



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 5J9W / pdb_00005j9w
Title : Crystal structure of the NuA4 core complex
Authors : Chen, Z.C.; Xu, P.
Deposited on : 2016-04-11
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

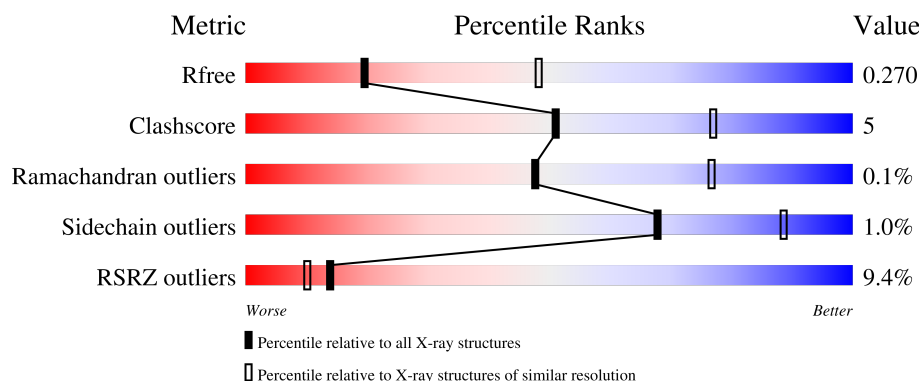
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	305	3% 79% 12% 9%
1	E	305	5% 75% 15% 9%
1	I	305	7% 79% 12% 9%
2	B	113	9% 58% 7% 35%
2	F	113	8% 56% 40%

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Mol	Chain	Length	Quality of chain
2	J	113	
3	C	280	
3	G	280	
3	K	280	
4	D	120	
4	H	120	
4	L	120	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18691 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 Histone acetyltransferase ESA1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	278	Total	C	N	O	S	0	0	0
			2355	1523	396	426	10			
1	A	278	Total	C	N	O	S	0	0	0
			2355	1523	396	426	10			
1	I	278	Total	C	N	O	S	0	0	0
			2355	1523	396	426	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	338	GLN	GLU	engineered mutation	UNP Q08649
A	338	GLN	GLU	engineered mutation	UNP Q08649
I	338	GLN	GLU	engineered mutation	UNP Q08649

- Molecule 2 is a protein called Chromatin modification-related protein EAF6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	68	Total	C	N	O		0	0	0
			570	355	96	119				
2	B	74	Total	C	N	O	S	0	0	0
			619	385	103	130	1			
2	J	70	Total	C	N	O		0	0	0
			587	367	99	121				

- Molecule 3 is a protein called Enhancer of polycomb-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	275	Total	C	N	O	S	0	0	0
			2307	1449	408	441	9			
3	C	267	Total	C	N	O	S	0	0	0
			2241	1410	392	430	9			

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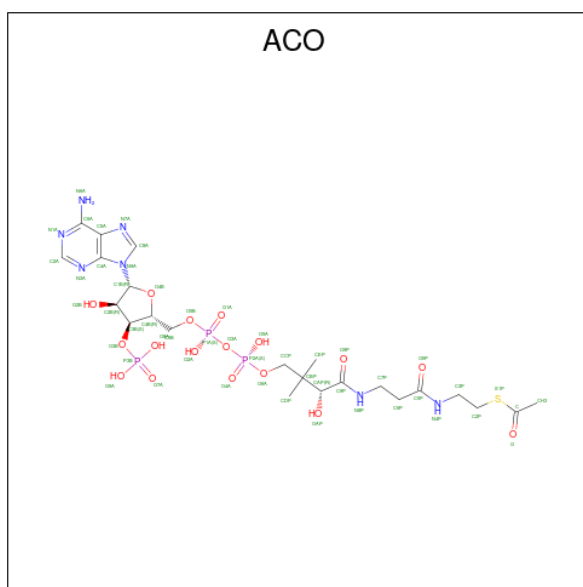
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	277	Total	C	N	O	S	0	0	0
			2321	1458	410	444	9			

- Molecule 4 is a protein called Chromatin modification-related protein YNG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	118	Total	C	N	O	S	0	0	0
			955	603	163	186	3			
4	D	119	Total	C	N	O	S	0	0	0
			962	608	164	187	3			
4	L	119	Total	C	N	O	S	0	0	0
			962	608	164	187	3			

- Molecule 5 is ACETYL COENZYME *A (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).

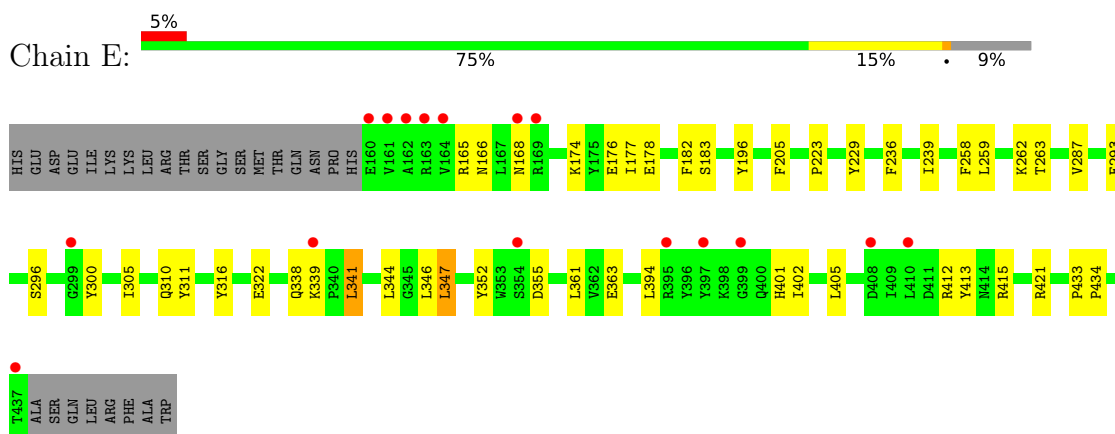


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
5	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

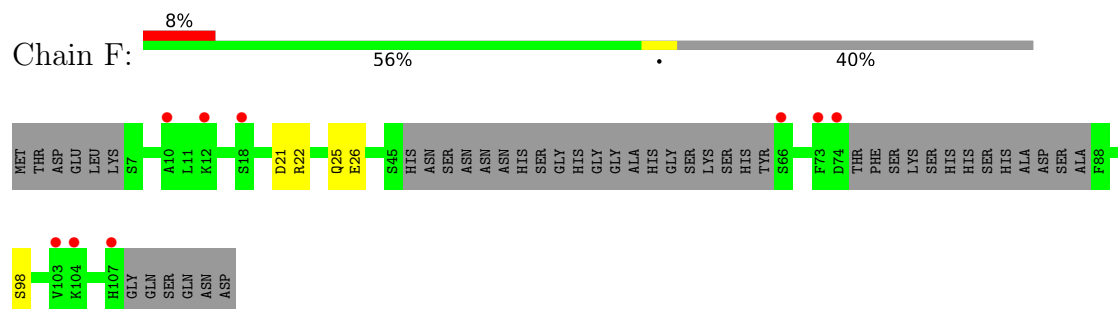
3 Residue-property plots [i](#)

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.

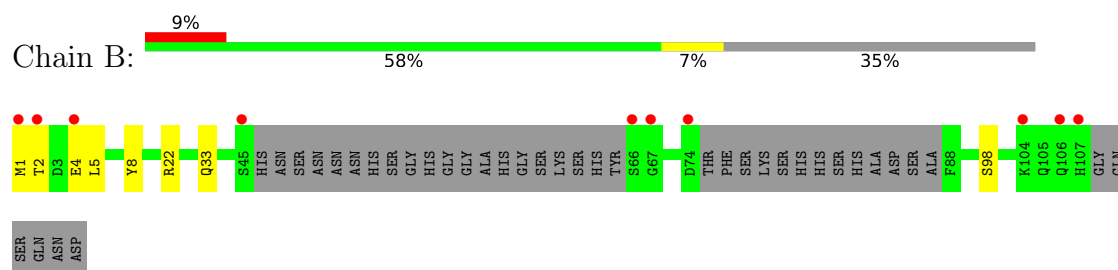
- Molecule 1: Histone acetyltransferase ESA1



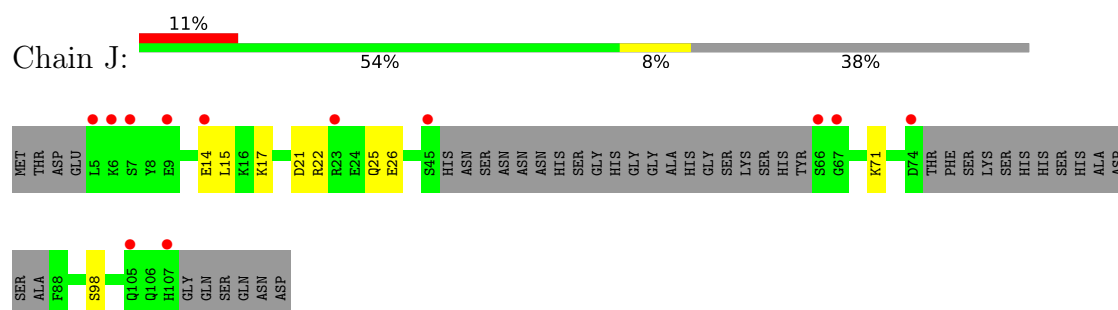
- Molecule 2: Chromatin modification-related protein EAF6



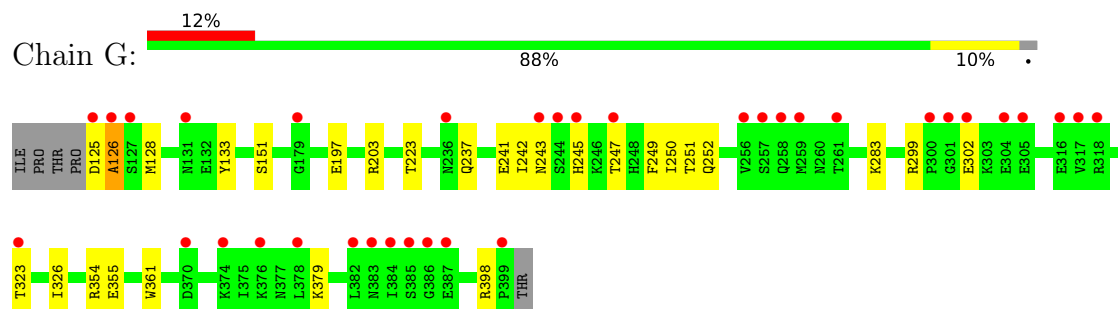
- Molecule 2: Chromatin modification-related protein EAF6



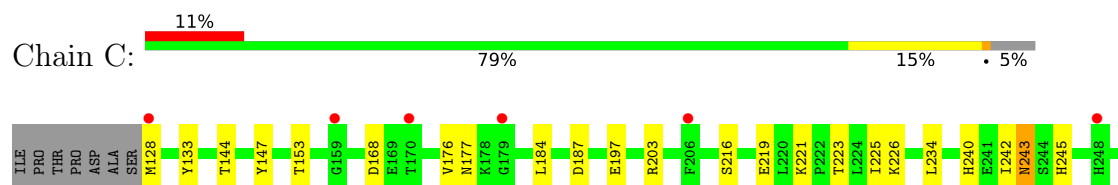
- Molecule 2: Chromatin modification-related protein EAF6

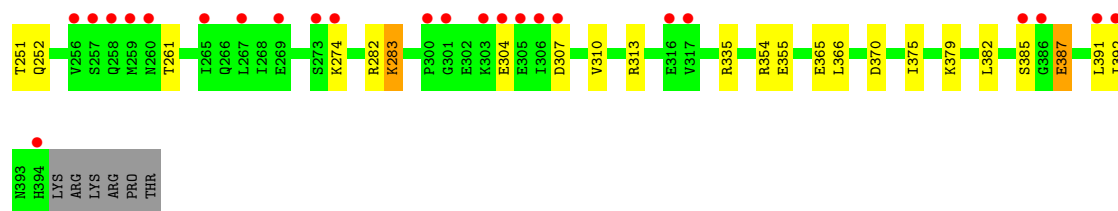


- Molecule 3: Enhancer of polycomb-like protein 1

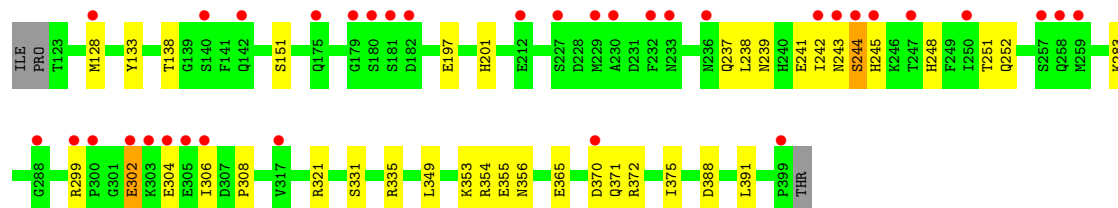
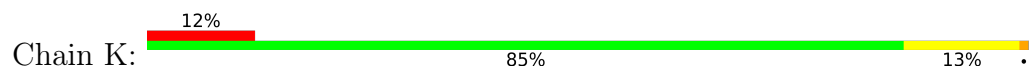


- Molecule 3: Enhancer of polycomb-like protein 1

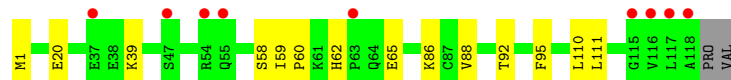
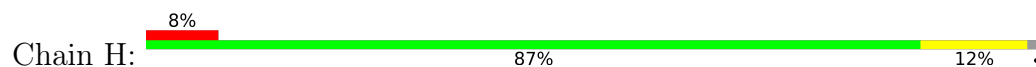




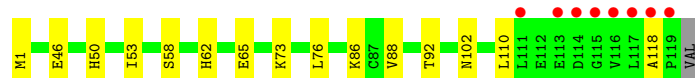
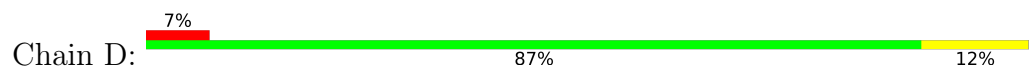
• Molecule 3: Enhancer of polycomb-like protein 1



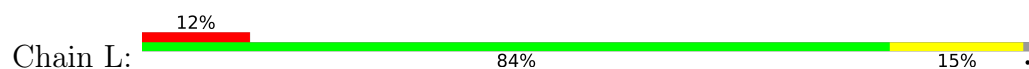
• Molecule 4: Chromatin modification-related protein YNG2



• Molecule 4: Chromatin modification-related protein YNG2



• Molecule 4: Chromatin modification-related protein YNG2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.26Å 138.57Å 167.87Å 90.00° 97.11° 90.00°	Depositor
Resolution (Å)	29.88 – 2.80 29.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	82.6 (29.88-2.80) 75.7 (29.88-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.80Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.227 , 0.271 0.227 , 0.270	Depositor DCC
R_{free} test set	2000 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	18691	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: ACO, ALY

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	0.17	0/2403	0.42	0/3246
1	E	0.18	0/2403	0.40	0/3246
1	I	0.17	0/2403	0.41	0/3246
2	B	0.13	0/626	0.40	0/834
2	F	0.11	0/577	0.36	0/769
2	J	0.11	0/594	0.41	0/791
3	C	0.18	0/2287	0.44	0/3080
3	G	0.16	0/2354	0.39	0/3168
3	K	0.18	0/2369	0.36	0/3190
4	D	0.13	0/974	0.35	0/1307
4	H	0.12	0/966	0.35	0/1295
4	L	0.12	0/974	0.36	0/1307
All	All	0.16	0/18930	0.40	0/25479

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	1
2	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	338	GLN	Peptide
2	B	4	GLU	Peptide

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	2355	0	2343	25	0
1	E	2355	0	2343	36	0
1	I	2355	0	2343	25	0
2	B	619	0	584	5	0
2	F	570	0	531	4	0
2	J	587	0	555	9	0
3	C	2241	0	2182	40	0
3	G	2307	0	2255	29	0
3	K	2321	0	2269	33	0
4	D	962	0	994	16	0
4	H	955	0	987	15	0
4	L	962	0	994	17	0
5	E	51	0	34	5	0
5	I	51	0	34	3	0
All	All	18691	0	18448	192	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 5.

All (192) 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:E:178:GLU:HB3	3:G:125:ASP:HB3	1.59	0.82
1:E:176:GLU:HB3	3:G:128:MET:HB2	1.62	0.80
1:E:341:LEU:HD23	1:E:346:LEU:HA	1.63	0.79
4:L:62:HIS:HB3	4:L:65:GLU:HB2	1.65	0.79
1:I:165:ARG:NH2	1:I:168:ASN:O	2.18	0.75
3:C:379:LYS:NZ	4:D:58:SER:OG	2.20	0.75
1:E:412:ARG:HG2	1:E:415:ARG:HH21	1.55	0.72
1:I:364:HIS:CE1	1:I:366:LYS:HB2	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:166:ASN:ND2	1:I:183:SER:O	2.24	0.69
3:G:251:THR:HB	4:H:92:THR:HG22	1.75	0.68
1:A:397:TYR:HB3	1:A:402:ILE:HD13	1.75	0.68
3:K:299:ARG:NE	3:K:302:GLU:OE2	2.26	0.68
3:K:251:THR:HB	4:L:92:THR:HG22	1.75	0.67
1:A:361:LEU:HB3	1:A:405:LEU:HD21	1.77	0.65
4:H:62:HIS:HB3	4:H:65:GLU:HB2	1.80	0.64
1:A:398:LYS:H	4:L:114:ASP:HA	1.63	0.64
3:G:197:GLU:OE2	3:G:283:LYS:NZ	2.31	0.63
3:C:391:LEU:HD21	4:D:53:ILE:HB	1.81	0.62
1:I:394:LEU:HD11	1:I:401:HIS:HB3	1.80	0.62
1:A:165:ARG:NH2	1:A:168:ASN:O	2.28	0.62
3:K:197:GLU:OE2	3:K:283:LYS:NZ	2.32	0.62
1:I:344:LEU:HG	5:I:500:ACO:H133	1.83	0.61
3:C:197:GLU:OE2	3:C:283:LYS:NZ	2.33	0.61
1:I:361:LEU:HB3	1:I:405:LEU:HD21	1.83	0.60
1:E:300:TYR:OH	1:E:339:LYS:HD2	2.03	0.59
1:E:229:TYR:HB3	1:E:236:PHE:HB2	1.85	0.59
2:F:98:SER:HB2	3:G:354:ARG:HH22	1.68	0.59
3:G:379:LYS:NZ	4:H:58:SER:OG	2.34	0.58
1:E:165:ARG:NH2	1:E:168:ASN:O	2.30	0.58
1:I:355:ASP:OD2	1:I:421:ARG:NH1	2.37	0.58
4:L:1:MET:HB3	4:L:111:LEU:HD23	1.86	0.58
2:J:98:SER:HB2	3:K:354:ARG:HH22	1.68	0.57
2:B:22:ARG:NH1	3:C:365:GLU:OE2	2.36	0.57
1:E:394:LEU:HD11	1:E:401:HIS:HB3	1.86	0.57
3:C:370:ASP:OD2	4:D:73:LYS:NZ	2.38	0.56
3:G:299:ARG:NH2	3:G:302:GLU:HG3	2.20	0.56
3:C:252:GLN:H	4:D:92:THR:HG22	1.71	0.56
3:C:240:HIS:HB2	3:C:245:HIS:HE1	1.70	0.56
4:D:62:HIS:HB3	4:D:65:GLU:HB2	1.88	0.55
1:E:176:GLU:O	3:G:126:ALA:HA	2.06	0.55
3:C:240:HIS:HB2	3:C:245:HIS:CE1	2.42	0.55
1:I:176:GLU:HB3	3:K:128:MET:HB2	1.88	0.55
1:A:174:LYS:HB3	3:C:133:TYR:CG	2.42	0.55
3:G:237:GLN:NE2	3:G:241:GLU:OE2	2.39	0.55
4:H:1:MET:HB3	4:H:111:LEU:HD23	1.88	0.55
1:E:361:LEU:HB3	1:E:405:LEU:HD21	1.89	0.54
1:E:363:GLU:OE2	1:E:413:TYR:OH	2.16	0.54
2:J:15:LEU:HD11	3:K:372:ARG:HD2	1.88	0.54
3:K:237:GLN:NE2	3:K:241:GLU:OE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:ILE:HD12	1:E:258:PHE:HZ	1.72	0.54
4:D:88:VAL:O	4:D:92:THR:HG23	2.08	0.54
3:K:335:ARG:NH2	4:L:112:GLU:OE2	2.41	0.53
3:C:392:ILE:O	3:C:392:ILE:HG23	2.09	0.53
2:B:98:SER:HB2	3:C:354:ARG:HH22	1.73	0.53
3:C:392:ILE:HG22	4:D:50:HIS:CD2	2.44	0.53
3:G:242:ILE:O	3:G:243:ASN:HB2	2.08	0.53
1:I:229:TYR:HB3	1:I:236:PHE:HB2	1.91	0.53
1:E:177:ILE:HG22	3:G:126:ALA:HB2	1.91	0.52
1:A:230:ARG:NH2	3:C:144:THR:O	2.42	0.52
1:E:177:ILE:HA	3:G:125:ASP:O	2.10	0.52
1:I:168:ASN:ND2	1:I:192:GLU:O	2.42	0.52
4:L:56:GLN:HB3	4:L:60:PRO:HG2	1.92	0.52
1:A:394:LEU:HD11	1:A:401:HIS:HB3	1.92	0.52
3:C:366:LEU:HD12	4:D:76:LEU:HG	1.92	0.52
1:E:166:ASN:HB2	1:E:182:PHE:HA	1.91	0.51
3:G:252:GLN:H	4:H:92:THR:HG22	1.75	0.51
3:K:242:ILE:HB	3:K:244:SER:HB3	1.92	0.51
1:E:322:GLU:HG2	1:E:352:TYR:HE1	1.75	0.51
1:I:347:LEU:HD12	5:I:500:ACO:H1B	1.92	0.51
1:A:213:ARG:NH2	3:C:187:ASP:OD2	2.42	0.51
1:I:365:GLN:C	1:I:366:LYS:HG3	2.36	0.51
1:A:229:TYR:HB3	1:A:236:PHE:HB2	1.92	0.51
3:K:370:ASP:OD2	4:L:73:LYS:NZ	2.44	0.51
3:C:375:ILE:O	3:C:379:LYS:HG3	2.11	0.50
2:B:5:LEU:HD23	3:C:382:LEU:HD13	1.92	0.50
3:C:251:THR:HB	4:D:92:THR:HG22	1.93	0.50
1:I:201:THR:HG22	1:I:220:LEU:HD23	1.93	0.50
2:J:14:GLU:HA	2:J:17:LYS:HD3	1.93	0.49
3:K:239:ASN:HD21	3:K:248:HIS:HA	1.77	0.49
1:I:341:LEU:HG	5:I:500:ACO:HH33	1.94	0.49
3:C:335:ARG:NH2	4:D:118:ALA:O	2.45	0.49
3:K:197:GLU:HG3	3:K:201:HIS:CE1	2.47	0.49
1:A:172:MET:HE2	1:A:254:LEU:HD11	1.95	0.49
2:J:15:LEU:HD13	3:K:375:ILE:HD12	1.95	0.48
1:E:223:PRO:HB3	1:E:239:ILE:HD11	1.96	0.48
3:K:304:GLU:HG3	3:K:306:ILE:H	1.78	0.48
1:E:177:ILE:HG22	3:G:126:ALA:CB	2.44	0.48
1:E:300:TYR:CE2	1:E:338:GLN:HG3	2.49	0.48
3:K:331:SER:HB3	4:L:117:LEU:HD13	1.96	0.47
3:K:355:GLU:OE2	4:L:86:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:ARG:HG2	1:E:415:ARG:NH2	2.27	0.47
3:C:304:GLU:CD	3:C:313:ARG:HH12	2.22	0.47
2:J:15:LEU:HD12	3:K:371:GLN:HB3	1.95	0.47
3:K:242:ILE:O	3:K:243:ASN:HB2	2.15	0.47
3:C:307:ASP:HB3	3:C:310:VAL:HG23	1.95	0.47
1:A:166:ASN:ND2	1:A:183:SER:O	2.45	0.47
1:A:232:ASP:OD1	1:A:232:ASP:N	2.47	0.47
3:C:379:LYS:HE2	3:C:379:LYS:HB3	1.61	0.47
2:F:26:GLU:HB3	3:G:398:ARG:NH1	2.30	0.47
3:C:252:GLN:H	4:D:92:THR:CG2	2.27	0.47
3:K:197:GLU:HG3	3:K:201:HIS:HE1	1.78	0.47
2:F:22:ARG:O	2:F:26:GLU:HG3	2.14	0.46
3:G:249:PHE:HE2	4:H:95:PHE:HB2	1.80	0.46
3:G:252:GLN:H	4:H:92:THR:CG2	2.28	0.46
4:H:88:VAL:O	4:H:92:THR:HG23	2.16	0.46
3:G:361:TRP:CZ3	4:H:39:LYS:HE3	2.50	0.46
1:A:223:PRO:HB3	1:A:239:ILE:HD11	1.98	0.46
3:K:252:GLN:H	4:L:92:THR:CG2	2.28	0.46
3:K:252:GLN:H	4:L:92:THR:HG22	1.80	0.46
1:E:355:ASP:OD2	1:E:421:ARG:NH1	2.49	0.46
1:E:421:ARG:NH2	5:E:500:ACO:O9A	2.47	0.46
1:I:322:GLU:HG2	1:I:352:TYR:HE1	1.79	0.46
3:C:168:ASP:OD1	3:C:282:ARG:NH1	2.48	0.46
3:G:323:THR:HG23	3:G:326:ILE:H	1.80	0.45
1:A:339:LYS:O	1:A:341:LEU:N	2.49	0.45
4:L:88:VAL:O	4:L:92:THR:HG23	2.16	0.45
1:E:344:LEU:HD23	5:E:500:ACO:HN8	1.80	0.45
1:E:347:LEU:HD12	5:E:500:ACO:H1B	1.98	0.45
3:C:216:SER:HB3	3:C:219:GLU:HG3	1.98	0.45
3:K:238:LEU:O	3:K:242:ILE:HG13	2.16	0.45
1:I:174:LYS:HB3	3:K:133:TYR:CG	2.52	0.45
1:I:182:PHE:CE2	3:K:308:PRO:HB2	2.51	0.45
1:E:344:LEU:HG	5:E:500:ACO:H133	1.99	0.45
1:E:174:LYS:HB3	3:G:133:TYR:CG	2.52	0.44
3:C:387:GLU:HG2	4:D:58:SER:OG	2.17	0.44
4:D:46:GLU:HG2	4:D:50:HIS:NE2	2.32	0.44
3:K:304:GLU:HA	3:K:304:GLU:OE1	2.17	0.44
1:I:232:ASP:OD1	1:I:232:ASP:N	2.50	0.44
3:K:151:SER:OG	4:L:20:GLU:OE2	2.29	0.44
4:D:1:MET:HE3	4:D:110:LEU:HB3	2.00	0.44
1:E:305:ILE:HG23	5:E:500:ACO:H31	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:ASN:ND2	1:E:183:SER:O	2.49	0.44
1:E:310:GLN:HB3	3:G:126:ALA:HB1	2.00	0.44
3:C:391:LEU:HD23	3:C:391:LEU:HA	1.74	0.44
3:K:321:ARG:NH2	4:L:1:MET:O	2.51	0.43
3:G:299:ARG:HH21	3:G:302:GLU:HG3	1.82	0.43
1:A:169:ARG:NE	1:A:176:GLU:OE2	2.50	0.43
1:E:310:GLN:HG2	1:E:311:TYR:CD2	2.54	0.43
1:A:213:ARG:HH22	3:C:187:ASP:CG	2.25	0.43
1:A:230:ARG:HB3	3:C:147:TYR:CE1	2.54	0.43
3:G:379:LYS:NZ	4:H:58:SER:HG	2.16	0.43
1:A:166:ASN:HB2	1:A:182:PHE:HA	2.01	0.43
1:A:177:ILE:HD12	1:A:258:PHE:HZ	1.83	0.43
1:A:388:ALA:HB1	1:A:394:LEU:HB2	2.00	0.43
1:I:166:ASN:HB2	1:I:182:PHE:HA	2.01	0.43
2:J:22:ARG:NH1	3:K:365:GLU:OE1	2.48	0.43
4:H:1:MET:HE3	4:H:110:LEU:HB3	2.00	0.43
2:B:8:TYR:HE1	3:C:379:LYS:HG2	1.83	0.43
3:C:221:LYS:O	3:C:225:ILE:HG12	2.19	0.43
1:I:258:PHE:CE1	1:I:309:PRO:HG2	2.53	0.43
1:A:244:GLN:OE1	3:C:153:THR:HA	2.19	0.43
3:C:176:VAL:HG22	3:C:274:LYS:HE3	2.01	0.43
2:B:8:TYR:CE1	3:C:379:LYS:HG2	2.54	0.42
1:A:177:ILE:HD12	1:A:258:PHE:CZ	2.54	0.42
4:L:76:LEU:HD12	4:L:76:LEU:HA	1.91	0.42
3:C:355:GLU:OE2	4:D:86:LYS:HE2	2.20	0.42
1:I:228:ILE:HD13	1:I:238:GLU:HB2	2.01	0.42
3:K:244:SER:HB2	3:K:356:ASN:ND2	2.34	0.42
3:K:349:LEU:HG	3:K:353:LYS:HE2	2.00	0.42
2:F:21:ASP:O	2:F:25:GLN:HG2	2.19	0.42
3:G:355:GLU:OE2	4:H:86:LYS:HE2	2.18	0.42
1:A:183:SER:O	1:A:185:TYR:N	2.51	0.42
1:A:417:LYS:HA	1:A:417:LYS:HD2	1.86	0.42
3:C:177:ASN:ND2	3:C:184:LEU:O	2.48	0.42
3:K:388:ASP:HA	3:K:391:LEU:HD23	2.02	0.42
3:C:203:ARG:HD2	3:C:223:THR:OG1	2.19	0.42
1:E:293:GLU:HB2	1:E:296:SER:HB2	2.02	0.41
3:G:250:ILE:HG23	4:H:88:VAL:HG22	2.02	0.41
3:G:302:GLU:HA	3:G:302:GLU:OE1	2.20	0.41
1:E:311:TYR:HB3	1:E:316:TYR:CD2	2.55	0.41
3:C:242:ILE:HG22	3:C:243:ASN:HD22	1.85	0.41
1:I:221:ARG:NH2	3:K:138:THR:O	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:ARG:O	2:J:26:GLU:HG3	2.21	0.41
2:J:71:LYS:HD3	2:J:71:LYS:HA	1.84	0.41
4:L:93:ALA:O	4:L:97:ILE:HG22	2.19	0.41
1:I:223:PRO:HB3	1:I:239:ILE:HD11	2.03	0.41
1:A:318:LYS:HE2	1:A:322:GLU:OE2	2.21	0.41
1:I:177:ILE:HD12	1:I:258:PHE:HZ	1.86	0.41
3:C:226:LYS:H	3:C:226:LYS:HG3	1.68	0.41
4:H:59:ILE:HB	4:H:60:PRO:HD3	2.03	0.41
1:I:221:ARG:HD3	1:I:282:LEU:O	2.21	0.41
2:J:21:ASP:O	2:J:25:GLN:HG2	2.21	0.40
1:E:196:TYR:HB2	1:E:205:PHE:HB2	2.02	0.40
1:E:433:PRO:HA	1:E:434:PRO:HD3	1.98	0.40
3:G:203:ARG:HD2	3:G:223:THR:OG1	2.22	0.40
1:E:259:LEU:HD12	1:E:262:ALY:HG2	2.03	0.40
3:G:151:SER:OG	4:H:20:GLU:OE2	2.31	0.40
3:G:243:ASN:HA	3:G:245:HIS:CE1	2.56	0.40
3:C:234:LEU:HD13	4:D:102:ASN:ND2	2.35	0.40
3:K:372:ARG:HG3	3:K:391:LEU:HD13	2.02	0.40
1:E:287:VAL:HA	1:E:311:TYR:CD2	2.55	0.40
4:L:59:ILE:HB	4:L:60:PRO:HD3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/305 (90%)	264 (96%)	11 (4%)	0	100	100
1	E	275/305 (90%)	265 (96%)	10 (4%)	0	100	100
1	I	275/305 (90%)	264 (96%)	11 (4%)	0	100	100
2	B	68/113 (60%)	65 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	62/113 (55%)	60 (97%)	2 (3%)	0	100	100
2	J	64/113 (57%)	62 (97%)	2 (3%)	0	100	100
3	C	265/280 (95%)	255 (96%)	9 (3%)	1 (0%)	30	60
3	G	273/280 (98%)	262 (96%)	10 (4%)	1 (0%)	30	60
3	K	275/280 (98%)	264 (96%)	11 (4%)	0	100	100
4	D	117/120 (98%)	117 (100%)	0	0	100	100
4	H	116/120 (97%)	116 (100%)	0	0	100	100
4	L	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
All	All	2182/2454 (89%)	2110 (97%)	70 (3%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	126	ALA
3	C	243	ASN

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	259/283 (92%)	256 (99%)	3 (1%)	63	87
1	E	259/283 (92%)	255 (98%)	4 (2%)	57	84
1	I	259/283 (92%)	257 (99%)	2 (1%)	73	90
2	B	69/100 (69%)	66 (96%)	3 (4%)	26	60
2	F	63/100 (63%)	63 (100%)	0	100	100
2	J	65/100 (65%)	65 (100%)	0	100	100
3	C	253/265 (96%)	248 (98%)	5 (2%)	48	80
3	G	260/265 (98%)	259 (100%)	1 (0%)	84	94
3	K	262/265 (99%)	259 (99%)	3 (1%)	65	87
4	D	110/111 (99%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	109/111 (98%)	109 (100%)	0	100	100
4	L	110/111 (99%)	110 (100%)	0	100	100
All	All	2078/2277 (91%)	2057 (99%)	21 (1%)	68	88

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	263	THR
1	E	341	LEU
1	E	347	LEU
1	E	402	ILE
3	G	247	THR
1	A	263	THR
1	A	347	LEU
1	A	402	ILE
2	B	1	MET
2	B	2	THR
2	B	33	GLN
3	C	128	MET
3	C	261	THR
3	C	283	LYS
3	C	385	SER
3	C	387	GLU
1	I	263	THR
1	I	347	LEU
3	K	244	SER
3	K	245	HIS
3	K	302	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
2	F	25	GLN
2	F	33	GLN
3	G	163	ASN
3	G	248	HIS
3	G	252	GLN
3	G	339	GLN
4	H	100	HIS
4	H	102	ASN

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Mol	Chain	Res	Type
3	C	163	ASN
3	C	201	HIS
3	C	240	HIS
3	C	371	GLN
3	C	383	ASN
4	D	44	GLN
4	D	48	GLN
4	D	50	HIS
4	D	102	ASN
3	K	236	ASN
3	K	245	HIS
3	K	252	GLN
3	K	266	GLN
3	K	338	HIS
3	K	339	GLN
3	K	356	ASN
3	K	383	ASN
4	L	100	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	ALY	A	262	1	10,11,12	1.08	0	7,12,14	0.94	0
1	ALY	E	262	1	10,11,12	1.05	0	7,12,14	1.02	0
1	ALY	I	262	1	10,11,12	1.06	1 (10%)	7,12,14	0.94	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
1	ALY	A	262	1	-	4/9/10/12	-
1	ALY	E	262	1	-	4/9/10/12	-
1	ALY	I	262	1	-	5/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	262	ALY	CH-NZ	2.10	1.39	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	E	262	ALY	N-CA-CB-CG
1	E	262	ALY	C-CA-CB-CG
1	A	262	ALY	N-CA-CB-CG
1	A	262	ALY	C-CA-CB-CG
1	I	262	ALY	N-CA-CB-CG
1	I	262	ALY	C-CA-CB-CG
1	I	262	ALY	O-C-CA-CB
1	A	262	ALY	CG-CD-CE-NZ
1	E	262	ALY	CG-CD-CE-NZ
1	I	262	ALY	CG-CD-CE-NZ
1	E	262	ALY	CA-CB-CG-CD
1	I	262	ALY	CA-CB-CG-CD
1	A	262	ALY	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	262	ALY	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACO	I	500	-	51,53,53	1.80	13 (25%)	73,79,79	1.74	16 (21%)
5	ACO	E	500	-	51,53,53	1.82	14 (27%)	73,79,79	1.64	10 (13%)

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
5	ACO	I	500	-	-	9/51/67/67	0/3/3/3
5	ACO	E	500	-	-	9/51/67/67	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	500	ACO	C5P-N4P	6.36	1.48	1.33
5	I	500	ACO	C5P-N4P	6.27	1.48	1.33
5	I	500	ACO	C2B-C3B	-4.30	1.43	1.53
5	E	500	ACO	C9P-N8P	4.28	1.43	1.33
5	E	500	ACO	C2B-C3B	-4.27	1.43	1.53
5	I	500	ACO	C9P-N8P	4.20	1.43	1.33
5	I	500	ACO	C6A-N6A	3.96	1.44	1.34
5	E	500	ACO	C6A-N6A	3.96	1.44	1.34
5	E	500	ACO	C5A-N7A	-2.83	1.33	1.39
5	I	500	ACO	C5A-N7A	-2.75	1.34	1.39
5	I	500	ACO	C2B-C1B	-2.53	1.45	1.53
5	E	500	ACO	C3B-C4B	-2.49	1.46	1.52
5	E	500	ACO	C2B-C1B	-2.48	1.45	1.53
5	I	500	ACO	C3B-C4B	-2.47	1.46	1.52
5	E	500	ACO	CEP-CBP	-2.45	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	500	ACO	CEP-CBP	-2.43	1.48	1.53
5	I	500	ACO	C1B-N9A	-2.30	1.40	1.46
5	E	500	ACO	C1B-N9A	-2.25	1.40	1.46
5	E	500	ACO	O4B-C1B	2.21	1.47	1.42
5	E	500	ACO	P2A-O3A	2.18	1.61	1.59
5	I	500	ACO	O4B-C1B	2.15	1.47	1.42
5	I	500	ACO	C5B-C4B	-2.13	1.45	1.51
5	E	500	ACO	C5B-C4B	-2.05	1.45	1.51
5	I	500	ACO	P2A-O3A	2.04	1.61	1.59
5	E	500	ACO	OAP-CAP	-2.02	1.38	1.42
5	I	500	ACO	P3B-O3B	-2.02	1.56	1.59
5	E	500	ACO	P3B-O3B	-2.01	1.56	1.59

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	500	ACO	N3A-C2A-N1A	-5.63	120.06	128.58
5	I	500	ACO	N3A-C2A-N1A	-5.62	120.08	128.58
5	E	500	ACO	C5A-C4A-N3A	-5.32	119.39	126.72
5	I	500	ACO	C5A-C4A-N3A	-5.09	119.71	126.72
5	E	500	ACO	N3A-C4A-N9A	4.52	134.85	127.17
5	I	500	ACO	N3A-C4A-N9A	4.29	134.46	127.17
5	E	500	ACO	C5A-N7A-C8A	3.87	109.54	103.45
5	I	500	ACO	C5A-N7A-C8A	3.87	109.53	103.45
5	E	500	ACO	C2A-N3A-C4A	3.63	120.69	111.83
5	I	500	ACO	C2A-N3A-C4A	3.58	120.58	111.83
5	I	500	ACO	N9A-C8A-N7A	-3.22	109.37	113.94
5	E	500	ACO	N9A-C8A-N7A	-3.13	109.50	113.94
5	I	500	ACO	C4A-C5A-N7A	-2.95	107.21	110.58
5	E	500	ACO	C4A-C5A-N7A	-2.94	107.22	110.58
5	I	500	ACO	CEP-CBP-CAP	2.77	113.49	108.77
5	I	500	ACO	C4B-O4B-C1B	-2.77	103.35	109.47
5	I	500	ACO	C3B-C2B-C1B	2.44	105.26	99.89
5	E	500	ACO	C3B-C2B-C1B	2.43	105.24	99.89
5	I	500	ACO	C4A-N9A-C8A	2.22	108.06	105.74
5	I	500	ACO	C6P-C5P-N4P	2.20	120.35	116.34
5	E	500	ACO	C4B-O4B-C1B	-2.20	104.61	109.47
5	E	500	ACO	C4A-N9A-C8A	2.14	107.98	105.74
5	I	500	ACO	O9P-C9P-N8P	-2.12	118.48	122.98
5	I	500	ACO	C3P-N4P-C5P	-2.07	118.97	122.82
5	I	500	ACO	C7P-N8P-C9P	-2.06	118.84	122.55
5	I	500	ACO	O4B-C1B-N9A	2.02	111.97	108.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

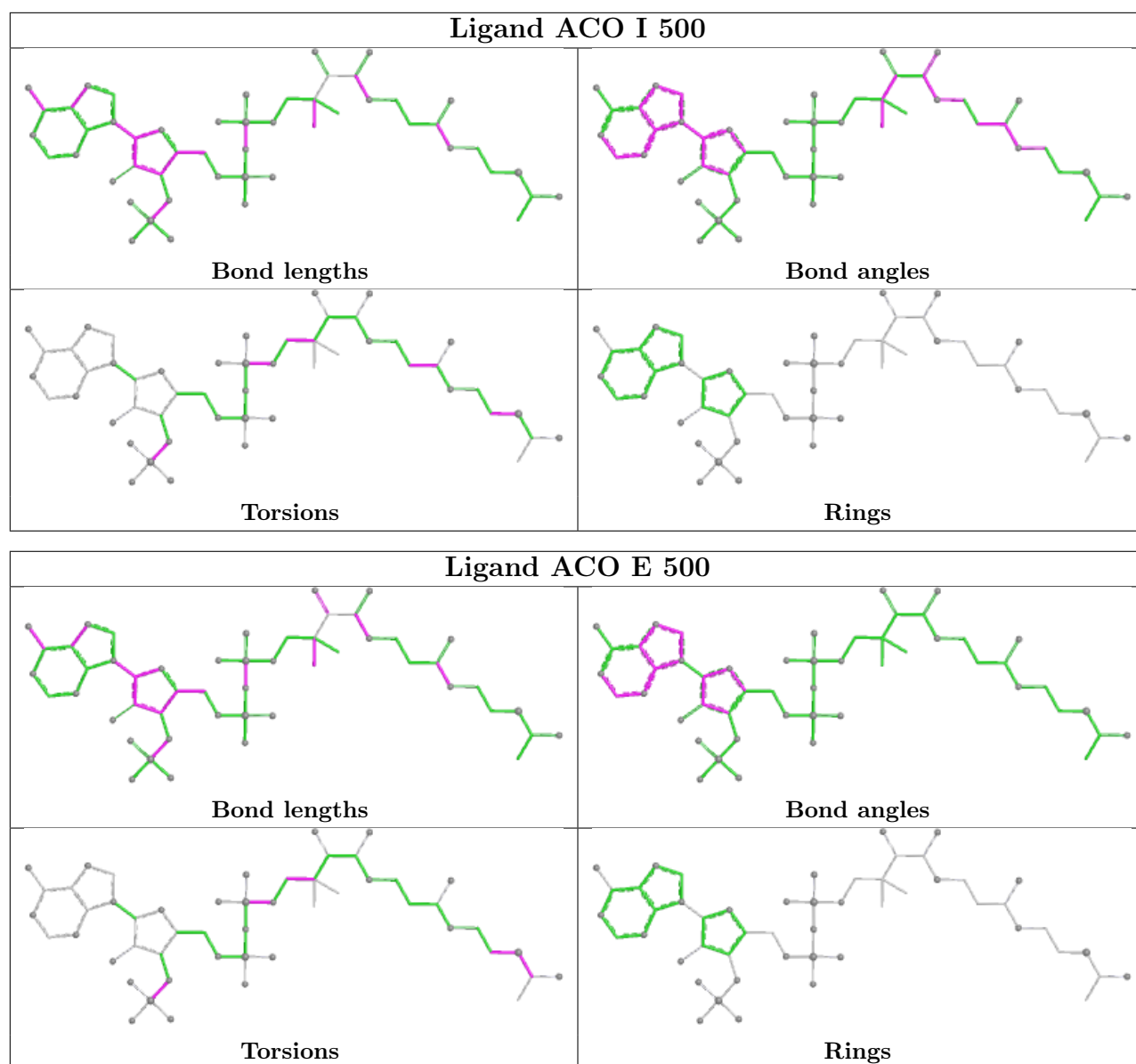
Mol	Chain	Res	Type	Atoms
5	E	500	ACO	CCP-O6A-P2A-O3A
5	E	500	ACO	CCP-O6A-P2A-O4A
5	E	500	ACO	CDP-CBP-CCP-O6A
5	E	500	ACO	O-C-S1P-C2P
5	E	500	ACO	CH3-C-S1P-C2P
5	I	500	ACO	CCP-O6A-P2A-O3A
5	I	500	ACO	CCP-O6A-P2A-O4A
5	E	500	ACO	CEP-CBP-CCP-O6A
5	I	500	ACO	CDP-CBP-CCP-O6A
5	I	500	ACO	CEP-CBP-CCP-O6A
5	E	500	ACO	C3P-C2P-S1P-C
5	I	500	ACO	C3P-C2P-S1P-C
5	E	500	ACO	CAP-CBP-CCP-O6A
5	I	500	ACO	CAP-CBP-CCP-O6A
5	E	500	ACO	C3B-O3B-P3B-O9A
5	I	500	ACO	O5P-C5P-C6P-C7P
5	I	500	ACO	N4P-C5P-C6P-C7P
5	I	500	ACO	C3B-O3B-P3B-O8A

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	500	ACO	3	0
5	E	500	ACO	5	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	277/305 (90%)	0.08	9 (3%) 50 40	21, 40, 73, 96	0
1	E	277/305 (90%)	0.37	16 (5%) 29 22	26, 52, 91, 111	0
1	I	277/305 (90%)	0.51	22 (7%) 18 13	29, 56, 110, 141	0
2	B	74/113 (65%)	0.71	10 (13%) 7 5	33, 52, 91, 129	0
2	F	68/113 (60%)	0.91	9 (13%) 7 6	32, 63, 105, 124	0
2	J	70/113 (61%)	0.91	12 (17%) 4 3	37, 57, 96, 104	0
3	C	267/280 (95%)	0.68	30 (11%) 10 7	20, 56, 98, 130	0
3	G	275/280 (98%)	0.60	35 (12%) 8 6	26, 55, 99, 116	0
3	K	277/280 (98%)	0.82	35 (12%) 8 6	32, 61, 100, 132	0
4	D	119/120 (99%)	0.19	8 (6%) 24 17	23, 41, 100, 130	0
4	H	118/120 (98%)	0.50	9 (7%) 20 14	34, 55, 92, 112	0
4	L	119/120 (99%)	0.58	14 (11%) 9 7	26, 52, 100, 107	0
All	All	2218/2454 (90%)	0.52	209 (9%) 14 10	20, 53, 99, 141	0

All (209) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	115	GLY	7.7
3	C	317	VAL	6.8
4	L	118	ALA	6.0
3	C	258	GLN	5.2
3	K	244	SER	5.0
3	K	306	ILE	5.0
1	I	397	TYR	4.9
2	B	66	SER	4.8
3	K	258	GLN	4.8
4	H	117	LEU	4.8
3	K	300	PRO	4.6

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Mol	Chain	Res	Type	RSRZ
4	L	119	PRO	4.6
4	L	58	SER	4.5
3	C	256	VAL	4.5
4	L	61	LYS	4.5
2	F	12	LYS	4.4
3	C	305	GLU	4.3
1	E	160	GLU	4.3
3	K	317	VAL	4.2
1	I	339	LYS	4.2
3	G	258	GLN	4.1
1	A	339	LYS	4.1
3	C	304	GLU	4.1
1	E	161	VAL	4.0
4	H	116	VAL	4.0
3	K	243	ASN	4.0
1	E	437	THR	3.9
2	J	66	SER	3.9
2	J	74	ASP	3.9
2	J	5	LEU	3.8
4	H	37	GLU	3.8
1	I	295	GLU	3.8
3	C	316	GLU	3.8
3	G	125	ASP	3.7
4	D	119	PRO	3.7
4	D	114	ASP	3.7
3	G	257	SER	3.7
3	G	385	SER	3.7
4	L	115	GLY	3.7
2	B	67	GLY	3.6
4	L	59	ILE	3.6
3	G	386	GLY	3.5
1	I	437	THR	3.5
2	F	107	HIS	3.5
3	G	383	ASN	3.5
2	B	107	HIS	3.5
3	G	126	ALA	3.5
3	G	305	GLU	3.5
3	C	259	MET	3.5
3	C	391	LEU	3.5
2	J	7	SER	3.5
3	K	399	PRO	3.5
4	D	118	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
3	K	230	ALA	3.4
3	K	232	PHE	3.4
1	E	397	TYR	3.4
3	G	317	VAL	3.4
1	I	375	SER	3.4
3	G	259	MET	3.4
3	K	229	MET	3.4
3	G	245	HIS	3.4
2	B	104	LYS	3.4
3	C	257	SER	3.4
3	K	303	LYS	3.4
2	J	9	GLU	3.3
2	F	10	ALA	3.3
2	J	107	HIS	3.3
2	B	45	SER	3.3
1	A	415	ARG	3.3
2	F	66	SER	3.3
3	K	257	SER	3.3
3	C	303	LYS	3.2
3	G	399	PRO	3.2
3	C	386	GLY	3.2
4	D	117	LEU	3.2
1	A	437	THR	3.2
4	L	117	LEU	3.1
1	I	398	LYS	3.1
1	I	407	GLU	3.1
3	C	306	ILE	3.1
1	A	194	PHE	3.1
2	J	23	ARG	3.1
3	G	127	SER	3.1
1	E	410	LEU	3.1
1	I	400	GLN	3.0
3	G	378	LEU	3.0
3	K	236	ASN	3.0
3	C	300	PRO	3.0
1	I	408	ASP	3.0
4	D	116	VAL	3.0
2	F	104	LYS	2.9
1	I	163	ARG	2.9
4	L	49	ILE	2.9
3	G	301	GLY	2.9
1	I	392	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	128	MET	2.9
3	G	256	VAL	2.9
3	G	382	LEU	2.9
3	C	301	GLY	2.8
1	A	397	TYR	2.8
2	B	2	THR	2.8
4	H	55	GLN	2.8
3	C	179	GLY	2.7
2	F	103	VAL	2.7
1	I	405	LEU	2.7
1	I	166	ASN	2.7
3	C	385	SER	2.7
4	L	40	LYS	2.7
3	K	302	GLU	2.7
3	G	374	LYS	2.6
1	I	415	ARG	2.6
4	H	54	ARG	2.6
1	I	411	ASP	2.6
2	B	106	GLN	2.6
3	C	267	LEU	2.6
3	K	242	ILE	2.6
4	L	51	LYS	2.6
3	K	305	GLU	2.6
1	E	408	ASP	2.6
2	B	1	MET	2.6
3	G	304	GLU	2.6
1	A	406	ASN	2.6
1	E	354	SER	2.5
3	K	304	GLU	2.5
3	G	243	ASN	2.5
3	K	259	MET	2.5
2	J	14	GLU	2.5
3	G	244	SER	2.5
3	G	300	PRO	2.5
1	E	162	ALA	2.5
3	G	236	ASN	2.5
2	B	74	ASP	2.5
4	L	60	PRO	2.5
1	E	399	GLY	2.5
2	F	74	ASP	2.4
3	C	307	ASP	2.4
3	C	392	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	K	181	SER	2.4
4	H	47	SER	2.4
1	E	163	ARG	2.4
3	K	233	ASN	2.4
3	C	206	PHE	2.4
3	G	247	THR	2.4
3	K	245	HIS	2.4
1	E	169	ARG	2.4
2	F	18	SER	2.4
3	G	376	LYS	2.4
4	L	66	ASP	2.4
3	K	180	SER	2.4
3	K	247	THR	2.4
3	G	384	ILE	2.4
1	A	407	GLU	2.3
4	H	118	ALA	2.3
1	I	344	LEU	2.3
1	E	395	ARG	2.3
3	C	159	GLY	2.3
3	K	182	ASP	2.3
3	C	265	ILE	2.3
3	K	212	GLU	2.3
1	A	366	LYS	2.3
1	I	369	THR	2.3
1	I	161	VAL	2.3
3	K	128	MET	2.3
1	I	394	LEU	2.3
3	K	227	SER	2.3
1	E	168	ASN	2.2
3	G	318	ARG	2.2
3	C	269	GLU	2.2
2	J	6	LYS	2.2
3	C	394	HIS	2.2
3	G	370	ASP	2.2
2	J	45	SER	2.2
3	K	288	GLY	2.2
3	G	131	ASN	2.2
4	L	63	PRO	2.2
3	G	179	GLY	2.2
3	K	179	GLY	2.2
1	I	160	GLU	2.1
2	B	4	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	248	HIS	2.1
1	A	280	ASP	2.1
3	C	170	THR	2.1
1	I	162	ALA	2.1
3	K	299	ARG	2.1
4	L	54	ARG	2.1
3	K	140	SER	2.1
3	K	250	ILE	2.1
1	E	339	LYS	2.1
3	C	274	LYS	2.1
4	H	115	GLY	2.1
3	G	261	THR	2.1
3	G	323	THR	2.1
2	J	105	GLN	2.1
3	K	142	GLN	2.1
1	E	164	VAL	2.1
3	C	260	ASN	2.1
2	F	73	PHE	2.1
3	G	302	GLU	2.1
4	D	113	GLU	2.1
3	K	175	GLN	2.0
1	I	435	VAL	2.0
4	D	111	LEU	2.0
3	G	316	GLU	2.0
3	C	273	SER	2.0
4	H	63	PRO	2.0
1	E	299	GLY	2.0
2	J	67	GLY	2.0
3	G	387	GLU	2.0
3	K	370	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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
1	ALY	I	262	12/13	0.92	0.13	35,46,54,56	0
1	ALY	A	262	12/13	0.95	0.11	23,36,42,51	0
1	ALY	E	262	12/13	0.95	0.10	29,38,51,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

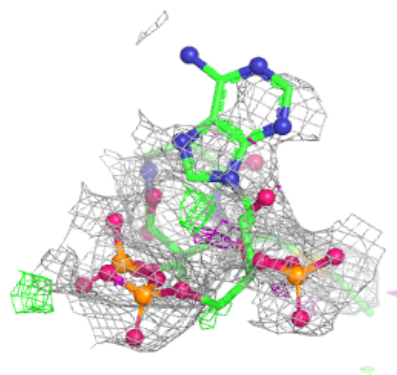
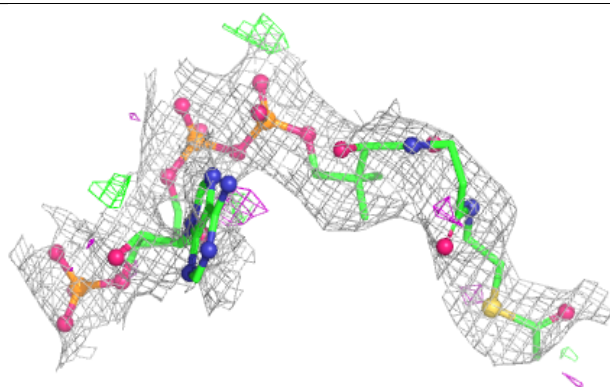
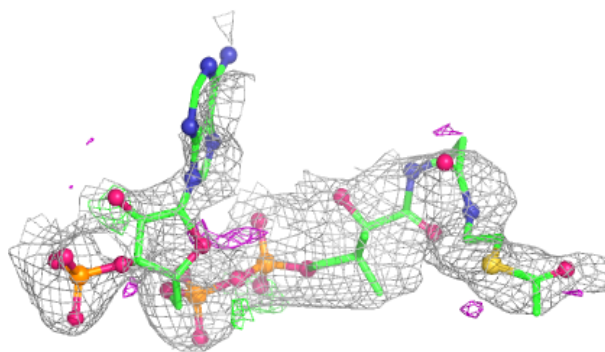
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

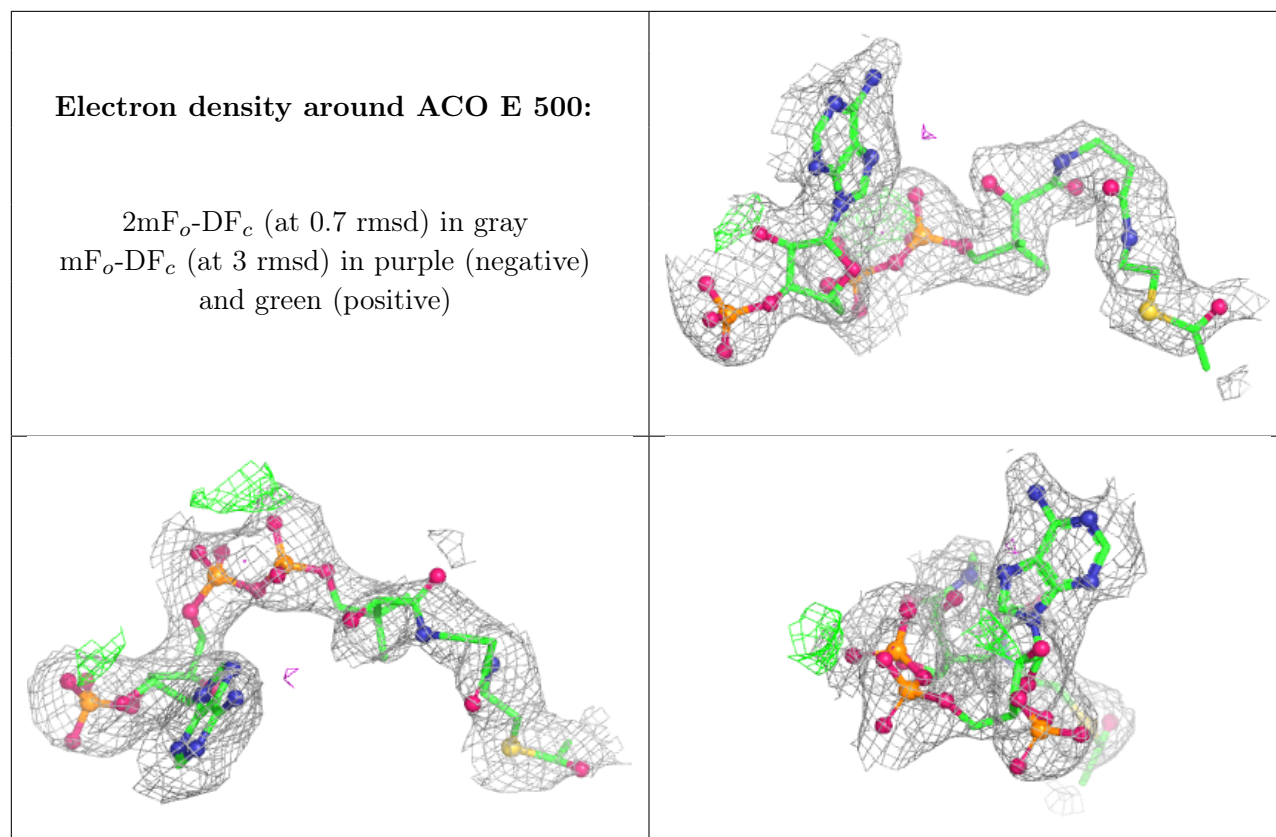
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACO	I	500	51/51	0.89	0.15	42,78,105,112	0
5	ACO	E	500	51/51	0.90	0.14	38,69,95,98	0

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 ACO I 500:

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.