



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:14 PM UTC

PDB ID : 6UV5 / pdb_00006uv5
EMDB ID : EMD-20904
Title : Structure of human ATP citrate lyase in complex with acetyl-CoA and oxaloacetate
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2019-11-01
Resolution : 3.40 Å(reported)
Based on initial model : 3MWD

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

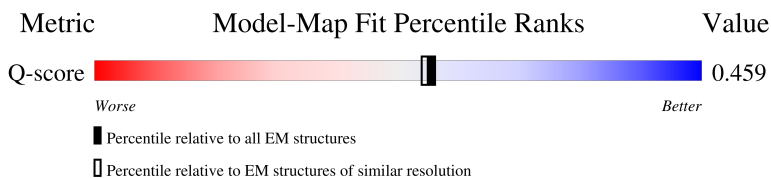
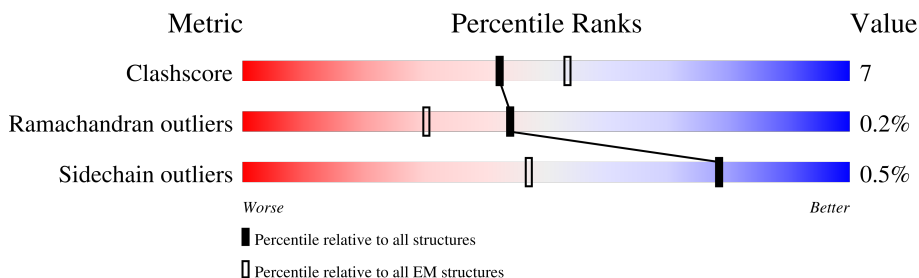
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1100	
1	B	1100	
1	C	1100	
1	D	1100	

2 Entry composition [i](#)

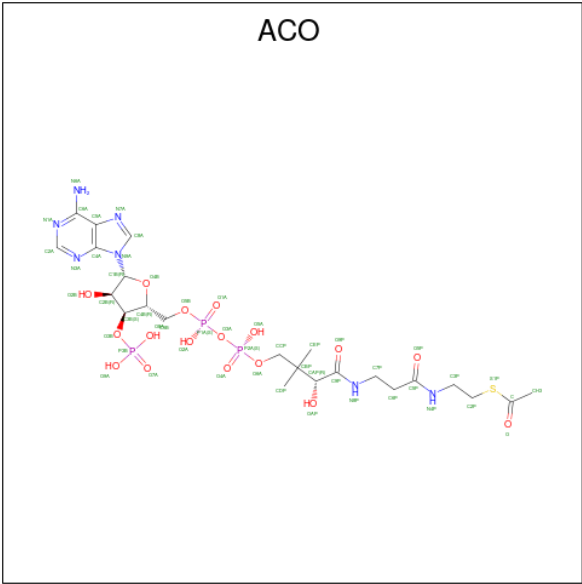
There are 4 unique types of molecules in this entry. The entry contains 31954 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 ATP citrate lyase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1021	Total 7906	5064	1340	1458	44	2	0
1	B	1021	Total 7906	5064	1340	1458	44	2	0
1	C	1021	Total 7906	5064	1340	1458	44	2	0
1	D	1021	Total 7906	5064	1340	1458	44	2	0

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



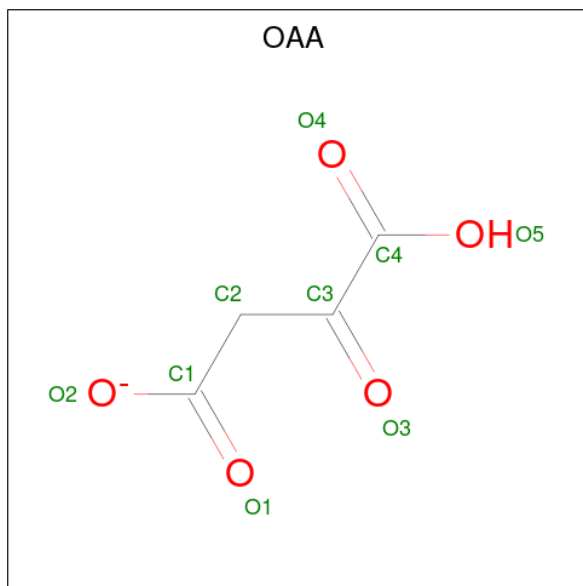
Mol	Chain	Residues	Atoms						AltConf
			Total	C	N	O	P	S	
2	A	1	Total 51	23	7	17	3	1	0
2	A	1	Total 102	46	14	34	6	2	1

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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	S
			51	23	7	17	3	1
2	D	1	Total	C	N	O	P	S
			51	23	7	17	3	1

- Molecule 3 is OXALOACETATE ION (CCD ID: OAA) (formula: $C_4H_3O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			9	4	5	
3	A	1	Total	C	O	0
			9	4	5	
3	B	1	Total	C	O	0
			9	4	5	
3	B	1	Total	C	O	0
			9	4	5	
3	C	1	Total	C	O	0
			9	4	5	
3	C	1	Total	C	O	0
			9	4	5	
3	D	1	Total	C	O	0
			9	4	5	
3	D	1	Total	C	O	0
			9	4	5	

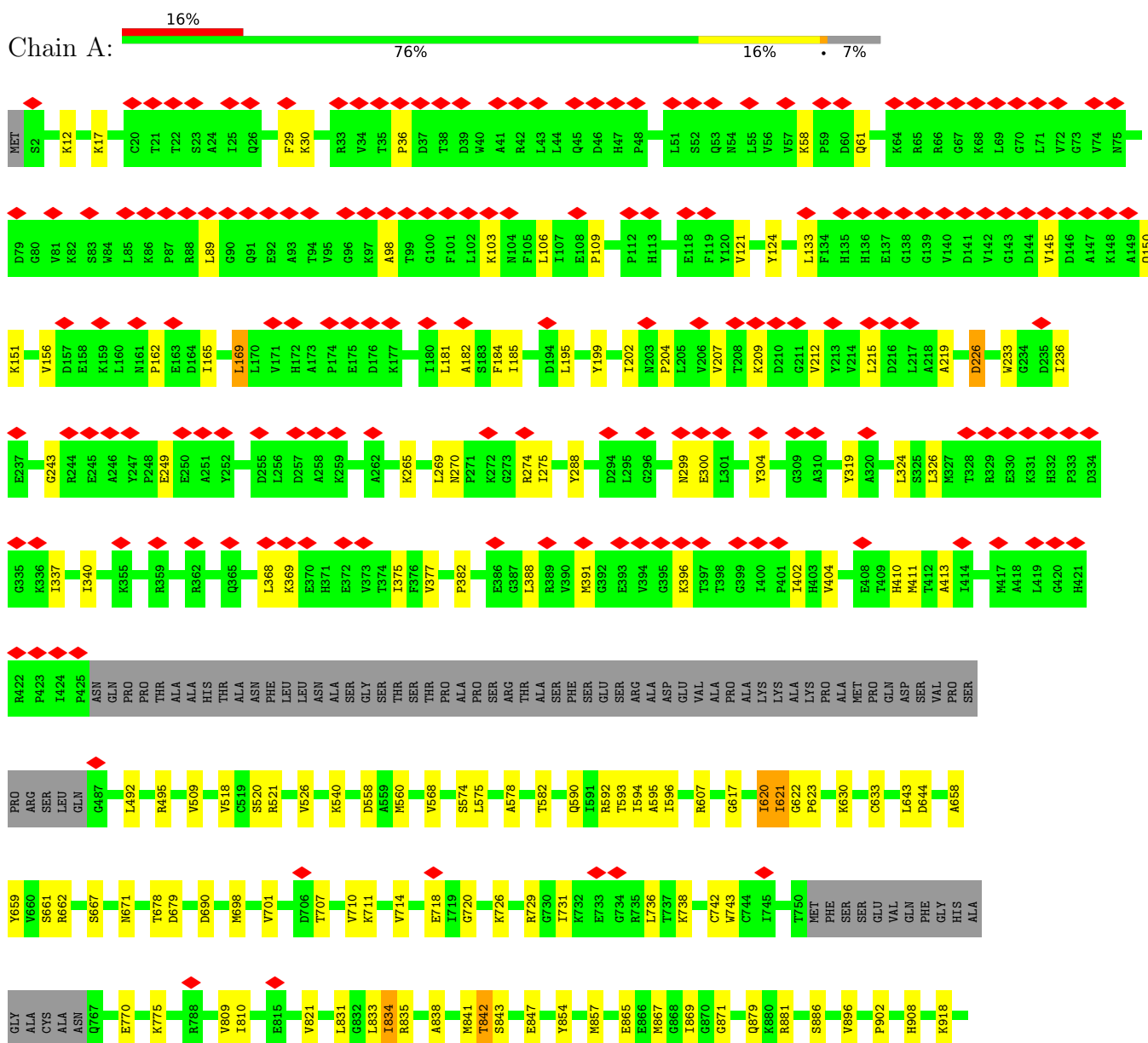
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total 1	O 1	0
4	B	1	Total 1	O 1	0
4	C	1	Total 1	O 1	0

3 Residue-property plots

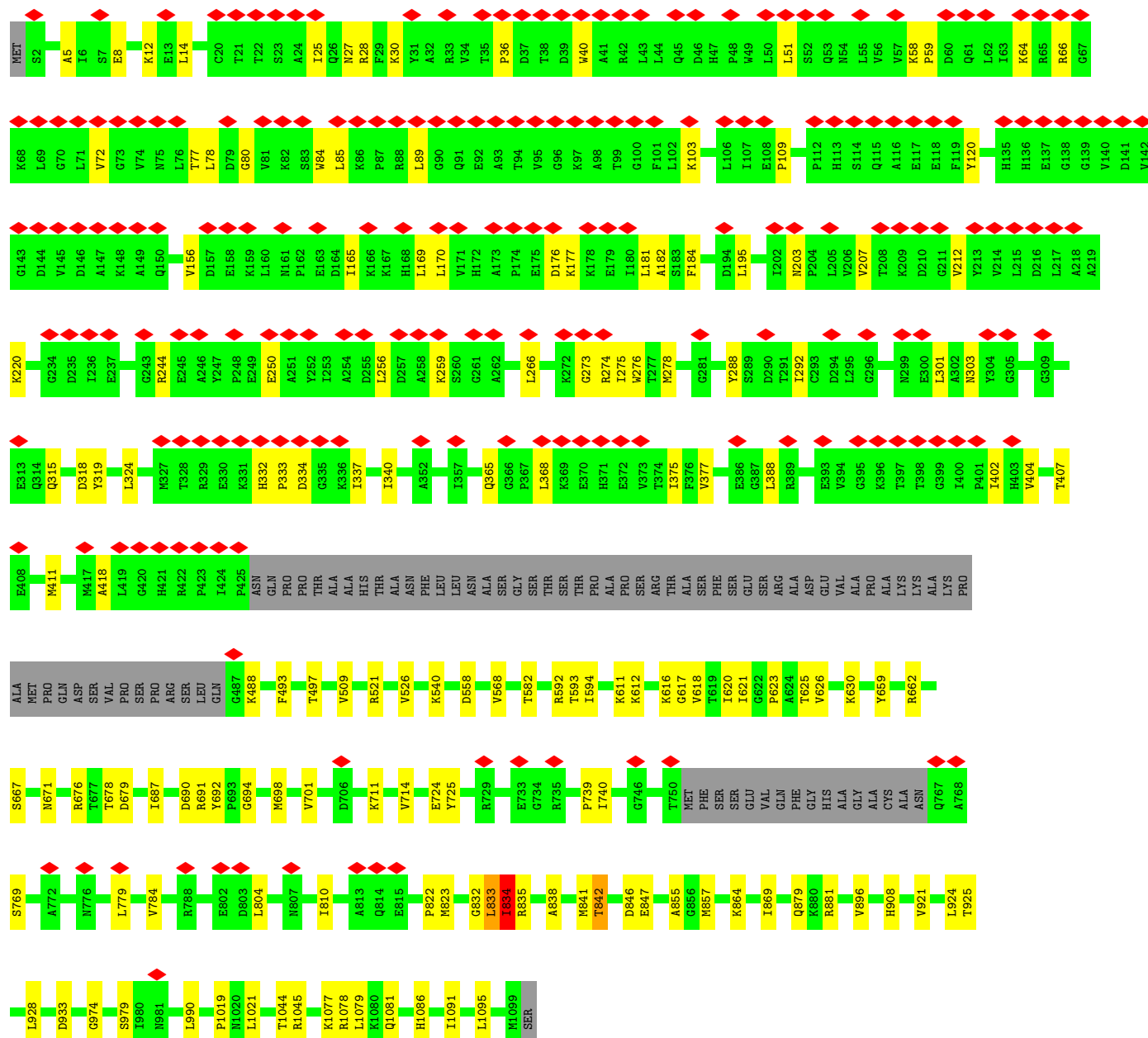
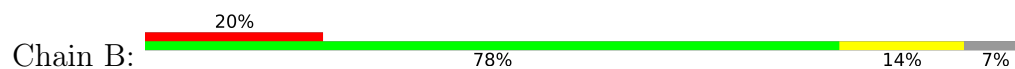
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: ATP citrate lyase





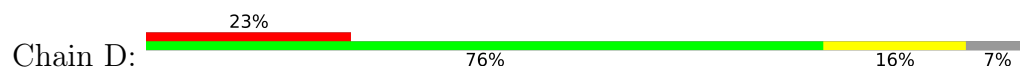
• Molecule 1: ATP citrate lyase



• Molecule 1: ATP citrate lyase



L928	D940	K944	M945	D951	S952	P956	E966	G967	K968	G974	K978	S979	I980	N981	D984	V987	E989	V1010	T1014	P1019	M1020	L1021	L1028	I1029	F1033	V1034	D1035	M1036	N1039	T1044	R1045	I1054	D1075	R1078	H1086	P1087	W1088																													
Q798	Y801	E802	D803	L804	V805	A806	N807	G808	V809	I810	V811	P812	A813	Q814	E815	V816	P817	Y825	R829	E830	L831	G832	I833	I834	R835	K836	M841	N1020	T842	S843	D846	M867	G868	I869	G870	G871	Q879	S886	M892	V896	P902	H908	N909	V921	L924	T925																				
K738	P739	I740	C741	C742	C743	C744	I745	G746	T747	C748	A749	T750	MET	PHE	SER	SER	GLU	VAL	GLN	PHE	GLY	HIS	ALA	GLY	ALA	ALA	ASN	Q767	A768	S769	E770	T771	A772	V773	A774	N775	Q777	A778	L779	K780	E781	A782	G783	V784	F785	V786	F787	S788	S789	F790	D791	E792	L793	G794	E795	I796	I797									
M666	E669	L670	M671	M672	S675	R676	T677	T678	V681	I687	G688	G689	D690	R691	T696	F697	M698	Q705	D706	T707	P708	G709	V710	M711	I712	I713	V714	V715	L716	G717	E718	I719	G720	G721	T722	E723	E724	Y725	K726	I727	C728	R729	G730	I731	K732	E733	G734	R735	L736	T737																
E584	T585	M586	N587	Y588	A589	I597	A598	E599	G600	I601	P602	E603	A604	L605	T606	R607	K608	L609	I610	K611	K612	A613	D614	Q615	K616	G617	I620	P623	G628	I629	K630	P631	G632	C633	I636	G637	M638	D644	A648	S649	M650	L651	S656	V657	Y658	Y659	R662	S663	G664	G665																
SER	PRO	ARG	SER	LEU	GLN	G487	K488	S489	T490	T491	L492	F493	H496	T497	M504	R507	A508	V509	D514	E521	D522	E523	V526	M529	D536	K540	F541	Y542	K546	E547	V552	N555	M556	A557	D558	A559	M560	R561	L569	A578	Y579	D580	S581	T582	M583																					
H421	R422	F423	I424	F425	ASN	GLN	PRO	PRO	THR	ALA	ALA	HIS	THR	ALA	ASN	PHE	LEU	LEU	ASN	ALA	SER	GLY	SER	THR	THR	PRO	ALA	SER	ARG	THR	ALA	SER	GLU	SER	GLU	ARG	ALA	ASP	GLU	VAL	ALA	PRO	ALA	LYS	LYS	LYS	PRO	ALA	H403	V404	F405	G406	T407	E408	T409	H410	M411	T412	A413	I414	V415	G416	M417	A418	L419	G420
I361	R362	D363	Y364	Q365	G366	P367	L368	K369	E370	H371	E372	V373	T374	I375	F376	V377	R378	R379	G380	G381	P382	N383	Y384	Q385	E386	G387	L388	R389	V390	M391	G392	H393	P393	D394	G395	K396	T397	G399	F401	I402	H403	V404	F405	G406	T407	E408	T409	H410	M411	T412	A413	I414	V415	G416	M417	A418	L419	G420								
L301	A302	N303	Y304	G305	E306	Y307	S308	G309	A310	P311	S312	E313	Q314	Q315	T316	Y317	D318	Y319	A320	G321	T322	I323	L324	S325	L326	N327	T328	R329	E330	K331	G332	H333	P333	D334	G335	K336	T337	L338	I339	I340	G341	G342	S343	I344	A345	N346	F347	T348	N349	V350	A351	A352	T353	F354	K355	G356	I357	R358	R359	A360						
P241	F242	G243	R244	E245	A246	Y247	P248	E249	E250	A251	Y252	I253	A254	D255	L256	D257	K258	E259	S260	G261	A262	S263	L264	K265	L266	T267	L268	L269	M270	P271	K272	G273	R274	I275	W276	T277	M278	V279	G281	G282	G283	A284	S285	V286	V287	Y288	S289	D290	T291	I292	C293	D294	L295	G296	G297	N298	E300									
L181	A182	S183	F184	I185	S186	G187	L188	F189	M190	F191	Y192	E193	D194	L195	Y196	F197	T198	Y199	L200	E201	I202	N203	P204	G143	D144	V145	D146	A147	K148	A149	Q150	K151	E152	L153	V154	G155	V156	D157	E158	K159	L160	M161	P162	E163	D164	I165	K166	I167	H168	L169	L170	V171	H172	A173	P174	E175	D176	K177	E178	E179	I180					
Q61	L62	I63	K64	R65	R66	G67	K68	L69	G70	L71	V72	G73	V74	M75	L76	T77	L78	D79	G80	W81	K82	S83	W84	L85	K86	P87	R88	L89	G90	Q91	E92	A93	T94	V95	G96	K97	A98	T99	G100	F101	L102	K103	L104	F105	L106	I107	E108	P109	F110	V111	P112	H113	S114	Q115	A116	E117	E118	F119	Y120							
MET	S2	A3	K4	A5	T6	S7	E8	Q9	T10	G11	K12	E13	L14	L15	Y16	K17	F18	I19	C20	T21	T22	S23	A24	T25	Q26	W27	R28	F29	K30	V31	A32	R33	V34	T35	P36	D37	T38	D39	W40	A41	R42	L43	L44	Q45	D46	H47	P48	W49	L50	L51	S52	Q53	N54	L55	V56	V57	K58	P59	D60							



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	108738	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	191.4, 191.4, 191.4	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86999995, 0.86999995, 0.86999995	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OAA, ACO

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	0.35	0/8083	0.59	5/10942 (0.0%)
1	B	0.35	0/8083	0.56	1/10942 (0.0%)
1	C	0.32	0/8083	0.57	1/10942 (0.0%)
1	D	0.34	0/8083	0.57	5/10942 (0.0%)
All	All	0.34	0/32332	0.57	12/43768 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	622	GLY	CA-C-N	9.72	131.99	119.84
1	A	622	GLY	C-N-CA	9.72	131.99	119.84
1	D	835	ARG	N-CA-C	-7.71	98.80	110.14
1	A	169	LEU	N-CA-C	6.77	121.20	113.15
1	B	842	THR	N-CA-C	5.59	122.71	110.80
1	D	622	GLY	CA-C-N	5.24	125.97	120.11
1	D	622	GLY	C-N-CA	5.24	125.97	120.11
1	A	842	THR	N-CA-C	5.23	121.95	110.80
1	D	842	THR	N-CA-C	5.20	121.86	110.80
1	D	833	LEU	N-CA-C	-5.13	107.68	114.04
1	A	952	SER	N-CA-C	-5.09	105.37	112.45
1	C	952	SER	N-CA-C	-5.00	105.50	112.45

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	7906	0	7956	129	0
1	B	7906	0	7956	104	0
1	C	7906	0	7956	117	0
1	D	7906	0	7956	116	0
2	A	153	0	102	5	0
2	B	51	0	34	1	0
2	D	51	0	34	1	0
3	A	18	0	4	0	0
3	B	18	0	4	0	0
3	C	18	0	4	0	0
3	D	18	0	4	0	0
4	A	1	0	0	0	0
4	B	1	0	0	2	0
4	C	1	0	0	0	0
All	All	31954	0	32010	430	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 (430) 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:B:833:LEU:HD11	4:B:1301:HOH:O	1.35	1.23
2:B:1201:ACO:O4B	2:B:1201:ACO:C1B	1.64	1.21
1:A:1018:LYS:HE3	2:A:1202[B]:ACO:O2A	1.38	1.19
2:D:1201:ACO:O4B	2:D:1201:ACO:C1B	1.64	1.17
1:A:831:LEU:CD1	1:A:833:LEU:HD23	1.78	1.14
2:A:1201:ACO:O4B	2:A:1201:ACO:C1B	1.64	1.10
1:C:831:LEU:HD11	1:C:833:LEU:HD23	1.47	0.96
1:D:623:PRO:HG2	1:D:690:ASP:CB	1.95	0.96
1:D:623:PRO:HD2	1:D:693:PRO:HA	1.45	0.95
1:A:831:LEU:HD12	1:A:833:LEU:HD23	1.47	0.95
1:B:623:PRO:HD2	1:B:690:ASP:OD2	1.65	0.93
1:B:36:PRO:HG2	1:B:103:LYS:HG2	1.50	0.92
1:A:831:LEU:HD11	1:A:833:LEU:CD2	2.05	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:623:PRO:HG2	1:C:690:ASP:OD2	1.78	0.83
1:A:831:LEU:HD11	1:A:833:LEU:HD23	1.58	0.82
1:D:623:PRO:HG2	1:D:690:ASP:HB3	1.60	0.81
1:A:831:LEU:CD1	1:A:833:LEU:CD2	2.57	0.81
1:D:623:PRO:HG2	1:D:690:ASP:HB2	1.62	0.80
1:A:150:GLN:CB	1:A:169:LEU:HD12	2.13	0.78
1:A:150:GLN:HB2	1:A:169:LEU:HD12	1.67	0.77
1:C:651:LEU:HD11	1:C:671:ASN:HD21	1.49	0.76
1:D:622:GLY:HA2	1:D:694:GLY:H	1.51	0.76
1:A:182:ALA:O	1:A:185:ILE:HB	1.89	0.72
1:D:831:LEU:HD11	1:D:833:LEU:HD23	1.71	0.72
1:C:831:LEU:CD1	1:C:833:LEU:HD23	2.20	0.70
1:A:833:LEU:HD12	1:A:833:LEU:O	1.92	0.68
1:C:833:LEU:HD12	1:C:833:LEU:O	1.92	0.68
1:D:622:GLY:HA3	1:D:687:ILE:O	1.94	0.67
1:B:80:GLY:O	1:B:84:TRP:HB2	1.95	0.66
1:A:36:PRO:HG2	1:A:103:LYS:HE3	1.79	0.65
1:C:153:LEU:HD23	1:C:153:LEU:C	2.22	0.64
1:C:834:ILE:HD13	1:D:834:ILE:HD12	1.79	0.64
1:A:169:LEU:HG	1:A:169:LEU:O	1.95	0.64
1:C:186:SER:O	1:C:189:PHE:HB3	1.98	0.64
1:D:623:PRO:CD	1:D:693:PRO:HA	2.24	0.63
1:B:497:THR:O	1:B:521:ARG:NH2	2.31	0.63
1:A:831:LEU:HD11	1:A:833:LEU:HD21	1.80	0.63
1:A:896:VAL:HG21	1:A:990:LEU:HD11	1.81	0.63
1:A:181:LEU:O	1:A:184:PHE:HB3	1.99	0.63
1:A:181:LEU:HD12	1:A:207:VAL:HG21	1.81	0.63
1:C:80:GLY:O	1:C:84:TRP:HB2	2.00	0.62
1:B:207:VAL:HG22	1:B:212:VAL:HG12	1.81	0.62
1:B:896:VAL:HG21	1:B:990:LEU:HD11	1.81	0.61
1:C:497:THR:O	1:C:521:ARG:NH2	2.34	0.61
1:C:1044:THR:OG1	1:C:1045:ARG:N	2.34	0.61
1:B:833:LEU:O	1:B:833:LEU:HD12	2.00	0.60
1:A:925:THR:HG23	1:C:925:THR:HG23	1.83	0.60
1:A:595:ALA:HA	1:A:621:ILE:HB	1.83	0.60
1:D:27:ASN:HD21	1:D:109:PRO:HD2	1.67	0.60
1:D:62:LEU:HD12	1:D:62:LEU:O	2.02	0.60
1:D:156:VAL:HG23	1:D:611:LYS:HD2	1.84	0.60
1:C:715:VAL:O	1:C:742:CYS:HA	2.02	0.59
1:B:925:THR:HG23	1:D:925:THR:HG23	1.83	0.59
1:B:181:LEU:O	1:B:184:PHE:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:924:LEU:O	1:B:928:LEU:HB2	2.02	0.59
1:B:1078:ARG:HH22	1:D:879:GLN:HE22	1.52	0.58
1:A:377:VAL:HG21	1:A:391:MET:HE2	1.84	0.58
1:C:663:SER:HB3	1:C:666:MET:HE2	1.85	0.58
1:C:825:TYR:HD1	1:D:834:ILE:HD11	1.68	0.58
1:A:1044:THR:OG1	1:A:1045:ARG:N	2.37	0.57
1:B:58:LYS:HB3	1:B:72:VAL:HG23	1.86	0.57
1:C:726:LYS:HD3	1:C:729:ARG:HE	1.70	0.57
1:D:32:ALA:HB3	1:D:107:ILE:HB	1.85	0.57
1:A:678:THR:OG1	1:A:679:ASP:N	2.38	0.57
1:A:834:ILE:HD13	1:B:834:ILE:HD12	1.86	0.57
1:D:1029:ILE:O	1:D:1033:PHE:HB2	2.04	0.57
1:C:909:ASN:ND2	1:D:913:CYS:SG	2.78	0.57
1:A:1079:LEU:HD13	1:C:841:MET:HB3	1.87	0.56
1:B:823:MET:SD	1:B:833:LEU:HD21	2.45	0.56
1:C:896:VAL:HG21	1:C:990:LEU:HD11	1.86	0.56
1:D:742:CYS:SG	1:D:743:TRP:N	2.79	0.56
1:A:662:ARG:NH2	1:A:690:ASP:O	2.38	0.56
1:A:908:HIS:HE1	1:B:908:HIS:HE1	1.53	0.56
1:A:707:THR:O	1:A:738:LYS:NZ	2.39	0.56
1:A:150:GLN:HB3	1:A:169:LEU:HD12	1.87	0.56
1:D:924:LEU:O	1:D:928:LEU:HB2	2.05	0.56
1:D:58:LYS:NZ	1:D:215:LEU:O	2.38	0.56
1:D:84:TRP:O	1:D:88:ARG:NH1	2.38	0.56
1:A:658:ALA:HB2	1:A:710:VAL:HG11	1.88	0.56
1:B:739:PRO:HG2	1:B:804:LEU:HD21	1.88	0.56
1:D:623:PRO:O	1:D:688:GLY:HA3	2.06	0.56
1:C:829:ARG:HH12	1:C:836:LYS:HB3	1.71	0.55
1:D:622:GLY:CA	1:D:687:ILE:O	2.54	0.55
1:A:270:ASN:ND2	1:A:299:ASN:O	2.39	0.55
1:D:150:GLN:NE2	1:D:168:HIS:O	2.40	0.55
1:D:343:SER:O	1:D:379:ARG:NH1	2.39	0.55
1:B:8:GLU:O	1:B:12:LYS:HB2	2.06	0.55
1:D:269:LEU:HD23	1:D:301:LEU:HB3	1.88	0.55
1:D:662:ARG:NH1	1:D:718:GLU:OE1	2.40	0.55
1:C:509:VAL:HG13	1:C:526:VAL:HG21	1.88	0.55
1:A:847:GLU:OE2	1:D:1088:TRP:NE1	2.35	0.55
1:B:170:LEU:HD11	1:B:182:ALA:HB2	1.89	0.55
1:C:940:ASP:OD2	1:C:944:LYS:NZ	2.39	0.54
1:D:987:VAL:HG13	1:D:1028:LEU:HD13	1.89	0.54
1:C:55:LEU:HD22	1:C:81:VAL:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LEU:HD21	1:C:303:ASN:HD21	1.72	0.54
1:D:12:LYS:HE2	1:D:106:LEU:HD21	1.88	0.54
1:C:966:GLU:O	1:C:968:LYS:NZ	2.38	0.54
1:D:407:THR:OG1	1:D:676:ARG:NH2	2.41	0.54
1:A:720:GLY:HA2	1:A:770:GLU:HB3	1.89	0.54
1:A:731:ILE:HG22	1:A:736:LEU:HB2	1.90	0.54
1:C:924:LEU:O	1:C:928:LEU:HB2	2.08	0.54
1:C:974:GLY:HA2	1:C:1021:LEU:HA	1.89	0.54
1:A:382:PRO:HA	1:A:644:ASP:OD2	2.08	0.54
1:B:488:LYS:NZ	1:B:618:VAL:O	2.41	0.54
1:C:657:VAL:HG13	1:C:712:MET:HG3	1.90	0.54
1:A:924:LEU:O	1:A:928:LEU:HB2	2.08	0.53
1:C:194:ASP:OD1	1:C:232:LYS:NZ	2.40	0.53
1:D:41:ALA:O	1:D:45:GLN:HB2	2.09	0.53
1:A:1038:ARG:NH2	1:A:1049:ASP:OD1	2.41	0.53
1:A:124:TYR:OH	1:A:151:LYS:NZ	2.41	0.53
1:B:933:ASP:OD1	1:B:933:ASP:N	2.41	0.53
1:B:974:GLY:HA2	1:B:1021:LEU:HA	1.89	0.53
1:C:540:LYS:NZ	1:D:838:ALA:O	2.36	0.53
1:D:940:ASP:OD2	1:D:944:LYS:NZ	2.35	0.53
1:C:16:TYR:O	1:C:28:ARG:NH1	2.42	0.53
1:D:181:LEU:O	1:D:184:PHE:HB3	2.09	0.53
1:B:667:SER:O	1:B:671:ASN:ND2	2.42	0.53
1:B:1077:LYS:HG3	1:D:1054:ILE:HD12	1.90	0.53
1:C:529:MET:HB2	1:C:552:VAL:HG22	1.90	0.52
1:C:708:PRO:O	1:C:711:LYS:NZ	2.42	0.52
1:C:631:PRO:HG2	1:C:681:VAL:HB	1.90	0.52
1:A:388:LEU:HD22	1:A:404:VAL:HB	1.92	0.52
1:D:275:ILE:HD11	1:D:419:LEU:HD21	1.91	0.52
1:D:831:LEU:CD1	1:D:833:LEU:HD23	2.39	0.52
1:A:659:TYR:HA	1:A:714:VAL:O	2.09	0.52
1:B:1079:LEU:HD13	1:D:841:MET:HB3	1.91	0.52
1:D:198:THR:OG1	1:D:222:ASP:OD1	2.28	0.52
1:D:262:ALA:HA	1:D:309:GLY:HA3	1.92	0.52
1:A:842:THR:HG21	1:C:902:PRO:HG3	1.92	0.51
1:A:156:VAL:HG11	1:A:607:ARG:HB3	1.93	0.51
1:A:661:SER:OG	1:A:662:ARG:N	2.42	0.51
1:C:314:GLN:HE21	1:C:315:GLN:HE21	1.56	0.51
1:C:886:SER:OG	1:C:1036:MET:SD	2.64	0.51
1:D:183:SER:O	1:D:186:SER:HB3	2.10	0.51
1:A:133:LEU:HD21	1:A:145:VAL:HB	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:PRO:HG3	1:C:842:THR:HG21	1.92	0.51
1:A:1078:ARG:HH22	1:C:879:GLN:HE22	1.59	0.51
1:B:842:THR:HG21	1:D:902:PRO:HG3	1.92	0.51
1:C:177:LYS:HD3	1:C:207:VAL:HB	1.93	0.51
1:B:85:LEU:HB2	1:B:89:LEU:HB2	1.93	0.51
1:B:711:LYS:HG3	1:B:810:ILE:HG12	1.93	0.51
1:A:518:VAL:HG11	1:A:643:LEU:HD11	1.92	0.51
1:B:165:ILE:HG23	1:B:169:LEU:HD23	1.93	0.51
1:D:653:ARG:NH2	1:D:679:ASP:O	2.43	0.51
1:D:662:ARG:HG2	1:D:687:ILE:HD11	1.93	0.51
1:D:697:PHE:HB2	1:D:723:GLU:HG3	1.92	0.51
1:D:165:ILE:HG23	1:D:169:LEU:HD23	1.92	0.50
1:A:509:VAL:HG13	1:A:526:VAL:HG21	1.93	0.50
1:B:869:ILE:HD13	1:D:869:ILE:HD13	1.94	0.50
1:C:58:LYS:CG	1:C:106:LEU:HD11	2.42	0.50
1:C:367:PRO:HA	1:C:370:GLU:HG2	1.93	0.50
1:B:509:VAL:HG13	1:B:526:VAL:HG21	1.93	0.50
1:C:122:CYS:O	1:C:132:VAL:HA	2.12	0.50
1:C:521:ARG:NH1	1:C:633:CYS:O	2.44	0.50
1:B:59:PRO:O	1:B:66:ARG:NH1	2.45	0.50
1:B:324:LEU:HD22	1:B:368:LEU:HD21	1.92	0.50
1:C:58:LYS:O	1:C:106:LEU:HG	2.11	0.50
1:D:622:GLY:C	1:D:687:ILE:O	2.55	0.50
1:A:698:MET:HA	1:A:701:VAL:HG22	1.93	0.50
1:C:1029:ILE:O	1:C:1033:PHE:HB2	2.12	0.50
1:D:707:THR:O	1:D:738:LYS:NZ	2.41	0.50
1:A:30:LYS:HB3	1:A:109:PRO:HG2	1.92	0.50
1:A:1077:LYS:HG3	1:C:1054:ILE:HD12	1.94	0.50
1:A:869:ILE:HD13	1:C:869:ILE:HD13	1.94	0.50
1:B:612:LYS:HE2	1:B:616:LYS:HE3	1.94	0.50
1:D:16:TYR:O	1:D:28:ARG:NH1	2.44	0.50
1:D:938:ALA:O	1:D:942:ALA:HB3	2.12	0.50
1:A:582:THR:HG23	1:A:594:ILE:HG21	1.94	0.49
1:A:592:ARG:NH2	1:A:617:GLY:O	2.45	0.49
1:C:542:TYR:OH	1:D:836:LYS:O	2.31	0.49
1:A:568:VAL:HG13	1:A:593:THR:HG23	1.94	0.49
1:B:337:ILE:HD13	1:B:418:ALA:HB1	1.94	0.49
1:D:558:ASP:N	1:D:558:ASP:OD1	2.44	0.49
1:A:908:HIS:HE1	1:B:908:HIS:CE1	2.31	0.49
1:B:176:ASP:OD1	1:B:177:LYS:NZ	2.45	0.49
1:C:394:VAL:O	1:C:398:THR:OG1	2.23	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:582:THR:HG23	1:D:594:ILE:HG21	1.95	0.49
1:D:896:VAL:HG21	1:D:990:LEU:HD11	1.93	0.49
1:A:98:ALA:HB1	1:A:243:GLY:HA2	1.93	0.49
1:A:207:VAL:HG22	1:A:212:VAL:HG22	1.95	0.49
1:C:394:VAL:HA	1:C:397:THR:HG22	1.94	0.49
1:A:61:GLN:HE22	1:A:103:LYS:H	1.60	0.49
1:A:375:ILE:HB	1:A:402:ILE:HG12	1.94	0.49
1:A:867:MET:HB2	1:A:871:GLY:HA3	1.93	0.49
1:D:886:SER:OG	1:D:1036:MET:SD	2.69	0.49
1:B:592:ARG:NH2	1:B:617:GLY:O	2.45	0.49
1:D:377:VAL:HG21	1:D:391:MET:HE2	1.93	0.49
1:D:560:MET:SD	1:D:590:GLN:NE2	2.82	0.49
1:A:288:TYR:OH	1:A:411:MET:O	2.29	0.49
1:A:838:ALA:O	1:B:540:LYS:NZ	2.36	0.49
1:A:540:LYS:NZ	1:B:838:ALA:O	2.35	0.49
1:C:410:HIS:HB3	1:C:413:ALA:HB2	1.94	0.49
1:D:509:VAL:HG13	1:D:526:VAL:HG21	1.95	0.49
1:A:726:LYS:HG2	1:A:729:ARG:HH21	1.77	0.49
2:A:1202[B]:ACO:HH33	2:A:1202[B]:ACO:H31	1.95	0.49
1:B:1044:THR:OG1	1:B:1045:ARG:N	2.34	0.49
1:C:56:VAL:HG13	1:C:110:PHE:HB2	1.94	0.49
1:C:522:ASP:OD1	1:C:522:ASP:N	2.44	0.49
1:C:921:VAL:O	1:C:925:THR:HB	2.13	0.49
1:B:278:MET:HE3	1:B:319:TYR:HD2	1.78	0.48
1:C:835:ARG:HG3	1:D:822:PRO:HG2	1.95	0.48
1:D:1044:THR:OG1	1:D:1045:ARG:N	2.46	0.48
1:A:1021:LEU:HD21	2:A:1202[B]:ACO:C1B	2.42	0.48
1:B:841:MET:HB3	1:D:1079:LEU:HD13	1.96	0.48
1:A:275:ILE:HG12	1:A:337:ILE:HD11	1.96	0.48
1:B:288:TYR:OH	1:B:411:MET:O	2.30	0.48
1:C:30:LYS:HB3	1:C:109:PRO:HG3	1.96	0.48
1:A:233:TRP:HB3	1:A:236:ILE:HD13	1.94	0.48
1:A:558:ASP:OD1	1:A:558:ASP:N	2.45	0.48
1:C:58:LYS:HG3	1:C:106:LEU:HD11	1.95	0.48
1:D:61:GLN:NE2	1:D:103:LYS:H	2.11	0.48
1:D:181:LEU:HD11	1:D:207:VAL:HG11	1.96	0.48
1:B:14:LEU:HD12	1:B:195:LEU:HD21	1.94	0.48
1:B:340:ILE:HB	1:B:377:VAL:HG22	1.95	0.48
1:B:558:ASP:N	1:B:558:ASP:OD1	2.45	0.48
1:B:847:GLU:OE2	1:C:1088:TRP:NE1	2.47	0.48
1:B:857:MET:HE1	1:B:881:ARG:HE	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:779:LEU:HD12	1:D:784:VAL:HG21	1.95	0.48
1:A:1086:HIS:HD2	1:A:1091:ILE:HD11	1.79	0.48
1:C:264:LEU:HA	1:C:306:GLU:O	2.13	0.48
1:A:17:LYS:HE2	1:A:29:PHE:HE2	1.79	0.48
1:C:956:PRO:HB3	1:C:1010:VAL:HG22	1.96	0.48
1:B:156:VAL:HG23	1:B:611:LYS:HD2	1.96	0.47
1:D:102:LEU:HB3	1:D:105:PHE:HE1	1.78	0.47
1:A:742:CYS:SG	1:A:743:TRP:N	2.87	0.47
1:A:1035:ASP:O	1:A:1039:ASN:CB	2.62	0.47
1:D:388:LEU:HD22	1:D:404:VAL:HB	1.95	0.47
1:C:979:SER:OG	1:C:1019:PRO:O	2.30	0.47
1:D:177:LYS:HB3	1:D:181:LEU:HD13	1.97	0.47
1:D:867:MET:HB2	1:D:871:GLY:HA3	1.97	0.47
1:C:716:LEU:HD21	1:C:745:ILE:HD12	1.96	0.47
1:D:780:LYS:HD2	1:D:786:VAL:HB	1.97	0.47
1:A:835:ARG:HG3	1:B:822:PRO:HG2	1.97	0.47
1:B:407:THR:O	1:B:676:ARG:NE	2.46	0.47
1:B:659:TYR:HA	1:B:714:VAL:O	2.15	0.47
1:C:39:ASP:OD1	1:C:39:ASP:N	2.45	0.47
1:A:718:GLU:O	1:A:775:LYS:NZ	2.47	0.47
1:A:857:MET:HE1	1:A:881:ARG:HE	1.80	0.47
1:A:1051:TYR:OH	1:C:1078:ARG:NH1	2.48	0.47
1:B:365:GLN:HA	1:B:368:LEU:HD12	1.95	0.47
1:B:493:PHE:HB2	1:B:630:LYS:HD3	1.97	0.47
1:B:879:GLN:HE22	1:D:1078:ARG:HH22	1.62	0.47
1:D:184:PHE:O	1:D:188:LEU:N	2.40	0.47
1:A:879:GLN:OE1	1:C:1078:ARG:NH2	2.46	0.47
1:A:886:SER:OG	1:A:1036:MET:SD	2.73	0.47
1:A:195:LEU:HG	1:A:233:TRP:HE1	1.80	0.47
1:C:908:HIS:HE1	1:D:908:HIS:HE1	1.63	0.47
1:A:199:TYR:O	1:A:219:ALA:HA	2.15	0.47
1:C:324:LEU:HD22	1:C:368:LEU:HD11	1.97	0.47
1:D:79:ASP:N	1:D:79:ASP:OD1	2.48	0.46
1:D:268:LEU:HG	1:D:303:ASN:HB3	1.97	0.46
1:D:668:ASN:HA	1:D:671:ASN:HD22	1.80	0.46
1:B:8:GLU:O	1:B:12:LYS:CB	2.63	0.46
1:B:274:ARG:NH2	1:B:334:ASP:O	2.48	0.46
1:C:662:ARG:HH11	1:C:718:GLU:HG3	1.80	0.46
1:D:260:SER:OG	1:D:315:GLN:NE2	2.44	0.46
1:D:721:GLY:N	1:D:770:GLU:OE1	2.48	0.46
1:D:407:THR:O	1:D:676:ARG:NE	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:974:GLY:HA2	1:D:1021:LEU:HA	1.97	0.46
1:A:410:HIS:HB3	1:A:413:ALA:HB2	1.97	0.46
1:B:740:ILE:HB	1:B:784:VAL:HG13	1.98	0.46
1:B:678:THR:OG1	1:B:679:ASP:N	2.48	0.46
1:D:208:THR:OG1	1:D:209:LYS:N	2.48	0.46
1:C:789:SER:OG	1:C:790:PHE:N	2.48	0.46
1:D:30:LYS:HB3	1:D:109:PRO:HG2	1.97	0.46
1:D:120:TYR:HB3	1:D:135:HIS:HB3	1.97	0.46
1:C:318:ASP:O	1:C:322:THR:OG1	2.30	0.46
1:A:121:VAL:HG12	1:A:202:ILE:HB	1.98	0.46
1:A:834:ILE:CD1	1:B:834:ILE:HD12	2.46	0.46
1:B:388:LEU:HD22	1:B:404:VAL:HB	1.97	0.45
1:C:133:LEU:HA	1:C:150:GLN:O	2.16	0.45
1:B:691:ARG:NH1	1:B:692:TYR:OH	2.49	0.45
1:C:987:VAL:HG13	1:C:1028:LEU:HD13	1.97	0.45
1:C:1092:SER:O	1:C:1092:SER:OG	2.29	0.45
1:C:663:SER:OG	1:C:664:GLY:N	2.49	0.45
1:D:135:HIS:ND1	1:D:137:GLU:O	2.45	0.45
1:C:787:PRO:HG3	1:C:793:LEU:HD13	1.99	0.45
1:A:690:ASP:OD1	1:A:690:ASP:N	2.48	0.45
1:B:244:ARG:NH1	1:B:250:GLU:OE2	2.46	0.45
1:C:678:THR:HG23	1:C:801:TYR:HB2	1.97	0.45
1:D:274:ARG:HA	1:D:336:LYS:HG2	1.98	0.45
1:D:582:THR:HG21	1:D:596:ILE:HD11	1.99	0.45
1:A:582:THR:HG21	1:A:596:ILE:HD11	1.99	0.45
1:A:667:SER:O	1:A:671:ASN:ND2	2.50	0.45
1:A:249:GLU:HG3	1:A:326:LEU:HD11	1.99	0.45
1:C:30:LYS:HD3	1:C:109:PRO:HG3	1.98	0.45
1:D:1086:HIS:HD2	1:D:1091:ILE:HD11	1.82	0.45
1:B:582:THR:HG23	1:B:594:ILE:HG21	1.99	0.45
1:B:568:VAL:HG13	1:B:593:THR:HG23	1.99	0.45
1:D:711:LYS:HG3	1:D:810:ILE:HG12	1.98	0.45
1:C:244:ARG:NH2	1:C:269:LEU:O	2.40	0.44
1:A:274:ARG:HG3	1:A:275:ILE:HG13	1.99	0.44
1:A:340:ILE:HB	1:A:377:VAL:HG22	1.99	0.44
1:C:21:THR:HG23	1:C:23:SER:H	1.83	0.44
1:C:274:ARG:HA	1:C:336:LYS:HG2	1.99	0.44
1:D:635:LYS:NZ	1:D:639:THR:O	2.42	0.44
1:D:857:MET:HE1	1:D:881:ARG:HE	1.81	0.44
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.85	0.44
1:C:181:LEU:HD13	1:C:207:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:833:LEU:HD12	1:C:833:LEU:C	2.43	0.44
1:B:120:TYR:HD1	1:B:203:ASN:HB2	1.82	0.44
1:B:846:ASP:H	1:C:1095:LEU:HD21	1.81	0.44
1:C:892:MET:HE3	1:C:892:MET:HB2	1.91	0.44
1:A:324:LEU:HB2	1:A:368:LEU:HD11	1.99	0.44
1:B:274:ARG:HG3	1:B:275:ILE:HG13	1.99	0.44
1:A:1065:ARG:HA	1:A:1065:ARG:HD3	1.87	0.44
1:A:1075:ASP:OD1	1:C:843:SER:OG	2.36	0.44
1:C:979:SER:OG	1:C:980:ILE:N	2.51	0.44
1:A:396:LYS:HA	1:A:396:LYS:HD3	1.80	0.43
1:A:620:ILE:O	1:A:620:ILE:HG22	2.16	0.43
1:B:1095:LEU:HD22	1:C:846:ASP:HB2	1.99	0.43
1:C:742:CYS:SG	1:C:743:TRP:N	2.91	0.43
1:D:659:TYR:HA	1:D:714:VAL:O	2.17	0.43
1:D:938:ALA:O	1:D:942:ALA:CB	2.66	0.43
1:B:40:TRP:HE1	1:B:85:LEU:HD21	1.83	0.43
1:C:1035:ASP:O	1:C:1039:ASN:CB	2.66	0.43
1:D:321:LYS:HA	1:D:324:LEU:HG	2.00	0.43
1:D:529:MET:HB2	1:D:552:VAL:HG22	2.00	0.43
1:B:30:LYS:HB3	1:B:109:PRO:HG2	1.99	0.43
1:B:5:ALA:HA	1:B:220:LYS:HA	2.01	0.43
1:A:36:PRO:HG3	1:A:89:LEU:HG	2.00	0.43
1:A:265:LYS:O	1:A:319:TYR:OH	2.37	0.43
1:A:574:SER:OG	1:A:575:LEU:N	2.51	0.43
1:A:643:LEU:HD23	1:A:821:VAL:HG21	2.01	0.43
1:A:809:VAL:HG13	1:A:810:ILE:HG13	2.01	0.43
1:A:929:LEU:HD21	1:C:925:THR:HG21	2.01	0.43
1:B:1086:HIS:HD2	1:B:1091:ILE:HD11	1.83	0.43
1:D:252:TYR:O	1:D:256:LEU:HB2	2.18	0.43
1:B:156:VAL:O	1:B:611:LYS:NZ	2.43	0.43
1:B:625:THR:OG1	1:B:626:VAL:N	2.52	0.43
1:C:181:LEU:O	1:C:184:PHE:HB3	2.17	0.43
1:A:711:LYS:HG3	1:A:810:ILE:HG12	2.00	0.43
1:B:621:ILE:HG22	1:B:621:ILE:O	2.17	0.43
1:B:662:ARG:HE	1:B:687:ILE:HD11	1.82	0.43
1:C:569:LEU:HD22	1:C:585:THR:HG21	2.00	0.43
1:B:292:ILE:HG21	1:B:301:LEU:HD13	2.00	0.43
1:B:620:ILE:HG22	1:B:694:GLY:HA3	2.01	0.43
1:D:77:THR:HG22	1:D:78:LEU:H	1.84	0.43
1:D:290:ASP:OD2	1:D:747:THR:N	2.51	0.43
1:A:974:GLY:HA2	1:A:1021:LEU:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ASN:OD1	1:B:303:ASN:N	2.52	0.42
1:C:867:MET:HB2	1:C:871:GLY:HA3	2.00	0.42
1:C:1086:HIS:HD2	1:C:1091:ILE:HD11	1.83	0.42
1:D:276:TRP:CE2	1:D:327:MET:HB3	2.54	0.42
1:D:344:ILE:HG13	1:D:668:ASN:HB3	2.00	0.42
1:A:1014:THR:HB	1:A:1021:LEU:HD23	2.00	0.42
1:C:375:ILE:HB	1:C:402:ILE:HG12	2.01	0.42
1:C:1014:THR:HB	1:C:1021:LEU:HD23	2.01	0.42
1:C:631:PRO:HB3	1:C:651:LEU:HB3	2.01	0.42
1:C:662:ARG:HG2	1:C:687:ILE:HD11	2.01	0.42
1:B:259:LYS:HE3	1:B:315:GLN:HE21	1.84	0.42
1:D:265:LYS:HB2	1:D:306:GLU:HG2	2.01	0.42
1:A:521:ARG:NH1	1:A:633:CYS:O	2.51	0.42
1:B:864:LYS:HE2	1:B:864:LYS:HB3	1.87	0.42
1:B:921:VAL:O	1:B:925:THR:HB	2.19	0.42
1:C:713:ILE:O	1:C:740:ILE:HA	2.20	0.42
1:D:516:ASP:OD2	1:D:525:SER:OG	2.30	0.42
1:A:58:LYS:HE3	1:A:106:LEU:HD23	2.02	0.42
1:A:933:ASP:OD1	1:A:933:ASP:N	2.49	0.42
1:B:25:ILE:H	1:B:28:ARG:HH21	1.68	0.42
1:B:27:ASN:HD22	1:B:30:LYS:HD2	1.85	0.42
1:B:375:ILE:O	1:B:402:ILE:HA	2.20	0.42
1:C:978:LYS:HE2	1:C:984:ASP:HA	2.01	0.42
1:D:369:LYS:HE2	1:D:369:LYS:HB3	1.93	0.42
1:A:560:MET:SD	1:A:590:GLN:NE2	2.91	0.42
1:B:725:TYR:OH	1:B:769:SER:O	2.29	0.42
1:B:979:SER:OG	1:B:1019:PRO:O	2.29	0.42
1:C:586:MET:HE3	1:C:612:LYS:HD3	2.01	0.42
1:C:628:GLY:H	1:C:636:ILE:HB	1.84	0.42
1:D:715:VAL:O	1:D:742:CYS:HA	2.18	0.42
1:D:292:ILE:HG12	1:D:415:VAL:HG21	2.01	0.42
1:A:1029:ILE:O	1:A:1033:PHE:HB2	2.19	0.42
1:C:183:SER:O	1:C:186:SER:HB2	2.20	0.42
1:A:834:ILE:HD11	1:B:834:ILE:HG21	2.01	0.42
1:D:259:LYS:NZ	1:D:314:GLN:OE1	2.53	0.42
1:D:1031:VAL:O	1:D:1035:ASP:HB2	2.20	0.42
1:A:209:LYS:HB2	1:A:209:LYS:HE2	1.84	0.41
1:A:204:PRO:HG2	1:A:215:LEU:HD13	2.01	0.41
1:A:1020:ASN:HB3	1:A:1021:LEU:H	1.70	0.41
1:B:332:HIS:HA	1:B:333:PRO:HD3	1.93	0.41
1:B:698:MET:HA	1:B:701:VAL:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:LEU:C	1:C:153:LEU:CD2	2.92	0.41
1:B:623:PRO:CD	1:B:690:ASP:OD2	2.51	0.41
1:B:833:LEU:CD1	4:B:1301:HOH:O	2.20	0.41
1:D:65:ARG:HG3	1:D:68:LYS:HD3	2.02	0.41
1:A:492:LEU:HD23	1:A:492:LEU:HA	1.91	0.41
1:B:256:LEU:HD21	1:B:318:ASP:HB2	2.03	0.41
1:B:273:GLY:O	1:B:276:TRP:NE1	2.51	0.41
1:B:337:ILE:HG21	1:B:418:ALA:HB1	2.02	0.41
1:A:269:LEU:HD11	1:A:304:TYR:HD2	1.84	0.41
1:C:5:ALA:HA	1:C:220:LYS:HA	2.02	0.41
1:C:199:TYR:O	1:C:219:ALA:HA	2.20	0.41
1:C:340:ILE:HB	1:C:377:VAL:HG22	2.03	0.41
1:C:493:PHE:O	1:C:630:LYS:NZ	2.51	0.41
1:C:659:TYR:HA	1:C:714:VAL:O	2.21	0.41
1:D:278:MET:HE2	1:D:323:ILE:HG21	2.02	0.41
1:A:12:LYS:HZ1	1:A:106:LEU:HD11	1.86	0.41
1:B:266:LEU:HD11	1:B:303:ASN:HD22	1.85	0.41
1:C:705:GLN:HE22	1:C:738:LYS:H	1.67	0.41
1:B:77:THR:HG22	1:B:78:LEU:H	1.85	0.41
1:C:369:LYS:HG3	1:C:400:ILE:HG13	2.01	0.41
1:C:825:TYR:OH	1:C:829:ARG:NH1	2.54	0.41
1:A:274:ARG:HG2	1:A:300:GLU:HB3	2.03	0.41
1:A:865:GLU:OE2	1:A:881:ARG:NH2	2.54	0.41
1:A:1077:LYS:HA	1:A:1077:LYS:HD3	1.87	0.41
1:C:196:TYR:HE2	1:C:228:ILE:HD12	1.85	0.41
1:A:495:ARG:NH2	1:A:520:SER:O	2.43	0.41
1:A:540:LYS:HE2	1:B:841:MET:HE2	2.01	0.41
1:A:843:SER:OG	1:C:1075:ASP:OD1	2.38	0.41
1:B:1081:GLN:HE22	1:D:841:MET:HE3	1.86	0.41
1:C:726:LYS:HD3	1:C:726:LYS:HA	1.91	0.41
1:D:493:PHE:HB2	1:D:630:LYS:HD3	2.03	0.41
1:A:162:PRO:HA	1:A:165:ILE:HD12	2.02	0.40
2:A:1202[B]:ACO:H31	2:A:1202[B]:ACO:H61	1.50	0.40
1:D:908:HIS:O	1:D:912:ILE:HG12	2.21	0.40
1:D:698:MET:HE1	1:D:736:LEU:HD11	2.02	0.40
1:D:1038:ARG:NH2	1:D:1049:ASP:OD1	2.55	0.40
1:A:150:GLN:O	1:A:169:LEU:HD11	2.21	0.40
1:A:578:ALA:O	1:A:582:THR:OG1	2.25	0.40
1:A:841:MET:HE2	1:A:841:MET:HB3	1.89	0.40
1:B:724:GLU:HB3	1:B:779:LEU:HD21	2.04	0.40
1:D:203:ASN:HA	1:D:204:PRO:HA	1.83	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LYS:HE3	1:A:369:LYS:HB2	1.85	0.40
1:A:411:MET:HE2	1:A:411:MET:HB3	1.96	0.40
1:A:630:LYS:HG2	1:A:633:CYS:HB2	2.03	0.40
1:C:945:MET:HE3	1:C:945:MET:HB2	1.98	0.40
1:A:918:LYS:HA	1:A:918:LYS:HD2	1.84	0.40
1:B:64:LYS:HA	1:B:64:LYS:HD3	1.92	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 PDB entries followed by that with respect to all EM entries.

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	1017/1100 (92%)	953 (94%)	61 (6%)	3 (0%)	36	65
1	B	1017/1100 (92%)	945 (93%)	69 (7%)	3 (0%)	36	65
1	C	1017/1100 (92%)	947 (93%)	70 (7%)	0	100	100
1	D	1017/1100 (92%)	953 (94%)	62 (6%)	2 (0%)	43	71
All	All	4068/4400 (92%)	3798 (93%)	262 (6%)	8 (0%)	44	71

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	854	TYR
1	B	834	ILE
1	D	854	TYR
1	D	1020	ASN
1	A	981	ASN
1	B	855	ALA
1	A	623	PRO
1	B	832	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 PDB entries followed by that with respect to all EM entries.

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	842/908 (93%)	834 (99%)	8 (1%)	68	75
1	B	842/908 (93%)	839 (100%)	3 (0%)	84	83
1	C	842/908 (93%)	837 (99%)	5 (1%)	78	80
1	D	842/908 (93%)	838 (100%)	4 (0%)	81	81
All	All	3368/3632 (93%)	3348 (99%)	20 (1%)	78	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	226[A]	ASP
1	A	226[B]	ASP
1	A	620	ILE
1	A	621	ILE
1	A	834	ILE
1	A	952	SER
1	A	976	ARG
1	A	1018	LYS
1	B	833	LEU
1	B	834	ILE
1	B	835	ARG
1	C	226[A]	ASP
1	C	226[B]	ASP
1	C	597	ILE
1	C	620	ILE
1	C	678	THR
1	D	62	LEU
1	D	226[A]	ASP
1	D	226[B]	ASP
1	D	834	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	104	ASN
1	A	346	ASN
1	A	403	HIS
1	A	410	HIS
1	A	563	HIS
1	A	668	ASN
1	A	671	ASN
1	A	900	HIS
1	A	908	HIS
1	A	961	ASN
1	A	1024	ASN
1	A	1081	GLN
1	B	27	ASN
1	B	136	HIS
1	B	150	GLN
1	B	190	ASN
1	B	315	GLN
1	B	403	HIS
1	B	668	ASN
1	B	671	ASN
1	B	961	ASN
1	B	1081	GLN
1	B	1086	HIS
1	B	1098	HIS
1	C	9	GLN
1	C	26	GLN
1	C	47	HIS
1	C	75	ASN
1	C	270	ASN
1	C	303	ASN
1	C	315	GLN
1	C	645	ASN
1	C	668	ASN
1	C	671	ASN
1	C	705	GLN
1	C	879	GLN
1	C	900	HIS
1	C	908	HIS
1	C	909	ASN
1	D	27	ASN
1	D	61	GLN
1	D	190	ASN

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Mol	Chain	Res	Type
1	D	203	ASN
1	D	270	ASN
1	D	299	ASN
1	D	315	GLN
1	D	403	HIS
1	D	563	HIS
1	D	671	ASN
1	D	700	HIS
1	D	705	GLN
1	D	961	ASN
1	D	1081	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
3	OAA	A	1203	-	8,8,8	1.39	1 (12%)	8,10,10	1.38	1 (12%)
3	OAA	C	1202	-	8,8,8	1.38	1 (12%)	8,10,10	1.38	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ACO	A	1201	-	51,53,53	3.11	16 (31%)	73,79,79	1.89	14 (19%)
3	OAA	B	1202	-	8,8,8	1.36	1 (12%)	8,10,10	1.42	1 (12%)
3	OAA	A	1204	-	8,8,8	1.33	1 (12%)	8,10,10	1.41	1 (12%)
2	ACO	D	1201	-	51,53,53	3.14	16 (31%)	73,79,79	1.88	14 (19%)
3	OAA	D	1203	-	8,8,8	1.35	1 (12%)	8,10,10	1.39	1 (12%)
2	ACO	A	1202[A]	-	51,53,53	1.16	5 (9%)	73,79,79	1.47	9 (12%)
2	ACO	A	1202[B]	-	51,53,53	1.15	4 (7%)	73,79,79	1.48	9 (12%)
2	ACO	B	1201	-	51,53,53	3.12	16 (31%)	73,79,79	1.93	13 (17%)
3	OAA	D	1202	-	8,8,8	1.35	1 (12%)	8,10,10	1.52	1 (12%)
3	OAA	C	1201	-	8,8,8	1.40	1 (12%)	8,10,10	1.46	1 (12%)
3	OAA	B	1203	-	8,8,8	1.37	1 (12%)	8,10,10	1.38	1 (12%)

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
3	OAA	A	1203	-	-	3/8/8/8	-
3	OAA	C	1202	-	-	0/8/8/8	-
2	ACO	A	1201	-	-	12/51/67/67	0/3/3/3
3	OAA	B	1202	-	-	6/8/8/8	-
3	OAA	A	1204	-	-	6/8/8/8	-
2	ACO	D	1201	-	-	17/51/67/67	0/3/3/3
3	OAA	D	1203	-	-	4/8/8/8	-
2	ACO	A	1202[A]	-	-	21/51/67/67	0/3/3/3
2	ACO	A	1202[B]	-	-	12/51/67/67	0/3/3/3
2	ACO	B	1201	-	-	15/51/67/67	0/3/3/3
3	OAA	D	1202	-	-	6/8/8/8	-
3	OAA	C	1201	-	-	6/8/8/8	-
3	OAA	B	1203	-	-	5/8/8/8	-

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	ACO	O4B-C1B	9.78	1.64	1.42
2	B	1201	ACO	O4B-C1B	9.73	1.64	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	ACO	O4B-C1B	9.65	1.64	1.42
2	B	1201	ACO	P1A-O3A	8.51	1.68	1.59
2	D	1201	ACO	P1A-O3A	8.46	1.68	1.59
2	A	1201	ACO	P1A-O3A	8.20	1.68	1.59
2	A	1201	ACO	C2B-C1B	-7.10	1.31	1.53
2	B	1201	ACO	C2B-C1B	-7.07	1.31	1.53
2	D	1201	ACO	C2B-C1B	-7.02	1.31	1.53
2	B	1201	ACO	O4B-C4B	-7.00	1.29	1.45
2	D	1201	ACO	O4B-C4B	-6.92	1.29	1.45
2	A	1201	ACO	O4B-C4B	-6.92	1.29	1.45
2	D	1201	ACO	C9P-N8P	6.75	1.49	1.33
2	B	1201	ACO	C9P-N8P	6.74	1.49	1.33
2	A	1201	ACO	C9P-N8P	6.64	1.49	1.33
2	D	1201	ACO	P2A-O3A	5.63	1.65	1.59
2	B	1201	ACO	P2A-O3A	5.38	1.65	1.59
2	D	1201	ACO	C5P-N4P	5.22	1.45	1.33
2	A	1201	ACO	P2A-O3A	5.20	1.65	1.59
2	B	1201	ACO	C5P-N4P	5.18	1.45	1.33
2	A	1201	ACO	C5P-N4P	5.17	1.45	1.33
2	D	1201	ACO	P3B-O3B	4.78	1.67	1.59
2	A	1202[B]	ACO	C5A-C4A	4.74	1.47	1.39
2	A	1202[A]	ACO	C5A-C4A	4.70	1.47	1.39
2	A	1201	ACO	P3B-O3B	4.66	1.67	1.59
2	B	1201	ACO	P3B-O3B	4.56	1.67	1.59
2	D	1201	ACO	C6A-N6A	3.73	1.43	1.34
2	A	1201	ACO	C6A-N6A	3.69	1.43	1.34
2	B	1201	ACO	C6A-N6A	3.69	1.43	1.34
2	A	1201	ACO	C5A-C4A	-3.57	1.32	1.39
2	B	1201	ACO	C5A-C4A	-3.48	1.32	1.39
2	D	1201	ACO	C5A-C4A	-3.46	1.32	1.39
2	D	1201	ACO	O5P-C5P	-3.37	1.16	1.23
2	B	1201	ACO	O5P-C5P	-3.30	1.16	1.23
2	A	1201	ACO	O5P-C5P	-3.20	1.16	1.23
2	B	1201	ACO	O3B-C3B	-2.98	1.33	1.44
2	A	1201	ACO	O3B-C3B	-2.96	1.34	1.44
2	D	1201	ACO	O3B-C3B	-2.93	1.34	1.44
2	A	1201	ACO	CCP-CBP	2.80	1.57	1.52
2	A	1202[A]	ACO	C5A-C6A	2.76	1.48	1.41
2	A	1202[B]	ACO	C5A-C6A	2.74	1.48	1.41
2	D	1201	ACO	C3P-N4P	2.69	1.52	1.46
2	B	1201	ACO	C3P-N4P	2.63	1.52	1.46
2	A	1201	ACO	C3P-N4P	2.61	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	ACO	CCP-CBP	2.57	1.56	1.52
2	D	1201	ACO	CCP-CBP	2.55	1.56	1.52
2	B	1201	ACO	C6P-C5P	2.51	1.56	1.51
2	A	1201	ACO	C6P-C5P	2.42	1.56	1.51
2	A	1202[B]	ACO	C8A-N7A	2.36	1.36	1.31
2	D	1201	ACO	C6P-C5P	2.35	1.56	1.51
3	A	1203	OAA	O3-C3	-2.34	1.18	1.23
2	A	1202[A]	ACO	C8A-N7A	2.33	1.36	1.31
2	A	1202[B]	ACO	C5A-N7A	-2.28	1.34	1.39
3	C	1201	OAA	O3-C3	-2.26	1.18	1.23
2	A	1201	ACO	C3B-C4B	2.23	1.58	1.52
2	D	1201	ACO	C3B-C4B	2.22	1.58	1.52
2	A	1202[A]	ACO	C5A-N7A	-2.22	1.35	1.39
3	D	1203	OAA	O3-C3	-2.20	1.18	1.23
3	C	1202	OAA	O3-C3	-2.16	1.18	1.23
3	B	1202	OAA	O3-C3	-2.15	1.18	1.23
3	B	1203	OAA	O3-C3	-2.15	1.18	1.23
3	D	1202	OAA	O3-C3	-2.14	1.18	1.23
2	B	1201	ACO	C3B-C4B	2.10	1.58	1.52
2	A	1202[A]	ACO	P1A-O3A	2.06	1.61	1.59
3	A	1204	OAA	O3-C3	-2.06	1.18	1.23

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	ACO	N6A-C6A-N1A	-6.85	103.13	118.38
2	D	1201	ACO	N6A-C6A-N1A	-6.68	103.50	118.38
2	A	1201	ACO	N6A-C6A-N1A	-6.60	103.67	118.38
2	D	1201	ACO	N3A-C2A-N1A	-6.13	119.30	128.58
2	A	1201	ACO	N3A-C2A-N1A	-6.05	119.43	128.58
2	B	1201	ACO	N3A-C2A-N1A	-5.92	119.62	128.58
2	A	1202[A]	ACO	C5A-C4A-N3A	-5.86	118.65	126.72
2	A	1202[B]	ACO	C5A-C4A-N3A	-5.84	118.68	126.72
2	B	1201	ACO	C5A-C6A-N6A	5.23	136.23	123.29
2	D	1201	ACO	C5A-C6A-N6A	5.19	136.15	123.29
2	A	1201	ACO	C5A-C6A-N6A	5.17	136.07	123.29
2	B	1201	ACO	C5A-C4A-N3A	-4.83	120.07	126.72
2	A	1201	ACO	C5A-C4A-N3A	-4.66	120.30	126.72
2	A	1202[B]	ACO	N3A-C4A-N9A	4.61	135.01	127.17
2	A	1202[A]	ACO	N3A-C4A-N9A	4.60	134.99	127.17
2	D	1201	ACO	C5A-C4A-N3A	-4.55	120.45	126.72
2	B	1201	ACO	N9A-C8A-N7A	-4.37	107.73	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ACO	N9A-C8A-N7A	-4.36	107.75	113.94
2	D	1201	ACO	N9A-C8A-N7A	-4.34	107.77	113.94
2	A	1202[A]	ACO	C2A-N3A-C4A	3.72	120.91	111.83
2	A	1202[B]	ACO	C2A-N3A-C4A	3.71	120.89	111.83
2	A	1202[A]	ACO	C4A-C5A-N7A	-3.53	106.54	110.58
2	A	1202[B]	ACO	C4A-C5A-N7A	-3.50	106.58	110.58
2	B	1201	ACO	C2A-N3A-C4A	3.43	120.20	111.83
2	D	1201	ACO	C2A-N3A-C4A	3.40	120.14	111.83
2	A	1201	ACO	C2A-N3A-C4A	3.39	120.11	111.83
2	A	1202[B]	ACO	N3A-C2A-N1A	-3.23	123.69	128.58
2	A	1202[A]	ACO	N3A-C2A-N1A	-3.22	123.71	128.58
2	B	1201	ACO	N3A-C4A-N9A	3.00	132.27	127.17
2	A	1201	ACO	N3A-C4A-N9A	2.90	132.09	127.17
2	B	1201	ACO	C5A-N7A-C8A	2.84	107.91	103.45
2	A	1201	ACO	C4B-O4B-C1B	-2.82	103.23	109.47
2	B	1201	ACO	CAP-C9P-N8P	2.80	121.80	116.48
2	D	1201	ACO	N3A-C4A-N9A	2.77	131.88	127.17
2	A	1201	ACO	C5A-N7A-C8A	2.75	107.78	103.45
2	D	1201	ACO	C5A-N7A-C8A	2.73	107.74	103.45
2	A	1202[B]	ACO	C4A-N9A-C8A	2.61	108.48	105.74
2	A	1201	ACO	C4A-N9A-C8A	2.60	108.47	105.74
2	A	1202[B]	ACO	C3B-C2B-C1B	2.59	105.58	99.89
2	A	1202[A]	ACO	C4A-N9A-C8A	2.59	108.45	105.74
2	A	1202[B]	ACO	C5A-N7A-C8A	2.58	107.50	103.45
2	A	1202[A]	ACO	C5A-N7A-C8A	2.58	107.50	103.45
2	B	1201	ACO	C4A-N9A-C8A	2.49	108.35	105.74
2	D	1201	ACO	C4B-O4B-C1B	-2.48	103.99	109.47
2	A	1201	ACO	CAP-C9P-N8P	2.47	121.17	116.48
3	D	1202	OAA	O5-C4-C3	2.47	120.43	113.59
2	D	1201	ACO	C4A-N9A-C8A	2.45	108.31	105.74
2	A	1202[A]	ACO	C3B-C2B-C1B	2.41	105.19	99.89
2	B	1201	ACO	C1B-N9A-C8A	-2.37	121.84	127.09
2	D	1201	ACO	CAP-C9P-N8P	2.33	120.90	116.48
2	B	1201	ACO	C4B-O4B-C1B	-2.32	104.34	109.47
3	B	1202	OAA	O5-C4-C3	2.32	120.02	113.59
2	A	1201	ACO	C1B-N9A-C8A	-2.30	121.98	127.09
3	A	1204	OAA	O5-C4-C3	2.30	119.97	113.59
3	C	1201	OAA	O5-C4-C3	2.28	119.91	113.59
3	A	1203	OAA	O5-C4-C3	2.27	119.90	113.59
2	D	1201	ACO	C6P-C5P-N4P	2.27	120.49	116.34
3	D	1203	OAA	O5-C4-C3	2.27	119.89	113.59
3	C	1202	OAA	O5-C4-C3	2.26	119.85	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1201	ACO	O4B-C1B-C2B	-2.23	101.84	106.62
3	B	1203	OAA	O5-C4-C3	2.23	119.77	113.59
2	B	1201	ACO	C6P-C5P-N4P	2.15	120.26	116.34
2	A	1202[B]	ACO	C6A-C5A-N7A	2.11	136.16	132.09
2	A	1202[A]	ACO	C6A-C5A-N7A	2.09	136.12	132.09
2	D	1201	ACO	C1B-N9A-C8A	-2.09	122.45	127.09
2	A	1201	ACO	O4B-C1B-C2B	-2.07	102.18	106.62
2	A	1201	ACO	CEP-CBP-CAP	2.05	112.26	108.77

There are no chirality outliers.

All (113) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ACO	CDP-CBP-CCP-O6A
2	A	1201	ACO	CEP-CBP-CCP-O6A
2	A	1201	ACO	CAP-CBP-CCP-O6A
2	A	1201	ACO	OAP-CAP-CBP-CCP
2	A	1201	ACO	C9P-CAP-CBP-CCP
2	A	1201	ACO	OAP-CAP-CBP-CDP
2	A	1201	ACO	C9P-CAP-CBP-CDP
2	A	1201	ACO	OAP-CAP-CBP-CEP
2	A	1201	ACO	C9P-CAP-CBP-CEP
2	A	1201	ACO	O-C-S1P-C2P
2	A	1201	ACO	CH3-C-S1P-C2P
2	A	1202[A]	ACO	C5B-O5B-P1A-O1A
2	A	1202[A]	ACO	C5B-O5B-P1A-O2A
2	A	1202[A]	ACO	CCP-O6A-P2A-O3A
2	A	1202[A]	ACO	CCP-O6A-P2A-O5A
2	A	1202[A]	ACO	OAP-CAP-CBP-CCP
2	A	1202[A]	ACO	C9P-CAP-CBP-CCP
2	A	1202[A]	ACO	OAP-CAP-CBP-CDP
2	A	1202[A]	ACO	C9P-CAP-CBP-CDP
2	A	1202[A]	ACO	C9P-CAP-CBP-CEP
2	A	1202[A]	ACO	CAP-C9P-N8P-C7P
2	A	1202[A]	ACO	O9P-C9P-N8P-C7P
2	A	1202[A]	ACO	C6P-C5P-N4P-C3P
2	A	1202[A]	ACO	O5P-C5P-N4P-C3P
2	A	1202[A]	ACO	O-C-S1P-C2P
2	A	1202[A]	ACO	CH3-C-S1P-C2P
2	A	1202[B]	ACO	C5B-O5B-P1A-O1A
2	A	1202[B]	ACO	CCP-O6A-P2A-O4A
2	A	1202[B]	ACO	O-C-S1P-C2P

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Mol	Chain	Res	Type	Atoms
2	A	1202[B]	ACO	CH3-C-S1P-C2P
2	B	1201	ACO	C5B-O5B-P1A-O3A
2	B	1201	ACO	CCP-O6A-P2A-O4A
2	B	1201	ACO	CCP-O6A-P2A-O5A
2	B	1201	ACO	CDP-CBP-CCP-O6A
2	B	1201	ACO	CEP-CBP-CCP-O6A
2	B	1201	ACO	CAP-CBP-CCP-O6A
2	B	1201	ACO	S1P-C2P-C3P-N4P
2	B	1201	ACO	O-C-S1P-C2P
2	D	1201	ACO	C5B-O5B-P1A-O2A
2	D	1201	ACO	CDP-CBP-CCP-O6A
2	D	1201	ACO	CEP-CBP-CCP-O6A
2	D	1201	ACO	CAP-CBP-CCP-O6A
2	D	1201	ACO	OAP-CAP-CBP-CCP
2	D	1201	ACO	C9P-CAP-CBP-CCP
2	D	1201	ACO	OAP-CAP-CBP-CDP
2	D	1201	ACO	C9P-CAP-CBP-CDP
2	D	1201	ACO	OAP-CAP-CBP-CEP
2	D	1201	ACO	C9P-CAP-CBP-CEP
2	D	1201	ACO	C3P-C2P-S1P-C
2	D	1201	ACO	O-C-S1P-C2P
2	D	1201	ACO	CH3-C-S1P-C2P
3	A	1203	OAA	C2-C3-C4-O4
3	A	1203	OAA	C2-C3-C4-O5
3	A	1204	OAA	O2-C1-C2-C3
3	A	1204	OAA	C2-C3-C4-O4
3	A	1204	OAA	C2-C3-C4-O5
3	B	1203	OAA	O3-C3-C4-O4
3	B	1203	OAA	O3-C3-C4-O5
3	B	1203	OAA	C2-C3-C4-O5
3	C	1201	OAA	O3-C3-C4-O4
3	C	1201	OAA	O3-C3-C4-O5
3	C	1201	OAA	C2-C3-C4-O5
3	D	1202	OAA	O3-C3-C4-O4
3	D	1202	OAA	O3-C3-C4-O5
3	D	1202	OAA	C2-C3-C4-O5
3	D	1203	OAA	C2-C3-C4-O5
2	A	1202[B]	ACO	C6P-C5P-N4P-C3P
2	A	1202[B]	ACO	O5P-C5P-N4P-C3P
2	D	1201	ACO	S1P-C2P-C3P-N4P
2	B	1201	ACO	CH3-C-S1P-C2P
2	A	1202[A]	ACO	OAP-CAP-CBP-CEP

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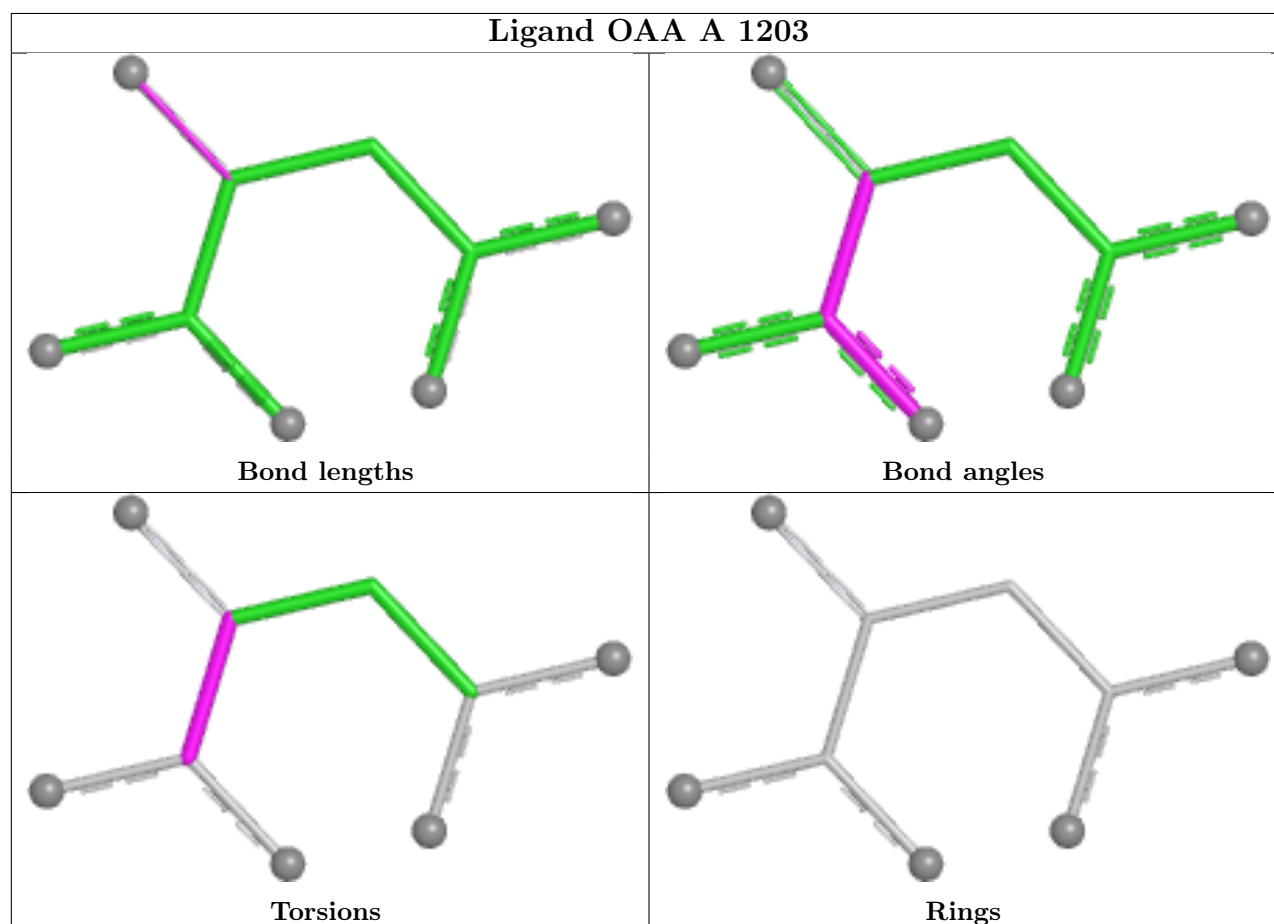
Mol	Chain	Res	Type	Atoms
2	B	1201	ACO	O9P-C9P-CAP-CBP
2	A	1202[A]	ACO	C3B-O3B-P3B-O8A
2	A	1202[A]	ACO	S1P-C2P-C3P-N4P
2	B	1201	ACO	N8P-C9P-CAP-OAP
2	A	1202[B]	ACO	O4B-C4B-C5B-O5B
3	D	1202	OAA	O2-C1-C2-C3
3	A	1203	OAA	O3-C3-C4-O4
3	A	1204	OAA	C1-C2-C3-O3
3	A	1204	OAA	O3-C3-C4-O4
3	B	1202	OAA	O3-C3-C4-O4
3	D	1203	OAA	C1-C2-C3-O3
3	B	1202	OAA	C2-C3-C4-O4
3	B	1203	OAA	C2-C3-C4-O4
3	C	1201	OAA	C2-C3-C4-O4
3	D	1202	OAA	C2-C3-C4-O4
3	D	1202	OAA	O1-C1-C2-C3
2	A	1202[B]	ACO	CDP-CBP-CCP-O6A
2	A	1202[A]	ACO	C5B-O5B-P1A-O3A
2	B	1201	ACO	C5B-O5B-P1A-O2A
2	B	1201	ACO	CCP-O6A-P2A-O3A
2	D	1201	ACO	C5B-O5B-P1A-O1A
2	D	1201	ACO	C5B-O5B-P1A-O3A
3	B	1202	OAA	O3-C3-C4-O5
3	B	1202	OAA	O1-C1-C2-C3
2	A	1202[A]	ACO	C5P-C6P-C7P-N8P
3	B	1202	OAA	C2-C3-C4-O5
3	D	1203	OAA	O1-C1-C2-C3
2	A	1202[B]	ACO	C3B-O3B-P3B-O7A
3	B	1202	OAA	O2-C1-C2-C3
3	B	1203	OAA	C1-C2-C3-O3
3	C	1201	OAA	C1-C2-C3-O3
3	C	1201	OAA	O1-C1-C2-C3
3	D	1203	OAA	C2-C3-C4-O4
2	A	1202[B]	ACO	C3B-C4B-C5B-O5B
2	A	1202[B]	ACO	C3B-O3B-P3B-O8A
2	A	1202[B]	ACO	CEP-CBP-CCP-O6A
2	B	1201	ACO	C9P-CAP-CBP-CCP
2	B	1201	ACO	N8P-C9P-CAP-CBP
2	A	1201	ACO	N8P-C9P-CAP-OAP
2	A	1202[A]	ACO	N8P-C9P-CAP-OAP
2	D	1201	ACO	N8P-C9P-CAP-OAP
3	A	1204	OAA	C1-C2-C3-C4

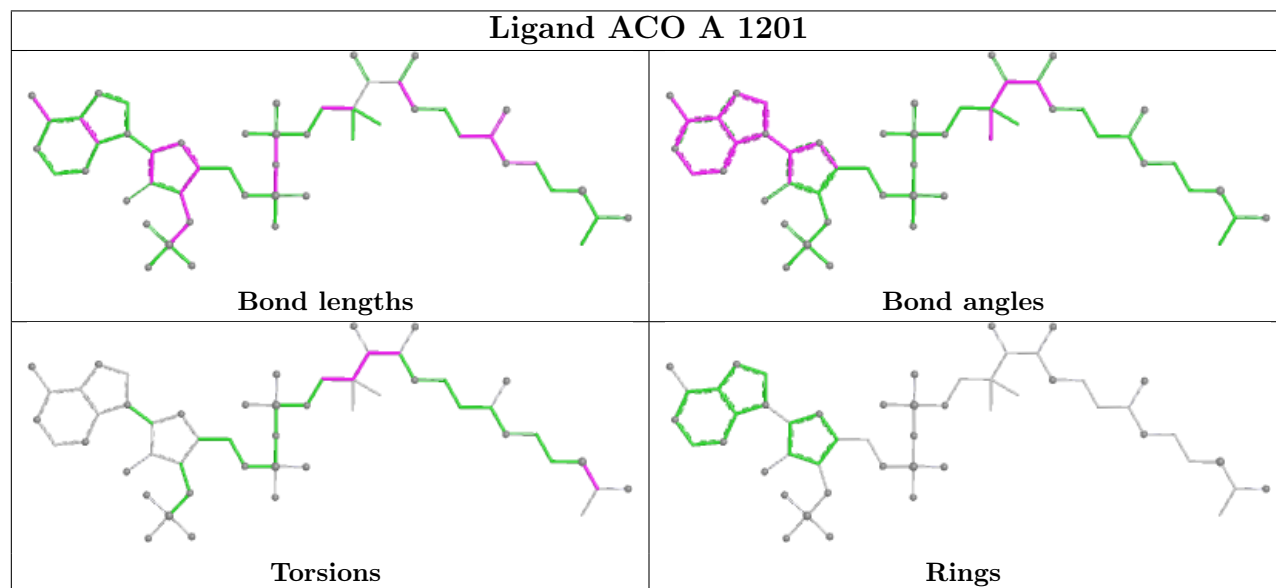
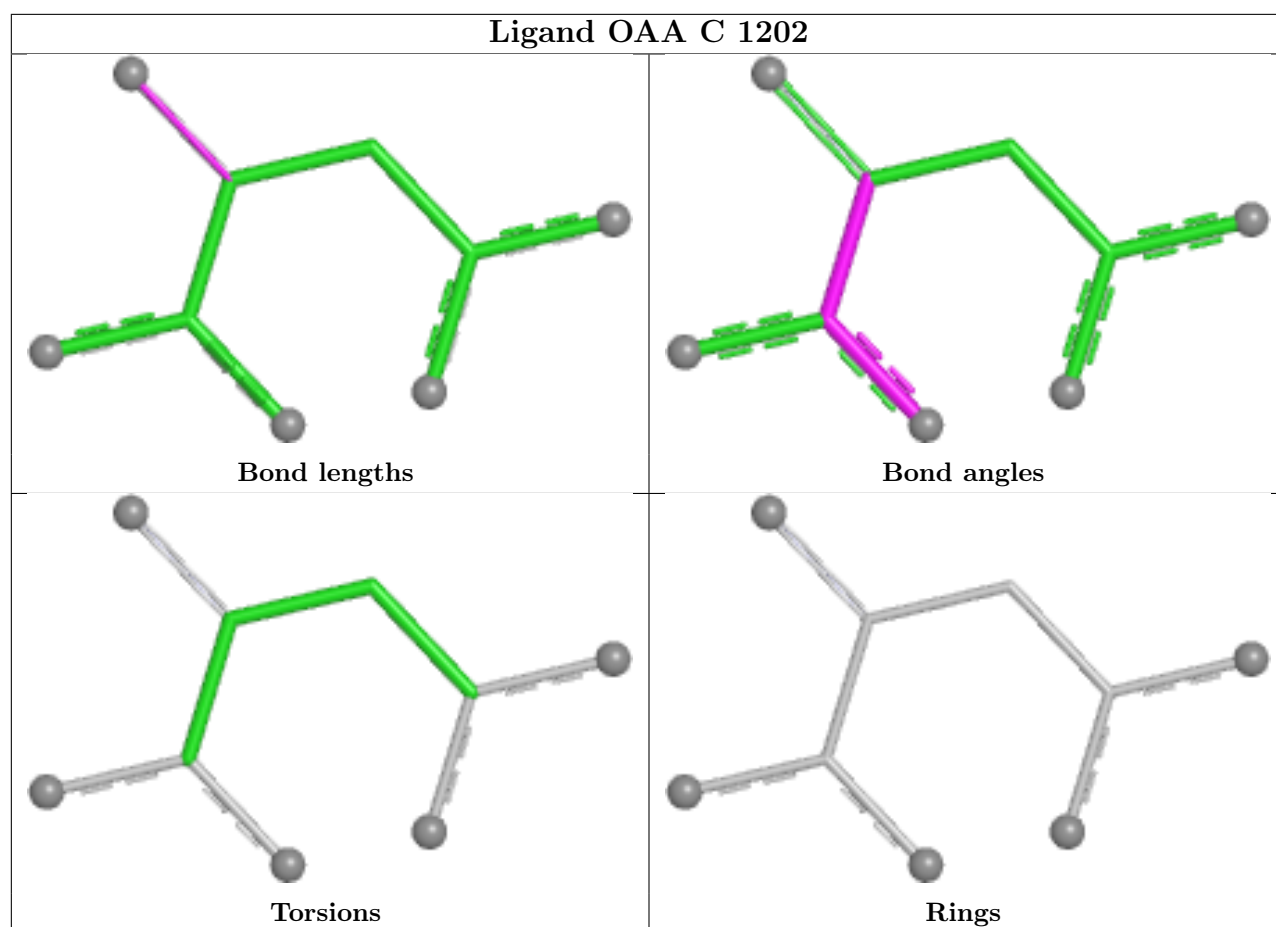
There are no ring outliers.

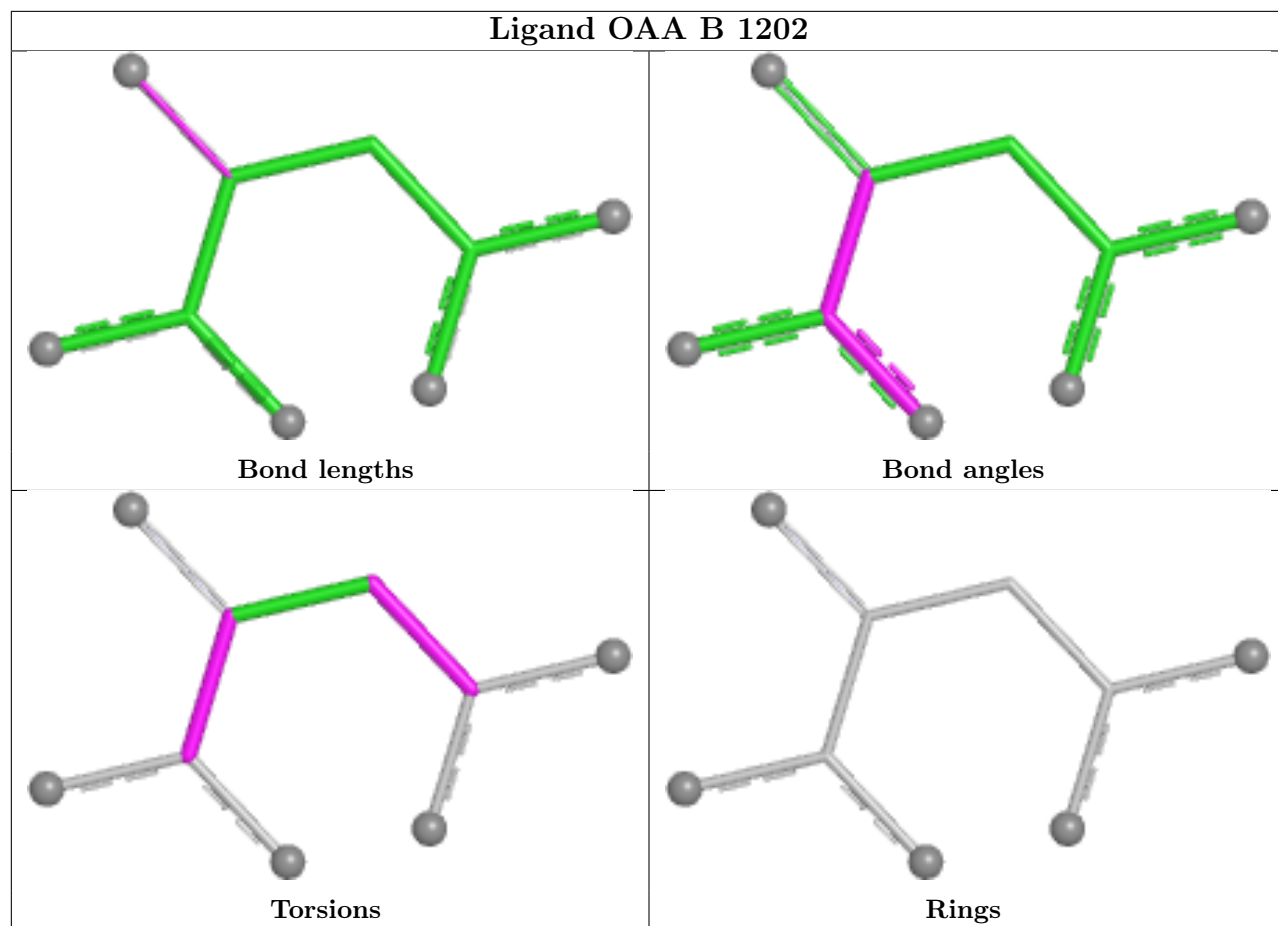
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	ACO	1	0
2	D	1201	ACO	1	0
2	A	1202[B]	ACO	4	0
2	B	1201	ACO	1	0

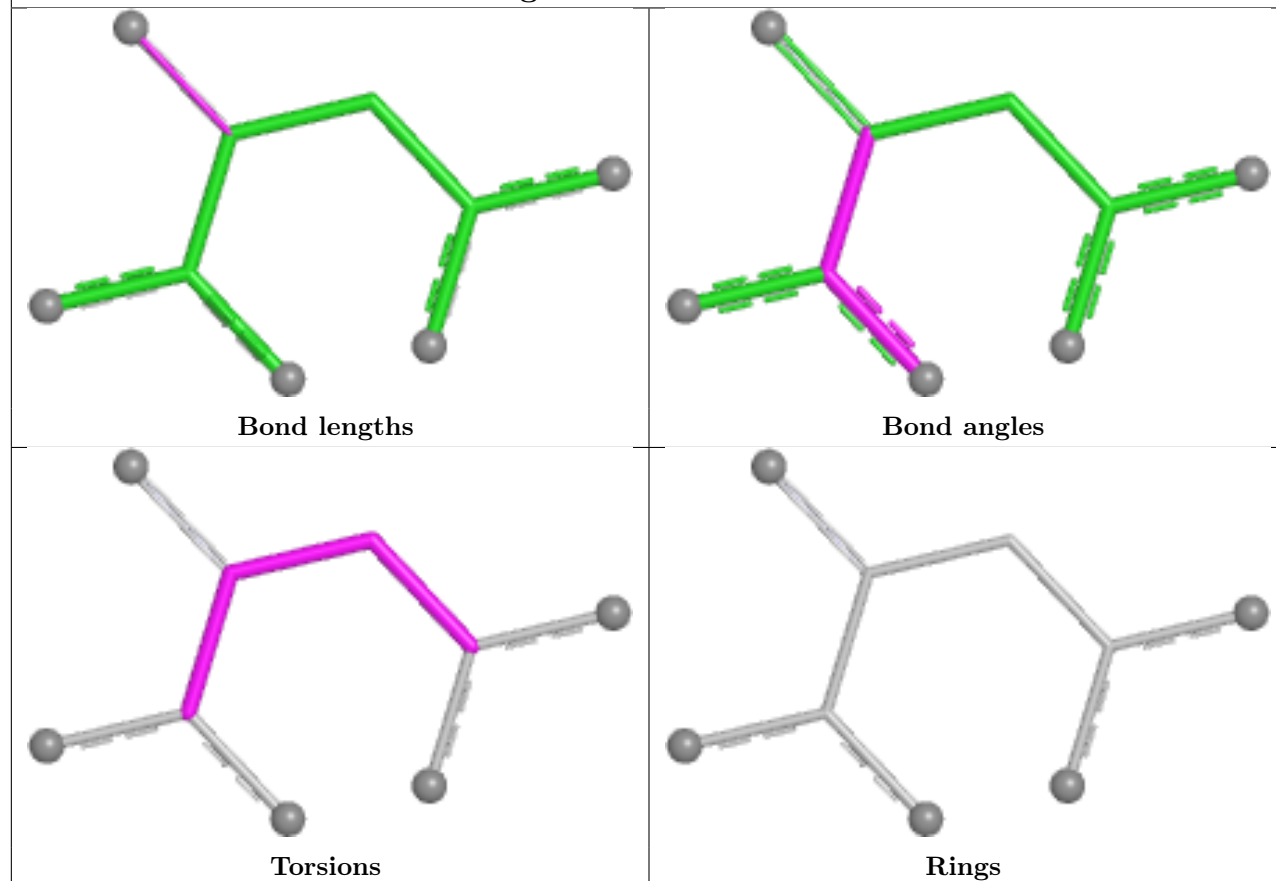
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



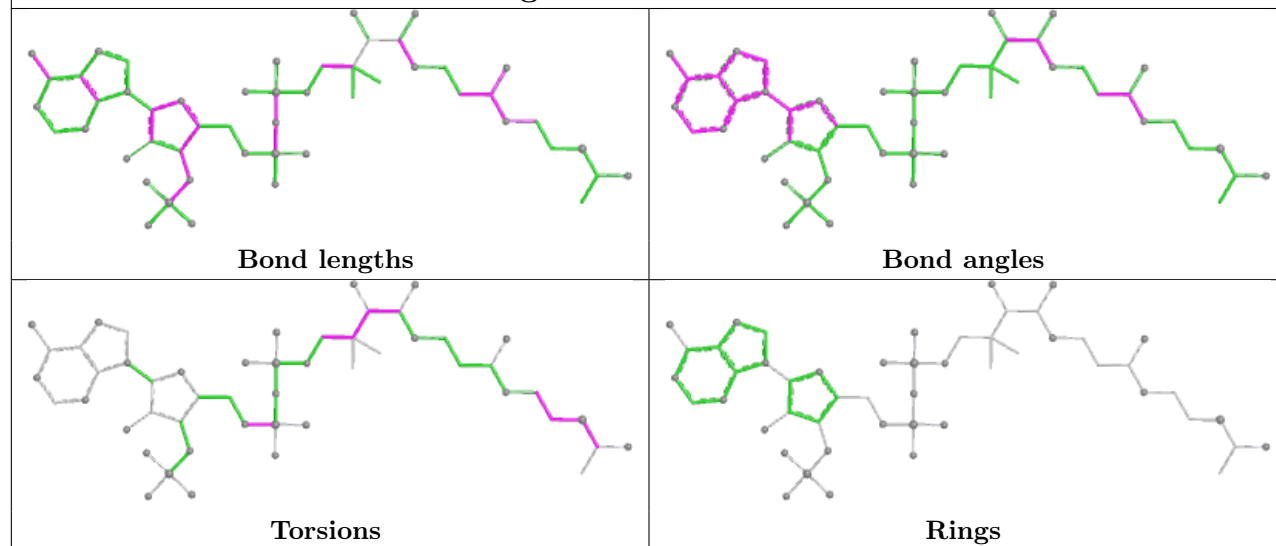




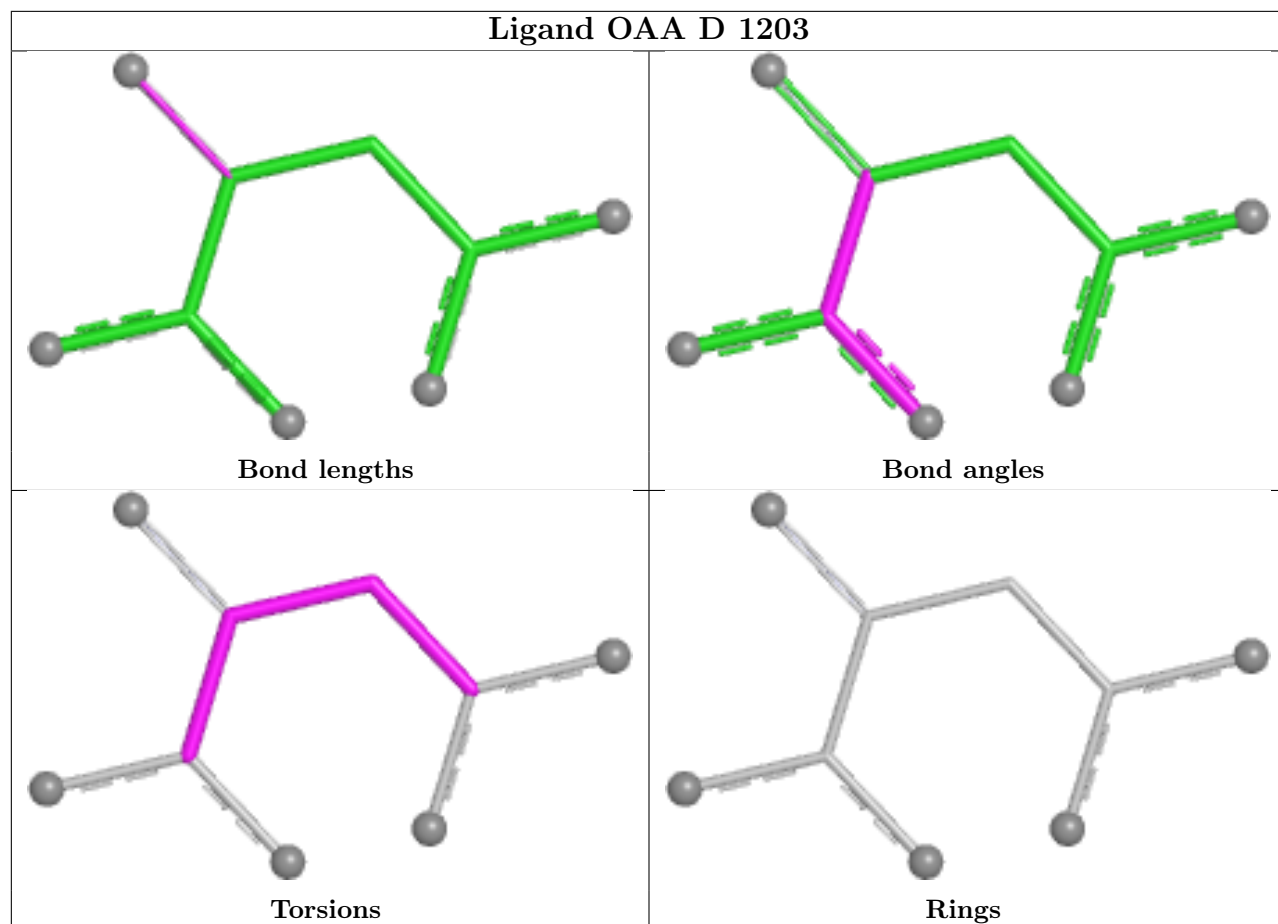
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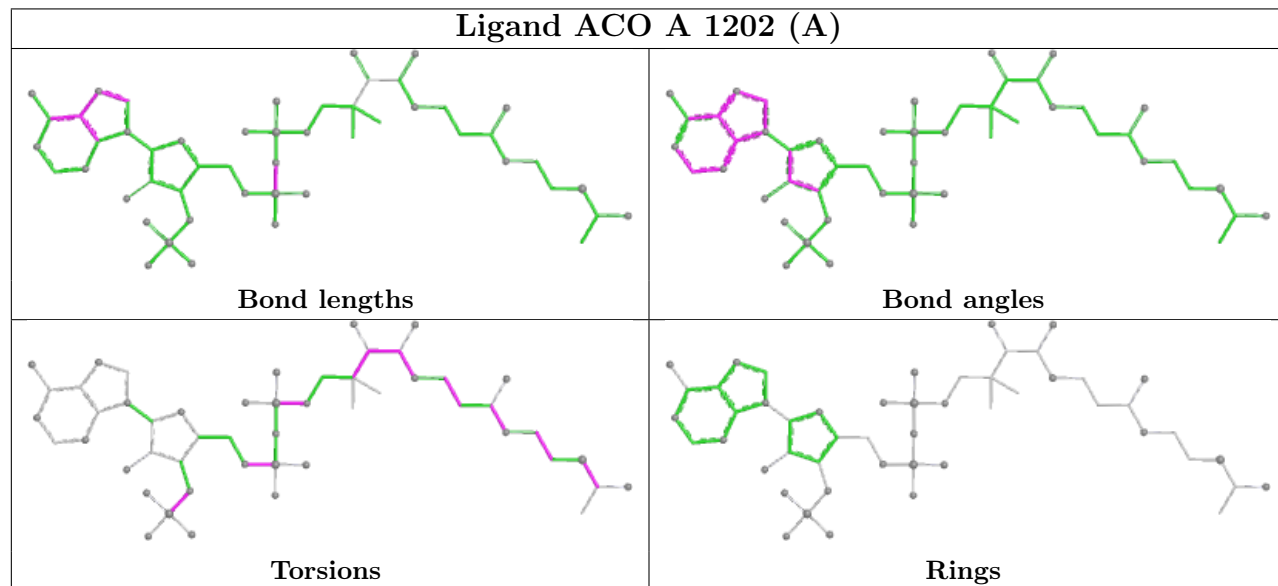
Ligand ACO D 1201

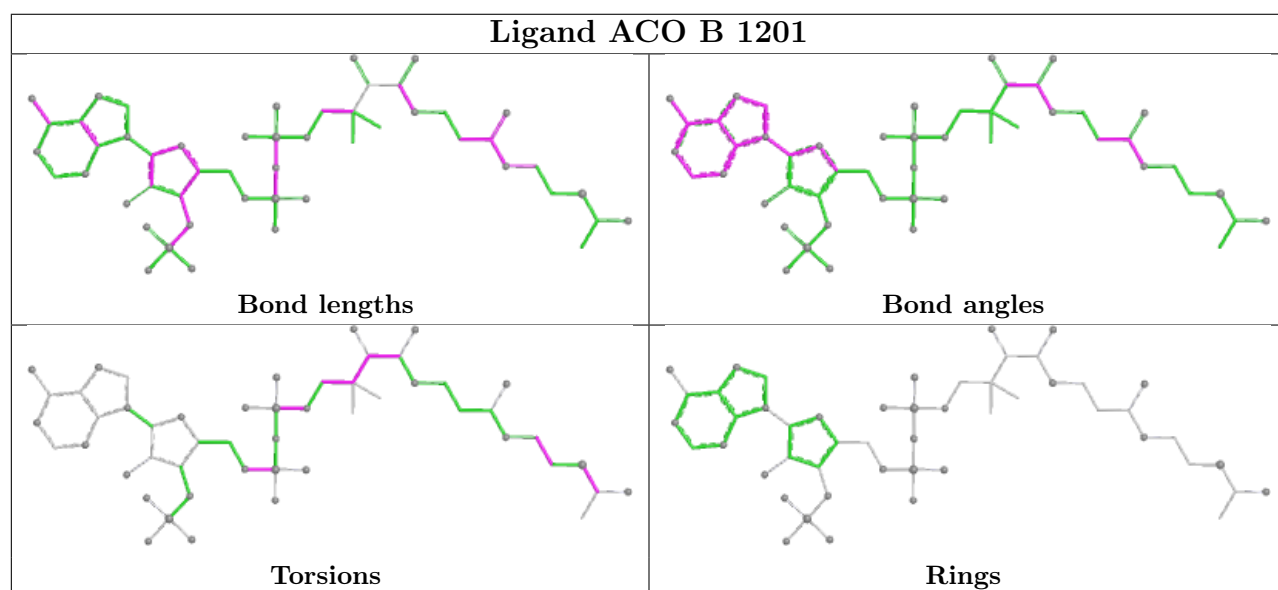
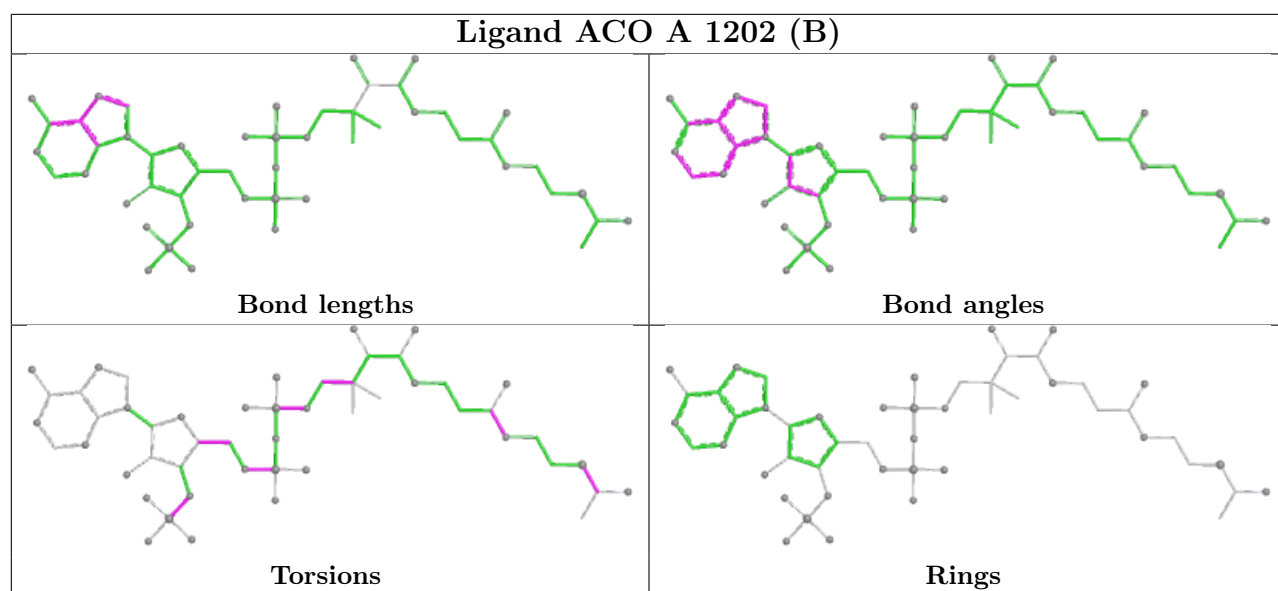


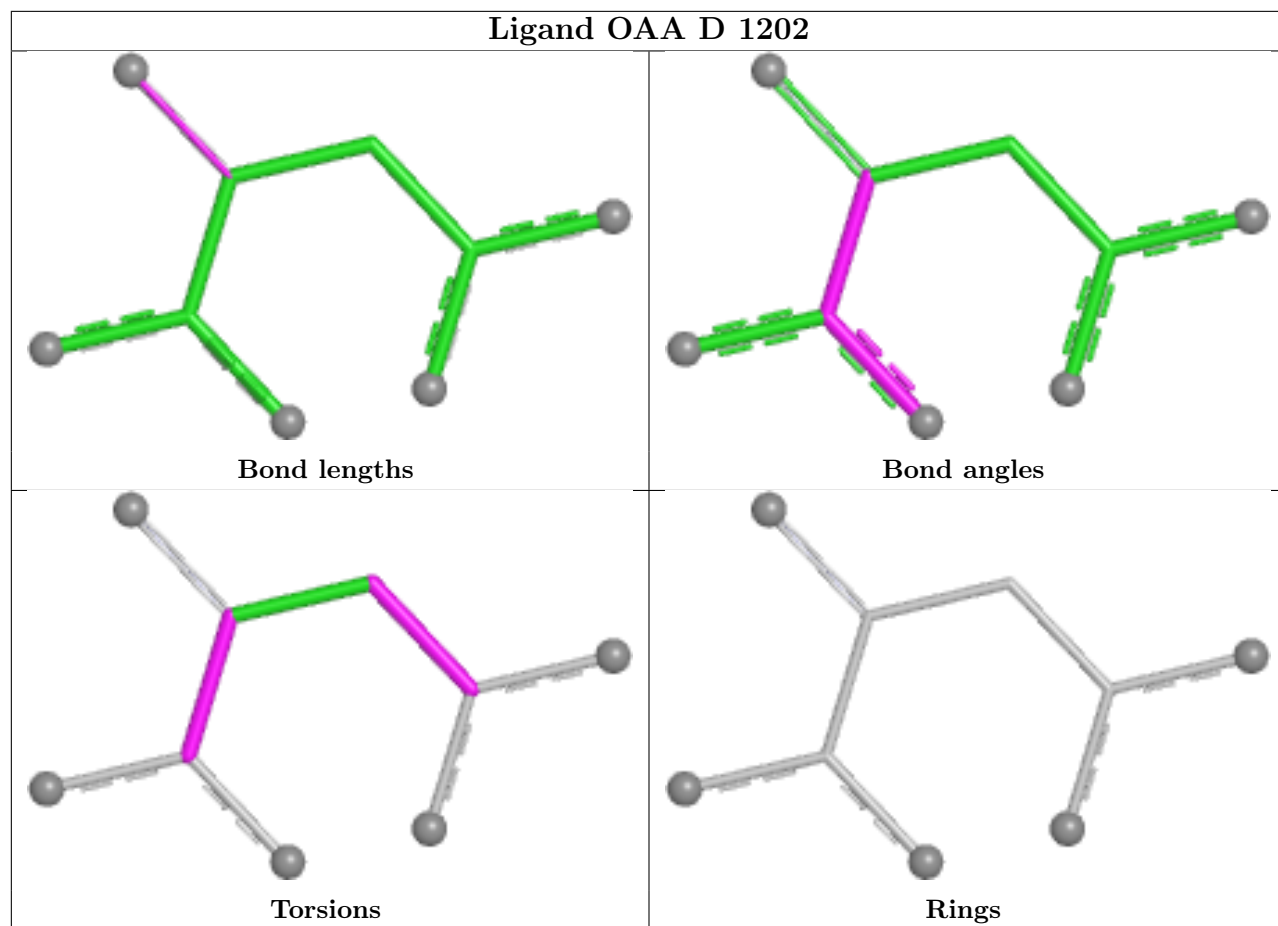
Ligand OAA D 1203

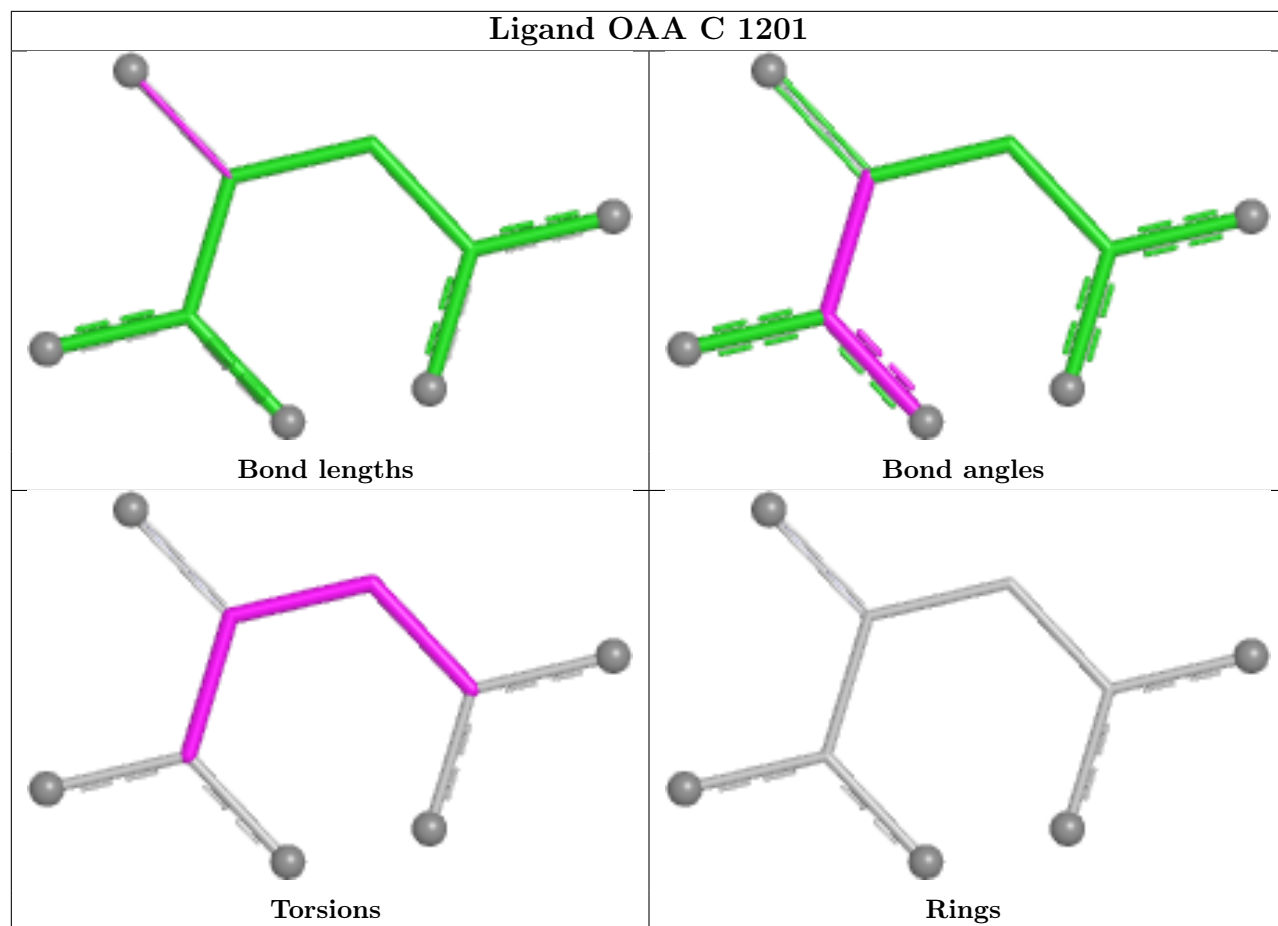


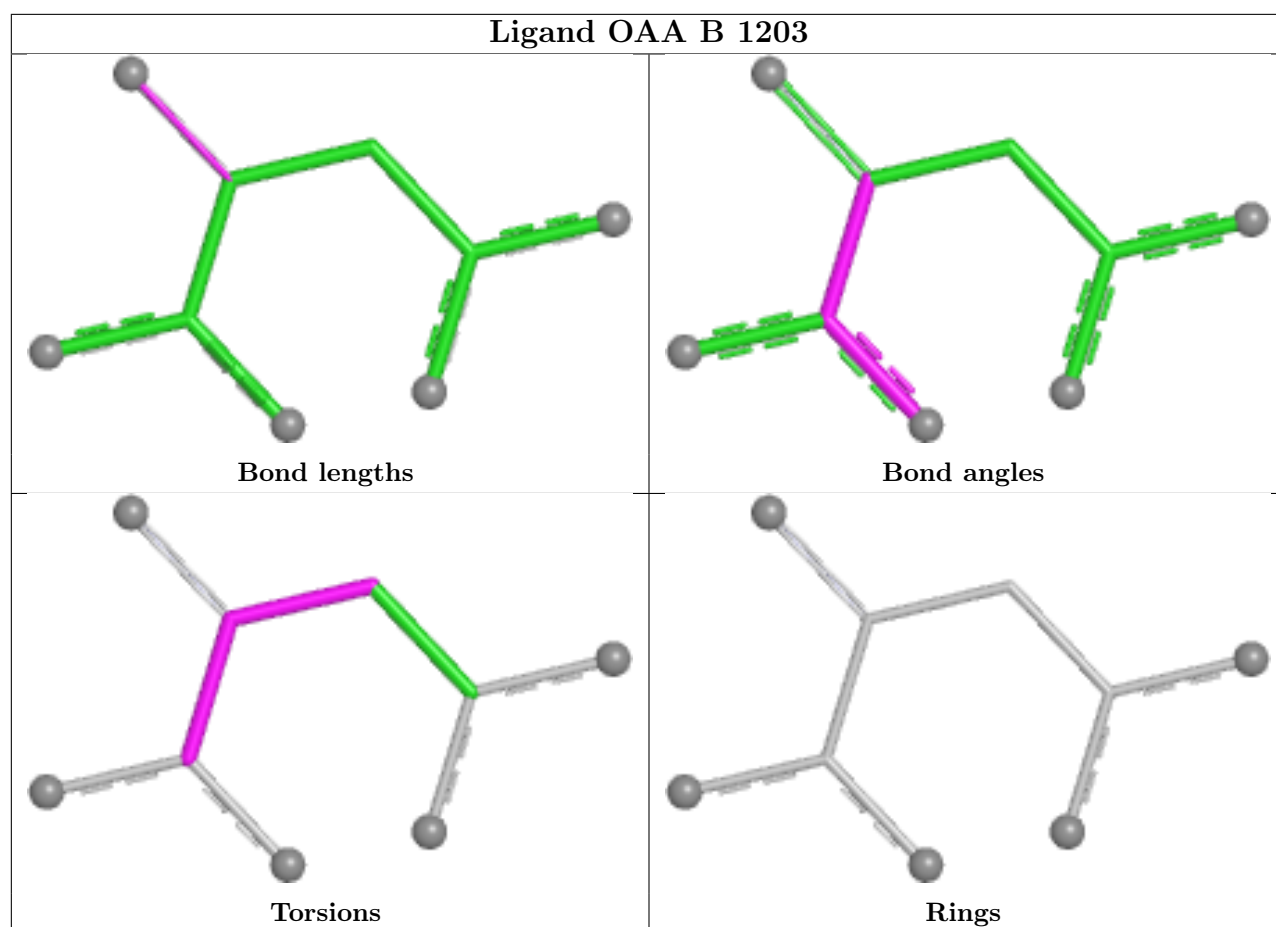
Ligand ACO A 1202 (A)











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.

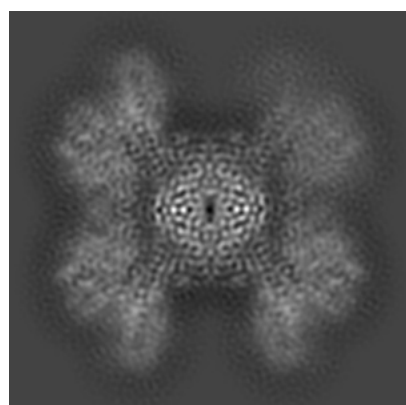
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20904. These allow visual inspection of the internal detail of the map and identification of artifacts.

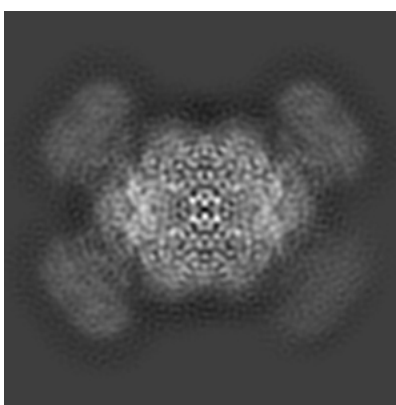
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

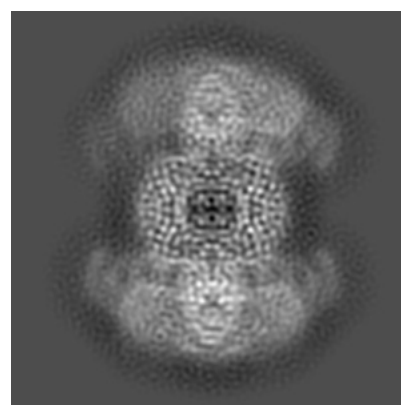
6.1.1 Primary map



X



Y

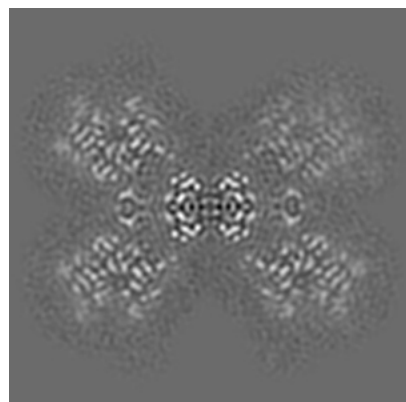


Z

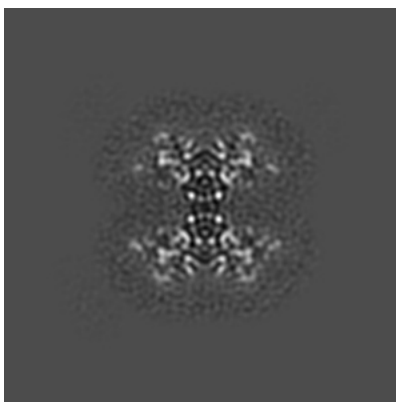
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

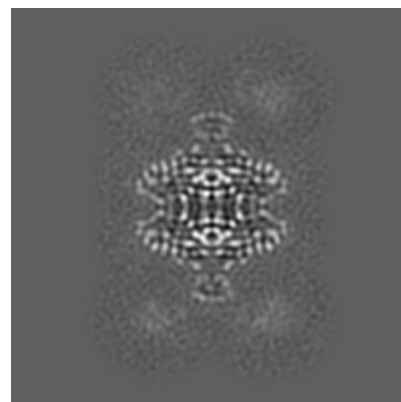
6.2.1 Primary map



X Index: 110



Y Index: 110

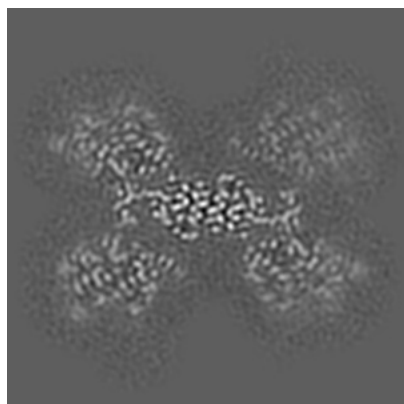


Z Index: 110

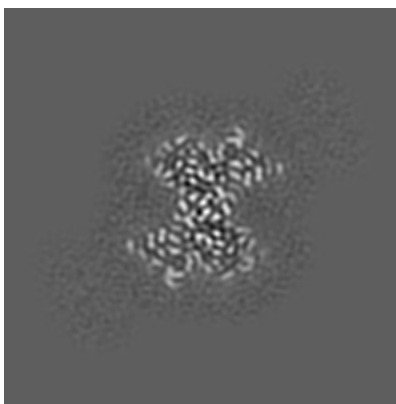
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

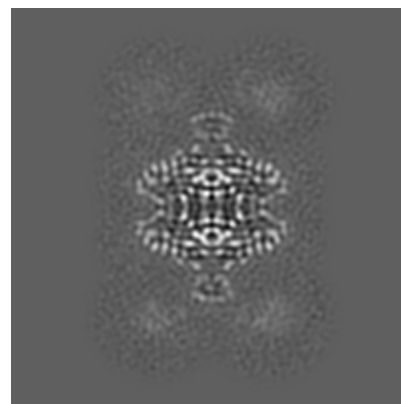
6.3.1 Primary map



X Index: 105



Y Index: 103

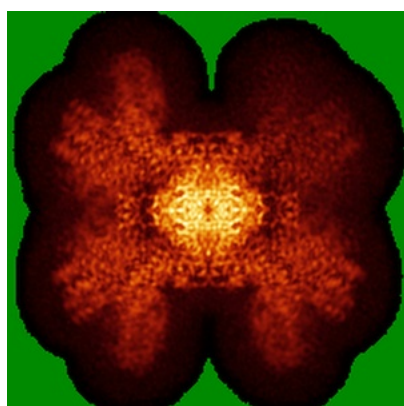


Z Index: 110

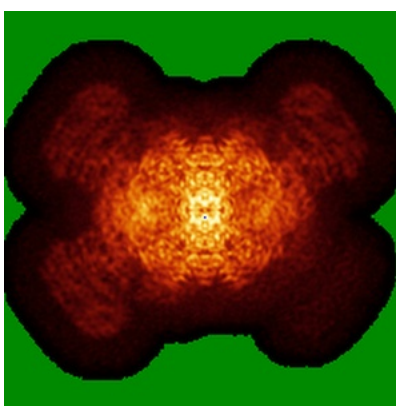
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

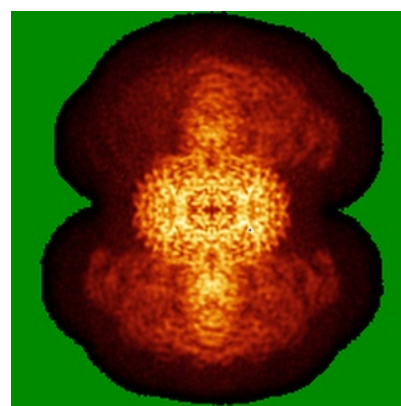
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

This section was not generated.

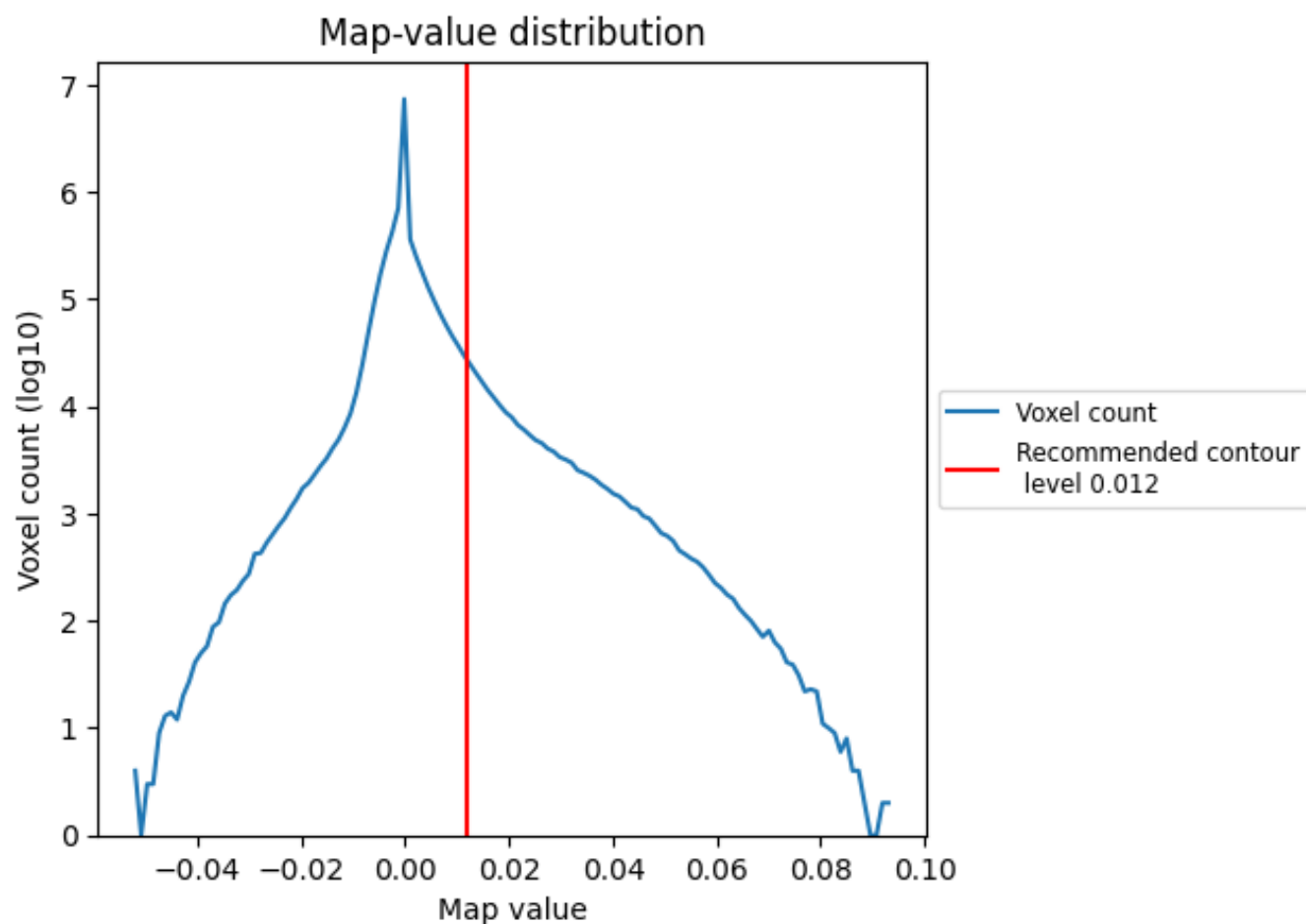
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

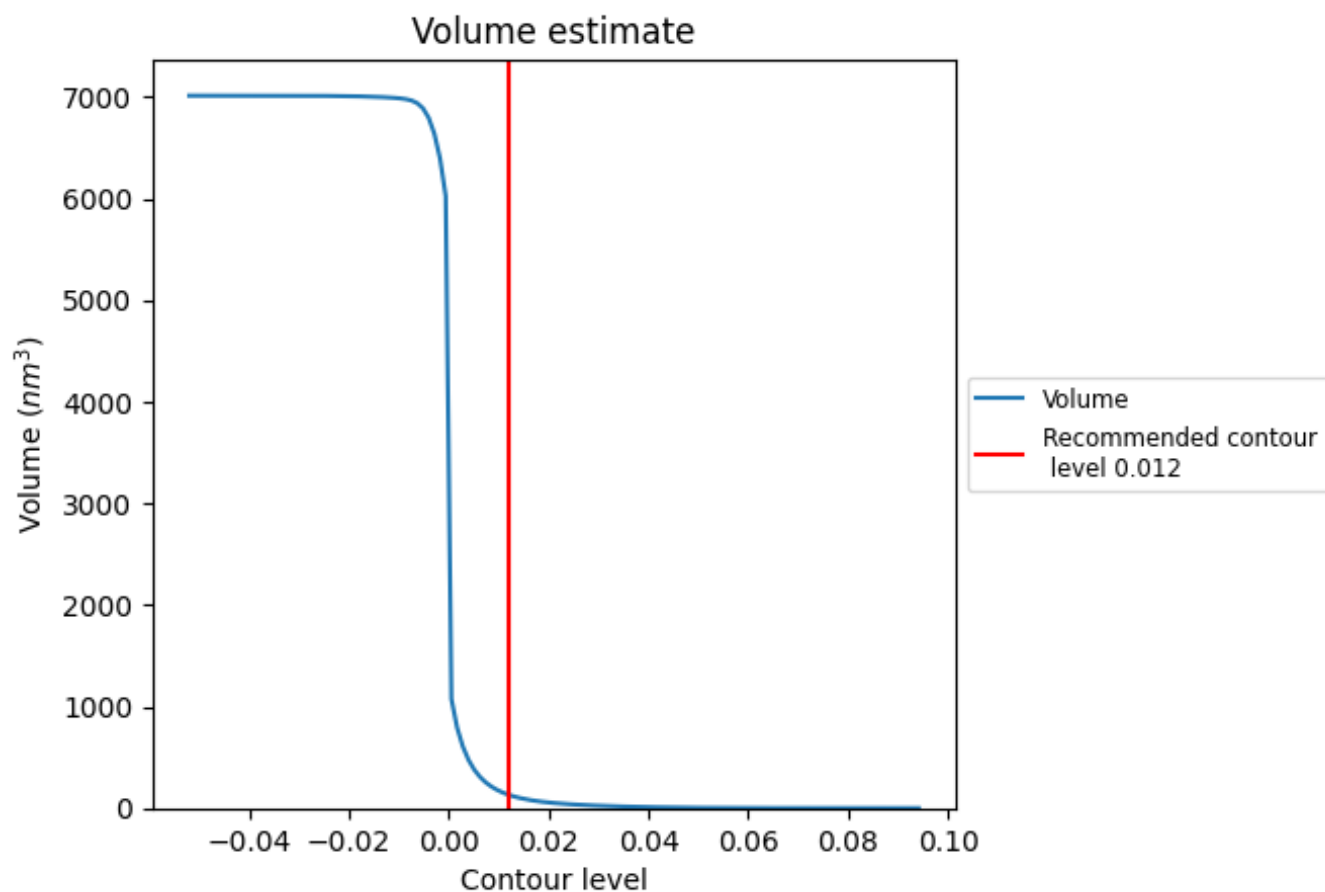
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

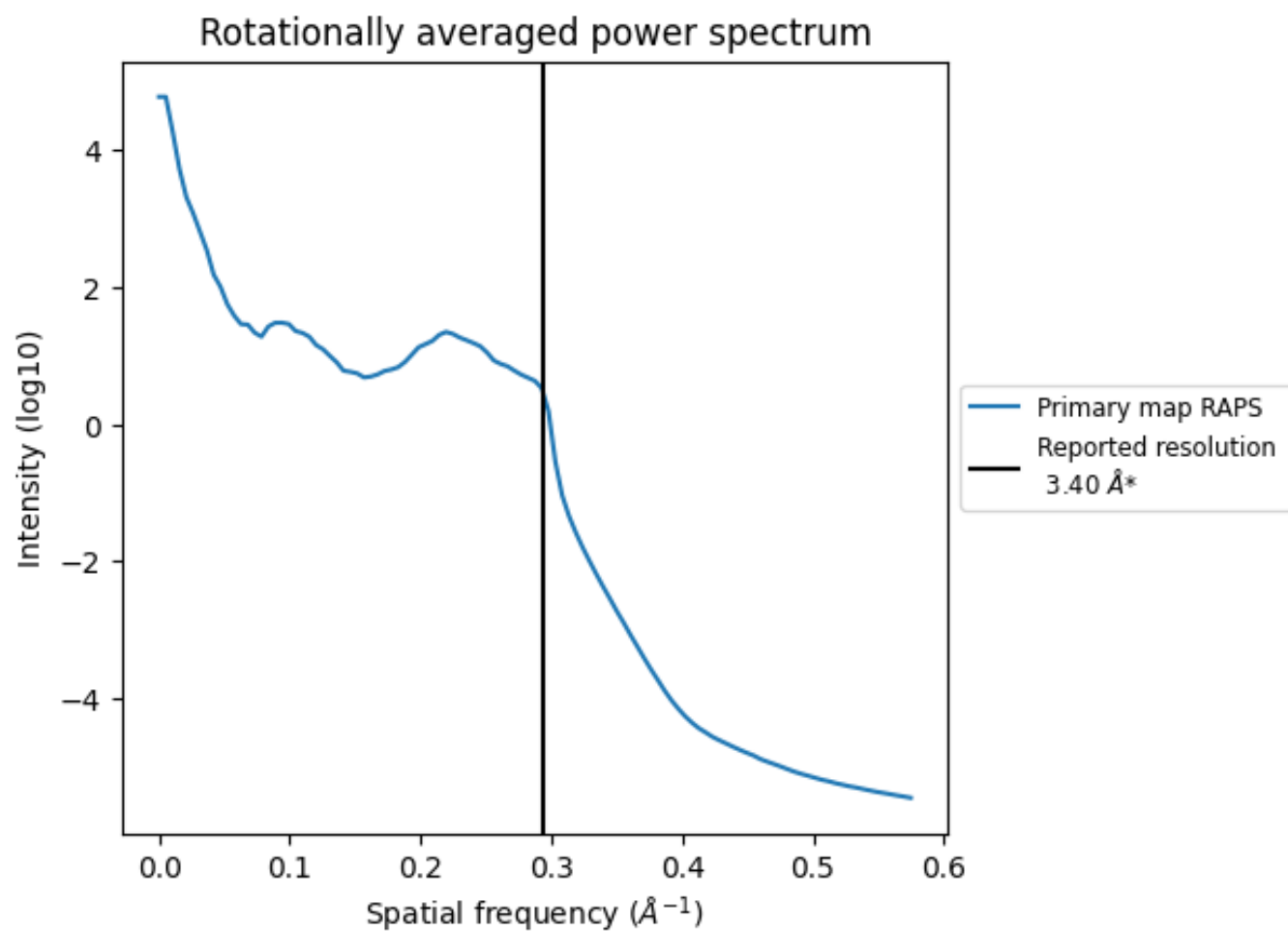
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 132 nm^3 ; this corresponds to an approximate mass of 119 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

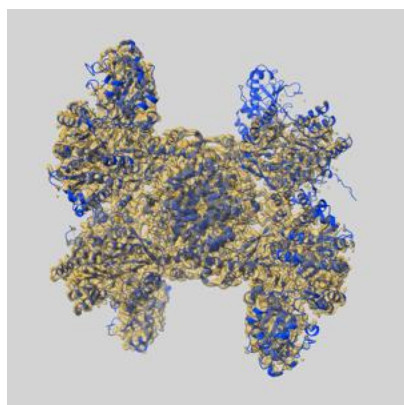
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

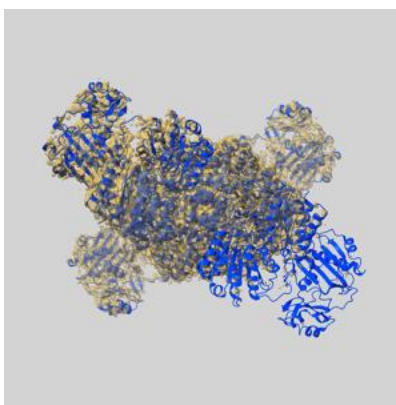
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20904 and PDB model 6UV5. Per-residue inclusion information can be found in section [3](#) on page [6](#).

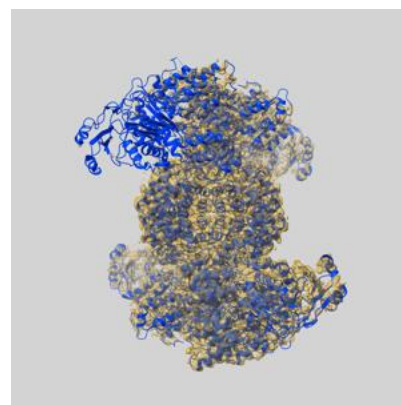
9.1 Map-model overlay [i](#)



X



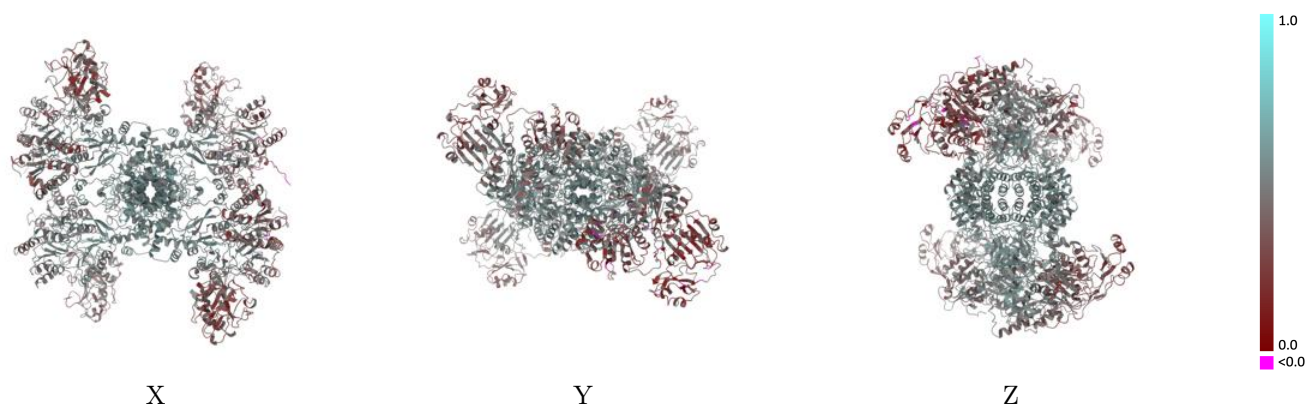
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)

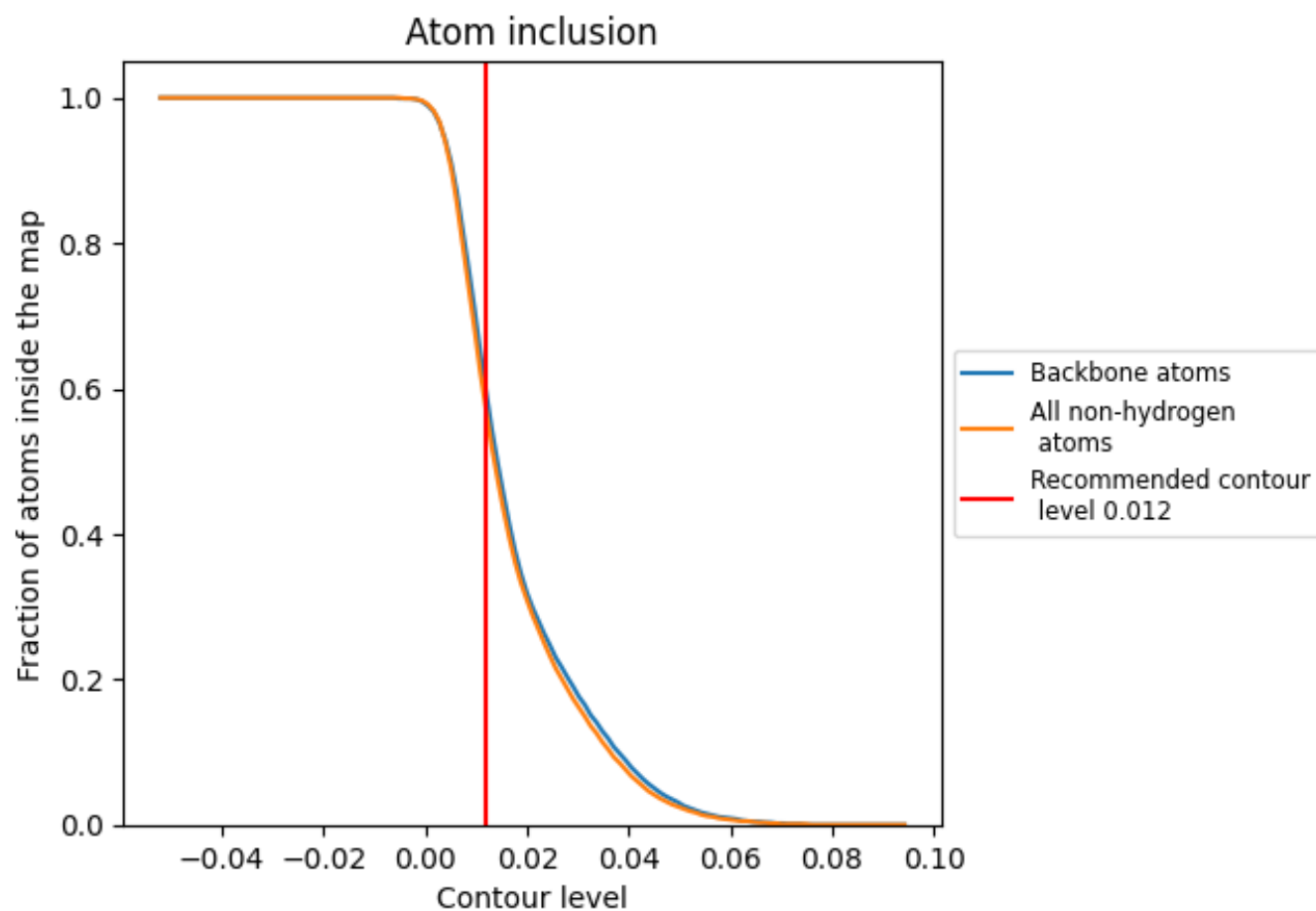


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 57% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5690	0.4590
A	0.6620	0.4780
B	0.6480	0.4760
C	0.3740	0.4210
D	0.6120	0.4640

