1	D	90	ASN
1	D	92	LYS
1	D	136	VAL
1	D	142	GLN
1	D	162	ARG
1	D	196	ARG
1	D	213	VAL
1	D	233	LEU
1	D	243	VAL
1	D	248	GLN
1	D	250	LEU
1	D	276	VAL
1	D	334	VAL
1	D	394	LEU
1	D	409	THR
1	D	420	LYS
1	D	437	LYS
1	D	442	ARG
1	D	470	GLN
1	D	473	LYS
1	D	475	THR
1	D	477	VAL
1	D	489	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	77	ASN
1	A	97	GLN
1	A	110	GLN
1	A	253	HIS
1	A	382	ASN
1	A	419	ASN
1	A	421	ASN
1	A	438	HIS
1	A	470	GLN
1	A	483	ASN

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Mol	Chain	Res	Type
1	B	47	GLN
1	B	97	GLN
1	B	208	GLN
1	B	248	GLN
1	B	290	ASN
1	B	313	ASN
1	B	382	ASN
1	B	421	ASN
1	C	77	ASN
1	C	97	GLN
1	C	142	GLN
1	C	208	GLN
1	C	248	GLN
1	C	306	ASN
1	D	47	GLN
1	D	77	ASN
1	D	97	GLN
1	D	208	GLN
1	D	344	GLN
1	D	417	HIS
1	D	470	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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
4	SIN	B	501	-	7,7,7	1.20	0	8,8,8	1.45	2 (25%)
4	SIN	D	501	-	7,7,7	1.15	0	8,8,8	1.29	1 (12%)
2	SCA	A	601	-	49,57,57	1.20	3 (6%)	61,84,84	2.06	12 (19%)

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
4	SIN	B	501	-	-	0/5/5/5	-
4	SIN	D	501	-	-	2/5/5/5	-
2	SCA	A	601	-	-	12/52/72/72	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	SCA	CS1-S	-2.77	1.69	1.76
2	A	601	SCA	OS4-CS4	-2.36	1.22	1.30
2	A	601	SCA	C4-N3	-2.02	1.32	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	SCA	CS2-CS1-S	7.97	122.73	113.46
2	A	601	SCA	OS1-CS1-CS2	-7.88	114.68	123.99
2	A	601	SCA	CP1-CP2-NP1	-4.37	103.24	112.42
2	A	601	SCA	CS3-CS2-CS1	-3.58	107.03	112.41
2	A	601	SCA	C4-C5-N7	-3.12	106.15	109.40
2	A	601	SCA	CS2-CS3-CS4	-3.08	106.98	113.60
4	D	501	SIN	C2-C3-C4	-3.00	107.16	113.60
2	A	601	SCA	O3'-C3'-C2'	-2.45	102.81	111.68
2	A	601	SCA	N3-C2-N1	-2.37	124.98	128.68
2	A	601	SCA	C2'-C3'-C4'	2.11	106.96	103.22
2	A	601	SCA	P2-O6-P1	-2.10	125.61	132.83
4	B	501	SIN	O2-C1-O1	-2.07	118.15	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	SCA	O33-P3-O32	2.05	115.45	107.64
4	B	501	SIN	O4-C4-C3	2.01	120.50	114.03
2	A	601	SCA	O2'-C2'-C3'	-2.00	105.48	111.17

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	SCA	CPB-O7-P2-O6
2	A	601	SCA	CPB-O7-P2-O21
2	A	601	SCA	CPB-O7-P2-O22
2	A	601	SCA	OP2-CP6-CP7-CPA
2	A	601	SCA	NP2-CP6-CP7-CPA
2	A	601	SCA	NP2-CP6-CP7-OP3
2	A	601	SCA	OP1-CP3-NP1-CP2
2	A	601	SCA	CP4-CP3-NP1-CP2
2	A	601	SCA	OP2-CP6-CP7-OP3
4	D	501	SIN	C2-C3-C4-O4
2	A	601	SCA	S-CP1-CP2-NP1
4	D	501	SIN	C2-C3-C4-O3
2	A	601	SCA	CS2-CS3-CS4-OS5
2	A	601	SCA	CS2-CS3-CS4-OS4

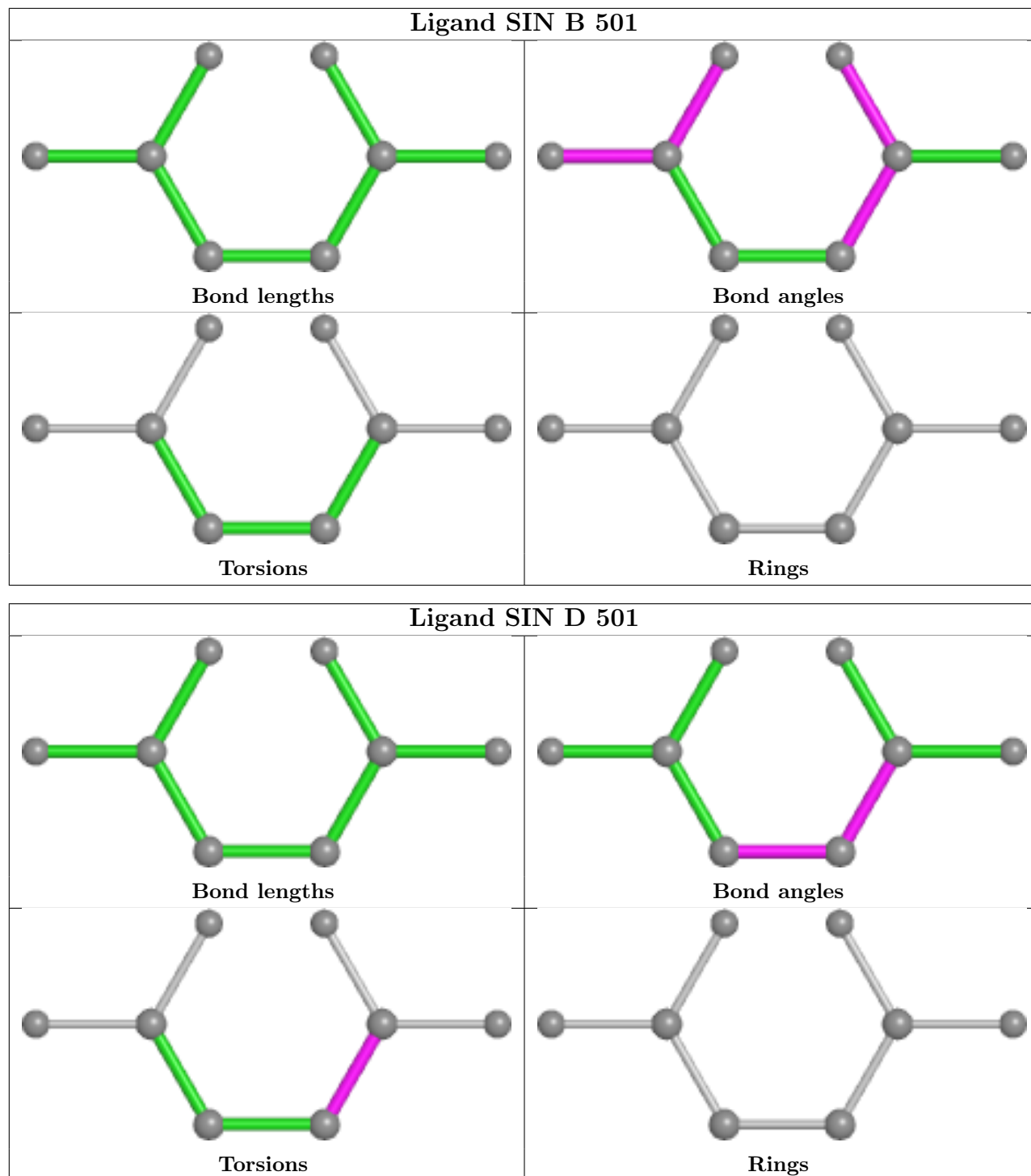
There are no ring outliers.

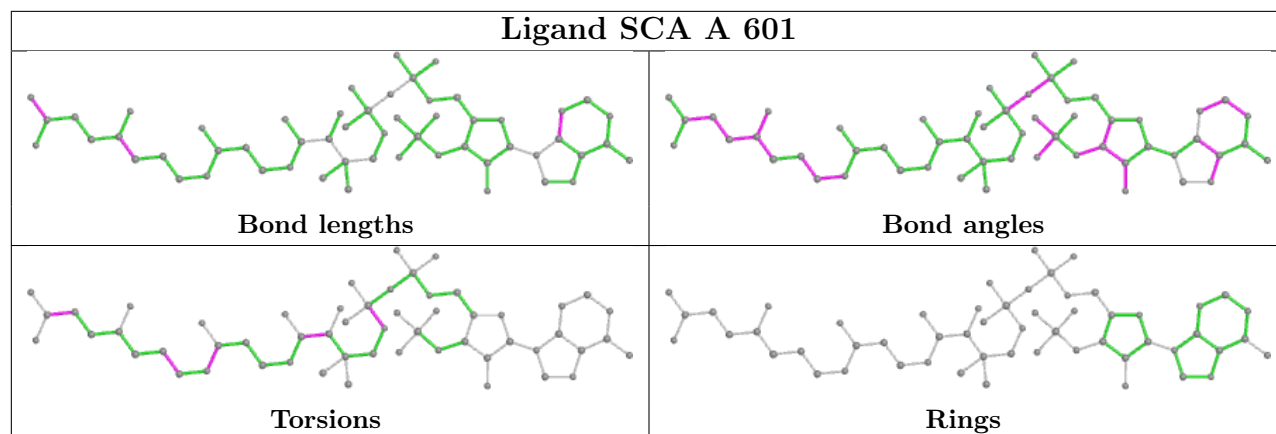
3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	501	SIN	2	0
4	D	501	SIN	1	0
2	A	601	SCA	14	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	459/483 (95%)	0.33	62 (13%) 3 2	23, 39, 100, 153	1 (0%)
1	B	470/483 (97%)	-0.32	1 (0%) 95 94	23, 35, 56, 91	1 (0%)
1	C	464/483 (96%)	0.16	40 (8%) 10 9	24, 45, 92, 146	1 (0%)
1	D	471/483 (97%)	-0.29	3 (0%) 89 88	23, 37, 58, 110	1 (0%)
All	All	1864/1932 (96%)	-0.03	106 (5%) 23 22	23, 38, 86, 153	4 (0%)

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	486	THR	11.6
1	A	458	VAL	6.7
1	A	464	GLU	6.5
1	C	147	ASP	6.2
1	A	483	ASN	5.3
1	A	473	LYS	5.3
1	C	310	ALA	5.2
1	A	477	VAL	5.1
1	C	276	VAL	5.1
1	A	465	ASP	4.9
1	A	449	VAL	4.8
1	A	466	THR	4.8
1	A	455	GLY	4.7
1	A	467	THR	4.7
1	A	463	ALA	4.6
1	A	478	GLY	4.5
1	A	471	VAL	4.4
1	A	469	ASP	4.3
1	A	453	VAL	4.3
1	A	381	ALA	4.3
1	C	311	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	468	VAL	4.2
1	A	310	ALA	3.9
1	A	454	ASP	3.9
1	C	480	ASP	3.9
1	A	452	VAL	3.9
1	A	481	ALA	3.8
1	A	311	GLY	3.8
1	A	476	GLY	3.8
1	A	428	GLU	3.8
1	C	454	ASP	3.6
1	C	277	ARG	3.6
1	C	423	ASP	3.6
1	A	309	PRO	3.5
1	C	379	VAL	3.5
1	A	484	VAL	3.4
1	C	465	ASP	3.4
1	A	485	ILE	3.3
1	A	459	LEU	3.3
1	A	475	THR	3.3
1	A	472	LYS	3.3
1	A	470	GLN	3.3
1	C	473	LYS	3.2
1	A	279	ARG	3.2
1	A	420	LYS	3.2
1	C	309	PRO	3.2
1	C	447	TYR	3.1
1	C	257	THR	3.1
1	A	149	ASN	3.1
1	C	332	ASP	3.0
1	C	424	PRO	3.0
1	C	444	ILE	3.0
1	C	298	ILE	3.0
1	C	307	TYR	2.9
1	C	455	GLY	2.9
1	A	421	ASN	2.9
1	A	438	HIS	2.9
1	C	478	GLY	2.8
1	C	484	VAL	2.8
1	C	308	ILE	2.7
1	D	248	GLN	2.7
1	C	430	CYS	2.7
1	C	477	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	480	ASP	2.7
1	A	443	ILE	2.6
1	C	278	GLN	2.6
1	C	305	SER	2.6
1	C	482	ASP	2.6
1	A	416	THR	2.5
1	A	479	PHE	2.5
1	A	415	THR	2.4
1	C	448	ALA	2.4
1	A	286	LEU	2.4
1	C	248	GLN	2.4
1	C	491	PRO	2.4
1	A	418	CYS	2.4
1	C	149	ASN	2.3
1	A	488	PRO	2.3
1	C	468	VAL	2.3
1	B	165	GLY	2.3
1	A	307	TYR	2.3
1	A	308	ILE	2.2
1	D	391	PRO	2.2
1	A	312	VAL	2.2
1	C	443	ILE	2.2
1	A	446	GLU	2.2
1	A	246	ARG	2.2
1	D	258	ARG	2.2
1	A	431	ARG	2.2
1	C	282	ARG	2.2
1	C	419	ASN	2.1
1	A	288	PHE	2.1
1	A	425	LYS	2.1
1	A	303	GLU	2.1
1	A	281	ALA	2.1
1	A	447	TYR	2.1
1	C	471	VAL	2.1
1	A	384	ASP	2.1
1	A	445	THR	2.1
1	A	451	ASP	2.1
1	A	296	LEU	2.1
1	A	427	VAL	2.0
1	C	428	GLU	2.0
1	C	258	ARG	2.0
1	C	490	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	487	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

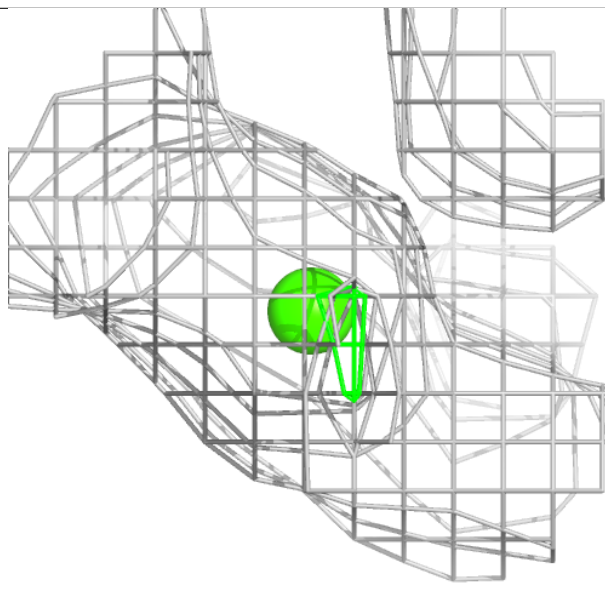
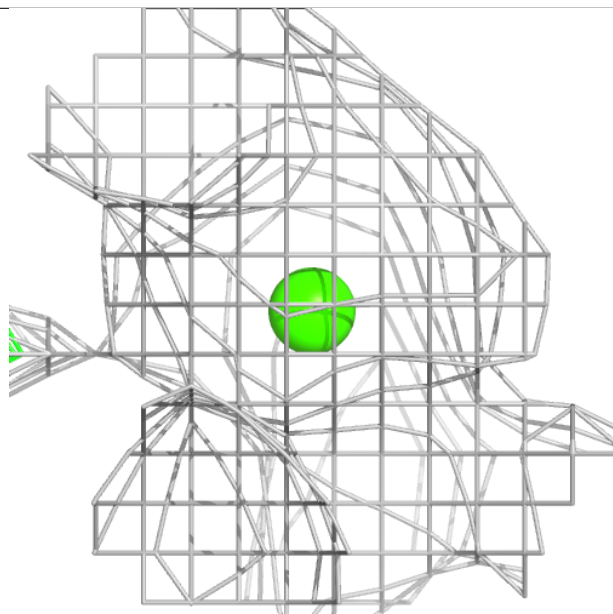
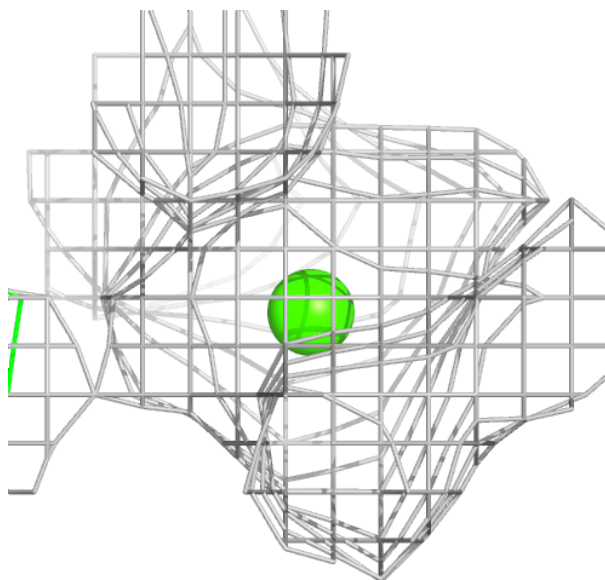
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	D	502	1/1	0.72	0.17	84,84,84,84	0
4	SIN	D	501	8/8	0.78	0.21	60,65,69,75	0
3	CA	B	502	1/1	0.80	0.09	70,70,70,70	0
2	SCA	A	601	55/55	0.84	0.23	65,79,98,108	0
3	CA	C	701	1/1	0.85	0.08	69,69,69,69	0
4	SIN	B	501	8/8	0.87	0.25	55,58,63,65	0
3	CA	A	602	1/1	0.94	0.06	61,61,61,61	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.

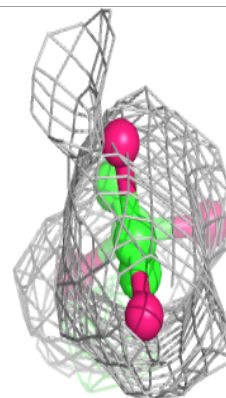
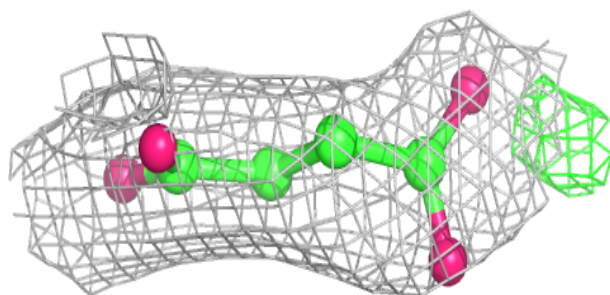
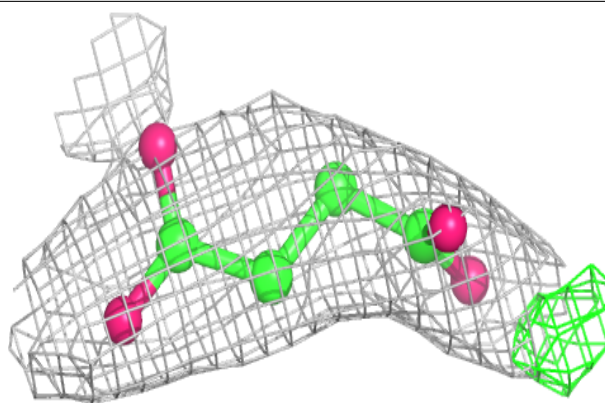
Electron density around CA D 502:

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



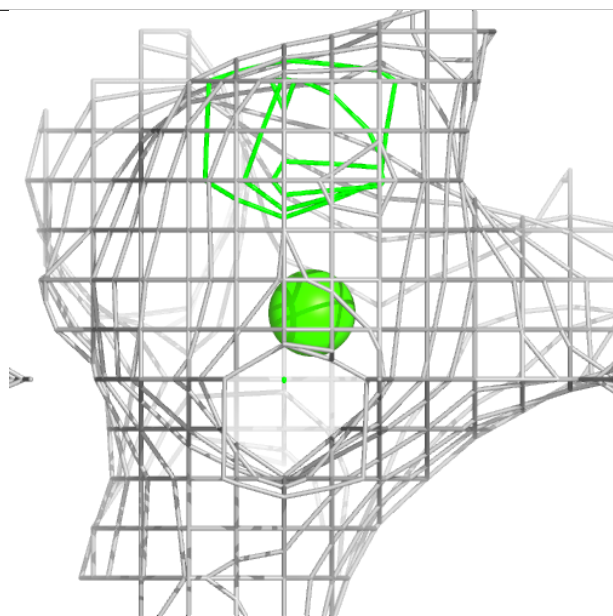
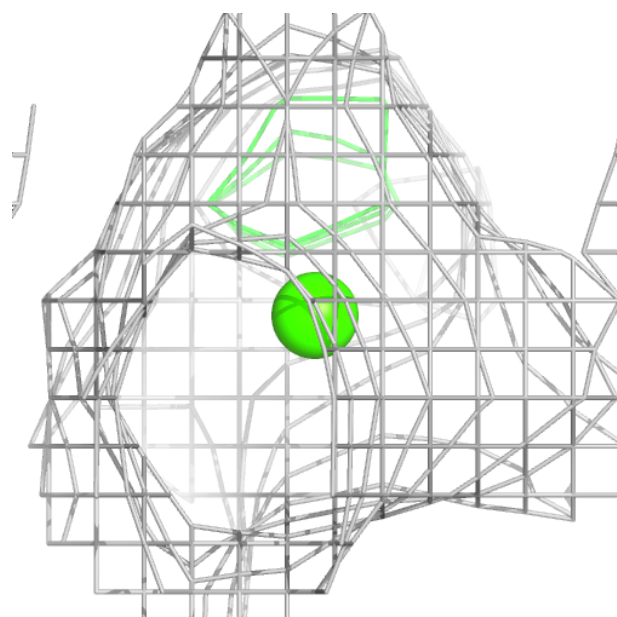
Electron density around SIN D 501:

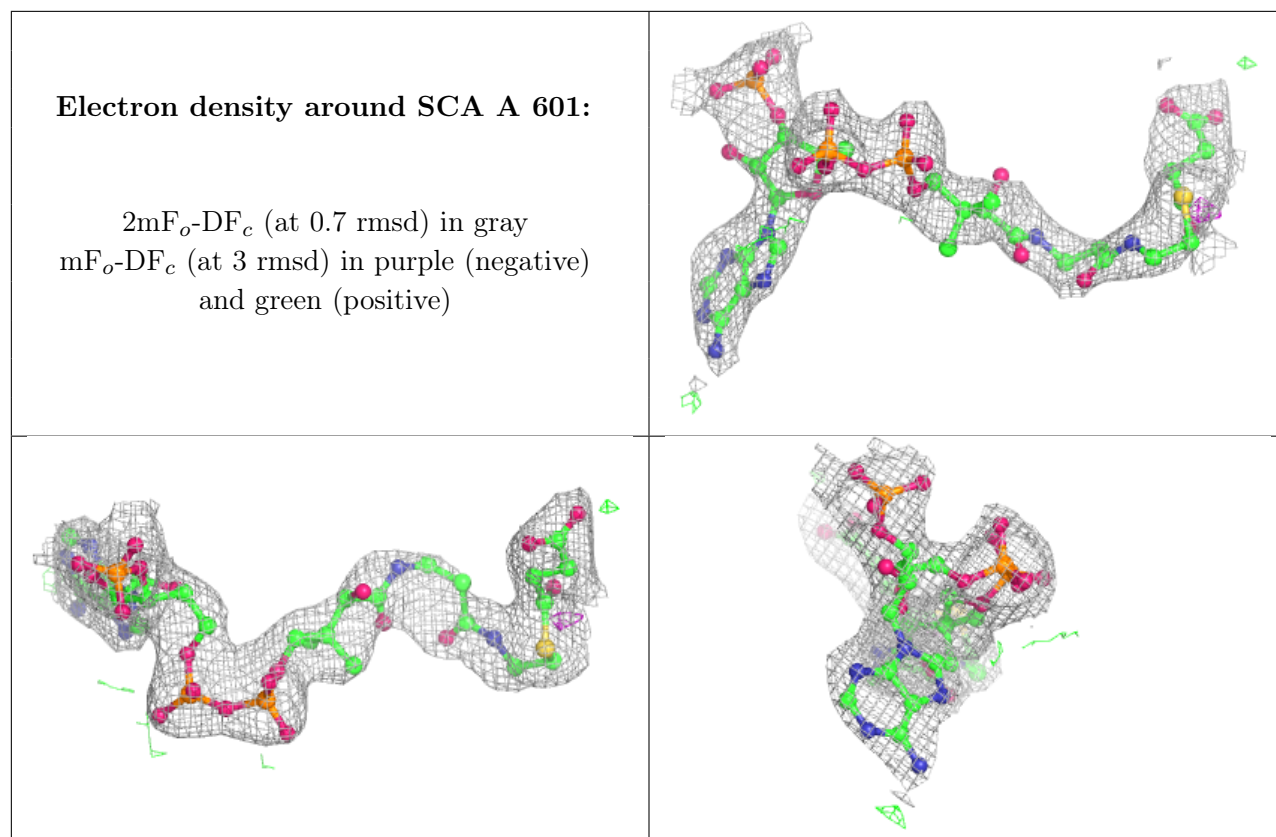
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 502:

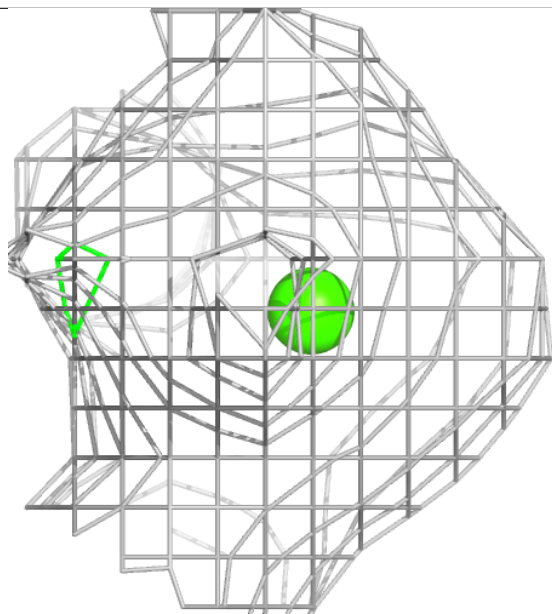
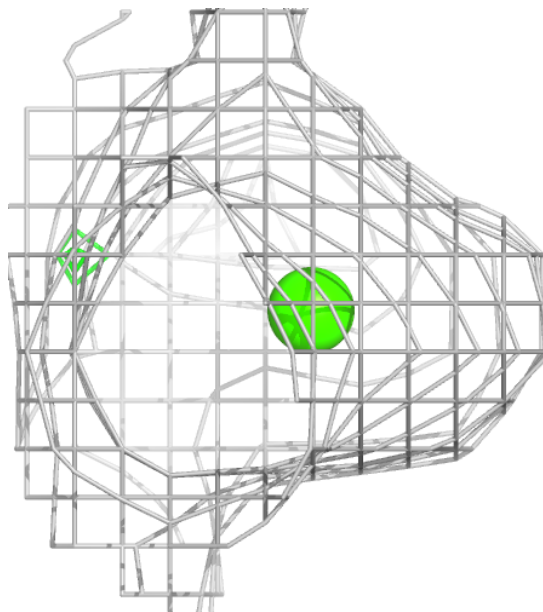
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





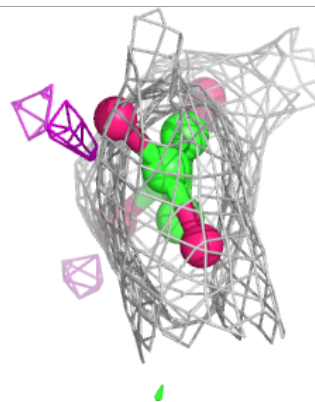
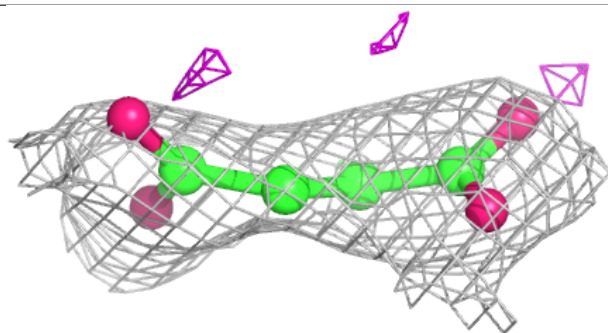
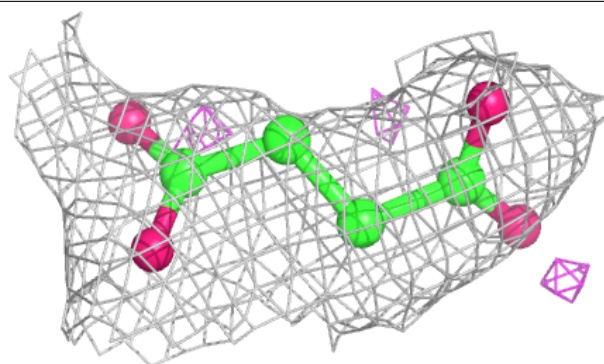
Electron density around CA C 701:

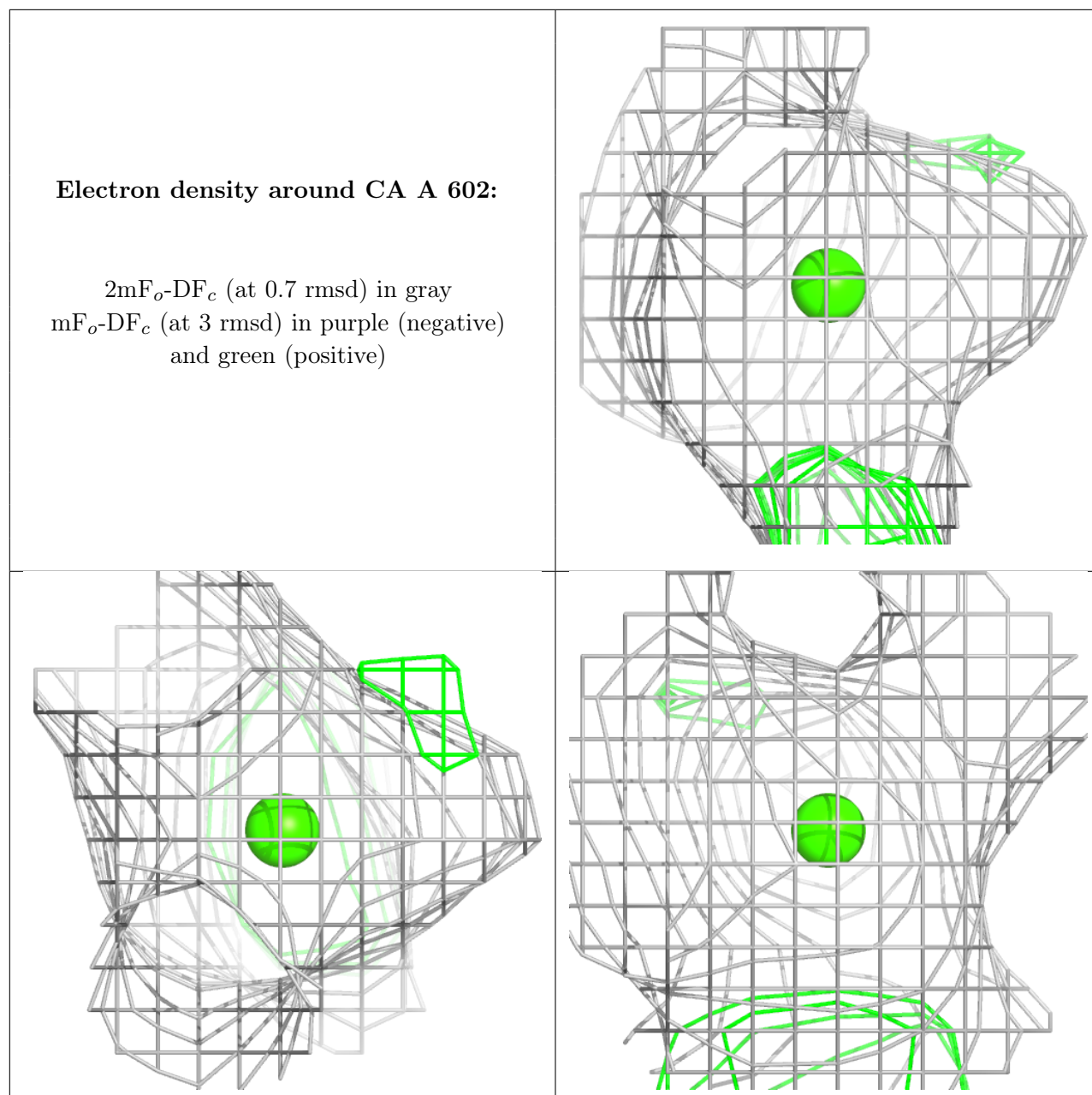
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SIN B 501:

$2mF_o-DF_c$ (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.