



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:25 AM UTC

PDB ID : 9XMY / pdb_00009xmy
Title : Crystal structure of ASCT D62N mutant from Trypanosoma brucei in complex with succinyl-CoA and acetylacetone.
Authors : Mochizuki, K.; Inaoka, D.K.; Fukuda, K.; Kurasawa, H.; Iyoda, K.; Nakai, U.; Harada, S.; Balogun, E.O.; Mazet, M.; Millerieux, Y.; Bringaud, F.; Boshart, M.; Hirayama, K.; Kita, K.; Shiba, T.
Deposited on : 2025-11-11
Resolution : 2.60 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

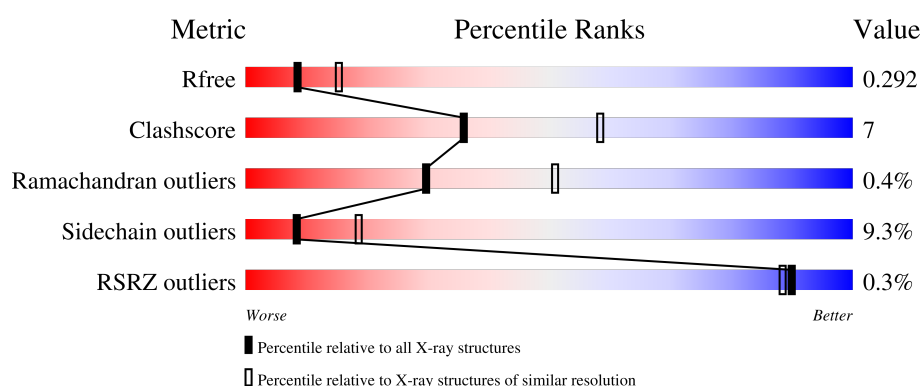
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	493	
1	B	493	
1	C	493	
1	D	493	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14398 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.

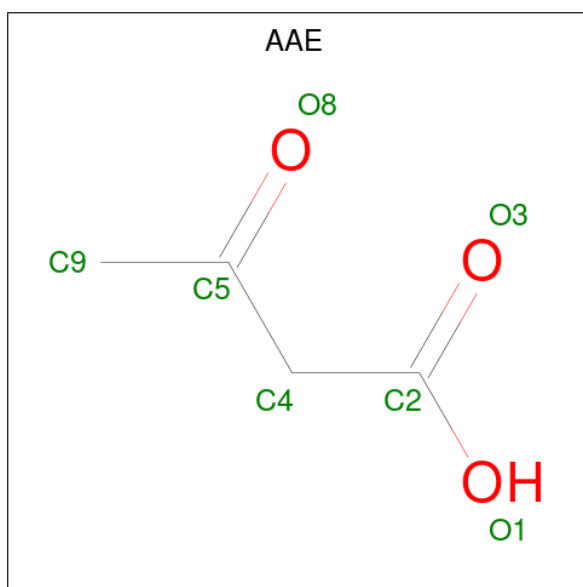
- Molecule 1 is a protein called Succinyl-CoA:3-ketoacid-coenzyme A transferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	1	0
			3569	2241	628	677	23			
1	B	468	Total	C	N	O	S	0	0	0
			3523	2215	617	668	23			
1	C	473	Total	C	N	O	S	0	0	0
			3560	2237	625	675	23			
1	D	471	Total	C	N	O	S	0	0	0
			3549	2228	625	673	23			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	ASN	ASP	engineered mutation	UNP Q386P1
A	419	ASN	SER	conflict	UNP Q386P1
B	62	ASN	ASP	engineered mutation	UNP Q386P1
B	419	ASN	SER	conflict	UNP Q386P1
C	62	ASN	ASP	engineered mutation	UNP Q386P1
C	419	ASN	SER	conflict	UNP Q386P1
D	62	ASN	ASP	engineered mutation	UNP Q386P1
D	419	ASN	SER	conflict	UNP Q386P1

- Molecule 2 is ACETOACETIC ACID (CCD ID: AAE) (formula: C₄H₆O₃) (labeled as "Ligand of Interest" by depositor).

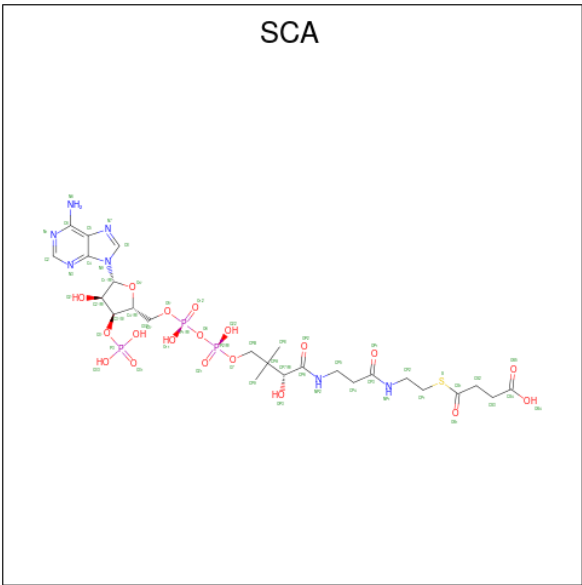


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is CALCIUM ION (CCD ID: 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 SUCCINYL-COENZYME A (CCD ID: SCA) (formula: C₂₅H₄₀N₇O₁₉P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	S	0	0
			55	25	7	19	3	1		
4	D	1	Total	C	N	O	P	S	0	0
			55	25	7	19	3	1		

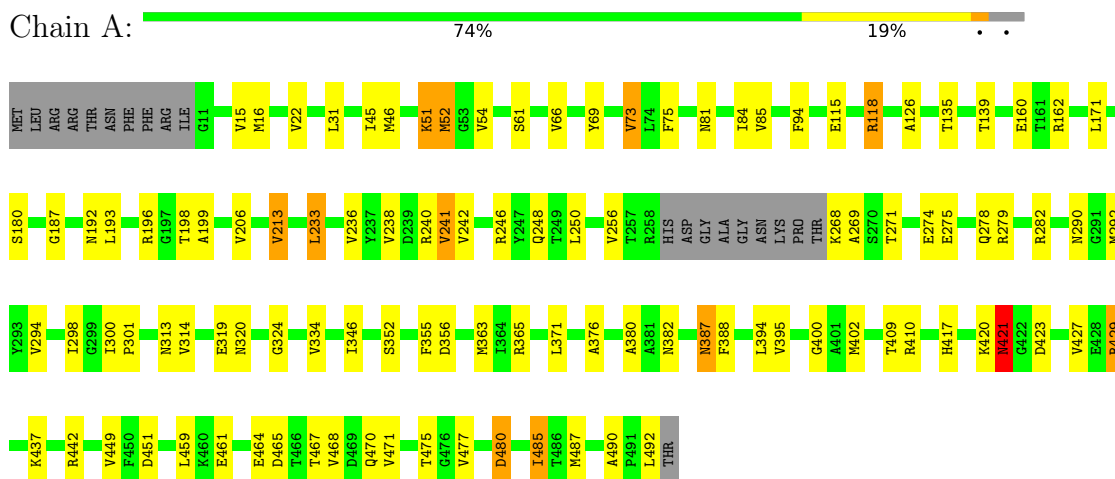
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total	O	0	0
			16	16		
5	B	17	Total	O	0	0
			17	17		
5	C	19	Total	O	0	0
			19	19		
5	D	17	Total	O	0	0
			17	17		

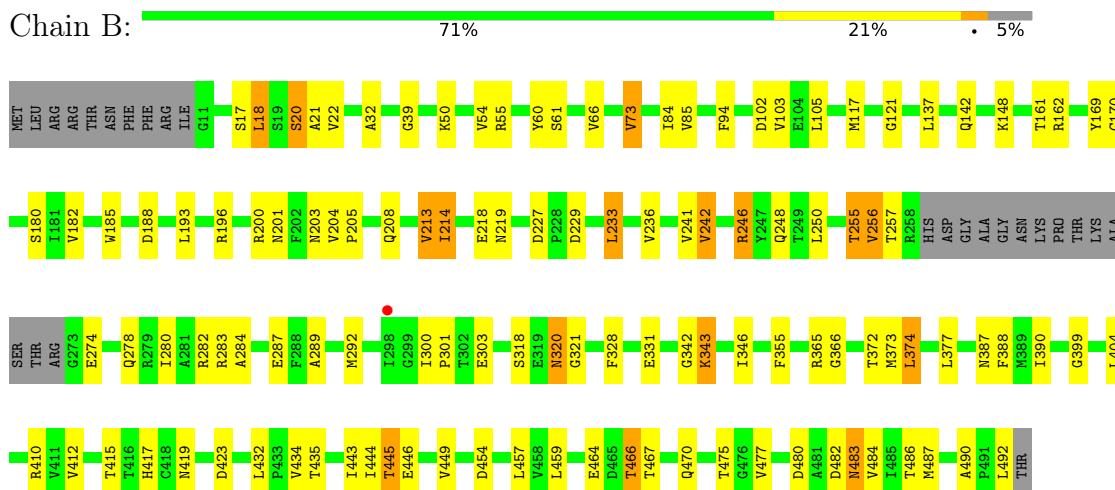
3 Residue-property plots

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

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

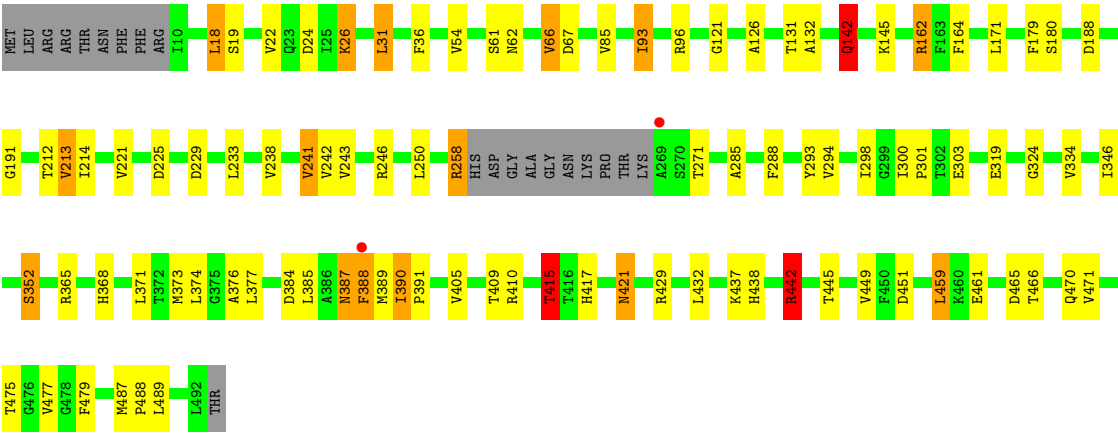


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase

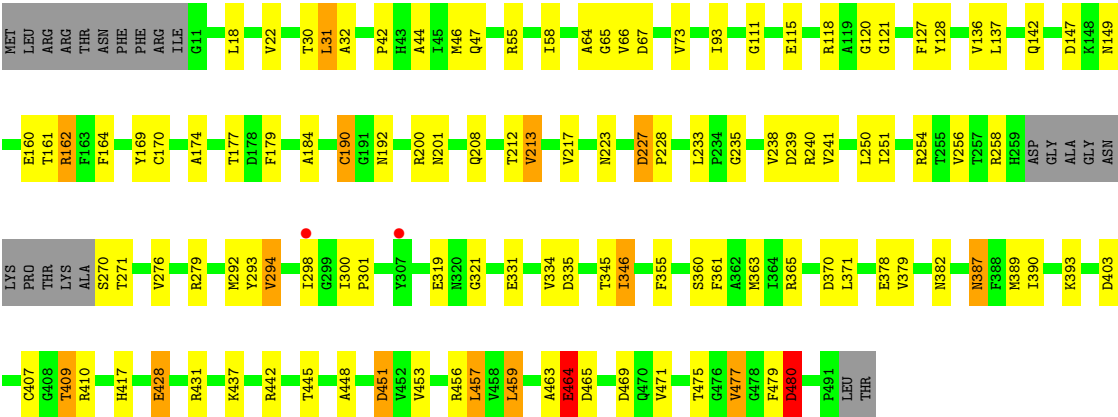


- Molecule 1: Succinyl-CoA:3-ketoacid-coenzyme A transferase





● 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	60.22Å 164.83Å 189.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.60) 99.3 (20.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.207 , 0.296 0.210 , 0.292	Depositor DCC
R_{free} test set	2968 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 21.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14398	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AAE, 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	0.58	0/3626	1.17	12/4905 (0.2%)
1	B	0.57	0/3580	1.12	8/4844 (0.2%)
1	C	0.58	0/3617	1.17	11/4894 (0.2%)
1	D	0.57	0/3607	1.14	10/4880 (0.2%)
All	All	0.58	0/14430	1.15	41/19523 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	9

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ASN	CB-CA-C	-7.16	98.86	110.74
1	D	465	ASP	CA-CB-CG	7.07	119.67	112.60
1	D	18	LEU	N-CA-CB	-6.85	99.79	110.06
1	B	388	PHE	CA-CB-CG	6.81	120.61	113.80
1	A	480	ASP	CA-CB-CG	6.74	119.34	112.60
1	A	464	GLU	CA-C-N	6.71	130.17	120.38
1	A	464	GLU	C-N-CA	6.71	130.17	120.38
1	D	480	ASP	CA-CB-CG	6.21	118.81	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	LYS	N-CA-CB	-5.97	101.17	110.55
1	D	147	ASP	CA-CB-CG	5.94	118.54	112.60
1	D	335	ASP	CA-CB-CG	5.92	118.53	112.60
1	D	239	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	467	THR	CA-CB-OG1	-5.88	100.78	109.60
1	C	18	LEU	N-CA-CB	-5.70	101.81	110.07
1	B	242	VAL	N-CA-CB	-5.65	102.18	111.44
1	A	409	THR	CA-CB-OG1	-5.64	101.13	109.60
1	B	170	CYS	CB-CA-C	-5.62	99.11	109.46
1	C	246	ARG	CB-CA-C	5.58	118.99	109.72
1	C	241	VAL	N-CA-CB	5.53	118.77	111.25
1	C	465	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	384	ASP	CA-CB-CG	5.38	117.98	112.60
1	C	415	THR	CA-CB-OG1	-5.35	101.58	109.60
1	C	225	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	423	ASP	CA-CB-CG	5.33	117.93	112.60
1	B	18	LEU	N-CA-CB	-5.32	102.29	110.01
1	C	229	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	465	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	73	VAL	N-CA-CB	-5.26	102.28	110.54
1	D	393	LYS	CB-CA-C	5.26	119.03	110.24
1	A	51	LYS	N-CA-CB	5.26	118.31	110.22
1	B	102	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	442	ARG	CD-NE-CZ	5.21	131.70	124.40
1	A	139	THR	CA-CB-OG1	-5.21	101.79	109.60
1	B	435	THR	CA-CB-OG1	-5.17	101.85	109.60
1	B	188	ASP	CA-CB-CG	5.14	117.74	112.60
1	B	480	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	160	GLU	CB-CA-C	-5.06	101.45	109.80
1	D	240	ARG	CB-CA-C	-5.05	102.37	110.14
1	C	142	GLN	CB-CA-C	5.04	118.08	109.72
1	C	442	ARG	CG-CD-NE	5.03	123.06	112.00
1	D	361	PHE	CA-CB-CG	-5.02	108.78	113.80

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	118	ARG	Sidechain
1	A	410	ARG	Sidechain
1	A	429	ARG	Sidechain
1	B	283	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	365	ARG	Sidechain
1	C	410	ARG	Sidechain
1	C	442	ARG	Sidechain
1	D	365	ARG	Sidechain
1	D	456	ARG	Sidechain

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	3569	0	3588	49	0
1	B	3523	0	3540	54	0
1	C	3560	0	3581	56	0
1	D	3549	0	3561	56	0
2	A	7	0	5	0	0
2	C	7	0	5	1	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	55	0	35	4	0
4	D	55	0	35	3	0
5	A	16	0	0	2	0
5	B	17	0	0	0	0
5	C	19	0	0	1	0
5	D	17	0	0	1	0
All	All	14398	0	14350	208	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 7.

All (208) 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:417:HIS:NE2	1:C:475:THR:HG22	1.80	0.96
1:C:18:LEU:HD13	1:C:242:VAL:HG11	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:HIS:NE2	1:C:475:THR:CG2	2.46	0.78
1:A:279:ARG:HH11	1:A:279:ARG:HB3	1.55	0.70
1:B:342:GLY:C	1:B:343:LYS:HG2	2.18	0.68
1:A:126:ALA:HB1	1:A:171:LEU:HD11	1.75	0.67
1:A:417:HIS:NE2	1:A:475:THR:HG22	2.08	0.67
1:B:399:GLY:HA3	4:B:501:SCA:S	2.35	0.67
1:C:31:LEU:HD22	1:C:179:PHE:HB2	1.77	0.66
1:D:55:ARG:HH11	1:D:55:ARG:HG2	1.60	0.65
1:A:420:LYS:O	1:A:421:ASN:HB3	1.97	0.63
1:D:457:LEU:HD23	1:D:457:LEU:H	1.63	0.63
1:A:319:GLU:OE1	1:A:400:GLY:HA3	1.97	0.63
1:D:270:SER:O	1:D:271:THR:OG1	2.17	0.63
1:C:24:ASP:O	1:C:26:LYS:HD3	1.99	0.62
1:D:319:GLU:OE1	4:D:501:SCA:H11	2.00	0.61
1:D:213:VAL:HG22	1:D:238:VAL:HA	1.82	0.61
1:C:162:ARG:HD2	1:C:164:PHE:CZ	2.36	0.61
1:B:21:ALA:HB1	1:B:214:ILE:HD12	1.83	0.60
1:C:421:ASN:C	1:C:421:ASN:HD22	2.08	0.60
1:B:193:LEU:HD12	1:B:233:LEU:HD12	1.82	0.60
1:B:372:THR:HG21	1:B:404:LEU:HB3	1.82	0.60
1:A:22:VAL:O	1:A:52:MET:HE2	2.02	0.59
1:A:282:ARG:NH1	1:A:490:ALA:O	2.36	0.59
1:B:60:TYR:CE2	1:B:84:ILE:HD13	2.37	0.59
1:A:442:ARG:HG3	1:A:451:ASP:OD1	2.02	0.58
1:B:417:HIS:NE2	1:B:475:THR:HG22	2.19	0.58
1:C:390:ILE:HG22	1:C:391:PRO:HD2	1.83	0.58
1:B:377:LEU:HD21	4:B:501:SCA:H93	1.85	0.57
1:A:290:ASN:HD22	1:A:313:ASN:H	1.52	0.57
1:C:131:THR:O	1:C:132:ALA:HB3	2.04	0.57
1:D:417:HIS:NE2	1:D:475:THR:HG22	2.19	0.57
1:A:118:ARG:NH2	1:D:115:GLU:OE2	2.36	0.57
1:A:420:LYS:O	1:A:421:ASN:CB	2.52	0.57
1:A:279:ARG:HB3	1:A:279:ARG:NH1	2.20	0.56
1:A:198:THR:HB	1:A:320:ASN:ND2	2.20	0.56
1:A:213:VAL:HG22	1:A:238:VAL:HA	1.87	0.56
1:C:387:ASN:O	1:C:389:MET:N	2.39	0.56
1:D:251:ILE:HG21	1:D:254:ARG:HG3	1.87	0.56
1:C:93:ILE:HG12	1:C:96:ARG:HH22	1.71	0.55
1:C:376:ALA:HB2	1:C:385:LEU:HD11	1.87	0.55
1:B:373:MET:HG2	1:B:412:VAL:HB	1.89	0.55
1:A:294:VAL:HG12	1:A:371:LEU:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ALA:HB1	1:A:274:GLU:HG3	1.88	0.55
1:D:319:GLU:OE2	4:D:501:SCA:HS21	2.07	0.55
1:C:429:ARG:HH21	1:C:429:ARG:HG3	1.72	0.54
1:D:448:ALA:HB1	1:D:459:LEU:HD21	1.90	0.54
1:C:387:ASN:O	1:C:388:PHE:C	2.50	0.53
1:D:471:VAL:O	1:D:475:THR:HG23	2.09	0.53
1:D:128:TYR:HA	1:D:170:CYS:O	2.09	0.53
1:A:356:ASP:C	1:A:356:ASP:OD1	2.50	0.53
1:A:449:VAL:HG23	1:A:487:MET:HE2	1.91	0.53
1:B:50:LYS:HD3	1:B:73:VAL:HG13	1.90	0.52
1:A:380:ALA:HA	1:A:427:VAL:O	2.09	0.52
1:B:483:ASN:O	1:B:484:VAL:HG23	2.10	0.52
1:D:387:ASN:HB2	4:D:501:SCA:H81	1.92	0.52
1:C:258:ARG:HH11	1:C:258:ARG:C	2.17	0.52
1:A:278:GLN:O	1:A:282:ARG:HG3	2.10	0.52
1:B:94:PHE:CZ	1:B:105:LEU:HD13	2.45	0.52
1:B:204:VAL:O	1:B:208:GLN:HG3	2.10	0.51
1:A:196:ARG:O	1:A:199:ALA:HB3	2.10	0.51
1:A:471:VAL:O	1:A:475:THR:HG23	2.11	0.51
1:A:461:GLU:HA	1:A:485:ILE:O	2.10	0.51
1:C:180:SER:HB2	1:C:213:VAL:HB	1.93	0.50
1:A:115:GLU:OE2	1:D:118:ARG:NH2	2.44	0.50
1:C:191:GLY:O	1:C:238:VAL:HG21	2.11	0.50
1:A:75:PHE:CE1	1:A:94:PHE:HD1	2.29	0.50
1:A:300:ILE:HB	1:A:301:PRO:HD3	1.93	0.50
1:B:161:THR:HA	1:B:169:TYR:O	2.11	0.50
1:B:342:GLY:O	1:B:343:LYS:HG2	2.12	0.50
1:A:16:MET:SD	1:A:240:ARG:HD3	2.52	0.49
1:B:300:ILE:HB	1:B:301:PRO:HD3	1.95	0.49
1:D:42:PRO:O	1:D:46:MET:HG2	2.12	0.49
1:D:66:VAL:O	1:D:67:ASP:C	2.55	0.49
1:C:459:LEU:HD12	1:C:479:PHE:CE1	2.48	0.49
1:D:442:ARG:NH1	1:D:451:ASP:OD1	2.46	0.49
1:A:292:MET:HB2	1:A:314:VAL:HG12	1.94	0.49
1:A:420:LYS:O	1:A:421:ASN:ND2	2.45	0.49
1:D:120:GLY:HA2	1:D:174:ALA:HB1	1.94	0.49
1:D:294:VAL:HG12	1:D:371:LEU:HB3	1.95	0.48
1:C:188:ASP:HA	1:C:221:VAL:O	2.13	0.48
1:B:17:SER:HG	1:B:20:SER:HG	1.59	0.48
1:D:192:ASN:OD1	1:D:235:GLY:N	2.47	0.48
1:B:366:GLY:HA3	1:C:121:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LEU:CD2	4:B:501:SCA:H93	2.43	0.48
1:B:256:VAL:HG21	1:B:331:GLU:HG2	1.96	0.47
1:D:463:ALA:O	1:D:464:GLU:C	2.57	0.47
1:B:321:GLY:HA2	1:B:355:PHE:CE2	2.49	0.47
1:C:179:PHE:HA	1:C:212:THR:O	2.14	0.47
1:D:321:GLY:HA2	1:D:355:PHE:CE2	2.50	0.47
1:D:428:GLU:HB3	1:D:477:VAL:CG1	2.44	0.47
1:D:457:LEU:H	1:D:457:LEU:CD2	2.28	0.47
1:B:284:ALA:O	1:B:287:GLU:HB2	2.15	0.46
1:D:292:MET:HA	1:D:370:ASP:OD2	2.15	0.46
1:D:200:ARG:O	1:D:201:ASN:C	2.58	0.46
1:D:480:ASP:OD1	1:D:480:ASP:C	2.58	0.46
1:A:324:GLY:HA3	1:A:352:SER:HB3	1.97	0.46
1:C:389:MET:O	1:C:390:ILE:HG13	2.15	0.46
1:A:61:SER:O	1:A:85:VAL:HA	2.15	0.46
1:D:111:GLY:HA3	1:D:403:ASP:OD1	2.15	0.46
1:C:66:VAL:HG22	1:C:67:ASP:N	2.31	0.46
1:B:60:TYR:CE2	1:B:84:ILE:CD1	2.99	0.46
1:C:243:VAL:HG12	1:C:243:VAL:O	2.16	0.46
1:B:18:LEU:O	1:B:22:VAL:HG23	2.15	0.46
1:C:61:SER:O	1:C:85:VAL:HG12	2.16	0.46
1:D:30:THR:C	1:D:31:LEU:HD23	2.41	0.45
1:D:32:ALA:HB2	1:D:177:THR:HG21	1.98	0.45
1:A:365:ARG:NH2	5:A:702:HOH:O	2.49	0.45
1:C:301:PRO:HB3	1:C:373:MET:HB3	1.98	0.45
1:C:461:GLU:OE1	1:C:488:PRO:HD2	2.17	0.45
1:D:407:CYS:SG	1:D:409:THR:HB	2.56	0.45
1:B:374:LEU:HD23	1:B:374:LEU:N	2.31	0.45
1:C:319:GLU:OE2	2:C:601:AAE:O1	2.33	0.45
1:D:64:ALA:O	1:D:65:GLY:C	2.60	0.45
1:B:443:ILE:HD12	1:B:457:LEU:HD11	1.98	0.45
1:C:442:ARG:NH1	1:C:451:ASP:OD1	2.48	0.45
1:D:137:LEU:HD12	1:D:137:LEU:N	2.31	0.45
1:D:378:GLU:OE1	1:D:431:ARG:N	2.50	0.45
1:A:271:THR:O	1:A:275:GLU:HB2	2.17	0.44
1:B:185:TRP:HA	1:B:218:GLU:OE1	2.17	0.44
1:B:466:THR:HG22	1:B:470:GLN:HG2	1.99	0.44
1:A:160:GLU:OE2	1:B:162:ARG:HG2	2.17	0.44
1:C:285:ALA:HA	1:C:288:PHE:CD2	2.52	0.44
1:C:324:GLY:HA3	1:C:352:SER:HB3	1.99	0.44
1:C:365:ARG:NH1	5:C:704:HOH:O	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:LEU:HD23	1:D:31:LEU:N	2.32	0.44
1:D:161:THR:HA	1:D:169:TYR:O	2.16	0.44
1:D:162:ARG:HD2	1:D:164:PHE:CE1	2.52	0.44
1:B:180:SER:HB2	1:B:213:VAL:HB	2.00	0.44
1:B:182:VAL:HB	1:B:203:ASN:OD1	2.18	0.44
1:B:415:THR:O	1:B:445:THR:HA	2.17	0.44
1:B:318:SER:OG	1:B:320:ASN:OD1	2.35	0.44
1:C:471:VAL:O	1:C:475:THR:HG23	2.17	0.44
1:D:410:ARG:HH22	1:D:442:ARG:HE	1.64	0.44
1:C:390:ILE:HD12	1:C:390:ILE:N	2.32	0.44
1:A:187:GLY:HA2	1:A:192:ASN:O	2.18	0.44
1:B:121:GLY:O	1:C:368:HIS:NE2	2.50	0.44
1:C:294:VAL:HG12	1:C:371:LEU:HB3	1.99	0.44
1:C:377:LEU:HG	1:C:387:ASN:HA	2.00	0.44
1:D:294:VAL:HG11	1:D:371:LEU:HD23	2.00	0.44
1:C:442:ARG:HG3	1:C:451:ASP:OD1	2.18	0.43
1:B:55:ARG:CZ	1:B:55:ARG:HB3	2.48	0.43
1:C:126:ALA:HB1	1:C:171:LEU:HD11	2.00	0.43
1:A:135:THR:HG21	1:A:402:MET:HE2	2.00	0.43
1:A:376:ALA:HA	1:A:387:ASN:HB3	2.00	0.43
1:C:36:PHE:CD2	1:C:62:ASN:ND2	2.86	0.43
1:D:30:THR:HG22	1:D:58:ILE:HB	2.00	0.43
1:D:44:ALA:HA	1:D:47:GLN:HE21	1.83	0.43
1:B:236:VAL:HA	1:C:293:TYR:CZ	2.54	0.43
1:D:121:GLY:HA3	1:D:208:GLN:O	2.18	0.43
1:D:300:ILE:N	1:D:301:PRO:CD	2.82	0.43
1:B:387:ASN:O	4:B:501:SCA:OP1	2.37	0.43
1:A:365:ARG:NH1	5:A:703:HOH:O	2.51	0.43
1:C:374:LEU:HD11	1:C:385:LEU:HD21	2.00	0.43
1:A:355:PHE:CE1	1:A:363:MET:HE1	2.53	0.42
1:A:15:VAL:HG22	1:A:241:VAL:HG22	2.00	0.42
1:B:280:ILE:HG23	1:B:444:ILE:HG22	2.01	0.42
1:B:282:ARG:HD2	1:B:490:ALA:O	2.19	0.42
1:C:258:ARG:C	1:C:258:ARG:NH1	2.77	0.42
1:D:184:ALA:O	1:D:217:VAL:HA	2.19	0.42
1:A:300:ILE:N	1:A:301:PRO:CD	2.82	0.42
1:D:457:LEU:HG	1:D:479:PHE:HB3	2.00	0.42
1:B:289:ALA:HB3	1:B:292:MET:HE3	2.02	0.42
1:D:360:SER:O	1:D:363:MET:HB3	2.18	0.42
1:D:200:ARG:HB3	5:D:610:HOH:O	2.18	0.42
1:A:180:SER:HB2	1:A:213:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:THR:O	1:C:445:THR:HA	2.20	0.42
1:B:282:ARG:NH2	1:B:490:ALA:O	2.43	0.42
1:B:446:GLU:OE1	1:B:446:GLU:N	2.45	0.42
1:D:227:ASP:OD1	1:D:228:PRO:HD2	2.20	0.42
1:B:449:VAL:HG23	1:B:487:MET:HE2	2.02	0.41
1:B:21:ALA:HB1	1:B:214:ILE:CD1	2.50	0.41
1:B:32:ALA:HA	1:B:60:TYR:O	2.20	0.41
1:B:61:SER:O	1:B:85:VAL:HA	2.20	0.41
1:D:190:CYS:HB3	1:D:223:ASN:ND2	2.35	0.41
1:A:236:VAL:HA	1:D:293:TYR:CE1	2.56	0.41
1:C:421:ASN:C	1:C:421:ASN:ND2	2.76	0.41
1:D:346:ILE:HD12	1:D:346:ILE:HA	1.92	0.41
1:B:320:ASN:OD1	1:B:320:ASN:N	2.53	0.41
1:B:32:ALA:HB1	1:B:117:MET:HE2	2.03	0.41
1:D:179:PHE:HA	1:D:212:THR:O	2.20	0.41
1:C:142:GLN:HE21	1:C:142:GLN:HB2	1.58	0.41
1:C:300:ILE:N	1:C:301:PRO:CD	2.84	0.41
1:C:417:HIS:CD2	1:C:475:THR:HG22	2.54	0.41
1:C:437:LYS:O	1:C:438:HIS:C	2.63	0.41
1:D:115:GLU:HB3	1:D:127:PHE:CZ	2.55	0.41
1:D:137:LEU:N	1:D:137:LEU:CD1	2.83	0.41
1:D:334:VAL:HG13	1:D:345:THR:HG21	2.02	0.41
1:A:84:ILE:HD12	1:A:84:ILE:N	2.35	0.41
1:A:193:LEU:HD12	1:A:233:LEU:HD12	2.03	0.41
1:A:395:VAL:O	1:A:395:VAL:HG13	2.20	0.41
1:B:390:ILE:HG23	1:B:432:LEU:HD22	2.02	0.41
1:B:200:ARG:O	1:B:201:ASN:C	2.63	0.41
1:A:66:VAL:HG12	1:A:69:TYR:HB3	2.03	0.41
1:C:131:THR:O	1:C:132:ALA:CB	2.68	0.41
1:D:459:LEU:HD12	1:D:479:PHE:CE1	2.56	0.41
1:A:45:ILE:O	1:A:46:MET:C	2.64	0.41
1:B:227:ASP:C	1:B:229:ASP:H	2.28	0.41
1:C:162:ARG:HD2	1:C:164:PHE:CE1	2.55	0.41
1:C:390:ILE:HG23	1:C:432:LEU:HD22	2.03	0.41
1:C:449:VAL:HG23	1:C:487:MET:HE2	2.03	0.41
1:B:246:ARG:H	1:B:246:ARG:HG2	1.76	0.40
1:C:66:VAL:CG2	1:C:67:ASP:N	2.84	0.40
1:A:246:ARG:HA	1:A:246:ARG:HD2	1.97	0.40
1:B:255:THR:HB	1:B:328:PHE:CD2	2.56	0.40
1:C:385:LEU:HD23	1:C:405:VAL:HG11	2.03	0.40
1:C:300:ILE:HB	1:C:301:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:PRO:HA	1:B:208:GLN:HE21	1.87	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	470/493 (95%)	439 (93%)	29 (6%)	2 (0%)	30	51
1	B	464/493 (94%)	438 (94%)	23 (5%)	3 (1%)	21	42
1	C	469/493 (95%)	442 (94%)	26 (6%)	1 (0%)	43	66
1	D	467/493 (95%)	437 (94%)	28 (6%)	2 (0%)	30	51
All	All	1870/1972 (95%)	1756 (94%)	106 (6%)	8 (0%)	30	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	ASN
1	C	388	PHE
1	D	464	GLU
1	A	387	ASN
1	B	39	GLY
1	D	387	ASN
1	B	410	ARG
1	B	482	ASP

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	381/397 (96%)	350 (92%)	31 (8%)	11	24
1	B	376/397 (95%)	335 (89%)	41 (11%)	6	13
1	C	380/397 (96%)	348 (92%)	32 (8%)	10	23
1	D	379/397 (96%)	341 (90%)	38 (10%)	7	16
All	All	1516/1588 (96%)	1374 (91%)	142 (9%)	8	18

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	51	LYS
1	A	52	MET
1	A	54	VAL
1	A	73	VAL
1	A	81[A]	ASN
1	A	81[B]	ASN
1	A	162	ARG
1	A	206	VAL
1	A	213	VAL
1	A	233	LEU
1	A	241	VAL
1	A	242	VAL
1	A	248	GLN
1	A	250	LEU
1	A	256	VAL
1	A	268	LYS
1	A	298	ILE
1	A	334	VAL
1	A	346	ILE
1	A	388	PHE
1	A	394	LEU
1	A	421	ASN
1	A	429	ARG
1	A	459	LEU
1	A	468	VAL
1	A	470	GLN
1	A	477	VAL
1	A	480	ASP
1	A	485	ILE

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Mol	Chain	Res	Type
1	A	492	LEU
1	B	20	SER
1	B	54	VAL
1	B	66	VAL
1	B	73	VAL
1	B	103	VAL
1	B	137	LEU
1	B	142	GLN
1	B	148	LYS
1	B	196	ARG
1	B	213	VAL
1	B	214	ILE
1	B	219	ASN
1	B	233	LEU
1	B	241	VAL
1	B	242	VAL
1	B	246	ARG
1	B	248	GLN
1	B	250	LEU
1	B	255	THR
1	B	256	VAL
1	B	257	THR
1	B	274	GLU
1	B	278	GLN
1	B	303	GLU
1	B	320	ASN
1	B	343	LYS
1	B	346	ILE
1	B	374	LEU
1	B	419	ASN
1	B	423	ASP
1	B	434	VAL
1	B	445	THR
1	B	454	ASP
1	B	459	LEU
1	B	464	GLU
1	B	466	THR
1	B	467	THR
1	B	477	VAL
1	B	483	ASN
1	B	486	THR
1	B	492	LEU

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Mol	Chain	Res	Type
1	C	19	SER
1	C	22	VAL
1	C	26	LYS
1	C	31	LEU
1	C	54	VAL
1	C	66	VAL
1	C	93	ILE
1	C	142	GLN
1	C	145	LYS
1	C	162	ARG
1	C	213	VAL
1	C	214	ILE
1	C	233	LEU
1	C	241	VAL
1	C	250	LEU
1	C	258	ARG
1	C	271	THR
1	C	298	ILE
1	C	303	GLU
1	C	334	VAL
1	C	346	ILE
1	C	352	SER
1	C	387	ASN
1	C	390	ILE
1	C	409	THR
1	C	415	THR
1	C	421	ASN
1	C	459	LEU
1	C	466	THR
1	C	470	GLN
1	C	477	VAL
1	C	489	LEU
1	D	22	VAL
1	D	31	LEU
1	D	73	VAL
1	D	93	ILE
1	D	136	VAL
1	D	142	GLN
1	D	149	ASN
1	D	162	ARG
1	D	190	CYS
1	D	213	VAL

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Mol	Chain	Res	Type
1	D	227	ASP
1	D	233	LEU
1	D	241	VAL
1	D	250	LEU
1	D	256	VAL
1	D	258	ARG
1	D	276	VAL
1	D	279	ARG
1	D	294	VAL
1	D	298	ILE
1	D	331	GLU
1	D	346	ILE
1	D	379	VAL
1	D	382	ASN
1	D	389	MET
1	D	390	ILE
1	D	409	THR
1	D	428	GLU
1	D	437	LYS
1	D	445	THR
1	D	451	ASP
1	D	453	VAL
1	D	457	LEU
1	D	459	LEU
1	D	464	GLU
1	D	469	ASP
1	D	477	VAL
1	D	480	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	ASN
1	A	97	GLN
1	A	110	GLN
1	A	208	GLN
1	A	248	GLN
1	A	290	ASN
1	A	295	ASN
1	A	306	ASN
1	A	382	ASN
1	A	419	ASN

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Mol	Chain	Res	Type
1	A	470	GLN
1	B	81	ASN
1	B	142	GLN
1	B	208	GLN
1	B	248	GLN
1	B	278	GLN
1	B	290	ASN
1	B	313	ASN
1	B	348	HIS
1	B	419	ASN
1	B	470	GLN
1	B	483	ASN
1	C	47	GLN
1	C	62	ASN
1	C	110	GLN
1	C	142	GLN
1	C	208	GLN
1	C	306	ASN
1	C	419	ASN
1	C	421	ASN
1	C	438	HIS
1	D	27	ASN
1	D	47	GLN
1	D	77	ASN
1	D	81	ASN
1	D	97	GLN
1	D	110	GLN
1	D	208	GLN
1	D	348	HIS
1	D	382	ASN
1	D	421	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	AAE	C	601	-	6,6,6	1.06	0	7,7,7	0.98	0
2	AAE	A	601	-	6,6,6	1.20	1 (16%)	7,7,7	1.38	1 (14%)
4	SCA	D	501	-	55,57,57	0.81	2 (3%)	78,84,84	1.20	4 (5%)
4	SCA	B	501	-	55,57,57	0.72	2 (3%)	78,84,84	1.23	4 (5%)

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	AAE	C	601	-	-	3/4/4/4	-
2	AAE	A	601	-	-	3/4/4/4	-
4	SCA	D	501	-	-	22/56/72/72	0/3/3/3
4	SCA	B	501	-	-	27/56/72/72	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	501	SCA	P1-O6	2.98	1.62	1.59
4	D	501	SCA	P2-O6	2.88	1.62	1.59
4	B	501	SCA	P2-O6	2.26	1.61	1.59
2	A	601	AAE	C4-C2	2.23	1.54	1.51
4	B	501	SCA	P1-O6	2.21	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	501	SCA	CP1-S-CS1	7.67	124.52	101.84
4	B	501	SCA	CP1-S-CS1	7.19	123.11	101.84
4	B	501	SCA	P3-O3'-C3'	-3.51	114.07	123.43
4	D	501	SCA	P3-O3'-C3'	-3.04	115.31	123.43
2	A	601	AAE	C5-C4-C2	3.01	119.21	112.35
4	B	501	SCA	CP5-CP4-CP3	2.95	117.31	112.39
4	D	501	SCA	C3'-C2'-C1'	2.14	104.60	99.89
4	B	501	SCA	CP4-CP3-NP1	2.04	120.05	116.34
4	D	501	SCA	CP2-NP1-CP3	2.02	126.58	122.82

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	AAE	C2-C4-C5-O8
2	A	601	AAE	C2-C4-C5-C9
2	C	601	AAE	C2-C4-C5-O8
2	C	601	AAE	C2-C4-C5-C9
4	B	501	SCA	C5'-O5'-P1-O11
4	B	501	SCA	C5'-O5'-P1-O12
4	B	501	SCA	C5'-O5'-P1-O6
4	B	501	SCA	CPB-O7-P2-O6
4	B	501	SCA	CPB-O7-P2-O21
4	B	501	SCA	OP3-CP7-CPA-CPB
4	B	501	SCA	CP6-CP7-CPA-CPB
4	B	501	SCA	OP3-CP7-CPA-CP9
4	B	501	SCA	CP6-CP7-CPA-CP9
4	B	501	SCA	OP3-CP7-CPA-CP8
4	B	501	SCA	CP6-CP7-CPA-CP8
4	B	501	SCA	CP7-CP6-NP2-CP5
4	B	501	SCA	CP3-CP4-CP5-NP2
4	B	501	SCA	CP4-CP3-NP1-CP2
4	B	501	SCA	OP1-CP3-NP1-CP2
4	D	501	SCA	O4'-C1'-N9-C8
4	D	501	SCA	O4'-C1'-N9-C4
4	D	501	SCA	C5'-O5'-P1-O11
4	D	501	SCA	C5'-O5'-P1-O12
4	D	501	SCA	C5'-O5'-P1-O6
4	D	501	SCA	CPB-O7-P2-O6
4	D	501	SCA	CPB-O7-P2-O21
4	D	501	SCA	CPB-O7-P2-O22

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Mol	Chain	Res	Type	Atoms
4	D	501	SCA	CP6-CP7-CPA-CPB
4	D	501	SCA	CP6-CP7-CPA-CP9
4	D	501	SCA	S-CP1-CP2-NP1
4	D	501	SCA	OS1-CS1-S-CP1
4	D	501	SCA	CS2-CS1-S-CP1
4	D	501	SCA	CP4-CP3-NP1-CP2
4	B	501	SCA	O4'-C4'-C5'-O5'
4	B	501	SCA	OP2-CP6-NP2-CP5
4	D	501	SCA	OP1-CP3-NP1-CP2
4	D	501	SCA	CS1-CS2-CS3-CS4
4	B	501	SCA	C3'-C4'-C5'-O5'
4	B	501	SCA	OP2-CP6-CP7-OP3
4	B	501	SCA	CS1-CS2-CS3-CS4
4	B	501	SCA	NP2-CP6-CP7-OP3
4	D	501	SCA	NP2-CP6-CP7-OP3
4	B	501	SCA	OS1-CS1-S-CP1
4	B	501	SCA	CS2-CS1-S-CP1
4	D	501	SCA	CP6-CP7-CPA-CP8
4	B	501	SCA	P2-O6-P1-O12
4	B	501	SCA	P1-O6-P2-O21
4	D	501	SCA	CP2-CP1-S-CS1
4	D	501	SCA	OP3-CP7-CPA-CPB
4	D	501	SCA	OP3-CP7-CPA-CP8
2	A	601	AAE	O3-C2-C4-C5
2	C	601	AAE	O3-C2-C4-C5
4	D	501	SCA	OP3-CP7-CPA-CP9
4	B	501	SCA	P2-O6-P1-O11
4	B	501	SCA	P1-O6-P2-O22

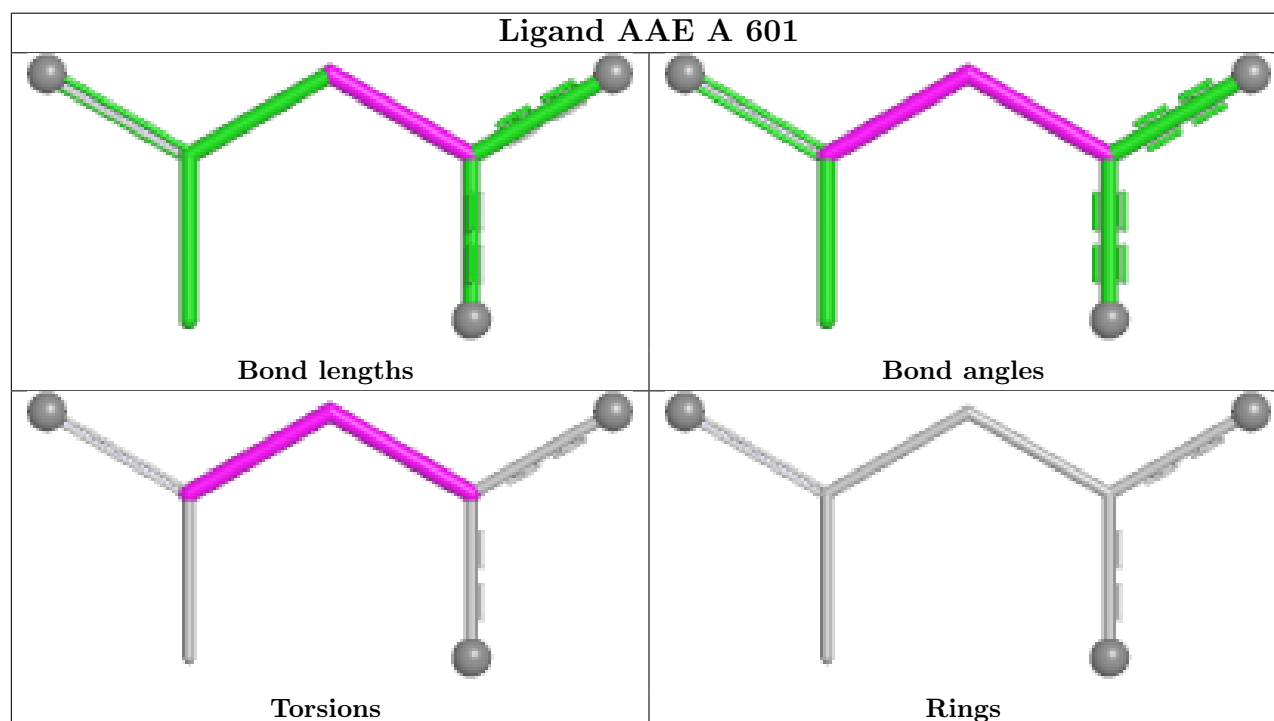
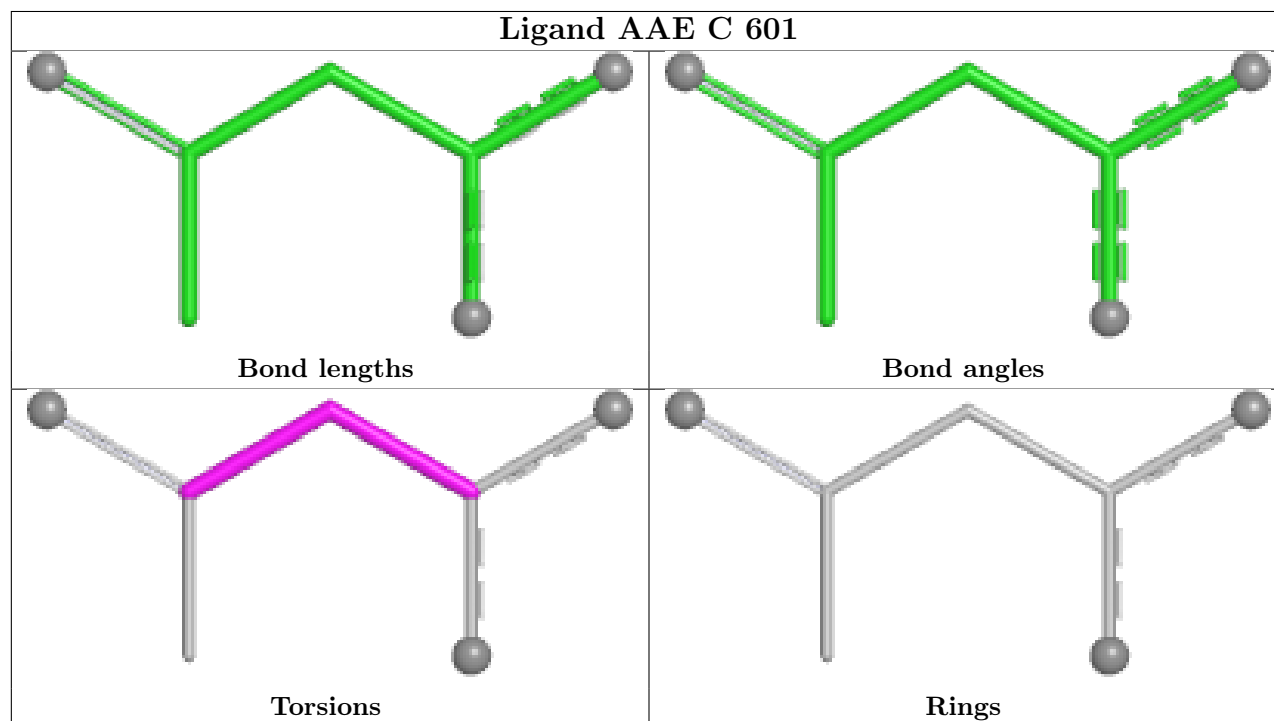
There are no ring outliers.

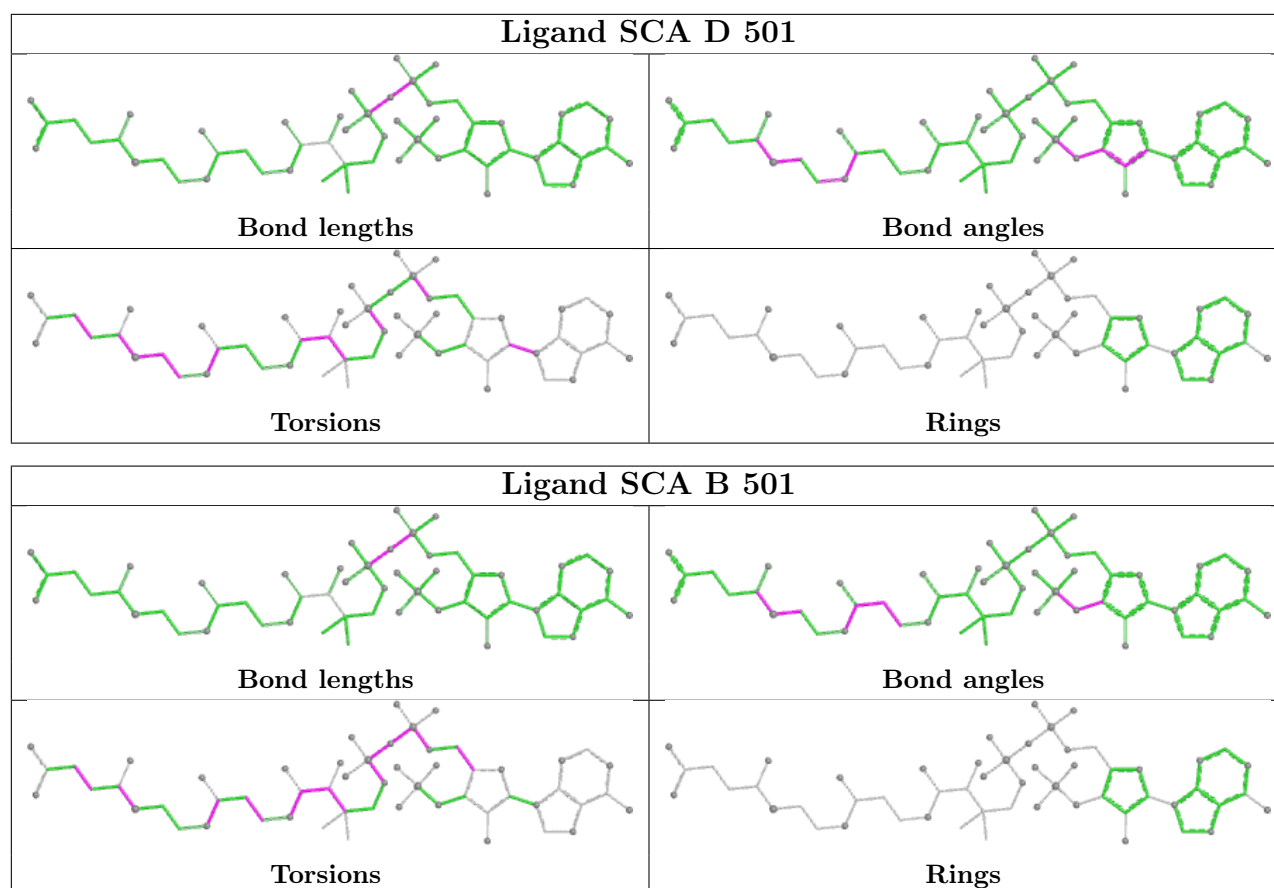
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	AAE	1	0
4	D	501	SCA	3	0
4	B	501	SCA	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	473/493 (95%)	-0.29	0	100 100	18, 44, 70, 122	2 (0%)
1	B	468/493 (94%)	-0.19	1 (0%)	91 90	29, 49, 83, 111	1 (0%)
1	C	473/493 (95%)	-0.30	2 (0%)	88 86	27, 44, 70, 117	1 (0%)
1	D	471/493 (95%)	-0.09	2 (0%)	88 86	27, 50, 94, 122	1 (0%)
All	All	1885/1972 (95%)	-0.22	5 (0%)	90 88	18, 47, 84, 122	5 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	298	ILE	2.2
1	C	388	PHE	2.2
1	C	269	ALA	2.1
1	D	298	ILE	2.0
1	D	307	TYR	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,

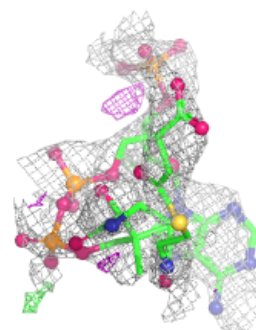
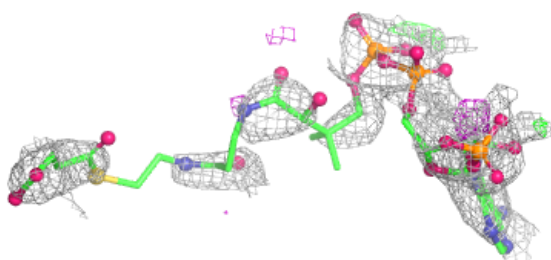
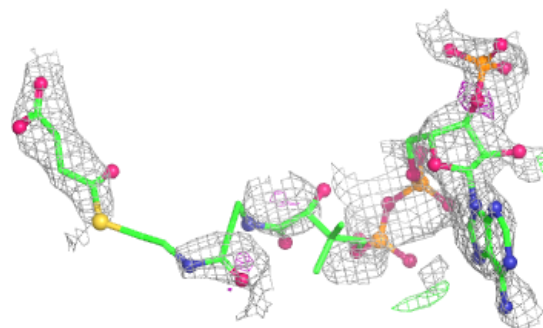
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SCA	B	501	55/55	0.60	0.14	75,134,171,174	0
4	SCA	D	501	55/55	0.65	0.15	78,124,148,150	0
2	AAE	A	601	7/7	0.80	0.13	57,61,69,70	0
3	CA	C	602	1/1	0.88	0.07	72,72,72,72	0
2	AAE	C	601	7/7	0.91	0.09	51,55,64,66	0
3	CA	A	602	1/1	0.92	0.07	58,58,58,58	0
3	CA	B	502	1/1	0.94	0.08	60,60,60,60	0
3	CA	D	502	1/1	0.94	0.08	65,65,65,65	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.

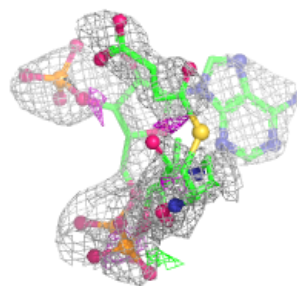
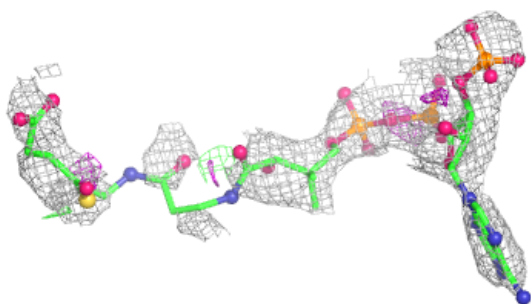
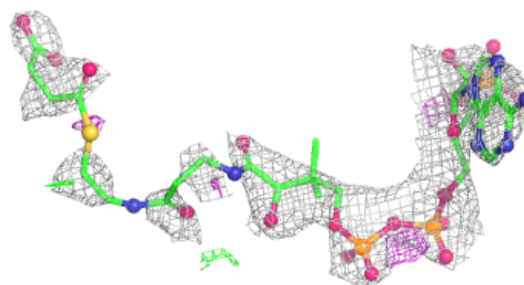
Electron density around SCA B 501:

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

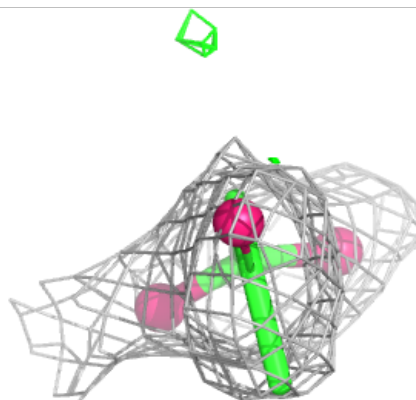
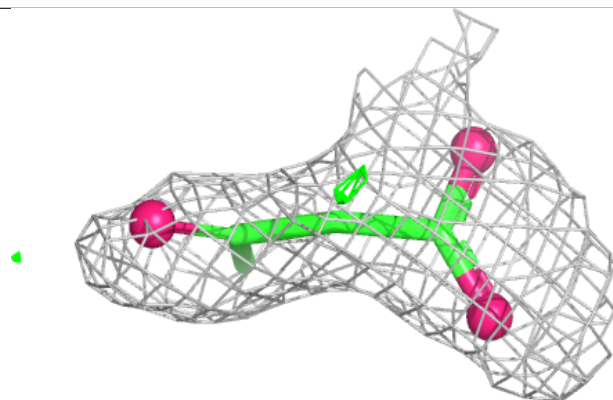
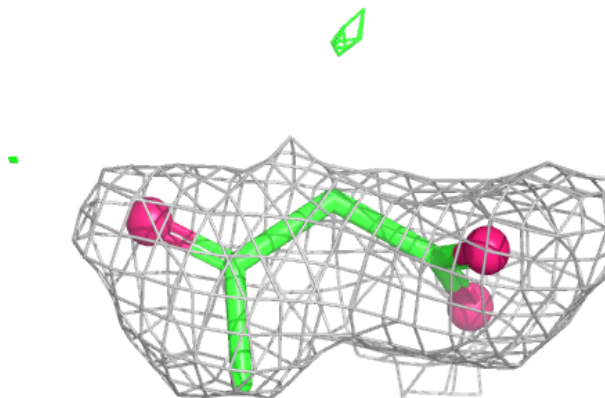


Electron density around SCA D 501:

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

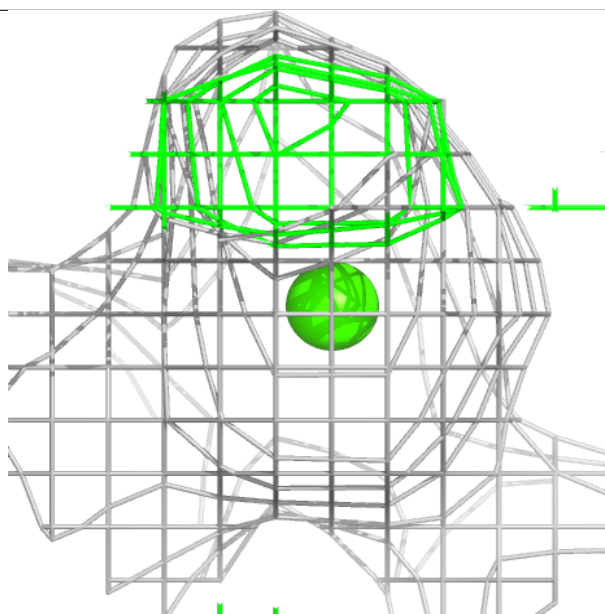
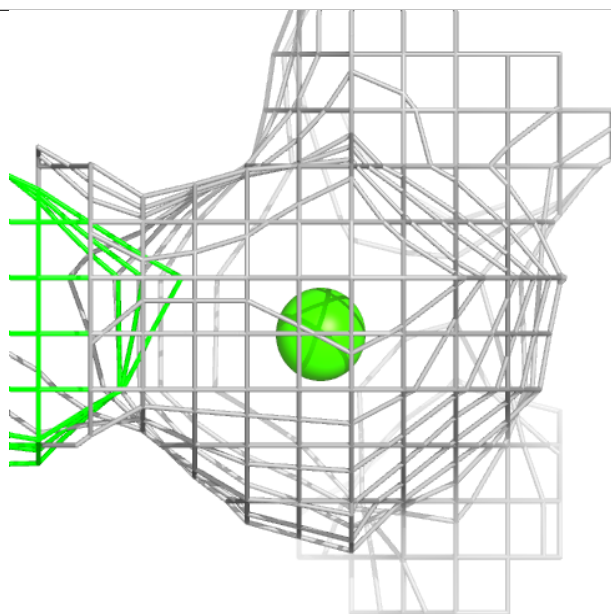
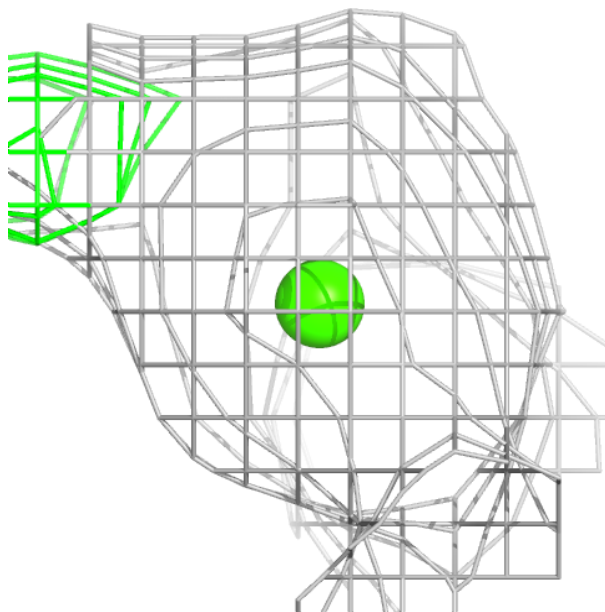
**Electron density around AAE A 601:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



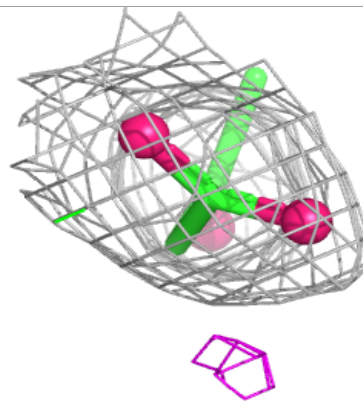
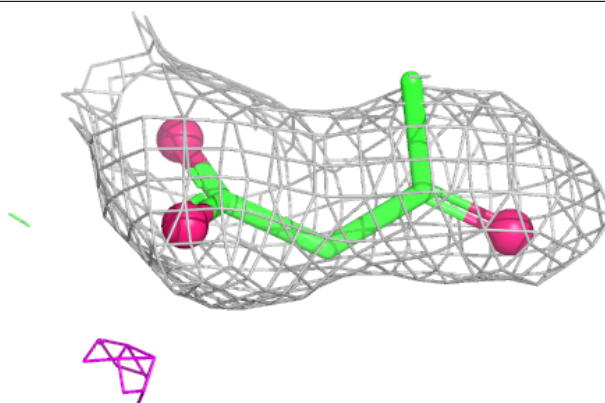
Electron density around CA C 602:

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



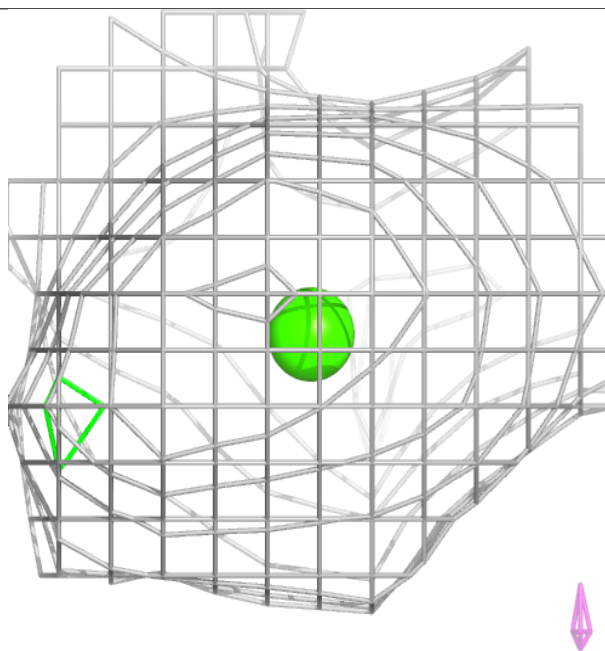
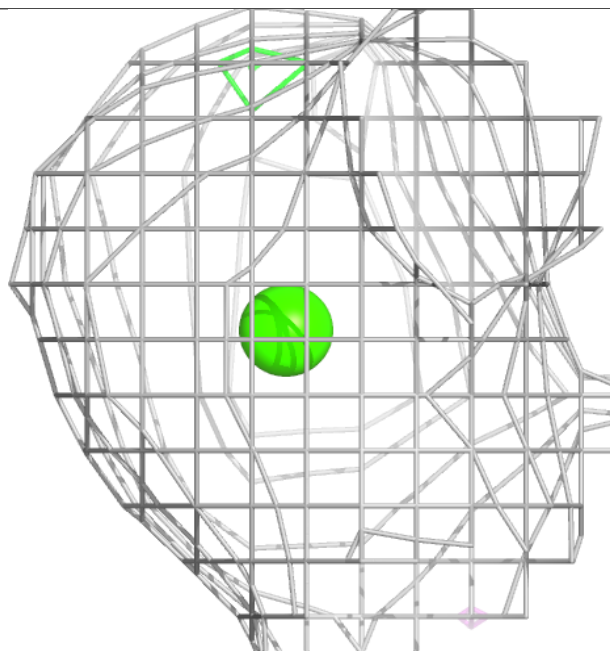
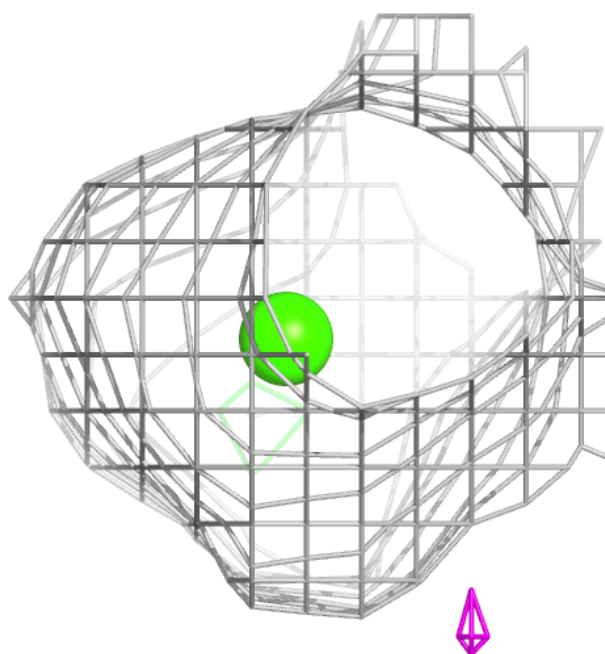
Electron density around AAE C 601:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



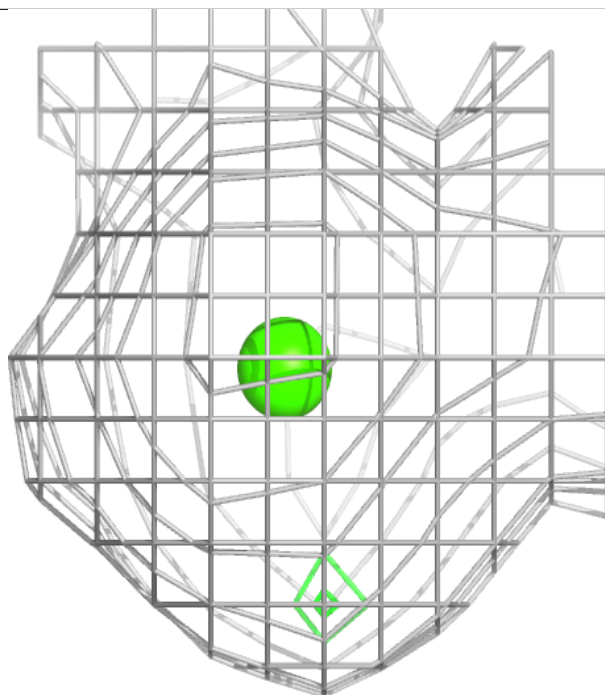
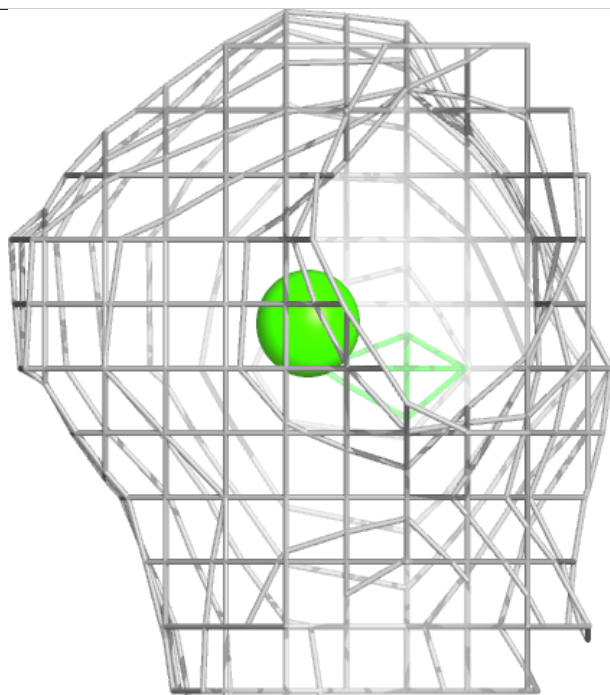
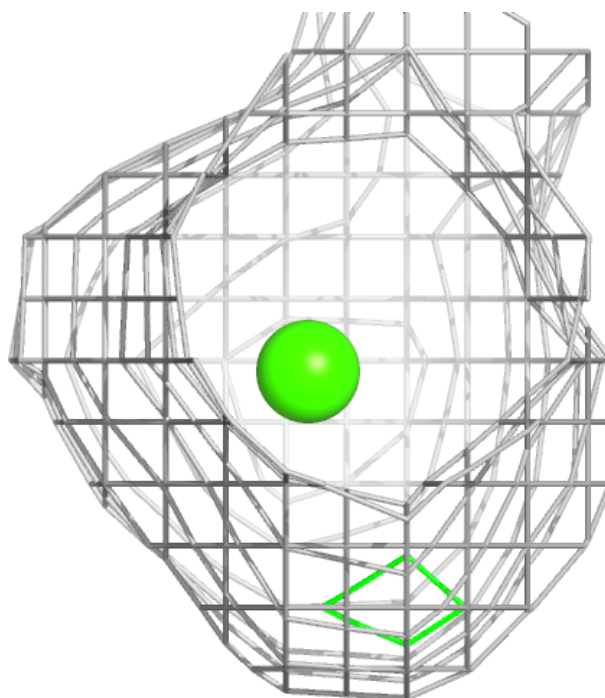
Electron density around CA A 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



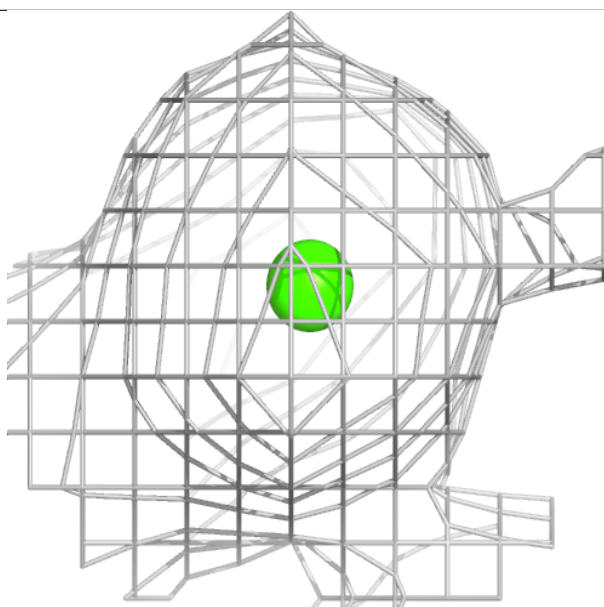
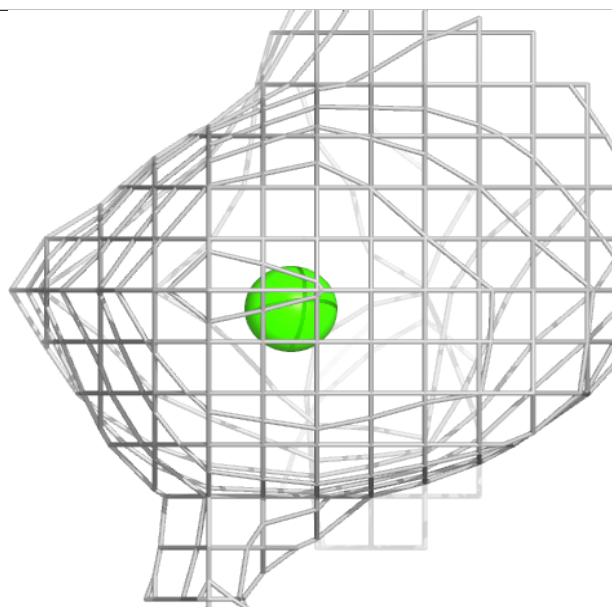
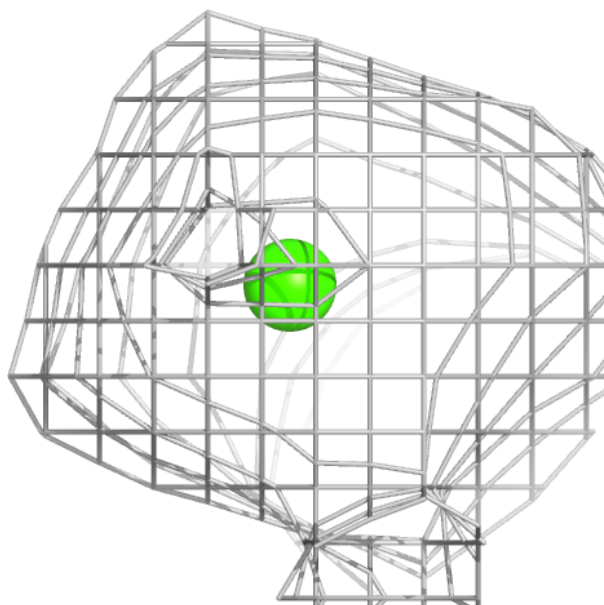
Electron density around CA B 502:

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



Electron density around CA 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.