



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 04:50 PM UTC

PDB ID : 6CSC / pdb_00006csc
Title : CHICKEN CITRATE SYNTHASE COMPLEX WITH TRIFLUOROACET
ONYL-COA AND CITRATE
Authors : Usher, K.C.; Remington, S.J.
Deposited on : 1997-06-19
Resolution : 2.25 Å(reported)

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

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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

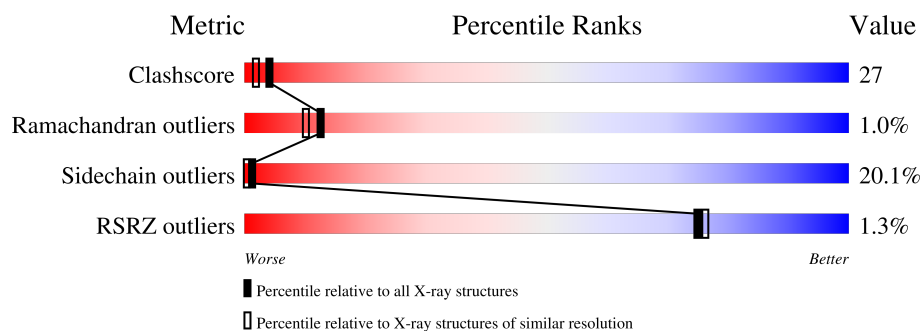
1 Overall quality at a glance

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))
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	437	51% 35% 11% .
1	B	437	50% 35% 12% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7101 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 CITRATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3402	2173	585	628	16			
1	B	434	Total	C	N	O	S	0	0	0
			3385	2164	582	623	16			

There are 52 discrepancies between the modelled and reference sequences:

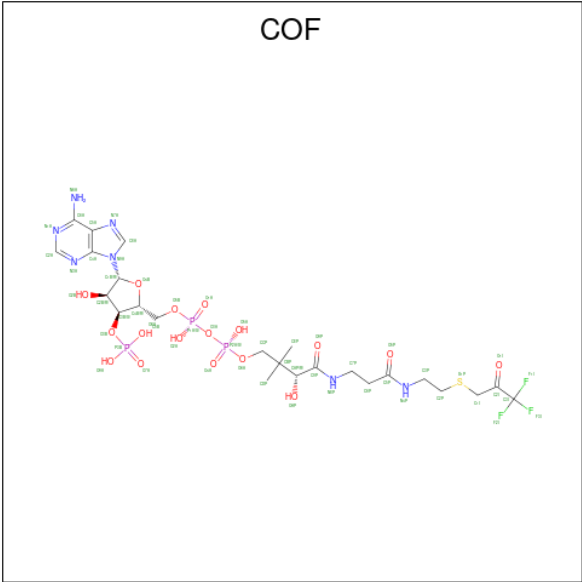
Chain	Residue	Modelled	Actual	Comment	Reference
A	12	SER	ALA	conflict	UNP P23007
A	30	ASN	GLY	conflict	UNP P23007
A	33	VAL	LEU	conflict	UNP P23007
A	52	ILE	VAL	conflict	UNP P23007
A	81	ALA	-	insertion	UNP P23007
A	85	GLU	GLY	conflict	UNP P23007
A	104	PRO	GLY	conflict	UNP P23007
A	105	GLU	ALA	conflict	UNP P23007
A	110	VAL	LEU	conflict	UNP P23007
A	163	ASN	LEU	conflict	UNP P23007
A	170	PHE	MET	conflict	UNP P23007
A	174	ASP	SER	conflict	UNP P23007
A	222	PRO	ALA	conflict	UNP P23007
A	283	LEU	GLY	conflict	UNP P23007
A	286	SER	ALA	conflict	UNP P23007
A	291	ASP	ALA	conflict	UNP P23007
A	292	LEU	ALA	conflict	UNP P23007
A	298	ASP	-	insertion	UNP P23007
A	299	GLU	-	insertion	UNP P23007
A	300	LYS	-	insertion	UNP P23007
A	343	SER	GLY	conflict	UNP P23007
A	366	LYS	ALA	conflict	UNP P23007
A	368	LYS	ALA	conflict	UNP P23007
A	428	ALA	ASP	conflict	UNP P23007
A	431	GLU	ILE	conflict	UNP P23007

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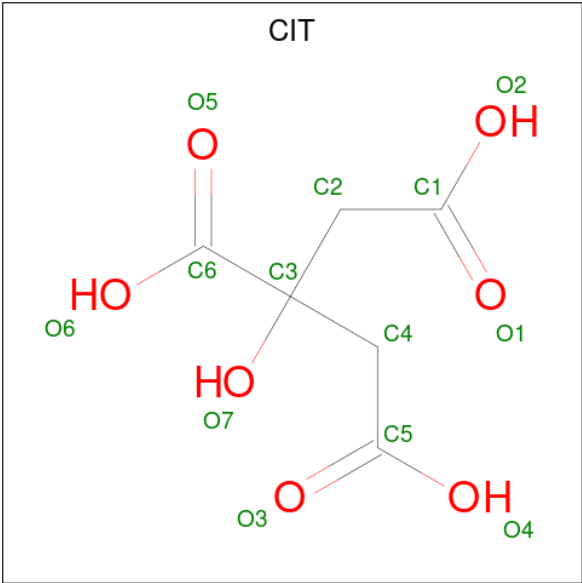
Chain	Residue	Modelled	Actual	Comment	Reference
A	432	LYS	ALA	conflict	UNP P23007
B	12	SER	ALA	conflict	UNP P23007
B	30	ASN	GLY	conflict	UNP P23007
B	33	VAL	LEU	conflict	UNP P23007
B	52	ILE	VAL	conflict	UNP P23007
B	81	ALA	-	insertion	UNP P23007
B	85	GLU	GLY	conflict	UNP P23007
B	104	PRO	GLY	conflict	UNP P23007
B	105	GLU	ALA	conflict	UNP P23007
B	110	VAL	LEU	conflict	UNP P23007
B	163	ASN	LEU	conflict	UNP P23007
B	170	PHE	MET	conflict	UNP P23007
B	174	ASP	SER	conflict	UNP P23007
B	222	PRO	ALA	conflict	UNP P23007
B	283	LEU	GLY	conflict	UNP P23007
B	286	SER	ALA	conflict	UNP P23007
B	291	ASP	ALA	conflict	UNP P23007
B	292	LEU	ALA	conflict	UNP P23007
B	298	ASP	-	insertion	UNP P23007
B	299	GLU	-	insertion	UNP P23007
B	300	LYS	-	insertion	UNP P23007
B	343	SER	GLY	conflict	UNP P23007
B	366	LYS	ALA	conflict	UNP P23007
B	368	LYS	ALA	conflict	UNP P23007
B	428	ALA	ASP	conflict	UNP P23007
B	431	GLU	ILE	conflict	UNP P23007
B	432	LYS	ALA	conflict	UNP P23007

- Molecule 2 is TRIFLUOROACETONYL COENZYME A (CCD ID: COF) (formula: $C_{24}H_{37}F_3N_7O_{17}P_3S$)



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	F	N	O	P	S		
2	A	1	71	32	6	9	19	3	2	0	1
2	B	1	71	32	6	9	19	3	2	0	1

- Molecule 3 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	13	6	7	0	0
3	B	1	13	6	7	0	0

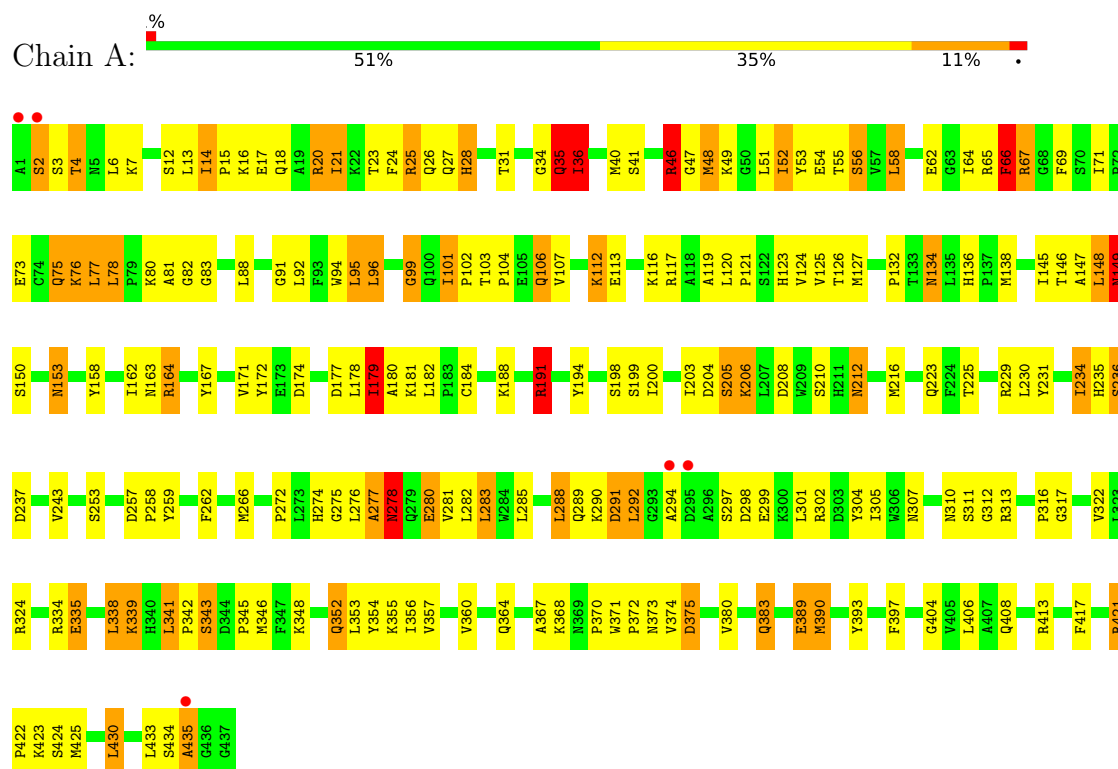
- Molecule 4 is water.

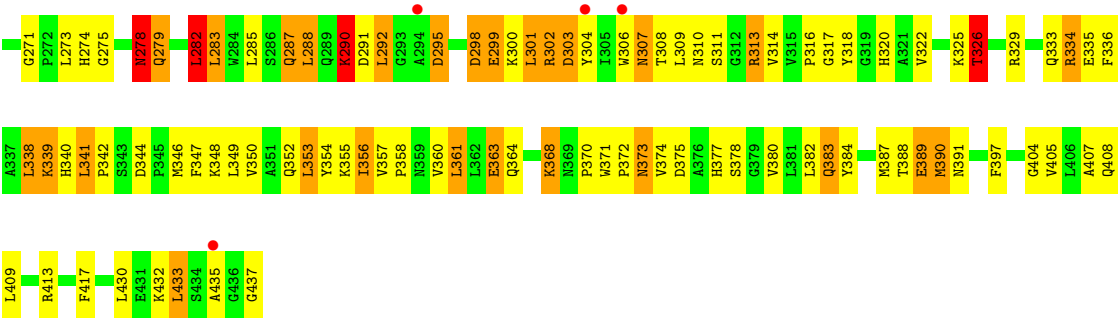
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total 72	O 72	0	0
4	B	74	Total 74	O 74	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CITRATE SYNTHASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.37Å 100.21Å 87.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.25 25.00 – 2.25	Depositor EDS
% Data completeness (in resolution range)	86.0 (25.00-2.25) 86.0 (25.00-2.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.22Å)	Xtriage
Refinement program	TNT 5F	Depositor
R, R_{free}	0.158 , (Not available) 0.148 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	14.2	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 107.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7101	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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: COF, CIT

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	1.23	2/3487 (0.1%)	1.67	57/4736 (1.2%)
1	B	1.18	2/3470 (0.1%)	1.60	32/4713 (0.7%)
All	All	1.20	4/6957 (0.1%)	1.64	89/9449 (0.9%)

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	1	0
1	B	1	0
All	All	2	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	SER	CA-C	6.29	1.60	1.52
1	A	357	VAL	CA-CB	-6.17	1.51	1.54
1	B	9	VAL	CA-CB	-5.55	1.48	1.54
1	B	191	ARG	C-N	-5.02	1.27	1.33

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	THR	N-CA-C	17.92	130.25	111.07
1	A	2	SER	N-CA-C	10.12	124.92	109.23
1	A	36	ILE	N-CA-CB	9.29	126.55	111.23
1	A	421	ARG	O-C-N	9.13	126.75	121.27
1	B	170	PHE	CA-CB-CG	-9.03	104.77	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	390	MET	N-CA-C	8.37	122.59	112.38
1	A	2	SER	CA-C-N	8.26	135.93	121.80
1	A	2	SER	C-N-CA	8.26	135.93	121.80
1	A	34	GLY	CA-C-N	8.12	137.06	121.54
1	A	34	GLY	C-N-CA	8.12	137.06	121.54
1	B	5	ASN	N-CA-CB	8.07	124.13	110.49
1	B	54	GLU	N-CA-C	7.58	122.99	112.45
1	A	46	ARG	CD-NE-CZ	-7.42	114.01	124.40
1	A	28	HIS	N-CA-C	7.40	122.03	112.41
1	A	35	GLN	N-CA-CB	-7.18	98.35	110.49
1	B	278	ASN	CB-CA-C	-7.06	99.13	110.84
1	A	46	ARG	N-CA-CB	6.98	120.54	109.51
1	B	229	ARG	NE-CZ-NH1	6.94	128.44	121.50
1	A	205	SER	N-CA-CB	-6.89	98.85	110.49
1	B	48	MET	N-CA-CB	6.75	121.16	110.23
1	A	35	GLN	CB-CA-C	-6.66	97.16	110.42
1	B	238	HIS	CA-CB-CG	-6.63	107.17	113.80
1	A	375	ASP	CA-CB-CG	6.61	119.21	112.60
1	A	55	THR	N-CA-C	6.60	118.47	111.28
1	B	356	ILE	N-CA-C	6.59	117.93	111.67
1	B	326	THR	N-CA-CB	6.50	119.78	109.51
1	A	54	GLU	N-CA-C	6.44	120.35	112.23
1	B	78	LEU	N-CA-C	6.25	117.76	109.83
1	A	67	ARG	N-CA-CB	6.24	121.04	110.49
1	B	71	ILE	N-CA-CB	6.24	114.43	110.50
1	A	35	GLN	CA-C-N	6.21	133.15	121.97
1	A	35	GLN	C-N-CA	6.21	133.15	121.97
1	A	48	MET	CA-C-N	-6.19	114.79	122.84
1	A	48	MET	C-N-CA	-6.19	114.79	122.84
1	A	180	ALA	N-CA-C	6.18	118.09	111.36
1	B	77	LEU	N-CA-C	6.09	117.71	111.14
1	A	393	TYR	N-CA-C	6.08	118.68	111.33
1	B	30	ASN	CA-CB-CG	-6.07	106.53	112.60
1	A	179	ILE	N-CA-CB	6.06	118.04	110.47
1	B	405	VAL	N-CA-C	6.01	116.67	110.36
1	A	294	ALA	N-CA-C	5.88	118.57	111.40
1	B	340	HIS	N-CA-C	5.82	121.25	114.04
1	A	66	PHE	CA-C-N	-5.80	110.47	121.54
1	A	66	PHE	C-N-CA	-5.80	110.47	121.54
1	A	47	GLY	CA-C-N	-5.75	114.78	122.72
1	A	47	GLY	C-N-CA	-5.75	114.78	122.72
1	A	78	LEU	N-CA-C	5.72	116.90	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	PRO	N-CA-CB	5.71	108.64	103.33
1	B	229	ARG	NE-CZ-NH2	-5.64	114.12	119.20
1	B	236	SER	N-CA-C	5.60	117.38	111.28
1	B	234	ILE	N-CA-C	5.59	118.08	111.09
1	A	343	SER	N-CA-CB	5.58	119.37	110.73
1	A	179	ILE	CA-CB-CG1	5.50	119.75	110.40
1	A	3	SER	CA-C-N	5.48	127.57	120.44
1	A	3	SER	C-N-CA	5.48	127.57	120.44
1	B	295	ASP	CA-CB-CG	5.48	118.08	112.60
1	A	367	ALA	N-CA-C	5.47	118.17	109.96
1	B	243	VAL	N-CA-C	5.46	116.10	110.36
1	B	271	GLY	CA-C-N	5.42	125.76	119.47
1	B	271	GLY	C-N-CA	5.42	125.76	119.47
1	B	282	LEU	N-CA-CB	5.39	117.98	109.94
1	A	278	ASN	CB-CA-C	-5.38	99.72	110.42
1	A	46	ARG	CA-CB-CG	-5.37	103.37	114.10
1	A	66	PHE	N-CA-CB	5.36	119.55	110.49
1	A	208	ASP	N-CA-CB	5.35	118.43	110.29
1	A	34	GLY	O-C-N	5.34	129.75	123.61
1	A	357	VAL	N-CA-C	5.32	119.31	112.67
1	A	307	ASN	CB-CA-C	-5.27	102.04	110.79
1	A	171	VAL	N-CA-C	-5.27	105.40	110.72
1	B	298	ASP	O-C-N	5.26	127.70	122.12
1	A	149	ASN	CA-C-N	5.24	127.82	120.28
1	A	149	ASN	C-N-CA	5.24	127.82	120.28
1	A	14	ILE	N-CA-C	5.23	120.19	108.88
1	A	191	ARG	CB-CA-C	-5.22	102.62	110.92
1	A	278	ASN	N-CA-CB	-5.18	101.74	110.49
1	A	95	LEU	CA-C-N	5.17	127.21	120.28
1	A	95	LEU	C-N-CA	5.17	127.21	120.28
1	A	99	GLY	N-CA-C	-5.17	108.11	115.30
1	A	52	ILE	N-CA-CB	5.16	117.18	110.99
1	A	225	THR	N-CA-CB	5.14	117.68	110.12
1	B	47	GLY	CA-C-N	-5.09	114.55	122.09
1	B	47	GLY	C-N-CA	-5.09	114.55	122.09
1	A	236	SER	N-CA-C	5.08	119.70	111.37
1	B	326	THR	CB-CA-C	5.06	117.44	110.16
1	B	185	VAL	CB-CA-C	-5.04	105.27	112.22
1	A	277	ALA	CB-CA-C	5.03	119.24	110.68
1	A	2	SER	CA-C-O	5.02	126.89	121.06
1	B	162	ILE	N-CA-C	5.01	115.87	110.21
1	B	290	LYS	N-CA-CB	5.01	117.27	110.01

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	4	THR	CA
1	B	5	ASN	CA

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	3402	0	3383	169	0
1	B	3385	0	3365	206	0
2	A	71	0	24	9	0
2	B	71	0	24	17	0
3	A	13	0	5	2	0
3	B	13	0	5	2	0
4	A	72	0	0	4	0
4	B	74	0	0	5	0
All	All	7101	0	6806	378	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 27.

All (378) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:VAL:HG21	2:B:700[A]:COF:H72	1.34	1.09
1:B:228:MET:HA	1:B:228:MET:HE2	1.33	1.06
1:B:124:VAL:HG21	1:B:148:LEU:HD13	1.40	1.02
1:A:124:VAL:HG21	1:A:148:LEU:HD13	1.40	1.02
1:A:24:PHE:HA	1:B:437:GLY:HA3	1.44	0.99
1:B:136:HIS:HD2	1:B:138:MET:H	1.10	0.98
1:B:314:VAL:HG21	2:B:700[B]:COF:H72	1.46	0.96
1:B:282:LEU:HD23	1:B:390:MET:HE3	1.46	0.95
2:B:700[A]:COF:HI12	3:B:701:CIT:O3	1.62	0.95
1:A:67:ARG:HD3	1:A:99:GLY:HA2	1.49	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:ASN:HD21	2:A:700[A]:COF:H32	1.31	0.95
1:A:20:ARG:HG2	1:A:20:ARG:HH11	1.32	0.94
1:B:164:ARG:HG3	1:B:164:ARG:HH11	1.32	0.94
1:A:204:ASP:H	1:A:212:ASN:HD21	0.94	0.93
1:A:136:HIS:HD2	1:A:138:MET:H	1.09	0.93
1:B:306:TRP:HH2	1:B:363:GLU:HG2	1.35	0.91
1:B:103:THR:H	1:B:106:GLN:HE21	1.16	0.90
1:B:88:LEU:HD23	1:B:229:ARG:HD2	1.56	0.88
1:A:346:MET:HG2	1:A:380:VAL:HG12	1.53	0.87
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.37	0.87
1:A:56:SER:HB2	1:A:64:ILE:HD11	1.54	0.87
1:B:292:LEU:HD21	1:B:304:TYR:CD2	2.09	0.86
1:B:288:LEU:HD13	1:B:292:LEU:HD23	1.58	0.85
1:A:136:HIS:CD2	1:A:138:MET:H	1.93	0.85
1:B:165:THR:HB	1:B:166:LYS:NZ	1.90	0.85
1:B:306:TRP:CH2	1:B:363:GLU:HG2	2.12	0.85
1:B:103:THR:H	1:B:106:GLN:NE2	1.76	0.83
1:B:204:ASP:H	1:B:212:ASN:HD21	1.22	0.83
1:A:204:ASP:H	1:A:212:ASN:ND2	1.75	0.82
1:B:228:MET:HA	1:B:228:MET:CE	2.09	0.81
1:B:136:HIS:CD2	1:B:138:MET:H	1.99	0.81
1:B:282:LEU:HD23	1:B:390:MET:CE	2.11	0.80
1:A:373:ASN:HD21	2:A:700[A]:COF:C3P	1.94	0.80
1:B:302:ARG:NH1	1:B:306:TRP:NE1	2.29	0.80
1:A:346:MET:HG2	1:A:380:VAL:CG1	2.11	0.80
1:B:302:ARG:HH11	1:B:306:TRP:HE1	1.30	0.79
1:A:204:ASP:N	1:A:212:ASN:HD21	1.79	0.78
1:B:166:LYS:HE3	1:B:166:LYS:N	1.97	0.78
2:B:700[A]:COF:HI12	3:B:701:CIT:C5	2.14	0.77
1:A:17:GLU:O	1:A:21:ILE:HD13	1.84	0.77
1:A:14:ILE:O	1:A:18:GLN:HG3	1.85	0.76
1:B:165:THR:HB	1:B:166:LYS:HZ2	1.47	0.76
1:B:112:LYS:HD2	1:B:112:LYS:N	1.98	0.76
1:A:301:LEU:HD22	1:A:352:GLN:OE1	1.84	0.76
1:A:352:GLN:HG2	1:A:355:LYS:HZ1	1.50	0.75
1:B:329:ARG:O	1:B:333:GLN:HG3	1.85	0.75
1:A:352:GLN:HG2	1:A:355:LYS:NZ	2.02	0.74
1:A:88:LEU:HD23	1:A:229:ARG:CD	2.19	0.73
1:B:204:ASP:OD1	1:B:206:LYS:HE3	1.90	0.72
1:A:132:PRO:HB2	1:A:134:ASN:ND2	2.06	0.71
1:B:19:ALA:O	1:B:23:THR:HG23	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:THR:HG21	1:B:354:TYR:OH	1.91	0.71
1:B:316:PRO:HA	2:B:700[B]:COF:O5P	1.91	0.71
1:B:166:LYS:HE3	1:B:166:LYS:CA	2.21	0.70
1:B:37:THR:OG1	1:B:40:MET:HG3	1.92	0.70
1:B:45:MET:HB3	1:B:48:MET:HG3	1.73	0.70
1:A:67:ARG:HD3	1:A:99:GLY:CA	2.22	0.70
1:A:103:THR:H	1:A:106:GLN:HE21	1.39	0.70
1:B:371:TRP:HB3	1:B:372:PRO:HD2	1.73	0.70
1:B:40:MET:HE3	1:B:48:MET:HG2	1.74	0.70
1:A:134:ASN:H	1:A:134:ASN:HD22	1.40	0.69
1:B:282:LEU:CD2	1:B:390:MET:HE3	2.22	0.69
1:A:334:ARG:HG2	1:A:338:LEU:CD2	2.23	0.69
1:A:14:ILE:HG22	1:A:15:PRO:HD3	1.76	0.69
1:A:35:GLN:O	1:A:36:ILE:HG13	1.93	0.68
1:B:72:PRO:O	1:B:76:LYS:HG2	1.94	0.68
1:B:342:PRO:O	1:B:348:LYS:HE2	1.92	0.68
1:A:181:LYS:O	1:A:184:CYS:HB2	1.94	0.67
1:B:292:LEU:HD21	1:B:304:TYR:HD2	1.58	0.67
1:B:325:LYS:HE3	1:B:326:THR:H	1.60	0.67
1:A:88:LEU:HD23	1:A:229:ARG:HD2	1.76	0.66
1:A:334:ARG:HG2	1:A:338:LEU:HD22	1.77	0.66
1:B:413:ARG:NH2	4:B:716:HOH:O	2.28	0.66
1:B:165:THR:C	1:B:166:LYS:HE3	2.21	0.66
1:A:425:MET:HE3	1:A:425:MET:HA	1.78	0.65
1:B:314:VAL:CG2	2:B:700[A]:COF:H72	2.20	0.65
1:A:231:TYR:O	1:A:234:ILE:HG22	1.97	0.65
1:B:156:ARG:HG3	1:B:156:ARG:NH1	2.08	0.65
1:A:46:ARG:NH1	1:A:46:ARG:HG2	2.13	0.64
1:B:204:ASP:H	1:B:212:ASN:ND2	1.93	0.64
1:B:112:LYS:HD2	1:B:112:LYS:H	1.62	0.63
1:A:430:LEU:O	1:A:430:LEU:HD12	1.98	0.63
1:B:302:ARG:HH11	1:B:306:TRP:NE1	1.91	0.63
1:B:40:MET:HE1	1:B:48:MET:HB3	1.80	0.63
1:A:20:ARG:HG2	1:A:20:ARG:NH1	2.02	0.63
1:A:277:ALA:HB1	2:A:700[A]:COF:HN4	1.65	0.62
1:B:67:ARG:HG2	1:B:99:GLY:HA2	1.81	0.62
1:A:153:ASN:ND2	1:A:174:ASP:OD1	2.29	0.62
1:A:88:LEU:HD23	1:A:229:ARG:HD3	1.81	0.62
1:B:336:PHE:HA	1:B:339:LYS:HD2	1.80	0.62
2:B:700[A]:COF:S1P	2:B:700[A]:COF:H62	2.40	0.62
1:B:40:MET:HE3	1:B:48:MET:CG	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD21	1:B:236:SER:OG	2.00	0.61
1:A:162:ILE:HD12	1:A:167:TYR:HD1	1.65	0.61
1:A:206:LYS:HB2	1:A:206:LYS:NZ	2.15	0.61
1:A:257:ASP:HB2	1:A:258:PRO:HD2	1.83	0.61
1:A:35:GLN:HG3	1:A:40:MET:HE1	1.81	0.61
1:A:311:SER:OG	1:A:313:ARG:HD3	2.00	0.61
1:A:316:PRO:HA	2:A:700[B]:COF:O5P	2.01	0.61
1:B:353:LEU:O	1:B:357:VAL:HG23	2.00	0.61
1:A:2:SER:HB3	1:A:106:GLN:OE1	2.00	0.61
1:A:283:LEU:HD13	1:A:390:MET:SD	2.41	0.60
1:A:289:GLN:NE2	1:A:346:MET:HE3	2.17	0.60
1:A:288:LEU:HD12	1:A:288:LEU:O	2.01	0.60
1:B:103:THR:N	1:B:106:GLN:HE21	1.95	0.60
1:A:136:HIS:HD2	1:A:138:MET:N	1.91	0.59
2:A:700[A]:COF:HI12	3:A:701:CIT:O4	2.02	0.59
1:A:257:ASP:OD1	1:A:259:TYR:HB2	2.01	0.59
1:B:373:ASN:C	1:B:373:ASN:HD22	2.09	0.59
1:A:153:ASN:HD22	1:A:153:ASN:H	1.49	0.59
1:A:24:PHE:HA	1:B:437:GLY:CA	2.28	0.59
1:A:413:ARG:NH1	1:A:417:PHE:O	2.29	0.59
1:B:132:PRO:HB2	1:B:134:ASN:OD1	2.03	0.59
1:B:177:ASP:O	1:B:181:LYS:HG3	2.03	0.58
1:A:413:ARG:NH2	4:A:709:HOH:O	2.28	0.58
1:B:298:ASP:HB3	1:B:356:ILE:HD11	1.85	0.58
1:A:288:LEU:HD12	1:A:288:LEU:C	2.27	0.58
1:B:136:HIS:HD2	1:B:138:MET:N	1.92	0.58
1:A:121:PRO:HD2	1:A:148:LEU:HD11	1.85	0.58
1:B:35:GLN:OE1	1:B:35:GLN:N	2.30	0.58
1:B:341:LEU:N	1:B:342:PRO:HD3	2.19	0.57
1:B:137:PRO:HG2	1:B:391:ASN:O	2.03	0.57
1:A:234:ILE:HG23	1:A:235:HIS:ND1	2.19	0.57
1:B:157:ALA:O	1:B:160:GLU:HB2	2.05	0.57
1:B:162:ILE:HD13	1:B:167:TYR:CE1	2.39	0.57
1:A:162:ILE:CD1	1:A:167:TYR:HD1	2.17	0.57
1:B:77:LEU:HB3	1:B:101:ILE:HD12	1.86	0.57
1:B:185:VAL:O	1:B:189:ILE:HG13	2.05	0.57
1:A:51:LEU:HD23	1:A:52:ILE:N	2.20	0.57
1:B:317:GLY:H	2:B:700[A]:COF:HN4	1.49	0.57
1:A:430:LEU:HD12	1:A:430:LEU:C	2.29	0.56
1:B:81:ALA:HB2	1:B:88:LEU:HD21	1.86	0.56
1:B:308:THR:O	1:B:313:ARG:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:PRO:HG3	2:B:700[B]:COF:HI11	1.87	0.56
1:B:28:HIS:O	1:B:29:GLY:C	2.48	0.56
1:B:162:ILE:HD13	1:B:167:TYR:HE1	1.71	0.56
1:B:164:ARG:HG3	1:B:164:ARG:NH1	2.08	0.56
1:B:124:VAL:HG21	1:B:148:LEU:CD1	2.26	0.56
1:B:166:LYS:HE3	1:B:166:LYS:HA	1.87	0.56
1:A:179:ILE:CD1	1:A:406:LEU:HD12	2.36	0.55
1:B:314:VAL:HG21	2:B:700[A]:COF:C7P	2.24	0.55
1:A:65:ARG:NH1	1:A:73:GLU:OE1	2.39	0.55
1:A:206:LYS:HB2	1:A:206:LYS:HZ2	1.71	0.55
1:B:54:GLU:H	1:B:408:GLN:HE22	1.54	0.55
1:A:46:ARG:HG2	1:A:46:ARG:HH11	1.72	0.54
1:A:81:ALA:O	1:A:83:GLY:N	2.40	0.54
1:A:23:THR:O	1:A:26:GLN:HB3	2.08	0.54
1:B:73:GLU:HA	1:B:76:LYS:HE3	1.88	0.54
1:A:66:PHE:N	1:A:69:PHE:O	2.38	0.54
1:B:335:GLU:O	1:B:339:LYS:HG3	2.08	0.54
1:A:288:LEU:HD22	1:A:304:TYR:CE2	2.42	0.54
1:B:4:THR:HG23	1:B:4:THR:O	2.08	0.54
1:B:300:LYS:HA	1:B:303:ASP:OD1	2.09	0.53
1:A:132:PRO:HB2	1:A:134:ASN:HD22	1.73	0.53
1:A:146:THR:O	1:A:149:ASN:HB3	2.07	0.53
1:B:16:LYS:HD2	1:B:16:LYS:N	2.22	0.53
1:B:88:LEU:HD23	1:B:229:ARG:CD	2.36	0.53
1:B:283:LEU:HD13	1:B:283:LEU:N	2.24	0.53
1:B:278:ASN:ND2	4:B:768:HOH:O	2.42	0.53
1:B:333:GLN:HE22	1:B:378:SER:HB3	1.74	0.53
1:A:53:TYR:CD1	1:A:408:GLN:HG2	2.44	0.53
1:B:292:LEU:H	1:B:292:LEU:HD22	1.74	0.53
1:B:357:VAL:HB	1:B:358:PRO:HD3	1.91	0.52
1:A:276:LEU:O	1:A:280:GLU:HG2	2.08	0.52
1:A:383:GLN:HG2	4:A:757:HOH:O	2.07	0.52
1:B:192:ASN:HD22	1:B:197:GLY:HA2	1.74	0.52
1:A:145:ILE:HD13	1:A:262:PHE:CE2	2.43	0.52
1:B:371:TRP:HB3	1:B:372:PRO:CD	2.39	0.52
1:A:262:PHE:CE1	1:A:266:MET:HE3	2.45	0.52
1:B:7:LYS:HD3	1:B:172:TYR:CE1	2.44	0.52
1:B:40:MET:CE	1:B:48:MET:HB3	2.40	0.52
1:A:194:TYR:CD2	1:A:389:GLU:HG3	2.45	0.52
1:A:101:ILE:HG12	1:A:102:PRO:HD2	1.92	0.52
1:B:228:MET:HE2	1:B:231:TYR:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:ASN:N	1:B:391:ASN:HD22	2.06	0.52
1:A:14:ILE:CG2	1:A:15:PRO:HD3	2.39	0.51
1:A:335:GLU:O	1:A:339:LYS:HD3	2.09	0.51
1:A:20:ARG:HH11	1:A:20:ARG:CG	2.13	0.51
1:A:113:GLU:O	1:A:117:ARG:HG3	2.10	0.51
1:B:275:GLY:O	1:B:278:ASN:HB2	2.10	0.51
1:A:277:ALA:HB1	2:A:700[A]:COF:N4P	2.25	0.51
1:A:177:ASP:HB3	1:A:181:LYS:HE3	1.93	0.51
1:A:28:HIS:O	1:B:38:VAL:HB	2.11	0.51
1:B:74:CYS:HB3	1:B:78:LEU:HD12	1.93	0.51
1:B:266:MET:HE2	1:B:266:MET:HA	1.93	0.51
1:B:301:LEU:HD23	1:B:352:GLN:HG2	1.92	0.51
1:B:347:PHE:HA	1:B:380:VAL:HG21	1.93	0.51
1:A:67:ARG:HD2	1:A:96:LEU:O	2.11	0.50
1:B:98:THR:OG1	1:B:100:GLN:HG2	2.11	0.50
1:B:204:ASP:HB3	1:B:207:LEU:HG	1.93	0.50
1:B:299:GLU:O	1:B:303:ASP:OD1	2.29	0.50
1:B:302:ARG:NH1	1:B:306:TRP:HE1	1.92	0.50
1:A:310:ASN:C	1:A:312:GLY:H	2.19	0.50
1:A:124:VAL:HG21	1:A:148:LEU:CD1	2.28	0.50
1:A:145:ILE:HD13	1:A:262:PHE:CD2	2.46	0.50
1:B:377:HIS:O	1:B:377:HIS:ND1	2.40	0.50
1:A:21:ILE:O	1:A:25:ARG:HB2	2.12	0.50
1:B:104:PRO:O	1:B:108:SER:OG	2.29	0.50
1:B:285:LEU:HD22	1:B:349:LEU:CD2	2.41	0.50
1:B:374:VAL:HG13	1:B:375:ASP:N	2.25	0.50
1:A:56:SER:OG	1:A:237:ASP:OD2	2.29	0.49
1:A:14:ILE:CB	1:A:15:PRO:HD3	2.42	0.49
1:A:24:PHE:CA	1:B:437:GLY:HA3	2.29	0.49
1:A:123:HIS:HE1	1:A:147:ALA:O	1.94	0.49
1:A:352:GLN:O	1:A:356:ILE:HG12	2.11	0.49
1:B:344:ASP:O	1:B:348:LYS:HG3	2.12	0.49
1:B:192:ASN:HA	1:B:197:GLY:HA2	1.93	0.49
1:A:305:ILE:HG22	1:A:360:VAL:HG11	1.94	0.49
1:B:123:HIS:HE1	1:B:147:ALA:O	1.96	0.49
1:B:214:THR:HG22	1:B:228:MET:HG3	1.95	0.49
1:A:46:ARG:HH11	1:A:46:ARG:CG	2.23	0.49
1:A:237:ASP:OD1	1:A:404:GLY:HA3	2.13	0.48
1:A:28:HIS:HB3	1:A:31:THR:HB	1.96	0.48
1:A:272:PRO:HA	1:A:276:LEU:HB3	1.95	0.48
1:A:95:LEU:O	1:A:99:GLY:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:O	1:A:116:LYS:HG3	2.13	0.48
1:A:364:GLN:O	1:A:364:GLN:HG2	2.11	0.48
1:A:257:ASP:HB2	1:A:258:PRO:CD	2.43	0.48
1:A:374:VAL:HG13	1:A:375:ASP:N	2.28	0.48
1:B:54:GLU:H	1:B:408:GLN:NE2	2.11	0.48
1:B:35:GLN:H	1:B:35:GLN:CD	2.19	0.48
1:B:165:THR:HB	1:B:166:LYS:HZ1	1.76	0.48
1:B:302:ARG:NH1	1:B:306:TRP:CD1	2.81	0.48
1:A:162:ILE:HD12	1:A:167:TYR:CD1	2.48	0.48
1:A:281:VAL:HG22	1:A:316:PRO:HB2	1.96	0.47
1:B:58:LEU:HD23	1:B:322:VAL:HG11	1.95	0.47
1:B:334:ARG:HG3	1:B:335:GLU:N	2.25	0.47
1:B:78:LEU:HB3	4:B:720:HOH:O	2.15	0.47
1:B:236:SER:O	1:B:404:GLY:HA3	2.15	0.47
1:A:164:ARG:CB	1:A:164:ARG:HH11	2.28	0.46
1:A:164:ARG:HH11	1:A:164:ARG:CG	2.28	0.46
1:A:153:ASN:ND2	1:A:153:ASN:N	2.63	0.46
1:A:292:LEU:N	1:A:292:LEU:CD2	2.79	0.46
1:B:112:LYS:HE3	1:B:205:SER:O	2.16	0.46
1:B:190:TYR:CE1	1:B:389:GLU:HG3	2.50	0.46
1:B:257:ASP:OD1	1:B:259:TYR:HB2	2.15	0.46
1:B:74:CYS:HB3	1:B:78:LEU:CD1	2.44	0.46
1:A:301:LEU:HD22	1:A:352:GLN:CD	2.40	0.46
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.68	0.46
1:B:341:LEU:N	1:B:342:PRO:CD	2.78	0.46
1:B:283:LEU:HD11	1:B:390:MET:CG	2.46	0.46
1:B:329:ARG:HB3	1:B:374:VAL:HG23	1.97	0.46
1:B:316:PRO:HB3	2:B:700[B]:COF:H21	1.97	0.46
1:A:53:TYR:CE1	1:A:408:GLN:HG2	2.51	0.45
1:B:80:LYS:HD3	1:B:87:PRO:HA	1.98	0.45
1:B:285:LEU:O	1:B:288:LEU:HB3	2.16	0.45
1:B:370:PRO:HD2	1:B:371:TRP:CD1	2.51	0.45
1:A:35:GLN:HG3	1:A:40:MET:SD	2.56	0.45
1:A:119:ALA:HB2	4:A:738:HOH:O	2.15	0.45
1:A:162:ILE:CD1	1:A:167:TYR:CD1	2.99	0.45
1:B:413:ARG:NH1	1:B:417:PHE:O	2.29	0.45
1:A:21:ILE:CD1	1:A:21:ILE:N	2.79	0.45
1:A:341:LEU:N	1:A:342:PRO:CD	2.79	0.45
1:A:46:ARG:HA	1:A:46:ARG:HD3	1.46	0.45
1:A:200:ILE:HB	1:A:216:MET:HB3	1.99	0.45
1:B:292:LEU:HD22	1:B:292:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:CG2	1:A:360:VAL:HG11	2.47	0.45
1:A:334:ARG:O	1:A:338:LEU:HD22	2.17	0.45
1:A:243:VAL:HB	1:A:274:HIS:CD2	2.51	0.45
1:A:297:SER:O	1:A:298:ASP:C	2.54	0.45
1:B:79:PRO:HG2	1:B:107:VAL:HG21	1.98	0.45
1:B:260:LEU:N	1:B:260:LEU:HD23	2.32	0.45
1:A:14:ILE:HG22	1:A:15:PRO:CD	2.45	0.45
1:B:338:LEU:CD1	1:B:347:PHE:CZ	3.00	0.44
1:B:154:PHE:HA	1:B:170:PHE:HB3	1.97	0.44
1:A:103:THR:HB	1:A:104:PRO:HD2	2.00	0.44
1:B:217:LEU:HD13	1:B:387:MET:HE1	1.98	0.44
1:B:189:ILE:O	1:B:193:LEU:HB2	2.17	0.44
1:B:279:GLN:O	1:B:283:LEU:HD22	2.16	0.44
1:B:338:LEU:HD12	1:B:338:LEU:HA	1.68	0.44
1:B:357:VAL:N	1:B:358:PRO:CD	2.80	0.44
1:A:35:GLN:HG3	1:A:40:MET:CE	2.48	0.44
1:A:354:TYR:CD1	1:A:372:PRO:HG3	2.53	0.44
1:B:14:ILE:HB	1:B:15:PRO:HD3	1.98	0.44
1:B:76:LYS:HG2	1:B:76:LYS:H	1.66	0.44
1:B:283:LEU:CD1	1:B:390:MET:HG3	2.48	0.44
1:A:25:ARG:HE	1:B:42:TYR:CB	2.30	0.44
1:B:214:THR:CG2	1:B:228:MET:HG3	2.48	0.44
1:B:301:LEU:HA	1:B:301:LEU:HD12	1.46	0.44
1:B:163:ASN:O	1:B:164:ARG:C	2.60	0.44
1:B:215:ASN:HD22	1:B:215:ASN:HA	1.59	0.44
1:A:121:PRO:O	1:A:125:VAL:HG23	2.17	0.44
1:A:21:ILE:CD1	1:A:21:ILE:H	2.31	0.43
1:A:413:ARG:HA	1:A:413:ARG:HD3	1.75	0.43
1:B:326:THR:HB	1:B:372:PRO:HD2	1.99	0.43
1:A:191:ARG:HG3	1:A:198:SER:O	2.18	0.43
1:B:97:VAL:HG23	1:B:407:ALA:HB1	2.00	0.43
1:B:279:GLN:HB2	1:B:390:MET:O	2.17	0.43
1:A:434:SER:O	1:A:435:ALA:HB2	2.18	0.43
1:B:283:LEU:HD13	1:B:390:MET:HG3	1.99	0.43
1:A:149:ASN:ND2	1:A:257:ASP:OD2	2.49	0.43
1:A:281:VAL:O	1:A:285:LEU:HG	2.18	0.43
1:A:397:PHE:O	1:A:397:PHE:HD1	2.01	0.43
1:B:16:LYS:N	1:B:16:LYS:CD	2.80	0.43
1:B:86:GLU:OE1	1:B:86:GLU:HA	2.19	0.43
1:A:71:ILE:O	1:A:75:GLN:HB2	2.19	0.43
1:B:40:MET:CE	1:B:48:MET:CG	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.75	0.43
1:A:153:ASN:ND2	1:A:153:ASN:H	2.15	0.43
1:A:345:PRO:HA	1:A:348:LYS:HD3	2.01	0.43
1:B:314:VAL:HG13	2:B:700[B]:COF:H22	2.00	0.43
1:A:163:ASN:O	1:A:164:ARG:C	2.62	0.43
1:A:20:ARG:O	1:A:21:ILE:C	2.61	0.43
1:A:24:PHE:HD1	1:B:437:GLY:HA3	1.84	0.43
1:B:221:ASP:OD1	1:B:222:PRO:HD2	2.19	0.43
1:A:76:LYS:HG3	1:A:77:LEU:HD13	2.01	0.42
1:A:124:VAL:HA	1:A:127:MET:HE2	2.00	0.42
1:A:317:GLY:HA2	2:A:700[A]:COF:H32	2.00	0.42
1:B:10:LEU:O	1:B:11:ALA:C	2.62	0.42
1:B:88:LEU:CD2	1:B:229:ARG:HD2	2.37	0.42
1:A:7:LYS:HD2	1:A:172:TYR:CE1	2.54	0.42
1:A:311:SER:CB	1:A:313:ARG:HH11	2.29	0.42
1:A:324:ARG:HA	1:A:324:ARG:HD3	1.70	0.42
1:B:298:ASP:CB	1:B:356:ILE:HD11	2.48	0.42
1:A:253:SER:HA	1:A:413:ARG:NH2	2.35	0.42
1:B:243:VAL:HB	1:B:274:HIS:CD2	2.55	0.42
1:B:283:LEU:HD12	1:B:283:LEU:HA	1.81	0.42
1:B:409:LEU:HD23	1:B:409:LEU:HA	1.93	0.42
1:A:91:GLY:HA3	4:A:713:HOH:O	2.19	0.42
1:B:164:ARG:HA	1:B:167:TYR:CE1	2.54	0.42
1:B:320:HIS:HA	2:B:700[A]:COF:F2I	2.10	0.42
1:B:357:VAL:O	1:B:361:LEU:HB2	2.19	0.42
1:B:40:MET:CE	1:B:48:MET:SD	3.08	0.42
1:B:110:VAL:O	1:B:111:SER:C	2.62	0.42
1:B:215:ASN:ND2	4:B:759:HOH:O	2.52	0.42
1:B:433:LEU:HD23	1:B:433:LEU:HA	1.82	0.42
1:B:228:MET:CE	1:B:231:TYR:HB3	2.50	0.42
1:B:288:LEU:HD22	1:B:304:TYR:CE1	2.55	0.42
1:A:421:ARG:HD3	1:A:422:PRO:O	2.20	0.41
1:B:5:ASN:C	1:B:5:ASN:HD22	2.28	0.41
1:A:275:GLY:O	1:A:278:ASN:HB2	2.20	0.41
1:A:310:ASN:C	1:A:312:GLY:N	2.77	0.41
1:A:234:ILE:HG21	1:A:234:ILE:HD13	1.36	0.41
1:B:48:MET:HB2	1:B:48:MET:HE3	1.84	0.41
1:B:153:ASN:ND2	4:B:749:HOH:O	2.28	0.41
1:B:374:VAL:CG1	1:B:375:ASP:N	2.83	0.41
1:B:397:PHE:C	1:B:397:PHE:CD1	2.98	0.41
1:A:112:LYS:HB3	1:A:112:LYS:HE2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASN:C	1:B:165:THR:N	2.78	0.41
1:B:373:ASN:HD21	1:B:375:ASP:HB2	1.86	0.41
1:A:58:LEU:HD13	1:A:322:VAL:CG1	2.50	0.41
1:A:370:PRO:HD2	1:A:371:TRP:CD1	2.56	0.41
1:B:182:LEU:HB2	1:B:183:PRO:HD3	2.03	0.41
1:A:92:LEU:HD21	1:A:236:SER:CB	2.50	0.41
1:A:103:THR:HG23	1:A:106:GLN:NE2	2.36	0.41
1:B:287:GLN:HA	1:B:290:LYS:HG3	2.01	0.41
1:A:91:GLY:HA2	1:A:107:VAL:HG22	2.03	0.41
1:B:7:LYS:HD3	1:B:172:TYR:CD1	2.56	0.41
1:B:40:MET:CE	1:B:48:MET:CB	2.99	0.41
1:B:306:TRP:CE2	1:B:360:VAL:HG22	2.56	0.41
1:B:397:PHE:HD1	1:B:397:PHE:O	2.03	0.41
1:A:178:LEU:O	1:A:179:ILE:C	2.63	0.41
1:A:274:HIS:CE1	3:A:701:CIT:H22	2.56	0.41
1:B:307:ASN:C	1:B:309:LEU:N	2.79	0.41
1:B:384:TYR:CD2	1:B:384:TYR:C	2.99	0.41
1:B:124:VAL:CG2	1:B:148:LEU:HD13	2.30	0.40
1:A:158:TYR:CD1	1:A:158:TYR:C	2.99	0.40
1:B:156:ARG:NH1	1:B:156:ARG:CG	2.80	0.40
1:B:156:ARG:HD2	1:B:156:ARG:HA	1.73	0.40
1:B:380:VAL:O	1:B:383:GLN:NE2	2.54	0.40
1:B:382:LEU:HD23	1:B:382:LEU:HA	1.88	0.40
1:A:230:LEU:O	1:A:234:ILE:HG22	2.22	0.40
1:A:291:ASP:HB3	1:A:292:LEU:HD22	2.03	0.40
1:A:51:LEU:HD23	1:A:51:LEU:C	2.46	0.40
1:B:273:LEU:O	2:B:700[A]:COF:S1P	2.79	0.40
1:B:338:LEU:CD1	1:B:347:PHE:HZ	2.34	0.40
1:A:94:TRP:HB3	1:A:102:PRO:HG3	2.02	0.40
1:A:283:LEU:CD1	1:A:390:MET:SD	3.09	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/437 (100%)	411 (94%)	19 (4%)	5 (1%)	11	8
1	B	432/437 (99%)	410 (95%)	18 (4%)	4 (1%)	14	12
All	All	867/874 (99%)	821 (95%)	37 (4%)	9 (1%)	12	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	36	ILE
1	A	435	ALA
1	B	311	SER
1	B	435	ALA
1	A	66	PHE
1	B	5	ASN
1	B	82	GLY
1	A	82	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/362 (100%)	291 (80%)	71 (20%)	1	0
1	B	360/362 (99%)	286 (79%)	74 (21%)	1	0
All	All	722/724 (100%)	577 (80%)	145 (20%)	1	0

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	6	LEU
1	A	12	SER
1	A	13	LEU

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Mol	Chain	Res	Type
1	A	16	LYS
1	A	20	ARG
1	A	21	ILE
1	A	25	ARG
1	A	27	GLN
1	A	35	GLN
1	A	41	SER
1	A	46	ARG
1	A	48	MET
1	A	49	LYS
1	A	56	SER
1	A	58	LEU
1	A	62	GLU
1	A	75	GLN
1	A	76	LYS
1	A	77	LEU
1	A	78	LEU
1	A	80	LYS
1	A	96	LEU
1	A	101	ILE
1	A	106	GLN
1	A	112	LYS
1	A	120	LEU
1	A	126	THR
1	A	134	ASN
1	A	148	LEU
1	A	149	ASN
1	A	150	SER
1	A	153	ASN
1	A	164	ARG
1	A	179	ILE
1	A	182	LEU
1	A	188	LYS
1	A	191	ARG
1	A	199	SER
1	A	203	ILE
1	A	205	SER
1	A	206	LYS
1	A	210	SER
1	A	212	ASN
1	A	223	GLN
1	A	234	ILE

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Mol	Chain	Res	Type
1	A	278	ASN
1	A	280	GLU
1	A	282	LEU
1	A	283	LEU
1	A	288	LEU
1	A	290	LYS
1	A	291	ASP
1	A	292	LEU
1	A	299	GLU
1	A	302	ARG
1	A	335	GLU
1	A	338	LEU
1	A	339	LYS
1	A	341	LEU
1	A	343	SER
1	A	352	GLN
1	A	353	LEU
1	A	368	LYS
1	A	383	GLN
1	A	389	GLU
1	A	390	MET
1	A	423	LYS
1	A	424	SER
1	A	430	LEU
1	A	433	LEU
1	B	5	ASN
1	B	7	LYS
1	B	13	LEU
1	B	16	LYS
1	B	20	ARG
1	B	21	ILE
1	B	22	LYS
1	B	35	GLN
1	B	40	MET
1	B	48	MET
1	B	49	LYS
1	B	51	LEU
1	B	62	GLU
1	B	67	ARG
1	B	76	LYS
1	B	78	LEU
1	B	85	GLU

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Mol	Chain	Res	Type
1	B	101	ILE
1	B	108	SER
1	B	112	LYS
1	B	116	LYS
1	B	148	LEU
1	B	149	ASN
1	B	156	ARG
1	B	160	GLU
1	B	162	ILE
1	B	164	ARG
1	B	165	THR
1	B	166	LYS
1	B	188	LYS
1	B	191	ARG
1	B	193	LEU
1	B	205	SER
1	B	206	LYS
1	B	223	GLN
1	B	227	LEU
1	B	228	MET
1	B	278	ASN
1	B	279	GLN
1	B	282	LEU
1	B	283	LEU
1	B	287	GLN
1	B	288	LEU
1	B	290	LYS
1	B	291	ASP
1	B	292	LEU
1	B	295	ASP
1	B	299	GLU
1	B	301	LEU
1	B	302	ARG
1	B	303	ASP
1	B	307	ASN
1	B	310	ASN
1	B	313	ARG
1	B	326	THR
1	B	334	ARG
1	B	338	LEU
1	B	339	LYS
1	B	341	LEU

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Mol	Chain	Res	Type
1	B	346	MET
1	B	350	VAL
1	B	353	LEU
1	B	355	LYS
1	B	361	LEU
1	B	363	GLU
1	B	364	GLN
1	B	368	LYS
1	B	373	ASN
1	B	383	GLN
1	B	388	THR
1	B	389	GLU
1	B	430	LEU
1	B	432	LYS
1	B	433	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	35	GLN
1	A	106	GLN
1	A	123	HIS
1	A	134	ASN
1	A	136	HIS
1	A	140	GLN
1	A	192	ASN
1	A	211	HIS
1	A	212	ASN
1	A	267	ASN
1	A	289	GLN
1	A	359	ASN
1	A	373	ASN
1	A	383	GLN
1	A	408	GLN
1	B	5	ASN
1	B	18	GLN
1	B	26	GLN
1	B	100	GLN
1	B	106	GLN
1	B	123	HIS
1	B	130	ASN

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Mol	Chain	Res	Type
1	B	136	HIS
1	B	140	GLN
1	B	192	ASN
1	B	211	HIS
1	B	212	ASN
1	B	215	ASN
1	B	267	ASN
1	B	287	GLN
1	B	289	GLN
1	B	333	GLN
1	B	340	HIS
1	B	373	ASN
1	B	383	GLN
1	B	391	ASN
1	B	408	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	COF	A	700[A]	-	55,57,57	1.54	7 (12%)	80,86,86	1.60	11 (13%)
3	CIT	A	701	-	12,12,12	1.03	0	17,17,17	2.21	7 (41%)
3	CIT	B	701	-	12,12,12	0.92	0	17,17,17	1.95	4 (23%)
2	COF	B	700[A]	-	55,57,57	1.28	6 (10%)	80,86,86	1.06	5 (6%)
2	COF	A	700[B]	-	55,57,57	1.31	4 (7%)	80,86,86	1.23	8 (10%)
2	COF	B	700[B]	-	55,57,57	1.10	4 (7%)	80,86,86	1.12	7 (8%)

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	COF	A	700[A]	-	-	11/58/74/74	0/3/3/3
3	CIT	A	701	-	-	6/16/16/16	-
3	CIT	B	701	-	-	3/16/16/16	-
2	COF	B	700[A]	-	-	11/58/74/74	0/3/3/3
2	COF	A	700[B]	-	-	5/58/74/74	0/3/3/3
2	COF	B	700[B]	-	-	6/58/74/74	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	700[A]	COF	O1I-C2I	4.39	1.28	1.21
2	A	700[A]	COF	P2A-O3A	3.78	1.63	1.59
2	A	700[B]	COF	P2A-O3A	3.78	1.63	1.59
2	B	700[A]	COF	C1I-C2I	3.74	1.56	1.51
2	A	700[A]	COF	C1I-C2I	3.31	1.56	1.51
2	A	700[A]	COF	P1A-O3A	3.25	1.63	1.59
2	A	700[B]	COF	P1A-O3A	3.25	1.63	1.59
2	A	700[A]	COF	C7P-N8P	-3.24	1.38	1.46
2	B	700[A]	COF	O1I-C2I	3.06	1.26	1.21
2	A	700[A]	COF	OAP-CAP	-3.01	1.37	1.42
2	A	700[B]	COF	OAP-CAP	-3.01	1.37	1.42
2	B	700[A]	COF	C9P-N8P	-2.91	1.26	1.33
2	A	700[A]	COF	CDP-CBP	-2.71	1.48	1.53
2	A	700[B]	COF	CDP-CBP	-2.71	1.48	1.53
2	B	700[A]	COF	C7P-N8P	-2.71	1.40	1.46
2	B	700[A]	COF	CCP-CBP	-2.68	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	700[B]	COF	CCP-CBP	-2.68	1.48	1.52
2	B	700[B]	COF	O1I-C2I	2.43	1.25	1.21
2	B	700[B]	COF	C7P-N8P	2.34	1.51	1.46
2	B	700[A]	COF	CDP-CBP	-2.30	1.49	1.53
2	B	700[B]	COF	CDP-CBP	-2.30	1.49	1.53

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700[A]	COF	O1I-C2I-C1I	8.63	129.51	120.96
2	A	700[A]	COF	OAP-CAP-CBP	6.07	124.25	110.18
2	A	700[B]	COF	OAP-CAP-CBP	6.07	124.25	110.18
3	A	701	CIT	O5-C6-C3	-4.16	114.03	122.09
3	B	701	CIT	O5-C6-C3	-4.10	114.15	122.09
3	A	701	CIT	O6-C6-C3	4.08	120.97	113.14
3	B	701	CIT	O7-C3-C6	3.98	114.60	108.96
2	B	700[B]	COF	C7P-N8P-C9P	-3.96	115.44	122.55
3	B	701	CIT	O6-C6-C3	3.75	120.33	113.14
3	A	701	CIT	O7-C3-C6	3.71	114.22	108.96
2	B	700[A]	COF	C7P-C6P-C5P	3.33	117.94	112.39
3	A	701	CIT	O3-C5-C4	-3.13	114.07	122.95
2	B	700[B]	COF	CAP-C9P-N8P	-3.01	110.78	116.48
2	B	700[A]	COF	O1I-C2I-C3I	2.93	123.75	116.37
2	B	700[A]	COF	C2P-S1P-C1I	-2.89	96.95	101.72
2	A	700[A]	COF	C7P-C6P-C5P	2.87	117.18	112.39
2	B	700[A]	COF	CDP-CBP-CCP	2.87	112.95	108.22
2	B	700[B]	COF	CDP-CBP-CCP	2.87	112.95	108.22
2	B	700[B]	COF	C2P-S1P-C1I	-2.80	97.11	101.72
2	B	700[B]	COF	O9P-C9P-N8P	2.79	128.88	122.98
2	B	700[B]	COF	O1I-C2I-C3I	2.71	123.21	116.37
2	B	700[A]	COF	O8A-P3B-O7A	2.64	121.11	110.83
2	B	700[B]	COF	O8A-P3B-O7A	2.64	121.11	110.83
2	A	700[A]	COF	O8A-P3B-O7A	2.64	121.10	110.83
2	A	700[B]	COF	O8A-P3B-O7A	2.64	121.10	110.83
2	A	700[A]	COF	O4B-C1B-C2B	-2.61	101.04	106.62
2	A	700[B]	COF	O4B-C1B-C2B	-2.61	101.04	106.62
2	A	700[A]	COF	O5A-P2A-O3A	2.56	114.18	107.27
2	A	700[B]	COF	O5A-P2A-O3A	2.56	114.18	107.27
3	A	701	CIT	C4-C3-C6	-2.54	104.41	110.03
2	A	700[A]	COF	C2B-C1B-N9A	-2.51	107.06	113.30
2	A	700[B]	COF	C2B-C1B-N9A	-2.51	107.06	113.30
3	A	701	CIT	O1-C1-C2	-2.50	115.88	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700[A]	COF	C2B-C3B-C4B	-2.47	98.92	103.24
2	A	700[B]	COF	C2B-C3B-C4B	-2.47	98.92	103.24
2	A	700[A]	COF	O1I-C2I-C3I	-2.42	110.27	116.37
2	A	700[A]	COF	C7P-N8P-C9P	2.36	126.78	122.55
3	B	701	CIT	O3-C5-C4	-2.19	116.74	122.95
3	A	701	CIT	O2-C1-C2	2.17	121.23	114.35
2	A	700[B]	COF	C3P-N4P-C5P	-2.15	118.81	122.82
2	A	700[A]	COF	O5A-P2A-O4A	2.08	122.14	112.44
2	A	700[B]	COF	O5A-P2A-O4A	2.08	122.14	112.44

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700[A]	COF	N8P-C9P-CAP-OAP
2	A	700[A]	COF	S1P-C2P-C3P-N4P
2	A	700[A]	COF	S1P-C1I-C2I-C3I
2	A	700[B]	COF	N8P-C9P-CAP-OAP
2	B	700[A]	COF	C5B-O5B-P1A-O3A
2	B	700[A]	COF	CDP-CBP-CCP-O6A
2	B	700[A]	COF	CEP-CBP-CCP-O6A
2	B	700[A]	COF	S1P-C2P-C3P-N4P
2	B	700[B]	COF	C5B-O5B-P1A-O3A
2	B	700[B]	COF	CDP-CBP-CCP-O6A
2	B	700[B]	COF	CEP-CBP-CCP-O6A
3	A	701	CIT	C2-C3-C6-O5
3	A	701	CIT	C2-C3-C6-O6
3	A	701	CIT	O7-C3-C6-O5
3	A	701	CIT	O7-C3-C6-O6
2	A	700[A]	COF	C6P-C5P-N4P-C3P
2	B	700[A]	COF	C6P-C5P-N4P-C3P
2	A	700[A]	COF	O5P-C5P-N4P-C3P
2	B	700[A]	COF	O5P-C5P-N4P-C3P
2	A	700[A]	COF	O9P-C9P-CAP-OAP
2	A	700[B]	COF	O9P-C9P-CAP-OAP
3	A	701	CIT	O2-C1-C2-C3
3	A	701	CIT	O1-C1-C2-C3
2	A	700[A]	COF	C5P-C6P-C7P-N8P
2	B	700[A]	COF	C5P-C6P-C7P-N8P
2	A	700[A]	COF	CEP-CBP-CCP-O6A
2	A	700[B]	COF	CEP-CBP-CCP-O6A
2	B	700[A]	COF	C5B-O5B-P1A-O1A

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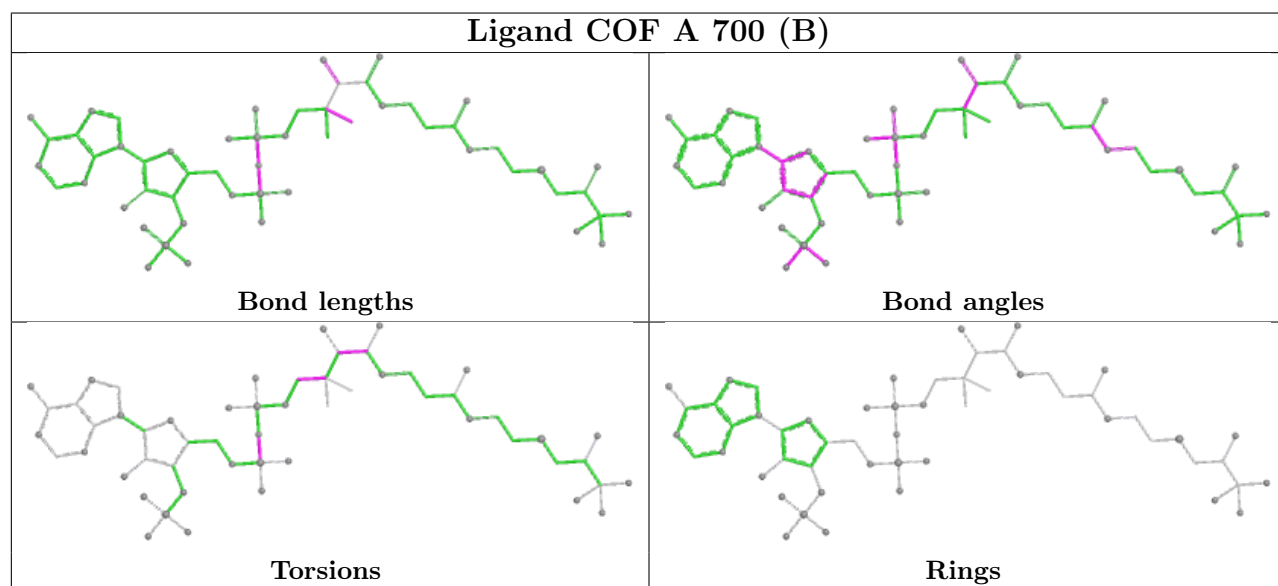
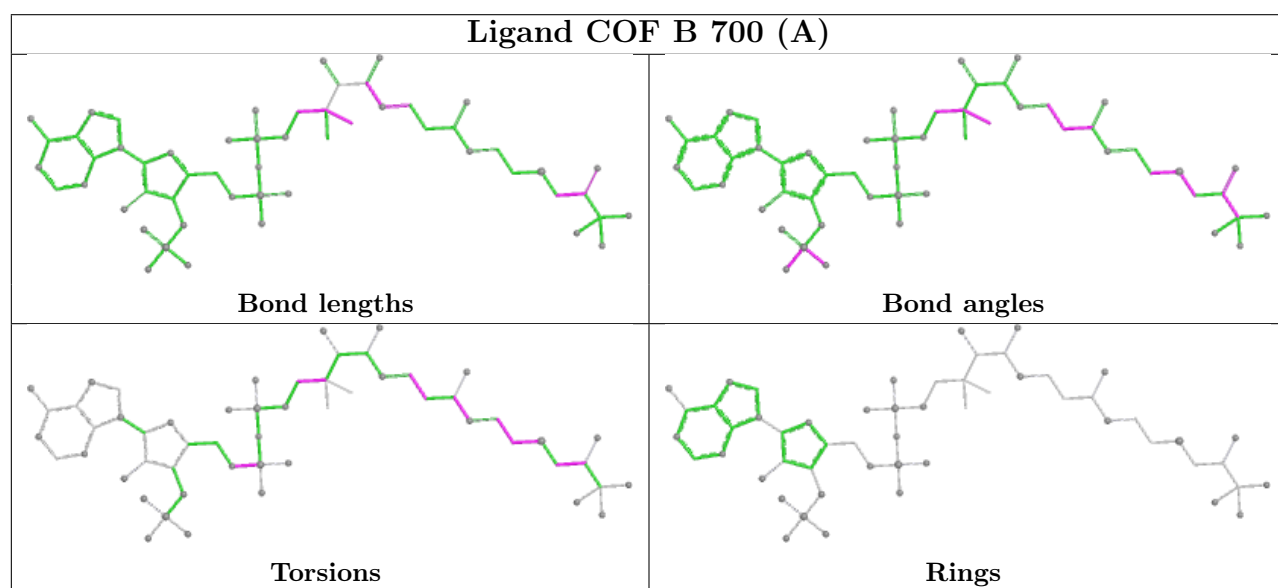
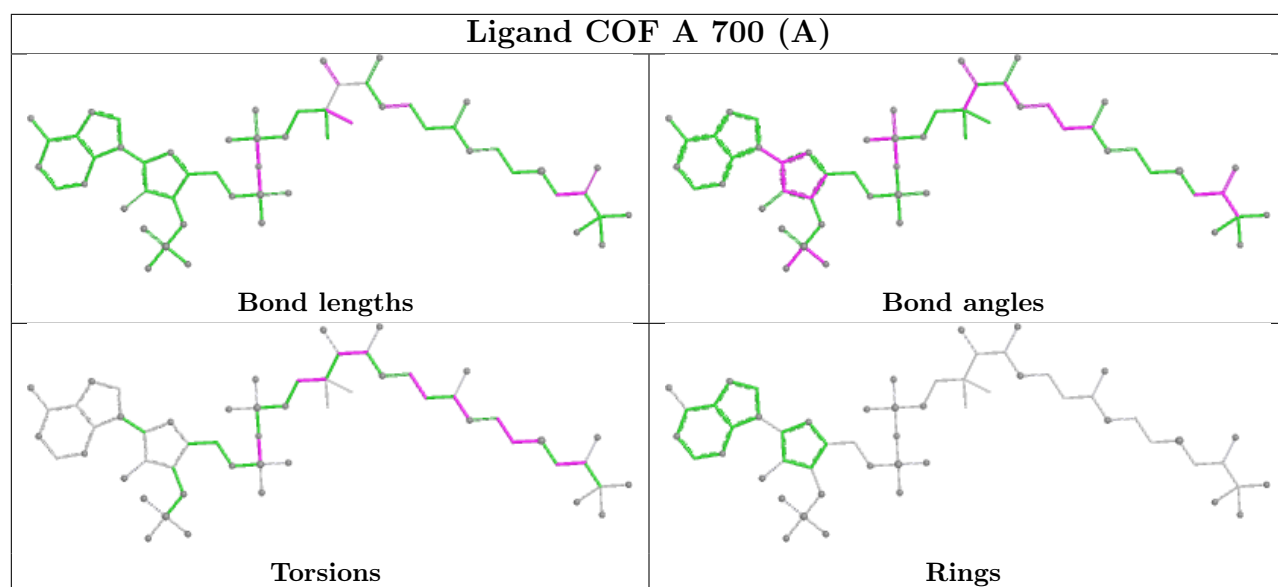
Mol	Chain	Res	Type	Atoms
2	B	700[B]	COF	C5B-O5B-P1A-O1A
3	B	701	CIT	C2-C3-C6-O5
3	B	701	CIT	C4-C3-C6-O5
2	B	700[B]	COF	S1P-C2P-C3P-N4P
2	B	700[A]	COF	C3P-C2P-S1P-C1I
3	B	701	CIT	O7-C3-C6-O5
2	B	700[A]	COF	S1P-C1I-C2I-C3I
2	A	700[A]	COF	C3P-C2P-S1P-C1I
2	A	700[A]	COF	CDP-CBP-CCP-O6A
2	A	700[B]	COF	CDP-CBP-CCP-O6A
2	B	700[A]	COF	CAP-CBP-CCP-O6A
2	B	700[B]	COF	CAP-CBP-CCP-O6A
2	A	700[A]	COF	P2A-O3A-P1A-O2A
2	A	700[B]	COF	P2A-O3A-P1A-O2A

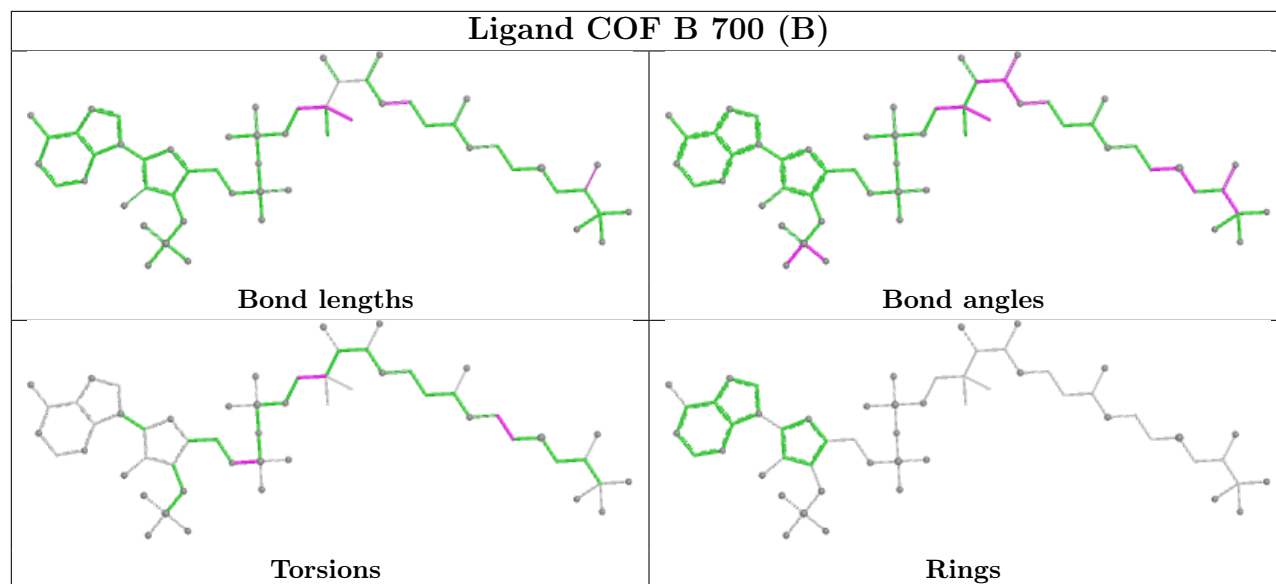
There are no ring outliers.

6 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	700[A]	COF	8	0
3	A	701	CIT	2	0
3	B	701	CIT	2	0
2	B	700[A]	COF	12	0
2	A	700[B]	COF	1	0
2	B	700[B]	COF	5	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	437/437 (100%)	-0.67	5 (1%) 78 79	1, 13, 51, 95	0
1	B	434/437 (99%)	-0.64	6 (1%) 73 74	2, 14, 53, 74	0
All	All	871/874 (99%)	-0.66	11 (1%) 75 76	1, 14, 53, 95	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	306	TRP	3.9
1	A	1	ALA	3.3
1	A	294	ALA	3.2
1	B	4	THR	3.0
1	B	294	ALA	3.0
1	A	2	SER	2.8
1	A	435	ALA	2.6
1	B	82	GLY	2.5
1	B	435	ALA	2.5
1	A	295	ASP	2.3
1	B	304	TYR	2.2

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 ⓘ

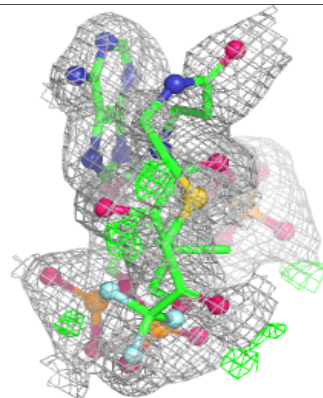
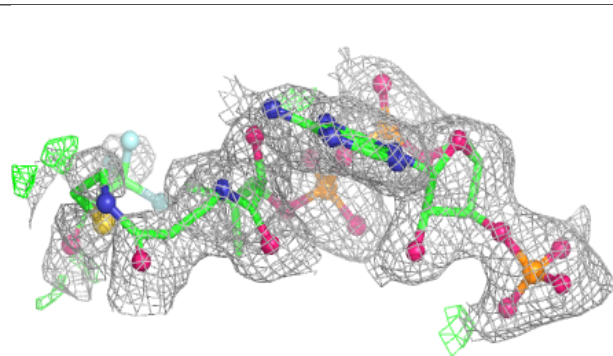
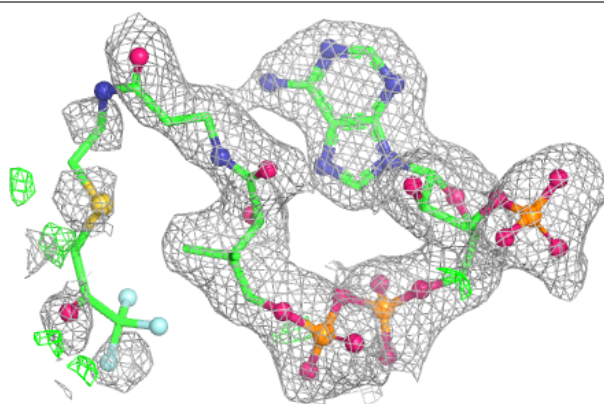
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COF	B	700[A]	55/55	0.97	0.10	1,23,100,100	16
2	COF	B	700[B]	55/55	0.97	0.10	1,21,100,100	16
2	COF	A	700[A]	55/55	0.98	0.07	1,13,74,100	16
2	COF	A	700[B]	55/55	0.98	0.07	1,13,81,100	16
3	CIT	A	701	13/13	0.98	0.05	1,4,29,46	0
3	CIT	B	701	13/13	0.99	0.04	1,5,26,29	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.

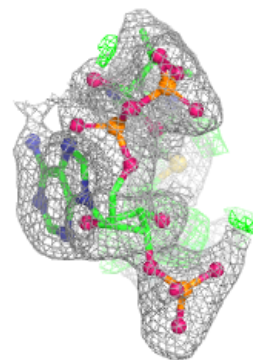
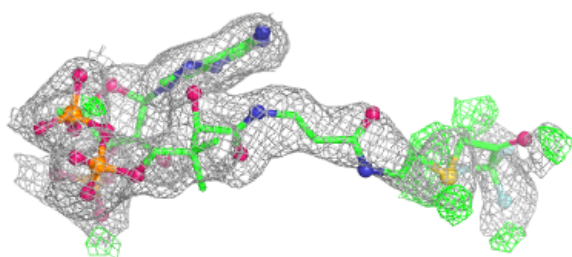
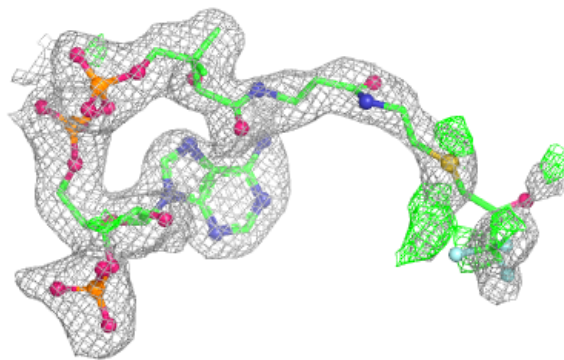
Electron density around COF B 700 (A):

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



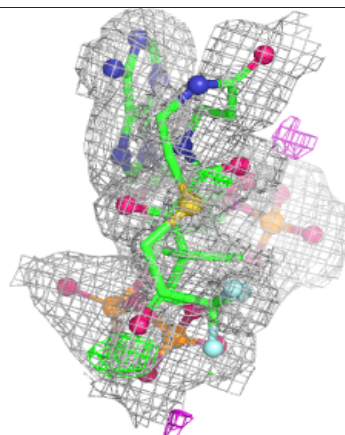
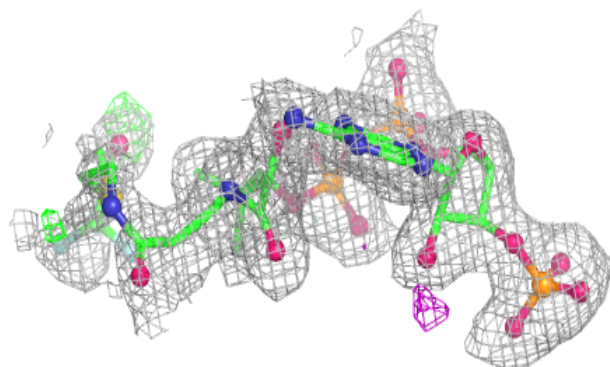
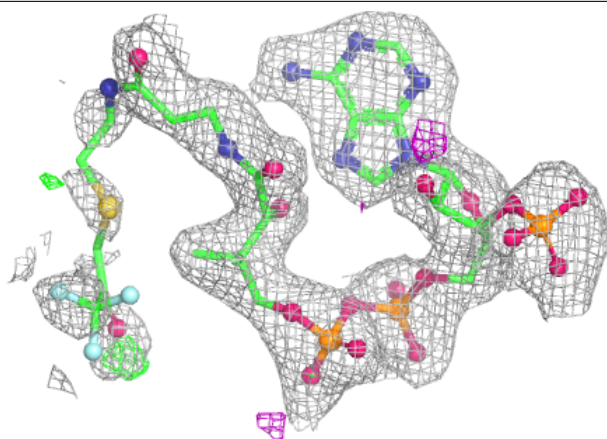
Electron density around COF B 700 (B):

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



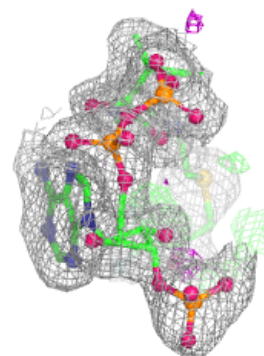
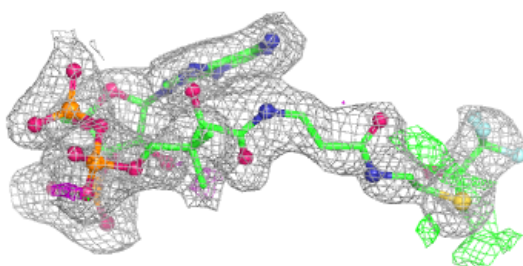
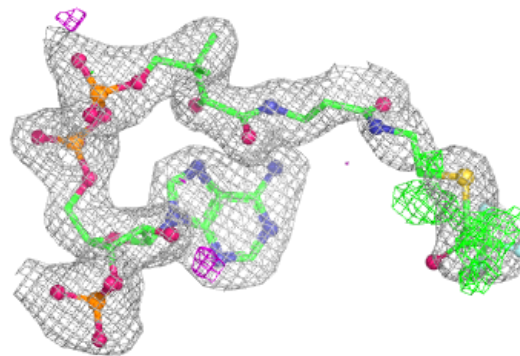
Electron density around COF A 700 (A):

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



Electron density around COF A 700 (B):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.