



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 AM UTC

PDB ID : 4PSX / pdb_00004psx
Title : Crystal structure of histone acetyltransferase complex
Authors : Yang, M.; Li, Y.
Deposited on : 2014-03-08
Resolution : 2.51 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

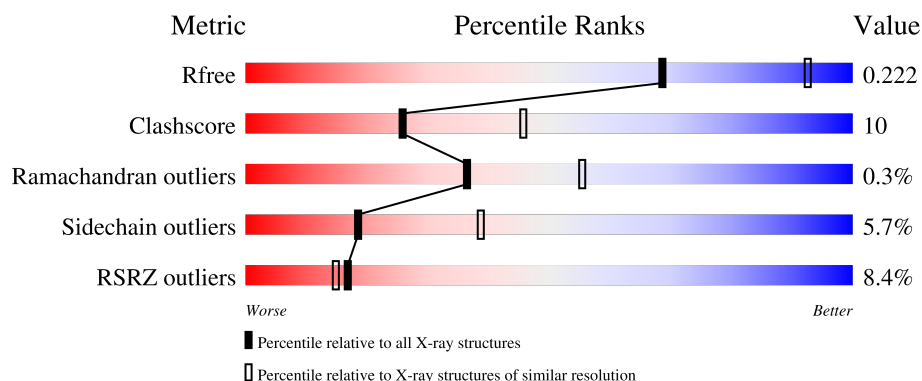
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	320	10% 78% 18% ..
1	D	320	8% 77% 18% ..
2	B	401	3% 69% 19% • 10%
2	E	401	4% 70% 18% • 10%
3	C	48	23% 48% 31% • 19%

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Mol	Chain	Length	Quality of chain
3	F	48	17% 48% 23% 6% 23%
4	P	15	33% 53% 7% 7% 33%
4	Y	15	40% 53% 20% 7% 20%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12392 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 type B catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2603	1679	426	494	4			
1	D	313	Total	C	N	O	S	0	0	0
			2603	1679	426	494	4			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q12341
A	2	SER	-	expression tag	UNP Q12341
A	3	ALA	-	expression tag	UNP Q12341
A	4	ASN	-	expression tag	UNP Q12341
A	5	ASP	-	expression tag	UNP Q12341
A	6	PHE	-	expression tag	UNP Q12341
A	320	SER	-	expression tag	UNP Q12341
D	1	MET	-	expression tag	UNP Q12341
D	2	SER	-	expression tag	UNP Q12341
D	3	ALA	-	expression tag	UNP Q12341
D	4	ASN	-	expression tag	UNP Q12341
D	5	ASP	-	expression tag	UNP Q12341
D	6	PHE	-	expression tag	UNP Q12341
D	320	SER	-	expression tag	UNP Q12341

- Molecule 2 is a protein called Histone acetyltransferase type B subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	361	Total	C	N	O	S	0	0	0
			2868	1808	484	566	10			
2	E	361	Total	C	N	O	S	0	0	0
			2868	1808	484	566	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	expression tag	UNP P39984
B	2	GLU	-	expression tag	UNP P39984
B	3	ASN	-	expression tag	UNP P39984
B	4	GLN	-	expression tag	UNP P39984
B	5	GLU	-	expression tag	UNP P39984
B	6	LYS	-	expression tag	UNP P39984
B	7	PRO	-	expression tag	UNP P39984
B	143	THR	VAL	engineered mutation	UNP P39984
B	390	GLY	-	expression tag	UNP P39984
B	391	GLY	-	expression tag	UNP P39984
B	392	PRO	-	expression tag	UNP P39984
B	393	PRO	-	expression tag	UNP P39984
B	394	LYS	-	expression tag	UNP P39984
B	395	VAL	-	expression tag	UNP P39984
B	396	ASN	-	expression tag	UNP P39984
B	397	LYS	-	expression tag	UNP P39984
B	398	ASP	-	expression tag	UNP P39984
B	399	ILE	-	expression tag	UNP P39984
B	400	ILE	-	expression tag	UNP P39984
B	401	SER	-	expression tag	UNP P39984
E	1	MET	-	expression tag	UNP P39984
E	2	GLU	-	expression tag	UNP P39984
E	3	ASN	-	expression tag	UNP P39984
E	4	GLN	-	expression tag	UNP P39984
E	5	GLU	-	expression tag	UNP P39984
E	6	LYS	-	expression tag	UNP P39984
E	7	PRO	-	expression tag	UNP P39984
E	143	THR	VAL	engineered mutation	UNP P39984
E	390	GLY	-	expression tag	UNP P39984
E	391	GLY	-	expression tag	UNP P39984
E	392	PRO	-	expression tag	UNP P39984
E	393	PRO	-	expression tag	UNP P39984
E	394	LYS	-	expression tag	UNP P39984
E	395	VAL	-	expression tag	UNP P39984
E	396	ASN	-	expression tag	UNP P39984
E	397	LYS	-	expression tag	UNP P39984
E	398	ASP	-	expression tag	UNP P39984
E	399	ILE	-	expression tag	UNP P39984
E	400	ILE	-	expression tag	UNP P39984
E	401	SER	-	expression tag	UNP P39984

- Molecule 3 is a protein called Histone H4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	39	Total	C	N	O	0	0	0
			294	180	70	44			
3	F	37	Total	C	N	O	0	0	0
			280	171	67	42			

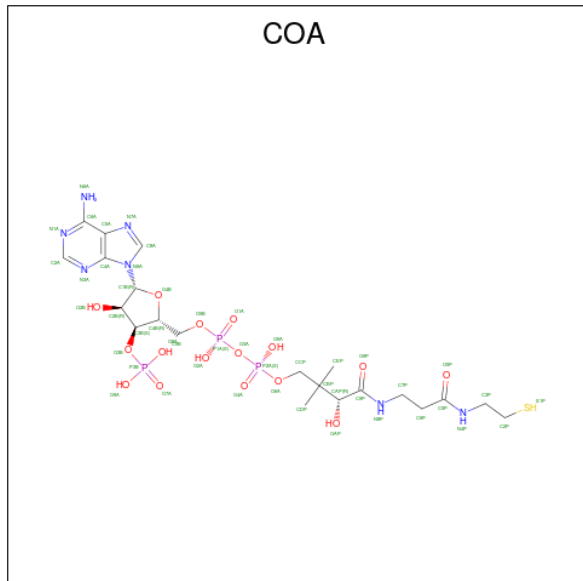
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	21	VAL	ILE	engineered mutation	UNP P02309
F	21	VAL	ILE	engineered mutation	UNP P02309

- Molecule 4 is a protein called Histone H3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	Y	12	Total	C	N	O	0	0	0
			90	52	21	17			
4	P	10	Total	C	N	O	0	0	0
			79	46	19	14			

- Molecule 5 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
5	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		

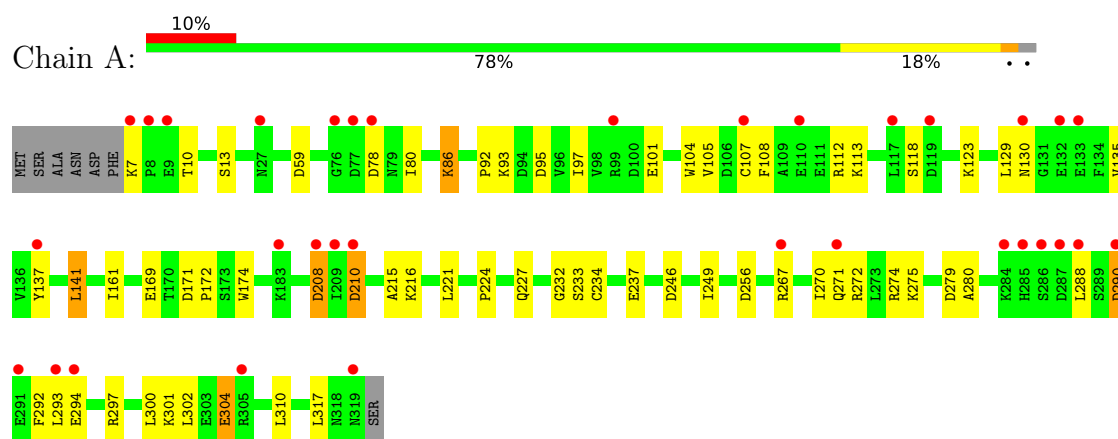
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	125	Total	O	0	0
			125	125		
7	B	153	Total	O	0	0
			153	153		
7	C	19	Total	O	0	0
			19	19		
7	D	122	Total	O	0	0
			122	122		
7	E	167	Total	O	0	0
			167	167		
7	F	18	Total	O	0	0
			18	18		
7	Y	1	Total	O	0	0
			1	1		
7	P	1	Total	O	0	0
			1	1		

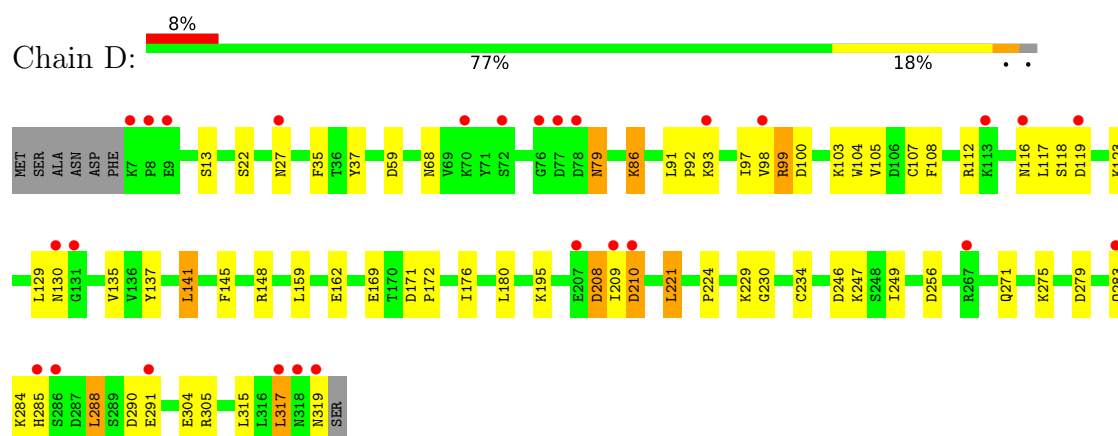
3 Residue-property plots [i](#)

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.

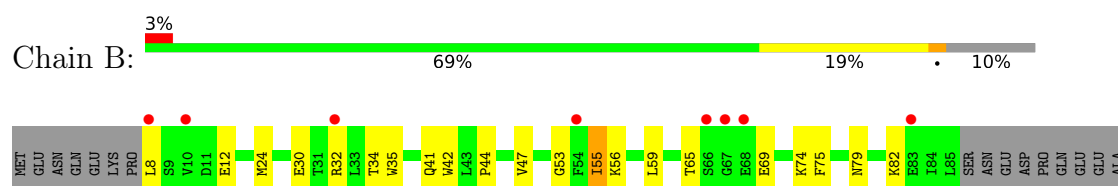
- Molecule 1: Histone acetyltransferase type B catalytic subunit

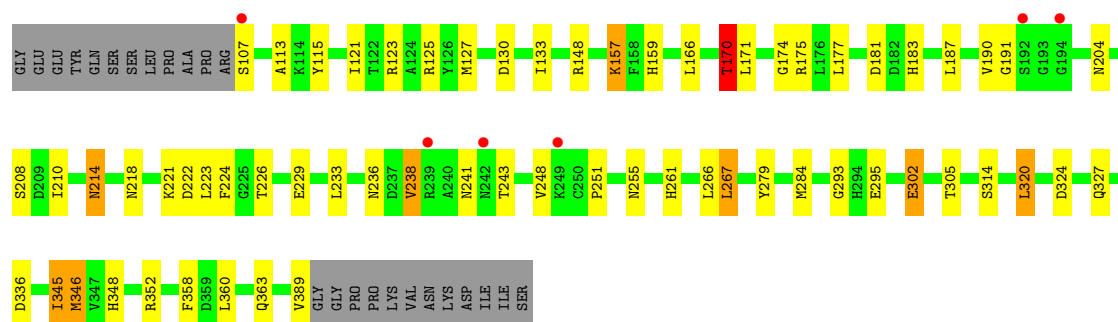


- Molecule 1: Histone acetyltransferase type B catalytic subunit

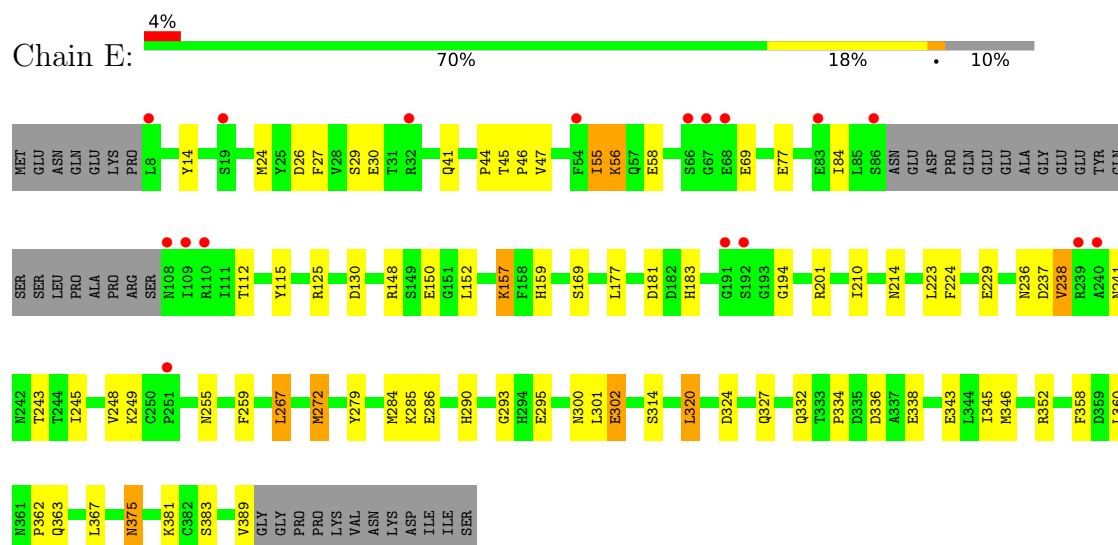


- Molecule 2: Histone acetyltransferase type B subunit 2

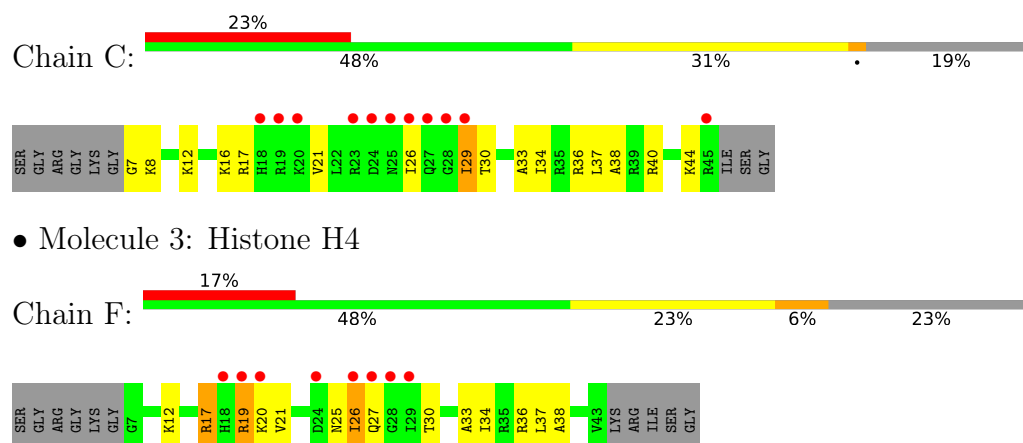




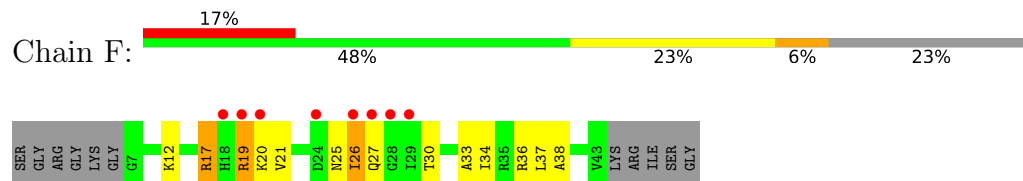
● Molecule 2: Histone acetyltransferase type B subunit 2



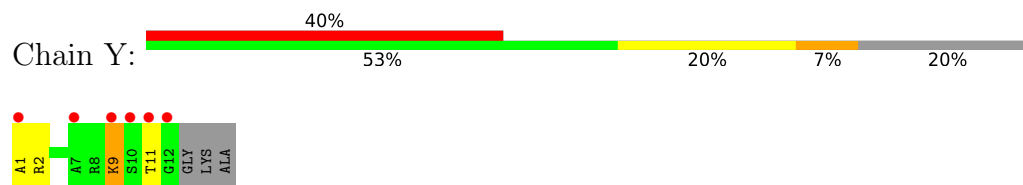
● Molecule 3: Histone H4



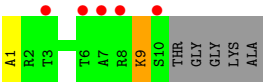
● Molecule 3: Histone H4



● Molecule 4: Histone H3



● Molecule 4: Histone H3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.55Å 85.33Å 114.51Å 75.97° 72.40° 66.06°	Depositor
Resolution (Å)	38.60 – 2.51 38.60 – 2.51	Depositor EDS
% Data completeness (in resolution range)	75.7 (38.60-2.51) 75.6 (38.60-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.181 , 0.223 0.182 , 0.222	Depositor DCC
R_{free} test set	3338 reflections (3.80%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12392	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: COA, SO4

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	0.51	0/2665	0.86	2/3602 (0.1%)
1	D	0.52	0/2665	0.84	4/3602 (0.1%)
2	B	0.53	0/2938	0.90	5/4001 (0.1%)
2	E	0.52	0/2938	0.89	4/4001 (0.1%)
3	C	0.55	0/295	1.02	0/386
3	F	0.59	0/281	1.12	2/368 (0.5%)
4	P	0.41	0/78	0.74	0/101
4	Y	0.42	0/89	0.78	0/116
All	All	0.52	0/11949	0.88	17/16177 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	79	ASN	N-CA-C	-6.38	104.75	113.30
2	E	345	ILE	CB-CA-C	-6.07	104.09	112.04
2	B	345	ILE	CB-CA-C	-5.95	104.45	111.94
2	E	130	ASP	CA-C-N	5.83	127.13	119.84
2	E	130	ASP	C-N-CA	5.83	127.13	119.84
2	B	130	ASP	CA-C-N	5.54	126.77	119.84
2	B	130	ASP	C-N-CA	5.54	126.77	119.84
2	B	133	ILE	N-CA-C	5.51	115.79	107.80
2	B	170	THR	N-CA-C	-5.51	106.56	113.28
1	A	224	PRO	N-CA-C	5.47	117.38	110.70
1	D	304	GLU	N-CA-C	5.41	117.17	111.28
3	F	26	ILE	N-CA-C	-5.37	105.30	110.72
1	D	224	PRO	N-CA-C	5.32	117.19	110.70
2	E	272	MET	N-CA-C	5.20	117.69	111.71
1	A	304	GLU	N-CA-C	5.20	116.95	111.28
1	D	98	VAL	N-CA-C	5.14	120.12	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	25	ASN	N-CA-C	5.10	116.58	108.67

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2603	0	2550	41	0
1	D	2603	0	2550	47	0
2	B	2868	0	2744	57	0
2	E	2868	0	2744	54	0
3	C	294	0	332	10	0
3	F	280	0	317	11	0
4	P	79	0	91	5	0
4	Y	90	0	101	5	0
5	A	48	0	32	5	0
5	D	48	0	32	8	0
6	B	5	0	0	0	0
7	A	125	0	0	10	0
7	B	153	0	0	18	0
7	C	19	0	0	3	0
7	D	122	0	0	18	0
7	E	167	0	0	17	0
7	F	18	0	0	4	0
7	P	1	0	0	0	0
7	Y	1	0	0	0	0
All	All	12392	0	11493	222	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 10.

All (222) 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:107:CYS:SG	7:A:592:HOH:O	2.25	0.94
3:F:17:ARG:HG3	7:F:103:HOH:O	1.71	0.89
2:E:194:GLY:O	7:E:620:HOH:O	1.95	0.83
1:A:232:GLY:HA3	5:A:401:COA:H132	1.62	0.82
2:B:327:GLN:OE1	7:B:644:HOH:O	1.97	0.81
2:E:169:SER:OG	7:E:524:HOH:O	1.97	0.81
1:A:234:CYS:SG	7:A:535:HOH:O	2.41	0.77
2:E:338:GLU:OE2	7:E:623:HOH:O	2.03	0.77
2:B:74:LYS:NZ	7:B:722:HOH:O	2.11	0.77
1:A:97:ILE:HD13	1:A:104:TRP:HA	1.66	0.76
5:D:401:COA:S1P	7:F:113:HOH:O	2.43	0.76
2:B:241:ASN:N	7:B:712:HOH:O	2.18	0.76
3:F:27:GLN:OE1	3:F:36:ARG:NH1	2.17	0.75
2:B:251:PRO:O	7:B:702:HOH:O	2.05	0.74
3:F:17:ARG:NH1	7:F:103:HOH:O	2.20	0.74
2:E:300:ASN:ND2	7:E:507:HOH:O	1.92	0.73
2:E:255:ASN:HD21	2:E:272:MET:HE2	1.51	0.73
2:E:286:GLU:OE2	7:E:598:HOH:O	2.07	0.73
1:D:137:TYR:OH	7:D:592:HOH:O	2.06	0.73
2:E:259:PHE:O	7:E:626:HOH:O	2.06	0.73
2:B:314:SER:HB3	2:B:320:LEU:HG	1.71	0.72
1:D:305:ARG:NH2	7:D:568:HOH:O	2.21	0.71
2:E:314:SER:HB3	2:E:320:LEU:HG	1.72	0.71
1:D:22:SER:OG	7:D:586:HOH:O	2.06	0.71
5:D:401:COA:O4A	7:D:595:HOH:O	2.09	0.71
2:E:285:LYS:O	7:E:563:HOH:O	2.08	0.71
2:B:236:ASN:HB3	2:B:243:THR:HG22	1.72	0.71
2:E:24:MET:HE3	3:F:38:ALA:HA	1.73	0.71
2:B:204:ASN:O	7:B:726:HOH:O	2.09	0.70
2:B:218:ASN:OD1	7:B:670:HOH:O	2.07	0.70
5:D:401:COA:O5A	7:D:530:HOH:O	2.10	0.70
1:D:171:ASP:O	7:D:587:HOH:O	2.11	0.69
2:B:69:GLU:OE1	4:Y:9:LYS:NZ	2.24	0.68
2:E:272:MET:HE3	4:P:1:ALA:N	2.07	0.68
2:E:115:TYR:OH	2:E:148:ARG:O	2.09	0.68
2:E:150:GLU:OE1	7:E:611:HOH:O	2.12	0.68
2:B:24:MET:HE3	3:C:38:ALA:HA	1.76	0.68
1:D:256:ASP:HB3	3:F:12:LYS:HD2	1.76	0.67
2:B:208:SER:O	7:B:747:HOH:O	2.13	0.67
2:E:58:GLU:OE2	7:E:538:HOH:O	2.13	0.66
1:D:234:CYS:SG	7:D:618:HOH:O	2.53	0.66
1:A:227:GLN:HG2	5:A:401:COA:H10	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:CYS:SG	7:D:606:HOH:O	2.53	0.65
2:E:236:ASN:HB3	2:E:243:THR:HG22	1.78	0.65
1:D:221:LEU:HA	5:D:401:COA:H72	1.78	0.64
2:B:181:ASP:HA	2:B:210:ILE:HG23	1.79	0.64
1:D:148:ARG:NH2	7:D:542:HOH:O	2.31	0.64
1:D:221:LEU:HD22	5:D:401:COA:H62	1.80	0.64
1:D:319:ASN:ND2	7:D:596:HOH:O	2.28	0.63
2:E:272:MET:HE3	4:P:1:ALA:H2	1.63	0.62
2:B:229:GLU:OE1	4:Y:1:ALA:HB2	2.00	0.61
2:B:352:ARG:HD3	7:B:742:HOH:O	1.99	0.61
2:B:115:TYR:OH	2:B:148:ARG:O	2.13	0.61
2:E:69:GLU:OE1	4:P:9:LYS:NZ	2.34	0.60
2:E:255:ASN:HD21	2:E:272:MET:CE	2.15	0.59
2:B:107:SER:N	7:B:709:HOH:O	2.36	0.58
1:A:7:LYS:HD3	1:A:10:THR:HG21	1.84	0.58
2:E:327:GLN:HB2	2:E:343:GLU:HA	1.84	0.58
2:B:255:ASN:OD1	4:Y:1:ALA:HB3	2.03	0.58
2:E:324:ASP:OD2	7:E:588:HOH:O	2.17	0.58
2:B:222:ASP:OD1	7:B:720:HOH:O	2.17	0.57
2:E:290:HIS:HD2	7:F:108:HOH:O	1.87	0.56
1:A:113:LYS:NZ	7:A:539:HOH:O	2.38	0.56
1:A:161:ILE:HG12	5:A:401:COA:H32	1.87	0.55
1:A:108:PHE:O	1:A:112:ARG:HG3	2.06	0.55
1:D:108:PHE:O	1:D:112:ARG:HG3	2.06	0.55
1:A:59:ASP:OD1	1:A:112:ARG:NH2	2.38	0.55
1:A:216:LYS:NZ	7:A:536:HOH:O	2.32	0.55
2:E:181:ASP:HA	2:E:210:ILE:HG23	1.88	0.55
1:A:141:LEU:HD13	1:A:169:GLU:HA	1.90	0.54
2:B:30:GLU:OE2	2:B:352:ARG:NH2	2.40	0.54
2:E:255:ASN:ND2	2:E:272:MET:HE2	2.20	0.54
2:B:177:LEU:HD21	2:B:224:PHE:CD2	2.42	0.54
1:D:285:HIS:HA	1:D:288:LEU:HD22	1.91	0.53
1:D:123:LYS:HE3	1:D:135:VAL:HG23	1.91	0.53
1:D:283:GLN:O	1:D:284:LYS:HG3	2.09	0.53
1:D:275:LYS:NZ	7:D:551:HOH:O	2.42	0.53
1:A:256:ASP:HB3	3:C:12:LYS:HD2	1.91	0.52
5:A:401:COA:O1A	7:A:594:HOH:O	2.18	0.52
2:E:84:ILE:HD11	2:E:367:LEU:HD13	1.92	0.52
2:E:30:GLU:OE2	2:E:352:ARG:NH2	2.43	0.52
1:A:227:GLN:HA	5:A:401:COA:H142	1.92	0.52
1:A:272:ARG:NH2	1:A:300:LEU:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:248:VAL:HG21	2:E:284:MET:HE3	1.91	0.51
1:D:117:LEU:HD22	1:D:180:LEU:HD11	1.93	0.51
1:A:290:ASP:HA	1:A:293:LEU:HD12	1.92	0.51
2:B:75:PHE:HB2	2:B:113:ALA:HB3	1.92	0.50
2:B:123:ARG:NH2	2:B:166:LEU:O	2.42	0.50
5:D:401:COA:O3A	7:D:598:HOH:O	2.19	0.50
2:B:302:GLU:OE2	7:B:708:HOH:O	2.19	0.50
2:E:267:LEU:HD13	2:E:279:TYR:HB2	1.93	0.50
2:B:24:MET:HE2	2:B:346:MET:HE2	1.93	0.49
3:C:30:THR:H	3:C:33:ALA:HB3	1.76	0.49
1:A:275:LYS:HE2	7:A:582:HOH:O	2.12	0.49
3:C:7:GLY:N	7:C:115:HOH:O	2.45	0.49
2:E:334:PRO:O	2:E:338:GLU:HG3	2.13	0.49
2:B:320:LEU:HB2	2:B:348:HIS:HB3	1.94	0.49
1:D:141:LEU:HD13	1:D:169:GLU:HA	1.95	0.49
2:B:255:ASN:O	4:Y:2:ARG:NH2	2.46	0.49
1:A:92:PRO:HG2	1:A:95:ASP:HB3	1.95	0.49
2:B:261:HIS:CD2	2:B:305:THR:HG22	2.48	0.49
3:F:30:THR:H	3:F:33:ALA:HB3	1.78	0.49
1:A:246:ASP:O	1:A:301:LYS:NZ	2.46	0.49
2:E:362:PRO:HG2	2:E:363:GLN:OE1	2.13	0.49
1:A:233:SER:O	1:A:237:GLU:HB2	2.13	0.48
1:D:291:GLU:HG3	7:D:536:HOH:O	2.12	0.48
2:B:53:GLY:O	2:B:82:LYS:HB2	2.13	0.48
1:D:100:ASP:HB3	1:D:103:LYS:HB3	1.95	0.48
3:C:40:ARG:HD3	3:C:44:LYS:HD2	1.95	0.48
1:A:279:ASP:OD1	1:A:280:ALA:N	2.45	0.48
2:B:170:THR:HG22	2:B:171:LEU:HG	1.95	0.48
2:B:175:ARG:NH1	7:B:720:HOH:O	2.13	0.48
1:A:267:ARG:HD3	7:A:581:HOH:O	2.12	0.48
1:D:209:ILE:O	7:D:590:HOH:O	2.19	0.48
1:A:210:ASP:OD2	1:A:210:ASP:N	2.26	0.48
2:B:241:ASN:HB2	7:B:712:HOH:O	2.13	0.48
2:B:79:ASN:O	2:B:107:SER:OG	2.29	0.47
1:D:246:ASP:HB3	1:D:249:ILE:HG12	1.95	0.47
1:A:297:ARG:HD2	1:A:304:GLU:HA	1.96	0.47
1:D:117:LEU:HG	1:D:145:PHE:HE2	1.79	0.47
2:E:177:LEU:HD21	2:E:224:PHE:CD2	2.49	0.47
2:E:301:LEU:HA	2:E:301:LEU:HD12	1.67	0.47
1:A:171:ASP:O	7:A:617:HOH:O	2.20	0.47
2:E:381:LYS:NZ	7:E:544:HOH:O	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:THR:O	3:C:34:ILE:HG12	2.14	0.47
2:E:229:GLU:CD	4:P:1:ALA:H1	2.22	0.47
2:B:324:ASP:HB2	2:B:345:ILE:HD11	1.96	0.47
1:A:215:ALA:HB2	1:A:249:ILE:HD12	1.96	0.47
3:C:36:ARG:HG3	7:C:110:HOH:O	2.14	0.47
1:D:317:LEU:HD12	1:D:317:LEU:HA	1.79	0.46
5:D:401:COA:O7A	5:D:401:COA:O2B	2.32	0.46
1:A:246:ASP:HB3	1:A:249:ILE:HG12	1.98	0.46
2:B:121:ILE:O	7:B:729:HOH:O	2.20	0.46
2:B:352:ARG:CD	7:B:742:HOH:O	2.59	0.46
1:D:229:LYS:N	7:D:598:HOH:O	2.48	0.46
2:B:248:VAL:HG21	2:B:284:MET:HE3	1.98	0.46
2:E:56:LYS:HD2	2:E:77:GLU:HG3	1.97	0.46
2:B:82:LYS:NZ	7:B:741:HOH:O	2.49	0.46
2:B:44:PRO:HA	2:B:363:GLN:OE1	2.15	0.45
1:D:97:ILE:HG21	1:D:104:TRP:HB2	1.98	0.45
2:E:14:TYR:OH	2:E:30:GLU:OE1	2.35	0.45
1:D:105:VAL:HA	1:D:108:PHE:CE2	2.50	0.45
1:D:118:SER:HA	1:D:137:TYR:CZ	2.51	0.45
1:D:59:ASP:OD1	1:D:112:ARG:NH2	2.49	0.45
1:A:129:LEU:HD23	1:A:129:LEU:HA	1.86	0.45
2:E:77:GLU:HB2	2:E:112:THR:HG21	1.98	0.45
2:B:34:THR:HG23	4:Y:9:LYS:HD3	1.97	0.45
1:D:208:ASP:OD1	1:D:208:ASP:N	2.49	0.45
1:D:279:ASP:O	1:D:283:GLN:HG2	2.17	0.45
2:E:201:ARG:NH1	2:E:238:VAL:O	2.50	0.45
2:E:47:VAL:HG13	2:E:55:ILE:HD13	1.99	0.45
5:D:401:COA:O1A	5:D:401:COA:H4B	2.17	0.44
2:E:302:GLU:HG3	7:E:625:HOH:O	2.17	0.44
2:B:175:ARG:NH2	7:B:720:HOH:O	2.48	0.44
1:D:171:ASP:HA	1:D:172:PRO:HD3	1.82	0.44
1:A:93:LYS:HB2	1:A:93:LYS:HE3	1.69	0.44
3:C:8:LYS:NZ	7:C:114:HOH:O	2.47	0.44
2:E:249:LYS:HG2	7:E:599:HOH:O	2.17	0.44
2:E:320:LEU:HD21	2:E:358:PHE:CG	2.53	0.44
2:B:35:TRP:CD2	2:B:65:THR:HG22	2.53	0.44
3:F:27:GLN:HB2	3:F:36:ARG:HH22	1.82	0.44
1:A:171:ASP:HA	1:A:172:PRO:HD3	1.82	0.44
1:D:68:ASN:ND2	1:D:99:ARG:HG3	2.31	0.44
2:E:45:THR:HA	2:E:46:PRO:HD3	1.86	0.44
2:B:8:LEU:HD22	2:B:12:GLU:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:PHE:CZ	2:E:29:SER:HB3	2.53	0.44
1:A:174:TRP:O	7:A:610:HOH:O	2.21	0.44
1:A:288:LEU:HD22	1:A:292:PHE:CD2	2.53	0.44
2:B:320:LEU:HD21	2:B:358:PHE:CG	2.52	0.43
2:E:157:LYS:NZ	2:E:159:HIS:O	2.45	0.43
2:B:41:GLN:OE1	2:B:125:ARG:HA	2.19	0.43
2:B:267:LEU:HD13	2:B:279:TYR:HB2	1.99	0.43
2:E:41:GLN:OE1	2:E:125:ARG:HA	2.19	0.43
2:B:214:ASN:HD22	2:B:214:ASN:C	2.27	0.43
1:D:210:ASP:OD1	1:D:210:ASP:N	2.25	0.43
1:A:171:ASP:HB3	1:A:174:TRP:CD1	2.54	0.43
1:A:208:ASP:OD1	1:A:208:ASP:N	2.51	0.43
1:D:315:LEU:HA	1:D:315:LEU:HD23	1.80	0.43
1:A:118:SER:HA	1:A:137:TYR:CZ	2.54	0.43
2:B:174:GLY:O	2:B:190:VAL:HG22	2.18	0.43
1:D:35:PHE:CZ	1:D:162:GLU:HB2	2.54	0.43
1:A:123:LYS:HE3	1:A:135:VAL:HG23	2.01	0.43
2:E:272:MET:HE3	4:P:1:ALA:H3	1.84	0.42
1:A:101:GLU:O	1:A:105:VAL:HG23	2.19	0.42
1:A:274:ARG:NH2	7:A:521:HOH:O	2.51	0.42
2:B:157:LYS:NZ	2:B:159:HIS:O	2.45	0.42
1:D:195:LYS:HE2	7:D:535:HOH:O	2.19	0.42
3:F:19:ARG:HD3	3:F:19:ARG:HA	1.85	0.42
2:B:42:TRP:CE3	2:B:59:LEU:HD13	2.54	0.42
2:B:42:TRP:HA	2:B:59:LEU:HD12	2.00	0.42
1:A:86:LYS:HA	1:A:86:LYS:HD3	1.79	0.42
2:B:174:GLY:HA3	2:B:191:GLY:N	2.35	0.42
2:E:44:PRO:HA	2:E:363:GLN:OE1	2.18	0.42
3:F:20:LYS:H	3:F:20:LYS:HG2	1.62	0.42
1:A:78:ASP:C	1:A:80:ILE:H	2.28	0.42
1:D:27:ASN:OD1	1:D:27:ASN:N	2.51	0.42
1:D:230:GLY:N	7:D:598:HOH:O	2.16	0.42
2:E:237:ASP:HB2	2:E:245:ILE:HD11	2.01	0.42
1:A:270:ILE:HG12	1:A:310:LEU:HD22	2.00	0.42
2:E:332:GLN:O	7:E:642:HOH:O	2.21	0.42
1:D:86:LYS:HA	1:D:86:LYS:HD3	1.76	0.41
1:D:93:LYS:HB2	1:D:93:LYS:HE3	1.79	0.41
1:D:319:ASN:HB2	7:D:596:HOH:O	2.19	0.41
2:E:375:ASN:OD1	2:E:375:ASN:N	2.51	0.41
2:B:127:MET:HE2	2:B:190:VAL:HG23	2.02	0.41
1:D:37:TYR:CD2	3:F:17:ARG:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:LEU:N	7:E:553:HOH:O	2.17	0.41
2:B:221:LYS:O	7:B:617:HOH:O	2.22	0.41
1:D:116:ASN:ND2	1:D:119:ASP:HB2	2.36	0.41
1:D:141:LEU:HG	1:D:176:ILE:HD11	2.03	0.41
3:F:30:THR:O	3:F:34:ILE:HG12	2.20	0.41
3:C:29:ILE:H	3:C:29:ILE:HG13	1.76	0.41
2:E:249:LYS:HE2	7:E:599:HOH:O	2.21	0.41
3:C:16:LYS:N	3:C:16:LYS:HD2	2.37	0.40
2:B:35:TRP:CE2	2:B:65:THR:HG22	2.56	0.40
2:B:222:ASP:O	2:B:238:VAL:HG22	2.21	0.40
1:D:91:LEU:HB3	1:D:92:PRO:HD2	2.04	0.40
2:B:47:VAL:HG13	2:B:55:ILE:HD13	2.03	0.40
2:B:175:ARG:HG3	2:B:187:LEU:HD11	2.02	0.40
1:D:129:LEU:HD23	1:D:129:LEU:HA	1.94	0.40
2:E:26:ASP:OD1	2:E:383:SER:HA	2.22	0.40
2:E:241:ASN:HB2	7:E:615:HOH:O	2.21	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	311/320 (97%)	300 (96%)	11 (4%)	0	100	100
1	D	311/320 (97%)	305 (98%)	5 (2%)	1 (0%)	36	55
2	B	357/401 (89%)	340 (95%)	16 (4%)	1 (0%)	36	55
2	E	357/401 (89%)	342 (96%)	14 (4%)	1 (0%)	36	55
3	C	37/48 (77%)	34 (92%)	3 (8%)	0	100	100
3	F	35/48 (73%)	33 (94%)	2 (6%)	0	100	100
4	P	8/15 (53%)	8 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	Y	10/15 (67%)	9 (90%)	0	1 (10%)	0 0
All	All	1426/1568 (91%)	1371 (96%)	51 (4%)	4 (0%)	36 55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	99	ARG
4	Y	11	THR
2	B	293	GLY
2	E	293	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	288/294 (98%)	276 (96%)	12 (4%)	26 52
1	D	288/294 (98%)	274 (95%)	14 (5%)	22 45
2	B	323/358 (90%)	303 (94%)	20 (6%)	16 34
2	E	323/358 (90%)	307 (95%)	16 (5%)	22 44
3	C	27/33 (82%)	22 (82%)	5 (18%)	1 3
3	F	26/33 (79%)	21 (81%)	5 (19%)	1 2
4	P	8/10 (80%)	7 (88%)	1 (12%)	4 9
4	Y	9/10 (90%)	8 (89%)	1 (11%)	6 12
All	All	1292/1390 (93%)	1218 (94%)	74 (6%)	18 39

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	86	LYS
1	A	130	ASN
1	A	141	LEU

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Mol	Chain	Res	Type
1	A	208	ASP
1	A	210	ASP
1	A	221	LEU
1	A	271	GLN
1	A	290	ASP
1	A	294	GLU
1	A	302	LEU
1	A	317	LEU
2	B	32	ARG
2	B	55	ILE
2	B	56	LYS
2	B	157	LYS
2	B	170	THR
2	B	183	HIS
2	B	214	ASN
2	B	223	LEU
2	B	226	THR
2	B	233	LEU
2	B	238	VAL
2	B	266	LEU
2	B	267	LEU
2	B	295	GLU
2	B	302	GLU
2	B	320	LEU
2	B	336	ASP
2	B	346	MET
2	B	360	LEU
2	B	389	VAL
3	C	17	ARG
3	C	21	VAL
3	C	26	ILE
3	C	29	ILE
3	C	37	LEU
1	D	13	SER
1	D	79	ASN
1	D	86	LYS
1	D	130	ASN
1	D	141	LEU
1	D	159	LEU
1	D	208	ASP
1	D	210	ASP
1	D	221	LEU

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Mol	Chain	Res	Type
1	D	247	LYS
1	D	271	GLN
1	D	288	LEU
1	D	290	ASP
1	D	317	LEU
2	E	55	ILE
2	E	56	LYS
2	E	157	LYS
2	E	183	HIS
2	E	214	ASN
2	E	223	LEU
2	E	238	VAL
2	E	267	LEU
2	E	295	GLU
2	E	302	GLU
2	E	320	LEU
2	E	336	ASP
2	E	346	MET
2	E	360	LEU
2	E	375	ASN
2	E	389	VAL
3	F	17	ARG
3	F	19	ARG
3	F	21	VAL
3	F	26	ILE
3	F	37	LEU
4	Y	9	LYS
4	P	9	LYS

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

Mol	Chain	Res	Type
1	A	55	HIS
2	B	214	ASN
2	B	283	ASN
2	B	290	HIS
2	B	306	HIS
1	D	116	ASN
1	D	268	ASN
1	D	271	GLN
1	D	319	ASN
2	E	71	ASN

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Mol	Chain	Res	Type
2	E	214	ASN
2	E	236	ASN
2	E	255	ASN
2	E	262	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	COA	A	401	-	47,50,50	1.72	6 (12%)	69,75,75	1.85	13 (18%)
6	SO4	B	501	-	4,4,4	0.35	0	6,6,6	0.10	0
5	COA	D	401	-	47,50,50	1.71	6 (12%)	69,75,75	2.18	20 (28%)

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	COA	A	401	-	-	19/48/64/64	0/3/3/3
5	COA	D	401	-	-	20/48/64/64	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401	COA	C5P-N4P	6.27	1.48	1.33
5	A	401	COA	C5P-N4P	6.09	1.47	1.33
5	D	401	COA	C6A-N6A	5.27	1.47	1.34
5	A	401	COA	C6A-N6A	5.21	1.47	1.34
5	A	401	COA	C9P-N8P	4.89	1.45	1.33
5	D	401	COA	C9P-N8P	4.29	1.43	1.33
5	A	401	COA	C5A-C4A	2.67	1.43	1.39
5	A	401	COA	C5A-N7A	-2.51	1.34	1.39
5	D	401	COA	C2B-C3B	-2.36	1.47	1.53
5	A	401	COA	C2B-C3B	-2.17	1.48	1.53
5	D	401	COA	C5A-N7A	-2.14	1.35	1.39
5	D	401	COA	C5A-C4A	2.11	1.42	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	401	COA	O4B-C1B-N9A	6.88	121.30	108.09
5	D	401	COA	N3A-C2A-N1A	-6.39	118.91	128.58
5	D	401	COA	C4B-O4B-C1B	-5.90	96.44	109.47
5	A	401	COA	C5A-C4A-N3A	-5.81	118.72	126.72
5	A	401	COA	N3A-C2A-N1A	-5.79	119.81	128.58
5	D	401	COA	C5A-C4A-N3A	-4.76	120.16	126.72
5	A	401	COA	N3A-C4A-N9A	4.70	135.16	127.17
5	A	401	COA	O6A-CCP-CBP	-4.40	103.48	110.55
5	D	401	COA	N3A-C4A-N9A	3.98	133.93	127.17
5	D	401	COA	C5A-N7A-C8A	3.91	109.59	103.45
5	A	401	COA	C5A-N7A-C8A	3.76	109.36	103.45
5	A	401	COA	C2A-N3A-C4A	3.60	120.63	111.83
5	D	401	COA	N9A-C8A-N7A	-3.48	109.00	113.94
5	D	401	COA	C6P-C5P-N4P	3.40	122.53	116.34
5	A	401	COA	CEP-CBP-CCP	-3.38	102.65	108.22
5	A	401	COA	O4B-C1B-N9A	3.14	114.11	108.09
5	A	401	COA	C4A-C5A-N7A	-3.08	107.06	110.58
5	D	401	COA	C4A-C5A-N7A	-3.04	107.11	110.58
5	D	401	COA	C2A-N3A-C4A	2.95	119.03	111.83
5	A	401	COA	C3B-C2B-C1B	2.65	105.72	99.89
5	D	401	COA	C4A-N9A-C8A	2.53	108.40	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	401	COA	C4A-N9A-C1B	-2.51	120.77	126.63
5	A	401	COA	CEP-CBP-CAP	2.48	113.00	108.77
5	D	401	COA	P3B-O3B-C3B	2.47	130.03	123.43
5	A	401	COA	C7P-C6P-C5P	-2.46	108.30	112.39
5	A	401	COA	N9A-C8A-N7A	-2.45	110.46	113.94
5	D	401	COA	C6P-C7P-N8P	-2.44	106.80	112.00
5	D	401	COA	C6A-C5A-N7A	2.39	136.70	132.09
5	D	401	COA	OAP-CAP-CBP	-2.38	104.68	110.18
5	D	401	COA	O4B-C1B-C2B	-2.35	101.60	106.62
5	D	401	COA	O5P-C5P-N4P	-2.19	118.72	123.03
5	D	401	COA	O4B-C4B-C5B	2.07	115.98	109.33
5	D	401	COA	CDP-CBP-CAP	-2.06	105.25	108.77

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	401	COA	CCP-O6A-P2A-O3A
5	A	401	COA	CCP-O6A-P2A-O5A
5	A	401	COA	OAP-CAP-CBP-CCP
5	A	401	COA	C9P-CAP-CBP-CCP
5	A	401	COA	OAP-CAP-CBP-CDP
5	A	401	COA	C9P-CAP-CBP-CDP
5	A	401	COA	OAP-CAP-CBP-CEP
5	A	401	COA	C9P-CAP-CBP-CEP
5	A	401	COA	C5P-C6P-C7P-N8P
5	A	401	COA	S1P-C2P-C3P-N4P
5	D	401	COA	P2A-O3A-P1A-O5B
5	D	401	COA	CDP-CBP-CCP-O6A
5	D	401	COA	CEP-CBP-CCP-O6A
5	D	401	COA	CAP-CBP-CCP-O6A
5	D	401	COA	N8P-C9P-CAP-OAP
5	D	401	COA	C5P-C6P-C7P-N8P
5	D	401	COA	S1P-C2P-C3P-N4P
5	A	401	COA	C3B-C4B-C5B-O5B
5	D	401	COA	C3B-C4B-C5B-O5B
5	D	401	COA	C4B-C5B-O5B-P1A
5	D	401	COA	C2B-C3B-O3B-P3B
5	A	401	COA	O4B-C4B-C5B-O5B
5	D	401	COA	C4B-C3B-O3B-P3B
5	D	401	COA	O9P-C9P-CAP-OAP
5	D	401	COA	O4B-C4B-C5B-O5B

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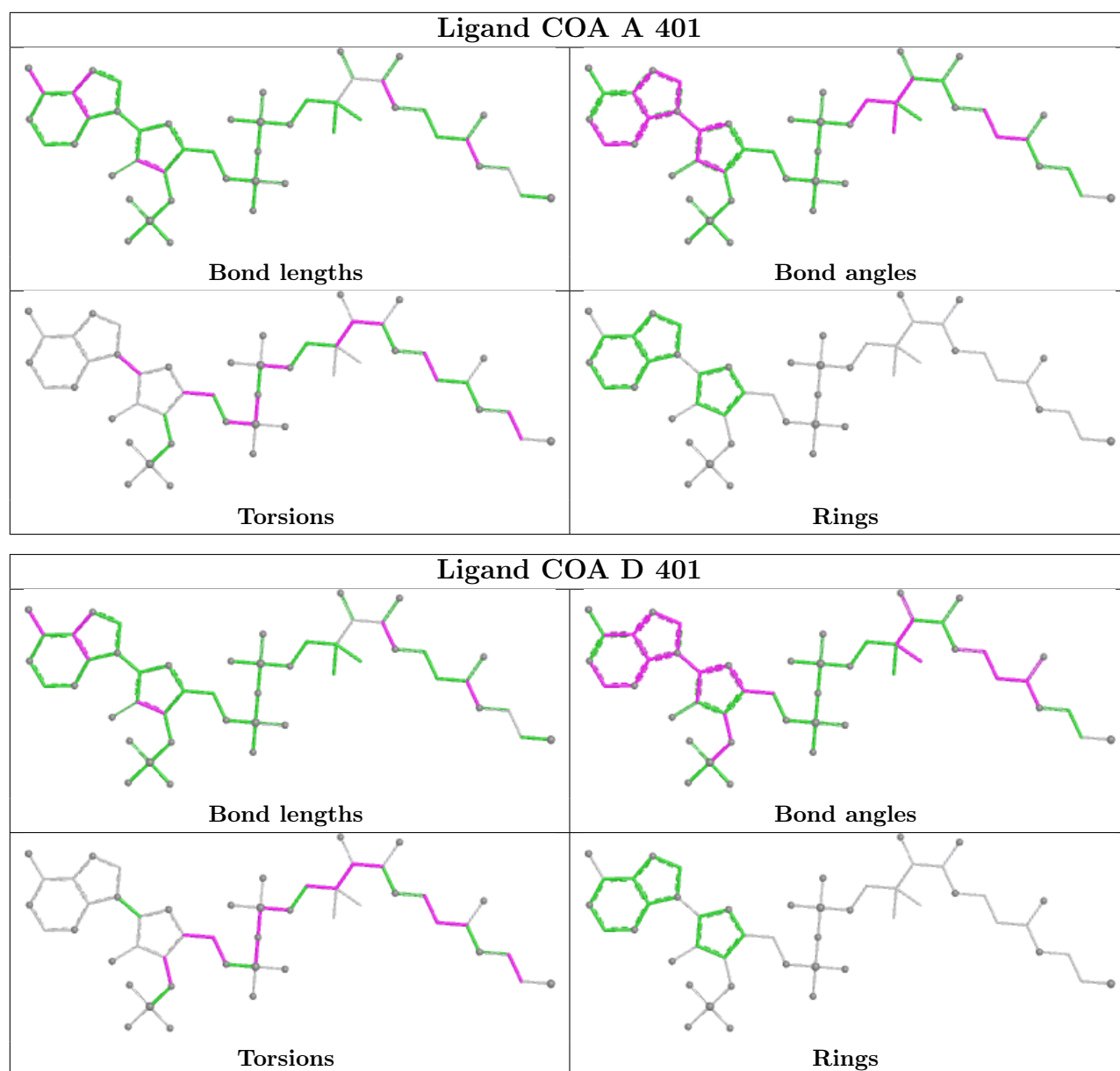
Mol	Chain	Res	Type	Atoms
5	A	401	COA	P2A-O3A-P1A-O5B
5	D	401	COA	P1A-O3A-P2A-O6A
5	D	401	COA	O5P-C5P-C6P-C7P
5	A	401	COA	C2B-C1B-N9A-C8A
5	A	401	COA	O9P-C9P-CAP-OAP
5	A	401	COA	C5B-O5B-P1A-O2A
5	A	401	COA	C5B-O5B-P1A-O3A
5	D	401	COA	CCP-O6A-P2A-O4A
5	D	401	COA	N4P-C5P-C6P-C7P
5	A	401	COA	O4B-C1B-N9A-C8A
5	D	401	COA	C9P-CAP-CBP-CDP
5	D	401	COA	C9P-CAP-CBP-CEP
5	D	401	COA	C9P-CAP-CBP-CCP
5	A	401	COA	N8P-C9P-CAP-OAP

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	401	COA	5	0
5	D	401	COA	8	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	313/320 (97%)	0.63	33 (10%)	11 10	52, 76, 122, 158	0
1	D	313/320 (97%)	0.55	27 (8%)	16 14	49, 75, 113, 149	0
2	B	361/401 (90%)	0.38	14 (3%)	43 38	51, 72, 110, 150	0
2	E	361/401 (90%)	0.36	17 (4%)	36 32	51, 73, 108, 152	0
3	C	39/48 (81%)	1.22	11 (28%)	1 1	59, 84, 154, 190	0
3	F	37/48 (77%)	1.20	8 (21%)	2 2	55, 81, 140, 175	0
4	P	10/15 (66%)	2.04	5 (50%)	0 0	85, 116, 128, 152	0
4	Y	12/15 (80%)	2.06	6 (50%)	0 0	90, 111, 132, 163	0
All	All	1446/1568 (92%)	0.54	121 (8%)	17 15	49, 75, 119, 190	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	26	ILE	7.2
1	D	286	SER	5.0
2	E	108	ASN	4.7
2	E	8	LEU	4.7
4	P	10	SER	4.6
3	F	26	ILE	4.4
3	C	29	ILE	4.4
1	A	271	GLN	4.3
2	E	86	SER	4.3
3	F	29	ILE	4.1
1	A	8	PRO	4.1
3	C	45	ARG	4.0
1	A	286	SER	4.0
1	D	285	HIS	4.0
1	A	287	ASP	3.9
2	B	107	SER	3.9

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Mol	Chain	Res	Type	RSRZ
3	C	27	GLN	3.7
3	F	27	GLN	3.7
1	D	291	GLU	3.6
3	F	19	ARG	3.6
1	A	284	LYS	3.5
2	E	251	PRO	3.4
1	A	209	ILE	3.4
2	B	8	LEU	3.3
4	Y	11	THR	3.3
1	D	210	ASP	3.3
1	D	119	ASP	3.3
1	A	119	ASP	3.2
4	Y	12	GLY	3.2
1	A	7	LYS	3.2
3	F	28	GLY	3.2
1	A	99	ARG	3.1
1	A	77	ASP	3.1
2	B	67	GLY	3.1
1	A	285	HIS	3.0
2	B	32	ARG	3.0
4	Y	10	SER	3.0
1	A	76	GLY	3.0
2	E	109	ILE	2.9
1	A	319	ASN	2.9
1	D	76	GLY	2.9
2	B	66	SER	2.9
2	E	32	ARG	2.9
1	D	318	ASN	2.8
2	E	192	SER	2.8
4	Y	1	ALA	2.8
2	B	54	PHE	2.8
3	F	18	HIS	2.8
1	D	283	GLN	2.8
1	A	210	ASP	2.8
1	A	208	ASP	2.7
1	A	78	ASP	2.7
3	C	25	ASN	2.7
2	B	192	SER	2.7
3	C	19	ARG	2.7
1	D	98	VAL	2.6
1	D	8	PRO	2.6
4	P	8	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	319	ASN	2.6
2	B	10	VAL	2.6
2	B	242	ASN	2.6
1	D	78	ASP	2.5
2	E	54	PHE	2.5
4	P	3	THR	2.5
2	B	239	ARG	2.5
1	D	70	LYS	2.5
1	D	116	ASN	2.5
2	B	68	GLU	2.5
1	A	288	LEU	2.5
2	E	240	ALA	2.5
4	P	6	THR	2.5
1	D	207	GLU	2.4
1	A	293	LEU	2.4
1	A	133	GLU	2.4
1	D	7	LYS	2.4
3	C	23	ARG	2.4
2	E	66	SER	2.3
1	A	267	ARG	2.3
1	A	291	GLU	2.3
2	E	68	GLU	2.3
2	E	83	GLU	2.3
1	A	305	ARG	2.3
1	A	290	ASP	2.3
1	A	130	ASN	2.3
1	A	183	LYS	2.3
3	F	24	ASP	2.3
1	D	27	ASN	2.2
3	C	18	HIS	2.2
2	B	83	GLU	2.2
2	E	191	GLY	2.2
4	Y	9	LYS	2.2
1	D	131	GLY	2.2
1	D	209	ILE	2.2
2	E	19	SER	2.2
1	D	77	ASP	2.2
1	A	110	GLU	2.2
2	E	110	ARG	2.2
1	D	113	LYS	2.2
3	F	20	LYS	2.2
1	A	27	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	317	LEU	2.2
1	D	72	SER	2.2
3	C	24	ASP	2.2
2	B	194	GLY	2.1
1	A	9	GLU	2.1
1	A	132	GLU	2.1
1	D	93	LYS	2.1
1	D	267	ARG	2.1
1	A	107	CYS	2.1
4	Y	7	ALA	2.1
1	A	294	GLU	2.1
1	D	9	GLU	2.1
2	B	249	LYS	2.1
2	E	239	ARG	2.1
4	P	7	ALA	2.0
1	A	117	LEU	2.0
2	E	67	GLY	2.0
3	C	28	GLY	2.0
3	C	20	LYS	2.0
1	D	130	ASN	2.0
1	A	137	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($\text{\AA}^2$)	Q<0.9
5	COA	A	401	48/48	0.68	0.30	137,138,141,141	0
5	COA	D	401	48/48	0.80	0.25	129,132,135,135	0

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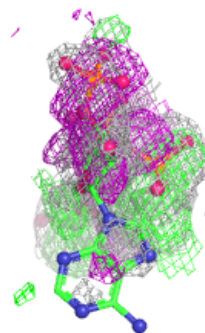
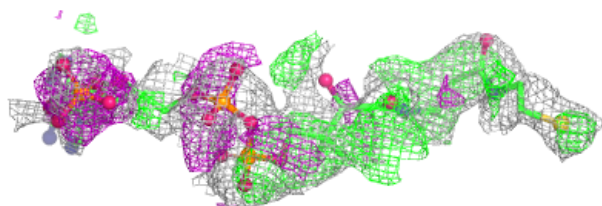
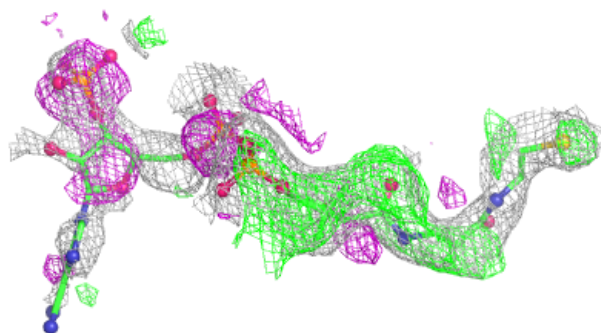
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	B	501	5/5	0.82	0.19	111,122,126,126	0

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.

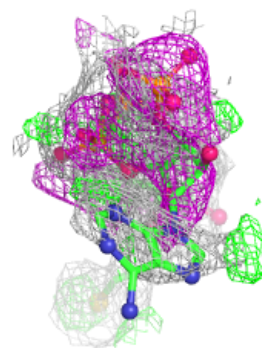
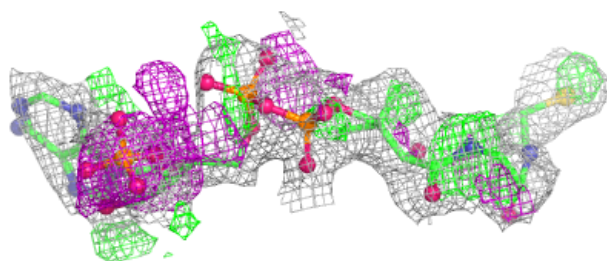
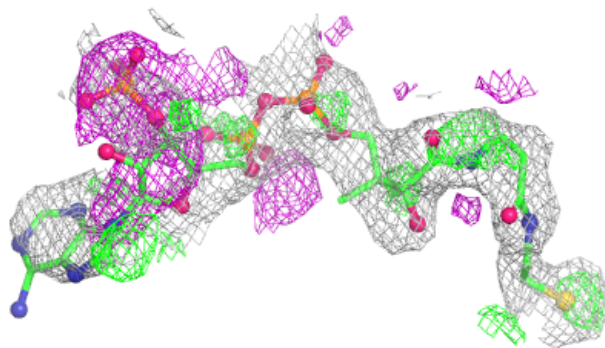
Electron density around COA A 401:

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 COA D 401:

$2mF_o-DF_c$ (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.