



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:52 PM UTC

PDB ID : 4JD3 / pdb_00004jd3
Title : Crystal Structure of Mycobacterium tuberculosis PKS11 Reveals Intermediates in the Synthesis of Methyl-branched Alkylpyrones
Authors : Gokulan, K.; Sacchettini, J.C.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)
Deposited on : 2013-02-22
Resolution : 2.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

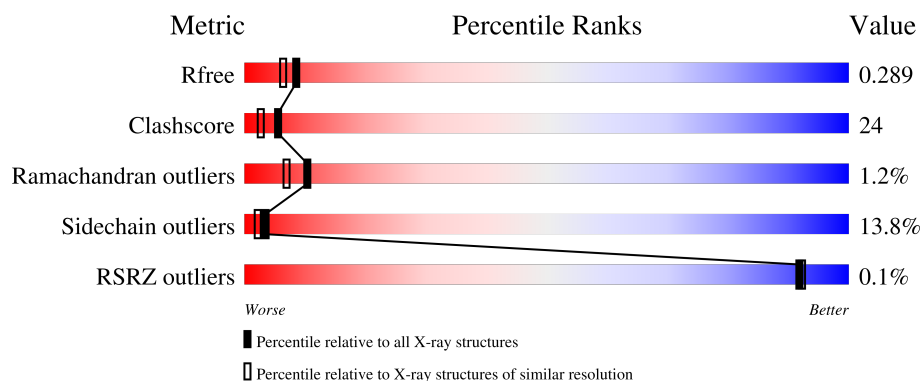
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	353	
1	B	353	
1	C	353	
1	D	353	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLM	A	400	-	-	X	-
2	PLM	B	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10842 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

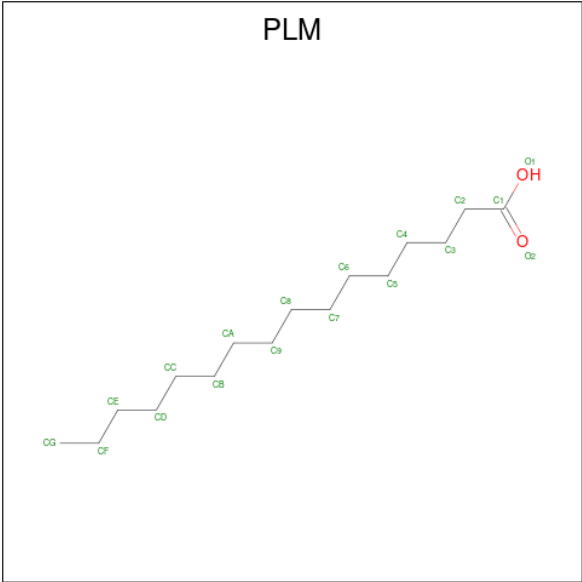
- Molecule 1 is a protein called Alpha-pyrone synthesis polyketide synthase-like Pks11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2642	1671	469	495	7			
1	C	352	Total	C	N	O	S	0	0	0
			2642	1671	469	495	7			
1	B	352	Total	C	N	O	S	0	1	0
			2652	1677	472	496	7			
1	D	352	Total	C	N	O	S	0	0	0
			2642	1671	469	495	7			

There are 4 discrepancies between the modelled and reference sequences:

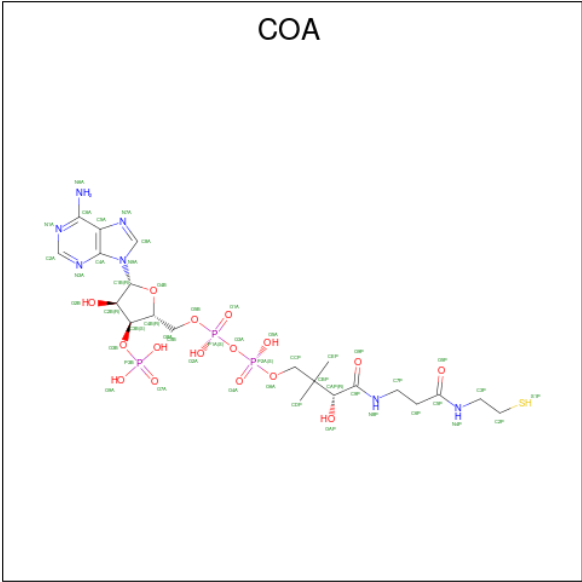
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	SER	CYS	engineered mutation	UNP O06587
C	138	SER	CYS	engineered mutation	UNP O06587
B	138	SER	CYS	engineered mutation	UNP O06587
D	138	SER	CYS	engineered mutation	UNP O06587

- Molecule 2 is PALMITIC ACID (CCD ID: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	16	2		
2	C	1	Total	C	O	0	0
			18	16	2		
2	B	1	Total	C	O	0	0
			18	16	2		
2	D	1	Total	C	O	0	0
			18	16	2		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

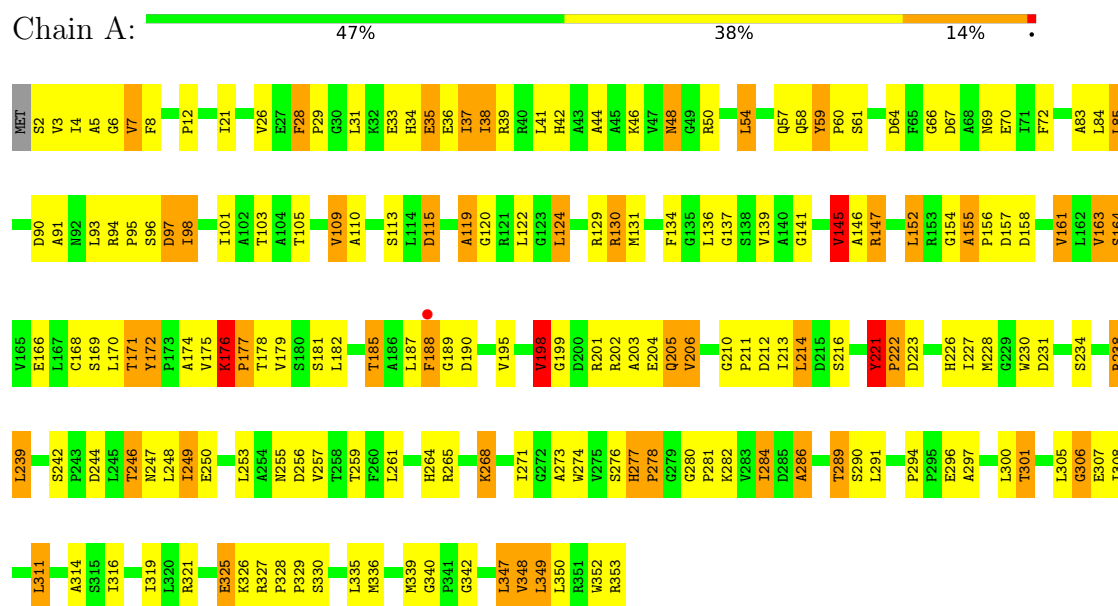
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total 20	O 20	0	0
4	C	25	Total 25	O 25	0	0
4	B	30	Total 30	O 30	0	0
4	D	21	Total 21	O 21	0	0

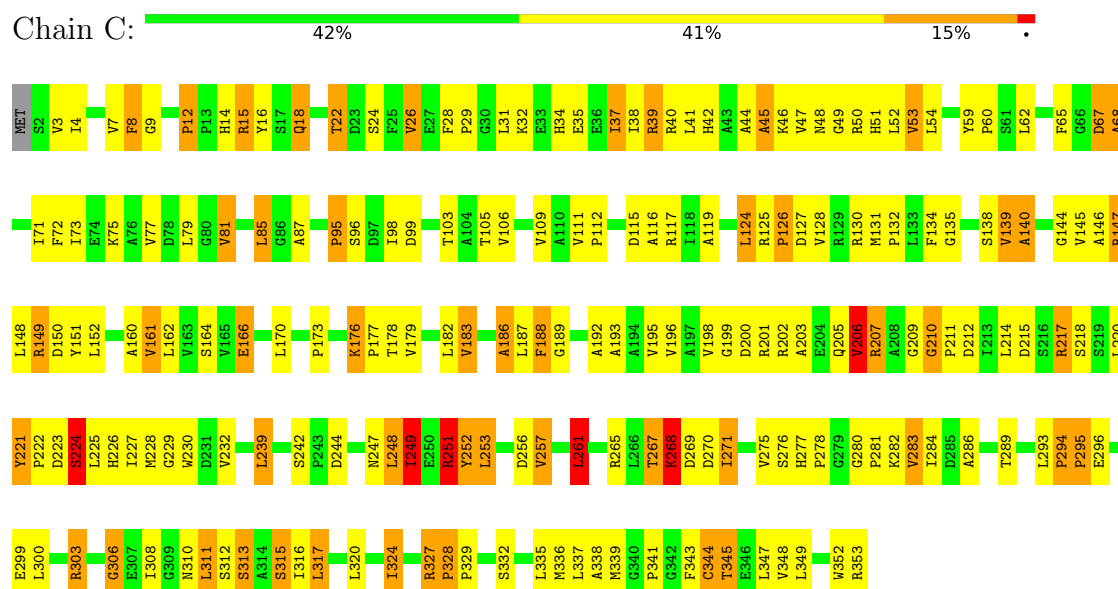
3 Residue-property plots

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 electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11



- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11



Chain B:

44% 39% 16%

Tokens (from left to right):

MET, S2, V3, T4, A5, G6, V7, F8, G9, A10, G11, T12, P13, A14, Q18, S19, E20, T21, V26, P29, E35, G36, T37, A38, G39, R40, L41, A42, A45, R50, H51, L52, V53, L54, P55, L56, Q57, F58, G59, P60, S61, D64, N69, E70, T71, F72, I73, K75, A76, V77, R78, V81, L84, A87, L88, D89, A91, N92, P95, I98, M100, I101, A102, T103, A104, T105, P106, T107, G108, V109, D115, A116, R117, I118, A119, L122, G123, L124, R125, R129, L130, M131, P132, L133, F134, G135, L136, G137, S138, V139, A140, G141, A142, V145, A146, R147, L148, A153, D158, V159, A160, V161, L162, V163, S164, V165, E166, L167, G168, S169, L170, T171, P173, A174, V175, S180, S181, A182, T185, A186, L187, F188, A193, A194, V195, V196, R201, E204, Q205, V206, R207, A208, G209, G210, P211, D212, L213, T213, L214, D215, S216, R217, L220, Y221, P222, D223, H226, T227, M228, G229, D231, V232, G233, S234, R235, R238, L239, S242, P243, D244, L245, T246, N247, R251, T252, L253, A254, N255, D256, V257, T258, T259, F260, L261, D262, A263, H264, T267, K268, D269, T270, T271, V274, W275, G276, P278, G279, G280, P281, K282, V283, T284, D285, A286, V287, A288, T289, S290, L291, A292, L293, P294, P295, E296, A297

Chain D:

Category	Value
L283	1
P294	1
P295	1
L298	1
E289	1
L300	1
T301	1
W302	1
K303	1
S304	1
L305	1
I308	1
G309	1
N310	1
L311	1
S312	1
S313	1
A314	1
S315	1
I319	1
L320	1
R321	1
D322	1
T323	1
I324	1
S325	1
K326	1
R327	1
P328	1
P329	1
S332	1
A333	1
G334	1
M336	1
L337	1
A338	1
M339	1
G340	1
P341	1
G342	1
F343	1
G344	1
T345	1
E346	1
L347	1
L350	1
R351	1
K352	1
R353	1
S224	1
L225	1
H226	1
I227	1
M228	1
G229	1
W230	1
D231	1
W232	1
G233	1
S234	1
H235	1
R240	1
G241	1
S242	1
T243	1
D244	1
T245	1
T246	1
N247	1
L248	1
R251	1
T252	1
L253	1
D256	1
T257	1
S258	1
T259	1
F260	1
L261	1
D262	1
A263	1
H264	1
R265	1
L266	1
T267	1
K268	1
L271	1
G272	1
S276	1
H277	1
T278	1
G279	1
G280	1
P281	1
K282	1
W283	1
L284	1
V287	1
A288	1
T289	1
S290	1
L291	1
A292	1
A146	1
R147	1
L148	1
R149	1
D150	1
Y151	1
L152	1
R153	1
G154	1
A155	1
P156	1
D157	1
D158	1
V159	1
A160	1
S164	1
V165	1
E166	1
L167	1
S168	1
L170	1
K176	1
P177	1
T178	1
V179	1
S180	1
S181	1
L182	1
V183	1
G184	1
L185	1
A186	1
L187	1
F188	1
A192	1
V198	1
G199	1
D200	1
R201	1
E202	1
A203	1
E204	1
Q205	1
V206	1
R207	1
A208	1
G209	1
G210	1
P211	1
D212	1
I213	1
L214	1
D215	1
S216	1
E217	1
V198	1
G199	1
D200	1
R201	1
E202	1
A203	1
E204	1
Q205	1
V206	1
R207	1
A208	1
G209	1
G210	1
P211	1
D212	1
I213	1
L214	1
D215	1
S216	1
E217	1
V198	1
G199	1
D200	1
R201	1
E202	1
A203	1
E204	1
Q205	1
V206	1
R207	1
A208	1
G209	1
G210	1
P211	1
D212	1
I213	1
L214	1
D215	1
S216	1
E217	1
V198	1
G199	1
D200	1

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.17Å 48.86Å 194.47Å 90.00° 97.82° 90.00°	Depositor
Resolution (Å)	32.11 – 2.25 32.11 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (32.11-2.25) 68.6 (32.11-2.25)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.24Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.194 , 0.294 0.201 , 0.289	Depositor DCC
R_{free} test set	2255 reflections (3.49%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10842	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, 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	1.79	30/2695 (1.1%)	1.86	89/3671 (2.4%)
1	B	1.85	36/2706 (1.3%)	1.80	53/3686 (1.4%)
1	C	1.92	55/2695 (2.0%)	1.83	66/3671 (1.8%)
1	D	1.86	37/2695 (1.4%)	1.85	75/3671 (2.0%)
All	All	1.86	158/10791 (1.5%)	1.84	283/14699 (1.9%)

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

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

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	VAL	CA-CB	9.68	1.66	1.54
1	C	249	ILE	CA-CB	9.42	1.64	1.54
1	D	145	VAL	CA-CB	9.23	1.66	1.54
1	C	81	VAL	C-O	-8.97	1.13	1.24
1	D	183	VAL	CA-CB	8.86	1.63	1.54
1	A	188	PHE	C-O	-8.71	1.13	1.23
1	A	7	VAL	C-O	8.61	1.32	1.24
1	A	110	ALA	C-N	8.47	1.43	1.33
1	C	41	LEU	C-O	8.44	1.34	1.24
1	B	76	ALA	CA-C	-8.30	1.42	1.52
1	C	12	PRO	C-O	-8.20	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	VAL	CA-CB	8.18	1.64	1.54
1	A	195	VAL	CA-CB	7.93	1.64	1.54
1	C	7	VAL	CA-CB	7.88	1.65	1.54
1	C	149	ARG	CA-C	7.64	1.62	1.52
1	D	119	ALA	C-O	7.47	1.32	1.24
1	C	203	ALA	CA-CB	-7.41	1.41	1.53
1	A	190	ASP	N-CA	7.37	1.55	1.46
1	A	21	ILE	CA-CB	7.17	1.61	1.54
1	C	139	VAL	CA-CB	7.02	1.64	1.54
1	D	104	ALA	CA-CB	-6.99	1.42	1.53
1	A	273	ALA	CA-C	6.99	1.60	1.52
1	D	324	ILE	CA-CB	6.97	1.62	1.54
1	C	39	ARG	CA-C	6.94	1.61	1.52
1	A	64	ASP	CA-C	6.94	1.61	1.52
1	C	81	VAL	C-N	6.92	1.42	1.33
1	D	102	ALA	CA-CB	6.91	1.63	1.53
1	C	283	VAL	CA-CB	6.87	1.62	1.54
1	D	12	PRO	C-O	-6.85	1.19	1.25
1	D	352	TRP	C-N	-6.73	1.24	1.33
1	C	195	VAL	CA-C	6.72	1.60	1.52
1	C	286	ALA	CA-CB	-6.70	1.42	1.53
1	A	98	ILE	CA-CB	6.69	1.62	1.53
1	B	289	THR	CA-CB	6.67	1.64	1.53
1	C	344	CYS	CA-C	6.64	1.60	1.52
1	B	227	ILE	C-O	6.63	1.32	1.24
1	D	276	SER	C-N	-6.62	1.22	1.33
1	C	68	ALA	CA-CB	6.60	1.63	1.53
1	D	146	ALA	CA-CB	6.58	1.64	1.53
1	C	222	PRO	C-O	6.57	1.31	1.23
1	D	59	TYR	C-O	-6.56	1.18	1.24
1	B	283	VAL	CA-C	6.55	1.61	1.52
1	A	124	LEU	C-O	6.52	1.31	1.23
1	C	140	ALA	CA-C	-6.50	1.43	1.52
1	D	155	ALA	C-N	6.49	1.41	1.34
1	D	257	VAL	CA-C	6.48	1.60	1.52
1	D	302	TRP	CA-C	-6.48	1.43	1.52
1	C	277	HIS	CA-C	6.47	1.60	1.52
1	C	130	ARG	CA-C	6.45	1.60	1.52
1	A	37	ILE	CA-CB	-6.44	1.45	1.54
1	A	105	THR	C-O	6.42	1.31	1.23
1	A	157	ASP	CA-C	-6.39	1.43	1.52
1	B	330	SER	CA-C	6.37	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	142	ALA	CA-CB	6.36	1.63	1.53
1	C	276	SER	N-CA	-6.16	1.38	1.46
1	C	85	LEU	N-CA	-6.16	1.38	1.46
1	B	281	PRO	CA-CB	6.12	1.62	1.53
1	B	182	LEU	C-O	6.08	1.31	1.24
1	C	67	ASP	N-CA	6.07	1.53	1.46
1	C	283	VAL	C-O	6.06	1.31	1.24
1	B	160	ALA	N-CA	6.05	1.53	1.46
1	B	98	ILE	CA-CB	6.04	1.62	1.53
1	B	233	GLY	CA-C	6.02	1.58	1.51
1	B	348	VAL	C-O	-6.00	1.17	1.24
1	A	146	ALA	CA-CB	5.97	1.62	1.53
1	C	200	ASP	CA-C	-5.96	1.45	1.52
1	D	231	ASP	N-CA	5.95	1.54	1.46
1	C	128	VAL	C-O	5.92	1.29	1.24
1	B	60	PRO	CA-C	5.91	1.62	1.52
1	B	168	CYS	CA-C	5.90	1.60	1.52
1	A	284	ILE	CA-CB	5.90	1.60	1.54
1	B	238	ARG	CA-C	5.89	1.60	1.52
1	A	188	PHE	C-N	5.88	1.42	1.33
1	D	224	SER	CA-C	5.87	1.59	1.52
1	D	281	PRO	CA-C	5.86	1.60	1.52
1	C	253	LEU	C-N	5.84	1.41	1.33
1	B	171	THR	CA-CB	5.83	1.63	1.53
1	B	129	ARG	C-O	-5.82	1.16	1.24
1	C	189	GLY	N-CA	5.81	1.49	1.44
1	A	163	VAL	CA-C	5.79	1.59	1.52
1	C	226	HIS	C-O	-5.79	1.16	1.24
1	C	161	VAL	CA-CB	5.78	1.64	1.54
1	D	84	LEU	CA-C	5.76	1.60	1.52
1	C	248	LEU	CA-C	-5.76	1.45	1.52
1	C	293	LEU	C-N	5.76	1.40	1.33
1	D	131	MET	C-O	-5.74	1.17	1.24
1	C	40	ARG	CA-C	5.68	1.60	1.52
1	C	295	PRO	N-CD	5.67	1.55	1.47
1	B	281	PRO	C-O	-5.61	1.17	1.24
1	C	37	ILE	CG1-CD1	-5.60	1.29	1.51
1	B	73	ILE	CA-CB	5.59	1.60	1.54
1	A	226	HIS	CA-C	5.56	1.60	1.52
1	B	5	ALA	CA-C	5.56	1.59	1.52
1	B	101	ILE	CA-CB	5.55	1.60	1.54
1	C	173	PRO	N-CD	5.53	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	275	VAL	CA-C	5.52	1.58	1.52
1	C	59	TYR	C-O	5.50	1.31	1.24
1	C	8	PHE	C-O	5.49	1.30	1.23
1	C	183	VAL	CA-C	5.49	1.59	1.52
1	A	198	VAL	C-O	-5.48	1.18	1.24
1	D	156	PRO	C-O	-5.47	1.17	1.24
1	D	210	GLY	C-N	5.47	1.41	1.33
1	A	234	SER	C-O	-5.47	1.17	1.24
1	A	221	TYR	C-O	5.46	1.30	1.23
1	D	304	SER	N-CA	5.46	1.53	1.46
1	D	217	ARG	CA-C	5.44	1.58	1.52
1	A	349	LEU	C-O	5.42	1.30	1.24
1	B	116	ALA	C-O	-5.41	1.17	1.24
1	B	238	ARG	NE-CZ	5.41	1.39	1.33
1	B	64	ASP	C-O	-5.39	1.17	1.24
1	A	90	ASP	CA-C	5.37	1.59	1.52
1	C	317	LEU	CA-C	5.36	1.59	1.52
1	B	10	ALA	C-O	-5.35	1.17	1.23
1	D	16	TYR	C-O	-5.34	1.17	1.24
1	D	142	ALA	CA-C	5.34	1.59	1.52
1	C	151	TYR	C-O	5.33	1.30	1.24
1	A	256	ASP	N-CA	5.33	1.52	1.46
1	C	54	LEU	C-N	5.31	1.40	1.33
1	B	316	ILE	CA-CB	5.31	1.60	1.54
1	A	238	ARG	C-O	-5.28	1.17	1.24
1	C	166	GLU	C-O	-5.27	1.18	1.24
1	A	5	ALA	CA-CB	5.27	1.62	1.53
1	D	118	ILE	C-O	-5.27	1.18	1.24
1	B	271	ILE	CA-C	-5.26	1.46	1.52
1	B	307	GLU	CA-C	5.26	1.59	1.52
1	A	249	ILE	CA-CB	-5.25	1.48	1.54
1	C	53	VAL	CA-CB	5.25	1.60	1.54
1	C	145	VAL	CA-CB	5.25	1.62	1.54
1	A	348	VAL	CA-CB	5.24	1.61	1.54
1	C	218	SER	CA-C	5.23	1.59	1.52
1	C	45	ALA	CA-CB	5.23	1.62	1.53
1	D	183	VAL	CA-C	5.19	1.58	1.52
1	C	117	ARG	CA-C	5.18	1.59	1.52
1	D	65	PHE	C-O	-5.18	1.18	1.24
1	D	140	ALA	CA-CB	5.17	1.61	1.53
1	D	64	ASP	C-O	-5.17	1.17	1.24
1	A	44	ALA	CA-CB	5.15	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	7	VAL	C-N	-5.14	1.27	1.33
1	D	323	THR	CA-CB	-5.14	1.45	1.53
1	D	283	VAL	CA-C	5.14	1.59	1.52
1	C	294	PRO	N-CD	5.11	1.54	1.47
1	B	142	ALA	CA-CB	-5.10	1.45	1.53
1	B	6	GLY	C-N	-5.10	1.26	1.33
1	B	52	LEU	C-O	-5.10	1.17	1.24
1	A	59	TYR	C-O	-5.10	1.17	1.24
1	D	106	VAL	C-O	-5.08	1.18	1.24
1	C	188	PHE	CA-C	5.06	1.59	1.52
1	D	45	ALA	C-O	-5.05	1.17	1.24
1	B	12	PRO	C-O	-5.05	1.18	1.24
1	C	306	GLY	C-O	-5.05	1.17	1.23
1	C	267	THR	CA-CB	5.04	1.63	1.54
1	C	119	ALA	C-O	-5.04	1.18	1.24
1	B	329	PRO	C-O	5.04	1.29	1.23
1	C	186	ALA	CA-CB	5.03	1.61	1.53
1	B	254	ALA	CA-CB	-5.03	1.45	1.53
1	C	177	PRO	N-CD	5.03	1.54	1.47
1	D	67	ASP	C-O	-5.02	1.18	1.24
1	C	166	GLU	N-CA	-5.01	1.40	1.46

All (283) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	ALA	CA-C-N	12.20	133.23	119.32
1	A	155	ALA	C-N-CA	12.20	133.23	119.32
1	D	352	TRP	CA-C-N	11.73	142.82	121.70
1	D	352	TRP	C-N-CA	11.73	142.82	121.70
1	A	177	PRO	CA-C-O	-11.49	112.53	121.38
1	B	71	ILE	N-CA-C	-10.19	100.43	110.72
1	C	59	TYR	CA-C-N	-10.00	109.36	119.56
1	C	59	TYR	C-N-CA	-10.00	109.36	119.56
1	D	131	MET	CA-C-N	9.76	132.03	119.84
1	D	131	MET	C-N-CA	9.76	132.03	119.84
1	D	22	THR	N-CA-C	-9.53	100.98	111.36
1	D	320	LEU	N-CA-C	9.49	122.60	111.02
1	D	283	VAL	N-CA-C	9.44	120.28	110.36
1	D	302	TRP	N-CA-C	-9.22	100.62	112.23
1	C	268	LYS	N-CA-C	-9.21	102.06	113.20
1	C	149	ARG	NE-CZ-NH1	-9.05	112.45	121.50
1	C	271	ILE	CB-CA-C	8.92	120.86	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	75	LYS	N-CA-C	8.64	122.32	111.69
1	B	307	GLU	N-CA-C	8.60	123.06	112.23
1	D	293	LEU	CA-C-N	8.55	129.18	120.38
1	D	293	LEU	C-N-CA	8.55	129.18	120.38
1	A	227	ILE	N-CA-C	8.23	118.32	110.42
1	B	106	VAL	CA-C-O	8.17	125.83	119.46
1	D	122	LEU	N-CA-C	-8.04	103.03	112.92
1	C	124	LEU	CA-C-O	8.02	130.05	121.55
1	A	307	GLU	N-CA-C	8.01	120.79	111.02
1	A	325	GLU	N-CA-C	8.01	119.64	111.07
1	A	152	LEU	N-CA-C	-7.96	103.14	113.17
1	D	180	SER	N-CA-C	7.82	120.56	111.02
1	B	158	ASP	N-CA-C	7.73	120.50	110.53
1	D	352	TRP	O-C-N	-7.66	112.70	122.20
1	A	97	ASP	N-CA-C	7.61	120.64	111.82
1	C	182	LEU	N-CA-C	7.55	119.52	111.28
1	A	280	GLY	N-CA-C	-7.35	97.35	112.34
1	D	319	ILE	N-CA-C	7.28	118.04	110.62
1	D	114	LEU	N-CA-C	7.27	120.13	111.33
1	B	319	ILE	N-CA-C	-7.22	102.16	112.35
1	A	350	LEU	N-CA-C	7.16	121.18	109.72
1	B	50	ARG	CA-C-N	-7.16	111.50	122.09
1	B	50	ARG	C-N-CA	-7.16	111.50	122.09
1	A	221	TYR	N-CA-C	7.11	118.75	109.93
1	D	230	TRP	CA-C-O	-7.11	113.17	120.71
1	D	344	CYS	N-CA-C	7.09	119.53	108.96
1	D	49	GLY	CA-C-O	-7.08	114.06	121.63
1	D	46	LYS	N-CA-C	7.05	121.13	111.54
1	D	202	ARG	NE-CZ-NH1	-7.03	114.47	121.50
1	B	263	ALA	N-CA-C	-7.00	102.80	111.75
1	D	277	HIS	N-CA-C	-7.00	100.94	109.83
1	D	130	ARG	N-CA-C	6.99	120.30	108.90
1	C	37	ILE	N-CA-C	-6.99	103.66	110.72
1	A	137	GLY	N-CA-C	6.96	123.97	111.02
1	A	28	PHE	CA-C-N	-6.94	111.16	119.84
1	A	28	PHE	C-N-CA	-6.94	111.16	119.84
1	B	294	PRO	CA-C-N	6.93	126.54	119.19
1	B	294	PRO	C-N-CA	6.93	126.54	119.19
1	A	261	LEU	N-CA-C	6.92	120.20	111.69
1	A	164	SER	CA-C-N	-6.89	114.21	123.10
1	A	164	SER	C-N-CA	-6.89	114.21	123.10
1	C	271	ILE	N-CA-C	6.88	118.38	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	LEU	N-CA-C	6.88	118.86	111.36
1	A	187	LEU	N-CA-C	6.86	121.92	112.04
1	C	251	ARG	NE-CZ-NH1	-6.77	114.73	121.50
1	B	325	GLU	N-CA-C	6.75	118.29	111.07
1	A	231	ASP	CA-C-N	6.74	130.96	121.66
1	A	231	ASP	C-N-CA	6.74	130.96	121.66
1	C	221	TYR	CA-C-N	-6.73	113.03	119.90
1	C	221	TYR	C-N-CA	-6.73	113.03	119.90
1	D	231	ASP	N-CA-CB	6.72	120.37	110.35
1	C	187	LEU	N-CA-C	6.70	121.50	113.12
1	A	255	ASN	N-CA-C	6.70	118.58	111.28
1	C	293	LEU	CA-C-N	-6.65	113.53	120.38
1	C	293	LEU	C-N-CA	-6.65	113.53	120.38
1	A	206	VAL	N-CA-C	-6.59	106.24	113.43
1	B	315	SER	N-CA-C	6.59	119.02	111.11
1	C	278	PRO	CA-C-O	-6.59	108.61	120.60
1	C	22	THR	N-CA-C	-6.57	103.32	112.45
1	C	149	ARG	NE-CZ-NH2	6.57	125.11	119.20
1	A	171	THR	CA-C-N	6.51	129.17	120.58
1	A	171	THR	C-N-CA	6.51	129.17	120.58
1	D	340	GLY	CA-C-N	6.50	126.27	119.76
1	D	340	GLY	C-N-CA	6.50	126.27	119.76
1	A	172	TYR	N-CA-C	6.50	122.49	113.45
1	C	52	LEU	CA-C-N	6.50	128.88	120.56
1	C	52	LEU	C-N-CA	6.50	128.88	120.56
1	C	261	LEU	N-CA-C	-6.49	104.05	112.23
1	A	64	ASP	N-CA-C	6.45	118.66	108.67
1	C	313	SER	N-CA-C	-6.43	104.69	112.54
1	A	174	ALA	N-CA-C	6.42	120.94	113.18
1	C	65	PHE	N-CA-C	6.40	117.92	111.07
1	A	109	VAL	CB-CA-C	-6.38	103.24	111.53
1	D	272	GLY	N-CA-C	6.32	122.49	114.66
1	D	42	HIS	N-CA-C	6.31	118.68	111.11
1	B	138	SER	N-CA-C	6.30	120.06	112.38
1	B	215	ASP	N-CA-C	6.28	117.77	108.60
1	D	210	GLY	CA-C-N	-6.28	114.26	120.98
1	D	210	GLY	C-N-CA	-6.28	114.26	120.98
1	C	344	CYS	N-CA-C	6.28	118.61	109.07
1	B	278	PRO	CB-CA-C	-6.27	104.56	113.09
1	A	306	GLY	CA-C-N	6.25	129.48	120.79
1	A	306	GLY	C-N-CA	6.25	129.48	120.79
1	B	54	LEU	CA-C-N	-6.24	113.85	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	LEU	C-N-CA	-6.24	113.85	120.03
1	B	212	ASP	N-CA-C	-6.24	100.34	110.20
1	A	308	ILE	N-CA-C	6.22	119.13	113.10
1	B	115	ASP	N-CA-C	-6.19	104.61	111.36
1	C	201	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	C	315	SER	CA-C-N	6.13	128.85	120.46
1	C	315	SER	C-N-CA	6.13	128.85	120.46
1	A	239	LEU	CA-CB-CG	-6.12	94.89	116.30
1	A	214	LEU	N-CA-C	6.09	120.91	112.45
1	D	207	ARG	N-CA-C	6.08	118.53	109.59
1	B	205	GLN	N-CA-C	6.07	117.77	111.03
1	D	150	ASP	N-CA-CB	6.02	118.75	110.01
1	C	85	LEU	N-CA-C	-6.02	104.06	111.40
1	C	140	ALA	N-CA-C	-6.02	104.65	112.23
1	C	252	TYR	N-CA-C	6.01	121.36	113.30
1	D	152	LEU	N-CA-C	6.01	118.79	111.82
1	C	328	PRO	CA-C-N	-5.99	113.52	119.93
1	C	328	PRO	C-N-CA	-5.99	113.52	119.93
1	B	217	ARG	NE-CZ-NH2	5.99	124.59	119.20
1	A	294	PRO	N-CA-C	-5.93	103.46	110.70
1	D	158	ASP	N-CA-C	5.92	119.60	110.42
1	C	251	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	D	138	SER	N-CA-C	5.91	119.96	112.87
1	B	280	GLY	CA-C-O	-5.91	113.07	121.52
1	C	15	ARG	N-CA-C	5.90	118.34	108.96
1	A	61	SER	CA-C-N	5.89	130.25	122.06
1	A	61	SER	C-N-CA	5.89	130.25	122.06
1	C	232	VAL	N-CA-C	5.89	117.83	108.87
1	D	130	ARG	CA-C-N	-5.88	116.51	122.74
1	D	130	ARG	C-N-CA	-5.88	116.51	122.74
1	D	340	GLY	N-CA-C	-5.88	100.35	112.34
1	A	259	THR	N-CA-C	-5.87	104.96	111.36
1	D	181	SER	N-CA-C	5.87	118.16	111.11
1	A	247	ASN	N-CA-C	5.86	119.69	112.54
1	D	148	LEU	N-CA-C	-5.86	104.81	111.14
1	A	282	LYS	CA-C-N	5.85	128.01	120.70
1	A	282	LYS	C-N-CA	5.85	128.01	120.70
1	A	6	GLY	N-CA-C	5.85	119.88	110.87
1	C	281	PRO	CA-C-N	5.83	128.90	120.79
1	C	281	PRO	C-N-CA	5.83	128.90	120.79
1	D	290	SER	N-CA-C	5.83	119.21	111.75
1	A	48	ASN	N-CA-C	5.82	120.52	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	PRO	CA-C-O	-5.82	113.22	122.82
1	A	257	VAL	N-CA-C	5.82	116.55	110.62
1	D	155	ALA	CA-C-N	-5.81	113.76	120.04
1	D	155	ALA	C-N-CA	-5.81	113.76	120.04
1	B	253	LEU	N-CA-C	5.79	117.40	111.14
1	B	280	GLY	O-C-N	5.79	127.56	121.77
1	A	273	ALA	N-CA-C	5.79	117.87	108.26
1	D	256	ASP	N-CA-CB	5.78	118.62	110.12
1	A	147	ARG	CA-C-N	5.78	128.29	120.44
1	A	147	ARG	C-N-CA	5.78	128.29	120.44
1	B	252	TYR	N-CA-C	5.75	120.42	113.17
1	C	257	VAL	N-CA-C	5.73	115.92	110.53
1	D	125	ARG	CA-C-N	-5.73	113.12	119.19
1	D	125	ARG	C-N-CA	-5.73	113.12	119.19
1	D	188	PHE	CA-C-N	5.72	127.26	122.17
1	D	188	PHE	C-N-CA	5.72	127.26	122.17
1	B	131	MET	CA-C-N	5.72	126.99	119.84
1	B	131	MET	C-N-CA	5.72	126.99	119.84
1	A	301	THR	O-C-N	-5.71	116.07	122.12
1	A	311	LEU	N-CA-C	-5.70	105.63	112.59
1	A	67	ASP	CB-CA-C	-5.70	101.90	110.90
1	C	148	LEU	N-CA-C	-5.70	105.15	111.36
1	A	176	LYS	CA-C-N	-5.68	115.91	121.65
1	A	176	LYS	C-N-CA	-5.68	115.91	121.65
1	D	265	ARG	NE-CZ-NH2	5.68	124.31	119.20
1	D	276	SER	N-CA-C	5.68	119.22	110.42
1	D	325	GLU	N-CA-C	5.67	118.19	111.33
1	A	305	LEU	CA-C-N	5.65	126.10	119.94
1	A	305	LEU	C-N-CA	5.65	126.10	119.94
1	B	287	VAL	CB-CA-C	-5.64	104.76	111.81
1	D	6	GLY	N-CA-C	5.63	119.36	111.14
1	A	145	VAL	N-CA-C	-5.63	104.05	111.09
1	C	230	TRP	CB-CA-C	-5.62	98.75	109.66
1	D	289	THR	CA-C-N	5.62	128.59	120.38
1	D	289	THR	C-N-CA	5.62	128.59	120.38
1	C	195	VAL	N-CA-C	5.61	116.03	108.17
1	B	147	ARG	N-CA-CB	5.60	119.53	110.40
1	D	89	ASP	N-CA-C	5.60	117.06	111.07
1	C	289	THR	CB-CA-C	-5.59	101.63	110.86
1	B	78	ASP	CB-CA-C	-5.58	102.05	110.92
1	A	286	ALA	N-CA-C	-5.57	104.84	111.69
1	D	243	PRO	CA-C-O	-5.56	112.20	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	278	PRO	CB-CA-C	-5.55	105.54	113.09
1	C	79	LEU	N-CA-C	5.54	118.24	111.82
1	D	137	GLY	N-CA-C	5.53	121.30	111.73
1	A	222	PRO	CA-C-O	-5.53	115.04	121.34
1	C	206	VAL	N-CA-C	-5.52	107.44	112.96
1	A	94	ARG	CA-C-N	-5.51	113.24	118.97
1	A	94	ARG	C-N-CA	-5.51	113.24	118.97
1	A	110	ALA	N-CA-C	5.50	118.21	109.24
1	B	37	ILE	CA-C-N	5.50	127.58	120.70
1	B	37	ILE	C-N-CA	5.50	127.58	120.70
1	A	98	ILE	N-CA-C	5.49	116.09	108.84
1	A	157	ASP	CB-CA-C	-5.48	101.30	110.56
1	D	215	ASP	N-CA-C	5.46	116.75	108.07
1	A	253	LEU	N-CA-C	5.45	117.31	111.36
1	B	56	LEU	N-CA-C	-5.44	105.43	111.36
1	D	59	TYR	N-CA-C	5.44	119.64	112.35
1	D	135	GLY	N-CA-C	-5.43	107.53	115.63
1	C	335	LEU	N-CA-C	5.42	117.79	109.07
1	A	98	ILE	N-CA-CB	-5.41	104.82	110.82
1	D	260	PHE	N-CA-C	-5.40	104.94	112.45
1	A	188	PHE	CA-C-O	5.40	127.21	121.05
1	C	267	THR	N-CA-C	-5.40	101.09	109.24
1	A	120	GLY	N-CA-C	-5.38	106.25	112.50
1	A	139	VAL	N-CA-C	-5.38	105.70	113.07
1	C	54	LEU	CA-C-O	5.37	125.44	120.60
1	C	217	ARG	CG-CD-NE	-5.37	100.18	112.00
1	D	41	LEU	N-CA-C	-5.36	105.35	111.14
1	A	246	THR	N-CA-C	5.35	116.79	111.07
1	A	213	ILE	N-CA-C	-5.34	98.22	106.72
1	C	289	THR	N-CA-CB	5.34	117.92	110.07
1	D	202	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	A	33	GLU	N-CA-C	-5.33	106.04	112.54
1	B	136	LEU	N-CA-C	-5.33	106.95	113.50
1	D	205	GLN	N-CA-C	5.33	118.00	111.82
1	C	16	TYR	N-CA-C	5.33	118.16	109.59
1	B	175	VAL	N-CA-CB	5.32	116.91	110.95
1	D	129	ARG	CG-CD-NE	-5.32	100.30	112.00
1	B	106	VAL	CB-CA-C	5.32	115.96	110.70
1	B	220	LEU	CA-C-N	5.27	128.57	121.20
1	B	220	LEU	C-N-CA	5.27	128.57	121.20
1	D	151	TYR	N-CA-C	5.26	117.10	111.36
1	C	40	ARG	O-C-N	-5.26	116.62	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	ASP	CA-C-N	5.25	127.63	120.54
1	D	89	ASP	C-N-CA	5.25	127.63	120.54
1	C	146	ALA	CA-C-N	5.24	129.59	120.68
1	C	146	ALA	C-N-CA	5.24	129.59	120.68
1	B	162	LEU	CA-C-N	-5.24	115.88	123.11
1	B	162	LEU	C-N-CA	-5.24	115.88	123.11
1	C	188	PHE	N-CA-C	5.24	118.09	109.76
1	B	168	CYS	N-CA-C	5.22	116.66	111.07
1	D	185	THR	N-CA-C	-5.22	106.42	112.89
1	D	308	ILE	N-CA-C	5.22	120.20	109.34
1	A	300	LEU	N-CA-C	5.21	116.96	111.28
1	C	278	PRO	CB-CA-C	-5.21	102.96	111.56
1	C	270	ASP	N-CA-C	-5.21	106.76	113.01
1	D	226	HIS	N-CA-C	-5.20	106.78	113.23
1	A	85	LEU	CA-C-N	5.20	125.75	119.98
1	A	85	LEU	C-N-CA	5.20	125.75	119.98
1	A	119	ALA	CA-C-N	5.20	125.71	119.94
1	A	119	ALA	C-N-CA	5.20	125.71	119.94
1	B	306	GLY	N-CA-C	-5.19	106.13	112.77
1	C	126	PRO	CB-CA-C	-5.18	104.49	111.85
1	C	116	ALA	N-CA-C	-5.17	105.09	111.40
1	A	130	ARG	CA-C-N	-5.17	117.73	122.28
1	A	130	ARG	C-N-CA	-5.17	117.73	122.28
1	B	292	ALA	CA-C-N	5.16	135.62	120.97
1	B	292	ALA	C-N-CA	5.16	135.62	120.97
1	B	89	ASP	CA-C-N	5.15	127.61	120.29
1	B	89	ASP	C-N-CA	5.15	127.61	120.29
1	A	12	PRO	CA-C-N	5.15	124.77	119.05
1	A	12	PRO	C-N-CA	5.15	124.77	119.05
1	C	67	ASP	CB-CG-OD1	5.15	130.24	118.40
1	B	220	LEU	O-C-N	-5.14	116.76	122.93
1	C	303	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	D	198	VAL	N-CA-C	5.13	116.75	108.85
1	B	74	GLU	CB-CA-C	-5.12	102.62	110.81
1	B	170	LEU	N-CA-C	-5.11	107.00	113.18
1	A	348	VAL	CB-CA-C	5.11	117.31	110.42
1	D	258	THR	N-CA-C	5.11	116.85	111.28
1	B	107	THR	N-CA-CB	-5.10	103.15	110.65
1	A	319	ILE	CA-C-N	5.09	127.11	120.28
1	A	319	ILE	C-N-CA	5.09	127.11	120.28
1	B	117	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	C	224	SER	CB-CA-C	-5.07	101.04	109.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	289	THR	CB-CA-C	5.07	118.76	110.96
1	A	249	ILE	N-CA-C	-5.06	104.97	110.23
1	D	345	THR	N-CA-C	-5.06	101.51	109.50
1	C	176	LYS	CA-C-N	-5.05	113.53	119.84
1	C	176	LYS	C-N-CA	-5.05	113.53	119.84
1	A	277	HIS	O-C-N	5.04	126.32	121.28
1	B	169	SER	CB-CA-C	-5.02	100.42	110.42
1	C	24	SER	CB-CA-C	-5.01	102.47	110.79
1	C	41	LEU	CA-C-N	5.01	127.40	120.29
1	C	41	LEU	C-N-CA	5.01	127.40	120.29
1	A	131	MET	CA-C-N	5.00	126.10	119.84
1	A	131	MET	C-N-CA	5.00	126.10	119.84
1	A	97	ASP	CA-C-N	5.00	128.68	121.18
1	A	97	ASP	C-N-CA	5.00	128.68	121.18

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	LYS	Peptide
1	C	239	LEU	Peptide
1	D	352	TRP	Peptide

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	2642	0	2675	113	0
1	B	2652	0	2681	145	0
1	C	2642	0	2675	145	0
1	D	2642	0	2674	133	1
2	A	18	0	31	11	0
2	B	18	0	31	9	0
2	C	18	0	31	4	0
2	D	18	0	31	5	0
3	B	48	0	32	4	0
3	C	48	0	32	6	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	20	0	0	0	0
4	B	30	0	0	5	0
4	C	25	0	0	3	0
4	D	21	0	0	2	0
All	All	10842	0	10893	511	1

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 24.

All (511) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:SER:HB3	1:C:343:PHE:H	1.10	1.11
1:B:353:ARG:HG2	1:B:353:ARG:HH11	1.12	1.07
1:B:107:THR:HG21	1:B:167:LEU:H	1.00	1.06
1:C:106:VAL:HG11	2:C:401:PLM:H21	1.36	1.04
1:C:34:HIS:HB3	1:C:37:ILE:HD11	1.37	1.03
1:A:182:LEU:O	1:A:185:THR:HG22	1.61	1.00
1:D:17:SER:OG	1:D:20:GLU:HG3	1.66	0.95
1:B:107:THR:HG21	1:B:167:LEU:N	1.83	0.94
1:B:267:THR:HG22	1:B:269:ASP:H	1.32	0.93
1:D:94:ARG:HB3	1:D:94:ARG:CZ	1.94	0.93
1:C:217:ARG:HG2	1:C:217:ARG:NH2	1.83	0.92
1:B:257:VAL:O	1:B:261:LEU:HD12	1.70	0.91
1:D:15:ARG:CG	1:D:15:ARG:HH21	1.82	0.91
1:C:18:GLN:NE2	1:C:50:ARG:HH21	1.70	0.89
1:A:42:HIS:NE2	1:A:185:THR:HG23	1.87	0.89
1:B:84:LEU:HD23	1:B:122:LEU:HD12	1.54	0.89
1:B:230:TRP:HH2	2:B:401:PLM:H62	1.33	0.88
1:D:17:SER:HG	1:D:20:GLU:HG3	1.36	0.88
1:C:249:ILE:HD11	1:C:339:MET:HG3	1.52	0.87
1:A:178:THR:HG23	1:A:181:SER:H	1.37	0.86
1:B:268:LYS:HD2	1:B:291:LEU:O	1.76	0.85
3:C:402:COA:H8A	3:C:402:COA:H52A	1.58	0.84
1:D:308:ILE:HD12	1:D:311:LEU:HD21	1.62	0.82
1:C:140:ALA:HB3	1:C:313:SER:HB2	1.62	0.81
1:C:224:SER:HB3	1:C:343:PHE:N	1.93	0.80
1:C:166:GLU:HG3	1:C:312:SER:HB3	1.63	0.80
1:B:103:THR:HG21	1:B:115:ASP:OD2	1.82	0.80
1:B:107:THR:CG2	1:B:167:LEU:H	1.91	0.80
1:A:69:ASN:HD21	1:A:109:VAL:H	1.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:GLN:HE22	1:C:50:ARG:HH21	1.29	0.79
1:D:15:ARG:HH21	1:D:15:ARG:HG3	1.46	0.79
1:B:26:VAL:HG11	1:B:35:GLU:OE1	1.83	0.78
1:B:353:ARG:HG2	1:B:353:ARG:NH1	1.92	0.78
1:C:217:ARG:HG2	1:C:217:ARG:HH21	1.47	0.78
1:C:67:ASP:O	1:C:71:ILE:HG13	1.84	0.78
1:D:211:PRO:HG3	1:D:352:TRP:CE3	2.18	0.78
1:B:141:GLY:O	1:B:145:VAL:HG23	1.83	0.77
1:B:230:TRP:CH2	2:B:401:PLM:H62	2.19	0.77
1:B:201:ARG:HD2	1:D:353:ARG:HB2	1.67	0.77
1:C:198:VAL:HG13	1:C:202:ARG:HB3	1.67	0.76
1:C:183:VAL:HG13	3:C:402:COA:CDP	2.16	0.76
1:B:103:THR:HG22	1:B:132:PRO:HA	1.68	0.76
1:B:201:ARG:HE	1:D:353:ARG:HH11	1.33	0.76
1:C:106:VAL:CG1	2:C:401:PLM:H21	2.15	0.76
1:B:69:ASN:HD21	1:B:109:VAL:H	1.35	0.75
1:C:337:LEU:HG	1:C:347:LEU:CD2	2.17	0.74
1:D:140:ALA:HB3	1:D:313:SER:HB3	1.69	0.74
1:D:308:ILE:HD12	1:D:311:LEU:CD2	2.18	0.74
1:D:201:ARG:HH11	1:D:204:GLU:CD	1.96	0.74
1:A:188:PHE:CZ	2:A:400:PLM:H62	2.23	0.73
1:C:294:PRO:HB2	1:C:295:PRO:HD2	1.71	0.73
1:A:188:PHE:CE1	2:A:400:PLM:H61	2.23	0.72
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.54	0.72
1:C:214:LEU:O	1:C:215:ASP:HB2	1.89	0.72
1:B:233:GLY:HA3	1:B:235[A]:HIS:CE1	2.25	0.72
1:D:310:ASN:HD22	1:D:312:SER:H	1.38	0.72
1:B:185:THR:HA	2:B:401:PLM:HB1	1.73	0.71
1:C:15:ARG:NH1	1:C:49:GLY:HA3	2.05	0.71
1:B:42:HIS:CD2	1:B:186:ALA:HB2	2.26	0.71
1:D:2:SER:N	1:D:200:ASP:OD1	2.23	0.71
1:D:42:HIS:HD2	1:D:186:ALA:HB2	1.54	0.71
1:C:135:GLY:HA2	1:D:111:VAL:HG22	1.71	0.70
1:C:28:PHE:HB2	1:C:31:LEU:HD12	1.73	0.70
1:D:119:ALA:HA	1:D:124:LEU:HG	1.72	0.70
1:A:274:TRP:CZ3	1:A:335:LEU:HD23	2.26	0.70
1:C:37:ILE:HG13	1:C:38:ILE:N	2.07	0.69
1:B:55:PRO:HD2	1:B:58:GLN:HE21	1.57	0.69
1:C:299:GLU:O	1:C:303:ARG:HG3	1.93	0.69
1:B:300:LEU:CD1	1:B:300:LEU:N	2.55	0.69
1:B:209:GLY:O	1:B:353:ARG:HG3	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:THR:O	1:D:182:LEU:HG	1.92	0.69
1:D:271:ILE:N	1:D:271:ILE:HD13	2.06	0.69
1:A:3:VAL:HG22	1:A:212:ASP:OD1	1.94	0.68
1:B:211:PRO:HG3	1:B:352:TRP:CZ3	2.28	0.68
1:C:311:LEU:HD11	4:C:504:HOH:O	1.94	0.68
1:B:255:ASN:O	1:B:259:THR:HG23	1.93	0.68
1:A:29:PRO:HD2	1:A:60:PRO:HB3	1.75	0.68
1:C:15:ARG:HB2	1:C:51:HIS:CD2	2.29	0.68
1:A:169:SER:HA	2:A:400:PLM:HF2	1.75	0.67
1:B:72:PHE:HE1	1:B:107:THR:HG22	1.58	0.67
1:B:283:VAL:HG23	3:B:402:COA:H61	1.76	0.67
1:D:310:ASN:ND2	1:D:312:SER:H	1.91	0.67
1:B:300:LEU:HD13	1:B:300:LEU:H	1.59	0.67
1:C:336:MET:HB2	1:C:348:VAL:HB	1.77	0.67
1:D:342:GLY:N	1:D:343:PHE:HA	2.09	0.67
1:B:84:LEU:HD23	1:B:122:LEU:CD1	2.24	0.67
1:C:280:GLY:O	1:C:284:ILE:HG13	1.95	0.67
1:B:188:PHE:CD2	2:B:401:PLM:H72	2.30	0.67
1:D:28:PHE:CD1	1:D:60:PRO:HG3	2.30	0.67
1:D:217:ARG:HB2	1:D:260:PHE:CD1	2.30	0.66
1:D:15:ARG:HD3	1:D:51:HIS:CE1	2.30	0.66
1:B:300:LEU:N	1:B:300:LEU:HD13	2.09	0.66
1:A:28:PHE:HB2	1:A:31:LEU:HD12	1.77	0.66
1:A:188:PHE:CE1	2:A:400:PLM:C6	2.79	0.66
1:B:257:VAL:O	1:B:261:LEU:CD1	2.43	0.65
1:C:251:ARG:HG2	1:C:252:TYR:CE2	2.31	0.65
1:C:15:ARG:HD2	1:C:51:HIS:CE1	2.31	0.65
1:D:268:LYS:HE2	1:D:268:LYS:H	1.62	0.65
1:B:336:MET:HB2	1:B:348:VAL:HB	1.79	0.65
1:A:119:ALA:HA	1:A:124:LEU:HG	1.79	0.64
1:C:4:ILE:O	1:C:210:GLY:HA3	1.97	0.64
1:C:135:GLY:CA	1:D:111:VAL:HG22	2.27	0.64
1:B:153:ARG:HD2	4:B:525:HOH:O	1.97	0.64
1:A:155:ALA:N	1:A:156:PRO:HD3	2.12	0.64
1:C:257:VAL:HG13	1:C:261:LEU:HD22	1.78	0.64
1:C:308:ILE:HD12	1:C:311:LEU:HD22	1.80	0.64
1:D:202:ARG:O	1:D:202:ARG:HG3	1.98	0.64
1:A:3:VAL:HG13	1:A:353:ARG:HH22	1.62	0.64
1:C:42:HIS:CD2	1:C:186:ALA:HA	2.34	0.63
1:C:140:ALA:HB3	1:C:313:SER:CB	2.27	0.63
1:B:55:PRO:HD2	1:B:58:GLN:NE2	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:TYR:HE2	1:B:169:SER:HB3	1.63	0.63
1:B:72:PHE:CE1	1:B:107:THR:HG22	2.33	0.63
1:D:94:ARG:CZ	1:D:94:ARG:CB	2.72	0.63
1:C:99:ASP:OD1	1:C:125:ARG:NH1	2.31	0.63
1:D:28:PHE:HB2	1:D:31:LEU:HD23	1.81	0.63
1:C:209:GLY:O	1:C:210:GLY:O	2.16	0.63
1:B:193:ALA:HB3	1:B:317:LEU:HD12	1.80	0.63
1:A:311:LEU:HB3	1:A:314:ALA:HB3	1.81	0.62
1:B:274:TRP:CZ2	1:B:293:LEU:HD21	2.34	0.62
1:C:220:LEU:HB2	4:D:513:HOH:O	1.99	0.62
1:C:53:VAL:CG2	1:C:75:LYS:HD2	2.29	0.62
1:C:244:ASP:HA	1:C:247:ASN:ND2	2.15	0.62
1:B:103:THR:CG2	1:B:115:ASP:OD2	2.47	0.62
1:B:310:ASN:HD22	1:B:312:SER:H	1.48	0.62
1:D:294:PRO:O	1:D:295:PRO:C	2.37	0.62
1:A:329:PRO:CD	1:C:265:ARG:NH2	2.63	0.61
1:B:59:TYR:CE2	1:B:169:SER:HB3	2.35	0.61
1:B:294:PRO:HB2	1:B:296:GLU:OE2	2.01	0.61
1:A:214:LEU:HB2	1:A:349:LEU:HD23	1.81	0.61
1:B:29:PRO:HD2	1:B:60:PRO:HB3	1.82	0.61
1:A:29:PRO:CD	1:A:60:PRO:HB3	2.30	0.61
1:C:221:TYR:CD1	1:C:221:TYR:N	2.68	0.61
1:C:239:LEU:HD13	2:C:401:PLM:H42	1.83	0.61
1:C:198:VAL:HG12	1:C:199:GLY:O	2.01	0.60
1:B:267:THR:N	1:B:270:ASP:OD2	2.32	0.60
1:C:18:GLN:HE22	1:C:50:ARG:NH2	1.97	0.60
1:D:111:VAL:HA	1:D:112:PRO:C	2.26	0.60
1:D:278:PRO:HG3	1:D:319:ILE:HD11	1.83	0.60
1:A:265:ARG:HG3	1:D:154:GLY:HA2	1.84	0.60
1:D:15:ARG:CG	1:D:15:ARG:NH2	2.50	0.60
1:C:339:MET:HA	1:C:344:CYS:O	2.02	0.59
1:D:15:ARG:HH21	1:D:15:ARG:HG2	1.65	0.59
1:D:271:ILE:N	1:D:271:ILE:CD1	2.64	0.59
1:D:69:ASN:O	1:D:73:ILE:HG13	2.01	0.59
1:A:28:PHE:O	1:A:29:PRO:C	2.42	0.59
1:C:35:GLU:O	1:C:39:ARG:HG3	2.03	0.59
1:B:329:PRO:HD2	1:B:332:SER:OG	2.03	0.59
1:A:34:HIS:O	1:A:38:ILE:HG13	2.02	0.59
1:C:111:VAL:HA	1:C:112:PRO:C	2.28	0.59
1:C:22:THR:O	1:C:26:VAL:HG13	2.03	0.59
1:D:15:ARG:NH2	1:D:15:ARG:HG2	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PHE:CZ	2:A:400:PLM:C6	2.86	0.58
1:C:125:ARG:NH2	1:C:127:ASP:OD2	2.37	0.58
1:C:294:PRO:HB2	1:C:295:PRO:CD	2.34	0.58
1:B:326:LYS:HG2	1:B:326:LYS:O	2.03	0.58
1:C:77:VAL:O	1:C:81:VAL:HG23	2.03	0.58
1:C:198:VAL:CG1	1:C:202:ARG:HB3	2.33	0.58
1:C:206:VAL:O	1:C:207:ARG:HB2	2.03	0.58
1:C:251:ARG:HG2	1:C:252:TYR:CZ	2.39	0.57
1:A:321:ARG:O	1:A:325:GLU:HG3	2.05	0.57
1:C:308:ILE:O	1:C:311:LEU:HD13	2.04	0.57
1:D:333:ALA:HA	1:D:350:LEU:O	2.04	0.57
1:B:166:GLU:HG3	1:B:312:SER:HB3	1.87	0.57
1:C:95:PRO:HB3	1:C:124:LEU:HD12	1.86	0.57
1:D:42:HIS:CD2	1:D:186:ALA:HB2	2.38	0.57
1:B:193:ALA:HB3	1:B:317:LEU:CD1	2.34	0.57
1:A:268:LYS:NZ	1:A:268:LYS:HB3	2.20	0.56
1:C:221:TYR:O	1:C:224:SER:HB2	2.05	0.56
1:B:227:ILE:HA	1:B:242:SER:HB2	1.86	0.56
1:B:275:VAL:HG11	1:B:320:LEU:HB2	1.86	0.56
1:C:221:TYR:N	1:C:221:TYR:HD1	2.01	0.56
1:D:88:LEU:HD21	1:D:98:ILE:HD11	1.85	0.56
1:D:283:VAL:O	1:D:287:VAL:HG23	2.05	0.56
1:B:339:MET:O	1:B:339:MET:HG2	2.05	0.56
1:A:155:ALA:N	1:A:156:PRO:CD	2.68	0.56
1:B:119:ALA:HA	1:B:124:LEU:HG	1.87	0.56
1:A:26:VAL:HB	1:A:35:GLU:HB2	1.88	0.56
1:B:283:VAL:CG2	3:B:402:COA:H61	2.34	0.56
1:D:240:ARG:HH21	1:D:240:ARG:HG3	1.70	0.56
1:A:136:LEU:HG	1:B:132:PRO:HG2	1.88	0.56
1:D:35:GLU:O	1:D:39:ARG:HG3	2.05	0.56
1:B:106:VAL:CG1	2:B:401:PLM:H31	2.36	0.56
1:A:176:LYS:HD3	1:A:238:ARG:CZ	2.36	0.56
1:A:329:PRO:HG3	1:C:265:ARG:HH21	1.72	0.55
1:D:94:ARG:CB	1:D:94:ARG:NH1	2.69	0.55
1:A:230:TRP:CH2	2:A:400:PLM:H72	2.42	0.55
1:C:283:VAL:HG21	3:C:402:COA:H22	1.88	0.55
1:D:28:PHE:CZ	1:D:60:PRO:HD3	2.41	0.55
1:D:94:ARG:HB3	1:D:94:ARG:NH1	2.22	0.55
1:B:87:ALA:HB1	1:B:196:VAL:HG23	1.88	0.54
1:A:188:PHE:CD2	2:A:400:PLM:H92	2.43	0.54
1:B:2:SER:HB2	1:B:213:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASN:N	1:A:306:GLY:O	2.34	0.54
1:B:18:GLN:HA	1:B:18:GLN:HE21	1.72	0.54
1:C:4:ILE:O	1:C:210:GLY:CA	2.55	0.54
1:C:229:GLY:HA2	1:D:111:VAL:HG12	1.90	0.54
1:D:7:VAL:HG12	1:D:321:ARG:HB2	1.89	0.53
1:D:280:GLY:O	1:D:284:ILE:HG13	2.08	0.53
1:A:4:ILE:HB	1:A:211:PRO:HD2	1.89	0.53
1:D:85:LEU:HD21	1:D:122:LEU:HD22	1.89	0.53
1:B:227:ILE:O	1:B:228:MET:HB3	2.07	0.53
1:A:329:PRO:CD	1:C:265:ARG:HH22	2.22	0.53
1:A:59:TYR:CE1	1:A:169:SER:HB2	2.43	0.53
1:D:140:ALA:HB3	1:D:313:SER:CB	2.37	0.53
1:A:178:THR:O	1:A:182:LEU:HG	2.09	0.53
1:A:268:LYS:NZ	1:A:268:LYS:CB	2.71	0.53
1:B:59:TYR:N	1:B:60:PRO:CD	2.72	0.53
1:B:312:SER:OG	2:B:401:PLM:H21	2.09	0.53
1:D:151:TYR:CD1	1:D:151:TYR:C	2.85	0.53
1:B:14:HIS:HD2	1:B:52:LEU:O	1.91	0.53
1:C:337:LEU:HG	1:C:347:LEU:HD23	1.90	0.53
1:A:216:SER:HA	1:A:347:LEU:O	2.08	0.53
1:C:320:LEU:O	1:C:324:ILE:HG13	2.09	0.52
1:C:295:PRO:HG2	1:C:296:GLU:H	1.74	0.52
1:B:35:GLU:O	1:B:39:ARG:HG3	2.09	0.52
1:B:247:ASN:HD21	1:B:251:ARG:HH21	1.57	0.52
1:B:353:ARG:HH11	1:B:353:ARG:CG	1.99	0.52
1:D:143:ALA:O	1:D:147:ARG:HG2	2.09	0.52
1:A:221:TYR:N	1:A:221:TYR:CD1	2.78	0.52
1:B:87:ALA:CB	1:B:196:VAL:HG23	2.40	0.52
1:A:188:PHE:CE2	2:A:400:PLM:H81	2.45	0.52
1:A:264:HIS:ND1	1:D:157:ASP:OD2	2.35	0.52
1:B:285:ASP:O	1:B:289:THR:N	2.39	0.52
1:A:178:THR:HG22	1:A:181:SER:HB2	1.91	0.51
1:D:59:TYR:C	1:D:61:SER:N	2.67	0.51
1:D:325:GLU:C	1:D:327:ARG:H	2.18	0.51
1:C:87:ALA:HB1	1:C:196:VAL:HG23	1.91	0.51
1:B:216:SER:HB2	4:B:513:HOH:O	2.11	0.51
1:D:265:ARG:O	1:D:266:LEU:HD23	2.11	0.51
1:B:330:SER:HB2	1:B:353:ARG:OXT	2.10	0.51
1:B:301:THR:HA	1:B:319:ILE:HD13	1.93	0.51
1:D:3:VAL:HG12	1:D:4:ILE:O	2.11	0.51
1:D:352:TRP:O	1:D:353:ARG:HG2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:TYR:N	1:A:221:TYR:HD1	2.08	0.51
1:D:188:PHE:CD2	2:D:400:PLM:H52	2.46	0.51
1:C:164:SER:O	1:C:192:ALA:HA	2.11	0.51
1:B:294:PRO:HB2	1:B:296:GLU:CD	2.36	0.51
1:D:230:TRP:CH2	2:D:400:PLM:H42	2.45	0.51
1:A:154:GLY:O	1:B:153:ARG:HD3	2.11	0.51
1:B:262:ASP:C	1:B:264:HIS:N	2.66	0.51
1:B:268:LYS:NZ	1:B:268:LYS:HB3	2.25	0.51
1:C:228:MET:HG2	1:C:341:PRO:HG3	1.92	0.50
1:B:296:GLU:O	1:B:297:ALA:C	2.54	0.50
1:D:81:VAL:HG13	1:D:122:LEU:HD21	1.93	0.50
1:C:37:ILE:HG13	1:C:38:ILE:H	1.74	0.50
1:C:251:ARG:CG	1:C:252:TYR:CZ	2.94	0.50
1:B:201:ARG:HE	1:D:353:ARG:NH1	2.05	0.50
1:B:262:ASP:O	1:B:263:ALA:C	2.54	0.50
1:D:201:ARG:HA	1:D:201:ARG:NE	2.27	0.50
1:A:188:PHE:CG	2:A:400:PLM:H92	2.46	0.50
1:B:51:HIS:HE1	4:B:511:HOH:O	1.94	0.50
1:B:75:LYS:O	1:B:78:ASP:HB2	2.11	0.50
1:D:247:ASN:O	1:D:251:ARG:HB2	2.12	0.50
1:B:106:VAL:HG11	2:B:401:PLM:H31	1.93	0.50
1:A:274:TRP:CD1	1:A:297:ALA:HB1	2.47	0.50
1:C:179:VAL:O	1:C:183:VAL:HG23	2.11	0.50
1:C:48:ASN:HB2	1:C:306:GLY:O	2.11	0.50
1:B:103:THR:HB	1:B:115:ASP:HB3	1.93	0.50
1:B:215:ASP:OD2	1:B:264:HIS:HE1	1.95	0.50
1:A:178:THR:CG2	1:A:181:SER:HB2	2.42	0.50
1:B:230:TRP:CH2	2:B:401:PLM:C6	2.94	0.50
1:A:182:LEU:O	1:A:185:THR:CG2	2.47	0.50
1:D:12:PRO:O	1:D:51:HIS:HD2	1.94	0.49
1:D:323:THR:O	1:D:323:THR:HG22	2.10	0.49
1:D:337:LEU:C	1:D:337:LEU:HD12	2.37	0.49
1:B:2:SER:C	1:B:3:VAL:HG23	2.37	0.49
1:B:310:ASN:HD22	1:B:311:LEU:N	2.09	0.49
1:D:12:PRO:HG3	1:D:79:LEU:HD11	1.94	0.49
1:D:165:VAL:HG13	1:D:192:ALA:HB2	1.94	0.49
1:D:200:ASP:O	1:D:204:GLU:HG3	2.11	0.49
1:A:134:PHE:O	1:A:136:LEU:N	2.43	0.49
1:A:66:GLY:O	1:A:70:GLU:HG2	2.13	0.49
1:C:14:HIS:O	1:C:51:HIS:HA	2.13	0.49
1:C:280:GLY:H	1:C:283:VAL:HB	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:VAL:O	1:B:26:VAL:CG1	2.59	0.49
1:B:131:MET:O	1:B:131:MET:HG2	2.13	0.49
1:A:329:PRO:HD2	1:C:265:ARG:HH22	1.78	0.49
1:C:152:LEU:HD11	1:C:160:ALA:HB3	1.95	0.49
1:B:275:VAL:HG13	1:B:319:ILE:HG22	1.93	0.49
1:A:198:VAL:HG13	1:A:202:ARG:HB3	1.94	0.48
1:C:18:GLN:HE21	1:C:18:GLN:HA	1.77	0.48
1:B:2:SER:C	1:B:3:VAL:CG2	2.86	0.48
1:D:230:TRP:HH2	2:D:400:PLM:H62	1.77	0.48
1:D:278:PRO:HG3	1:D:319:ILE:CD1	2.43	0.48
1:B:54:LEU:HB2	1:B:59:TYR:CZ	2.48	0.48
1:A:98:ILE:CD1	1:A:161:VAL:HG11	2.43	0.48
1:B:221:TYR:N	1:B:221:TYR:CD1	2.82	0.48
1:B:310:ASN:ND2	1:B:312:SER:H	2.10	0.48
1:B:243:PRO:HG3	3:B:402:COA:C2A	2.44	0.48
1:A:95:PRO:O	1:A:96:SER:C	2.56	0.48
1:A:59:TYR:N	1:A:60:PRO:CD	2.77	0.48
1:B:18:GLN:HE22	1:B:50:ARG:HH21	1.62	0.48
1:B:230:TRP:HZ3	1:B:239:LEU:HB2	1.78	0.48
1:D:47:VAL:HG22	1:D:305:LEU:CD1	2.43	0.48
1:C:62:LEU:HD11	1:C:68:ALA:HA	1.95	0.48
1:C:328:PRO:O	1:C:329:PRO:C	2.56	0.48
1:D:111:VAL:CA	1:D:112:PRO:C	2.87	0.48
1:A:155:ALA:O	1:A:158:ASP:HB2	2.14	0.47
1:A:329:PRO:CG	1:C:265:ARG:NH2	2.77	0.47
1:A:328:PRO:HB3	1:A:329:PRO:HD2	1.97	0.47
1:A:198:VAL:HG11	1:A:203:ALA:HA	1.95	0.47
1:D:7:VAL:CG1	1:D:321:ARG:HB2	2.44	0.47
1:A:58:GLN:O	1:A:58:GLN:HG2	2.14	0.47
1:A:152:LEU:HD22	1:A:199:GLY:N	2.29	0.47
1:A:276:SER:O	1:A:301:THR:CG2	2.63	0.47
1:C:251:ARG:HG3	1:C:252:TYR:CE1	2.50	0.47
1:D:328:PRO:HG2	1:D:352:TRP:CD2	2.49	0.47
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.28	0.47
1:C:207:ARG:HG2	1:C:207:ARG:HH21	1.80	0.47
1:C:328:PRO:HG2	1:C:352:TRP:CD2	2.50	0.47
1:B:7:VAL:HG12	1:B:8:PHE:N	2.29	0.47
1:D:244:ASP:HA	1:D:247:ASN:HD22	1.80	0.47
1:B:72:PHE:HE1	1:B:107:THR:CG2	2.28	0.47
1:A:57:GLN:CD	1:A:57:GLN:H	2.23	0.47
1:A:98:ILE:HG12	1:A:161:VAL:CG1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HE3	1:A:176:LYS:HB2	1.63	0.47
1:C:53:VAL:HG22	1:C:75:LYS:HD2	1.95	0.47
1:C:115:ASP:OD2	1:C:132:PRO:HB3	2.15	0.47
1:B:221:TYR:N	1:B:221:TYR:HD1	2.13	0.47
1:D:166:GLU:HG3	1:D:312:SER:HB3	1.95	0.47
1:C:224:SER:OG	1:C:343:PHE:HB3	2.15	0.46
1:C:308:ILE:CD1	1:C:311:LEU:HD22	2.43	0.46
1:B:29:PRO:CD	1:B:60:PRO:HB3	2.45	0.46
1:D:209:GLY:O	1:D:210:GLY:O	2.33	0.46
1:D:262:ASP:O	1:D:263:ALA:C	2.58	0.46
1:A:276:SER:O	1:A:301:THR:HG23	2.15	0.46
1:A:328:PRO:CB	1:A:329:PRO:HD2	2.46	0.46
1:B:5:ALA:O	1:B:91:ALA:HA	2.15	0.46
1:B:106:VAL:HB	1:B:137:GLY:HA2	1.97	0.46
1:C:188:PHE:HA	1:C:310:ASN:O	2.15	0.46
1:C:214:LEU:HD12	1:C:349:LEU:HG	1.97	0.46
1:C:256:ASP:OD2	1:C:345:THR:HG21	2.14	0.46
1:D:339:MET:HA	1:D:344:CYS:O	2.15	0.46
1:A:91:ALA:O	1:A:93:LEU:HG	2.14	0.46
1:C:98:ILE:HD12	1:C:124:LEU:HD21	1.97	0.46
1:B:40:ARG:HH22	3:B:402:COA:H52A	1.80	0.46
1:B:124:LEU:N	1:B:124:LEU:HD23	2.30	0.46
1:B:174:ALA:HB1	1:B:238:ARG:HB2	1.97	0.46
1:B:201:ARG:HD2	1:D:353:ARG:CB	2.41	0.46
1:D:59:TYR:C	1:D:61:SER:H	2.23	0.46
1:D:79:LEU:CD1	1:D:167:LEU:HD21	2.46	0.46
1:B:77:VAL:O	1:B:81:VAL:HG13	2.16	0.46
1:A:248:LEU:O	1:A:249:ILE:C	2.57	0.46
1:C:166:GLU:CG	1:C:312:SER:HB3	2.41	0.46
1:D:103:THR:HG21	1:D:114:LEU:HB2	1.97	0.46
1:A:145:VAL:HG12	1:A:348:VAL:HG11	1.96	0.46
1:C:8:PHE:CE1	1:C:9:GLY:O	2.69	0.46
1:B:45:ALA:HB1	1:B:187:LEU:CD2	2.46	0.46
1:D:310:ASN:HD22	1:D:311:LEU:N	2.12	0.46
1:A:98:ILE:O	1:A:98:ILE:HG22	2.16	0.45
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.74	0.45
1:A:141:GLY:HA3	1:A:316:ILE:CG2	2.46	0.45
1:A:168:CYS:HB2	1:A:189:GLY:O	2.16	0.45
1:A:188:PHE:CE1	2:A:400:PLM:H62	2.47	0.45
1:A:329:PRO:HG3	1:C:265:ARG:NH2	2.30	0.45
1:C:109:VAL:HG13	1:D:134:PHE:HE2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ARG:HH21	1:C:217:ARG:CG	2.16	0.45
1:B:353:ARG:NH1	1:B:353:ARG:CG	2.69	0.45
1:D:248:LEU:HD23	1:D:248:LEU:HA	1.73	0.45
1:C:183:VAL:HG13	3:C:402:COA:H131	1.95	0.45
1:C:131:MET:SD	1:D:131:MET:HE2	2.56	0.45
1:C:225:LEU:HD11	1:D:117:ARG:HG2	1.99	0.45
1:D:351:ARG:HD3	1:D:353:ARG:HE	1.82	0.45
1:C:225:LEU:HD13	1:D:117:ARG:NH1	2.32	0.45
1:C:227:ILE:HD13	1:C:242:SER:CB	2.46	0.45
1:D:234:SER:HB3	4:D:510:HOH:O	2.15	0.45
1:C:147:ARG:HA	1:C:147:ARG:HD3	1.78	0.45
1:C:267:THR:C	1:C:269:ASP:N	2.74	0.45
1:B:37:ILE:HG12	1:B:41:LEU:HD22	1.99	0.45
1:B:98:ILE:HG12	1:B:161:VAL:HG13	1.99	0.45
1:B:130:ARG:NE	4:B:528:HOH:O	2.42	0.45
1:D:79:LEU:HD13	1:D:167:LEU:HD21	1.98	0.45
1:D:241:LEU:HD11	1:D:245:LEU:CD1	2.47	0.45
1:C:29:PRO:CD	1:C:60:PRO:HB3	2.46	0.45
1:D:22:THR:HG23	1:D:42:HIS:ND1	2.32	0.45
1:D:304:SER:HB2	1:D:319:ILE:HG12	1.98	0.45
1:A:39:ARG:HG2	1:A:39:ARG:NH1	2.26	0.45
1:A:109:VAL:CG1	1:B:232:VAL:HG21	2.47	0.45
1:C:139:VAL:HA	1:C:338:ALA:HB1	1.99	0.45
1:B:226:HIS:H	1:B:226:HIS:CD2	2.34	0.45
1:A:271:ILE:HG21	1:A:274:TRP:CE2	2.51	0.45
1:C:109:VAL:HG13	1:D:134:PHE:CE2	2.52	0.45
1:C:327:ARG:HA	1:C:328:PRO:HD3	1.78	0.45
1:A:171:THR:OG1	2:A:400:PLM:HA2	2.17	0.45
1:B:211:PRO:HG3	1:B:352:TRP:HZ3	1.78	0.45
1:D:18:GLN:HE22	1:D:50:ARG:NE	2.15	0.45
1:C:211:PRO:HD3	1:C:324:ILE:HD13	1.98	0.44
1:B:84:LEU:O	1:B:88:LEU:HG	2.17	0.44
1:C:176:LYS:O	1:C:178:THR:N	2.46	0.44
1:D:85:LEU:HG	1:D:122:LEU:HD21	2.00	0.44
1:D:342:GLY:N	1:D:343:PHE:CA	2.79	0.44
1:C:161:VAL:HG12	1:C:196:VAL:HG13	2.00	0.44
1:C:268:LYS:HB2	1:C:268:LYS:HE3	1.33	0.44
1:B:50:ARG:HG2	1:B:309:GLY:HA3	1.98	0.44
1:D:201:ARG:NE	1:D:204:GLU:OE1	2.40	0.44
1:B:124:LEU:O	1:B:125:ARG:C	2.57	0.44
1:D:131:MET:HA	1:D:132:PRO:HD2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:MET:HB2	1:B:129:ARG:HB2	1.98	0.44
1:B:230:TRP:CZ3	1:B:239:LEU:HB2	2.52	0.44
1:D:214:LEU:HD11	1:D:351:ARG:HB2	2.00	0.44
1:D:166:GLU:OE1	1:D:166:GLU:HA	2.18	0.44
1:C:45:ALA:O	1:C:46:LYS:HB2	2.18	0.43
1:D:42:HIS:NE2	1:D:185:THR:CG2	2.81	0.43
1:C:4:ILE:O	1:C:210:GLY:N	2.51	0.43
1:D:94:ARG:O	1:D:97:ASP:HB2	2.18	0.43
1:A:289:THR:HG22	1:A:290:SER:N	2.32	0.43
1:A:336:MET:HB2	1:A:348:VAL:HB	2.00	0.43
1:C:32:LYS:NZ	1:C:35:GLU:OE1	2.49	0.43
1:C:253:LEU:HD11	1:C:337:LEU:HD21	1.99	0.43
1:B:10:ALA:HA	4:B:522:HOH:O	2.18	0.43
1:D:217:ARG:HH21	1:D:217:ARG:HD3	1.68	0.43
1:C:147:ARG:HA	1:C:150:ASP:HB2	2.00	0.43
1:C:227:ILE:HD13	1:C:242:SER:HB3	1.99	0.43
1:B:72:PHE:CE1	1:B:107:THR:CG2	3.01	0.43
1:D:105:THR:OG1	1:D:165:VAL:O	2.33	0.43
1:D:329:PRO:O	1:D:332:SER:OG	2.26	0.43
1:A:172:TYR:HA	1:A:175:VAL:HG23	2.01	0.43
1:B:26:VAL:HG22	1:B:35:GLU:HA	2.00	0.43
1:D:230:TRP:CH2	2:D:400:PLM:H62	2.53	0.43
1:A:274:TRP:CZ3	1:A:335:LEU:CD2	3.00	0.43
1:D:106:VAL:HG11	2:D:400:PLM:H22	2.01	0.43
1:A:277:HIS:HA	1:A:278:PRO:HD2	1.61	0.43
1:C:329:PRO:O	1:C:332:SER:OG	2.34	0.43
1:B:88:LEU:O	1:B:92:ASN:N	2.52	0.43
1:C:135:GLY:HA2	1:D:111:VAL:CG2	2.43	0.43
1:B:98:ILE:HG12	1:B:161:VAL:CG1	2.48	0.43
1:D:100:MET:HE3	1:D:160:ALA:HB1	2.00	0.43
1:A:37:ILE:O	1:A:37:ILE:HG12	2.19	0.42
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.83	0.42
1:C:311:LEU:HB2	1:C:315:SER:OG	2.19	0.42
1:B:100:MET:CB	1:B:129:ARG:HB2	2.49	0.42
1:C:138:SER:OG	2:C:401:PLM:O2	2.32	0.42
1:C:3:VAL:HG22	1:C:212:ASP:OD1	2.19	0.42
1:C:12:PRO:HD2	1:C:51:HIS:HB2	2.01	0.42
1:B:45:ALA:HB1	1:B:187:LEU:HD23	2.00	0.42
1:B:172:TYR:N	1:B:173:PRO:CD	2.83	0.42
1:A:3:VAL:HG11	1:A:353:ARG:HH12	1.84	0.42
1:D:291:LEU:O	1:D:292:ALA:HB3	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HB2	1:A:59:TYR:CZ	2.55	0.42
1:A:103:THR:HA	1:A:163:VAL:O	2.19	0.42
1:A:109:VAL:HG13	1:B:134:PHE:HE2	1.85	0.42
1:C:44:ALA:HA	4:C:502:HOH:O	2.19	0.42
1:C:282:LYS:HD2	1:C:282:LYS:HA	1.78	0.42
1:C:29:PRO:HD3	1:C:60:PRO:HB3	2.02	0.42
1:C:45:ALA:HB1	1:C:47:VAL:HG23	2.00	0.42
1:C:152:LEU:O	4:C:518:HOH:O	2.22	0.42
1:D:124:LEU:N	1:D:124:LEU:HD23	2.34	0.42
1:D:136:LEU:O	1:D:139:VAL:HG12	2.20	0.42
1:C:152:LEU:HA	1:C:152:LEU:HD23	1.85	0.42
1:D:31:LEU:HD12	1:D:31:LEU:HA	1.84	0.42
1:A:8:PHE:CD1	1:A:83:ALA:HA	2.55	0.42
1:A:228:MET:SD	1:A:340:GLY:HA2	2.60	0.42
1:C:338:ALA:O	1:C:345:THR:HA	2.20	0.42
1:B:138:SER:N	2:B:401:PLM:O1	2.43	0.42
1:D:233:GLY:C	1:D:235:HIS:H	2.27	0.42
1:A:46:LYS:HB2	1:A:281:PRO:HG3	2.02	0.41
1:A:95:PRO:O	1:A:97:ASP:N	2.53	0.41
1:A:50:ARG:NH1	1:A:188:PHE:O	2.36	0.41
1:B:21:ILE:HG21	1:B:21:ILE:HD13	1.67	0.41
1:B:77:VAL:O	1:B:78:ASP:C	2.62	0.41
1:A:115:ASP:OD2	1:A:130:ARG:HB3	2.20	0.41
1:B:58:GLN:C	1:B:60:PRO:HD2	2.45	0.41
1:B:294:PRO:CB	1:B:296:GLU:OE2	2.67	0.41
1:D:352:TRP:CD1	1:D:352:TRP:H	2.38	0.41
1:A:166:GLU:HA	1:A:166:GLU:OE1	2.19	0.41
1:A:250:GLU:HG2	1:A:286:ALA:HB1	2.03	0.41
1:B:339:MET:HE3	1:B:339:MET:HB3	1.53	0.41
1:D:59:TYR:O	1:D:60:PRO:C	2.61	0.41
1:A:205:GLN:O	1:A:205:GLN:HG3	2.13	0.41
1:C:251:ARG:HG3	1:C:252:TYR:CD1	2.56	0.41
1:B:300:LEU:N	1:B:300:LEU:HD12	2.33	0.41
1:D:52:LEU:HD23	1:D:52:LEU:HA	1.80	0.41
1:A:211:PRO:HG3	1:A:352:TRP:CZ3	2.55	0.41
1:C:248:LEU:HA	1:C:248:LEU:HD23	1.47	0.41
1:D:147:ARG:HE	1:D:147:ARG:HA	1.86	0.41
1:C:337:LEU:HG	1:C:347:LEU:HD21	2.00	0.41
1:B:136:LEU:O	1:B:139:VAL:HG12	2.20	0.41
1:B:205:GLN:C	1:B:207:ARG:H	2.27	0.41
1:A:330:SER:OG	1:A:353:ARG:OXT	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:PHE:O	1:C:73:ILE:C	2.61	0.41
1:C:124:LEU:O	1:C:125:ARG:C	2.62	0.41
1:C:144:GLY:C	1:C:162:LEU:HD22	2.46	0.41
1:D:156:PRO:O	1:D:199:GLY:HA3	2.21	0.41
1:D:271:ILE:HD12	1:D:271:ILE:HA	1.68	0.41
1:A:54:LEU:HB2	1:A:59:TYR:OH	2.21	0.41
1:A:58:GLN:O	1:A:58:GLN:CG	2.68	0.41
1:A:221:TYR:HA	1:A:222:PRO:HD3	1.89	0.41
1:C:228:MET:HE1	3:C:402:COA:S1P	2.61	0.41
1:B:311:LEU:HB2	1:B:315:SER:OG	2.21	0.41
1:A:178:THR:OG1	1:A:179:VAL:N	2.53	0.40
1:C:28:PHE:O	1:C:29:PRO:C	2.60	0.40
1:C:251:ARG:CG	1:C:252:TYR:CE1	3.04	0.40
1:B:7:VAL:HG22	1:B:195:VAL:HG22	2.03	0.40
1:D:84:LEU:HD23	1:D:84:LEU:HA	1.84	0.40
1:D:288:ALA:HA	1:D:293:LEU:HD12	2.02	0.40
1:A:239:LEU:HD12	1:A:239:LEU:HA	1.24	0.40
1:C:193:ALA:HB3	1:C:317:LEU:HD12	2.04	0.40
1:C:283:VAL:HG23	3:C:402:COA:C6P	2.51	0.40
1:B:168:CYS:SG	1:B:188:PHE:HB3	2.61	0.40
1:B:253:LEU:O	1:B:256:ASP:HB2	2.21	0.40
1:D:91:ALA:O	1:D:92:ASN:C	2.65	0.40
1:A:176:LYS:HB3	1:A:177:PRO:CD	2.51	0.40
1:C:134:PHE:CD1	1:C:134:PHE:C	2.99	0.40
1:A:72:PHE:CD1	1:A:72:PHE:C	2.99	0.40
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.78	0.40
1:A:250:GLU:HA	1:A:290:SER:OG	2.22	0.40
1:B:104:ALA:HB3	1:B:164:SER:HA	2.03	0.40
1:B:201:ARG:NE	1:D:353:ARG:HH11	2.08	0.40
1:D:119:ALA:HB1	1:D:124:LEU:HB2	2.04	0.40
1:D:310:ASN:HD22	1:D:312:SER:N	2.13	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:LYS:NZ	3:C:402:COA:O8A[2_555]	1.52	0.68

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	350/353 (99%)	320 (91%)	27 (8%)	3 (1%)	14	12
1	B	351/353 (99%)	317 (90%)	29 (8%)	5 (1%)	9	5
1	C	350/353 (99%)	313 (89%)	33 (9%)	4 (1%)	11	8
1	D	350/353 (99%)	314 (90%)	31 (9%)	5 (1%)	9	5
All	All	1401/1412 (99%)	1264 (90%)	120 (9%)	17 (1%)	10	7

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	327	ARG
1	B	169	SER
1	A	210	GLY
1	C	96	SER
1	C	210	GLY
1	D	210	GLY
1	A	244	ASP
1	C	207	ARG
1	D	263	ALA
1	D	326	LYS
1	D	209	GLY
1	D	327	ARG
1	B	210	GLY
1	B	327	ARG
1	A	342	GLY
1	B	95	PRO
1	B	342	GLY

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	280/281 (100%)	245 (88%)	35 (12%)	4	3
1	B	281/281 (100%)	237 (84%)	44 (16%)	2	1
1	C	280/281 (100%)	255 (91%)	25 (9%)	9	7
1	D	280/281 (100%)	229 (82%)	51 (18%)	2	0
All	All	1121/1124 (100%)	966 (86%)	155 (14%)	3	2

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	7	VAL
1	A	35	GLU
1	A	36	GLU
1	A	38	ILE
1	A	41	LEU
1	A	54	LEU
1	A	84	LEU
1	A	101	ILE
1	A	113	SER
1	A	115	ASP
1	A	129	ARG
1	A	145	VAL
1	A	147	ARG
1	A	161	VAL
1	A	164	SER
1	A	176	LYS
1	A	185	THR
1	A	198	VAL
1	A	201	ARG
1	A	204	GLU
1	A	205	GLN
1	A	206	VAL
1	A	221	TYR
1	A	223	ASP
1	A	242	SER
1	A	246	THR
1	A	268	LYS

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Mol	Chain	Res	Type
1	A	284	ILE
1	A	289	THR
1	A	291	LEU
1	A	296	GLU
1	A	327	ARG
1	A	339	MET
1	A	347	LEU
1	C	18	GLN
1	C	26	VAL
1	C	85	LEU
1	C	95	PRO
1	C	103	THR
1	C	105	THR
1	C	126	PRO
1	C	147	ARG
1	C	149	ARG
1	C	205	GLN
1	C	206	VAL
1	C	223	ASP
1	C	224	SER
1	C	249	ILE
1	C	251	ARG
1	C	261	LEU
1	C	268	LYS
1	C	271	ILE
1	C	275	VAL
1	C	300	LEU
1	C	311	LEU
1	C	316	ILE
1	C	324	ILE
1	C	345	THR
1	C	353	ARG
1	B	14	HIS
1	B	18	GLN
1	B	19	SER
1	B	35	GLU
1	B	39	ARG
1	B	41	LEU
1	B	61	SER
1	B	81	VAL
1	B	95	PRO
1	B	100	MET

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Mol	Chain	Res	Type
1	B	103	THR
1	B	105	THR
1	B	107	THR
1	B	115	ASP
1	B	124	LEU
1	B	133	LEU
1	B	147	ARG
1	B	148	LEU
1	B	153	ARG
1	B	180	SER
1	B	181	SER
1	B	204	GLU
1	B	207	ARG
1	B	213	ILE
1	B	216	SER
1	B	223	ASP
1	B	228	MET
1	B	245	LEU
1	B	246	THR
1	B	247	ASN
1	B	255	ASN
1	B	268	LYS
1	B	269	ASP
1	B	282	LYS
1	B	289	THR
1	B	300	LEU
1	B	311	LEU
1	B	320	LEU
1	B	321	ARG
1	B	327	ARG
1	B	337	LEU
1	B	339	MET
1	B	347	LEU
1	B	353	ARG
1	D	2	SER
1	D	15	ARG
1	D	18	GLN
1	D	24	SER
1	D	26	VAL
1	D	31	LEU
1	D	33	GLU
1	D	46	LYS

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Mol	Chain	Res	Type
1	D	54	LEU
1	D	61	SER
1	D	84	LEU
1	D	90	ASP
1	D	94	ARG
1	D	103	THR
1	D	105	THR
1	D	115	ASP
1	D	124	LEU
1	D	138	SER
1	D	147	ARG
1	D	148	LEU
1	D	153	ARG
1	D	164	SER
1	D	170	LEU
1	D	176	LYS
1	D	179	VAL
1	D	183	VAL
1	D	185	THR
1	D	187	LEU
1	D	206	VAL
1	D	213	ILE
1	D	228	MET
1	D	235	HIS
1	D	240	ARG
1	D	245	LEU
1	D	253	LEU
1	D	256	ASP
1	D	257	VAL
1	D	268	LYS
1	D	271	ILE
1	D	298	LEU
1	D	300	LEU
1	D	304	SER
1	D	311	LEU
1	D	315	SER
1	D	321	ARG
1	D	327	ARG
1	D	335	LEU
1	D	337	LEU
1	D	345	THR
1	D	347	LEU

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Mol	Chain	Res	Type
1	D	352	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	HIS
1	A	69	ASN
1	A	247	ASN
1	A	318	HIS
1	C	18	GLN
1	C	34	HIS
1	C	48	ASN
1	C	57	GLN
1	C	205	GLN
1	C	247	ASN
1	B	14	HIS
1	B	18	GLN
1	B	34	HIS
1	B	51	HIS
1	B	58	GLN
1	B	69	ASN
1	B	226	HIS
1	B	247	ASN
1	B	264	HIS
1	B	310	ASN
1	D	18	GLN
1	D	51	HIS
1	D	247	ASN
1	D	310	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
2	PLM	B	401	-	17,17,17	1.71	3 (17%)	17,17,17	1.97	4 (23%)
3	COA	B	402	-	47,50,50	1.38	8 (17%)	69,75,75	1.91	19 (27%)
2	PLM	D	400	-	17,17,17	1.22	1 (5%)	17,17,17	2.45	6 (35%)
2	PLM	A	400	-	17,17,17	0.82	1 (5%)	17,17,17	1.01	1 (5%)
3	COA	C	402	-	47,50,50	1.30	6 (12%)	69,75,75	2.05	16 (23%)
2	PLM	C	401	-	17,17,17	0.75	0	17,17,17	1.93	4 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLM	B	401	-	-	2/15/15/15	-
3	COA	B	402	-	-	22/48/64/64	0/3/3/3
2	PLM	D	400	-	-	4/15/15/15	-
2	PLM	A	400	-	-	10/15/15/15	-
3	COA	C	402	-	-	19/48/64/64	0/3/3/3
2	PLM	C	401	-	-	5/15/15/15	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLM	C2-C1	4.28	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	COA	C5A-N7A	-4.20	1.31	1.39
2	B	401	PLM	O2-C1	4.06	1.35	1.22
2	D	400	PLM	O2-C1	3.71	1.34	1.22
3	B	402	COA	C4A-N9A	-3.29	1.30	1.37
3	B	402	COA	C5A-N7A	-3.13	1.33	1.39
3	B	402	COA	C5A-C4A	3.13	1.44	1.39
3	C	402	COA	C5A-C4A	2.99	1.44	1.39
3	B	402	COA	O5P-C5P	-2.95	1.17	1.23
3	C	402	COA	C8A-N9A	-2.72	1.32	1.37
3	B	402	COA	C8A-N9A	-2.46	1.33	1.37
3	B	402	COA	P3B-O8A	-2.37	1.46	1.54
2	A	400	PLM	O1-C1	-2.23	1.23	1.30
3	B	402	COA	P3B-O3B	-2.17	1.55	1.59
3	C	402	COA	P3B-O9A	-2.14	1.46	1.54
3	C	402	COA	O9P-C9P	-2.12	1.19	1.23
2	B	401	PLM	O1-C1	-2.04	1.24	1.30
3	C	402	COA	C4A-N9A	-2.01	1.33	1.37
3	B	402	COA	P3B-O9A	-2.00	1.47	1.54

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	COA	C5A-C4A-N3A	-7.07	116.98	126.72
3	C	402	COA	N3A-C4A-N9A	6.94	138.98	127.17
2	D	400	PLM	O1-C1-C2	-5.78	95.73	114.00
2	B	401	PLM	C4-C3-C2	4.65	130.22	113.13
3	B	402	COA	N3A-C4A-N9A	4.57	134.93	127.17
2	B	401	PLM	C3-C2-C1	-4.40	103.03	114.51
3	B	402	COA	C5A-C4A-N3A	-4.35	120.73	126.72
2	C	401	PLM	C4-C3-C2	4.28	128.86	113.13
3	B	402	COA	C4A-N9A-C8A	4.27	110.22	105.74
2	D	400	PLM	C9-C8-C7	-4.26	92.85	114.37
3	B	402	COA	N3A-C2A-N1A	-4.10	122.37	128.58
3	C	402	COA	O6A-CCP-CBP	4.06	117.08	110.55
2	C	401	PLM	C6-C5-C4	-4.01	94.08	114.37
2	D	400	PLM	O1-C1-O2	3.93	133.44	123.33
3	B	402	COA	C7P-N8P-C9P	3.73	129.25	122.55
3	C	402	COA	C2A-N3A-C4A	3.70	120.88	111.83
3	C	402	COA	N6A-C6A-N1A	3.65	126.52	118.38
3	B	402	COA	O3B-P3B-O7A	-3.63	96.41	109.33
3	C	402	COA	O3B-C3B-C4B	-3.59	97.39	110.03
3	B	402	COA	C2A-N3A-C4A	3.55	120.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	PLM	CC-CB-CA	-3.32	97.60	114.37
3	B	402	COA	CDP-CBP-CCP	3.31	113.69	108.22
3	C	402	COA	C5A-C6A-N6A	-3.28	115.16	123.29
3	C	402	COA	C1B-N9A-C8A	-3.20	120.00	127.09
3	B	402	COA	O9A-P3B-O8A	3.08	119.35	107.80
2	B	401	PLM	C9-C8-C7	-3.06	98.88	114.37
3	B	402	COA	C6P-C5P-N4P	2.96	121.74	116.34
3	C	402	COA	C4A-N9A-C8A	2.89	108.77	105.74
3	B	402	COA	C7P-C6P-C5P	2.84	117.12	112.39
3	C	402	COA	P3B-O3B-C3B	2.81	130.94	123.43
2	D	400	PLM	C6-C5-C4	-2.79	100.24	114.37
2	C	401	PLM	O2-C1-C2	-2.78	114.28	123.09
3	C	402	COA	CEP-CBP-CCP	2.77	112.80	108.22
3	B	402	COA	O3A-P2A-O4A	-2.77	102.36	110.70
3	C	402	COA	N3A-C2A-N1A	-2.66	124.55	128.58
3	B	402	COA	N6A-C6A-N1A	2.60	124.17	118.38
3	B	402	COA	C5A-C6A-N6A	-2.49	117.12	123.29
2	A	400	PLM	O2-C1-C2	-2.29	115.83	123.09
3	C	402	COA	C3B-C2B-C1B	2.27	104.88	99.89
2	C	401	PLM	C5-C4-C3	-2.27	102.90	114.37
3	C	402	COA	C7P-N8P-C9P	2.27	126.62	122.55
3	B	402	COA	CDP-CBP-CAP	-2.26	104.92	108.77
3	C	402	COA	O2B-C2B-C3B	2.26	117.50	111.19
3	C	402	COA	C5A-N7A-C8A	2.25	106.99	103.45
2	B	401	PLM	C6-C5-C4	-2.25	102.99	114.37
3	B	402	COA	N9A-C8A-N7A	-2.18	110.84	113.94
3	B	402	COA	C2A-N1A-C6A	2.18	122.30	118.73
3	B	402	COA	O5A-P2A-O4A	2.16	122.51	112.44
3	B	402	COA	O3B-C3B-C2B	-2.11	104.12	111.68
2	D	400	PLM	CD-CC-CB	2.08	124.90	114.37

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	402	COA	C5B-O5B-P1A-O2A
3	C	402	COA	CCP-O6A-P2A-O5A
3	C	402	COA	CAP-C9P-N8P-C7P
3	C	402	COA	C5P-C6P-C7P-N8P
3	C	402	COA	C2P-C3P-N4P-C5P
3	B	402	COA	P2A-O3A-P1A-O5B
3	B	402	COA	CCP-O6A-P2A-O3A

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Mol	Chain	Res	Type	Atoms
3	B	402	COA	CCP-O6A-P2A-O4A
3	B	402	COA	CDP-CBP-CCP-O6A
3	B	402	COA	CEP-CBP-CCP-O6A
3	B	402	COA	CAP-CBP-CCP-O6A
3	B	402	COA	CAP-C9P-N8P-C7P
3	B	402	COA	O9P-C9P-N8P-C7P
3	B	402	COA	C5P-C6P-C7P-N8P
3	B	402	COA	C6P-C5P-N4P-C3P
3	B	402	COA	O5P-C5P-N4P-C3P
3	B	402	COA	S1P-C2P-C3P-N4P
3	C	402	COA	O9P-C9P-N8P-C7P
3	C	402	COA	C6P-C5P-N4P-C3P
3	C	402	COA	O4B-C4B-C5B-O5B
2	A	400	PLM	C3-C4-C5-C6
3	C	402	COA	O5P-C5P-N4P-C3P
3	C	402	COA	C2B-C3B-O3B-P3B
2	D	400	PLM	C8-C9-CA-CB
2	A	400	PLM	C2-C3-C4-C5
2	A	400	PLM	C4-C5-C6-C7
2	A	400	PLM	CC-CD-CE-CF
3	C	402	COA	C4B-C3B-O3B-P3B
2	D	400	PLM	C5-C6-C7-C8
3	B	402	COA	O9P-C9P-CAP-OAP
2	A	400	PLM	CA-CB-CC-CD
2	A	400	PLM	CD-CE-CF-CG
2	A	400	PLM	C7-C8-C9-CA
3	C	402	COA	C3B-C4B-C5B-O5B
2	A	400	PLM	C8-C9-CA-CB
3	C	402	COA	S1P-C2P-C3P-N4P
3	C	402	COA	C5B-O5B-P1A-O1A
3	C	402	COA	C5B-O5B-P1A-O3A
3	C	402	COA	CCP-O6A-P2A-O3A
3	C	402	COA	CCP-O6A-P2A-O4A
3	B	402	COA	CCP-O6A-P2A-O5A
3	B	402	COA	P1A-O3A-P2A-O4A
3	B	402	COA	O9P-C9P-CAP-CBP
3	B	402	COA	C3B-O3B-P3B-O9A
3	B	402	COA	N8P-C9P-CAP-CBP
2	B	401	PLM	C2-C3-C4-C5
2	C	401	PLM	C2-C3-C4-C5
2	C	401	PLM	O1-C1-C2-C3
3	B	402	COA	C4B-C5B-O5B-P1A

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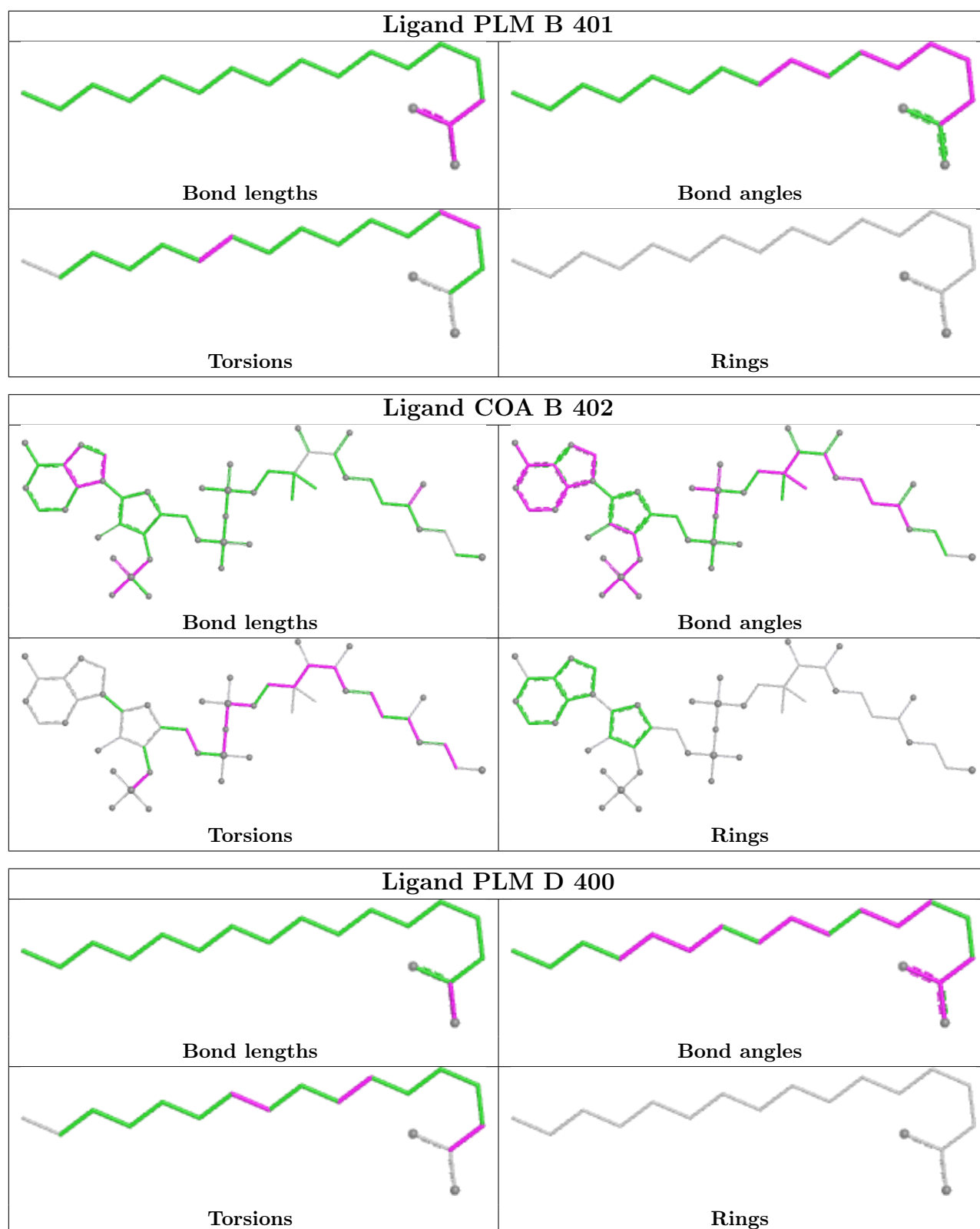
Mol	Chain	Res	Type	Atoms
2	D	400	PLM	O1-C1-C2-C3
2	C	401	PLM	O2-C1-C2-C3
2	D	400	PLM	O2-C1-C2-C3
2	A	400	PLM	O2-C1-C2-C3
3	B	402	COA	P1A-O3A-P2A-O6A
2	A	400	PLM	O1-C1-C2-C3
3	C	402	COA	P2A-O3A-P1A-O2A
3	B	402	COA	C9P-CAP-CBP-CCP
2	B	401	PLM	C9-CA-CB-CC
2	C	401	PLM	C1-C2-C3-C4
3	B	402	COA	N8P-C9P-CAP-OAP
3	C	402	COA	P1A-O3A-P2A-O5A
2	C	401	PLM	C3-C4-C5-C6

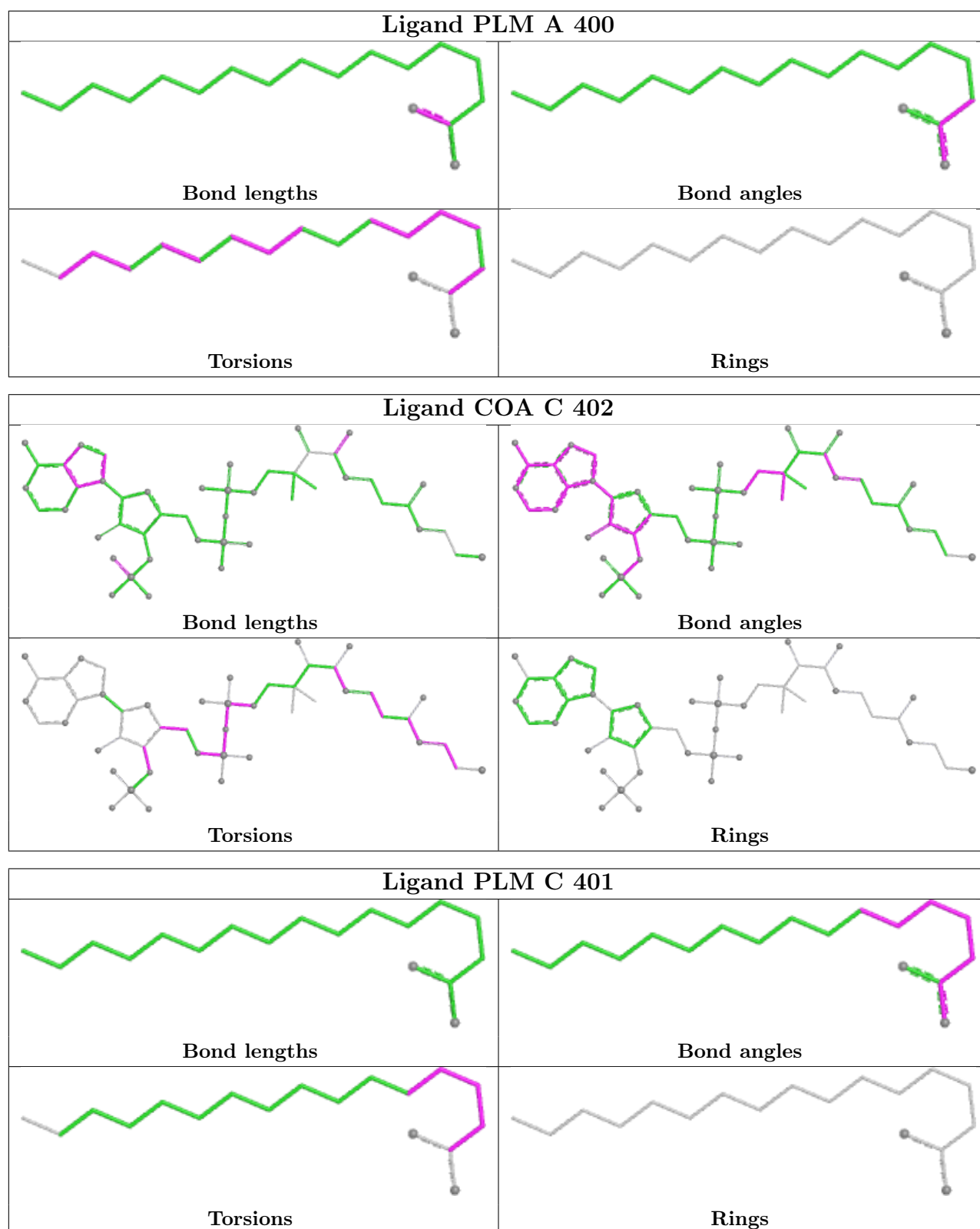
There are no ring outliers.

6 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	PLM	9	0
3	B	402	COA	4	0
2	D	400	PLM	5	0
2	A	400	PLM	11	0
3	C	402	COA	6	1
2	C	401	PLM	4	0

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





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	352/353 (99%)	-0.26	1 (0%) 90 90	21, 36, 48, 61	0
1	B	352/353 (99%)	-0.21	1 (0%) 90 90	18, 35, 50, 66	1 (0%)
1	C	352/353 (99%)	-0.30	0 100 100	21, 34, 49, 70	0
1	D	352/353 (99%)	-0.25	0 100 100	21, 35, 50, 65	0
All	All	1408/1412 (99%)	-0.26	2 (0%) 92 92	18, 35, 49, 70	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	235[A]	HIS	3.9
1	A	188	PHE	2.5

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

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

6.3 Carbohydrates [i](#)

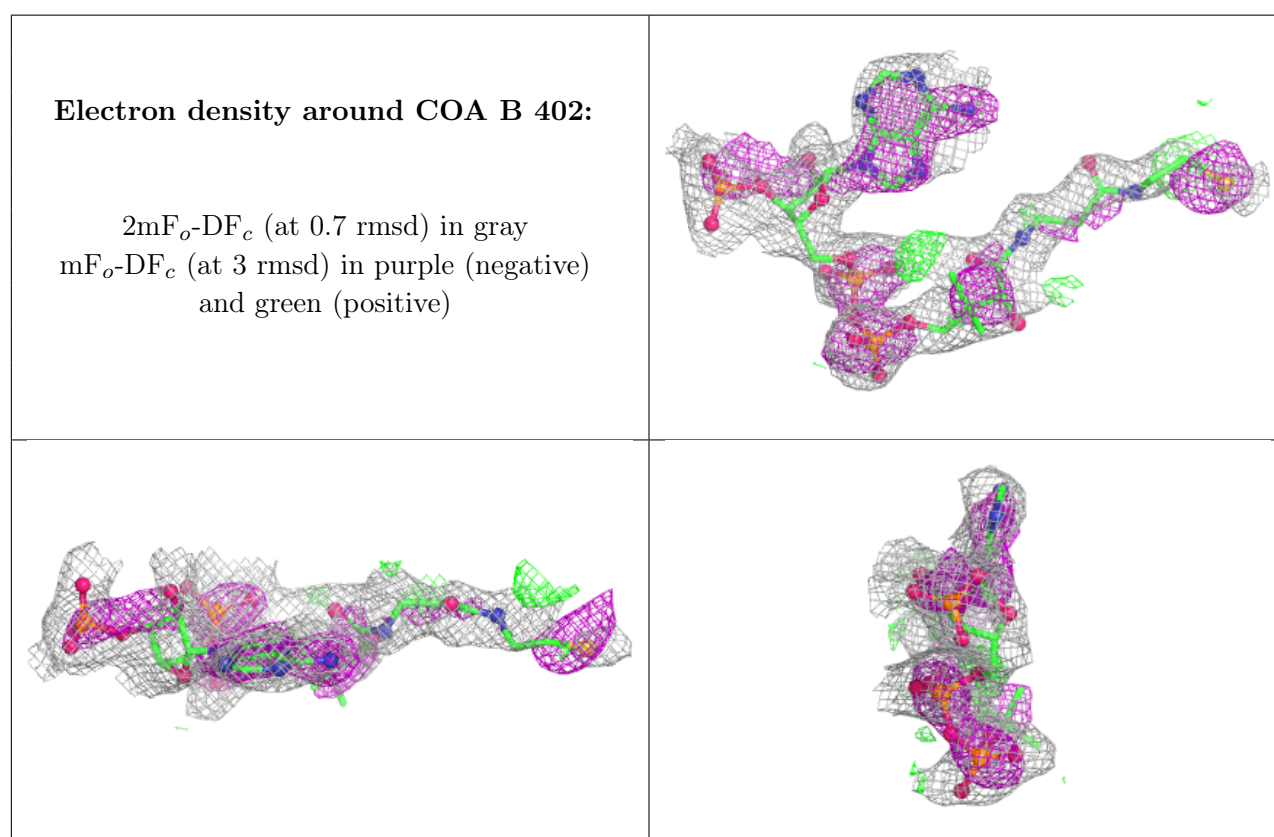
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

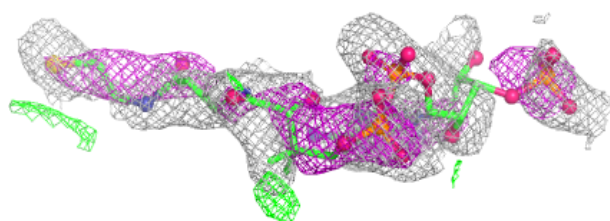
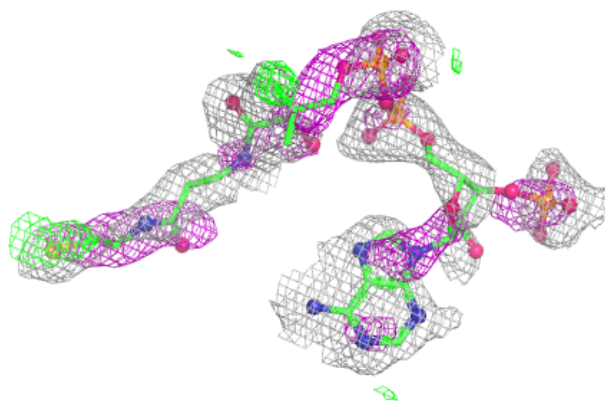
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	COA	B	402	48/48	0.75	0.14	24,37,50,56	0
3	COA	C	402	48/48	0.80	0.13	24,37,54,63	0
2	PLM	A	400	18/18	0.85	0.13	29,36,46,47	0
2	PLM	D	400	18/18	0.88	0.11	25,33,39,41	0
2	PLM	B	401	18/18	0.92	0.09	28,37,50,53	0
2	PLM	C	401	18/18	0.92	0.09	29,31,36,39	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

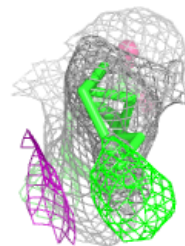
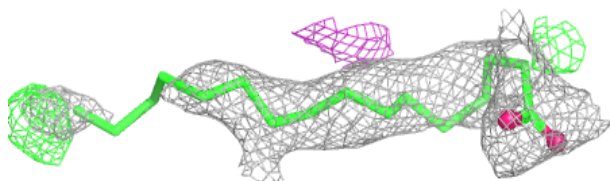
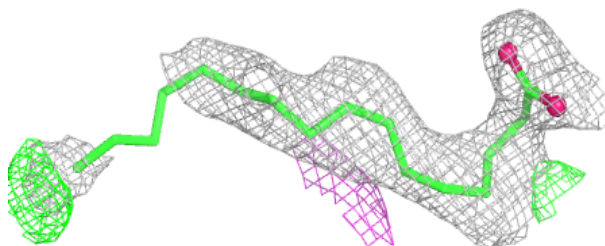


Electron density around COA C 402:

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

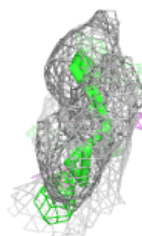
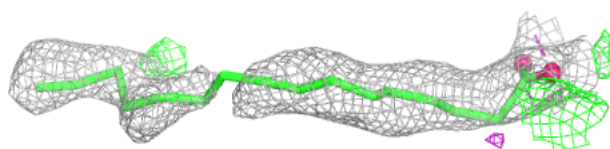
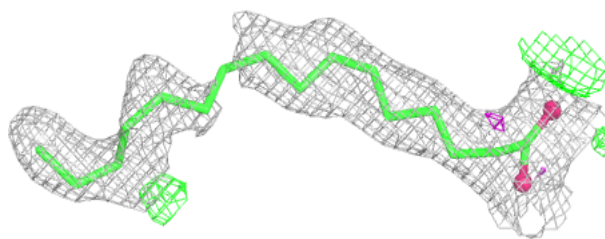
**Electron density around PLM A 400:**

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

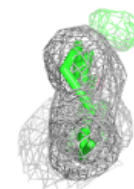
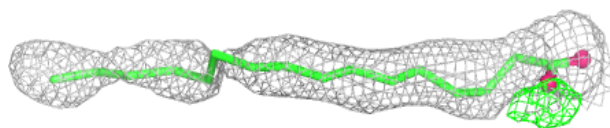
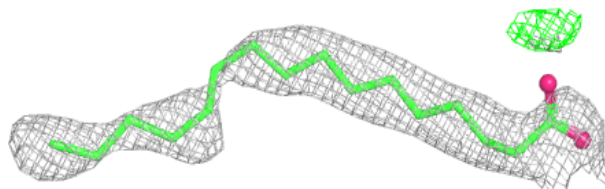


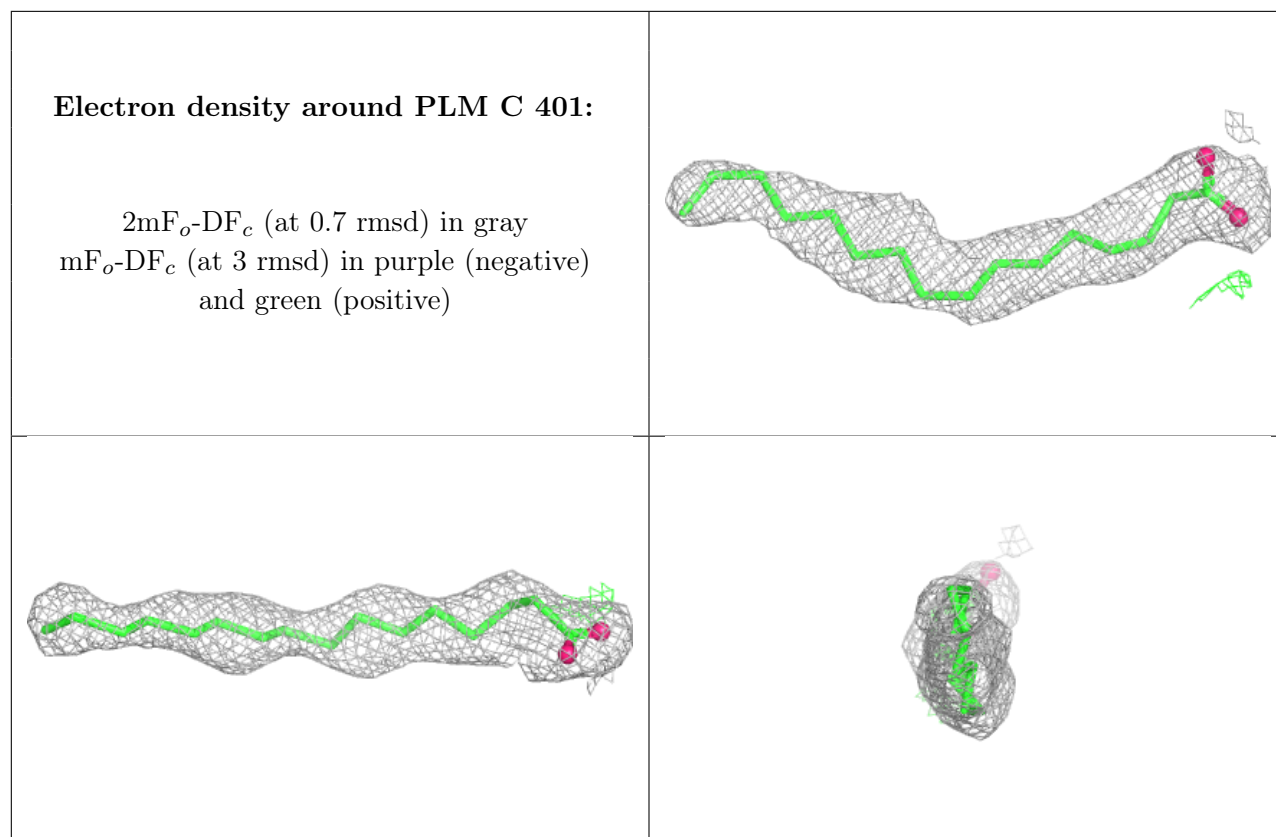
Electron density around PLM D 400:

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

**Electron density around PLM B 401:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.