



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:50 PM UTC

PDB ID : 7RKZ / pdb_00007rkz
EMDB ID : EMD-24511
Title : Structure of ACLY D1026A-substrates-asym-int
Authors : Wei, X.; Marmorstein, R.
Deposited on : 2021-07-22
Resolution : 2.60 Å(reported)

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:

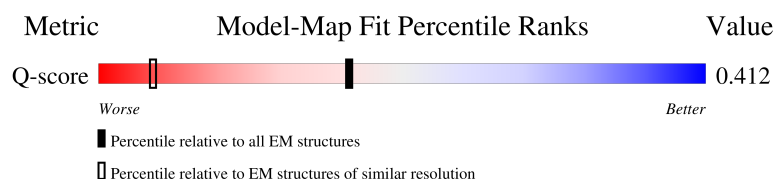
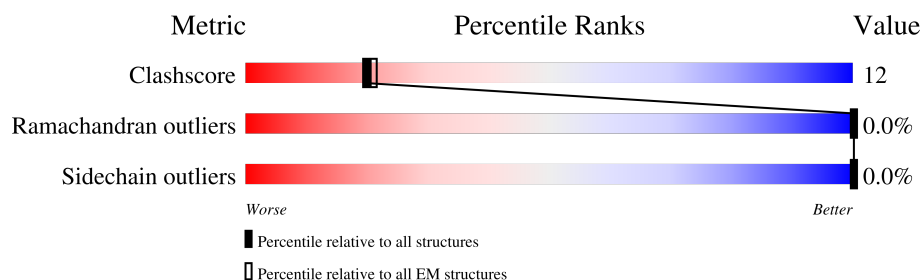
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	1101	
1	B	1101	
1	C	1101	
1	D	1101	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 32610 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.

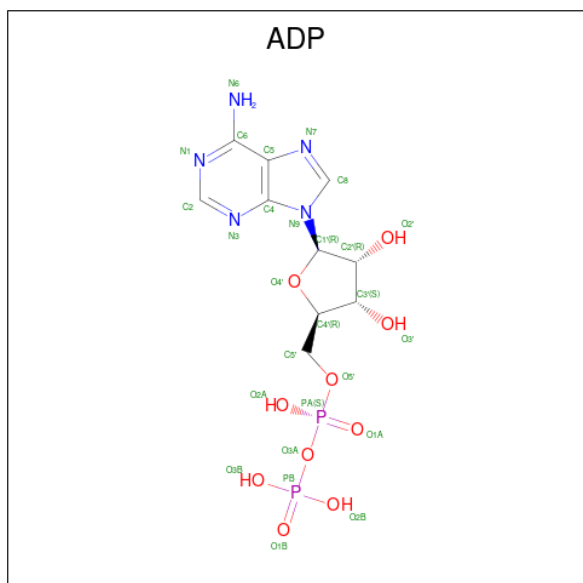
- Molecule 1 is a protein called ATP-citrate synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1032	Total	C	N	O	S	2	0
			7989	5114	1354	1474	47		
1	B	1032	Total	C	N	O	S	2	0
			7989	5114	1354	1474	47		
1	C	1032	Total	C	N	O	S	2	0
			7989	5114	1354	1474	47		
1	D	1030	Total	C	N	O	S	2	0
			7974	5105	1350	1472	47		

There are 4 discrepancies between the modelled and reference sequences:

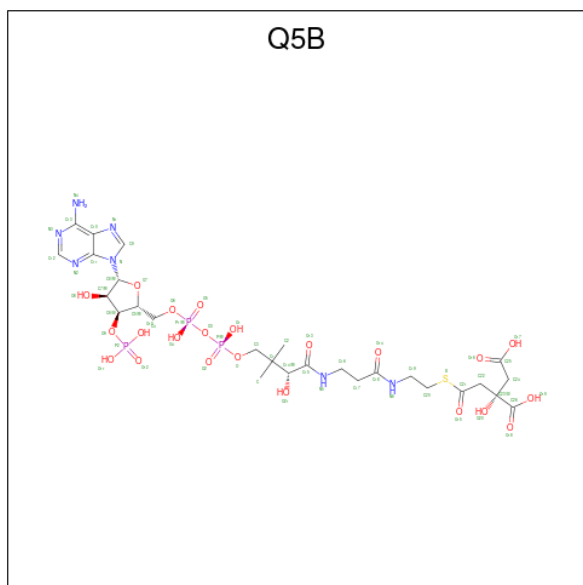
Chain	Residue	Modelled	Actual	Comment	Reference
A	1026	ALA	ASP	engineered mutation	UNP P53396
B	1026	ALA	ASP	engineered mutation	UNP P53396
C	1026	ALA	ASP	engineered mutation	UNP P53396
D	1026	ALA	ASP	engineered mutation	UNP P53396

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



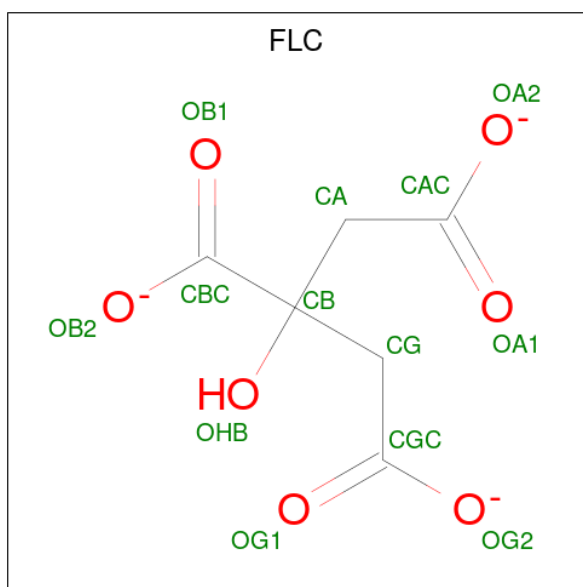
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
2	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 3 is (3S)-citryl-Coenzyme A (CCD ID: Q5B) (formula: $C_{27}H_{42}N_7O_{22}P_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
3	A	1	Total 60	C 27	N 7	O 22	P 3	S 1	0
3	B	1	Total 60	C 27	N 7	O 22	P 3	S 1	0
3	D	1	Total 60	C 27	N 7	O 22	P 3	S 1	0

- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).

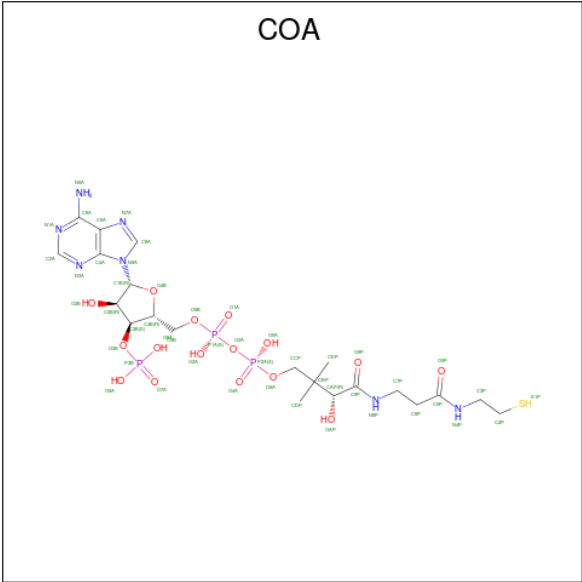


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			13	6	7	
4	B	1	Total	C	O	0
			13	6	7	
4	C	1	Total	C	O	0
			13	6	7	
4	D	1	Total	C	O	0
			13	6	7	

- Molecule 5 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	C	0
			1	1	
5	C	1	Total	C	0
			1	1	

- Molecule 6 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms					AltConf
6	A	1	Total	C	N	O	P	S
			48	21	7	16	3	1
6	B	1	Total	C	N	O	P	S
			48	21	7	16	3	1
6	C	1	Total	C	N	O	P	S
			48	21	7	16	3	1
6	C	1	Total	C	N	O	P	S
			48	21	7	16	3	1

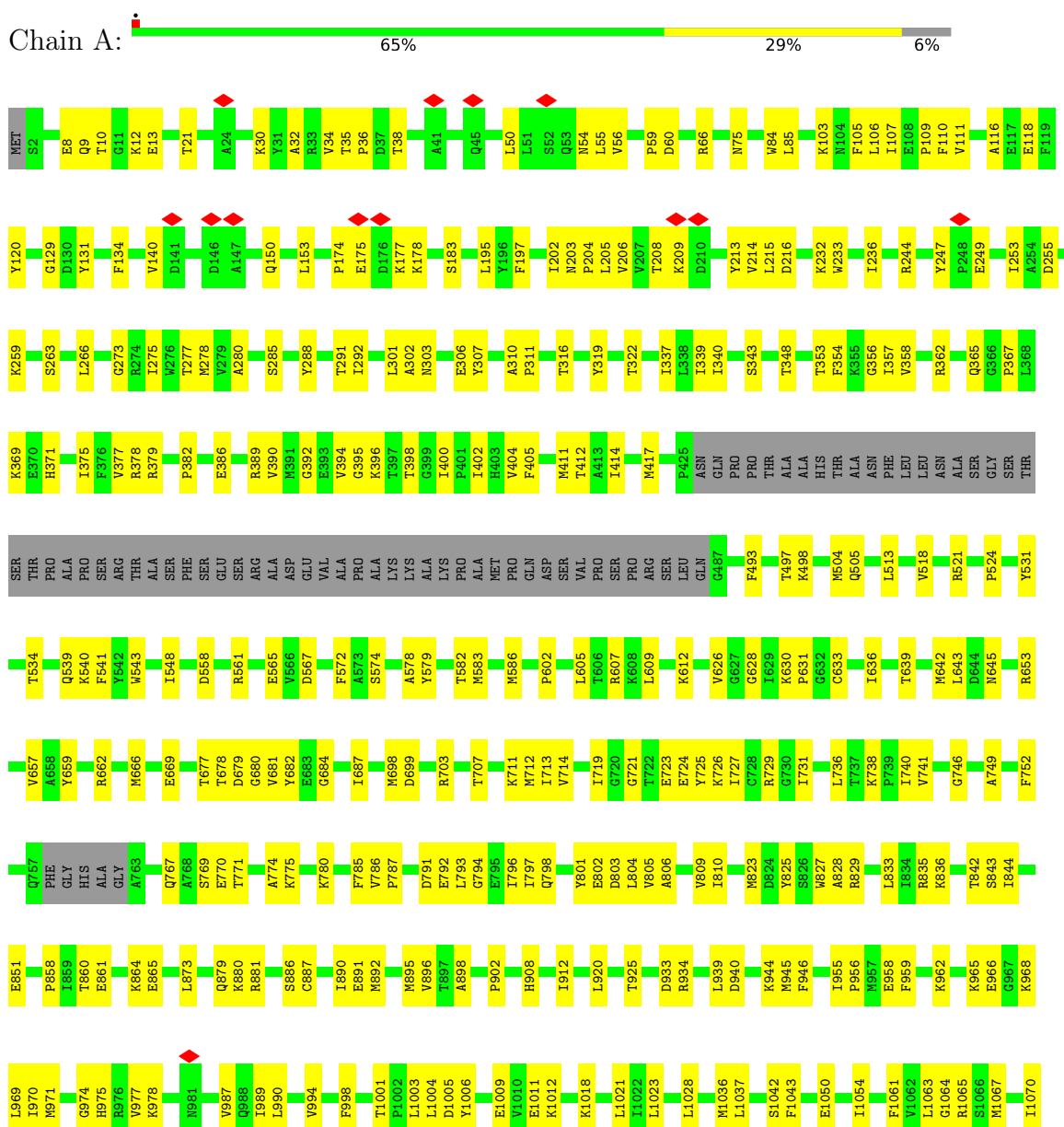
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		AltConf
7	A	35	Total	O	0
			35	35	
7	B	47	Total	O	0
			47	47	
7	C	37	Total	O	0
			37	37	
7	D	43	Total	O	0
			43	43	

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.

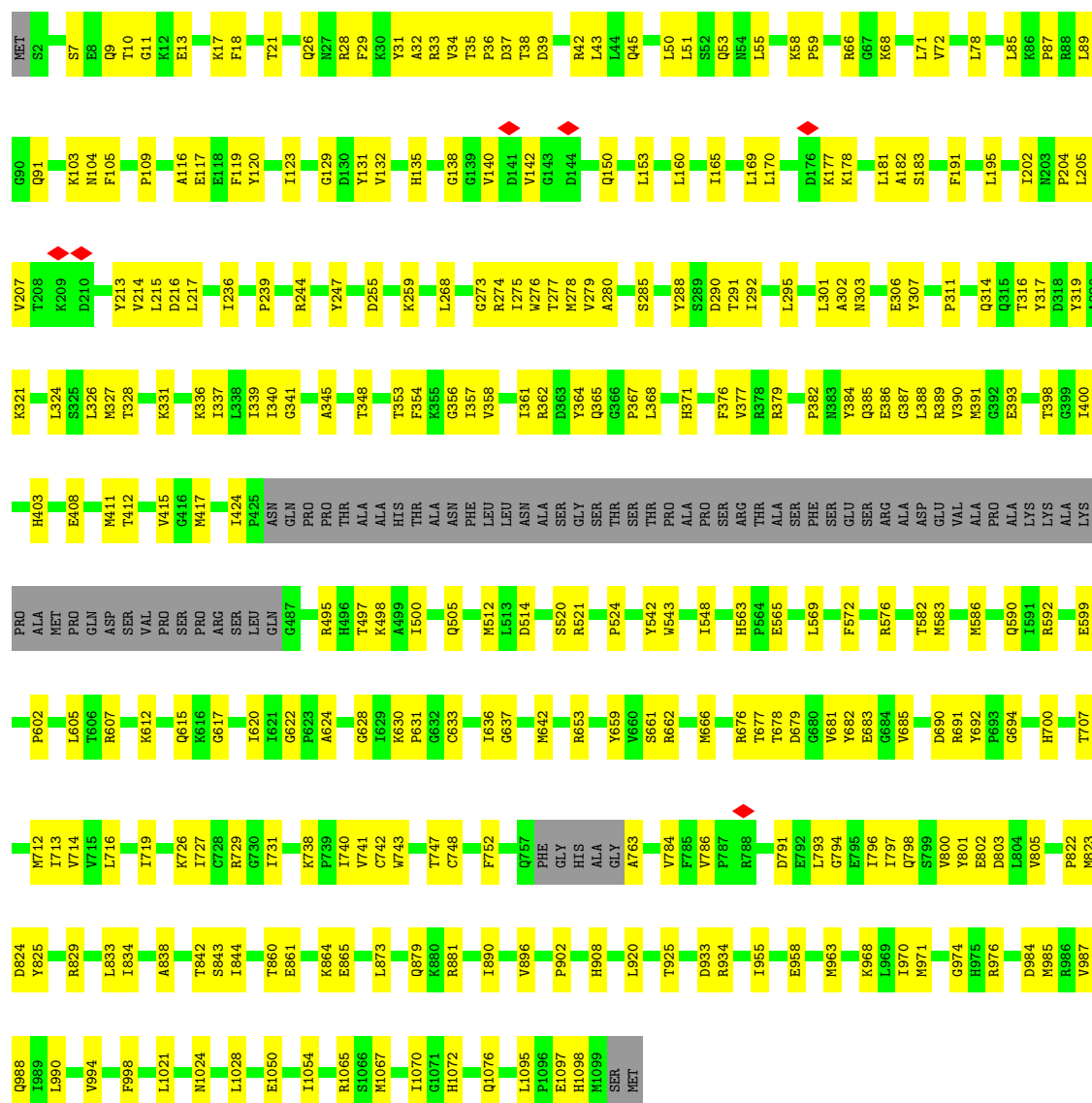
• Molecule 1: ATP-citrate synthase





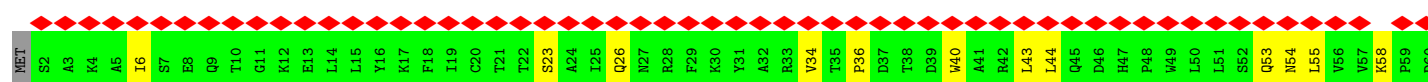
● Molecule 1: ATP-citrate synthase

Chain B: 67% 27% 6%



● Molecule 1: ATP-citrate synthase

Chain C: 46% 67% 27% 6%



L1008	E861	F785	V714	I629	H563	K488	PRO	G366	Y304	P241	L181	V121	Q61
I1013	V862	V786	V715	C633	P664	S489	PRO	P367	G305	F242	A182	C122	L62
S1016	F863	F787	L716	F634	E565	T490	THR	L368	E306	G243	S183	I123	I63
N1024	I869	R788	G717	K635	V566	T491	ALA	K369	S307	R244	F184	Y124	K64
L1028	L873	S789	E718	T636	D567	H496	HIS	E370	S308	E245	I185	A125	R65
F1043	F878	F790	I719	G637	V568	H499	THR	H371	G309	A246	S186	T126	R66
E1047	Q879	D791	G720	N638	L569	A499	ALA	A310	A310	Y247	G187	R127	G67
F1061	E792	E792	T722	L647	N571	V501	ASN	E372	F311	P248	L188	E128	K68
G1064	G794	G794	E723	A648	S574	V502	LEU	V374	S312	E249	F189	G129	L69
R1065	E795	S649	T725	A648	L575	G503	LEU	V375	E313	E250	L190	D130	G70
S1066	T796	K650	K726	K650	R576	M504	ASN	F376	Q314	A251	N191	Y131	L71
R1067	T797	L651	T727	L651	S577	L513	GLY	V377	Q315	Y252	F191	V132	V72
P902	Q798	Y652	C728	Y652	A578	Y517	THR	R379	T316	I253	G193	L133	G73
H908	Y601	R653	C728	R653	Y579	Y517	THR	G380	Y317	A254	D194	F134	V74
I912	D803	P654	R729	P654	D580	P382	THR	G381	D318	D255	L195	H135	N75
K918	L804	V657	G730	V657	S581	N383	PRO	P382	Y319	L256	Y196	H136	L76
T925	E802	G664	I731	G664	T582	E386	ALA	E386	A320	D257	F197	E137	T77
R1085	D803	G665	K732	G665	D522	G387	ALA	G387	K321	A258	T198	G138	L78
V1094	L804	G666	E733	G666	E523	E387	PRO	E387	T322	K259	Y199	G139	D79
S1099	A806	M666	G734	M666	P524	L388	SER	L388	I323	S260	L200	V140	G80
Q1076	R807	S667	R735	S667	S525	R389	ARG	R389	L324	G261	E201	D141	V81
K1077	G808	M668	L736	M668	V526	V390	THR	V390	S325	A262	I202	V142	K82
R1099	L810	E669	T737	E669	A527	K391	ALA	K391	L326	L264	N203	G143	S83
P956	V811	N671	K738	N671	A528	G392	SER	G392	T328	K265	P204	D144	W84
M957	P812	L674	P739	L674	M529	E393	GLU	E393	R329	L266	V206	V145	L85
F959	A813	T677	I740	T677	V530	G395	SER	G395	E330	L267	V207	D146	L86
V960	Q814	T678	V741	T678	V531	K396	ALA	K396	K331	L268	T208	K148	K86
K962	R816	T679	I745	T679	I591	T397	GLU	T397	H332	L269	K209	Q150	P87
M963	P817	G680	C748	G680	R592	G535	VAL	G535	P333	N270	D210	K151	L89
E966	L818	V681	A749	V681	T594	D536	ALA	D536	G335	P271	G211	L152	Q91
I970	P819	E682	T751	E682	A598	H537	PRO	H537	K336	K272	V212	L153	E92
M971	T820	E683	F752	E683	E599	K538	ALA	K538	I337	R274	Y213	V154	A93
G972	V821	G684	S753	G684	P602	K540	LYS	K540	L338	I275	V214	G155	T94
I973	D824	V685	S754	V685	E603	F541	LYS	F541	I339	W276	L215	V156	V95
G974	Y825	G688	E755	G688	A604	Y542	PRO	A604	G341	G277	D216	G156	G96
H975	S826	R691	E756	R691	L605	H543	ALA	L605	G342	T277	L217	D157	K97
R976	S826	Y692	V757	Y692	T606	G544	MET	G544	G342	M278	A218	E158	A98
M985	A828	P693	PHE	P693	R607	H545	GLN	H545	I344	V279	A219	K159	T99
R986	R829	F697	GLY	F697	K608	K546	ASP	K546	A345	G281	K220	L160	G100
V987	E830	M698	HIS	M698	L609	E547	SER	E547	N346	G282	V221	N161	F101
R995	L831	D699	ALA	D699	T610	I548	VAL	I548	F347	G283	D222	P162	L102
T1001	G832	H700	GLY	H700	K611	L549	SER	K611	T348	G283	A223	E163	K103
L1004	L833	V701	A763	V701	K612	I550	PRO	K612	A352	V286	T224	D164	N104
D1005	T894	L702	C764	T894	A613	P551	ARG	A613	T353	V287	A225	I165	F105
	R835	L702	A765	R835	D614	V552	SER	D614	F354	Y288	G226	K166	L106
	T842	Y704	M766	T842	Q615	F553	LEU	Q615	K355	S289	I228	K166	L106
	S843	Q705	Q767	S843	K616	K554	GLN	K616	K356	I292	Y227	K167	I107
	I844	Q705	A768	I844	G617	N555	GLN	G617	I357	L295	L228	H168	E108
	G856	K711	S769	G856	T620	N556		T620	L419	G296	C229	L169	P109
	M857	M712	E770	M857	I621	A559		I621	G420	G297	K230	L170	F110
	T860	I713	Q777	T860	A624	N560		A624	H421	V298	V171	H172	V111
					T625	R561		T625	A360	N299	K231	H172	P112
					G628	K562		G628	I361	E300	W233	A173	H113
									D363	L301	G234	P174	S114
									Y364	A302	D235	E175	Q115
									Q365	N303	I236	D176	A116
											E237	K177	E117
											F238	K178	E118
											P239	E179	F119
												I180	Y120

• Molecule 1: ATP-citrate synthase



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	237362	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	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	3.024	Depositor
Minimum map value	-1.514	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.157	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	182.59999, 182.59999, 182.59999	wwPDB
Map dimensions	220, 220, 220	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, UNL, Q5B, FLC, COA

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	0.14	0/8167	0.34	0/11054
1	B	0.17	0/8167	0.35	0/11054
1	C	0.13	0/8167	0.31	0/11054
1	D	0.15	0/8151	0.33	0/11032
All	All	0.15	0/32652	0.33	0/44194

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7989	0	8040	222	0
1	B	7989	0	8040	208	0
1	C	7989	0	8040	201	0
1	D	7974	0	8031	210	0
2	A	27	0	12	6	0
2	B	27	0	12	2	0
2	D	27	0	12	2	0
3	A	60	0	0	1	0
3	B	60	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	60	0	0	1	0
4	A	13	0	5	1	0
4	B	13	0	5	1	0
4	C	13	0	5	1	0
4	D	13	0	5	1	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	48	0	32	4	0
6	B	48	0	32	3	0
6	C	96	0	64	11	0
7	A	35	0	0	0	0
7	B	47	0	0	0	0
7	C	37	0	0	1	0
7	D	43	0	0	0	0
All	All	32610	0	32335	804	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 12.

All (804) 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:D:279:VAL:HG12	1:D:341:GLY:H	1.36	0.89
1:C:1085:ARG:HE	6:C:2102:COA:H62A	1.21	0.86
1:A:719:ILE:HD11	1:A:746:GLY:HA3	1.59	0.83
1:D:316:THR:HG21	1:D:353:THR:HA	1.60	0.82
1:C:835:ARG:HG3	1:D:822:PRO:HB2	1.62	0.81
1:A:316:THR:HG21	1:A:353:THR:HA	1.61	0.81
1:C:541:PHE:HA	1:D:835:ARG:HH22	1.46	0.80
1:B:268:LEU:HD11	1:B:326:LEU:HD11	1.65	0.79
1:D:55:LEU:HD21	1:D:107:ILE:HD12	1.65	0.78
1:D:583:MET:HE2	1:D:609:LEU:HD23	1.67	0.76
1:C:538:LYS:HB3	1:C:549:LEU:HB3	1.68	0.76
1:C:316:THR:HG21	1:C:353:THR:HA	1.65	0.75
1:C:713:ILE:HB	1:C:740:ILE:HG12	1.69	0.75
1:D:1065:ARG:HH22	4:D:1203:FLC:HA2	1.52	0.74
1:B:275:ILE:HG23	1:B:337:ILE:HD11	1.67	0.74
1:D:125:ALA:HB1	1:D:607:ARG:HH22	1.53	0.73
1:C:54:ASN:HD21	1:C:75:ASN:HA	1.53	0.72
1:D:490:THR:HA	1:D:703:ARG:HG2	1.71	0.72
1:A:1078:ARG:HH22	1:C:1047:GLU:HG2	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:LYS:NZ	1:B:838:ALA:O	2.20	0.71
1:D:611:LYS:O	1:D:615:GLN:NE2	2.22	0.71
1:C:896:VAL:HG13	1:C:986:ARG:HD2	1.71	0.71
1:D:773:VAL:O	1:D:777:GLN:NE2	2.23	0.71
1:C:628:GLY:H	1:C:636:ILE:HB	1.54	0.71
1:D:698:MET:HG2	1:D:726:LYS:HE3	1.71	0.71
1:C:170:LEU:HD23	1:C:178:LYS:HG3	1.73	0.70
1:A:1054:ILE:HD12	1:C:1077:LYS:HB3	1.74	0.69
1:C:374:THR:HG23	1:C:401:PRO:HB2	1.74	0.69
1:A:825:TYR:OH	1:A:829:ARG:NH1	2.23	0.69
1:A:583:MET:HE2	1:A:609:LEU:HD23	1.74	0.69
1:B:712:MET:HE1	1:B:797:ILE:HG23	1.72	0.69
1:C:199:TYR:HB3	1:C:220:LYS:HB2	1.74	0.69
1:B:825:TYR:OH	1:B:829:ARG:NH1	2.25	0.69
1:A:497:THR:O	1:A:521:ARG:NH2	2.26	0.68
1:A:50:LEU:HD12	1:A:55:LEU:HD21	1.74	0.68
1:D:382:PRO:HB3	1:D:642:MET:HE3	1.74	0.68
1:A:823:MET:HE1	1:A:833:LEU:HD12	1.75	0.68
1:C:354:PHE:HD1	1:C:391:MET:HE3	1.57	0.68
1:A:835:ARG:HG2	1:B:542:TYR:CE2	2.28	0.67
1:B:87:PRO:O	1:B:91:GLN:NE2	2.26	0.67
1:B:202:ILE:HG23	1:B:214:VAL:HG23	1.76	0.67
1:C:343:SER:O	1:C:379:ARG:NH1	2.25	0.67
1:D:59:PRO:HD2	1:D:66:ARG:HD3	1.77	0.67
1:B:1065:ARG:HH22	4:B:1203:FLC:HA2	1.59	0.67
3:B:1202:Q5B:N4	1:D:973:ILE:O	2.28	0.67
1:C:739:PRO:HG2	1:C:804:LEU:HD21	1.76	0.67
1:D:53:GLN:HE21	1:D:109:PRO:HB3	1.59	0.67
1:D:780:LYS:HE3	1:D:786:VAL:HB	1.77	0.66
1:B:497:THR:O	1:B:521:ARG:NH2	2.29	0.66
1:C:177:LYS:HD2	1:C:207:VAL:HG13	1.76	0.66
1:D:787:PRO:HG3	1:D:796:ILE:HD11	1.78	0.66
1:C:571:ASN:ND2	1:C:581:SER:OG	2.29	0.66
1:C:500:ILE:HG13	1:C:566:VAL:HG11	1.78	0.65
1:C:340:ILE:HD11	1:C:377:VAL:HG12	1.76	0.65
1:D:979:SER:HB2	1:D:1019:PRO:HB2	1.77	0.65
1:C:84:TRP:HE3	1:C:85:LEU:HD22	1.61	0.65
1:D:354:PHE:HE1	1:D:391:MET:HB2	1.60	0.65
1:A:310:ALA:H	1:A:348:THR:HG22	1.61	0.65
1:A:626:VAL:HG13	1:A:639:THR:HG22	1.79	0.65
1:C:1001:THR:HB	1:C:1004:LEU:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:726:LYS:HA	1:A:729:ARG:HG2	1.80	0.64
1:C:331:LYS:NZ	1:C:370:GLU:O	2.30	0.64
1:A:602:PRO:HG2	1:A:605:LEU:HD12	1.77	0.64
1:B:974:GLY:O	1:B:1024:ASN:ND2	2.22	0.64
1:B:39:ASP:HB3	1:B:42:ARG:HD2	1.79	0.64
1:C:995:ARG:NH2	1:C:1005:ASP:OD1	2.27	0.64
1:A:582:THR:HG22	1:A:586:MET:HE2	1.79	0.64
1:C:741:VAL:HG22	1:C:785:PHE:HB2	1.79	0.64
1:C:985:MET:HE3	1:C:985:MET:HA	1.80	0.63
1:A:835:ARG:NH2	1:B:514:ASP:OD1	2.30	0.63
1:C:995:ARG:HH21	1:C:1008:LEU:HD12	1.62	0.63
1:B:13:GLU:O	1:B:17:LYS:HG3	1.98	0.63
1:D:560:MET:SD	1:D:590:GLN:NE2	2.70	0.63
1:B:512:MET:HE2	1:B:637:GLY:H	1.63	0.63
1:A:987:VAL:HG13	1:A:1028:LEU:HD22	1.81	0.63
1:B:58:LYS:NZ	1:B:215:LEU:O	2.32	0.62
1:D:493:PHE:O	1:D:630:LYS:NZ	2.27	0.62
1:A:653:ARG:NH2	1:A:679:ASP:O	2.31	0.62
1:B:833:LEU:HD12	1:B:834:ILE:HG12	1.81	0.62
1:A:367:PRO:O	1:A:371:HIS:ND1	2.32	0.62
1:B:521:ARG:NH1	1:B:633:CYS:O	2.32	0.62
1:B:971:MET:HA	6:B:1204:COA:H62	1.82	0.62
1:D:336:LYS:HD2	1:D:371:HIS:HB3	1.80	0.62
1:B:120:TYR:HB3	1:B:135:HIS:HB3	1.82	0.62
1:B:68:LYS:HZ2	1:B:140:VAL:HG12	1.64	0.62
1:B:204:PRO:HB2	1:B:215:LEU:HB2	1.82	0.62
1:C:26:GLN:HB2	1:C:213:TYR:HE1	1.64	0.62
1:A:358:VAL:HG13	1:A:394:VAL:HG11	1.81	0.62
1:B:277:THR:HG22	1:B:339:ILE:HB	1.82	0.62
1:A:724:GLU:HB2	1:A:775:LYS:HE2	1.83	0.61
1:C:653:ARG:HH12	1:C:680:GLY:HA3	1.65	0.61
1:A:253:ILE:HD11	1:A:322:THR:HG21	1.81	0.61
1:A:558:ASP:OD1	1:A:561:ARG:NH2	2.34	0.61
1:A:707:THR:O	1:A:738:LYS:NZ	2.33	0.61
1:D:772:ALA:O	1:D:776:ASN:ND2	2.33	0.61
1:B:150:GLN:HG2	1:B:169:LEU:HA	1.82	0.61
1:C:354:PHE:HA	1:C:357:ILE:HG12	1.82	0.61
1:A:940:ASP:OD2	1:A:944:LYS:NZ	2.33	0.61
1:D:177:LYS:HD2	1:D:207:VAL:HG13	1.83	0.60
1:D:350:VAL:HG23	1:D:382:PRO:HD2	1.83	0.60
1:A:116:ALA:O	1:A:177:LYS:NZ	2.33	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:521:ARG:NH1	1:C:633:CYS:O	2.31	0.60
1:A:896:VAL:HG21	1:A:990:LEU:HD11	1.83	0.60
1:B:7:SER:HB3	1:B:239:PRO:HG3	1.83	0.60
1:B:412:THR:HG21	1:B:791:ASP:HA	1.83	0.60
1:D:54:ASN:HB3	1:D:110:PHE:HB3	1.83	0.60
1:D:581:SER:O	1:D:585:THR:HG23	2.00	0.60
1:D:991:LYS:HB2	1:D:1028:LEU:HD11	1.83	0.60
1:C:987:VAL:HG13	1:C:1028:LEU:HD22	1.82	0.60
1:B:411:MET:HE1	1:B:666:MET:HE1	1.82	0.60
1:B:691:ARG:NH1	1:B:692:TYR:OH	2.35	0.60
1:A:721:GLY:N	1:A:770:GLU:OE1	2.34	0.60
1:D:851:GLU:HG2	1:D:858:PRO:HB3	1.84	0.60
1:B:563:HIS:O	1:B:590:GLN:NE2	2.34	0.59
1:A:802:GLU:HA	1:A:805:VAL:HG22	1.84	0.59
1:C:256:LEU:HD21	1:C:318:ASP:HB2	1.83	0.59
1:D:125:ALA:HB1	1:D:607:ARG:NH2	2.16	0.59
1:D:206:VAL:HB	1:D:213:TYR:HB2	1.84	0.59
1:D:502:TRP:CD1	1:D:573:ALA:HB2	2.37	0.59
1:D:713:ILE:HB	1:D:740:ILE:HG12	1.83	0.59
1:D:974:GLY:O	1:D:1024:ASN:ND2	2.27	0.59
1:A:278:MET:HB2	1:A:319:TYR:HE2	1.67	0.59
1:B:9:GLN:HE22	1:B:31:TYR:HE1	1.50	0.59
1:D:77:THR:HG23	1:D:80:GLY:H	1.65	0.59
1:A:369:LYS:NZ	1:A:398:THR:O	2.36	0.59
1:D:354:PHE:CE1	1:D:391:MET:HB2	2.37	0.59
1:A:275:ILE:HG23	1:A:337:ILE:HD11	1.83	0.59
1:B:53:GLN:HE21	1:B:109:PRO:HB3	1.68	0.59
1:B:66:ARG:NH2	1:B:216:ASP:OD1	2.30	0.59
1:B:985:MET:HE2	1:B:985:MET:HA	1.85	0.59
1:C:64:LYS:HG2	1:C:65:ARG:HG3	1.85	0.58
1:C:120:TYR:HB3	1:C:135:HIS:HB3	1.84	0.58
1:B:896:VAL:HG21	1:B:990:LEU:HD11	1.84	0.58
1:D:284:ALA:HA	1:D:666:MET:HE3	1.84	0.58
1:D:287:VAL:HG22	1:D:745:ILE:HG12	1.84	0.58
1:B:382:PRO:HB3	1:B:642:MET:HE3	1.84	0.58
1:C:1065:ARG:HH22	4:C:2103:FLC:HA2	1.69	0.58
1:A:412:THR:HG21	1:A:791:ASP:HA	1.84	0.58
1:A:498:LYS:HD2	1:A:565:GLU:HG3	1.84	0.58
1:B:354:PHE:HA	1:B:357:ILE:HG12	1.85	0.58
1:C:697:PHE:HB2	1:C:723:GLU:HG2	1.85	0.58
1:A:835:ARG:HG3	1:B:822:PRO:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:974:GLY:O	6:C:2101:COA:H133	2.04	0.58
1:C:568:VAL:HG12	1:C:593:THR:HB	1.86	0.58
1:D:987:VAL:HG13	1:D:1028:LEU:HD13	1.85	0.58
1:A:861:GLU:HA	1:A:864:LYS:HG2	1.85	0.57
1:B:285:SER:HB2	1:B:306:GLU:HB3	1.85	0.57
1:C:55:LEU:HD11	1:C:107:ILE:HD12	1.86	0.57
1:C:53:GLN:HE21	1:C:109:PRO:HB3	1.67	0.57
1:C:731:ILE:HD11	1:C:740:ILE:HD12	1.86	0.57
1:C:268:LEU:HD11	1:C:326:LEU:HD21	1.85	0.57
1:C:513:LEU:HG	1:C:517:TYR:CE2	2.38	0.57
1:C:586:MET:HE1	1:C:620:ILE:HD11	1.86	0.57
1:D:77:THR:O	1:D:81:VAL:N	2.35	0.57
1:B:324:LEU:HB3	1:B:364:TYR:CE2	2.40	0.57
1:C:295:LEU:HD21	1:C:415:VAL:HG12	1.87	0.57
1:D:602:PRO:HG2	1:D:605:LEU:HD12	1.86	0.57
1:B:50:LEU:HD12	1:B:55:LEU:HD21	1.86	0.57
1:C:603:GLU:OE1	1:C:691:ARG:NH2	2.38	0.57
1:A:340:ILE:O	1:A:377:VAL:HA	2.03	0.57
1:C:23:SER:HA	1:C:180:ILE:HD11	1.87	0.57
1:D:199:TYR:O	1:D:219:ALA:HA	2.03	0.57
1:D:604:ALA:HA	1:D:607:ARG:HD3	1.86	0.57
1:B:273:GLY:C	1:B:276:TRP:HE1	2.13	0.56
1:B:311:PRO:HD2	1:B:348:THR:HG23	1.87	0.56
1:A:32:ALA:HB3	1:A:107:ILE:HG13	1.87	0.56
1:A:724:GLU:OE1	1:A:775:LYS:NZ	2.36	0.56
1:B:630:LYS:HG2	1:B:633:CYS:HB2	1.86	0.56
1:D:204:PRO:HD2	1:D:215:LEU:HB2	1.87	0.56
1:B:288:TYR:O	1:B:292:ILE:HG12	2.04	0.56
1:B:273:GLY:HA3	1:B:302:ALA:HB2	1.87	0.56
1:D:278:MET:HG3	1:D:319:TYR:HE2	1.71	0.56
1:D:610:ILE:HD11	1:D:692:TYR:O	2.06	0.56
1:D:976:ARG:HG3	1:D:977:VAL:HG13	1.88	0.56
1:A:34:VAL:HG23	1:A:105:PHE:HB2	1.87	0.56
1:A:405:PHE:HE2	1:A:417:MET:HG3	1.71	0.56
1:B:28:ARG:HG2	1:B:29:PHE:CD2	2.41	0.56
1:D:164:ASP:HA	1:D:168:HIS:HB2	1.88	0.56
1:A:657:VAL:HG22	1:A:712:MET:HB3	1.87	0.56
1:D:823:MET:HE3	1:D:828:ALA:HB2	1.88	0.56
1:C:823:MET:HE3	1:C:827:TRP:CZ3	2.40	0.56
1:C:1085:ARG:NE	6:C:2102:COA:H62A	1.98	0.56
1:B:576:ARG:HD2	1:D:1017:LYS:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:860:THR:HG22	1:D:989:ILE:HD11	1.88	0.56
1:C:570:ILE:HD13	1:C:636:ILE:HG23	1.89	0.55
1:A:12:LYS:NZ	1:A:214:VAL:O	2.40	0.55
1:A:962:LYS:HA	1:A:965:LYS:HE2	1.87	0.55
1:B:21:THR:HG1	1:B:183:SER:HG	1.54	0.55
1:D:61:GLN:HE22	1:D:242:PHE:HA	1.71	0.55
1:D:574:SER:OG	3:D:1202:Q5B:O12	2.23	0.55
1:D:659:TYR:HA	1:D:714:VAL:O	2.06	0.55
1:D:1004:LEU:O	1:D:1008:LEU:HG	2.06	0.55
1:C:135:HIS:HE1	1:C:137:GLU:HB3	1.70	0.55
1:A:354:PHE:HA	1:A:357:ILE:HG12	1.88	0.55
1:B:823:MET:HE1	1:B:833:LEU:HD21	1.89	0.55
1:D:707:THR:O	1:D:738:LYS:NZ	2.38	0.55
1:D:660:VAL:HG12	1:D:715:VAL:HG22	1.89	0.55
6:C:2102:COA:H62	1:D:972:GLY:H	1.70	0.55
1:A:278:MET:SD	1:A:340:ILE:HG22	2.46	0.55
1:A:395:GLY:HA3	1:A:402:ILE:HG13	1.89	0.55
1:B:38:THR:OG1	1:B:42:ARG:NH2	2.40	0.55
1:A:851:GLU:HG2	1:A:858:PRO:HB3	1.87	0.55
1:B:742:CYS:SG	1:B:743:TRP:N	2.80	0.55
1:C:1024:ASN:HD22	6:C:2101:COA:HN4	1.55	0.55
1:D:127:ARG:O	1:D:611:LYS:NZ	2.36	0.55
1:D:177:LYS:HA	1:D:180:ILE:HG22	1.89	0.55
1:D:788:ARG:N	1:D:792:GLU:OE2	2.40	0.54
1:A:175:GLU:HA	1:A:178:LYS:HD3	1.89	0.54
1:A:375:ILE:HB	1:A:402:ILE:HD13	1.88	0.54
1:A:677:THR:HB	1:A:798:GLN:HG3	1.89	0.54
1:B:280:ALA:HB2	1:B:307:TYR:CZ	2.42	0.54
1:B:719:ILE:O	1:B:763:ALA:N	2.41	0.54
1:A:843:SER:OG	1:C:1075:ASP:OD1	2.21	0.54
1:D:568:VAL:HG22	1:D:593:THR:HB	1.89	0.54
1:B:36:PRO:HG2	1:B:103:LYS:HD3	1.89	0.54
1:B:291:THR:HB	1:B:415:VAL:HG11	1.88	0.54
1:B:843:SER:HB2	1:D:1075:ASP:OD2	2.07	0.54
1:A:36:PRO:HG2	1:A:103:LYS:HD3	1.90	0.54
1:A:925:THR:HG23	1:C:925:THR:HG23	1.90	0.54
1:B:244:ARG:NE	1:B:247:TYR:OH	2.40	0.54
1:D:311:PRO:HD2	1:D:348:THR:HG23	1.89	0.54
1:A:835:ARG:N	1:B:823:MET:O	2.37	0.54
1:D:718:GLU:O	1:D:775:LYS:NZ	2.35	0.54
1:A:977:VAL:HG23	1:A:978:LYS:HD3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ILE:HG21	1:B:182:ALA:HA	1.90	0.54
1:D:122:CYS:HA	1:D:201:GLU:HG3	1.89	0.54
1:A:9:GLN:NE2	1:A:60:ASP:OD2	2.41	0.54
1:A:543:TRP:HB2	1:A:548:ILE:HD13	1.90	0.54
1:A:804:LEU:HD12	1:A:809:VAL:HG11	1.90	0.53
1:B:206:VAL:HG23	1:B:213:TYR:HB2	1.89	0.53
1:B:592:ARG:NH2	1:B:617:GLY:O	2.42	0.53
1:B:1054:ILE:HD12	1:D:1077:LYS:HB3	1.90	0.53
1:D:728:CYS:O	1:D:732:LYS:HG2	2.08	0.53
1:A:630:LYS:HG2	1:A:633:CYS:HB2	1.90	0.53
1:A:793:LEU:O	1:A:796:ILE:HG22	2.08	0.53
1:C:517:TYR:OH	1:C:543:TRP:HA	2.08	0.53
1:C:562:LYS:HD2	1:C:563:HIS:ND1	2.24	0.53
1:A:574:SER:OG	3:A:1202:Q5B:O12	2.20	0.53
1:A:886:SER:OG	1:A:1036:MET:SD	2.67	0.53
1:A:975:HIS:NE2	1:A:978:LYS:HE2	2.23	0.53
1:B:307:TYR:HD2	1:B:311:PRO:HG3	1.73	0.53
3:B:1202:Q5B:C10	1:D:969:LEU:HD22	2.39	0.53
1:C:188:LEU:HD21	1:C:200:LEU:HD22	1.89	0.53
1:D:55:LEU:HD13	1:D:81:VAL:HG21	1.90	0.53
1:A:9:GLN:HG2	1:A:106:LEU:HD21	1.90	0.53
1:A:513:LEU:HD22	1:A:524:PRO:HB3	1.90	0.53
1:A:971:MET:HA	6:A:1205:COA:H61	1.89	0.53
1:D:612:LYS:HE2	1:D:616:LYS:HE2	1.90	0.53
1:A:713:ILE:HB	1:A:740:ILE:HG12	1.89	0.53
1:B:45:GLN:OE1	1:B:45:GLN:N	2.37	0.53
1:C:517:TYR:OH	1:C:542:TYR:O	2.26	0.53
1:D:888:GLN:O	1:D:892:MET:HG3	2.09	0.53
1:A:129:GLY:O	1:A:607:ARG:NH1	2.42	0.52
1:A:288:TYR:O	1:A:292:ILE:HG12	2.09	0.52
1:B:377:VAL:HG11	1:B:391:MET:HE1	1.91	0.52
1:C:375:ILE:HB	1:C:402:ILE:HD13	1.91	0.52
1:C:823:MET:HE1	1:C:833:LEU:HD12	1.91	0.52
1:B:861:GLU:HA	1:B:864:LYS:HG2	1.92	0.52
1:D:65:ARG:NH2	2:D:1201:ADP:O3B	2.43	0.52
1:D:657:VAL:HG21	1:D:678:THR:HG21	1.92	0.52
1:A:628:GLY:H	1:A:636:ILE:HB	1.75	0.52
1:B:963:MET:HE1	1:B:968:LYS:HE2	1.91	0.52
1:C:345:ALA:HB3	1:C:381:GLY:HA3	1.91	0.52
1:D:292:ILE:HA	1:D:415:VAL:HG21	1.92	0.52
1:A:378:ARG:HB2	1:A:414:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ARG:HB2	1:B:824:ASP:HA	1.92	0.52
1:B:177:LYS:HD2	1:B:207:VAL:HG13	1.91	0.52
1:C:543:TRP:HB3	1:C:546:LYS:HE3	1.90	0.52
1:A:263:SER:O	1:A:307:TYR:HA	2.10	0.52
1:A:362:ARG:O	1:A:365:GLN:NE2	2.38	0.52
1:A:711:LYS:HG3	1:A:810:ILE:HG12	1.92	0.52
1:B:295:LEU:HD12	1:B:415:VAL:HG22	1.91	0.52
1:D:16:TYR:O	1:D:28:ARG:NH1	2.43	0.52
1:A:277:THR:O	1:A:303:ASN:ND2	2.42	0.52
1:A:316:THR:HG23	1:A:356:GLY:HA3	1.91	0.52
1:A:966:GLU:HG2	1:A:968:LYS:HE3	1.90	0.52
1:B:364:TYR:HE2	1:B:368:LEU:HD12	1.75	0.52
1:B:628:GLY:H	1:B:636:ILE:HB	1.74	0.52
1:C:40:TRP:O	1:C:44:LEU:HD12	2.10	0.52
1:D:268:LEU:HD21	1:D:326:LEU:HD21	1.91	0.52
1:D:412:THR:O	1:D:415:VAL:HG12	2.09	0.52
1:B:123:ILE:HG12	1:B:132:VAL:HG22	1.90	0.52
1:C:625:THR:HB	1:C:688:GLY:HA2	1.92	0.52
1:A:66:ARG:NE	2:A:1201:ADP:O1B	2.43	0.52
1:D:269:LEU:HD21	1:D:753:SER:H	1.73	0.51
1:D:386:GLU:HA	1:D:389:ARG:HG2	1.92	0.51
1:A:140:VAL:HG13	2:A:1201:ADP:H5'1	1.91	0.51
1:C:500:ILE:HG12	1:C:528:ALA:HB3	1.92	0.51
1:C:586:MET:HG3	1:C:612:LYS:HD3	1.92	0.51
1:B:602:PRO:HG2	1:B:605:LEU:HD12	1.93	0.51
1:B:987:VAL:HG13	1:B:1028:LEU:HD13	1.93	0.51
1:A:1018:LYS:NZ	6:A:1205:COA:O5B	2.43	0.51
1:C:87:PRO:O	1:C:91:GLN:NE2	2.44	0.51
1:D:884:LYS:O	1:D:888:GLN:HG2	2.10	0.51
1:A:631:PRO:HG2	1:A:681:VAL:O	2.10	0.51
1:A:892:MET:HG2	1:C:863:PHE:HE1	1.76	0.51
1:D:12:LYS:HD3	1:D:217:LEU:HD11	1.92	0.51
1:B:316:THR:HG23	1:B:356:GLY:HA3	1.93	0.51
1:D:288:TYR:HE1	1:D:412:THR:HA	1.75	0.51
1:A:698:MET:HE1	1:A:727:ILE:HG13	1.93	0.51
1:A:989:ILE:HD11	1:C:860:THR:HG22	1.93	0.51
1:B:116:ALA:O	1:B:177:LYS:NZ	2.34	0.51
1:C:343:SER:HB3	1:C:669:GLU:HB2	1.93	0.51
1:C:278:MET:HE3	1:C:340:ILE:HG21	1.91	0.51
1:B:58:LYS:HG2	1:B:72:VAL:HG23	1.92	0.51
1:B:277:THR:O	1:B:303:ASN:ND2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:199:TYR:HB3	1:D:220:LYS:HB2	1.92	0.51
1:D:362:ARG:NH2	1:D:398:THR:HB	2.26	0.51
1:A:698:MET:HG2	1:A:723:GLU:OE2	2.11	0.50
1:C:962:LYS:O	1:C:966:GLU:HG3	2.11	0.50
1:D:518:VAL:HG11	1:D:643:LEU:HD11	1.93	0.50
1:A:120:TYR:HD2	1:A:203:ASN:HB2	1.76	0.50
1:A:975:HIS:HD2	1:A:978:LYS:H	1.60	0.50
1:A:1009:GLU:HA	1:A:1012:LYS:HG2	1.93	0.50
1:B:181:LEU:HD11	1:B:207:VAL:HG11	1.92	0.50
1:B:612:LYS:HA	1:B:615:GLN:HG2	1.93	0.50
1:B:902:PRO:HG3	1:D:842:THR:HG21	1.93	0.50
1:D:743:TRP:HE1	1:D:745:ILE:HD13	1.75	0.50
1:C:167:LYS:O	1:C:168:HIS:ND1	2.43	0.50
1:D:493:PHE:HB2	1:D:630:LYS:HE2	1.92	0.50
1:A:504:MET:HG2	1:A:531:TYR:CG	2.47	0.50
1:B:933:ASP:OD1	1:B:934:ARG:N	2.43	0.50
1:D:668:ASN:HA	1:D:671:ASN:HD22	1.75	0.50
1:B:408:GLU:HA	1:B:676:ARG:HH22	1.77	0.50
1:C:354:PHE:CE2	1:C:379:ARG:HG2	2.47	0.50
1:A:505:GLN:HG3	1:A:572:PHE:CG	2.47	0.50
1:A:908:HIS:CE1	1:A:912:ILE:HD11	2.47	0.50
1:B:1097:GLU:HG2	1:B:1098:HIS:N	2.27	0.50
1:C:386:GLU:O	1:C:390:VAL:HG23	2.11	0.50
1:D:32:ALA:HB3	1:D:107:ILE:HB	1.93	0.50
1:D:653:ARG:NH1	1:D:679:ASP:O	2.44	0.50
1:C:225:ALA:HB2	1:C:602:PRO:HB3	1.93	0.50
1:C:657:VAL:HG12	1:C:712:MET:HB3	1.94	0.50
1:D:66:ARG:NH1	1:D:216:ASP:OD1	2.45	0.50
1:A:288:TYR:HA	1:A:291:THR:HG22	1.93	0.49
1:A:1075:ASP:OD1	1:C:843:SER:OG	2.27	0.49
1:B:274:ARG:HG3	1:B:336:LYS:HA	1.94	0.49
1:B:865:GLU:OE1	1:B:881:ARG:NH2	2.46	0.49
1:B:690:ASP:OD1	1:B:691:ARG:N	2.44	0.49
1:D:857:MET:HE2	1:D:862:VAL:HA	1.94	0.49
1:B:317:TYR:CE1	1:B:321:LYS:HE2	2.47	0.49
1:D:909:ASN:OD1	1:D:930:THR:HG21	2.12	0.49
1:B:398:THR:HG23	1:B:400:ILE:HG12	1.94	0.49
1:C:362:ARG:O	1:C:365:GLN:NE2	2.39	0.49
1:A:66:ARG:HE	2:A:1201:ADP:PB	2.36	0.49
1:A:288:TYR:CZ	1:A:292:ILE:HD11	2.48	0.49
1:C:629:ILE:HD13	1:C:651:LEU:HD13	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:ILE:HG22	1:B:879:GLN:OE1	2.12	0.49
1:C:54:ASN:HB3	1:C:110:PHE:HB3	1.95	0.49
1:C:135:HIS:CE1	1:C:137:GLU:HB3	2.47	0.49
1:C:502:TRP:NE1	1:C:556:MET:SD	2.73	0.49
1:C:383:ASN:HB2	1:C:827:TRP:HE1	1.76	0.49
1:B:653:ARG:NH2	1:B:679:ASP:O	2.44	0.48
1:D:82:LYS:O	1:D:86:LYS:NZ	2.44	0.48
1:D:640:GLY:HA2	1:D:668:ASN:OD1	2.13	0.48
1:D:127:ARG:NH2	1:D:693:PRO:O	2.45	0.48
1:D:573:ALA:O	1:D:598:ALA:HB2	2.13	0.48
1:B:129:GLY:O	1:B:607:ARG:NH1	2.46	0.48
1:B:800:VAL:O	1:B:803:ASP:HB3	2.13	0.48
1:C:346:ASN:ND2	1:C:665:GLY:HA2	2.29	0.48
1:C:844:ILE:HG22	1:C:879:GLN:OE1	2.14	0.48
1:D:256:LEU:HA	1:D:259:LYS:HG2	1.95	0.48
1:A:405:PHE:CE2	1:A:417:MET:HG3	2.47	0.48
1:B:976:ARG:HD2	6:B:1204:COA:H2B	1.95	0.48
1:C:281:GLY:HA2	1:C:308:SER:HB3	1.95	0.48
1:D:630:LYS:HD3	1:D:683:GLU:OE1	2.13	0.48
1:D:741:VAL:HG11	1:D:797:ILE:HG12	1.95	0.48
1:A:202:ILE:HG22	1:A:205:LEU:HB2	1.94	0.48
1:A:208:THR:HG22	1:A:209:LYS:H	1.79	0.48
1:C:63:ILE:HB	1:C:66:ARG:HE	1.79	0.48
1:D:288:TYR:O	1:D:292:ILE:HG13	2.14	0.48
1:D:994:VAL:HG13	1:D:998:PHE:CD2	2.48	0.48
1:A:771:THR:O	1:A:775:LYS:HG2	2.14	0.48
1:C:986:ARG:NH1	7:C:2202:HOH:O	2.47	0.48
1:D:364:TYR:CZ	1:D:367:PRO:HG2	2.48	0.48
1:A:955:ILE:HG13	1:A:958:GLU:H	1.79	0.48
1:C:36:PRO:HG3	1:C:89:LEU:HD21	1.94	0.48
1:C:414:ILE:HA	1:C:417:MET:HE2	1.95	0.48
1:D:249:GLU:OE2	1:D:325:SER:OG	2.32	0.48
1:A:933:ASP:OD1	1:A:934:ARG:N	2.46	0.48
1:B:202:ILE:HG21	1:B:205:LEU:HD12	1.96	0.48
1:B:842:THR:HG21	1:D:902:PRO:HG3	1.96	0.48
1:C:76:LEU:HD23	1:C:81:VAL:HA	1.95	0.48
1:D:788:ARG:HG2	1:D:792:GLU:OE2	2.14	0.48
1:A:195:LEU:HD13	1:A:232:LYS:HG2	1.95	0.47
1:A:204:PRO:HB2	1:A:215:LEU:HD22	1.95	0.47
1:A:994:VAL:HG13	1:A:998:PHE:CD2	2.49	0.47
1:D:120:TYR:HB3	1:D:135:HIS:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PHE:O	1:A:150:GLN:HB3	2.14	0.47
1:A:657:VAL:HG21	1:A:678:THR:HG21	1.96	0.47
1:B:599:GLU:HG3	1:B:624:ALA:HA	1.97	0.47
1:D:18:PHE:HD2	1:D:195:LEU:HD21	1.79	0.47
1:D:340:ILE:O	1:D:377:VAL:HA	2.14	0.47
1:A:244:ARG:HE	1:A:247:TYR:HE1	1.62	0.47
1:B:255:ASP:O	1:B:259:LYS:HG2	2.13	0.47
1:C:188:LEU:HD11	1:C:202:ILE:HD12	1.95	0.47
1:A:21:THR:HG1	1:A:183:SER:HG	1.62	0.47
1:A:120:TYR:CD2	1:A:203:ASN:HB2	2.49	0.47
1:A:803:ASP:O	1:A:806:ALA:HB3	2.13	0.47
1:B:793:LEU:O	1:B:796:ILE:HG22	2.15	0.47
1:C:504:MET:HE3	1:C:531:TYR:HE1	1.79	0.47
1:D:896:VAL:HG21	1:D:990:LEU:HD11	1.95	0.47
1:A:273:GLY:HA3	1:A:302:ALA:HB2	1.96	0.47
1:A:719:ILE:HG12	1:A:749:ALA:HB2	1.97	0.47
1:A:873:LEU:HD22	1:A:890:ILE:HG21	1.96	0.47
1:B:191:PHE:CE1	1:B:195:LEU:HD12	2.49	0.47
1:B:1067:MET:HE1	1:D:869:ILE:HG23	1.96	0.47
1:C:704:TYR:O	1:C:738:LYS:NZ	2.47	0.47
1:C:963:MET:HG3	1:C:970:ILE:HG12	1.97	0.47
1:D:174:PRO:CG	1:D:177:LYS:HE3	2.44	0.47
1:D:504:MET:HG2	1:D:531:TYR:CG	2.50	0.47
1:B:345:ALA:HB3	1:B:382:PRO:HD2	1.96	0.47
1:D:173:ALA:O	1:D:178:LYS:HE3	2.15	0.47
1:A:377:VAL:HG13	1:A:404:VAL:HA	1.97	0.47
1:A:842:THR:HG21	1:C:902:PRO:HG3	1.95	0.47
1:B:59:PRO:HG3	1:B:71:LEU:HB3	1.96	0.47
1:B:630:LYS:HD2	1:B:683:GLU:HG3	1.97	0.47
1:C:354:PHE:CD1	1:C:391:MET:HE3	2.45	0.47
1:C:376:PHE:HD1	1:C:403:HIS:HB2	1.79	0.47
1:C:787:PRO:HG3	1:C:793:LEU:HA	1.97	0.47
1:B:631:PRO:HG2	1:B:681:VAL:O	2.15	0.47
1:A:307:TYR:HD2	1:A:311:PRO:HG3	1.79	0.47
1:A:771:THR:HG23	1:A:774:ALA:H	1.80	0.47
1:A:920:LEU:HD11	1:A:1070:ILE:HG23	1.97	0.47
1:B:387:GLY:HA2	1:B:390:VAL:HG12	1.96	0.47
1:C:156:VAL:HB	1:C:611:LYS:HD2	1.97	0.47
1:C:543:TRP:O	1:C:546:LYS:HG3	2.15	0.47
1:D:77:THR:O	1:D:81:VAL:HG23	2.15	0.47
1:D:111:VAL:HG11	1:D:213:TYR:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:698:MET:HE3	1:D:702:LEU:HD21	1.97	0.47
1:B:367:PRO:O	1:B:371:HIS:ND1	2.48	0.47
1:B:994:VAL:O	1:B:998:PHE:HB2	2.15	0.47
1:D:268:LEU:HD11	1:D:326:LEU:HD21	1.97	0.47
6:A:1205:COA:H71	6:A:1205:COA:N6A	2.30	0.46
1:B:33:ARG:HE	1:B:104:ASN:ND2	2.14	0.46
6:C:2102:COA:OAP	1:D:974:GLY:HA3	2.16	0.46
1:A:946:PHE:HB3	1:A:1003:LEU:HD11	1.97	0.46
1:D:1018:LYS:HE2	1:D:1020:ASN:OD1	2.16	0.46
1:A:767:GLN:HG2	1:A:769:SER:H	1.80	0.46
1:B:10:THR:HG21	1:B:236:ILE:HG13	1.98	0.46
1:B:32:ALA:HB1	1:B:43:LEU:HD21	1.97	0.46
1:B:659:TYR:HA	1:B:714:VAL:O	2.15	0.46
1:B:677:THR:HB	1:B:798:GLN:HG3	1.98	0.46
1:B:984:ASP:O	1:B:988:GLN:HG2	2.16	0.46
1:C:327:MET:HE3	1:C:336:LYS:HD3	1.97	0.46
1:D:125:ALA:HB3	1:D:198:THR:HG23	1.97	0.46
1:D:336:LYS:O	1:D:373:VAL:HA	2.15	0.46
1:D:719:ILE:HG13	1:D:763:ALA:HA	1.97	0.46
1:C:666:MET:SD	1:C:716:LEU:HD23	2.55	0.46
1:C:685:VAL:HG11	1:C:700:HIS:CE1	2.50	0.46
1:C:835:ARG:NH2	1:D:824:ASP:OD1	2.49	0.46
1:C:908:HIS:O	1:C:912:ILE:HG12	2.16	0.46
1:B:42:ARG:NH1	1:B:43:LEU:HB2	2.30	0.46
1:B:582:THR:HG22	1:B:586:MET:HE3	1.96	0.46
1:C:664:GLY:O	1:C:667:SER:OG	2.24	0.46
1:D:505:GLN:HG3	1:D:572:PHE:CG	2.50	0.46
1:D:749:ALA:HA	1:D:755:GLU:HG3	1.98	0.46
1:A:131:TYR:CE1	1:A:153:LEU:HD13	2.51	0.46
1:C:712:MET:HE1	1:C:797:ILE:HG23	1.96	0.46
1:A:1063:LEU:HD21	1:C:1067:MET:HG2	1.97	0.46
1:B:390:VAL:O	1:B:393:GLU:HG3	2.16	0.46
1:C:529:MET:HB3	1:C:552:VAL:HG22	1.97	0.46
1:C:731:ILE:HG13	1:C:736:LEU:HD12	1.97	0.46
1:D:152:LEU:HD23	1:D:169:LEU:HD12	1.98	0.46
1:A:659:TYR:CE1	1:A:684:GLY:HA3	2.51	0.46
1:B:389:ARG:NH1	1:B:390:VAL:HB	2.31	0.46
1:C:582:THR:O	1:C:586:MET:HG2	2.16	0.46
1:D:87:PRO:O	1:D:91:GLN:NE2	2.48	0.46
1:D:330:GLU:HG3	1:D:336:LYS:HZ1	1.80	0.46
1:B:955:ILE:HG13	1:B:958:GLU:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:677:THR:HB	1:C:798:GLN:HB2	1.98	0.46
1:A:10:THR:HG21	1:A:236:ILE:HG13	1.98	0.46
1:A:66:ARG:N	2:A:1201:ADP:O2B	2.49	0.46
1:A:865:GLU:OE1	1:A:881:ARG:NH1	2.50	0.46
1:B:10:THR:HA	1:B:13:GLU:HG2	1.98	0.46
1:D:337:ILE:HD12	1:D:339:ILE:HD11	1.97	0.46
1:A:780:LYS:HE3	1:A:786:VAL:HG13	1.98	0.45
1:B:42:ARG:HA	1:B:45:GLN:HE22	1.81	0.45
1:B:290:ASP:OD2	1:B:747:THR:N	2.40	0.45
1:B:543:TRP:HB2	1:B:548:ILE:HD13	1.98	0.45
1:B:925:THR:HG23	1:D:925:THR:HG23	1.99	0.45
1:B:17:LYS:HB2	1:B:18:PHE:CD1	2.51	0.45
1:B:368:LEU:HD23	1:B:371:HIS:HB2	1.96	0.45
1:B:500:ILE:O	1:B:569:LEU:HD12	2.16	0.45
1:C:711:LYS:HG3	1:C:810:ILE:HG12	1.98	0.45
1:D:646:ILE:HG23	1:D:651:LEU:HB2	1.97	0.45
1:D:715:VAL:HB	1:D:742:CYS:HB2	1.98	0.45
1:A:195:LEU:HD23	1:A:197:PHE:CZ	2.52	0.45
1:A:288:TYR:CZ	1:A:339:ILE:HG21	2.52	0.45
1:B:379:ARG:HG3	1:B:379:ARG:HH11	1.82	0.45
1:B:622:GLY:HA3	1:B:694:GLY:H	1.80	0.45
1:C:975:HIS:CD2	1:C:976:ARG:H	2.34	0.45
1:B:713:ILE:HB	1:B:740:ILE:HG12	1.98	0.45
1:C:825:TYR:OH	1:C:829:ARG:NH1	2.49	0.45
1:D:317:TYR:HE1	1:D:359:ARG:NH1	2.15	0.45
1:A:518:VAL:HG11	1:A:643:LEU:HD11	1.97	0.45
1:A:787:PRO:HB2	1:A:792:GLU:HG3	1.98	0.45
1:B:726:LYS:HG2	1:B:729:ARG:NH1	2.31	0.45
1:B:920:LEU:HD11	1:B:1070:ILE:HG23	1.97	0.45
1:C:82:LYS:O	1:C:86:LYS:HG2	2.17	0.45
1:C:414:ILE:HG22	1:C:417:MET:HE2	1.98	0.45
1:C:532:PRO:O	1:C:554:LYS:HG3	2.16	0.45
1:D:173:ALA:H	1:D:178:LYS:HE3	1.82	0.45
1:D:384:TYR:CE2	1:D:385:GLN:NE2	2.80	0.45
1:D:386:GLU:O	1:D:390:VAL:HG22	2.17	0.45
1:D:488:LYS:HZ1	1:D:614:ASP:HA	1.81	0.45
1:D:498:LYS:HB3	1:D:527:ALA:HB2	1.99	0.45
1:C:320:ALA:HB2	1:C:357:ILE:HG22	1.98	0.45
1:D:411:MET:HE1	1:D:666:MET:HE1	1.99	0.45
1:D:705:GLN:NE2	1:D:737:THR:OG1	2.41	0.45
1:B:802:GLU:HA	1:B:805:VAL:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HA	1:C:239:PRO:HD2	1.99	0.45
1:C:279:VAL:HG22	1:C:341:GLY:H	1.82	0.45
1:C:324:LEU:HD11	1:C:361:ILE:HG22	1.98	0.45
1:D:661:SER:OG	1:D:662:ARG:N	2.50	0.45
1:D:718:GLU:N	1:D:718:GLU:OE1	2.50	0.45
1:A:844:ILE:HG22	1:A:879:GLN:OE1	2.17	0.45
1:B:314:GLN:O	1:B:317:TYR:HB3	2.17	0.45
1:B:666:MET:HB3	1:B:716:LEU:HD23	1.99	0.45
1:B:707:THR:O	1:B:738:LYS:NZ	2.48	0.45
1:C:186:SER:O	1:C:190:ASN:ND2	2.34	0.45
1:D:955:ILE:HG13	1:D:958:GLU:H	1.82	0.45
1:A:887:CYS:O	1:A:891:GLU:HG3	2.17	0.44
1:B:170:LEU:HB3	1:B:178:LYS:HE3	1.98	0.44
1:B:963:MET:HG3	1:B:970:ILE:HG12	1.99	0.44
1:C:54:ASN:OD1	1:C:55:LEU:N	2.46	0.44
1:C:297:GLY:HA2	1:C:300:GLU:HG2	1.99	0.44
1:C:405:PHE:CD2	1:C:409:THR:HG21	2.52	0.44
1:C:827:TRP:O	1:C:831:LEU:HG	2.16	0.44
1:D:278:MET:HB3	1:D:340:ILE:HG22	1.99	0.44
1:D:1001:THR:HB	1:D:1004:LEU:HB3	1.99	0.44
1:A:823:MET:HB3	1:B:834:ILE:HD13	1.99	0.44
1:B:26:GLN:HG2	1:B:213:TYR:HE1	1.81	0.44
1:C:163:GLU:O	1:C:167:LYS:HG2	2.17	0.44
1:C:513:LEU:HG	1:C:517:TYR:HE2	1.83	0.44
1:A:578:ALA:O	1:A:582:THR:OG1	2.27	0.44
1:A:851:GLU:OE2	1:A:860:THR:HG23	2.16	0.44
1:A:956:PRO:HD3	1:A:1006:TYR:CE1	2.52	0.44
1:B:727:ILE:O	1:B:731:ILE:HG13	2.17	0.44
1:D:301:LEU:HD23	1:D:752:PHE:HZ	1.82	0.44
1:D:704:TYR:HB3	1:D:710:VAL:HG11	1.98	0.44
1:A:8:GLU:O	1:A:12:LYS:HG2	2.17	0.44
1:B:339:ILE:HD13	1:B:376:PHE:HB2	2.00	0.44
1:B:524:PRO:HG3	1:B:543:TRP:CE3	2.53	0.44
1:D:731:ILE:HD12	1:D:740:ILE:HD12	1.99	0.44
1:D:787:PRO:HG3	1:D:796:ILE:CD1	2.46	0.44
1:A:30:LYS:HG3	1:A:109:PRO:HD3	2.00	0.44
1:B:631:PRO:HD2	1:B:682:TYR:O	2.17	0.44
1:D:326:LEU:HA	1:D:329:ARG:NH1	2.31	0.44
1:D:630:LYS:HG3	1:D:682:TYR:O	2.18	0.44
1:D:940:ASP:OD1	1:D:944:LYS:NZ	2.51	0.44
1:A:255:ASP:O	1:A:259:LYS:HG2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLU:HA	1:A:389:ARG:HG2	1.99	0.44
1:A:725:TYR:CE1	1:A:775:LYS:HD2	2.52	0.44
1:A:741:VAL:HG23	1:A:785:PHE:O	2.18	0.44
1:B:11:GLY:HA3	1:B:217:LEU:HD11	1.99	0.44
1:B:385:GLN:HG2	1:B:386:GLU:N	2.33	0.44
1:B:586:MET:HE2	1:B:620:ILE:HD11	2.00	0.44
1:B:873:LEU:HD22	1:B:890:ILE:HG21	1.99	0.44
1:A:825:TYR:OH	1:A:836:LYS:HE2	2.18	0.44
1:A:939:LEU:HD22	1:A:1061:PHE:HB2	2.00	0.44
1:A:945:MET:HE1	1:A:970:ILE:HA	1.99	0.44
1:A:1005:ASP:O	1:A:1009:GLU:OE1	2.35	0.44
1:B:968:LYS:HE2	1:B:968:LYS:HB2	1.76	0.44
1:C:339:ILE:HD13	1:C:376:PHE:HB2	2.00	0.44
1:C:386:GLU:O	1:C:389:ARG:HG3	2.18	0.44
6:C:2102:COA:H62	1:D:971:MET:HA	2.00	0.44
1:D:184:PHE:CE2	1:D:205:LEU:HD11	2.53	0.44
1:A:84:TRP:HE3	1:A:85:LEU:HD22	1.82	0.44
1:B:742:CYS:HB3	1:B:784:VAL:HG11	2.00	0.44
1:C:162:PRO:HA	1:C:165:ILE:HD12	1.99	0.44
1:D:529:MET:O	1:D:552:VAL:HA	2.17	0.44
1:A:678:THR:HG23	1:A:801:TYR:CD1	2.52	0.44
1:B:36:PRO:HG2	1:B:103:LYS:HA	1.99	0.44
1:C:674:ILE:O	1:C:678:THR:N	2.50	0.44
1:B:255:ASP:OD1	1:B:259:LYS:HE3	2.18	0.43
1:B:362:ARG:O	1:B:365:GLN:NE2	2.49	0.43
1:C:66:ARG:NH1	1:C:216:ASP:OD2	2.51	0.43
1:C:135:HIS:NE2	1:C:148:LYS:HE3	2.33	0.43
1:C:289:SER:HA	1:C:292:ILE:HG12	2.00	0.43
1:C:892:MET:HA	1:C:895:MET:HE3	1.99	0.43
1:A:823:MET:HE3	1:A:827:TRP:CD1	2.52	0.43
1:A:902:PRO:HG3	1:C:842:THR:HG21	2.00	0.43
1:C:518:VAL:HA	1:C:819:PRO:HD2	1.99	0.43
1:D:203:ASN:HA	1:D:204:PRO:HA	1.75	0.43
1:A:659:TYR:HA	1:A:714:VAL:O	2.17	0.43
1:A:974:GLY:HA2	1:A:1021:LEU:HA	1.99	0.43
1:B:331:LYS:HZ2	1:B:371:HIS:HA	1.82	0.43
1:C:123:ILE:HG23	1:C:132:VAL:HG12	2.00	0.43
1:D:390:VAL:HA	1:D:393:GLU:HG3	2.00	0.43
1:D:980:ILE:C	1:D:982:ASN:H	2.25	0.43
1:A:111:VAL:HG21	1:A:213:TYR:CE2	2.53	0.43
1:B:35:THR:HG22	1:B:37:ASP:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:HIS:CD2	1:B:424:ILE:HG21	2.53	0.43
1:D:556:MET:O	1:D:560:MET:HG2	2.18	0.43
1:D:628:GLY:H	1:D:636:ILE:HB	1.84	0.43
1:A:858:PRO:HD2	1:A:861:GLU:OE1	2.18	0.43
1:B:131:TYR:CE1	1:B:153:LEU:HD13	2.53	0.43
1:C:208:THR:HG22	1:C:209:LYS:N	2.34	0.43
1:C:892:MET:O	1:C:896:VAL:HG23	2.18	0.43
1:D:358:VAL:O	1:D:362:ARG:HG2	2.19	0.43
1:B:119:PHE:CD2	1:B:181:LEU:HD21	2.53	0.43
1:B:678:THR:HG23	1:B:801:TYR:CD1	2.54	0.43
1:C:287:VAL:HG22	1:C:745:ILE:HG21	2.00	0.43
1:C:310:ALA:H	1:C:348:THR:HG22	1.83	0.43
1:C:539:GLN:HB3	1:C:550:ILE:CG2	2.48	0.43
1:C:971:MET:HA	6:C:2101:COA:H62	2.00	0.43
1:D:771:THR:O	1:D:775:LYS:HG2	2.18	0.43
1:A:925:THR:HG23	1:C:925:THR:CG2	2.47	0.43
1:A:1001:THR:HB	1:A:1004:LEU:HB3	1.99	0.43
1:B:215:LEU:HD22	2:B:1201:ADP:N6	2.32	0.43
1:B:685:VAL:HG11	1:B:700:HIS:CD2	2.54	0.43
1:B:1072:HIS:O	1:B:1076:GLN:HG2	2.18	0.43
1:C:34:VAL:HG12	1:C:43:LEU:HD11	1.99	0.43
1:C:376:PHE:CD1	1:C:403:HIS:HB2	2.53	0.43
1:C:499:ALA:N	1:C:525:SER:O	2.51	0.43
1:D:192:TYR:CD1	1:D:197:PHE:HB2	2.53	0.43
1:A:873:LEU:HD22	1:A:890:ILE:HD13	2.01	0.43
1:B:417:MET:HB3	1:B:424:ILE:HG13	2.01	0.43
1:C:120:TYR:CZ	1:C:145:VAL:HG11	2.54	0.43
1:C:163:GLU:HB2	1:C:167:LYS:NZ	2.33	0.43
1:B:165:ILE:HD13	1:B:169:LEU:HD12	2.01	0.43
1:B:278:MET:HG2	1:B:319:TYR:CE2	2.53	0.43
1:B:358:VAL:HA	1:B:361:ILE:HG12	2.01	0.43
1:D:122:CYS:O	1:D:132:VAL:HA	2.19	0.43
1:D:692:TYR:O	1:D:693:PRO:C	2.61	0.43
1:A:636:ILE:O	1:A:639:THR:HG23	2.18	0.43
1:B:794:GLY:HA2	1:B:797:ILE:HD12	2.00	0.43
1:C:58:LYS:NZ	1:C:108:GLU:OE2	2.51	0.43
1:A:56:VAL:HG21	2:A:1201:ADP:C6	2.54	0.42
1:C:595:ALA:HA	1:C:621:ILE:HB	2.00	0.42
1:D:55:LEU:HD23	1:D:56:VAL:N	2.33	0.42
1:D:659:TYR:CE1	1:D:684:GLY:HA3	2.54	0.42
1:A:398:THR:HG23	1:A:400:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:MET:CG	1:A:726:LYS:HD2	2.49	0.42
1:A:698:MET:HG3	1:A:726:LYS:HD2	2.02	0.42
1:A:969:LEU:HD22	6:A:1205:COA:C4A	2.48	0.42
1:B:117:GLU:O	1:B:206:VAL:HA	2.19	0.42
1:B:512:MET:HE2	1:B:637:GLY:N	2.32	0.42
1:B:714:VAL:HA	1:B:741:VAL:O	2.19	0.42
1:C:286:VAL:HG22	1:C:304:TYR:OH	2.19	0.42
1:D:50:LEU:HD23	1:D:50:LEU:H	1.84	0.42
1:D:97:LYS:NZ	1:D:753:SER:HA	2.34	0.42
1:A:206:VAL:HG23	1:A:213:TYR:HB2	2.02	0.42
1:A:912:ILE:HD13	1:B:908:HIS:HD2	1.84	0.42
1:B:742:CYS:O	1:B:786:VAL:HG23	2.19	0.42
1:C:160:LEU:HG	1:C:165:ILE:HD11	2.00	0.42
1:A:54:ASN:HD21	1:A:75:ASN:HA	1.85	0.42
1:A:310:ALA:N	1:A:348:THR:HG22	2.33	0.42
1:A:579:TYR:CD1	1:A:605:LEU:HB3	2.55	0.42
1:A:631:PRO:HD2	1:A:682:TYR:O	2.19	0.42
1:C:822:PRO:HB2	1:D:835:ARG:HG3	2.00	0.42
1:D:127:ARG:HH12	1:D:693:PRO:HD2	1.83	0.42
1:A:174:PRO:O	1:A:178:LYS:HG3	2.20	0.42
1:A:232:LYS:HB2	1:A:232:LYS:HE3	1.82	0.42
1:A:382:PRO:HB3	1:A:642:MET:HE3	2.01	0.42
1:A:699:ASP:O	1:A:703:ARG:HG3	2.19	0.42
1:B:384:TYR:O	1:B:388:LEU:N	2.46	0.42
1:C:857:MET:HG2	1:C:862:VAL:HG23	2.01	0.42
1:D:332:HIS:CE1	1:D:334:ASP:HB3	2.54	0.42
1:A:54:ASN:HB3	1:A:110:PHE:HB3	2.02	0.42
1:A:118:GLU:OE2	1:A:204:PRO:HB3	2.19	0.42
1:A:567:ASP:OD1	1:A:567:ASP:N	2.53	0.42
1:B:275:ILE:C	1:B:276:TRP:HD1	2.27	0.42
1:B:386:GLU:O	1:B:389:ARG:HD3	2.20	0.42
1:C:77:THR:O	1:C:81:VAL:N	2.43	0.42
1:C:1094:VAL:HG23	1:C:1094:VAL:O	2.19	0.42
1:D:174:PRO:HG2	1:D:177:LYS:HE3	2.00	0.42
1:D:290:ASP:HB2	1:D:745:ILE:HD11	2.01	0.42
1:A:30:LYS:HG2	1:A:109:PRO:HG3	2.01	0.42
1:A:35:THR:O	1:A:38:THR:HG22	2.19	0.42
1:A:280:ALA:HB3	1:A:379:ARG:NH1	2.35	0.42
1:A:493:PHE:CZ	1:A:636:ILE:HD11	2.55	0.42
1:B:66:ARG:HG2	2:B:1201:ADP:O2B	2.20	0.42
1:B:160:LEU:HD21	1:B:165:ILE:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LYS:HG3	1:B:565:GLU:HG3	2.02	0.42
1:C:292:ILE:HD11	1:C:301:LEU:HD22	2.01	0.42
1:C:604:ALA:HA	1:C:607:ARG:HE	1.85	0.42
1:D:825:TYR:OH	1:D:836:LYS:HE3	2.19	0.42
1:B:34:VAL:HG23	1:B:105:PHE:HB2	2.01	0.42
1:B:340:ILE:O	1:B:377:VAL:HA	2.20	0.42
1:C:55:LEU:HD21	1:C:107:ILE:HB	2.01	0.42
1:D:354:PHE:CZ	1:D:390:VAL:HG23	2.54	0.42
1:D:728:CYS:SG	1:D:779:LEU:HD23	2.60	0.42
1:A:411:MET:HE1	1:A:666:MET:HE1	2.01	0.42
1:A:731:ILE:HG12	1:A:736:LEU:HB2	2.01	0.42
1:B:35:THR:O	1:B:38:THR:HG22	2.20	0.42
1:B:331:LYS:NZ	1:B:371:HIS:HA	2.35	0.42
1:C:972:GLY:H	6:C:2101:COA:H62	1.85	0.42
1:D:59:PRO:HA	1:D:105:PHE:CD1	2.54	0.42
1:D:278:MET:HG3	1:D:319:TYR:CE2	2.51	0.42
1:D:422:ARG:HG3	1:D:423:PRO:HD2	2.01	0.42
1:A:215:LEU:HD23	2:A:1201:ADP:C5	2.54	0.42
1:A:698:MET:CE	1:A:727:ILE:HG13	2.50	0.42
1:A:1037:LEU:HD12	1:A:1043:PHE:CE2	2.55	0.42
1:B:661:SER:OG	1:B:662:ARG:N	2.53	0.42
1:D:131:TYR:CE1	1:D:153:LEU:HB2	2.55	0.42
1:D:857:MET:HE3	1:D:861:GLU:HG2	2.01	0.42
1:B:495:ARG:NH2	1:B:520:SER:O	2.53	0.41
1:C:123:ILE:HG12	1:C:132:VAL:HG12	2.01	0.41
1:C:918:LYS:NZ	1:D:929:LEU:O	2.46	0.41
1:D:290:ASP:OD1	1:D:748:CYS:N	2.53	0.41
1:A:653:ARG:HH12	1:A:680:GLY:HA3	1.86	0.41
1:A:678:THR:HG22	1:A:679:ASP:N	2.35	0.41
1:A:891:GLU:O	1:A:895:MET:HG3	2.19	0.41
1:A:1065:ARG:HH22	4:A:1203:FLC:HA2	1.86	0.41
1:C:388:LEU:HD11	1:C:404:VAL:HG13	2.03	0.41
1:A:255:ASP:OD1	1:A:259:LYS:HE3	2.20	0.41
1:A:392:GLY:O	1:A:396:LYS:HE3	2.20	0.41
1:A:539:GLN:HG2	1:A:541:PHE:CE2	2.56	0.41
1:A:823:MET:HE2	1:A:828:ALA:HA	2.03	0.41
1:A:945:MET:HE2	1:A:959:PHE:HZ	1.85	0.41
1:B:583:MET:SD	1:B:612:LYS:HD3	2.60	0.41
1:C:63:ILE:O	1:C:66:ARG:NH2	2.53	0.41
1:C:203:ASN:HA	1:C:204:PRO:HA	1.75	0.41
6:C:2102:COA:H2B	1:D:976:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:TRP:O	1:D:572:PHE:HB2	2.20	0.41
1:A:280:ALA:HB2	1:A:307:TYR:CZ	2.55	0.41
1:B:379:ARG:HG3	1:B:379:ARG:NH1	2.35	0.41
1:C:161:ASN:OD1	1:C:161:ASN:N	2.52	0.41
1:D:522:ASP:OD1	1:D:522:ASP:N	2.52	0.41
1:A:195:LEU:HD11	1:A:233:TRP:HD1	1.85	0.41
1:B:301:LEU:HD11	1:B:752:PHE:HZ	1.85	0.41
1:B:976:ARG:NH2	1:D:848:ARG:O	2.54	0.41
1:C:504:MET:HB3	1:C:531:TYR:CE1	2.55	0.41
1:D:215:LEU:HD22	2:D:1201:ADP:C6	2.56	0.41
1:D:801:TYR:O	1:D:805:VAL:HG23	2.20	0.41
1:D:888:GLN:HB2	1:D:993:TYR:OH	2.20	0.41
1:C:278:MET:HB3	1:C:340:ILE:HG22	2.03	0.41
1:D:541:PHE:CD2	1:D:550:ILE:HD12	2.55	0.41
1:D:851:GLU:OE2	1:D:860:THR:HG23	2.21	0.41
1:A:285:SER:HB3	1:A:306:GLU:HB3	2.03	0.41
1:A:880:LYS:HD2	1:A:1042:SER:O	2.20	0.41
1:A:1050:GLU:O	1:A:1054:ILE:HG12	2.21	0.41
1:B:138:GLY:HA2	1:B:142:VAL:HG12	2.03	0.41
1:B:974:GLY:HA2	1:B:1021:LEU:HA	2.03	0.41
1:C:560:MET:HB3	1:C:590:GLN:NE2	2.35	0.41
1:C:939:LEU:HD22	1:C:1061:PHE:HB2	2.03	0.41
1:C:1013:ILE:O	1:C:1016:SER:OG	2.26	0.41
6:C:2102:COA:H133	1:D:974:GLY:O	2.20	0.41
1:A:253:ILE:HG13	1:A:266:LEU:HB3	2.03	0.41
1:A:343:SER:HB2	1:A:669:GLU:HB2	2.03	0.41
1:B:328:THR:HB	1:B:364:TYR:OH	2.20	0.41
1:C:530:VAL:HG11	1:C:556:MET:SD	2.61	0.41
1:A:662:ARG:HD3	1:A:687:ILE:HD11	2.03	0.41
1:B:278:MET:HE3	1:B:340:ILE:HG21	2.02	0.41
1:B:290:ASP:HA	1:B:748:CYS:SG	2.61	0.41
1:B:505:GLN:HG3	1:B:572:PHE:CG	2.56	0.41
1:B:925:THR:CG2	1:D:925:THR:HG23	2.51	0.41
1:B:1050:GLU:O	1:B:1054:ILE:HG12	2.20	0.41
1:C:133:LEU:HA	1:C:150:GLN:O	2.21	0.41
1:C:134:PHE:CE2	1:C:170:LEU:HD12	2.55	0.41
1:C:204:PRO:HG2	1:C:215:LEU:HD12	2.03	0.41
1:C:823:MET:HE2	1:C:828:ALA:HA	2.02	0.41
1:D:249:GLU:HG2	1:D:322:THR:HG23	2.02	0.41
1:D:316:THR:HG23	1:D:356:GLY:HA3	2.02	0.41
1:D:613:ALA:HB1	1:D:618:VAL:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:661:SER:HB2	1:D:716:LEU:HB2	2.02	0.41
1:A:645:ASN:C	1:A:645:ASN:HD22	2.28	0.41
1:A:794:GLY:O	1:A:797:ILE:HB	2.21	0.41
1:B:279:VAL:HG11	1:B:285:SER:HA	2.02	0.41
1:B:316:THR:HG21	1:B:353:THR:HA	2.02	0.41
1:B:976:ARG:CD	6:B:1204:COA:H2B	2.51	0.41
1:D:288:TYR:CE2	1:D:292:ILE:HD11	2.56	0.41
1:B:276:TRP:CH2	1:B:327:MET:HA	2.56	0.40
1:B:1095:LEU:HD23	1:C:856:GLY:H	1.86	0.40
1:C:247:TYR:CD1	1:C:268:LEU:HD12	2.57	0.40
1:C:354:PHE:HE2	1:C:379:ARG:HG2	1.84	0.40
1:C:599:GLU:HB2	1:C:624:ALA:HA	2.03	0.40
1:C:878:PHE:HB3	1:C:1043:PHE:HE2	1.86	0.40
1:C:956:PRO:O	1:C:960:VAL:HG23	2.21	0.40
1:D:120:TYR:CE2	1:D:122:CYS:HB2	2.56	0.40
1:D:946:PHE:HB3	1:D:1003:LEU:HD11	2.03	0.40
1:A:925:THR:CG2	1:C:925:THR:HG23	2.51	0.40
1:B:85:LEU:HD12	1:B:89:LEU:HD12	2.03	0.40
1:B:354:PHE:O	1:B:358:VAL:HG22	2.21	0.40
1:C:201:GLU:HB3	1:C:218:ALA:HB3	2.02	0.40
1:C:551:PRO:HB2	1:C:553:PHE:CE1	2.56	0.40
1:C:898:ALA:HA	1:C:1064:GLY:O	2.20	0.40
1:D:291:THR:OG1	1:D:790:PHE:HB3	2.20	0.40
1:A:203:ASN:O	1:A:216:ASP:HB2	2.22	0.40
1:A:208:THR:HG22	1:A:209:LYS:N	2.35	0.40
1:A:386:GLU:O	1:A:390:VAL:HG22	2.21	0.40
1:A:1067:MET:HE1	1:C:869:ILE:HG23	2.04	0.40
1:B:51:LEU:HA	1:B:78:LEU:HD21	2.04	0.40
3:B:1202:Q5B:O11	1:D:1017:LYS:NZ	2.41	0.40
1:C:77:THR:HG22	1:C:78:LEU:N	2.36	0.40
1:C:683:GLU:CD	1:C:703:ARG:HH12	2.30	0.40
1:C:955:ILE:HG13	1:C:958:GLU:H	1.87	0.40
1:A:301:LEU:HD11	1:A:752:PHE:CZ	2.57	0.40
1:A:1067:MET:HE2	1:C:873:LEU:HD12	2.03	0.40
1:B:288:TYR:CE2	1:B:341:GLY:HA3	2.56	0.40
1:A:10:THR:HA	1:A:13:GLU:HG2	2.02	0.40
1:A:59:PRO:HG2	1:A:66:ARG:HG2	2.03	0.40
1:A:249:GLU:O	1:A:253:ILE:HG12	2.22	0.40
1:A:531:TYR:CE2	1:A:534:THR:HG23	2.56	0.40
1:A:583:MET:SD	1:A:612:LYS:HD3	2.62	0.40
1:A:898:ALA:HA	1:A:1064:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1011:GLU:HG3	1:A:1023:LEU:N	2.37	0.40
1:B:36:PRO:HB3	1:B:89:LEU:HD21	2.02	0.40
1:C:84:TRP:O	1:C:87:PRO:HD2	2.22	0.40
1:D:515:PHE:CD2	1:D:635:LYS:HB2	2.56	0.40
1:D:579:TYR:CD2	1:D:605:LEU:HB3	2.56	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	1028/1101 (93%)	994 (97%)	34 (3%)	0	100	100
1	B	1028/1101 (93%)	997 (97%)	31 (3%)	0	100	100
1	C	1028/1101 (93%)	1002 (98%)	26 (2%)	0	100	100
1	D	1026/1101 (93%)	991 (97%)	34 (3%)	1 (0%)	48	70
All	All	4110/4404 (93%)	3984 (97%)	125 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	690	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	852/908 (94%)	852 (100%)	0	100	100
1	B	852/908 (94%)	852 (100%)	0	100	100
1	C	852/908 (94%)	852 (100%)	0	100	100
1	D	851/908 (94%)	850 (100%)	1 (0%)	88	96
All	All	3407/3632 (94%)	3406 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	691	ARG

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

Mol	Chain	Res	Type
1	A	9	GLN
1	A	314	GLN
1	A	315	GLN
1	A	385	GLN
1	A	539	GLN
1	A	807	ASN
1	A	908	HIS
1	A	1024	ASN
1	A	1039	ASN
1	B	9	GLN
1	B	203	ASN
1	B	555	ASN
1	B	908	HIS
1	B	1039	ASN
1	C	115	GLN
1	C	410	HIS
1	C	645	ASN
1	C	668	ASN
1	C	988	GLN
1	C	1039	ASN
1	D	365	GLN
1	D	615	GLN
1	D	777	GLN
1	D	909	ASN
1	D	988	GLN
1	D	1039	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 2 are unknown - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	FLC	C	2103	-	12,12,12	1.10	0	17,17,17	1.32	1 (5%)
4	FLC	D	1203	-	12,12,12	1.10	0	17,17,17	1.34	1 (5%)
6	COA	C	2101	-	47,50,50	1.17	5 (10%)	69,75,75	1.49	9 (13%)
3	Q5B	A	1202	-	60,62,62	2.97	19 (31%)	87,93,93	1.73	17 (19%)
2	ADP	B	1201	-	28,29,29	1.42	4 (14%)	43,45,45	1.83	8 (18%)
2	ADP	D	1201	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
6	COA	B	1204	-	47,50,50	1.15	5 (10%)	69,75,75	1.52	9 (13%)
4	FLC	A	1203	-	12,12,12	1.10	0	17,17,17	1.37	1 (5%)
4	FLC	B	1203	-	12,12,12	1.11	0	17,17,17	1.38	1 (5%)
3	Q5B	B	1202	-	60,62,62	2.88	21 (35%)	87,93,93	1.84	22 (25%)
2	ADP	A	1201	-	28,29,29	1.43	5 (17%)	43,45,45	1.83	9 (20%)
3	Q5B	D	1202	-	60,62,62	2.97	19 (31%)	87,93,93	1.73	17 (19%)
6	COA	A	1205	-	47,50,50	1.17	5 (10%)	69,75,75	1.50	10 (14%)
6	COA	C	2102	-	47,50,50	1.16	5 (10%)	69,75,75	1.57	11 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FLC	C	2103	-	-	12/16/16/16	-
4	FLC	D	1203	-	-	7/16/16/16	-
6	COA	C	2101	-	-	9/48/64/64	0/3/3/3
3	Q5B	A	1202	-	-	20/66/83/83	0/3/3/3
2	ADP	B	1201	-	-	6/16/32/32	0/3/3/3
2	ADP	D	1201	-	-	3/16/32/32	0/3/3/3
6	COA	B	1204	-	-	16/48/64/64	0/3/3/3
4	FLC	A	1203	-	-	7/16/16/16	-
4	FLC	B	1203	-	-	2/16/16/16	-
3	Q5B	B	1202	-	-	21/66/83/83	0/3/3/3
2	ADP	A	1201	-	-	3/16/32/32	0/3/3/3
3	Q5B	D	1202	-	-	22/66/83/83	0/3/3/3
6	COA	A	1205	-	-	19/48/64/64	0/3/3/3
6	COA	C	2102	-	-	14/48/64/64	0/3/3/3

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1202	Q5B	P1-O3	9.46	1.69	1.59
3	A	1202	Q5B	P1-O3	9.38	1.69	1.59
3	B	1202	Q5B	P1-O3	8.40	1.68	1.59
3	A	1202	Q5B	P-O3	8.26	1.68	1.59
3	D	1202	Q5B	P-O3	8.20	1.68	1.59
3	B	1202	Q5B	C6-C5	-7.91	1.32	1.52
3	D	1202	Q5B	C6-C5	-7.91	1.32	1.52
3	A	1202	Q5B	C6-C5	-7.90	1.32	1.52
3	D	1202	Q5B	C18-N6	7.33	1.50	1.33
3	A	1202	Q5B	C7-C6	7.33	1.69	1.53
3	A	1202	Q5B	C18-N6	7.33	1.50	1.33
3	B	1202	Q5B	C7-C6	7.26	1.68	1.53
3	B	1202	Q5B	P-O3	7.26	1.67	1.59
3	D	1202	Q5B	C7-C6	7.24	1.68	1.53
3	B	1202	Q5B	C18-N6	7.17	1.50	1.33
3	D	1202	Q5B	C15-N5	6.69	1.49	1.33
3	A	1202	Q5B	C15-N5	6.65	1.49	1.33
3	B	1202	Q5B	C15-N5	6.52	1.48	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1201	ADP	C5-C4	4.75	1.47	1.39
2	A	1201	ADP	C5-C4	4.74	1.47	1.39
2	B	1201	ADP	C5-C4	4.69	1.47	1.39
6	A	1205	COA	C5A-C4A	4.47	1.47	1.39
6	B	1204	COA	C5A-C4A	4.28	1.46	1.39
6	C	2101	COA	C5A-C4A	4.27	1.46	1.39
3	D	1202	Q5B	O7-C5	4.19	1.54	1.45
3	A	1202	Q5B	O7-C5	4.16	1.54	1.45
6	C	2102	COA	C5A-C4A	4.12	1.46	1.39
3	B	1202	Q5B	O7-C5	3.87	1.53	1.45
3	D	1202	Q5B	C21-S	3.73	1.85	1.76
3	B	1202	Q5B	C21-S	3.68	1.84	1.76
3	A	1202	Q5B	C21-S	3.67	1.84	1.76
3	B	1202	Q5B	O20-C23	-3.34	1.36	1.43
3	B	1202	Q5B	C9-N	-3.32	1.31	1.37
3	A	1202	Q5B	P2-O9	3.29	1.65	1.59
3	D	1202	Q5B	P2-O9	3.28	1.65	1.59
3	A	1202	Q5B	O20-C23	-3.23	1.37	1.43
3	D	1202	Q5B	C22-C23	3.14	1.57	1.54
3	D	1202	Q5B	O20-C23	-3.14	1.37	1.43
3	A	1202	Q5B	C22-C23	3.08	1.57	1.54
3	B	1202	Q5B	O13-C15	-2.94	1.17	1.23
3	B	1202	Q5B	P2-O9	2.82	1.64	1.59
2	A	1201	ADP	C5-C6	2.76	1.48	1.41
3	B	1202	Q5B	C23-C26	-2.75	1.50	1.53
3	A	1202	Q5B	C9-N	-2.75	1.32	1.37
2	B	1201	ADP	C5-C6	2.74	1.48	1.41
3	D	1202	Q5B	C9-N	-2.71	1.32	1.37
3	B	1202	Q5B	C22-C23	2.71	1.57	1.54
2	D	1201	ADP	C5-C6	2.70	1.48	1.41
6	C	2102	COA	C5A-C6A	2.63	1.48	1.41
3	D	1202	Q5B	O14-C18	-2.62	1.18	1.23
3	B	1202	Q5B	O14-C18	-2.61	1.18	1.23
3	A	1202	Q5B	O14-C18	-2.60	1.18	1.23
6	C	2101	COA	C5A-C6A	2.58	1.48	1.41
3	A	1202	Q5B	O13-C15	-2.57	1.18	1.23
3	D	1202	Q5B	C22-C21	2.55	1.56	1.51
3	D	1202	Q5B	O13-C15	-2.55	1.18	1.23
3	A	1202	Q5B	C22-C21	2.55	1.56	1.51
6	C	2102	COA	C5A-N7A	-2.51	1.34	1.39
6	B	1204	COA	C5A-N7A	-2.50	1.34	1.39
6	A	1205	COA	C5A-C6A	2.50	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1205	COA	C5A-N7A	-2.49	1.34	1.39
3	A	1202	Q5B	C2-C1	2.47	1.58	1.53
3	B	1202	Q5B	C-C1	-2.47	1.48	1.53
6	C	2101	COA	C5A-N7A	-2.46	1.34	1.39
3	D	1202	Q5B	C2-C1	2.45	1.58	1.53
6	B	1204	COA	C5A-C6A	2.42	1.47	1.41
2	B	1201	ADP	C8-N7	2.40	1.36	1.31
3	B	1202	Q5B	C2-C1	2.37	1.58	1.53
3	A	1202	Q5B	C23-C26	-2.36	1.51	1.53
3	D	1202	Q5B	C23-C26	-2.36	1.51	1.53
2	D	1201	ADP	C5-N7	-2.35	1.34	1.39
2	A	1201	ADP	C8-N7	2.32	1.36	1.31
3	B	1202	Q5B	C22-C21	2.31	1.55	1.51
2	B	1201	ADP	C5-N7	-2.31	1.34	1.39
2	A	1201	ADP	C5-N7	-2.30	1.34	1.39
2	D	1201	ADP	C8-N7	2.28	1.36	1.31
3	D	1202	Q5B	C13-N4	2.26	1.40	1.34
3	D	1202	Q5B	P1-O6	2.24	1.68	1.59
3	A	1202	Q5B	C13-N4	2.24	1.39	1.34
3	A	1202	Q5B	P1-O6	2.18	1.67	1.59
6	A	1205	COA	C8A-N7A	2.17	1.35	1.31
6	B	1204	COA	C4A-N9A	-2.15	1.33	1.37
6	A	1205	COA	C4A-N9A	-2.13	1.33	1.37
6	C	2102	COA	C4A-N9A	-2.12	1.33	1.37
6	C	2101	COA	C8A-N7A	2.12	1.35	1.31
3	B	1202	Q5B	C13-N3	-2.12	1.29	1.35
6	C	2101	COA	C4A-N9A	-2.10	1.33	1.37
3	B	1202	Q5B	O-C3	-2.07	1.37	1.43
2	A	1201	ADP	PA-O3A	2.05	1.61	1.59
6	B	1204	COA	C8A-N7A	2.04	1.35	1.31
3	B	1202	Q5B	P1-O6	2.01	1.67	1.59
6	C	2102	COA	C8A-N7A	2.01	1.35	1.31

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	ADP	C5-C4-N3	-5.98	118.48	126.72
2	D	1201	ADP	C5-C4-N3	-5.94	118.54	126.72
2	B	1201	ADP	C5-C4-N3	-5.81	118.72	126.72
6	A	1205	COA	C5A-C4A-N3A	-5.77	118.77	126.72
3	B	1202	Q5B	N3-C12-N2	-5.76	119.86	128.58
6	C	2102	COA	C5A-C4A-N3A	-5.67	118.91	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2101	COA	C5A-C4A-N3A	-5.61	118.99	126.72
3	D	1202	Q5B	C10-C11-N2	-5.56	119.07	126.72
6	B	1204	COA	C5A-C4A-N3A	-5.55	119.08	126.72
3	A	1202	Q5B	C10-C11-N2	-5.54	119.09	126.72
3	A	1202	Q5B	N3-C12-N2	-5.17	120.76	128.58
3	A	1202	Q5B	C22-C21-S	5.13	120.03	113.56
3	D	1202	Q5B	N3-C12-N2	-5.07	120.90	128.58
3	D	1202	Q5B	C22-C21-S	5.01	119.88	113.56
3	B	1202	Q5B	C22-C21-S	4.74	119.54	113.56
2	A	1201	ADP	N3-C4-N9	4.73	135.21	127.17
2	D	1201	ADP	N3-C4-N9	4.66	135.09	127.17
3	B	1202	Q5B	C10-C11-N2	-4.63	120.34	126.72
6	A	1205	COA	N3A-C4A-N9A	4.58	134.96	127.17
2	B	1201	ADP	N3-C4-N9	4.51	134.83	127.17
6	C	2101	COA	N3A-C4A-N9A	4.46	134.74	127.17
6	B	1204	COA	N3A-C4A-N9A	4.45	134.74	127.17
6	C	2102	COA	N3A-C4A-N9A	4.44	134.71	127.17
3	D	1202	Q5B	N2-C11-N	4.23	134.35	127.17
3	A	1202	Q5B	N2-C11-N	4.20	134.31	127.17
3	A	1202	Q5B	C12-N2-C11	4.18	122.05	111.83
3	D	1202	Q5B	C12-N2-C11	4.16	121.98	111.83
3	B	1202	Q5B	C11-N-C9	4.12	110.06	105.74
3	B	1202	Q5B	C12-N2-C11	4.08	121.80	111.83
3	B	1202	Q5B	N2-C11-N	3.89	133.78	127.17
6	C	2102	COA	C4A-C5A-N7A	-3.85	106.18	110.58
6	C	2102	COA	C2A-N3A-C4A	3.83	121.17	111.83
3	B	1202	Q5B	N-C9-N1	-3.75	108.61	113.94
6	C	2101	COA	C2A-N3A-C4A	3.74	120.97	111.83
2	A	1201	ADP	C2-N3-C4	3.71	120.90	111.83
3	A	1202	Q5B	C16-C17-C18	3.67	118.51	112.39
2	B	1201	ADP	C2-N3-C4	3.66	120.78	111.83
4	B	1203	FLC	OB2-CBC-CB	3.66	120.16	113.14
2	D	1201	ADP	C2-N3-C4	3.64	120.71	111.83
4	A	1203	FLC	OB2-CBC-CB	3.63	120.10	113.14
6	C	2102	COA	N3A-C2A-N1A	-3.61	123.11	128.58
6	A	1205	COA	C2A-N3A-C4A	3.61	120.66	111.83
3	D	1202	Q5B	O19-C26-C23	3.59	120.03	113.14
3	D	1202	Q5B	C16-C17-C18	3.59	118.37	112.39
6	B	1204	COA	C2A-N3A-C4A	3.59	120.59	111.83
4	D	1203	FLC	OB2-CBC-CB	3.58	120.02	113.14
4	C	2103	FLC	OB2-CBC-CB	3.58	120.01	113.14
3	A	1202	Q5B	O19-C26-C23	3.58	120.01	113.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	ADP	C4-C5-N7	-3.56	106.51	110.58
2	D	1201	ADP	C4-C5-N7	-3.56	106.51	110.58
6	C	2101	COA	C4A-C5A-N7A	-3.54	106.53	110.58
6	B	1204	COA	C4A-C5A-N7A	-3.51	106.57	110.58
2	A	1201	ADP	C4-C5-N7	-3.51	106.57	110.58
6	C	2101	COA	N3A-C2A-N1A	-3.46	123.34	128.58
3	B	1202	Q5B	C16-C17-C18	3.45	118.13	112.39
6	A	1205	COA	C4A-C5A-N7A	-3.39	106.71	110.58
6	B	1204	COA	N3A-C2A-N1A	-3.29	123.59	128.58
3	B	1202	Q5B	O7-C8-N	3.18	114.19	108.09
2	B	1201	ADP	N3-C2-N1	-3.13	123.84	128.58
6	A	1205	COA	N3A-C2A-N1A	-3.13	123.84	128.58
2	A	1201	ADP	N3-C2-N1	-3.08	123.92	128.58
3	B	1202	Q5B	O19-C26-C23	3.05	119.00	113.14
6	C	2102	COA	C4A-N9A-C8A	3.04	108.93	105.74
2	D	1201	ADP	N3-C2-N1	-3.01	124.03	128.58
6	B	1204	COA	C4A-N9A-C8A	2.95	108.84	105.74
6	C	2101	COA	C4A-N9A-C8A	2.93	108.81	105.74
6	C	2102	COA	C5A-N7A-C8A	2.92	108.04	103.45
3	D	1202	Q5B	N-C9-N1	-2.88	109.86	113.94
3	A	1202	Q5B	N-C9-N1	-2.86	109.88	113.94
3	B	1202	Q5B	C-C1-C14	2.84	113.61	108.77
3	B	1202	Q5B	C20-S-C21	2.75	109.98	101.84
6	A	1205	COA	C4A-N9A-C8A	2.73	108.61	105.74
3	A	1202	Q5B	C11-C10-N1	-2.72	107.47	110.58
3	B	1202	Q5B	C10-N1-C9	2.71	107.71	103.45
3	D	1202	Q5B	C10-N1-C9	2.71	107.71	103.45
3	D	1202	Q5B	C11-C10-N1	-2.70	107.49	110.58
3	A	1202	Q5B	C10-N1-C9	2.69	107.68	103.45
6	C	2101	COA	C5A-N7A-C8A	2.65	107.62	103.45
2	D	1201	ADP	C5-N7-C8	2.64	107.59	103.45
6	B	1204	COA	C5A-N7A-C8A	2.62	107.56	103.45
2	A	1201	ADP	C5-N7-C8	2.57	107.50	103.45
2	B	1201	ADP	C5-N7-C8	2.57	107.49	103.45
2	B	1201	ADP	C4-N9-C8	2.56	108.43	105.74
2	A	1201	ADP	C4-N9-C8	2.55	108.41	105.74
3	B	1202	Q5B	O15-C21-C22	-2.54	119.77	123.66
6	A	1205	COA	C5A-N7A-C8A	2.51	107.39	103.45
6	C	2102	COA	C7P-C6P-C5P	-2.51	108.22	112.39
3	D	1202	Q5B	C11-N-C9	2.50	108.37	105.74
3	A	1202	Q5B	C11-N-C9	2.50	108.36	105.74
2	A	1201	ADP	C3'-C2'-C1'	2.49	106.18	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	Q5B	C11-C10-N1	-2.49	107.74	110.58
2	D	1201	ADP	C4-N9-C8	2.48	108.34	105.74
6	C	2102	COA	C6A-C5A-N7A	2.46	136.83	132.09
6	C	2102	COA	N9A-C8A-N7A	-2.44	110.47	113.94
3	D	1202	Q5B	C20-S-C21	2.44	109.04	101.84
3	A	1202	Q5B	C20-S-C21	2.43	109.03	101.84
3	B	1202	Q5B	C14-C15-N5	2.37	120.98	116.48
3	B	1202	Q5B	C13-C10-N1	2.35	136.62	132.09
3	A	1202	Q5B	O15-C21-C22	-2.34	120.07	123.66
3	D	1202	Q5B	O15-C21-C22	-2.32	120.11	123.66
3	A	1202	Q5B	C-C1-C14	2.31	112.70	108.77
6	C	2101	COA	C6A-C5A-N7A	2.31	136.54	132.09
2	D	1201	ADP	C3'-C2'-C1'	2.28	105.78	101.46
6	A	1205	COA	C7P-C6P-C5P	-2.27	108.62	112.39
3	D	1202	Q5B	C-C1-C14	2.23	112.57	108.77
6	C	2101	COA	N9A-C8A-N7A	-2.23	110.77	113.94
3	D	1202	Q5B	O7-C8-N	2.22	112.35	108.09
6	B	1204	COA	C6A-C5A-N7A	2.20	136.33	132.09
3	A	1202	Q5B	O15-C21-S	-2.19	119.90	122.68
6	B	1204	COA	N9A-C8A-N7A	-2.18	110.85	113.94
2	B	1201	ADP	C6-C5-N7	2.13	136.19	132.09
3	B	1202	Q5B	C11-N-C8	-2.12	121.67	126.63
3	D	1202	Q5B	C17-C18-N6	2.11	120.19	116.34
3	D	1202	Q5B	O15-C21-S	-2.10	120.01	122.68
6	C	2102	COA	C2A-N1A-C6A	2.09	122.17	118.73
6	A	1205	COA	C6A-C5A-N7A	2.08	136.09	132.09
3	B	1202	Q5B	C17-C18-N6	2.06	120.11	116.34
3	B	1202	Q5B	O13-C15-N5	-2.06	118.62	122.98
6	A	1205	COA	N9A-C8A-N7A	-2.06	111.02	113.94
3	A	1202	Q5B	C14-C15-N5	2.04	120.35	116.48
2	A	1201	ADP	C6-C5-N7	2.03	136.01	132.09
3	B	1202	Q5B	C19-N6-C18	-2.03	119.04	122.82
3	A	1202	Q5B	C17-C18-N6	2.02	120.03	116.34
3	B	1202	Q5B	O7-C8-C7	-2.01	102.31	106.62
2	D	1201	ADP	C6-C5-N7	2.00	135.96	132.09

There are no chirality outliers.

All (161) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	ADP	O4'-C4'-C5'-O5'
2	B	1201	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	1201	ADP	C5'-O5'-PA-O3A
2	B	1201	ADP	O4'-C4'-C5'-O5'
2	B	1201	ADP	C3'-C4'-C5'-O5'
2	D	1201	ADP	C5'-O5'-PA-O3A
3	A	1202	Q5B	C3-O-P-O1
3	A	1202	Q5B	C3-O-P-O3
3	A	1202	Q5B	C-C1-C14-C15
3	A	1202	Q5B	C-C1-C14-O21
3	A	1202	Q5B	C2-C1-C14-C15
3	A	1202	Q5B	C2-C1-C14-O21
3	A	1202	Q5B	C3-C1-C14-C15
3	A	1202	Q5B	C3-C1-C14-O21
3	A	1202	Q5B	C14-C15-N5-C16
3	B	1202	Q5B	C3-O-P-O3
3	B	1202	Q5B	C-C1-C14-C15
3	B	1202	Q5B	C-C1-C14-O21
3	B	1202	Q5B	C2-C1-C14-C15
3	B	1202	Q5B	C2-C1-C14-O21
3	B	1202	Q5B	C3-C1-C14-C15
3	B	1202	Q5B	C3-C1-C14-O21
3	B	1202	Q5B	C-C1-C3-O
3	B	1202	Q5B	C14-C1-C3-O
3	B	1202	Q5B	C2-C1-C3-O
3	B	1202	Q5B	C14-C15-N5-C16
3	B	1202	Q5B	N6-C19-C20-S
3	B	1202	Q5B	O6-C4-C5-O7
3	D	1202	Q5B	C3-O-P-O1
3	D	1202	Q5B	C3-O-P-O2
3	D	1202	Q5B	C3-O-P-O3
3	D	1202	Q5B	C-C1-C14-C15
3	D	1202	Q5B	C-C1-C14-O21
3	D	1202	Q5B	C2-C1-C14-C15
3	D	1202	Q5B	C2-C1-C14-O21
3	D	1202	Q5B	C3-C1-C14-C15
3	D	1202	Q5B	C3-C1-C14-O21
3	D	1202	Q5B	C14-C15-N5-C16
3	D	1202	Q5B	C19-C20-S-C21
3	D	1202	Q5B	C22-C21-S-C20
3	D	1202	Q5B	O15-C21-S-C20
4	A	1203	FLC	CG-CB-CBC-OB1
4	A	1203	FLC	CG-CB-CBC-OB2
4	A	1203	FLC	OHB-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
4	A	1203	FLC	OHB-CB-CBC-OB2
4	C	2103	FLC	CAC-CA-CB-OHB
4	C	2103	FLC	CA-CB-CBC-OB1
4	C	2103	FLC	CA-CB-CBC-OB2
4	C	2103	FLC	OHB-CB-CBC-OB1
4	C	2103	FLC	OHB-CB-CBC-OB2
4	C	2103	FLC	CA-CB-CG-CGC
4	C	2103	FLC	OHB-CB-CG-CGC
6	A	1205	COA	C5B-O5B-P1A-O1A
6	A	1205	COA	C5B-O5B-P1A-O2A
6	A	1205	COA	C5B-O5B-P1A-O3A
6	A	1205	COA	CCP-O6A-P2A-O3A
6	A	1205	COA	OAP-CAP-CBP-CCP
6	A	1205	COA	C9P-CAP-CBP-CCP
6	A	1205	COA	OAP-CAP-CBP-CDP
6	A	1205	COA	C9P-CAP-CBP-CDP
6	A	1205	COA	OAP-CAP-CBP-CEP
6	A	1205	COA	C9P-CAP-CBP-CEP
6	A	1205	COA	CAP-C9P-N8P-C7P
6	A	1205	COA	C5P-C6P-C7P-N8P
6	A	1205	COA	C6P-C5P-N4P-C3P
6	B	1204	COA	C5B-O5B-P1A-O1A
6	B	1204	COA	C5B-O5B-P1A-O2A
6	B	1204	COA	P1A-O3A-P2A-O6A
6	B	1204	COA	CCP-O6A-P2A-O3A
6	B	1204	COA	CCP-O6A-P2A-O4A
6	B	1204	COA	CCP-O6A-P2A-O5A
6	B	1204	COA	CDP-CBP-CCP-O6A
6	B	1204	COA	CEP-CBP-CCP-O6A
6	B	1204	COA	CAP-CBP-CCP-O6A
6	B	1204	COA	S1P-C2P-C3P-N4P
6	C	2101	COA	O4B-C4B-C5B-O5B
6	C	2101	COA	C5B-O5B-P1A-O3A
6	C	2101	COA	CCP-O6A-P2A-O3A
6	C	2101	COA	CCP-O6A-P2A-O4A
6	C	2101	COA	CCP-O6A-P2A-O5A
6	C	2101	COA	S1P-C2P-C3P-N4P
6	C	2102	COA	C5B-O5B-P1A-O1A
6	C	2102	COA	C5B-O5B-P1A-O2A
6	C	2102	COA	C5B-O5B-P1A-O3A
6	C	2102	COA	CCP-O6A-P2A-O3A
6	C	2102	COA	CCP-O6A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
6	C	2102	COA	CCP-O6A-P2A-O5A
6	C	2102	COA	CDP-CBP-CCP-O6A
6	C	2102	COA	CEP-CBP-CCP-O6A
6	C	2102	COA	CAP-CBP-CCP-O6A
6	C	2102	COA	S1P-C2P-C3P-N4P
6	A	1205	COA	O5P-C5P-N4P-C3P
3	A	1202	Q5B	O13-C15-N5-C16
3	B	1202	Q5B	O13-C15-N5-C16
3	D	1202	Q5B	O13-C15-N5-C16
2	A	1201	ADP	C3'-C4'-C5'-O5'
4	C	2103	FLC	CAC-CA-CB-CG
4	C	2103	FLC	CBC-CB-CG-CGC
3	A	1202	Q5B	O6-C4-C5-O7
3	B	1202	Q5B	O6-C4-C5-C6
6	C	2101	COA	C3B-C4B-C5B-O5B
6	C	2102	COA	O4B-C4B-C5B-O5B
3	B	1202	Q5B	C16-C17-C18-O14
3	D	1202	Q5B	O6-C4-C5-O7
4	C	2103	FLC	CAC-CA-CB-CBC
3	A	1202	Q5B	O6-C4-C5-C6
3	B	1202	Q5B	C16-C17-C18-N6
2	A	1201	ADP	PA-O3A-PB-O1B
6	A	1205	COA	O9P-C9P-N8P-C7P
6	C	2102	COA	C3B-C4B-C5B-O5B
4	A	1203	FLC	CB-CG-CGC-OG1
3	A	1202	Q5B	O15-C21-S-C20
4	A	1203	FLC	CB-CG-CGC-OG2
3	A	1202	Q5B	P-O3-P1-O6
3	B	1202	Q5B	P1-O3-P-O
3	D	1202	Q5B	P-O3-P1-O6
6	C	2102	COA	P1A-O3A-P2A-O6A
3	A	1202	Q5B	C22-C21-S-C20
4	D	1203	FLC	CA-CB-CBC-OB1
4	D	1203	FLC	CG-CB-CBC-OB1
3	D	1202	Q5B	C-C1-C3-O
3	D	1202	Q5B	C2-C1-C3-O
3	B	1202	Q5B	C20-C19-N6-C18
4	D	1203	FLC	CAC-CA-CB-CG
4	D	1203	FLC	CAC-CA-CB-OHB
2	B	1201	ADP	C5'-O5'-PA-O2A
2	D	1201	ADP	C5'-O5'-PA-O1A
3	A	1202	Q5B	C3-O-P-O2

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Mol	Chain	Res	Type	Atoms
3	B	1202	Q5B	C3-O-P-O2
6	A	1205	COA	CCP-O6A-P2A-O4A
6	B	1204	COA	C5B-O5B-P1A-O3A
6	C	2101	COA	C5B-O5B-P1A-O1A
3	D	1202	Q5B	C16-C17-C18-O14
6	B	1204	COA	O4B-C4B-C5B-O5B
4	A	1203	FLC	CAC-CA-CB-OHB
4	C	2103	FLC	CG-CB-CBC-OB2
4	D	1203	FLC	CA-CB-CBC-OB2
4	D	1203	FLC	CG-CB-CBC-OB2
3	D	1202	Q5B	C16-C17-C18-N6
3	A	1202	Q5B	C6-O9-P2-O10
6	C	2101	COA	C2B-C1B-N9A-C8A
6	A	1205	COA	P1A-O3A-P2A-O4A
6	C	2102	COA	P2A-O3A-P1A-O2A
4	B	1203	FLC	CA-CB-CBC-OB2
4	C	2103	FLC	CG-CB-CBC-OB1
4	B	1203	FLC	CAC-CA-CB-OHB
2	D	1201	ADP	PA-O3A-PB-O1B
3	A	1202	Q5B	C16-C17-C18-O14
6	B	1204	COA	O5P-C5P-N4P-C3P
4	D	1203	FLC	OHB-CB-CBC-OB1
3	A	1202	Q5B	C16-C17-C18-N6
3	D	1202	Q5B	O6-C4-C5-C6
6	B	1204	COA	C2B-C1B-N9A-C8A
3	A	1202	Q5B	O21-C14-C15-N5
3	B	1202	Q5B	O21-C14-C15-N5
3	D	1202	Q5B	O21-C14-C15-N5
2	B	1201	ADP	PB-O3A-PA-O2A
6	A	1205	COA	P2A-O3A-P1A-O2A
6	A	1205	COA	P1A-O3A-P2A-O5A
6	B	1204	COA	P2A-O3A-P1A-O1A
6	B	1204	COA	P2A-O3A-P1A-O2A

There are no ring outliers.

14 monomers are involved in 37 short contacts:

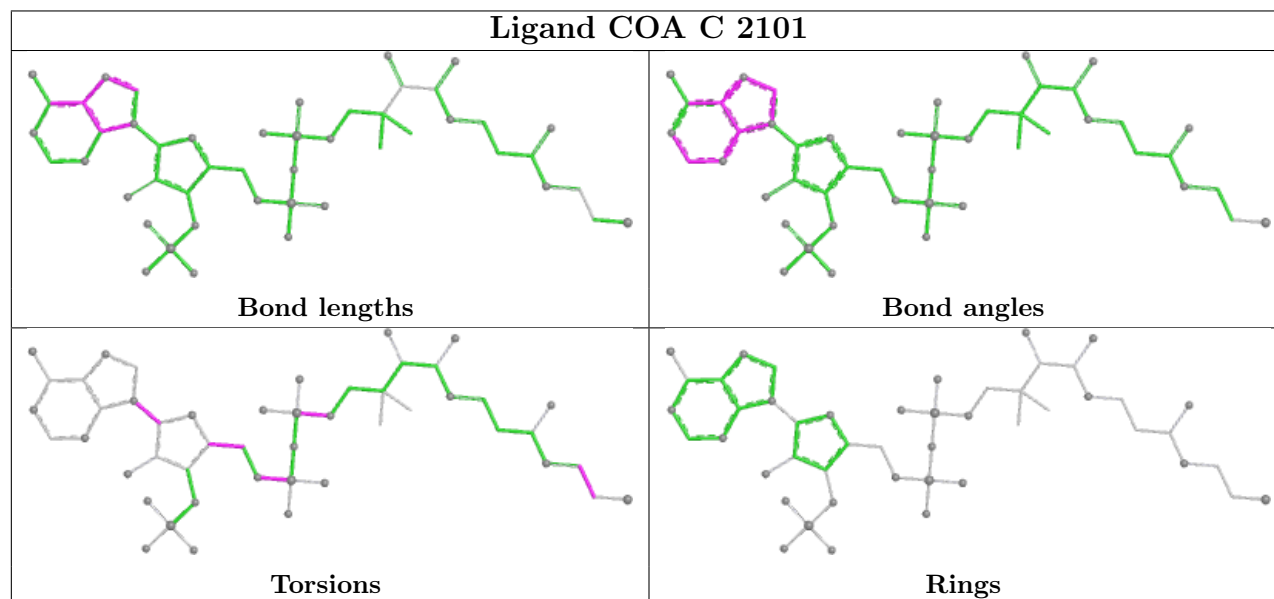
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2103	FLC	1	0
4	D	1203	FLC	1	0
6	C	2101	COA	4	0
3	A	1202	Q5B	1	0

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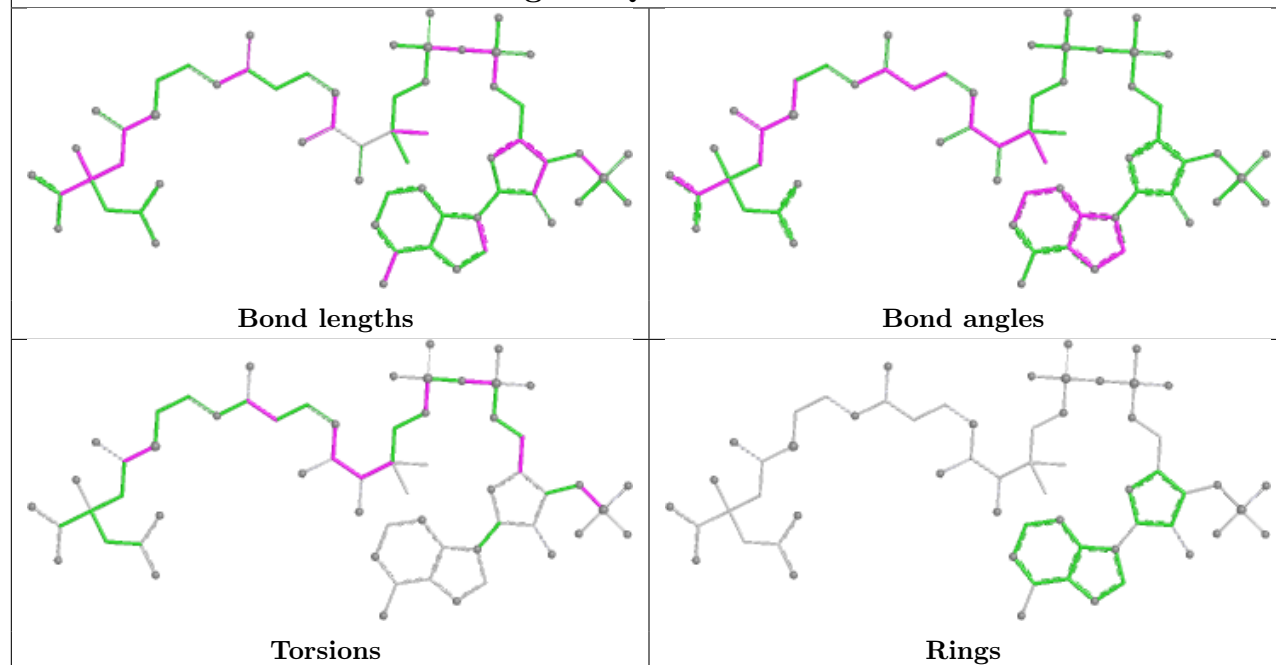
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1201	ADP	2	0
2	D	1201	ADP	2	0
6	B	1204	COA	3	0
4	A	1203	FLC	1	0
4	B	1203	FLC	1	0
3	B	1202	Q5B	3	0
2	A	1201	ADP	6	0
3	D	1202	Q5B	1	0
6	A	1205	COA	4	0
6	C	2102	COA	7	0

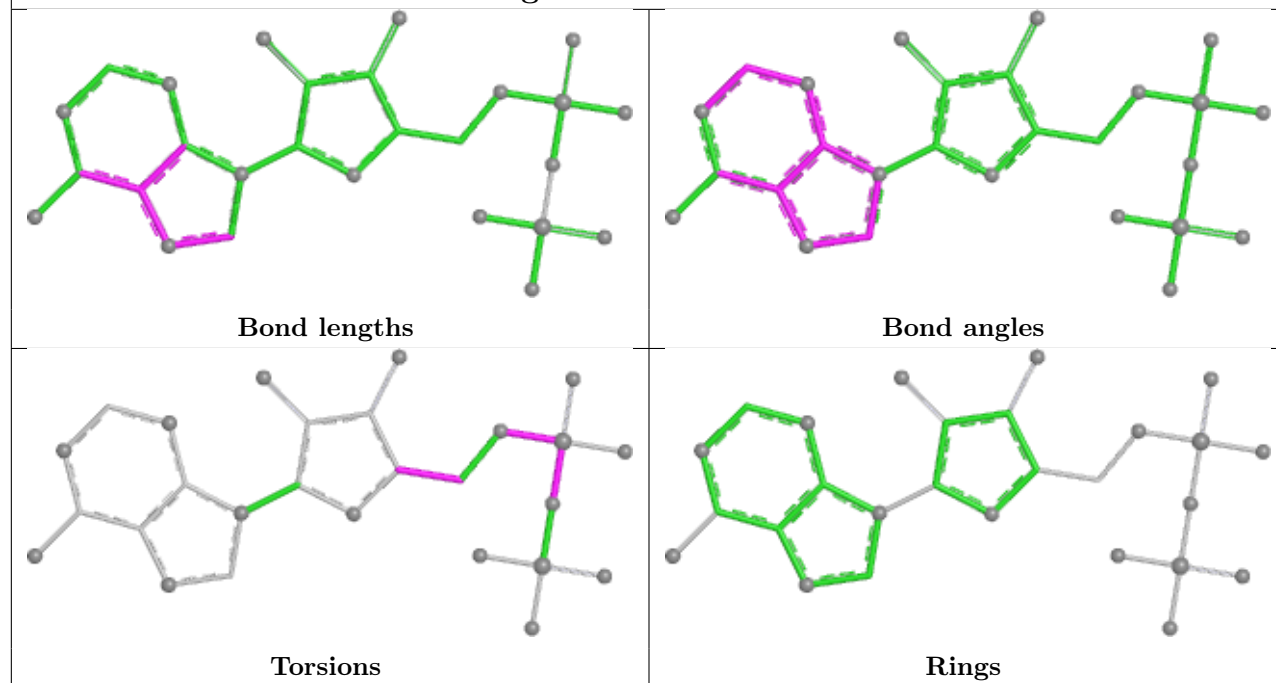
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

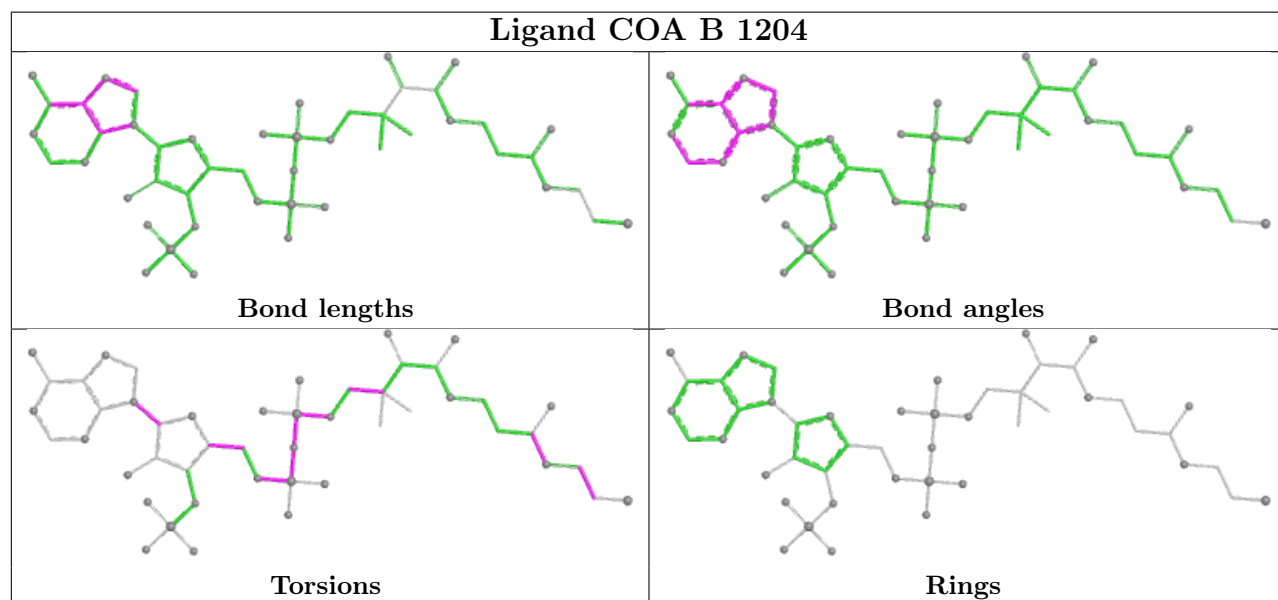
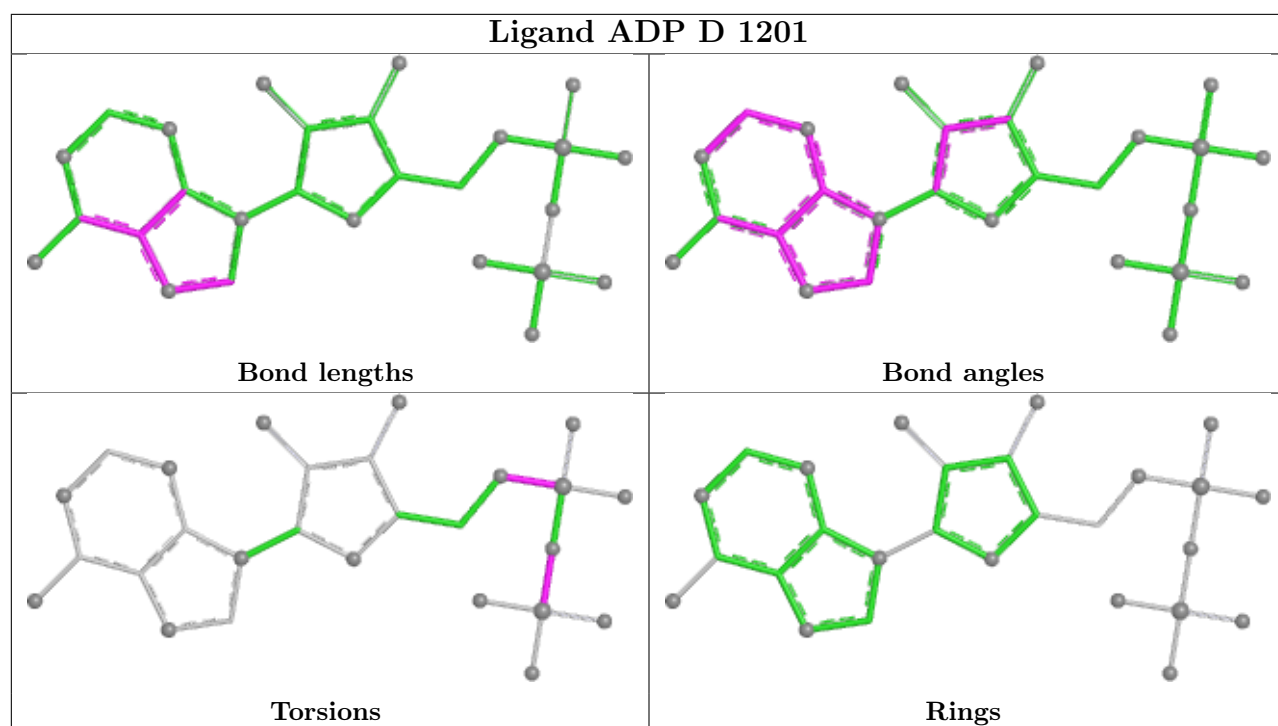


Ligand Q5B A 1202

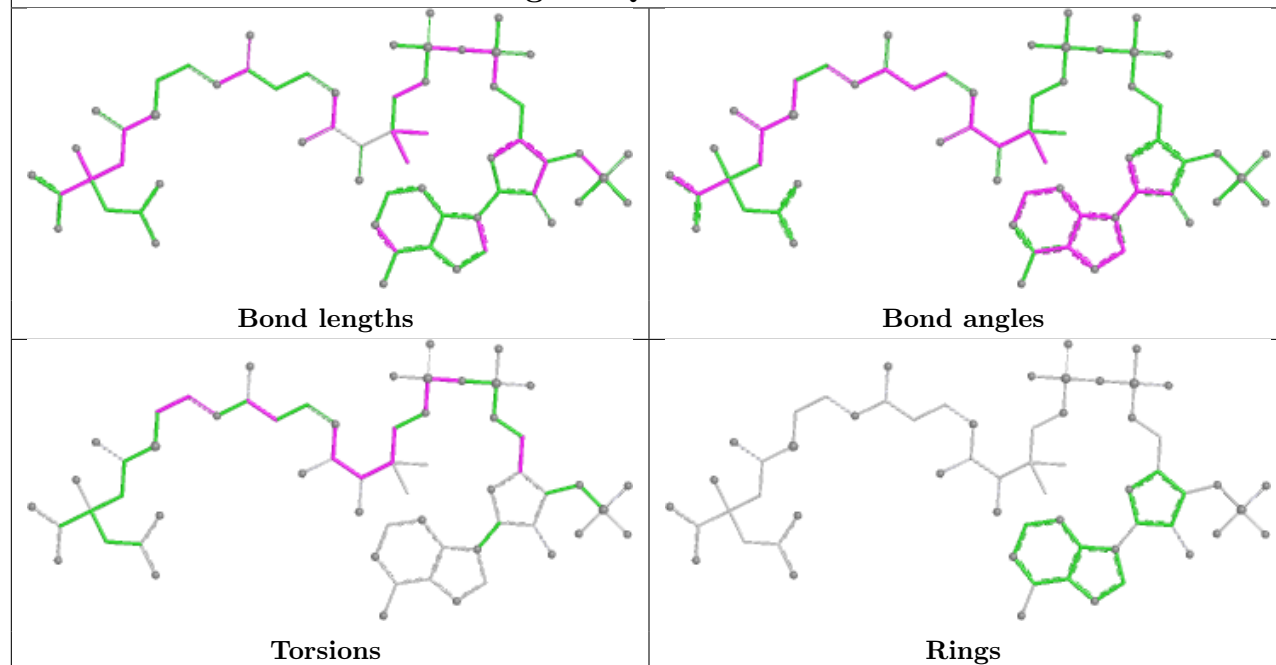


Ligand ADP B 1201

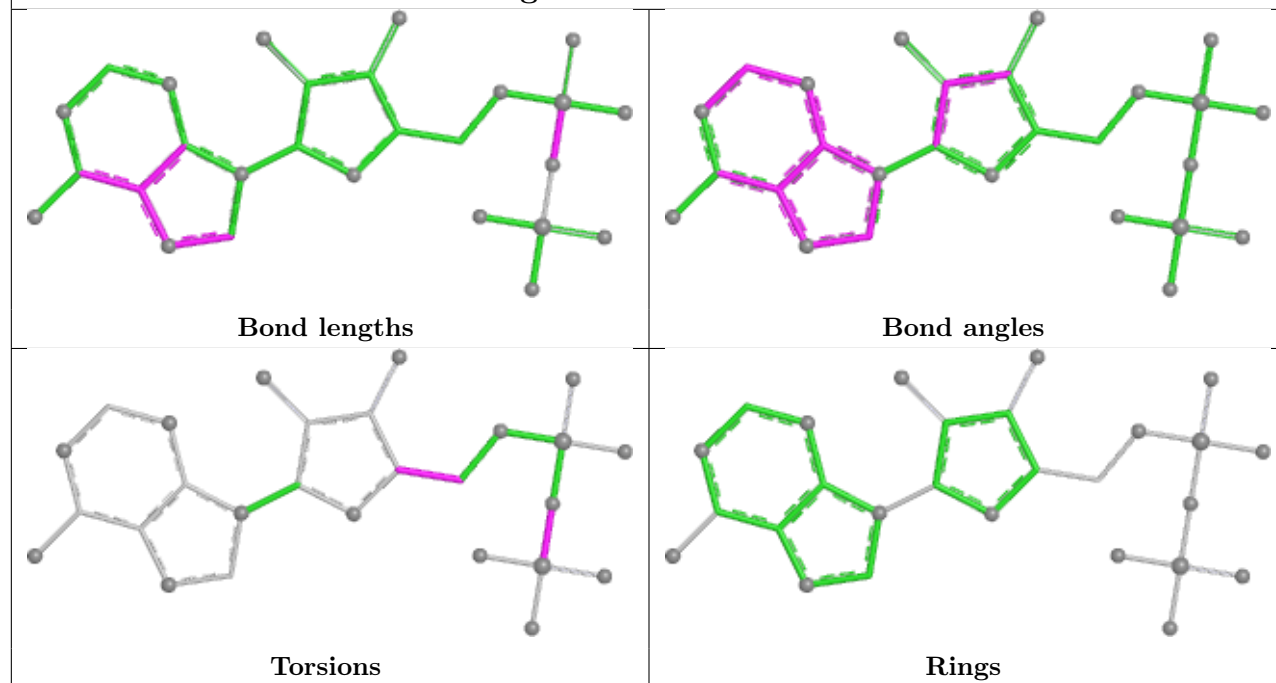


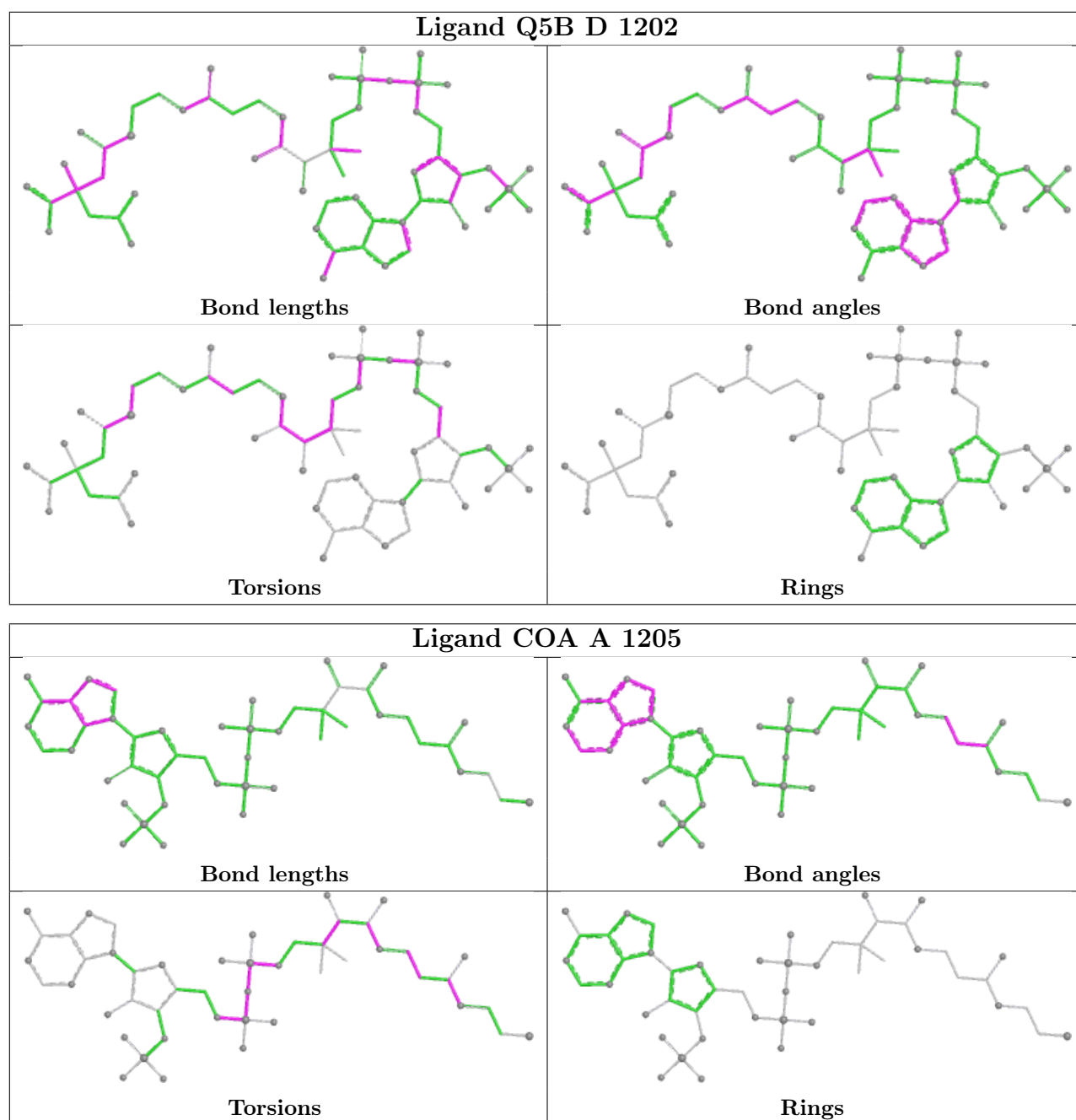


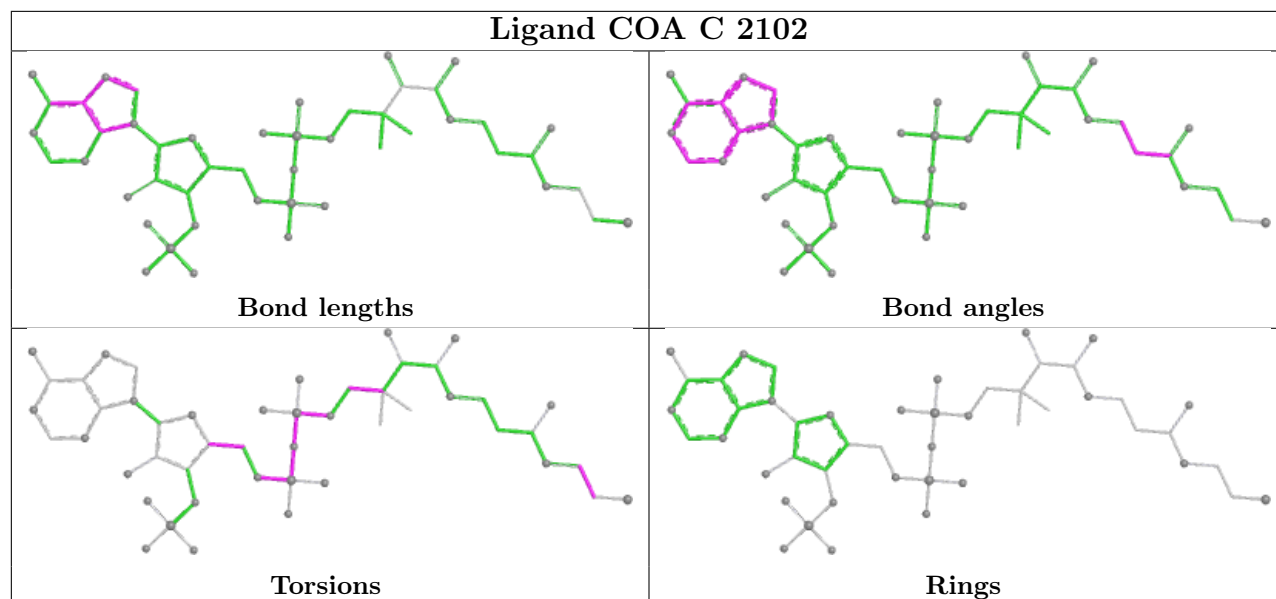
Ligand Q5B B 1202



Ligand ADP A 1201







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.

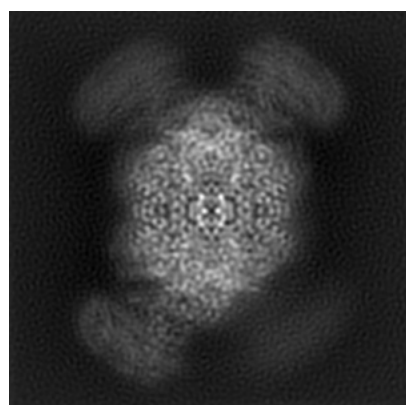
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-24511. These allow visual inspection of the internal detail of the map and identification of artifacts.

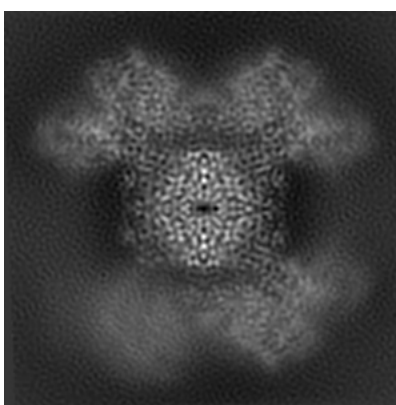
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

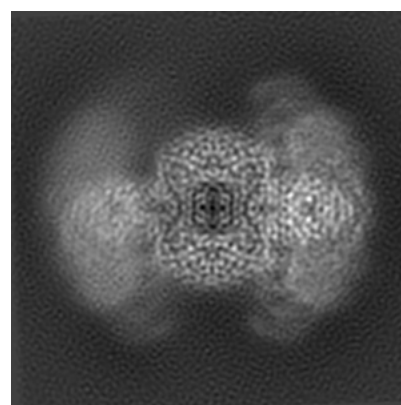
6.1.1 Primary map



X



Y

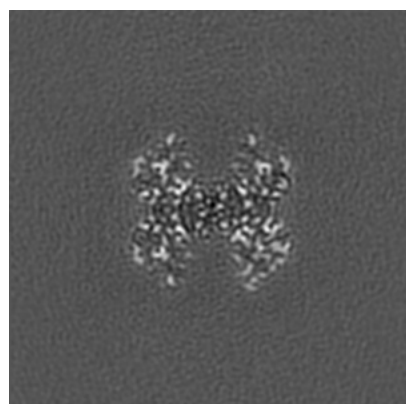


Z

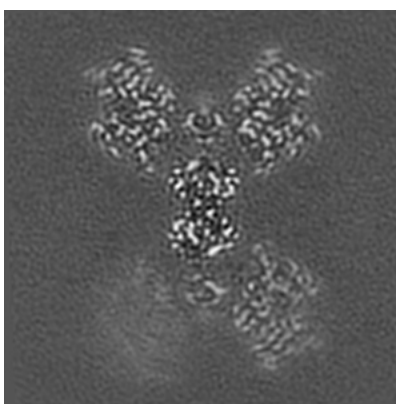
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

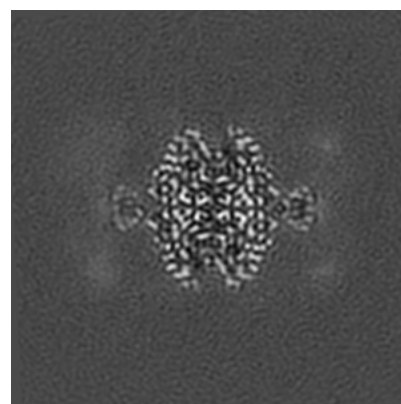
6.2.1 Primary map



X Index: 110



Y Index: 110

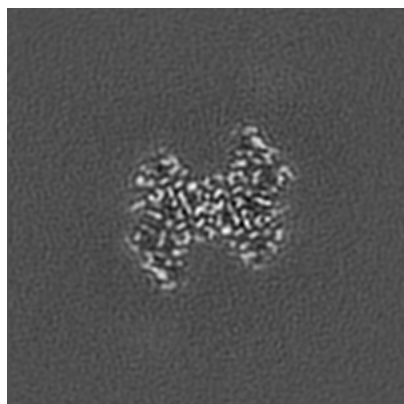


Z Index: 110

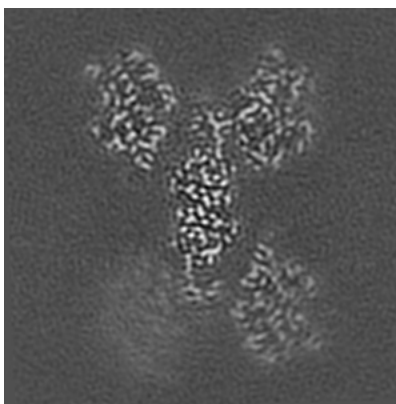
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

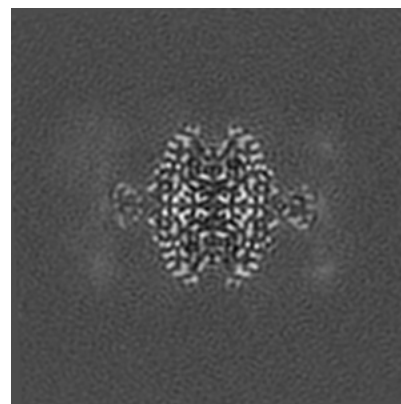
6.3.1 Primary map



X Index: 119



Y Index: 106

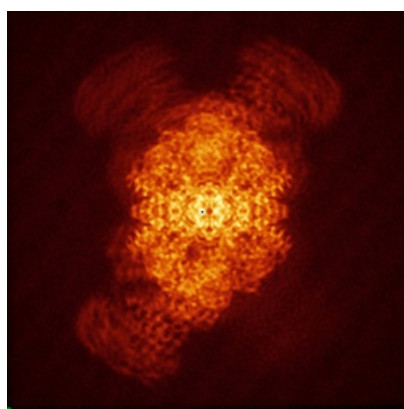


Z Index: 109

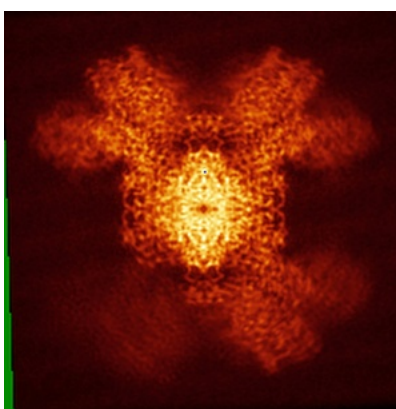
The images above show the largest variance slices of the map in three orthogonal directions.

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

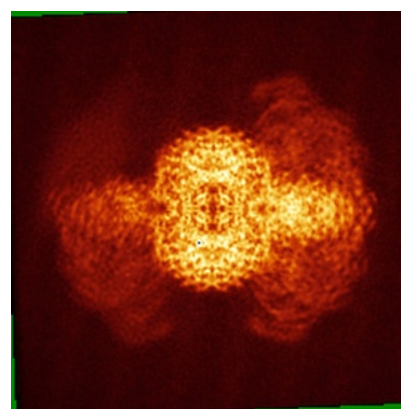
6.4.1 Primary map



X



Y

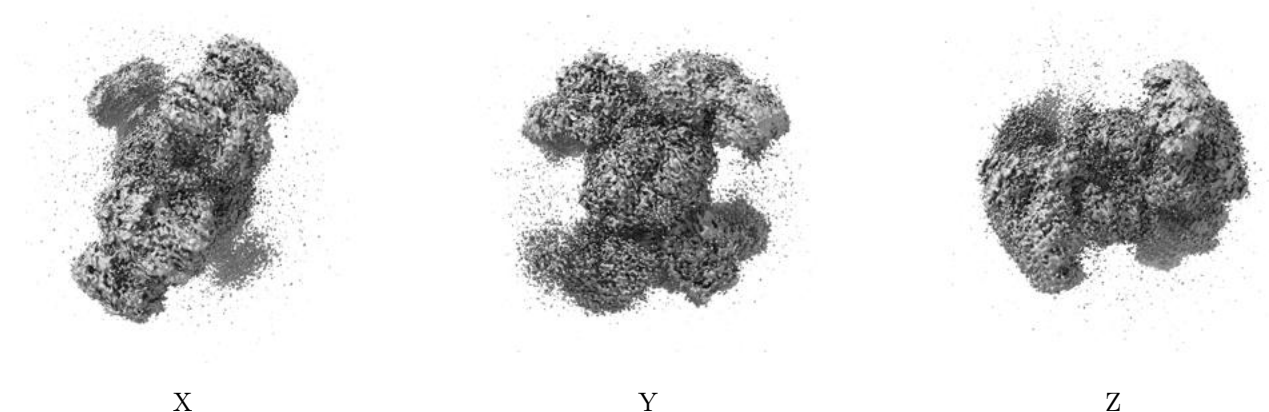


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

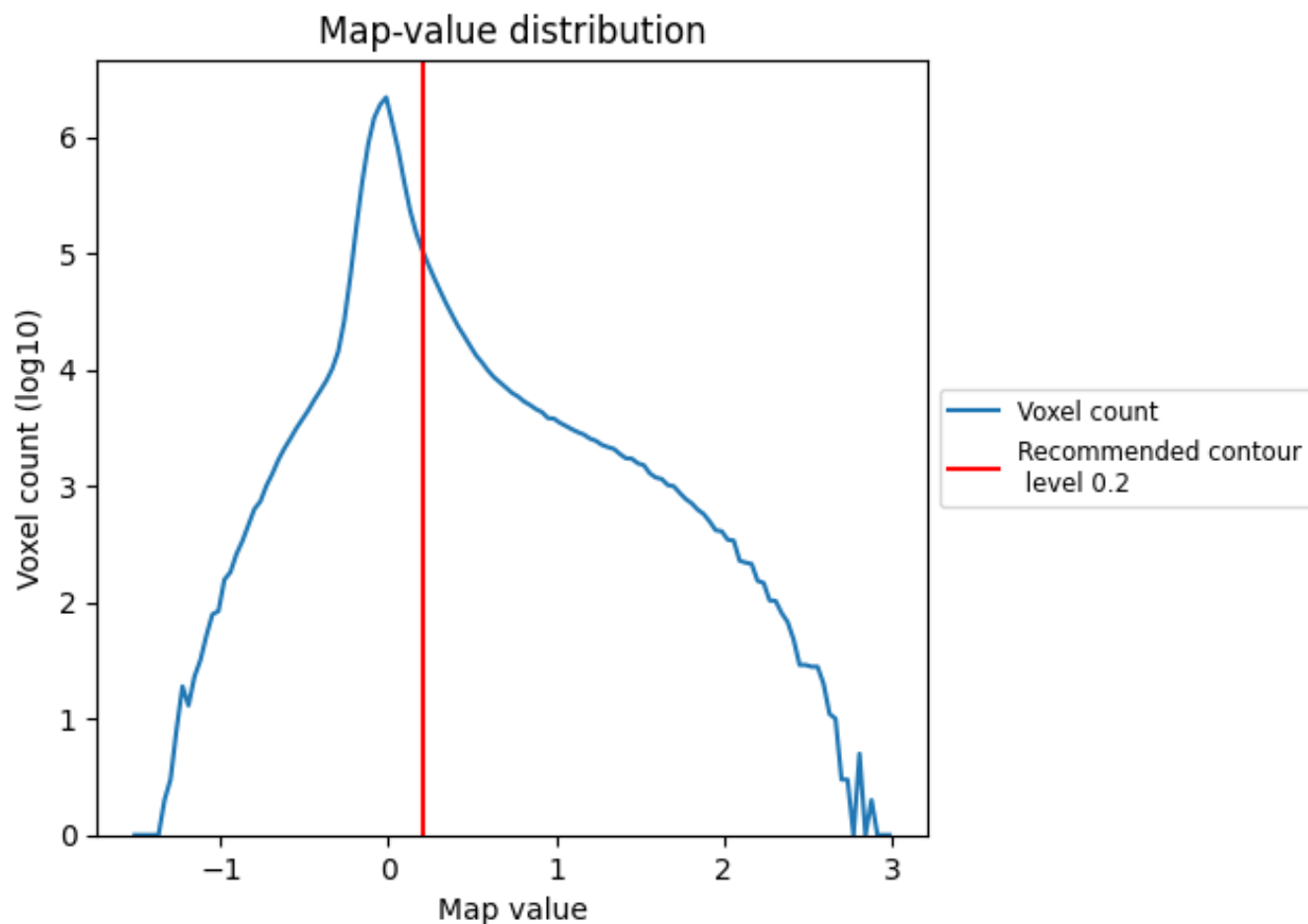
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

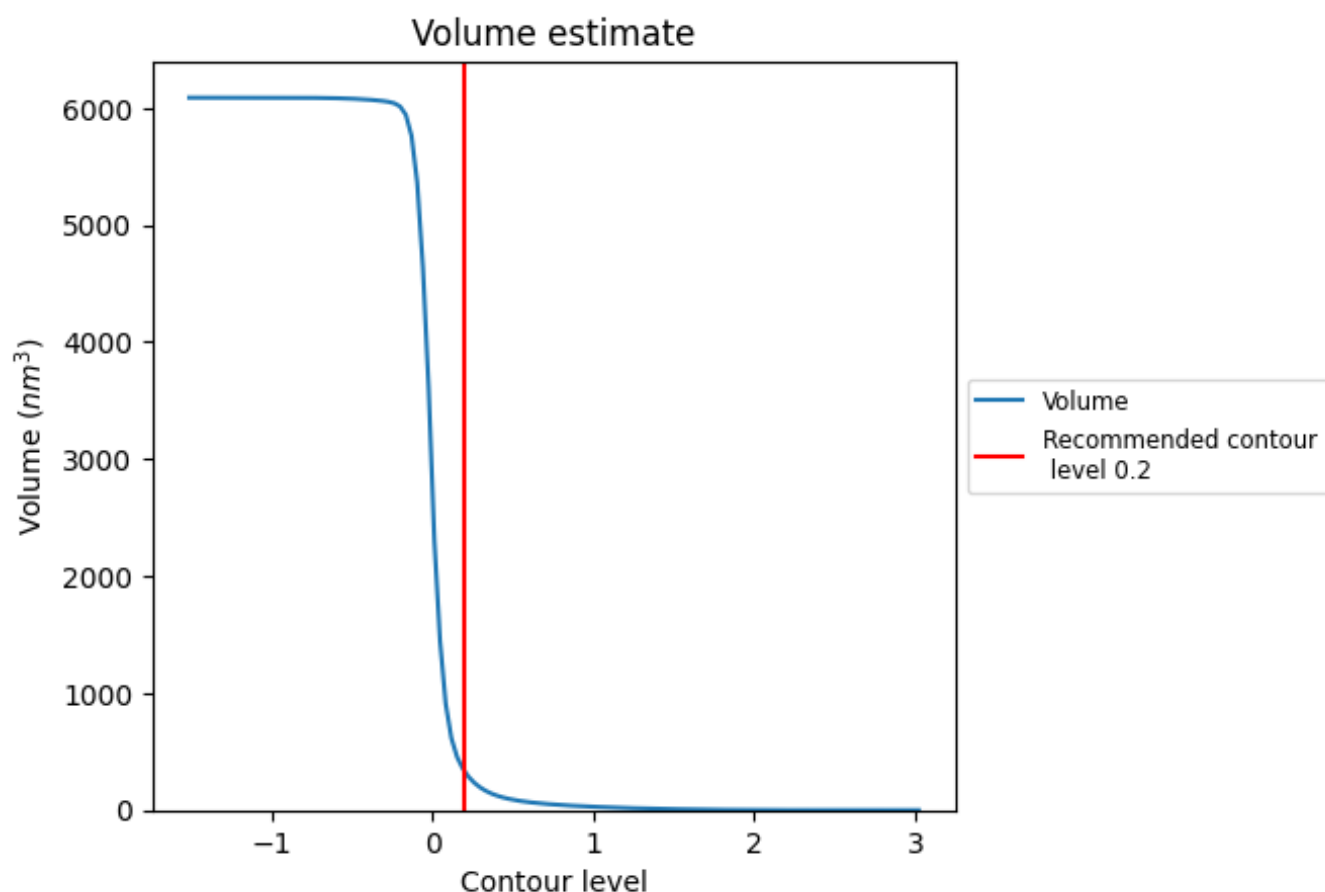
This section contains the results of statistical analysis of the map.

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.

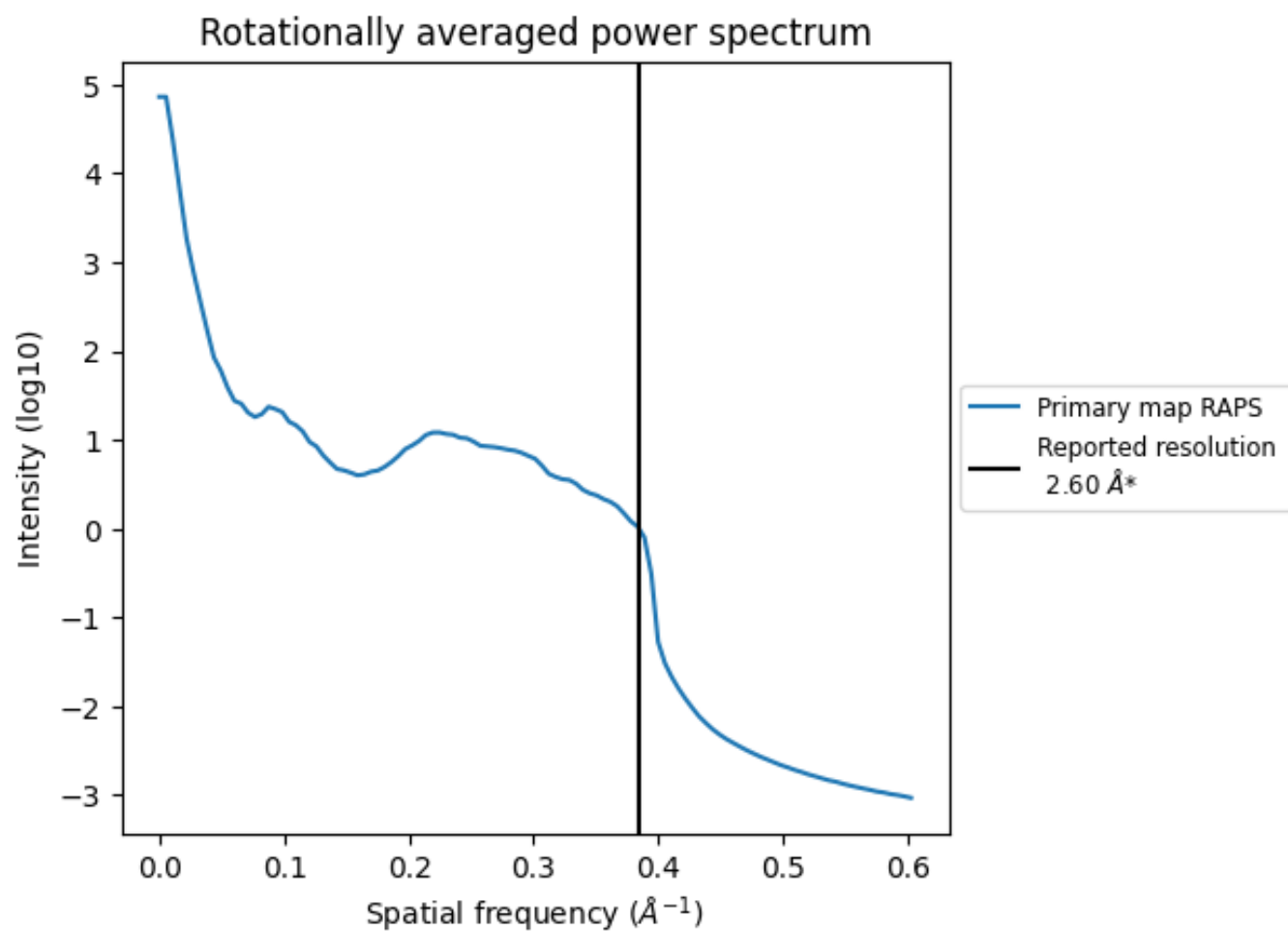
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm³; this corresponds to an approximate mass of 299 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 0.385 Å⁻¹

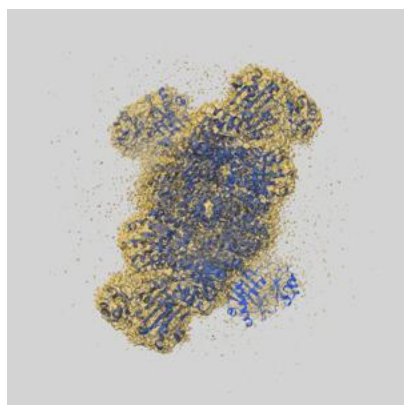
8 Fourier-Shell correlation ⓘ

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

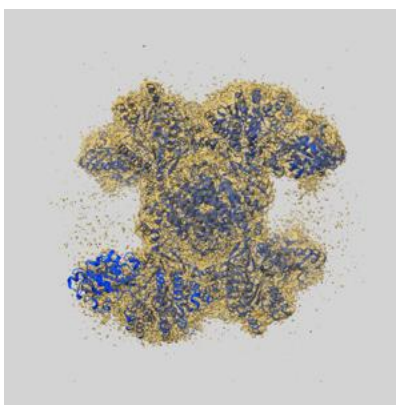
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-24511 and PDB model 7RKZ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

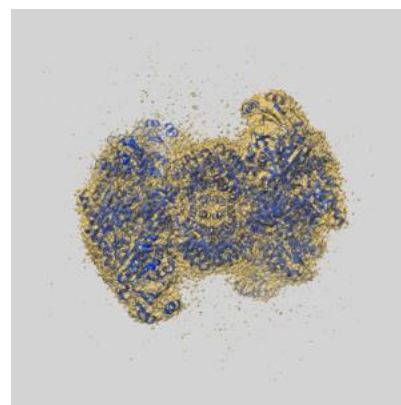
9.1 Map-model overlay [i](#)



X



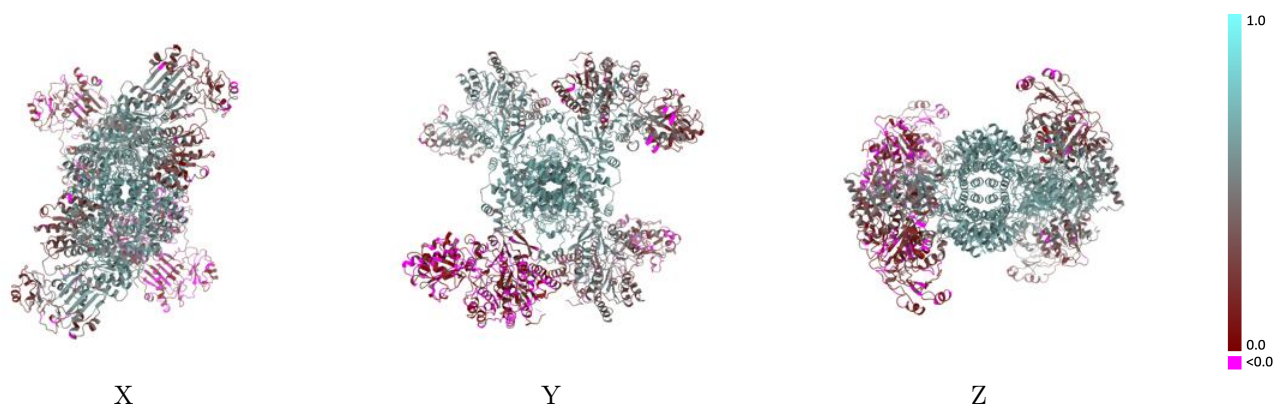
Y



Z

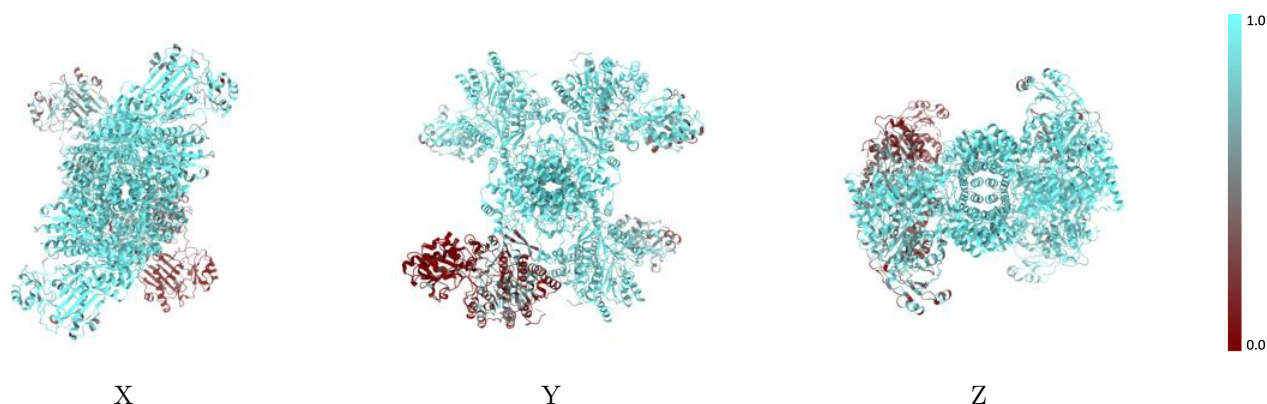
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



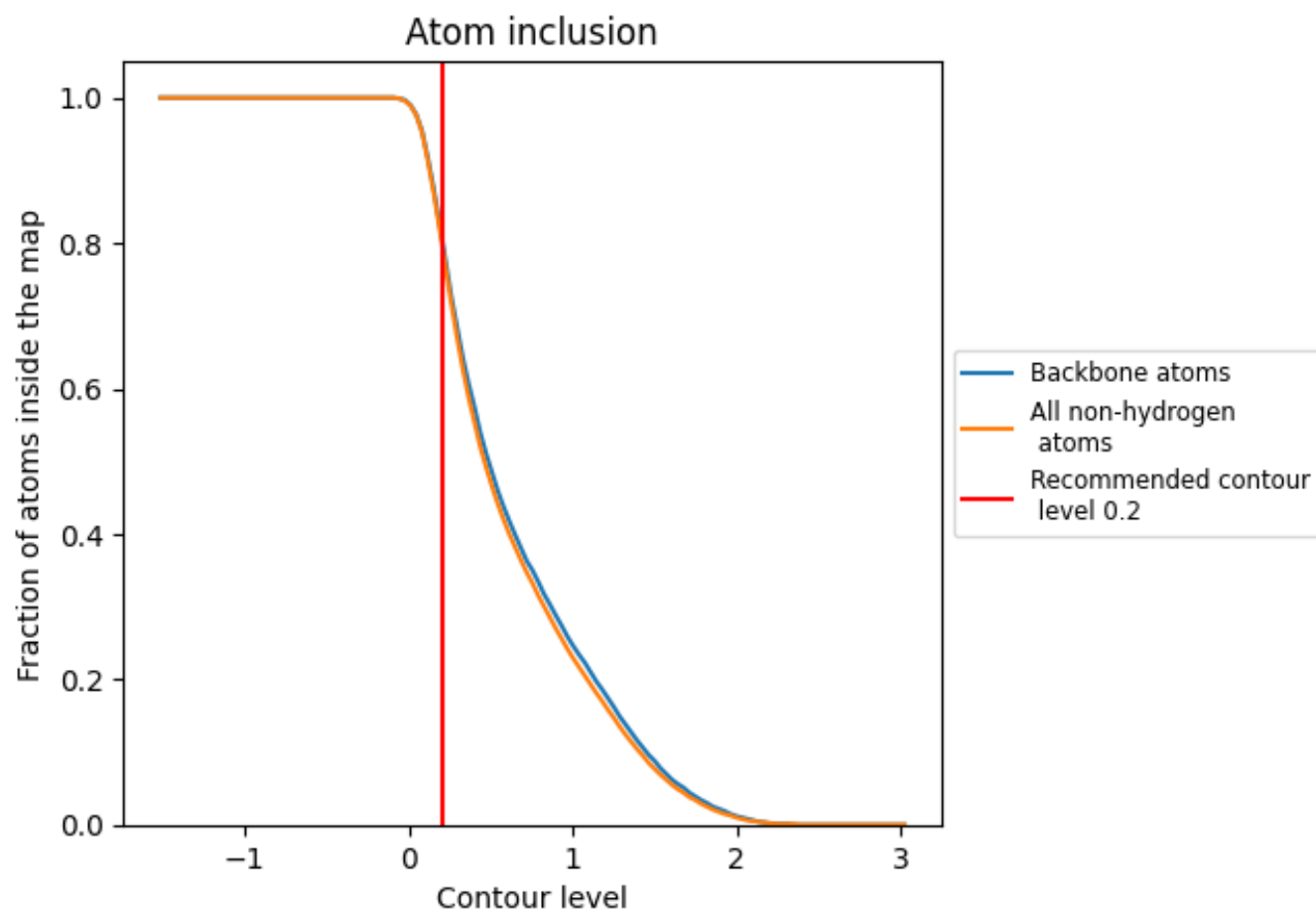
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.2).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 80% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8030	0.4120
A	0.9280	0.4910
B	0.9450	0.5230
C	0.4900	0.2380
D	0.8530	0.3970

