



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:34 PM UTC

PDB ID : 1QFL / pdb_00001qfl
Title : BIOSYNTHETIC THIOLASE FROM ZOOGLOEA RAMIGERA IN COM-
PLEX WITH A REACTION INTERMEDIATE.
Authors : Modis, Y.; Wierenga, R.K.
Deposited on : 1999-04-12
Resolution : 1.92 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

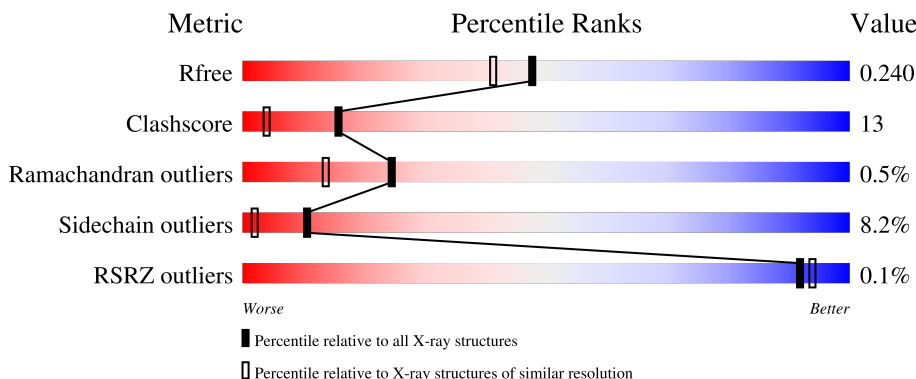
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	389	
1	B	389	
1	C	389	
1	D	389	

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
1	SCY	A	89	-	-	X	-
1	SCY	B	89	-	-	X	-
1	SCY	C	89	-	-	X	-
1	SCY	D	89	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12204 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.

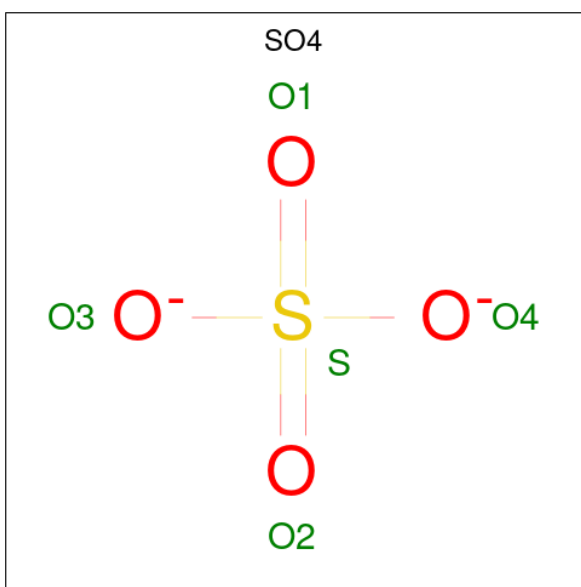
- Molecule 1 is a protein called PROTEIN (ACETOACETYL-COA THIOLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2816	1748	509	538	21			
1	B	389	Total	C	N	O	S	0	0	0
			2816	1748	509	538	21			
1	C	389	Total	C	N	O	S	0	0	0
			2816	1748	509	538	21			
1	D	389	Total	C	N	O	S	0	0	0
			2816	1748	509	538	21			

There are 12 discrepancies between the modelled and reference sequences:

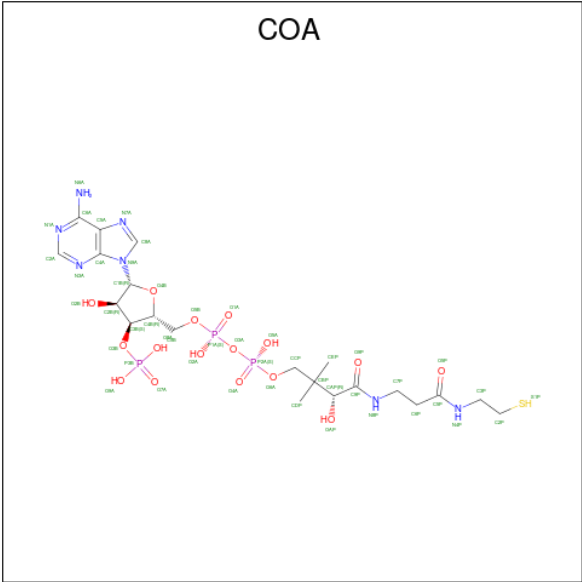
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	insertion	UNP P07097
A	89	SCY	CYS	modified residue	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	11	ALA	-	insertion	UNP P07097
B	89	SCY	CYS	modified residue	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	11	ALA	-	insertion	UNP P07097
C	89	SCY	CYS	modified residue	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
D	11	ALA	-	insertion	UNP P07097
D	89	SCY	CYS	modified residue	UNP P07097
D	129	ARG	ALA	conflict	UNP P07097

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



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

- Molecule 4 is water.

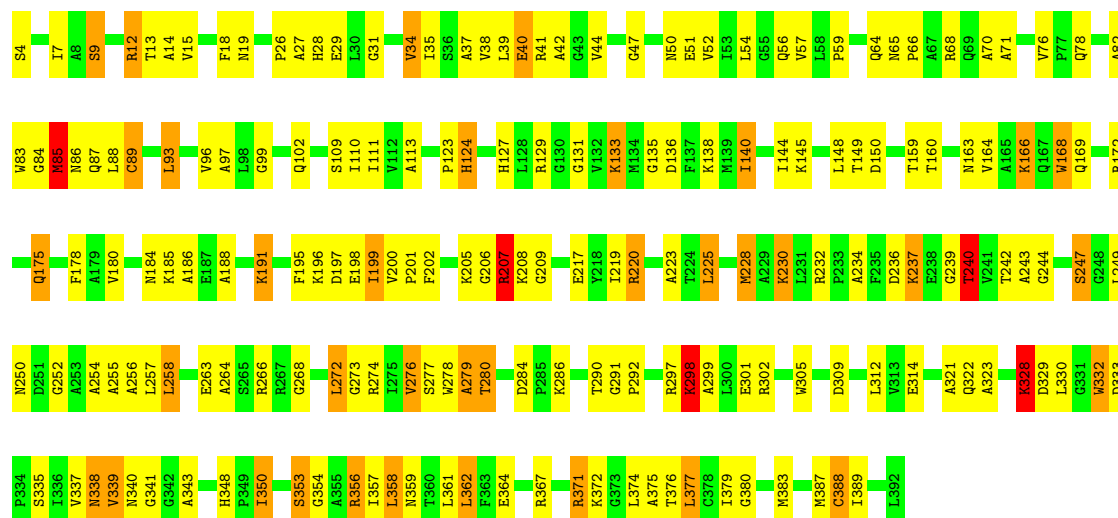
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total	O	0	0
			287	287		
4	B	275	Total	O	0	0
			275	275		
4	C	94	Total	O	0	0
			94	94		
4	D	62	Total	O	0	0
			62	62		

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.

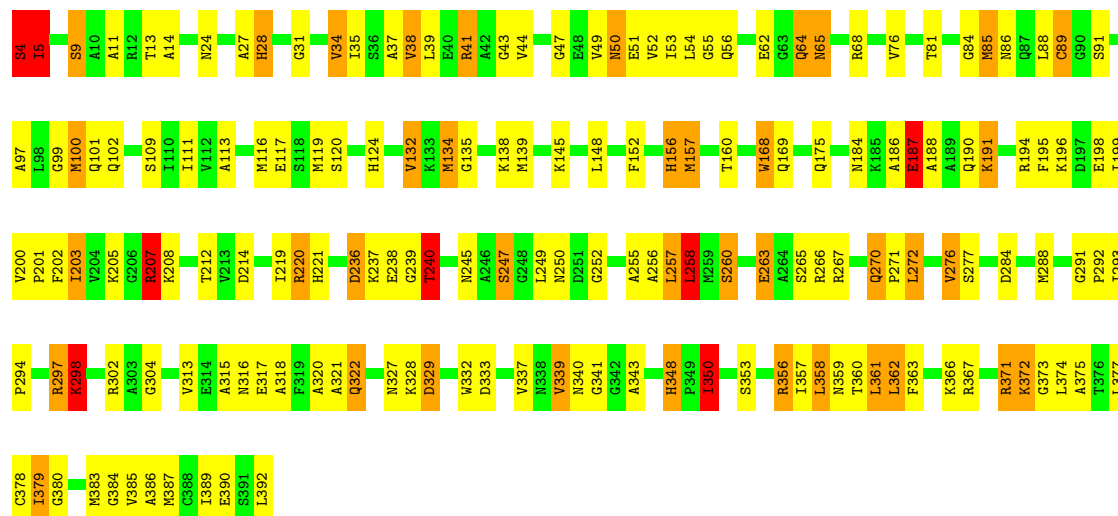
• Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)

Chain A: 

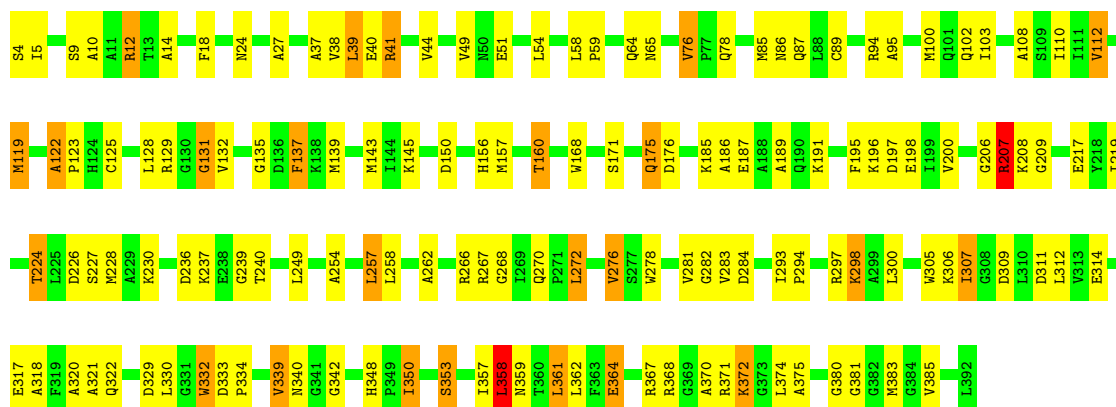


• Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)

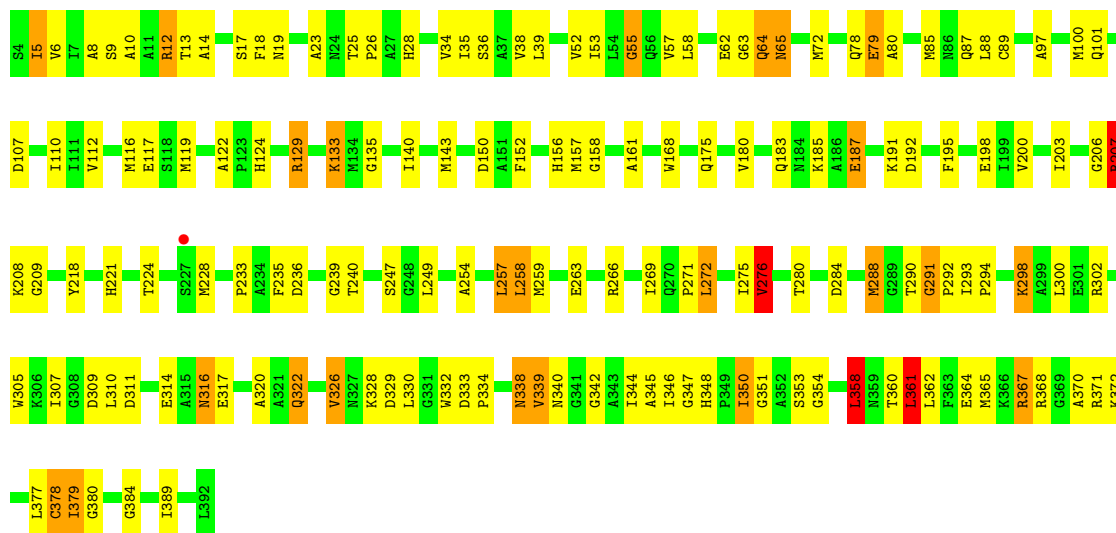
Chain B: 



● Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)

Chain C:  63% 30% 6% ●

● Molecule 1: PROTEIN (ACETOACETYL-COA THIOLASE)

Chain D:  60% 33% 6% ●

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.46Å 78.86Å 149.75Å 90.00° 93.43° 90.00°	Depositor
Resolution (Å)	50.00 – 1.92 50.00 – 1.93	Depositor EDS
% Data completeness (in resolution range)	85.5 (50.00-1.92) 79.2 (50.00-1.93)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	8.40	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.92Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.209 , 0.256 0.235 , 0.240	Depositor DCC
R_{free} test set	7058 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.700	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 26.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12204	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.96% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: COA, SO4, SCY

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	1.49	14/2847 (0.5%)	2.57	204/3842 (5.3%)
1	B	1.52	16/2847 (0.6%)	2.50	201/3842 (5.2%)
1	C	0.80	0/2847	1.90	70/3842 (1.8%)
1	D	0.71	0/2847	1.77	50/3842 (1.3%)
All	All	1.19	30/11388 (0.3%)	2.21	525/15368 (3.4%)

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	56	GLN	N-CA	7.89	1.55	1.46
1	A	290	THR	C-N	-7.52	1.29	1.34
1	A	35	ILE	C-O	-6.77	1.16	1.24
1	A	274	ARG	N-CA	-6.72	1.37	1.46
1	B	386	ALA	C-O	6.50	1.31	1.23
1	B	84	GLY	N-CA	6.47	1.50	1.44
1	A	71	ALA	N-CA	-6.39	1.38	1.46
1	A	199	ILE	N-CA	-6.38	1.38	1.46
1	B	361	LEU	C-N	6.15	1.42	1.33
1	B	356	ARG	N-CA	5.84	1.53	1.46
1	B	11	ALA	N-CA	-5.82	1.38	1.46
1	B	255	ALA	N-CA	-5.81	1.39	1.46
1	B	252	GLY	N-CA	5.78	1.51	1.45
1	A	254	ALA	N-CA	-5.72	1.39	1.46
1	B	188	ALA	C-O	5.70	1.30	1.24
1	A	362	LEU	N-CA	-5.53	1.39	1.46
1	B	117	GLU	N-CA	5.51	1.52	1.46
1	A	54	LEU	CA-CB	5.47	1.61	1.53
1	B	54	LEU	N-CA	-5.47	1.39	1.46
1	B	52	VAL	N-CA	-5.45	1.39	1.46
1	A	197	ASP	N-CA	-5.43	1.40	1.46
1	B	379	ILE	C-N	-5.33	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	GLY	N-CA	5.29	1.53	1.45
1	B	271	PRO	C-O	-5.28	1.17	1.23
1	B	384	GLY	N-CA	5.21	1.50	1.45
1	B	341	GLY	C-O	-5.20	1.18	1.23
1	A	86	ASN	N-CA	-5.13	1.40	1.46
1	A	54	LEU	CB-CG	5.05	1.63	1.53
1	B	86	ASN	N-CA	-5.03	1.40	1.46
1	A	64	GLN	CA-CB	5.00	1.61	1.53

All (525) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	ARG	CD-NE-CZ	23.01	156.61	124.40
1	B	4	SER	CA-C-O	-13.23	98.31	120.80
1	A	240	THR	N-CA-CB	-12.65	94.17	111.00
1	A	228	MET	CA-CB-CG	11.88	137.86	114.10
1	A	198	GLU	O-C-N	-11.59	109.84	122.12
1	B	240	THR	N-CA-CB	-11.01	96.36	111.00
1	C	59	PRO	CB-CA-C	-10.84	98.00	109.92
1	A	57	VAL	O-C-N	10.69	132.71	122.23
1	A	110	ILE	O-C-N	-10.48	112.28	123.18
1	B	86	ASN	OD1-CG-ND2	-10.34	112.27	122.60
1	A	34	VAL	CA-C-O	-10.00	110.25	120.85
1	A	200	VAL	CA-C-O	9.97	126.16	119.38
1	A	54	LEU	CA-C-O	9.96	130.85	120.40
1	A	124	HIS	CA-C-O	-9.87	109.85	120.80
1	B	350	ILE	CA-CB-CG1	9.73	126.95	110.40
1	B	367	ARG	NE-CZ-NH2	-9.64	110.52	119.20
1	A	266	ARG	CD-NE-CZ	9.54	137.75	124.40
1	B	200	VAL	N-CA-C	-9.46	97.58	107.89
1	A	99	GLY	CA-C-O	9.42	130.45	120.75
1	C	348	HIS	N-CA-CB	-9.37	99.47	111.09
1	B	41	ARG	NH1-CZ-NH2	9.37	131.48	119.30
1	A	297	ARG	CD-NE-CZ	9.30	137.41	124.40
1	A	339	VAL	CA-CB-CG2	9.26	126.15	110.40
1	C	207	ARG	CD-NE-CZ	9.26	137.37	124.40
1	B	371	ARG	CG-CD-NE	9.24	132.34	112.00
1	A	86	ASN	CA-CB-CG	9.24	121.84	112.60
1	A	207	ARG	CD-NE-CZ	9.21	137.29	124.40
1	A	196	LYS	O-C-N	-9.19	112.38	122.12
1	B	54	LEU	CA-C-O	-9.12	110.54	120.30
1	B	5	ILE	N-CA-C	9.08	120.96	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	VAL	CA-C-O	9.07	130.39	120.95
1	B	11	ALA	O-C-N	8.97	133.02	123.42
1	D	207	ARG	CD-NE-CZ	8.96	136.94	124.40
1	A	13	THR	CA-CB-OG1	8.95	123.03	109.60
1	D	347	GLY	CA-C-O	-8.94	115.85	122.37
1	A	338	ASN	OD1-CG-ND2	-8.91	113.69	122.60
1	A	65	ASN	OD1-CG-ND2	-8.87	113.73	122.60
1	A	200	VAL	O-C-N	-8.84	113.45	121.41
1	A	70	ALA	O-C-N	-8.83	112.97	122.07
1	B	157	MET	CA-C-N	8.69	129.62	119.98
1	B	157	MET	C-N-CA	8.69	129.62	119.98
1	B	51	GLU	O-C-N	-8.68	113.52	123.33
1	B	86	ASN	CB-CG-ND2	8.67	129.41	116.40
1	C	76	VAL	N-CA-C	-8.66	100.47	108.95
1	B	240	THR	CB-CA-C	8.65	122.63	109.13
1	A	198	GLU	CA-C-O	8.60	129.67	120.55
1	B	378	CYS	O-C-N	-8.56	113.29	122.96
1	B	379	ILE	CA-C-N	8.54	128.12	119.92
1	B	379	ILE	C-N-CA	8.54	128.12	119.92
1	A	44	VAL	CA-C-O	8.50	129.66	120.57
1	A	70	ALA	CA-C-N	8.37	131.32	120.44
1	A	70	ALA	C-N-CA	8.37	131.32	120.44
1	A	47	GLY	O-C-N	-8.36	113.36	122.73
1	A	40	GLU	CB-CG-CD	8.35	126.79	112.60
1	B	252	GLY	CA-C-O	-8.33	113.25	121.75
1	B	116	MET	O-C-N	8.20	132.66	123.48
1	B	250	ASN	CB-CG-ND2	8.19	128.69	116.40
1	B	270	GLN	OE1-CD-NE2	-8.15	114.45	122.60
1	B	341	GLY	N-CA-C	-8.15	102.47	112.33
1	A	50	ASN	CB-CG-ND2	8.11	128.56	116.40
1	B	245	ASN	CA-CB-CG	8.10	120.70	112.60
1	B	348	HIS	N-CA-CB	-8.07	101.08	111.09
1	A	12	ARG	NE-CZ-NH1	8.05	129.55	121.50
1	D	14	ALA	N-CA-C	-8.01	99.74	110.55
1	D	200	VAL	N-CA-CB	7.96	122.35	111.21
1	B	200	VAL	O-C-N	-7.94	114.26	121.41
1	C	24	ASN	CA-CB-CG	-7.94	104.66	112.60
1	B	341	GLY	CA-C-O	-7.91	116.27	122.52
1	B	187	GLU	CB-CG-CD	-7.91	99.15	112.60
1	B	85	MET	CA-C-O	7.87	129.83	121.33
1	A	247	SER	CA-C-N	-7.85	114.53	122.69
1	A	247	SER	C-N-CA	-7.85	114.53	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	238	GLU	CA-C-O	7.83	130.58	121.34
1	C	139	MET	N-CA-C	-7.72	95.93	108.52
1	A	228	MET	CA-C-O	7.68	128.56	120.42
1	A	302	ARG	NE-CZ-NH2	-7.66	112.31	119.20
1	A	277	SER	O-C-N	7.65	131.29	123.26
1	B	359	ASN	OD1-CG-ND2	-7.64	114.96	122.60
1	B	236	ASP	CA-CB-CG	7.62	120.22	112.60
1	B	360	THR	CA-C-O	-7.62	112.48	120.55
1	B	313	VAL	CA-C-O	7.57	129.09	120.76
1	B	138	LYS	CA-C-N	7.51	132.61	122.84
1	B	138	LYS	C-N-CA	7.51	132.61	122.84
1	A	136	ASP	CA-C-O	-7.50	112.84	121.47
1	B	277	SER	O-C-N	7.47	130.76	123.29
1	B	207	ARG	CD-NE-CZ	7.46	134.84	124.40
1	B	329	ASP	CA-CB-CG	-7.43	105.17	112.60
1	B	190	GLN	CA-C-O	7.41	128.60	120.82
1	B	357	ILE	CA-C-O	-7.41	112.47	120.47
1	B	255	ALA	O-C-N	7.40	131.03	123.26
1	C	131	GLY	CA-C-O	-7.40	117.12	122.23
1	B	343	ALA	N-CA-C	7.39	121.40	112.38
1	C	12	ARG	CA-C-O	-7.38	112.50	121.06
1	A	186	ALA	O-C-N	7.37	131.34	122.27
1	A	76	VAL	CA-C-O	-7.35	113.01	119.62
1	B	327	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	A	97	ALA	CA-C-N	7.32	130.09	120.28
1	A	97	ALA	C-N-CA	7.32	130.09	120.28
1	A	27	ALA	N-CA-C	7.30	120.16	111.33
1	A	356	ARG	NE-CZ-NH2	7.29	125.76	119.20
1	D	12	ARG	CA-C-O	-7.28	113.47	121.33
1	A	367	ARG	CD-NE-CZ	-7.27	114.22	124.40
1	B	5	ILE	CB-CA-C	-7.27	100.34	110.96
1	B	202	PHE	CA-CB-CG	-7.25	106.55	113.80
1	B	124	HIS	CA-CB-CG	-7.24	106.56	113.80
1	B	50	ASN	CB-CG-ND2	7.22	127.23	116.40
1	B	184	ASN	CA-C-O	7.22	128.21	120.55
1	D	64	GLN	CA-C-O	7.21	129.08	121.15
1	C	249	LEU	CA-C-O	-7.21	112.58	120.43
1	A	29	GLU	CA-C-O	7.19	128.24	119.97
1	A	217	GLU	CA-C-O	-7.17	109.93	119.11
1	C	135	GLY	CA-C-O	7.16	127.46	121.88
1	A	202	PHE	CA-CB-CG	-7.14	106.66	113.80
1	A	41	ARG	CA-C-N	-7.13	110.78	122.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ARG	C-N-CA	-7.13	110.78	122.54
1	D	316	ASN	CA-CB-CG	-7.06	105.54	112.60
1	B	76	VAL	N-CA-C	-7.05	101.27	108.96
1	C	94	ARG	CD-NE-CZ	7.03	134.24	124.40
1	A	268	GLY	CA-C-O	7.02	128.56	119.44
1	C	58	LEU	N-CA-CB	-7.02	99.65	111.30
1	A	4	SER	CA-C-O	-7.01	108.88	120.80
1	A	129	ARG	CG-CD-NE	-7.00	96.59	112.00
1	D	52	VAL	CA-C-N	6.97	132.48	123.13
1	D	52	VAL	C-N-CA	6.97	132.48	123.13
1	D	367	ARG	CD-NE-CZ	6.96	134.14	124.40
1	A	149	THR	CA-C-O	-6.95	113.34	120.71
1	C	372	LYS	CA-C-N	-6.94	114.20	121.35
1	C	372	LYS	C-N-CA	-6.94	114.20	121.35
1	A	87	GLN	N-CA-C	-6.92	102.02	110.88
1	B	31	GLY	O-C-N	6.91	128.87	122.17
1	C	306	LYS	CA-C-O	-6.90	113.14	121.28
1	A	362	LEU	N-CA-C	6.88	118.44	111.07
1	B	337	VAL	O-C-N	-6.88	115.95	123.18
1	A	85	MET	N-CA-C	-6.88	98.71	108.96
1	A	14	ALA	N-CA-C	-6.88	101.42	110.43
1	D	129	ARG	CG-CD-NE	-6.86	96.92	112.00
1	A	102	GLN	OE1-CD-NE2	6.83	129.43	122.60
1	C	41	ARG	NE-CZ-NH2	-6.81	113.07	119.20
1	A	250	ASN	N-CA-C	6.78	118.42	108.86
1	A	341	GLY	O-C-N	6.78	130.48	122.68
1	A	252	GLY	N-CA-C	6.77	120.63	110.75
1	B	38	VAL	N-CA-CB	6.76	119.74	110.54
1	A	196	LYS	CA-C-N	6.75	129.22	120.44
1	A	196	LYS	C-N-CA	6.75	129.22	120.44
1	A	230	LYS	N-CA-CB	-6.75	100.11	110.44
1	A	228	MET	CG-SD-CE	-6.75	86.05	100.90
1	B	367	ARG	CD-NE-CZ	6.73	133.82	124.40
1	B	256	ALA	CA-C-O	6.72	128.97	121.11
1	D	135	GLY	CA-C-O	6.72	126.87	122.23
1	A	198	GLU	N-CA-C	6.72	118.60	111.28
1	B	44	VAL	CA-C-O	6.71	127.59	120.48
1	B	198	GLU	CA-C-O	-6.71	111.87	119.79
1	B	361	LEU	O-C-N	6.69	128.96	122.07
1	B	200	VAL	CA-C-O	6.68	123.92	119.38
1	B	377	LEU	O-C-N	6.68	130.88	123.33
1	A	195	PHE	CA-CB-CG	-6.66	107.14	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	GLY	CA-C-N	6.65	131.89	122.72
1	A	273	GLY	C-N-CA	6.65	131.89	122.72
1	A	129	ARG	NE-CZ-NH2	-6.62	113.24	119.20
1	B	267	ARG	CD-NE-CZ	-6.62	115.13	124.40
1	A	273	GLY	O-C-N	-6.62	115.58	123.46
1	B	91	SER	N-CA-C	6.62	119.05	111.11
1	A	148	LEU	CA-C-N	-6.61	113.35	122.93
1	A	148	LEU	C-N-CA	-6.61	113.35	122.93
1	B	41	ARG	NE-CZ-NH2	-6.61	113.25	119.20
1	A	51	GLU	N-CA-C	6.60	119.35	108.99
1	D	5	ILE	CB-CG1-CD1	6.59	127.63	113.80
1	D	353	SER	N-CA-C	6.58	119.30	111.33
1	A	65	ASN	N-CA-C	6.57	124.34	109.81
1	A	86	ASN	OD1-CG-ND2	-6.54	116.06	122.60
1	A	172	ARG	CA-C-O	-6.53	113.62	120.55
1	A	166	LYS	CA-C-O	6.53	127.43	120.70
1	B	362	LEU	N-CA-C	6.49	118.35	111.28
1	A	44	VAL	O-C-N	-6.47	115.85	123.03
1	B	332	TRP	CA-C-O	6.46	128.60	121.56
1	A	50	ASN	CA-C-O	6.45	127.87	120.00
1	A	15	VAL	CB-CA-C	6.45	118.77	110.96
1	A	199	ILE	CB-CA-C	-6.45	102.77	111.15
1	B	41	ARG	NE-CZ-NH1	-6.43	115.07	121.50
1	A	219	ILE	CA-C-N	-6.43	113.85	122.72
1	A	219	ILE	C-N-CA	-6.43	113.85	122.72
1	B	55	GLY	N-CA-C	-6.41	103.86	111.36
1	D	346	ILE	N-CA-C	6.41	117.19	110.72
1	B	64	GLN	CA-C-O	-6.39	114.00	120.96
1	C	112	VAL	N-CA-CB	6.38	120.22	111.41
1	D	133	LYS	N-CA-C	6.38	118.24	111.28
1	B	9	SER	O-C-N	6.37	129.66	123.29
1	A	76	VAL	N-CA-C	-6.36	103.10	109.02
1	B	111	ILE	CA-C-N	-6.36	114.85	123.12
1	B	111	ILE	C-N-CA	-6.36	114.85	123.12
1	B	28	HIS	CA-C-O	-6.35	111.81	119.49
1	D	247	SER	N-CA-CB	6.34	119.06	110.38
1	B	148	LEU	N-CA-C	6.32	121.85	112.94
1	A	110	ILE	CA-C-O	6.30	126.64	120.27
1	A	159	THR	N-CA-C	-6.30	104.29	112.23
1	B	84	GLY	N-CA-C	-6.29	100.65	112.10
1	B	221	HIS	CA-CB-CG	-6.28	107.52	113.80
1	A	97	ALA	CA-C-O	6.28	127.07	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	35	ILE	CA-C-O	6.27	127.50	120.85
1	B	247	SER	CA-C-N	-6.26	116.18	122.69
1	B	247	SER	C-N-CA	-6.26	116.18	122.69
1	B	145	LYS	CA-C-O	6.26	127.39	120.82
1	B	339	VAL	N-CA-CB	-6.25	98.40	110.78
1	B	152	PHE	CA-CB-CG	-6.25	107.55	113.80
1	A	65	ASN	CA-C-N	6.24	126.71	119.47
1	A	65	ASN	C-N-CA	6.24	126.71	119.47
1	A	29	GLU	O-C-N	-6.24	114.60	122.27
1	C	51	GLU	CA-C-O	6.23	128.29	121.06
1	A	12	ARG	CD-NE-CZ	6.22	133.11	124.40
1	B	132	VAL	CA-C-O	-6.21	113.40	120.66
1	C	156	HIS	CA-CB-CG	6.20	120.00	113.80
1	B	86	ASN	N-CA-C	6.18	117.56	107.23
1	C	18	PHE	CA-CB-CG	6.17	119.97	113.80
1	B	37	ALA	CA-C-O	6.16	126.94	120.42
1	A	136	ASP	O-C-N	6.15	129.91	122.96
1	B	361	LEU	CA-CB-CG	6.15	137.81	116.30
1	A	26	PRO	CA-C-O	-6.14	114.44	121.56
1	C	284	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	343	ALA	CA-C-O	-6.12	113.19	120.10
1	A	109	SER	CA-CB-OG	-6.11	98.88	111.10
1	D	378	CYS	CA-C-O	-6.11	114.03	121.36
1	A	4	SER	N-CA-CB	6.11	120.88	110.50
1	A	135	GLY	N-CA-C	-6.10	105.82	112.04
1	A	78	GLN	OE1-CD-NE2	-6.08	116.52	122.60
1	A	83	TRP	O-C-N	6.08	130.29	123.48
1	A	28	HIS	CA-C-O	-6.07	113.24	120.10
1	D	12	ARG	CG-CD-NE	6.07	125.36	112.00
1	B	100	MET	CG-SD-CE	-6.07	87.55	100.90
1	A	333	ASP	CA-CB-CG	6.06	118.66	112.60
1	A	99	GLY	O-C-N	-6.06	116.37	122.19
1	B	387	MET	CA-C-O	-6.06	113.33	120.60
1	A	268	GLY	O-C-N	-6.06	114.81	122.32
1	B	375	ALA	CA-C-O	-6.06	114.16	120.70
1	B	54	LEU	O-C-N	6.04	130.28	123.27
1	C	122	ALA	O-C-N	6.02	127.80	121.42
1	A	335	SER	CA-C-O	-6.01	112.22	119.49
1	C	381	GLY	N-CA-C	-6.01	107.40	115.21
1	D	55	GLY	N-CA-C	-6.00	103.37	111.54
1	A	286	LYS	CA-C-O	-6.00	113.32	120.10
1	C	298	LYS	CA-CB-CG	6.00	126.09	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	GLU	CA-C-O	5.99	127.45	120.14
1	B	339	VAL	CA-CB-CG2	5.99	120.58	110.40
1	A	220	ARG	N-CA-CB	5.98	120.18	110.43
1	B	199	ILE	N-CA-CB	5.98	117.05	110.53
1	C	102	GLN	OE1-CD-NE2	-5.97	116.63	122.60
1	A	197	ASP	N-CA-CB	5.97	118.67	110.01
1	B	317	GLU	N-CA-CB	5.95	117.79	110.53
1	B	373	GLY	O-C-N	5.95	128.77	123.60
1	B	302	ARG	CD-NE-CZ	5.93	132.70	124.40
1	C	383	MET	O-C-N	5.93	129.92	123.10
1	D	316	ASN	CA-C-O	5.93	126.88	120.95
1	B	302	ARG	NE-CZ-NH2	-5.92	113.87	119.20
1	A	196	LYS	N-CA-C	5.92	117.73	111.28
1	B	363	PHE	CA-C-O	-5.92	112.81	119.79
1	A	247	SER	CA-C-O	-5.92	115.25	121.99
1	B	49	VAL	CA-CB-CG1	5.91	120.45	110.40
1	C	139	MET	N-CA-CB	5.91	119.83	110.55
1	C	257	LEU	CA-C-O	-5.91	114.04	120.36
1	A	228	MET	N-CA-CB	-5.91	101.42	110.16
1	A	323	ALA	CA-C-O	-5.90	114.62	120.82
1	A	186	ALA	CA-C-O	-5.90	113.19	119.97
1	C	217	GLU	N-CA-C	5.89	120.33	113.20
1	A	68	ARG	O-C-N	5.89	128.36	122.12
1	A	19	ASN	CA-C-N	5.88	135.83	123.12
1	A	19	ASN	C-N-CA	5.88	135.83	123.12
1	A	367	ARG	O-C-N	-5.88	115.89	122.12
1	D	150	ASP	CA-CB-CG	-5.88	106.72	112.60
1	C	318	ALA	N-CA-C	-5.88	104.96	111.36
1	B	117	GLU	O-C-N	-5.87	116.73	123.42
1	A	50	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	B	297	ARG	NE-CZ-NH1	5.86	127.36	121.50
1	B	168	TRP	CA-C-N	5.86	130.68	122.36
1	B	168	TRP	C-N-CA	5.86	130.68	122.36
1	A	184	ASN	O-C-N	-5.85	115.91	122.12
1	B	298	LYS	CA-C-O	5.85	126.62	120.42
1	D	140	ILE	N-CA-C	5.84	116.99	108.58
1	B	249	LEU	N-CA-C	-5.84	99.01	108.52
1	B	276	VAL	CB-CA-C	5.83	119.87	111.65
1	B	5	ILE	CB-CG1-CD1	5.82	126.01	113.80
1	A	175	GLN	O-C-N	5.81	128.06	122.07
1	A	312	LEU	CA-C-O	-5.81	114.48	120.99
1	A	242	THR	CA-C-O	-5.81	114.75	121.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	HIS	N-CA-CB	5.80	119.16	110.22
1	B	250	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	B	56	GLN	CB-CG-CD	-5.79	102.76	112.60
1	C	27	ALA	CA-C-O	-5.79	114.71	120.90
1	D	361	LEU	CB-CA-C	-5.79	101.55	110.81
1	A	278	TRP	N-CA-C	-5.79	100.34	108.96
1	C	283	VAL	N-CA-CB	5.76	120.73	111.23
1	A	57	VAL	CA-C-O	-5.75	113.68	119.20
1	B	13	THR	N-CA-C	-5.74	102.02	110.52
1	C	321	ALA	CA-C-O	-5.74	114.46	120.55
1	B	43	GLY	N-CA-C	-5.74	106.25	115.08
1	D	338	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	B	219	ILE	O-C-N	-5.71	117.25	122.79
1	A	239	GLY	CA-C-O	5.71	127.92	121.92
1	A	220	ARG	NE-CZ-NH2	-5.70	114.07	119.20
1	B	357	ILE	N-CA-C	-5.70	103.97	111.09
1	B	371	ARG	CA-C-N	-5.70	113.97	122.74
1	B	371	ARG	C-N-CA	-5.70	113.97	122.74
1	A	178	PHE	CA-CB-CG	5.69	119.49	113.80
1	C	150	ASP	CA-CB-CG	-5.69	106.91	112.60
1	C	219	ILE	CA-C-N	-5.66	114.91	122.72
1	C	219	ILE	C-N-CA	-5.66	114.91	122.72
1	B	76	VAL	CA-C-O	-5.64	114.40	119.82
1	A	42	ALA	N-CA-CB	-5.64	102.14	110.49
1	B	284	ASP	CA-C-N	5.64	126.01	119.47
1	B	284	ASP	C-N-CA	5.64	126.01	119.47
1	A	9	SER	O-C-N	-5.63	117.34	123.26
1	B	135	GLY	N-CA-C	-5.63	104.63	112.18
1	B	100	MET	N-CA-CB	-5.63	101.83	110.16
1	B	266	ARG	CD-NE-CZ	5.63	132.28	124.40
1	B	333	ASP	CA-C-O	5.63	125.03	119.51
1	A	41	ARG	NH1-CZ-NH2	5.63	126.62	119.30
1	B	24	ASN	CB-CG-ND2	5.63	124.84	116.40
1	A	70	ALA	CA-C-O	5.62	126.72	120.82
1	A	284	ASP	CA-C-N	5.62	125.72	119.32
1	A	284	ASP	C-N-CA	5.62	125.72	119.32
1	B	361	LEU	CA-C-N	-5.62	112.75	120.28
1	B	361	LEU	C-N-CA	-5.62	112.75	120.28
1	B	265	SER	CB-CA-C	5.61	119.69	110.88
1	A	87	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	B	260	SER	N-CA-CB	5.60	118.23	110.17
1	A	367	ARG	N-CA-C	5.60	117.38	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	LEU	CA-C-N	-5.59	114.60	120.31
1	A	54	LEU	C-N-CA	-5.59	114.60	120.31
1	A	353	SER	CA-CB-OG	-5.59	99.92	111.10
1	D	79	GLU	CB-CG-CD	5.59	122.10	112.60
1	B	184	ASN	O-C-N	-5.58	116.21	122.12
1	D	119	MET	CA-C-N	5.57	127.69	120.44
1	D	119	MET	C-N-CA	5.57	127.69	120.44
1	A	350	ILE	N-CA-C	5.57	120.93	109.34
1	B	255	ALA	N-CA-C	5.57	116.73	108.60
1	B	4	SER	N-CA-CB	5.57	119.97	110.50
1	B	348	HIS	N-CA-C	5.57	119.96	108.71
1	C	86	ASN	N-CA-CB	-5.56	102.22	110.90
1	B	195	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	302	ARG	CA-CB-CG	-5.56	102.98	114.10
1	B	35	ILE	O-C-N	-5.55	116.11	121.83
1	B	187	GLU	CA-CB-CG	-5.55	103.00	114.10
1	C	339	VAL	CB-CA-C	5.54	119.29	112.04
1	D	326	VAL	CB-CA-C	-5.54	104.89	111.81
1	C	270	GLN	OE1-CD-NE2	5.53	128.13	122.60
1	D	87	GLN	N-CA-CB	5.53	119.39	111.65
1	B	284	ASP	CA-C-O	-5.52	114.28	119.80
1	A	138	LYS	CA-C-N	5.52	130.52	122.85
1	A	138	LYS	C-N-CA	5.52	130.52	122.85
1	B	250	ASN	CA-CB-CG	-5.51	107.08	112.60
1	D	36	SER	CA-C-O	-5.51	114.71	120.55
1	A	35	ILE	O-C-N	-5.51	116.51	121.91
1	B	348	HIS	CA-C-N	5.51	126.72	119.84
1	B	348	HIS	C-N-CA	5.51	126.72	119.84
1	A	41	ARG	CD-NE-CZ	-5.50	116.70	124.40
1	B	200	VAL	N-CA-CB	5.50	117.49	111.61
1	C	87	GLN	N-CA-C	-5.50	103.44	111.30
1	B	196	LYS	N-CA-C	5.49	117.26	111.28
1	B	156	HIS	N-CA-C	5.48	117.77	110.53
1	A	168	TRP	N-CA-C	-5.48	106.26	113.17
1	D	378	CYS	N-CA-C	-5.48	101.61	110.32
1	C	137	PHE	CA-CB-CG	5.47	119.27	113.80
1	B	205	LYS	N-CA-CB	5.46	118.12	109.71
1	A	93	LEU	CA-C-N	5.46	127.59	120.28
1	A	93	LEU	C-N-CA	5.46	127.59	120.28
1	B	318	ALA	N-CA-C	-5.45	105.24	111.07
1	B	14	ALA	N-CA-C	-5.45	102.94	110.35
1	B	339	VAL	CG1-CB-CG2	5.44	122.77	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	322	GLN	CA-CB-CG	5.43	124.97	114.10
1	A	359	ASN	N-CA-C	-5.43	105.44	111.36
1	A	19	ASN	OD1-CG-ND2	5.42	128.02	122.60
1	A	110	ILE	N-CA-C	5.42	115.79	107.77
1	B	113	ALA	CA-C-O	-5.42	114.77	121.11
1	B	99	GLY	O-C-N	5.42	127.44	122.19
1	A	111	ILE	CA-CB-CG2	5.41	119.70	110.50
1	C	175	GLN	N-CA-C	-5.41	105.81	112.90
1	D	58	LEU	N-CA-C	5.40	118.43	109.79
1	A	140	ILE	N-CA-C	5.39	116.01	108.89
1	B	139	MET	N-CA-C	-5.39	98.99	108.20
1	B	64	GLN	O-C-N	5.38	129.52	123.06
1	C	86	ASN	N-CA-C	5.38	117.11	107.80
1	C	85	MET	CA-C-N	-5.38	114.64	122.44
1	C	85	MET	C-N-CA	-5.38	114.64	122.44
1	D	112	VAL	N-CA-CB	5.37	118.55	111.25
1	B	389	ILE	CA-CB-CG1	5.36	119.52	110.40
1	C	339	VAL	N-CA-CB	-5.35	103.78	110.47
1	C	359	ASN	CB-CA-C	-5.35	102.48	110.88
1	B	68	ARG	NE-CZ-NH2	5.35	124.01	119.20
1	D	13	THR	N-CA-C	-5.34	102.08	110.36
1	C	119	MET	N-CA-C	-5.34	105.50	112.23
1	A	31	GLY	CA-C-O	-5.34	115.00	120.66
1	A	264	ALA	N-CA-C	-5.34	105.54	111.36
1	C	278	TRP	CA-C-O	-5.34	115.56	121.33
1	A	57	VAL	CB-CA-C	-5.34	103.05	110.95
1	A	28	HIS	CA-C-N	-5.33	112.21	120.31
1	A	28	HIS	C-N-CA	-5.33	112.21	120.31
1	A	185	LYS	N-CA-CB	5.33	118.04	110.16
1	B	120	SER	CB-CA-C	-5.32	101.96	110.79
1	A	175	GLN	CA-C-O	-5.32	115.23	120.82
1	A	339	VAL	CB-CA-C	5.32	121.94	111.79
1	B	315	ALA	N-CA-C	-5.32	99.74	108.41
1	C	131	GLY	N-CA-C	-5.32	106.33	112.29
1	A	223	ALA	CA-C-O	-5.31	115.21	121.16
1	A	188	ALA	O-C-N	-5.30	116.50	122.12
1	C	267	ARG	CD-NE-CZ	5.30	131.83	124.40
1	C	14	ALA	N-CA-C	-5.30	103.89	110.41
1	A	97	ALA	O-C-N	-5.30	116.11	122.15
1	B	373	GLY	CA-C-O	-5.29	115.90	121.57
1	A	172	ARG	O-C-N	5.29	127.73	122.12
1	A	145	LYS	O-C-N	5.28	127.80	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	228	MET	O-C-N	-5.28	116.13	122.15
1	B	194	ARG	CD-NE-CZ	5.28	131.78	124.40
1	B	47	GLY	O-C-N	-5.27	116.82	122.73
1	B	362	LEU	N-CA-CB	-5.27	102.37	110.12
1	B	97	ALA	O-C-N	-5.27	116.14	122.15
1	D	150	ASP	N-CA-CB	5.27	117.75	109.69
1	A	113	ALA	CA-C-O	5.27	127.17	121.06
1	D	276	VAL	CB-CA-C	5.26	120.74	112.16
1	A	37	ALA	CA-C-O	-5.26	114.84	120.42
1	B	119	MET	CA-CB-CG	-5.26	103.58	114.10
1	A	180	VAL	CB-CA-C	-5.26	104.96	112.22
1	B	56	GLN	CA-CB-CG	-5.25	103.59	114.10
1	A	144	ILE	CA-C-O	5.25	126.74	121.17
1	D	112	VAL	N-CA-C	-5.25	100.82	108.17
1	C	12	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	A	42	ALA	O-C-N	-5.25	115.78	122.34
1	B	372	LYS	CA-C-N	-5.25	117.41	121.82
1	B	372	LYS	C-N-CA	-5.25	117.41	121.82
1	B	11	ALA	CA-C-N	-5.24	113.72	122.21
1	B	11	ALA	C-N-CA	-5.24	113.72	122.21
1	B	53	ILE	O-C-N	-5.24	117.38	122.99
1	B	195	PHE	CA-C-O	5.24	125.42	119.18
1	B	145	LYS	N-CA-C	5.24	116.68	111.07
1	D	344	ILE	CA-C-O	-5.24	115.62	121.17
1	A	321	ALA	O-C-N	-5.23	116.68	122.07
1	B	102	GLN	CG-CD-OE1	-5.22	110.35	120.80
1	B	54	LEU	N-CA-C	5.22	116.92	108.41
1	B	258	LEU	CB-CA-C	-5.22	99.82	109.37
1	B	337	VAL	CA-C-N	5.21	129.81	122.46
1	B	337	VAL	C-N-CA	5.21	129.81	122.46
1	A	234	ALA	CA-C-O	-5.20	113.42	119.14
1	B	350	ILE	N-CA-C	5.20	120.16	109.34
1	C	385	VAL	N-CA-CB	5.20	119.89	111.36
1	A	340	ASN	N-CA-C	5.19	118.92	112.59
1	B	304	GLY	O-C-N	-5.19	115.88	122.32
1	D	316	ASN	N-CA-C	5.19	118.00	110.42
1	A	96	VAL	N-CA-CB	5.19	118.36	110.58
1	B	14	ALA	CA-C-N	5.18	128.85	122.37
1	B	14	ALA	C-N-CA	5.18	128.85	122.37
1	B	160	THR	N-CA-C	-5.18	105.63	111.28
1	A	127	HIS	CA-C-N	5.17	130.51	122.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	HIS	C-N-CA	5.17	130.51	122.49
1	B	187	GLU	OE1-CD-OE2	5.17	135.32	122.90
1	C	95	ALA	CB-CA-C	-5.17	102.54	110.81
1	C	207	ARG	N-CA-C	-5.17	106.11	112.72
1	D	309	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	258	LEU	N-CA-C	5.16	118.15	109.95
1	C	358	LEU	CA-C-O	5.16	126.02	120.55
1	B	288	MET	CA-C-O	5.15	125.97	120.20
1	B	116	MET	CA-C-N	-5.15	112.88	121.64
1	B	116	MET	C-N-CA	-5.15	112.88	121.64
1	C	364	GLU	N-CA-CB	5.15	117.88	110.20
1	C	196	LYS	N-CA-C	5.15	117.29	111.11
1	C	266	ARG	CA-CB-CG	5.15	124.39	114.10
1	A	279	ALA	CB-CA-C	-5.14	101.07	110.62
1	B	27	ALA	N-CA-C	5.13	116.88	111.28
1	A	280	THR	N-CA-CB	5.13	119.43	110.81
1	A	240	THR	OG1-CB-CG2	5.13	119.56	109.30
1	B	201	PRO	CB-CA-C	-5.13	104.39	111.21
1	D	10	ALA	N-CA-CB	-5.13	103.61	111.56
1	D	64	GLN	OE1-CD-NE2	5.13	127.73	122.60
1	B	34	VAL	CA-C-O	-5.13	114.93	120.47
1	A	309	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	10	ALA	CA-C-O	5.12	126.71	121.23
1	B	109	SER	CA-CB-OG	-5.12	100.86	111.10
1	D	358	LEU	N-CA-C	-5.12	105.40	111.69
1	C	54	LEU	N-CA-CB	5.12	119.11	110.77
1	B	220	ARG	N-CA-CB	5.11	118.52	110.23
1	B	378	CYS	CB-CA-C	5.11	118.87	109.46
1	A	168	TRP	CB-CA-C	5.11	118.62	110.09
1	A	200	VAL	N-CA-CB	5.11	117.07	111.61
1	B	65	ASN	CA-C-N	5.10	125.39	119.47
1	B	65	ASN	C-N-CA	5.10	125.39	119.47
1	C	24	ASN	OD1-CG-ND2	5.10	127.70	122.60
1	A	56	GLN	OE1-CD-NE2	-5.10	117.50	122.60
1	A	328	LYS	CA-CB-CG	5.09	124.29	114.10
1	B	38	VAL	N-CA-C	5.09	115.81	110.62
1	D	161	ALA	N-CA-C	-5.09	105.64	111.14
1	B	102	GLN	N-CA-C	-5.09	105.73	111.28
1	A	298	LYS	N-CA-CB	-5.08	102.65	110.12
1	C	276	VAL	CB-CA-C	5.08	119.05	112.24
1	B	276	VAL	CA-CB-CG2	5.08	119.03	110.40
1	D	379	ILE	CA-C-O	-5.07	114.99	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	PHE	N-CA-CB	5.07	118.42	110.46
1	D	53	ILE	CB-CG1-CD1	5.07	124.45	113.80
1	D	152	PHE	CA-CB-CG	-5.07	108.73	113.80
1	A	364	GLU	N-CA-C	-5.06	105.46	111.69
1	A	371	ARG	CD-NE-CZ	5.06	131.49	124.40
1	C	262	ALA	CA-C-O	5.06	126.64	121.07
1	C	65	ASN	CA-C-N	5.06	125.34	119.47
1	C	65	ASN	C-N-CA	5.06	125.34	119.47
1	A	201	PRO	CB-CA-C	-5.06	104.76	111.23
1	A	64	GLN	CA-C-O	-5.05	115.16	120.92
1	B	160	THR	N-CA-CB	5.05	117.55	110.12
1	B	332	TRP	O-C-N	-5.05	116.90	122.86
1	C	367	ARG	N-CA-C	5.05	116.79	111.28
1	D	192	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	68	ARG	CA-C-O	-5.04	115.20	120.55
1	D	107	ASP	N-CA-CB	-5.04	103.12	110.53
1	B	203	ILE	CA-C-O	-5.04	114.89	120.74
1	A	250	ASN	CA-CB-CG	-5.04	107.56	112.60
1	B	353	SER	N-CA-C	5.03	117.42	111.33
1	A	86	ASN	CB-CG-ND2	5.03	123.94	116.40
1	C	132	VAL	CB-CA-C	5.03	118.18	111.19
1	A	41	ARG	NE-CZ-NH2	-5.03	114.68	119.20
1	A	254	ALA	O-C-N	5.02	129.21	123.48
1	A	357	ILE	O-C-N	-5.02	116.33	122.06
1	A	377	LEU	CA-C-N	5.02	129.72	121.39
1	A	377	LEU	C-N-CA	5.02	129.72	121.39
1	A	135	GLY	CA-C-O	5.02	126.06	122.45
1	B	187	GLU	CG-CD-OE1	-5.01	106.87	118.40
1	C	123	PRO	N-CA-C	5.01	118.23	111.22
1	A	299	ALA	O-C-N	-5.00	116.82	122.12
1	B	214	ASP	CA-C-O	5.00	124.71	119.51
1	B	385	VAL	CA-C-O	-5.00	115.98	121.28
1	A	388	CYS	CA-C-O	5.00	126.35	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2816	0	2821	77	0
1	B	2816	0	2821	67	0
1	C	2816	0	2821	78	0
1	D	2816	0	2821	96	0
2	A	15	0	0	0	0
2	B	15	0	0	2	0
3	A	48	0	32	4	0
3	B	48	0	31	0	0
3	C	48	0	31	1	0
3	D	48	0	31	2	0
4	A	287	0	0	10	0
4	B	275	0	0	20	0
4	C	94	0	0	9	0
4	D	62	0	0	7	0
All	All	12204	0	11409	305	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 13.

All (305) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LEU:HG	4:A:770:HOH:O	1.45	1.12
1:B:258:LEU:HG	4:B:939:HOH:O	1.53	1.07
1:D:88:LEU:HB3	1:D:89:SCY:HE2	1.39	1.03
1:D:89:SCY:HE1	1:D:380:GLY:H	1.24	1.03
1:D:258:LEU:HG	4:D:421:HOH:O	1.62	0.98
1:C:89:SCY:HE1	1:C:380:GLY:H	1.31	0.92
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.30	0.92
1:A:93:LEU:HD11	1:A:387:MET:HE2	1.53	0.89
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.11	0.85
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.39	0.84
1:C:5:ILE:HG13	1:C:100:MET:HG2	1.58	0.84
1:B:247:SER:HB2	4:B:840:HOH:O	1.77	0.83
1:D:89:SCY:CE	1:D:380:GLY:H	1.94	0.79
1:B:390:GLU:OE2	4:B:961:HOH:O	2.01	0.79
1:C:89:SCY:CE	1:C:380:GLY:H	1.96	0.79
1:D:89:SCY:HE1	1:D:380:GLY:N	1.97	0.79
1:B:134:MET:HG3	4:C:401:HOH:O	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:SCY:HE1	1:A:380:GLY:H	1.47	0.78
1:A:175:GLN:HE22	1:A:240:THR:CG2	1.95	0.77
1:B:372:LYS:HE3	4:B:928:HOH:O	1.84	0.77
1:A:387:MET:SD	4:A:887:HOH:O	2.43	0.76
1:D:88:LEU:CB	1:D:89:SCY:HE2	2.15	0.75
1:B:356:ARG:C	1:B:356:ARG:HD2	2.13	0.74
1:D:300:LEU:HD21	1:D:310:LEU:HD11	1.67	0.74
1:B:89:SCY:HE1	1:B:380:GLY:H	1.52	0.74
1:D:88:LEU:HB3	1:D:89:SCY:CE	2.14	0.73
1:D:5:ILE:HG13	1:D:100:MET:HG2	1.71	0.72
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.54	0.72
1:C:89:SCY:HE1	1:C:380:GLY:N	2.04	0.72
1:D:298:LYS:HE2	1:D:302:ARG:HG3	1.72	0.72
1:A:88:LEU:HB3	1:A:89:SCY:HE2	1.73	0.70
1:A:298:LYS:HA	1:A:298:LYS:NZ	2.07	0.70
1:B:207:ARG:HG2	1:B:207:ARG:HH11	1.57	0.70
1:A:279:ALA:HB1	1:A:298:LYS:HG3	1.75	0.69
1:D:290:THR:HA	4:D:444:HOH:O	1.92	0.68
1:A:247:SER:HB2	4:A:951:HOH:O	1.93	0.67
1:B:392:LEU:HD12	4:B:854:HOH:O	1.95	0.67
1:D:292:PRO:HD3	1:D:378:CYS:HA	1.76	0.67
1:A:279:ALA:CB	1:A:298:LYS:HG3	2.25	0.66
1:C:64:GLN:HE22	1:D:157:MET:HE3	1.60	0.66
1:D:326:VAL:HG22	4:D:444:HOH:O	1.95	0.66
1:D:203:ILE:HB	4:D:448:HOH:O	1.95	0.66
1:D:89:SCY:HE2	1:D:89:SCY:H	1.61	0.65
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.61	0.65
1:B:392:LEU:HB2	4:B:854:HOH:O	1.96	0.65
1:A:163:ASN:HA	1:A:166:LYS:NZ	2.12	0.65
1:A:12:ARG:HD2	1:A:356:ARG:HG2	1.79	0.65
1:A:163:ASN:HA	1:A:166:LYS:HZ1	1.61	0.65
1:B:41:ARG:HD2	4:B:907:HOH:O	1.96	0.65
1:B:257:LEU:HD23	1:B:258:LEU:N	2.11	0.64
1:B:5:ILE:HG13	1:B:100:MET:HG2	1.79	0.64
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.11	0.64
1:A:225:LEU:HG	4:A:926:HOH:O	1.98	0.63
1:B:4:SER:CA	4:B:999:HOH:O	2.46	0.63
1:D:322:GLN:O	1:D:326:VAL:HG23	1.99	0.63
1:B:88:LEU:HB3	1:B:89:SCY:HE2	1.82	0.62
1:C:297:ARG:HG2	1:C:297:ARG:HH11	1.62	0.62
1:A:358:LEU:HD21	1:A:387:MET:HE3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:LEU:HB2	1:D:379:ILE:HG23	1.80	0.62
1:A:89:SCY:CE	1:A:380:GLY:H	2.12	0.61
1:A:175:GLN:NE2	1:A:240:THR:HG23	2.13	0.61
1:B:257:LEU:HD23	1:B:257:LEU:C	2.26	0.61
1:B:186:ALA:HA	1:B:340:ASN:O	2.00	0.61
1:A:247:SER:HB2	1:A:348:HIS:HB2	1.83	0.60
1:D:175:GLN:HE22	1:D:240:THR:CG2	2.15	0.60
1:A:89:SCY:HE1	1:A:380:GLY:N	2.16	0.60
1:D:55:GLY:HA2	1:D:85:MET:O	2.01	0.60
1:D:305:TRP:CE2	1:D:372:LYS:HD3	2.37	0.60
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.14	0.59
1:A:228:MET:HE1	1:A:244:GLY:HA3	1.83	0.59
1:C:207:ARG:HG2	1:C:207:ARG:HH11	1.68	0.59
1:A:228:MET:HE1	1:A:244:GLY:C	2.28	0.59
1:A:52:VAL:O	1:A:82:ALA:HA	2.03	0.58
1:B:41:ARG:HB2	4:B:907:HOH:O	2.02	0.58
1:A:191:LYS:NZ	4:A:736:HOH:O	2.36	0.58
1:C:236:ASP:HB3	1:C:239:GLY:HA3	1.86	0.58
1:D:97:ALA:O	1:D:101:GLN:HG3	2.04	0.58
1:C:37:ALA:HB2	1:C:200:VAL:HG21	1.86	0.57
1:C:374:LEU:C	1:C:374:LEU:HD23	2.29	0.57
1:C:89:SCY:SG	1:C:350:ILE:HG23	2.44	0.57
1:A:133:LYS:HA	4:C:464:HOH:O	2.04	0.57
1:A:387:MET:HE3	1:A:389:ILE:HD11	1.86	0.56
1:D:180:VAL:HG22	1:D:228:MET:HE3	1.86	0.56
1:C:129:ARG:NH2	1:D:122:ALA:O	2.35	0.56
1:A:354:GLY:HA2	1:A:377:LEU:HD11	1.87	0.56
1:A:40:GLU:HG3	4:A:1010:HOH:O	2.05	0.56
1:B:348:HIS:HB2	4:B:840:HOH:O	2.05	0.56
1:A:276:VAL:HG22	1:A:388:CYS:HB2	1.87	0.56
1:C:41:ARG:NH1	1:C:197:ASP:O	2.39	0.56
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.30	0.56
1:B:41:ARG:CD	4:B:907:HOH:O	2.53	0.56
1:D:358:LEU:HD22	1:D:362:LEU:HG	1.88	0.56
1:B:4:SER:N	4:B:999:HOH:O	2.38	0.56
1:B:89:SCY:HE1	1:B:380:GLY:N	2.21	0.55
1:D:9:SER:HA	1:D:272:LEU:CD2	2.36	0.55
1:D:236:ASP:HB3	1:D:239:GLY:HA3	1.88	0.55
1:A:12:ARG:O	1:A:199:ILE:HA	2.07	0.54
1:B:4:SER:CB	4:B:999:HOH:O	2.55	0.54
1:D:207:ARG:HG2	1:D:207:ARG:HH11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ARG:HD2	1:B:356:ARG:O	2.06	0.54
1:A:9:SER:HA	1:A:272:LEU:HD22	1.90	0.54
1:D:275:ILE:HA	1:D:389:ILE:HD13	1.90	0.54
1:B:203:ILE:CD1	1:B:212:THR:OG1	2.56	0.54
1:A:206:GLY:HA3	1:A:209:GLY:O	2.08	0.54
1:A:298:LYS:HA	1:A:298:LYS:HZ3	1.70	0.54
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.73	0.54
1:B:100:MET:C	1:B:100:MET:HE2	2.32	0.53
1:C:129:ARG:HD3	1:D:18:PHE:CZ	2.43	0.53
1:D:311:ASP:HB2	1:D:370:ALA:HB1	1.89	0.53
1:D:291:GLY:O	1:D:294:PRO:HD2	2.09	0.53
1:B:257:LEU:C	1:B:257:LEU:CD2	2.82	0.53
1:D:133:LYS:HD3	4:D:426:HOH:O	2.08	0.53
1:B:50:ASN:HB3	4:B:953:HOH:O	2.08	0.53
1:B:132:VAL:O	1:D:129:ARG:HA	2.08	0.53
1:C:103:ILE:HA	1:C:108:ALA:O	2.07	0.53
1:C:168:TRP:CH2	1:C:329:ASP:HB2	2.43	0.53
1:D:314:GLU:OE2	1:D:338:ASN:HA	2.09	0.53
1:A:34:VAL:HG12	1:A:255:ALA:HB3	1.90	0.53
1:B:260:SER:OG	2:B:721:SO4:O2	2.24	0.53
1:C:176:ASP:CG	1:C:228:MET:HG3	2.34	0.53
1:C:358:LEU:HD22	1:C:362:LEU:HG	1.91	0.52
1:D:187:GLU:HG3	1:D:221:HIS:HA	1.91	0.52
1:D:258:LEU:HD22	1:D:258:LEU:N	2.24	0.52
1:A:372:LYS:HE3	4:A:922:HOH:O	2.08	0.52
1:D:72:MET:HE1	1:D:78:GLN:HB3	1.92	0.52
1:A:257:LEU:C	1:A:257:LEU:HD23	2.35	0.52
1:C:300:LEU:HD13	1:C:307:ILE:HG12	1.90	0.52
1:B:316:ASN:HB3	4:B:744:HOH:O	2.09	0.52
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.45	0.52
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.45	0.52
1:D:263:GLU:OE1	1:D:266:ARG:NH1	2.43	0.52
1:D:57:VAL:HG21	1:D:350:ILE:HG22	1.91	0.52
1:D:64:GLN:O	1:D:65:ASN:C	2.53	0.52
1:A:228:MET:HE1	1:A:244:GLY:CA	2.40	0.51
1:B:237:LYS:HB2	4:B:855:HOH:O	2.09	0.51
1:B:293:ILE:HB	1:B:294:PRO:HD3	1.91	0.51
1:C:272:LEU:HG	4:C:430:HOH:O	2.10	0.51
1:A:207:ARG:HG2	1:A:208:LYS:H	1.75	0.51
1:B:89:SCY:CE	1:B:380:GLY:H	2.21	0.51
1:C:293:ILE:HB	1:C:294:PRO:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HB2	1:B:379:ILE:HG23	1.93	0.51
1:D:206:GLY:HA3	1:D:209:GLY:O	2.10	0.51
1:A:258:LEU:N	1:A:258:LEU:HD22	2.26	0.51
1:C:12:ARG:HA	1:C:254:ALA:HA	1.93	0.51
1:B:4:SER:N	4:B:862:HOH:O	2.43	0.51
1:B:236:ASP:O	1:B:239:GLY:N	2.43	0.51
1:D:35:ILE:O	1:D:38:VAL:HG22	2.11	0.51
1:B:89:SCY:HE2	1:B:89:SCY:H	1.75	0.50
1:C:39:LEU:HD12	1:C:44:VAL:O	2.12	0.50
1:C:207:ARG:HG2	1:C:208:LYS:H	1.77	0.50
1:B:293:ILE:HB	1:B:294:PRO:CD	2.41	0.50
1:C:293:ILE:HB	1:C:294:PRO:CD	2.41	0.50
1:A:298:LYS:HA	1:A:298:LYS:HZ2	1.77	0.50
1:B:207:ARG:HG2	1:B:208:LYS:H	1.75	0.50
1:C:122:ALA:O	1:D:129:ARG:NH2	2.42	0.50
1:D:207:ARG:HG2	1:D:208:LYS:H	1.77	0.50
1:B:134:MET:O	1:B:134:MET:HG2	2.11	0.50
1:A:305:TRP:CZ3	1:A:388:CYS:HB3	2.47	0.50
1:D:18:PHE:O	1:D:19:ASN:HB2	2.12	0.50
1:D:288:MET:HE1	3:D:393:COA:S1P	2.52	0.50
1:C:128:LEU:HD21	1:C:137:PHE:CZ	2.47	0.50
1:C:187:GLU:OE1	1:C:191:LYS:HE2	2.11	0.50
1:C:157:MET:HE2	1:C:157:MET:HA	1.94	0.49
1:A:85:MET:HA	1:B:85:MET:HA	1.94	0.49
1:C:145:LYS:O	1:D:63:GLY:HA2	2.12	0.49
1:B:89:SCY:SG	1:B:350:ILE:HG23	2.53	0.49
1:A:258:LEU:CG	4:A:770:HOH:O	2.27	0.49
1:C:353:SER:O	1:C:357:ILE:HG23	2.13	0.49
1:C:305:TRP:CE2	1:C:372:LYS:HD3	2.47	0.49
1:D:195:PHE:O	1:D:198:GLU:HG2	2.12	0.49
1:D:293:ILE:HB	1:D:294:PRO:HD3	1.95	0.49
1:C:258:LEU:N	1:C:258:LEU:HD22	2.26	0.49
4:B:899:HOH:O	1:C:145:LYS:HB2	2.12	0.48
1:D:272:LEU:HD21	4:D:430:HOH:O	2.12	0.48
1:A:298:LYS:NZ	1:A:301:GLU:OE1	2.47	0.48
1:D:168:TRP:CH2	1:D:329:ASP:HB2	2.48	0.48
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.75	0.48
1:A:371:ARG:HG3	4:A:932:HOH:O	2.12	0.48
1:D:276:VAL:HG11	1:D:305:TRP:CZ2	2.49	0.48
1:C:312:LEU:HD21	1:C:364:GLU:HB3	1.95	0.47
1:B:9:SER:HA	1:B:272:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:LYS:NZ	1:B:191:LYS:HB3	2.30	0.47
1:C:143:MET:CG	4:C:421:HOH:O	2.61	0.47
1:A:314:GLU:O	1:A:375:ALA:HA	2.15	0.47
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.50	0.47
1:B:298:LYS:HE2	2:B:719:SO4:O1	2.13	0.47
1:C:333:ASP:O	1:C:334:PRO:C	2.57	0.47
1:D:240:THR:HA	4:D:436:HOH:O	2.14	0.47
1:A:280:THR:HG23	1:B:81:THR:HG21	1.97	0.47
1:A:236:ASP:O	1:A:237:LYS:C	2.57	0.47
1:A:374:LEU:HD21	1:A:376:THR:HB	1.97	0.46
1:A:358:LEU:HD11	1:A:387:MET:HE1	1.96	0.46
1:C:89:SCY:OCD	3:C:393:COA:S1P	2.72	0.46
1:C:189:ALA:CB	1:C:340:ASN:HB3	2.46	0.46
1:D:292:PRO:HD3	1:D:378:CYS:CA	2.44	0.46
3:A:393:COA:H52A	3:A:393:COA:H2B	1.54	0.46
1:C:305:TRP:CZ3	1:C:372:LYS:HB3	2.51	0.46
1:C:311:ASP:HB2	1:C:370:ALA:HB1	1.97	0.46
1:C:312:LEU:HD23	1:C:361:LEU:CD2	2.46	0.46
1:D:175:GLN:HB3	1:D:320:ALA:HB3	1.96	0.46
1:B:350:ILE:HG21	1:B:350:ILE:HD13	1.69	0.45
1:C:175:GLN:HB3	1:C:320:ALA:HB3	1.97	0.45
1:C:206:GLY:HA3	1:C:209:GLY:O	2.16	0.45
1:A:243:ALA:CB	3:A:393:COA:H51A	2.46	0.45
1:C:186:ALA:HA	1:C:340:ASN:O	2.17	0.45
1:D:110:ILE:HG23	1:D:257:LEU:HD21	1.98	0.45
1:A:88:LEU:HB2	1:A:379:ILE:HG23	1.98	0.45
1:C:38:VAL:HG21	1:C:112:VAL:HG13	1.98	0.45
1:C:185:LYS:NZ	4:C:429:HOH:O	2.49	0.45
1:D:361:LEU:HD22	1:D:365:MET:SD	2.57	0.45
1:A:328:LYS:HE3	1:A:328:LYS:HB2	1.69	0.45
1:C:49:VAL:HB	1:C:76:VAL:HG13	1.99	0.45
1:C:125:CYS:HA	1:D:124:HIS:O	2.16	0.45
1:A:168:TRP:O	1:A:169:GLN:HB2	2.16	0.45
1:C:297:ARG:HG2	1:C:297:ARG:NH1	2.30	0.45
1:C:364:GLU:O	1:C:368:ARG:HG2	2.17	0.45
1:B:64:GLN:O	1:B:65:ASN:C	2.60	0.45
1:D:207:ARG:N	1:D:207:ARG:HD3	2.32	0.45
1:B:236:ASP:O	1:B:237:LYS:C	2.59	0.45
1:C:309:ASP:HB3	1:C:372:LYS:HD2	1.99	0.45
1:D:143:MET:HE3	1:D:249:LEU:HD22	1.99	0.45
1:D:354:GLY:HA2	1:D:377:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:O	1:A:164:VAL:HG23	2.16	0.45
1:A:379:ILE:HB	1:A:383:MET:HB2	2.00	0.44
1:B:374:LEU:HD23	1:B:374:LEU:C	2.41	0.44
1:C:268:GLY:HA2	4:C:486:HOH:O	2.17	0.44
1:D:28:HIS:ND1	1:D:62:GLU:OE2	2.42	0.44
1:D:293:ILE:N	1:D:294:PRO:HD2	2.32	0.44
1:C:281:VAL:HG12	1:C:282:GLY:N	2.32	0.44
1:C:119:MET:HE3	1:C:350:ILE:HG13	1.99	0.44
1:A:298:LYS:HD3	1:A:298:LYS:C	2.43	0.44
1:B:320:ALA:O	1:B:321:ALA:C	2.59	0.44
1:C:78:GLN:NE2	1:D:284:ASP:HA	2.32	0.44
1:C:143:MET:HB2	4:C:421:HOH:O	2.16	0.44
1:C:157:MET:HE1	4:C:419:HOH:O	2.16	0.44
1:D:117:GLU:OE2	1:D:351:GLY:N	2.50	0.44
1:D:293:ILE:HG21	1:D:329:ASP:OD2	2.17	0.44
1:A:93:LEU:CD1	1:A:387:MET:HE2	2.35	0.44
1:C:330:LEU:HD13	1:C:332:TRP:CH2	2.52	0.44
1:C:171:SER:OG	4:C:417:HOH:O	2.04	0.44
1:D:158:GLY:HA3	1:D:235:PHE:CD2	2.53	0.44
1:A:337:VAL:O	1:A:338:ASN:C	2.60	0.44
1:B:358:LEU:O	1:B:362:LEU:HG	2.17	0.44
1:C:110:ILE:HG23	1:C:257:LEU:HD21	2.00	0.44
1:A:247:SER:OG	3:A:393:COA:H61	2.18	0.43
1:C:226:ASP:O	1:C:230:LYS:HG3	2.18	0.43
1:C:282:GLY:N	1:D:79:GLU:O	2.47	0.43
1:D:28:HIS:HA	1:D:116:MET:SD	2.58	0.43
1:D:333:ASP:HA	1:D:334:PRO:HD2	1.83	0.43
1:D:317:GLU:CD	1:D:342:GLY:HA3	2.43	0.43
1:A:133:LYS:H	1:A:133:LYS:HG2	1.67	0.43
1:D:233:PRO:HB2	1:D:236:ASP:O	2.18	0.43
1:A:131:GLY:HA2	1:C:131:GLY:HA2	2.00	0.43
1:C:157:MET:HA	1:C:160:THR:HG23	2.00	0.43
1:B:38:VAL:HA	4:B:907:HOH:O	2.18	0.43
1:D:364:GLU:O	1:D:368:ARG:HG2	2.19	0.43
1:B:263:GLU:CD	4:B:929:HOH:O	2.62	0.43
1:D:8:ALA:HB2	1:D:259:MET:HE3	2.01	0.43
1:A:124:HIS:HA	1:A:140:ILE:O	2.17	0.42
1:A:358:LEU:O	1:A:362:LEU:HG	2.18	0.42
1:B:28:HIS:ND1	1:B:62:GLU:OE2	2.40	0.42
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.37	0.42
1:D:157:MET:HG3	3:D:393:COA:S1P	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.81	0.42
1:B:379:ILE:HB	1:B:383:MET:HB2	2.00	0.42
1:A:237:LYS:HD3	1:A:237:LYS:HA	1.51	0.42
1:A:330:LEU:HD13	1:A:332:TRP:CH2	2.53	0.42
1:D:89:SCY:O	1:D:377:LEU:HD22	2.20	0.42
1:A:291:GLY:N	1:A:292:PRO:CD	2.82	0.42
1:B:371:ARG:HH11	1:B:371:ARG:HD2	1.55	0.42
1:D:339:VAL:HG12	1:D:340:ASN:OD1	2.20	0.42
1:B:291:GLY:N	1:B:292:PRO:CD	2.83	0.42
1:B:100:MET:HE2	1:B:101:GLN:N	2.34	0.42
1:A:18:PHE:HB2	1:A:249:LEU:O	2.20	0.42
1:D:290:THR:O	1:D:291:GLY:C	2.63	0.42
1:D:12:ARG:HA	1:D:254:ALA:HA	2.01	0.42
1:D:183:GLN:HA	1:D:345:ALA:HB2	2.02	0.42
1:B:187:GLU:O	1:B:191:LYS:HG3	2.20	0.41
1:C:9:SER:HA	1:C:272:LEU:HD22	2.02	0.41
1:C:89:SCY:HE2	1:C:89:SCY:H	1.85	0.41
1:C:293:ILE:CB	1:C:294:PRO:CD	2.98	0.41
1:D:175:GLN:HE22	1:D:240:THR:HG23	1.84	0.41
1:D:185:LYS:HD2	1:D:339:VAL:O	2.19	0.41
1:C:224:THR:HG1	1:C:227:SER:H	1.65	0.41
1:D:269:ILE:O	1:D:271:PRO:HD3	2.21	0.41
1:A:243:ALA:HB3	3:A:393:COA:H51A	2.01	0.41
1:B:156:HIS:ND1	1:B:157:MET:N	2.69	0.41
1:A:7:ILE:HG23	1:A:256:ALA:HB1	2.03	0.41
1:C:64:GLN:HE22	1:D:157:MET:CE	2.32	0.41
1:B:5:ILE:CG1	1:B:100:MET:HG2	2.48	0.41
1:C:64:GLN:NE2	1:D:157:MET:HE3	2.33	0.41
1:C:195:PHE:O	1:C:198:GLU:HG2	2.21	0.41
1:D:156:HIS:ND1	1:D:157:MET:N	2.69	0.41
1:D:25:THR:HA	1:D:26:PRO:HD3	1.86	0.41
1:D:6:VAL:HG22	1:D:259:MET:O	2.21	0.40
1:D:187:GLU:OE1	1:D:191:LYS:HG3	2.21	0.40
1:A:191:LYS:HE2	1:A:191:LYS:HB3	1.86	0.40
1:A:358:LEU:HD21	1:A:387:MET:CE	2.50	0.40
1:A:225:LEU:CG	4:A:926:HOH:O	2.64	0.40
1:B:298:LYS:HD3	1:B:298:LYS:C	2.47	0.40
1:C:314:GLU:O	1:C:375:ALA:HA	2.21	0.40
1:D:17:SER:HG	1:D:218:TYR:HD1	1.70	0.40
1:D:280:THR:HA	1:D:384:GLY:O	2.21	0.40
1:C:350:ILE:HD13	1:C:350:ILE:HG21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:SCY:HE1	1:D:380:GLY:CA	2.51	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 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	386/389 (99%)	374 (97%)	11 (3%)	1 (0%)	36	26
1	B	386/389 (99%)	373 (97%)	12 (3%)	1 (0%)	36	26
1	C	386/389 (99%)	367 (95%)	18 (5%)	1 (0%)	36	26
1	D	386/389 (99%)	366 (95%)	15 (4%)	5 (1%)	9	2
All	All	1544/1556 (99%)	1480 (96%)	56 (4%)	8 (0%)	24	14

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	350	ILE
1	D	350	ILE
1	B	350	ILE
1	D	23	ALA
1	D	80	ALA
1	A	350	ILE
1	D	291	GLY
1	D	65	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/275 (100%)	248 (90%)	27 (10%)	7	1
1	B	275/275 (100%)	250 (91%)	25 (9%)	9	1
1	C	275/275 (100%)	257 (94%)	18 (6%)	15	4
1	D	275/275 (100%)	255 (93%)	20 (7%)	13	3
All	All	1100/1100 (100%)	1010 (92%)	90 (8%)	10	2

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	59	PRO
1	A	66	PRO
1	A	85	MET
1	A	123	PRO
1	A	133	LYS
1	A	191	LYS
1	A	205	LYS
1	A	207	ARG
1	A	220	ARG
1	A	225	LEU
1	A	230	LYS
1	A	232	ARG
1	A	237	LYS
1	A	240	THR
1	A	258	LEU
1	A	263	GLU
1	A	272	LEU
1	A	276	VAL
1	A	298	LYS
1	A	322	GLN
1	A	328	LYS
1	A	332	TRP
1	A	339	VAL
1	A	353	SER
1	A	358	LEU
1	A	361	LEU
1	B	4	SER
1	B	5	ILE
1	B	34	VAL

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	134	MET
1	B	169	GLN
1	B	187	GLU
1	B	191	LYS
1	B	207	ARG
1	B	220	ARG
1	B	240	THR
1	B	257	LEU
1	B	258	LEU
1	B	263	GLU
1	B	270	GLN
1	B	272	LEU
1	B	276	VAL
1	B	297	ARG
1	B	298	LYS
1	B	322	GLN
1	B	328	LYS
1	B	339	VAL
1	B	358	LEU
1	B	361	LEU
1	B	366	LYS
1	C	4	SER
1	C	39	LEU
1	C	40	GLU
1	C	160	THR
1	C	207	ARG
1	C	224	THR
1	C	237	LYS
1	C	272	LEU
1	C	276	VAL
1	C	298	LYS
1	C	307	ILE
1	C	322	GLN
1	C	332	TRP
1	C	339	VAL
1	C	353	SER
1	C	358	LEU
1	C	361	LEU
1	C	371	ARG
1	D	34	VAL
1	D	39	LEU

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Mol	Chain	Res	Type
1	D	187	GLU
1	D	207	ARG
1	D	224	THR
1	D	257	LEU
1	D	258	LEU
1	D	272	LEU
1	D	276	VAL
1	D	288	MET
1	D	298	LYS
1	D	307	ILE
1	D	322	GLN
1	D	328	LYS
1	D	339	VAL
1	D	358	LEU
1	D	360	THR
1	D	361	LEU
1	D	367	ARG
1	D	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	184	ASN
1	B	24	ASN
1	B	175	GLN
1	B	184	ASN
1	C	64	GLN
1	C	78	GLN
1	C	175	GLN
1	C	184	ASN
1	C	316	ASN
1	D	19	ASN
1	D	78	GLN
1	D	127	HIS
1	D	175	GLN
1	D	316	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SCY	D	89	1	7,8,9	0.65	0	4,9,11	0.42	0
1	SCY	A	89	1	7,8,9	1.31	1 (14%)	4,9,11	1.28	0
1	SCY	B	89	1	7,8,9	1.25	1 (14%)	4,9,11	1.24	0
1	SCY	C	89	1	7,8,9	1.13	0	4,9,11	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SCY	D	89	1	-	2/5/7/9	-
1	SCY	A	89	1	-	2/5/7/9	-
1	SCY	B	89	1	-	2/5/7/9	-
1	SCY	C	89	1	-	2/5/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	SCY	CB-CA	2.55	1.59	1.53
1	B	89	SCY	CB-CA	2.17	1.58	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	89	SCY	OCD-CD-SG-CB

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Mol	Chain	Res	Type	Atoms
1	A	89	SCY	CE-CD-SG-CB
1	B	89	SCY	OCD-CD-SG-CB
1	B	89	SCY	CE-CD-SG-CB
1	C	89	SCY	OCD-CD-SG-CB
1	C	89	SCY	CE-CD-SG-CB
1	D	89	SCY	OCD-CD-SG-CB
1	D	89	SCY	CE-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	89	SCY	9	0
1	A	89	SCY	4	0
1	B	89	SCY	6	0
1	C	89	SCY	6	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	SO4	A	720	-	4,4,4	0.59	0	6,6,6	0.14	0
3	COA	C	393	-	47,50,50	2.28	13 (27%)	69,75,75	1.79	15 (21%)
2	SO4	B	724	-	4,4,4	0.66	0	6,6,6	0.38	0
3	COA	B	393	-	47,50,50	2.28	12 (25%)	69,75,75	2.30	19 (27%)
3	COA	D	393	-	47,50,50	2.24	15 (31%)	69,75,75	1.81	11 (15%)
2	SO4	B	721	-	4,4,4	0.67	0	6,6,6	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	722	-	4,4,4	0.72	0	6,6,6	0.36	0
2	SO4	B	719	-	4,4,4	0.77	0	6,6,6	0.22	0
2	SO4	A	723	-	4,4,4	0.93	0	6,6,6	0.54	0
3	COA	A	393	-	47,50,50	2.59	19 (40%)	69,75,75	2.48	19 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	B	393	-	-	7/48/64/64	0/3/3/3
3	COA	A	393	-	-	6/48/64/64	0/3/3/3
3	COA	D	393	-	-	11/48/64/64	0/3/3/3
3	COA	C	393	-	-	11/48/64/64	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	393	COA	P1A-O3A	-9.83	1.48	1.59
3	B	393	COA	P1A-O3A	-8.03	1.50	1.59
3	C	393	COA	O9P-C9P	6.85	1.36	1.23
3	A	393	COA	O9P-C9P	6.69	1.36	1.23
3	D	393	COA	O9P-C9P	6.58	1.36	1.23
3	C	393	COA	P1A-O3A	-6.33	1.52	1.59
3	D	393	COA	P1A-O3A	-5.91	1.53	1.59
3	B	393	COA	P2A-O3A	5.73	1.65	1.59
3	B	393	COA	O9P-C9P	5.50	1.34	1.23
3	D	393	COA	P3B-O3B	5.02	1.68	1.59
3	D	393	COA	P2A-O3A	4.75	1.64	1.59
3	A	393	COA	P3B-O3B	4.73	1.67	1.59
3	C	393	COA	P2A-O3A	4.59	1.64	1.59
3	C	393	COA	P3B-O3B	4.52	1.67	1.59
3	B	393	COA	P3B-O3B	4.45	1.67	1.59
3	A	393	COA	P2A-O3A	4.31	1.64	1.59
3	C	393	COA	C3P-N4P	3.84	1.54	1.46
3	C	393	COA	O5P-C5P	3.70	1.30	1.23
3	A	393	COA	P3B-O7A	3.60	1.61	1.50
3	D	393	COA	C3P-N4P	3.42	1.53	1.46
3	D	393	COA	O5P-C5P	3.29	1.29	1.23
3	A	393	COA	C3P-N4P	3.20	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	393	COA	P3B-O7A	3.14	1.60	1.50
3	D	393	COA	P3B-O7A	3.11	1.60	1.50
3	A	393	COA	OAP-CAP	2.97	1.47	1.42
3	A	393	COA	CCP-CBP	2.93	1.57	1.52
3	B	393	COA	P3B-O7A	2.89	1.59	1.50
3	A	393	COA	P2A-O6A	2.86	1.70	1.59
3	B	393	COA	C9P-N8P	-2.79	1.27	1.33
3	D	393	COA	C5A-C6A	2.76	1.48	1.41
3	C	393	COA	C5A-C6A	2.69	1.48	1.41
3	A	393	COA	C5A-C6A	2.61	1.48	1.41
3	A	393	COA	C2A-N1A	2.58	1.38	1.33
3	D	393	COA	C2A-N1A	2.55	1.38	1.33
3	C	393	COA	C2A-N1A	2.54	1.38	1.33
3	B	393	COA	C3P-N4P	2.54	1.51	1.46
3	D	393	COA	O4B-C4B	2.54	1.50	1.45
3	A	393	COA	O5P-C5P	2.44	1.28	1.23
3	A	393	COA	O4B-C4B	2.42	1.50	1.45
3	D	393	COA	C7P-N8P	-2.40	1.40	1.46
3	A	393	COA	C7P-C6P	-2.38	1.43	1.51
3	B	393	COA	C5A-C6A	2.36	1.47	1.41
3	B	393	COA	C8A-N7A	2.32	1.36	1.31
3	A	393	COA	CDP-CBP	2.27	1.58	1.53
3	B	393	COA	O4B-C4B	2.23	1.50	1.45
3	C	393	COA	O4B-C4B	2.20	1.49	1.45
3	C	393	COA	CCP-CBP	2.19	1.56	1.52
3	B	393	COA	CDP-CBP	2.17	1.58	1.53
3	D	393	COA	C8A-N7A	2.13	1.35	1.31
3	A	393	COA	C5A-N7A	-2.13	1.35	1.39
3	D	393	COA	CCP-CBP	2.09	1.56	1.52
3	B	393	COA	C5A-N7A	-2.06	1.35	1.39
3	A	393	COA	C8A-N7A	2.06	1.35	1.31
3	D	393	COA	C9P-N8P	-2.06	1.28	1.33
3	C	393	COA	C9P-N8P	-2.04	1.28	1.33
3	C	393	COA	C8A-N7A	2.04	1.35	1.31
3	A	393	COA	O3B-C3B	-2.03	1.37	1.44
3	A	393	COA	C5A-C4A	2.03	1.42	1.39
3	D	393	COA	O4B-C1B	2.01	1.46	1.42

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	393	COA	C2P-C3P-N4P	-9.66	90.40	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	393	COA	C7P-N8P-C9P	7.73	136.44	122.55
3	B	393	COA	C7P-C6P-C5P	7.55	124.98	112.39
3	B	393	COA	C6P-C5P-N4P	-7.55	102.59	116.34
3	A	393	COA	C6P-C7P-N8P	7.11	127.13	112.00
3	D	393	COA	C7P-N8P-C9P	6.88	134.90	122.55
3	D	393	COA	P3B-O3B-C3B	-6.17	106.96	123.43
3	A	393	COA	C7P-N8P-C9P	-6.14	111.51	122.55
3	B	393	COA	C7P-N8P-C9P	5.91	133.17	122.55
3	B	393	COA	O5P-C5P-C6P	5.76	132.46	122.02
3	A	393	COA	O6A-CCP-CBP	-5.75	101.31	110.55
3	B	393	COA	C2P-C3P-N4P	-5.43	99.99	112.31
3	A	393	COA	C2B-C3B-C4B	-4.79	94.84	103.24
3	A	393	COA	O4B-C4B-C5B	-4.45	95.07	109.33
3	D	393	COA	CEP-CBP-CCP	-4.40	100.96	108.22
3	D	393	COA	C6P-C7P-N8P	4.30	121.16	112.00
3	C	393	COA	C2P-C3P-N4P	-4.30	102.55	112.31
3	B	393	COA	O6A-CCP-CBP	-4.00	104.11	110.55
3	B	393	COA	P3B-O3B-C3B	-3.95	112.88	123.43
3	A	393	COA	CAP-C9P-N8P	3.89	123.86	116.48
3	A	393	COA	C6P-C5P-N4P	-3.84	109.35	116.34
3	D	393	COA	O4B-C1B-C2B	-3.78	98.53	106.62
3	A	393	COA	P3B-O3B-C3B	-3.62	113.76	123.43
3	D	393	COA	CDP-CBP-CCP	3.30	113.67	108.22
3	A	393	COA	N6A-C6A-N1A	3.28	125.68	118.38
3	B	393	COA	C5B-C4B-C3B	3.26	125.23	114.38
3	C	393	COA	CEP-CBP-CCP	-3.14	103.05	108.22
3	A	393	COA	O5B-C5B-C4B	-3.08	98.49	108.99
3	C	393	COA	P3B-O3B-C3B	-3.08	115.20	123.43
3	C	393	COA	CEP-CBP-CAP	3.02	113.92	108.77
3	B	393	COA	C2A-N1A-C6A	2.97	123.61	118.73
3	B	393	COA	O9P-C9P-N8P	2.96	129.24	122.98
3	C	393	COA	O4B-C1B-C2B	-2.93	100.36	106.62
3	A	393	COA	CEP-CBP-CAP	2.87	113.67	108.77
3	C	393	COA	O6A-CCP-CBP	-2.85	105.97	110.55
3	C	393	COA	C6P-C5P-N4P	2.84	121.53	116.34
3	D	393	COA	C4B-O4B-C1B	-2.77	103.35	109.47
3	B	393	COA	O9P-C9P-CAP	-2.52	113.85	120.89
3	C	393	COA	CDP-CBP-CCP	2.51	112.37	108.22
3	B	393	COA	C2B-C3B-C4B	-2.48	98.89	103.24
3	B	393	COA	OAP-CAP-CBP	2.48	115.92	110.18
3	C	393	COA	O5A-P2A-O3A	2.47	113.95	107.27
3	C	393	COA	CAP-C9P-N8P	-2.47	111.80	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	393	COA	O5A-P2A-O3A	2.46	113.93	107.27
3	C	393	COA	O4B-C1B-N9A	2.39	112.67	108.09
3	B	393	COA	O3B-C3B-C4B	2.39	118.44	110.03
3	A	393	COA	O9P-C9P-CAP	-2.37	114.28	120.89
3	A	393	COA	O9A-P3B-O8A	2.33	116.53	107.80
3	A	393	COA	CEP-CBP-CDP	2.32	113.83	109.20
3	A	393	COA	OAP-CAP-CBP	2.25	115.39	110.18
3	B	393	COA	N6A-C6A-N1A	2.24	123.38	118.38
3	B	393	COA	O4B-C1B-C2B	-2.22	101.86	106.62
3	B	393	COA	C4A-C5A-N7A	2.21	113.11	110.58
3	C	393	COA	C5B-C4B-C3B	2.19	121.69	114.38
3	D	393	COA	CAP-C9P-N8P	-2.16	112.39	116.48
3	A	393	COA	O8A-P3B-O3B	2.15	114.22	105.85
3	A	393	COA	C5B-C4B-C3B	-2.14	107.23	114.38
3	C	393	COA	O3B-C3B-C4B	2.10	117.44	110.03
3	D	393	COA	CEP-CBP-CAP	2.10	112.34	108.77
3	D	393	COA	O2A-P1A-O3A	2.08	112.90	107.27
3	B	393	COA	C5A-C4A-N9A	-2.08	103.55	105.81
3	D	393	COA	O5A-P2A-O3A	2.04	112.79	107.27
3	C	393	COA	O5P-C5P-C6P	-2.03	118.35	122.02
3	B	393	COA	O5A-P2A-O3A	2.02	112.72	107.27

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	393	COA	C5B-O5B-P1A-O1A
3	A	393	COA	C5B-O5B-P1A-O2A
3	A	393	COA	C5B-O5B-P1A-O3A
3	B	393	COA	C5B-O5B-P1A-O1A
3	B	393	COA	C5B-O5B-P1A-O3A
3	B	393	COA	S1P-C2P-C3P-N4P
3	C	393	COA	C5B-O5B-P1A-O1A
3	C	393	COA	C5B-O5B-P1A-O2A
3	C	393	COA	C5B-O5B-P1A-O3A
3	C	393	COA	S1P-C2P-C3P-N4P
3	D	393	COA	C5B-O5B-P1A-O1A
3	D	393	COA	C5B-O5B-P1A-O2A
3	D	393	COA	C5B-O5B-P1A-O3A
3	D	393	COA	CCP-O6A-P2A-O4A
3	D	393	COA	C5P-C6P-C7P-N8P
3	D	393	COA	S1P-C2P-C3P-N4P

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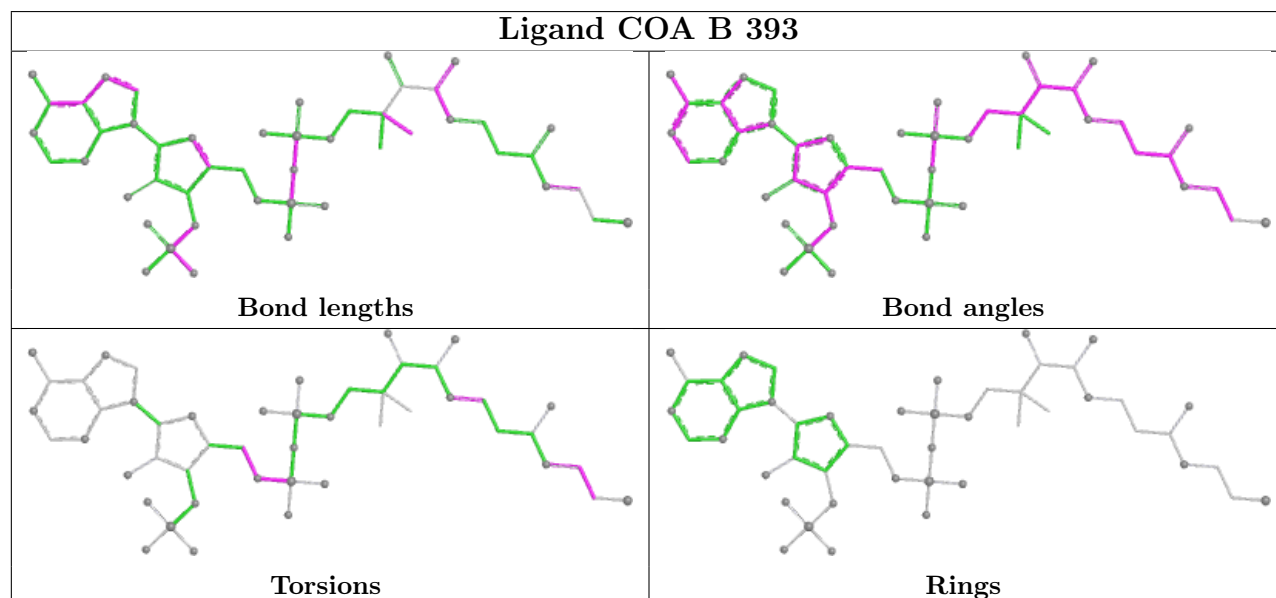
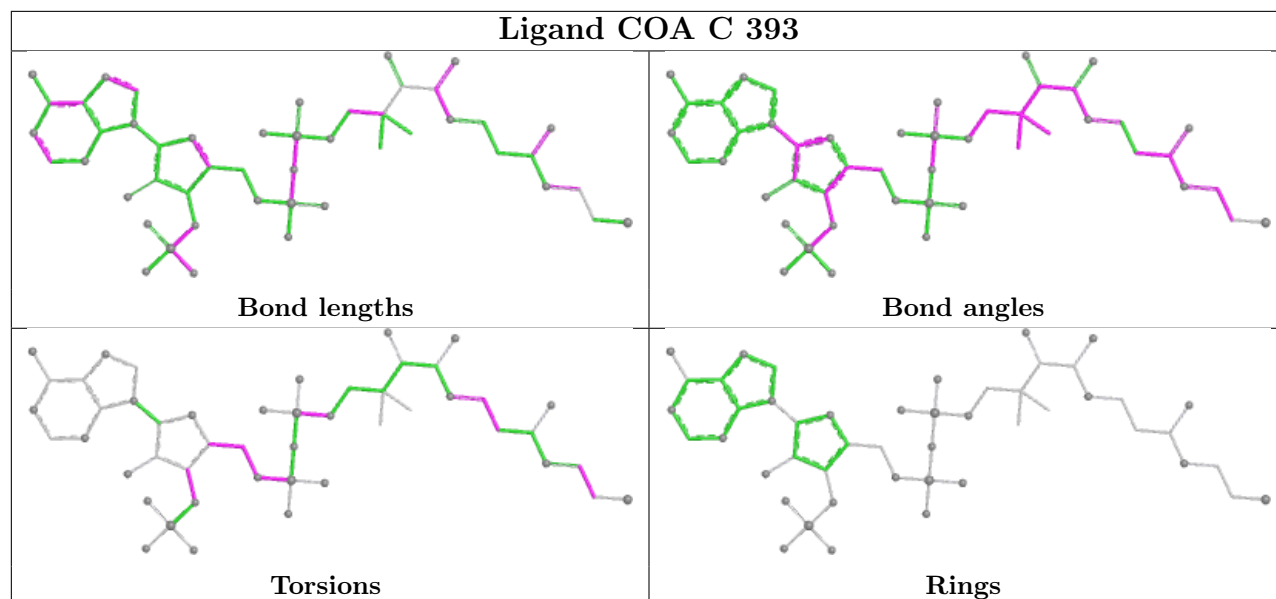
Mol	Chain	Res	Type	Atoms
3	B	393	COA	C6P-C7P-N8P-C9P
3	D	393	COA	O4B-C4B-C5B-O5B
3	C	393	COA	C6P-C7P-N8P-C9P
3	A	393	COA	C3B-C4B-C5B-O5B
3	D	393	COA	C3B-C4B-C5B-O5B
3	D	393	COA	O5P-C5P-C6P-C7P
3	C	393	COA	C4B-C3B-O3B-P3B
3	A	393	COA	S1P-C2P-C3P-N4P
3	B	393	COA	C5B-O5B-P1A-O2A
3	C	393	COA	CCP-O6A-P2A-O4A
3	C	393	COA	C4B-C5B-O5B-P1A
3	A	393	COA	O4B-C4B-C5B-O5B
3	C	393	COA	C5P-C6P-C7P-N8P
3	D	393	COA	C3B-O3B-P3B-O9A
3	D	393	COA	N4P-C5P-C6P-C7P
3	C	393	COA	C2B-C3B-O3B-P3B
3	C	393	COA	C3B-C4B-C5B-O5B
3	B	393	COA	C4B-C5B-O5B-P1A
3	B	393	COA	C2P-C3P-N4P-C5P

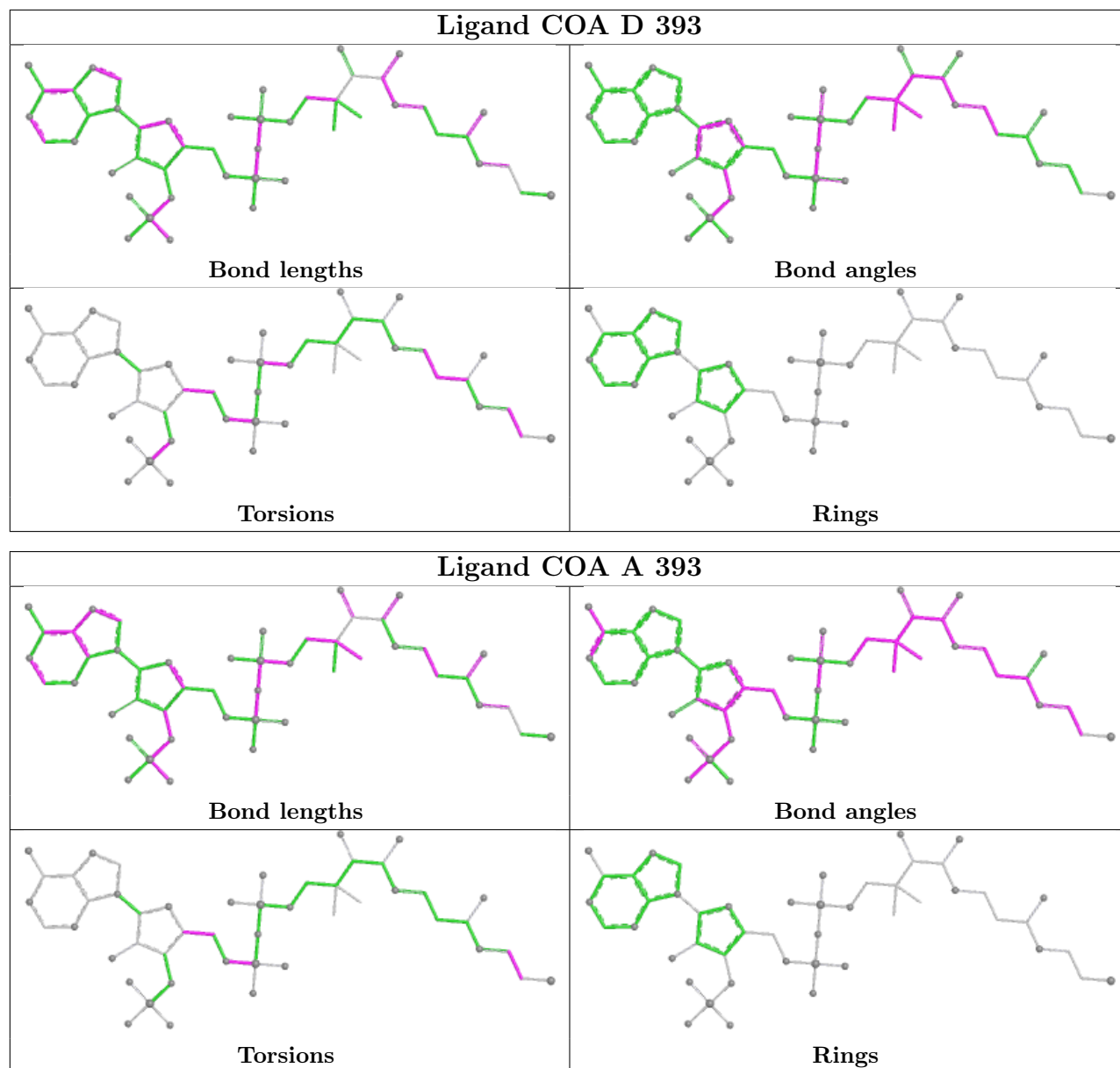
There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	393	COA	1	0
3	D	393	COA	2	0
2	B	721	SO4	1	0
2	B	719	SO4	1	0
3	A	393	COA	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	388/389 (99%)	-1.09	0	100	100	12, 21, 44, 87	0
1	B	388/389 (99%)	-1.05	0	100	100	11, 20, 42, 97	0
1	C	388/389 (99%)	-0.40	0	100	100	25, 45, 77, 119	0
1	D	388/389 (99%)	-0.10	1 (0%)	90	93	22, 52, 115, 138	0
All	All	1552/1556 (99%)	-0.66	1 (0%)	92	94	11, 36, 84, 138	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	227	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q < 0.9
1	SCY	C	89	9/10	0.98	0.09	33,40,55,57	0
1	SCY	D	89	9/10	0.98	0.08	35,39,63,69	0
1	SCY	A	89	9/10	0.99	0.06	14,18,31,34	0
1	SCY	B	89	9/10	0.99	0.04	13,16,28,31	0

6.3 Carbohydrates [i](#)

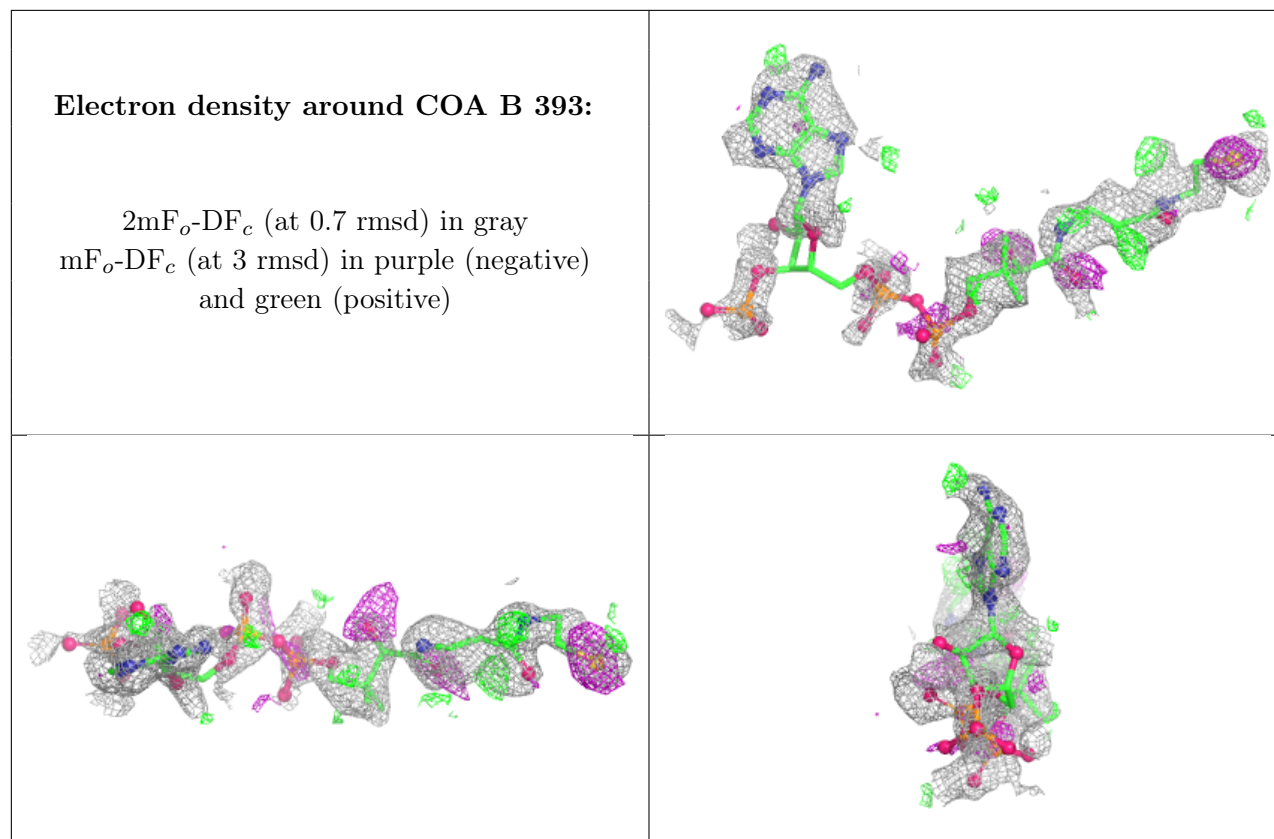
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

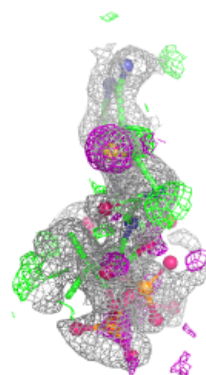
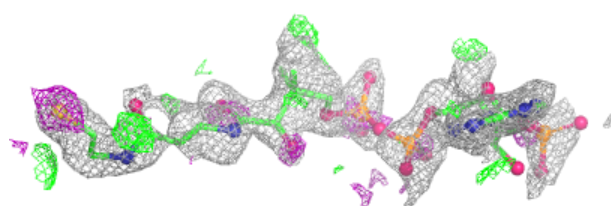
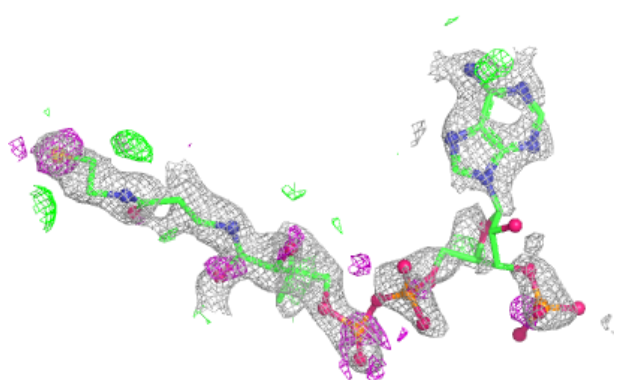
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	COA	B	393	48/48	0.94	0.08	26,36,62,64	0
3	COA	A	393	48/48	0.95	0.08	25,37,51,55	0
3	COA	C	393	48/48	0.95	0.10	68,82,96,97	0
3	COA	D	393	48/48	0.95	0.12	88,117,126,126	0
2	SO4	A	723	5/5	0.97	0.07	44,46,52,53	0
2	SO4	A	722	5/5	0.98	0.06	50,51,56,58	0
2	SO4	A	720	5/5	0.98	0.07	60,60,62,63	0
2	SO4	B	719	5/5	0.98	0.06	58,58,59,60	0
2	SO4	B	724	5/5	0.98	0.07	45,48,50,52	0
2	SO4	B	721	5/5	0.99	0.06	53,56,61,62	0

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

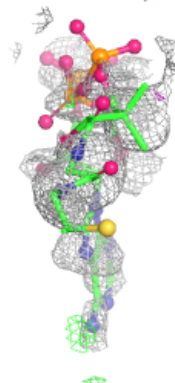
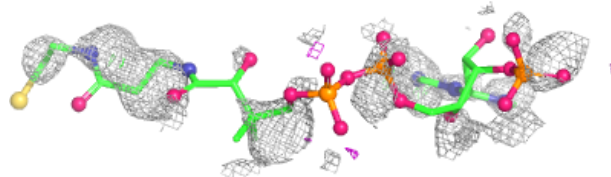
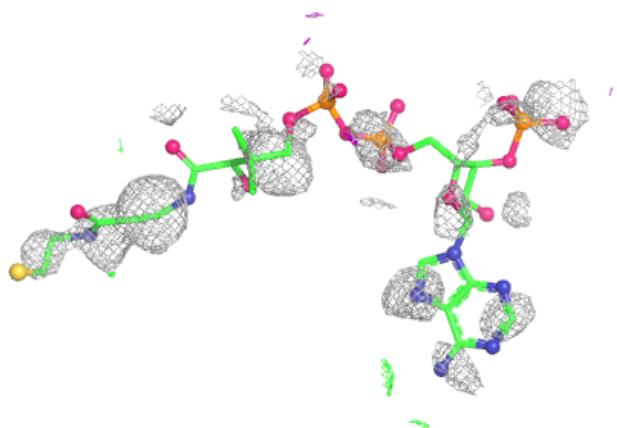


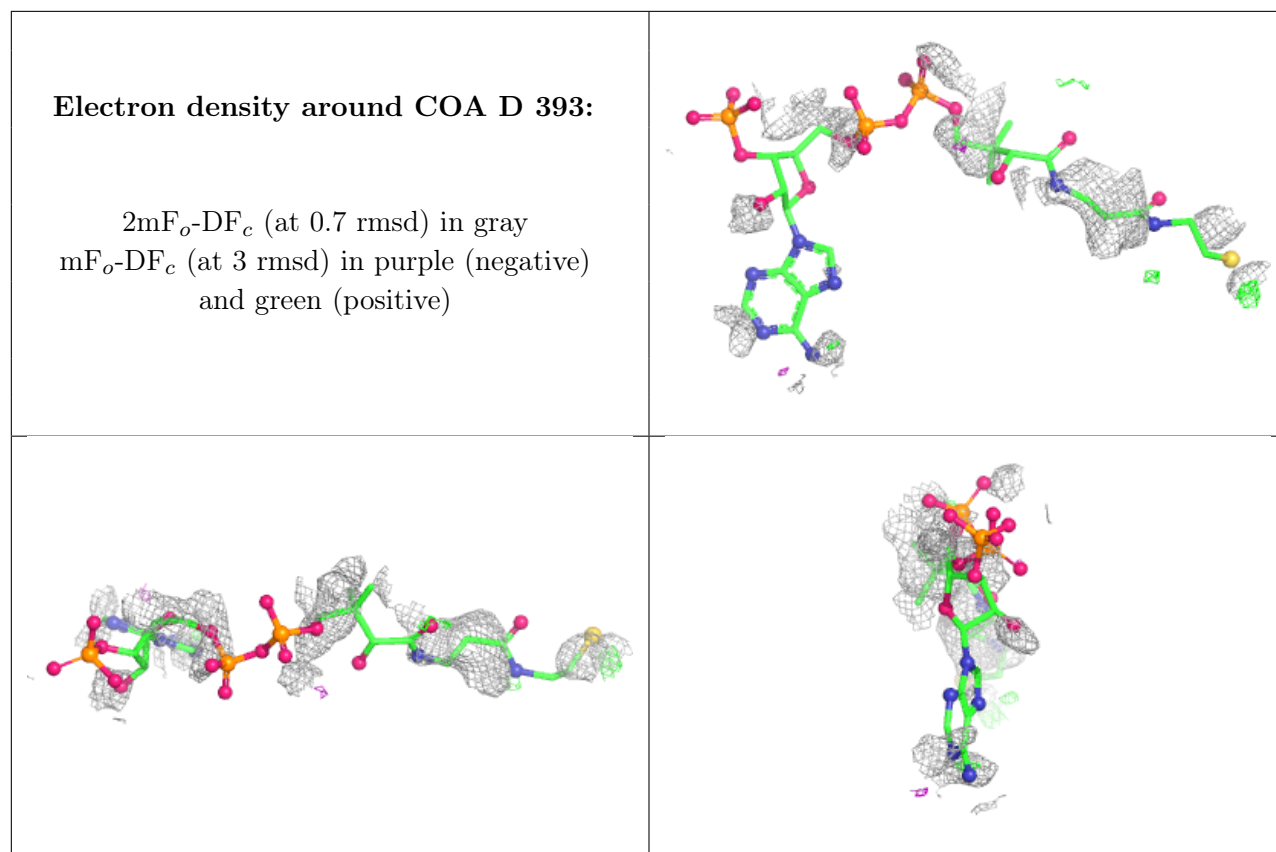
Electron density around COA A 393:

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

**Electron density around COA C 393:**

$2mF_o-DF_c$ (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.