Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:00 PM GMT

PDB ID	:	1DLV
Title	:	BIOSYNTHETIC THIOLASE FROM ZOOGLOEA RAMIGERA IN COMPLEX WITH COA
Authors	:	Modis, Y.; Wierenga, R.K.
Deposited on	:	1999-12-12
Resolution	:	2.29 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

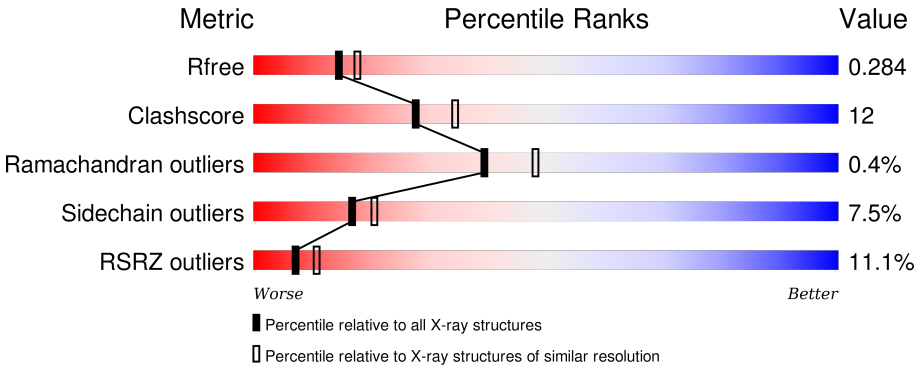
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	% 57% 34% 8% ·
1	B	389	% 61% 30% 7% ·
1	C	389	14% 70% 24% 5%
1	D	389	28% 69% 26% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12192 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.

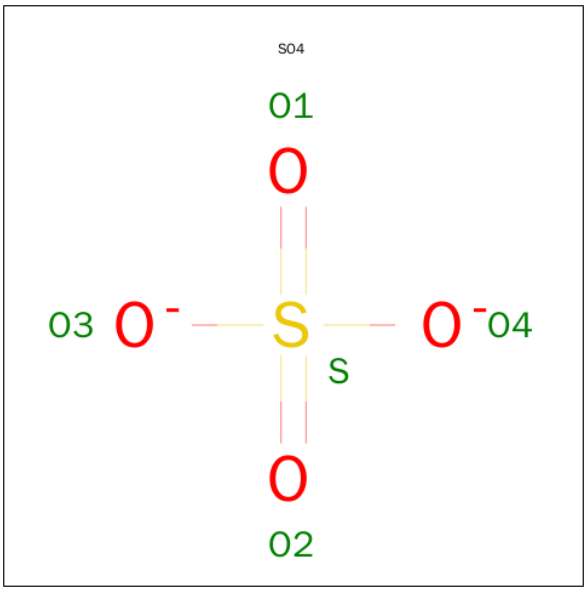
- Molecule 1 is a protein called BIOSYNTHETIC THIOLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	B	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	C	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			
1	D	389	Total	C	N	O	S	0	0	0
			2813	1746	509	537	21			

There are 8 discrepancies between the modelled and reference sequences:

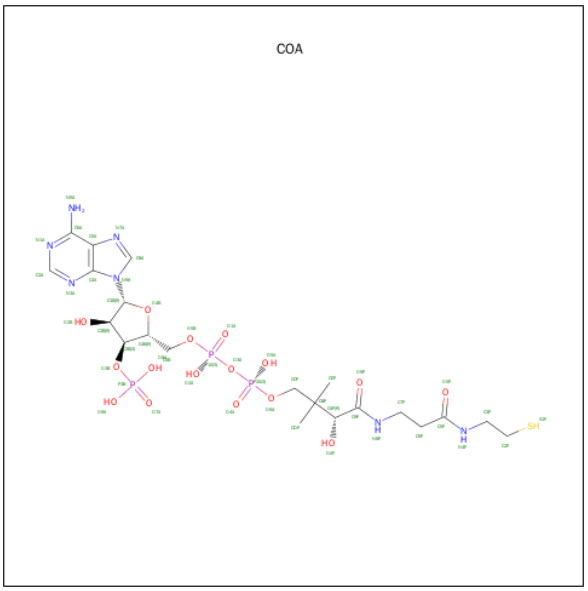
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	INSERTION	UNP P07097
A	129	ARG	ALA	CONFLICT	UNP P07097
B	11	ALA	-	INSERTION	UNP P07097
B	129	ARG	ALA	CONFLICT	UNP P07097
C	11	ALA	-	INSERTION	UNP P07097
C	129	ARG	ALA	CONFLICT	UNP P07097
D	11	ALA	-	INSERTION	UNP P07097
D	129	ARG	ALA	CONFLICT	UNP P07097

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is COENZYME A (three-letter code: 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.

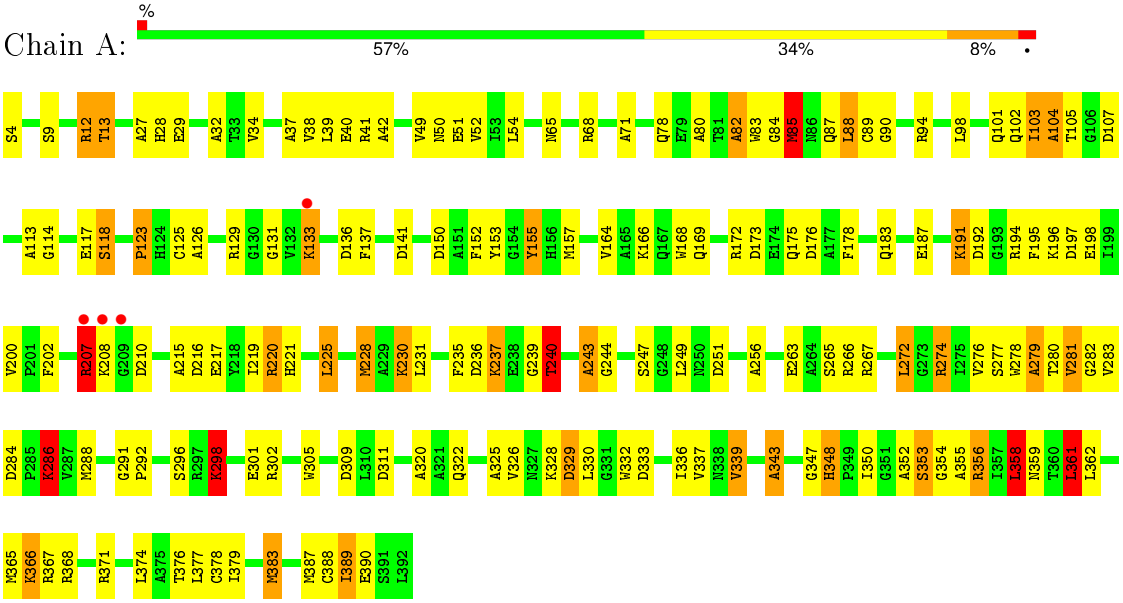
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	287	Total	O	1	0
			287	287		
4	B	276	Total	O	3	0
			276	276		
4	C	96	Total	O	0	0
			96	96		
4	D	59	Total	O	1	0
			59	59		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

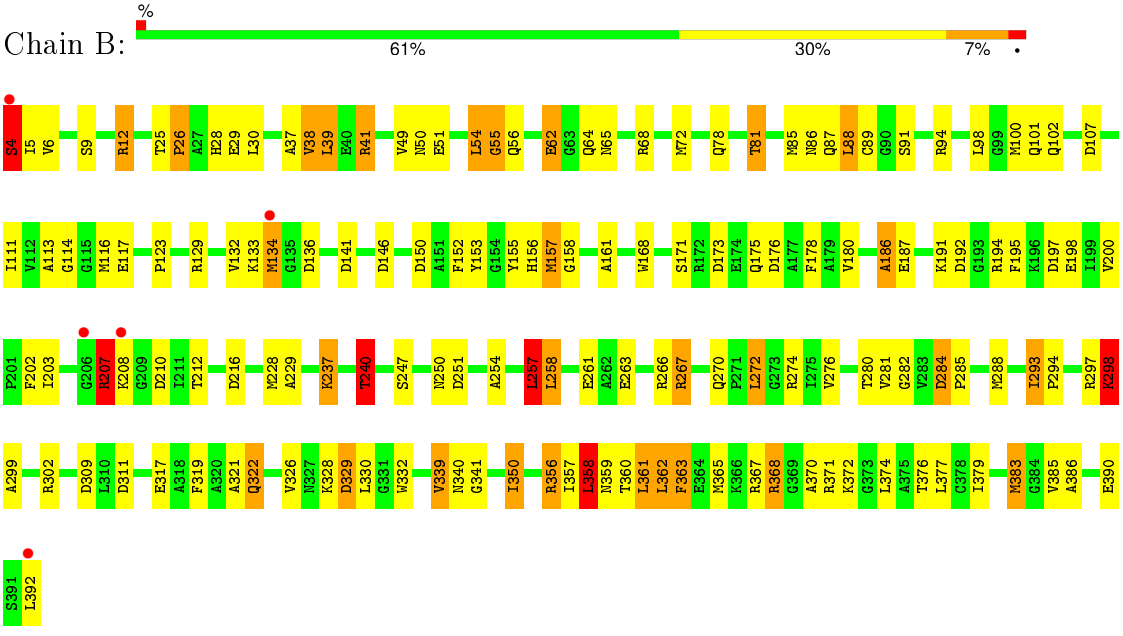
- Molecule 1: BIOSYNTHETIC THIOLASE

Chain A:



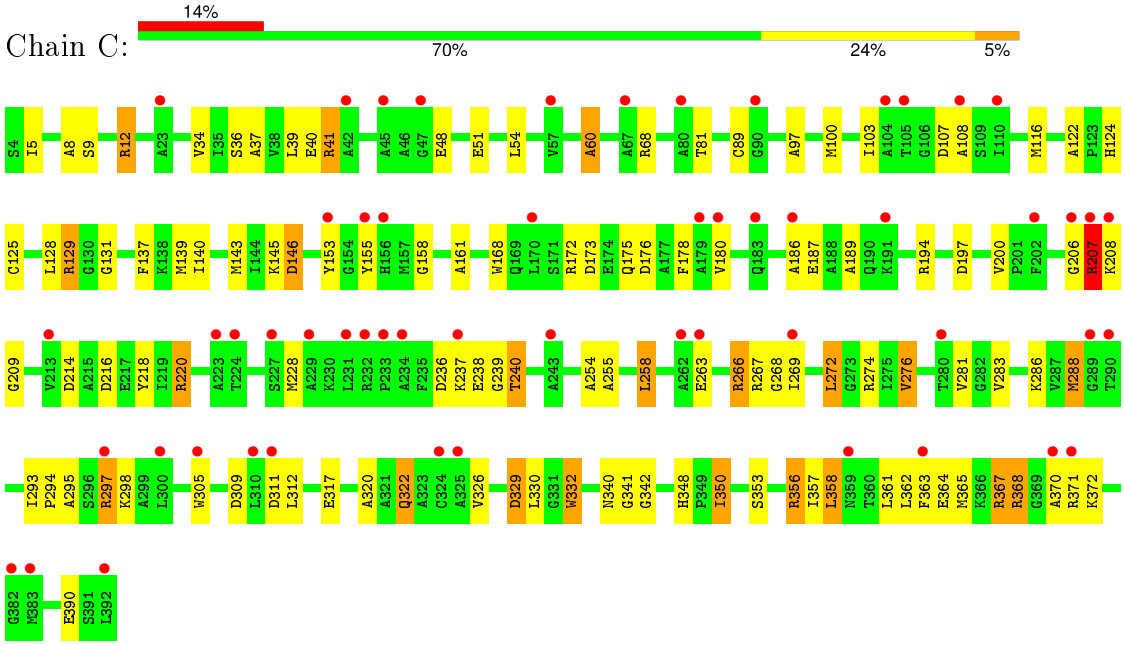
- Molecule 1: BIOSYNTHETIC THIOLASE

Chain B:



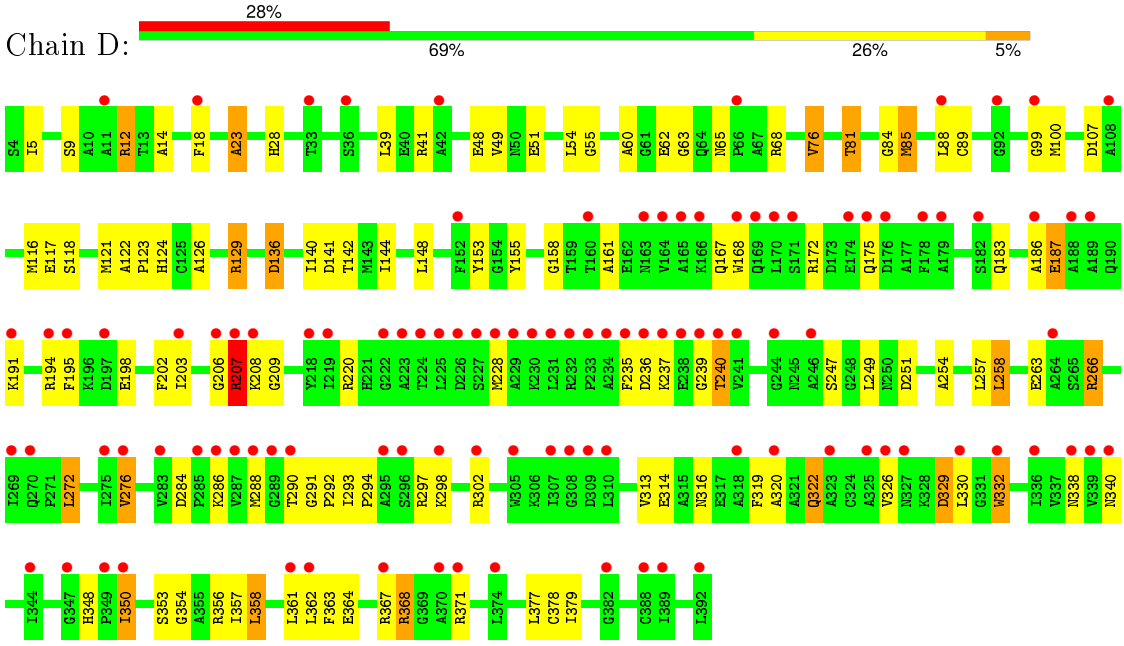
• Molecule 1: BIOSYNTHETIC THIOLASE

Chain C:



• Molecule 1: BIOSYNTHETIC THIOLASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	84.82Å 79.30Å 149.98Å 90.00° 93.49° 90.00°	Depositor
Resolution (Å)	30.00 – 2.29 29.51 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.0 (30.00-2.29) 82.2 (29.51-2.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.05 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.242 , 0.293 0.238 , 0.284	Depositor DCC
R_{free} test set	4441 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	19.1	Xtriage
Anisotropy	0.727	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 58.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Outliers	0 of 99352 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	12192	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: COA, SO4

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	1.24	7/2854 (0.2%)	2.64	181/3853 (4.7%)
1	B	1.22	7/2854 (0.2%)	2.32	142/3853 (3.7%)
1	C	0.61	0/2854	1.67	46/3853 (1.2%)
1	D	0.60	0/2854	1.71	55/3853 (1.4%)
All	All	0.97	14/11416 (0.1%)	2.12	424/15412 (2.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	54	LEU	C-N	20.46	1.69	1.33
1	A	278	TRP	CZ2-CH2	-12.08	1.14	1.37
1	A	118	SER	CA-CB	11.31	1.70	1.52
1	A	278	TRP	CZ3-CH2	10.95	1.57	1.40
1	A	90	GLY	N-CA	8.92	1.59	1.46
1	A	278	TRP	CE3-CZ3	-8.52	1.24	1.38
1	B	195	PHE	CE2-CZ	7.67	1.51	1.37
1	B	55	GLY	N-CA	-6.56	1.36	1.46
1	B	367	ARG	NE-CZ	-5.65	1.25	1.33
1	B	367	ARG	CZ-NH2	5.61	1.40	1.33
1	A	68	ARG	NE-CZ	5.51	1.40	1.33
1	B	194	ARG	C-O	5.42	1.33	1.23
1	B	356	ARG	CG-CD	-5.05	1.39	1.51
1	A	80	ALA	N-CA	5.00	1.56	1.46

All (424) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	ARG	NE-CZ-NH1	22.74	131.67	120.30
1	A	367	ARG	NE-CZ-NH1	22.35	131.47	120.30
1	A	251	ASP	CB-CG-OD1	21.21	137.39	118.30
1	C	266	ARG	NE-CZ-NH2	20.53	130.57	120.30
1	D	329	ASP	CB-CG-OD2	20.18	136.46	118.30
1	D	117	GLU	OE1-CD-OE2	-18.75	100.81	123.30
1	A	216	ASP	CB-CG-OD1	18.41	134.87	118.30
1	A	274	ARG	CD-NE-CZ	18.03	148.84	123.60
1	B	367	ARG	NE-CZ-NH1	17.75	129.17	120.30
1	B	216	ASP	CB-CG-OD1	17.35	133.91	118.30
1	A	371	ARG	NE-CZ-NH1	17.21	128.91	120.30
1	A	356	ARG	NE-CZ-NH1	-17.01	111.79	120.30
1	B	266	ARG	NE-CZ-NH2	16.78	128.69	120.30
1	B	367	ARG	NE-CZ-NH2	-16.33	112.13	120.30
1	A	12	ARG	NE-CZ-NH1	16.25	128.43	120.30
1	B	41	ARG	CD-NE-CZ	16.18	146.25	123.60
1	A	94	ARG	NE-CZ-NH2	-16.03	112.28	120.30
1	A	333	ASP	CB-CG-OD1	15.10	131.89	118.30
1	B	356	ARG	NE-CZ-NH1	-15.01	112.80	120.30
1	A	51	GLU	OE1-CD-OE2	14.76	141.02	123.30
1	D	266	ARG	NE-CZ-NH2	14.76	127.68	120.30
1	B	266	ARG	CD-NE-CZ	14.48	143.87	123.60
1	A	368	ARG	NE-CZ-NH1	14.28	127.44	120.30
1	D	48	GLU	OE1-CD-OE2	-14.25	106.20	123.30
1	A	178	PHE	CB-CG-CD2	-14.22	110.85	120.80
1	A	228	MET	CA-CB-CG	14.06	137.19	113.30
1	B	368	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	A	194	ARG	NE-CZ-NH1	13.82	127.21	120.30
1	A	129	ARG	NE-CZ-NH1	13.59	127.09	120.30
1	B	155	TYR	CB-CG-CD2	13.16	128.89	121.00
1	B	356	ARG	NE-CZ-NH2	-13.00	113.80	120.30
1	A	41	ARG	NE-CZ-NH2	12.93	126.77	120.30
1	A	284	ASP	CB-CG-OD1	12.84	129.86	118.30
1	A	94	ARG	CD-NE-CZ	12.79	141.51	123.60
1	A	195	PHE	CB-CG-CD2	-12.77	111.86	120.80
1	B	356	ARG	NH1-CZ-NH2	12.59	133.25	119.40
1	B	367	ARG	CD-NE-CZ	12.55	141.18	123.60
1	B	317	GLU	OE1-CD-OE2	12.55	138.36	123.30
1	A	178	PHE	CB-CG-CD1	12.47	129.53	120.80
1	B	363	PHE	CB-CG-CD1	12.28	129.40	120.80
1	A	390	GLU	OE1-CD-OE2	12.04	137.75	123.30
1	B	68	ARG	NE-CZ-NH2	11.83	126.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	41	ARG	NE-CZ-NH2	-11.81	114.40	120.30
1	D	367	ARG	NE-CZ-NH1	11.60	126.10	120.30
1	B	309	ASP	CB-CG-OD2	11.54	128.69	118.30
1	A	150	ASP	CB-CG-OD2	11.25	128.42	118.30
1	A	217	GLU	OE1-CD-OE2	-11.22	109.84	123.30
1	B	153	TYR	CB-CG-CD2	11.15	127.69	121.00
1	C	172	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	A	192	ASP	CB-CG-OD1	10.88	128.10	118.30
1	A	4	SER	CA-CB-OG	10.82	140.43	111.20
1	C	356	ARG	NE-CZ-NH2	10.75	125.67	120.30
1	D	302	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	D	329	ASP	OD1-CG-OD2	-10.72	102.93	123.30
1	A	195	PHE	CB-CG-CD1	10.62	128.24	120.80
1	B	266	ARG	NH1-CZ-NH2	-10.52	107.82	119.40
1	B	150	ASP	CB-CG-OD2	-10.34	109.00	118.30
1	A	172	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	A	42	ALA	N-CA-CB	-10.32	95.64	110.10
1	B	68	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	A	368	ARG	NE-CZ-NH2	-10.12	115.24	120.30
1	A	207	ARG	CD-NE-CZ	10.10	137.73	123.60
1	B	68	ARG	NH1-CZ-NH2	-10.01	108.39	119.40
1	B	192	ASP	CB-CG-OD1	9.98	127.28	118.30
1	A	197	ASP	CB-CG-OD1	-9.96	109.34	118.30
1	B	386	ALA	CB-CA-C	9.89	124.94	110.10
1	A	266	ARG	NE-CZ-NH1	-9.86	115.37	120.30
1	D	41	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	A	371	ARG	CD-NE-CZ	9.81	137.34	123.60
1	C	207	ARG	CD-NE-CZ	9.76	137.27	123.60
1	A	117	GLU	OE1-CD-OE2	9.74	134.99	123.30
1	B	41	ARG	NE-CZ-NH1	-9.64	115.48	120.30
1	B	361	LEU	CB-CG-CD2	9.52	127.18	111.00
1	B	141	ASP	CB-CG-OD2	-9.50	109.75	118.30
1	D	367	ARG	NE-CZ-NH2	-9.45	115.57	120.30
1	D	12	ARG	NE-CZ-NH1	-9.42	115.59	120.30
1	A	173	ASP	CB-CG-OD1	9.40	126.76	118.30
1	C	216	ASP	CB-CG-OD1	9.40	126.76	118.30
1	A	302	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	274	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	B	178	PHE	CB-CG-CD2	9.29	127.30	120.80
1	B	297	ARG	CD-NE-CZ	9.28	136.59	123.60
1	A	367	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	B	146	ASP	CB-CG-OD2	9.17	126.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	363	PHE	CB-CG-CD2	9.17	127.22	120.80
1	A	267	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	B	302	ARG	NE-CZ-NH2	-9.11	115.74	120.30
1	C	367	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	D	284	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	D	207	ARG	CD-NE-CZ	8.99	136.18	123.60
1	A	12	ARG	NH1-CZ-NH2	-8.98	109.52	119.40
1	C	266	ARG	NH1-CZ-NH2	-8.87	109.64	119.40
1	D	48	GLU	CG-CD-OE2	8.87	136.04	118.30
1	B	81	THR	CA-CB-CG2	8.86	124.81	112.40
1	B	356	ARG	CG-CD-NE	8.85	130.38	111.80
1	A	117	GLU	CG-CD-OE1	-8.84	100.61	118.30
1	A	4	SER	N-CA-CB	8.82	123.74	110.50
1	B	251	ASP	CB-CG-OD1	8.61	126.05	118.30
1	B	129	ARG	NE-CZ-NH1	-8.59	116.00	120.30
1	B	94	ARG	CD-NE-CZ	8.57	135.60	123.60
1	A	65	ASN	OD1-CG-ND2	-8.54	102.26	121.90
1	C	267	ARG	NE-CZ-NH2	-8.53	116.04	120.30
1	B	141	ASP	CB-CG-OD1	8.47	125.92	118.30
1	A	68	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	B	207	ARG	CD-NE-CZ	8.40	135.35	123.60
1	A	240	THR	N-CA-CB	-8.35	94.43	110.30
1	A	266	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	D	68	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	A	266	ARG	NH1-CZ-NH2	8.23	128.45	119.40
1	D	172	ARG	NE-CZ-NH2	-8.19	116.20	120.30
1	B	329	ASP	CB-CG-OD2	8.19	125.67	118.30
1	D	194	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	C	220	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	107	ASP	CB-CG-OD1	-8.06	111.05	118.30
1	D	12	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	B	284	ASP	CB-CG-OD2	-8.03	111.07	118.30
1	A	210	ASP	CB-CG-OD2	-8.02	111.08	118.30
1	B	194	ARG	CD-NE-CZ	8.02	134.82	123.60
1	C	48	GLU	OE1-CD-OE2	-8.01	113.69	123.30
1	C	60	ALA	CB-CA-C	8.00	122.10	110.10
1	B	302	ARG	CD-NE-CZ	7.93	134.70	123.60
1	A	235	PHE	CB-CG-CD2	-7.86	115.30	120.80
1	B	339	VAL	CG1-CB-CG2	7.83	123.44	110.90
1	B	321	ALA	CB-CA-C	-7.68	98.57	110.10
1	D	136	ASP	CB-CG-OD1	-7.68	111.39	118.30
1	A	207	ARG	NE-CZ-NH1	7.66	124.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	129	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	B	152	PHE	CB-CG-CD1	-7.62	115.47	120.80
1	A	89	CYS	CA-C-O	-7.59	104.15	120.10
1	B	363	PHE	CB-CG-CD2	-7.55	115.51	120.80
1	B	155	TYR	CB-CG-CD1	-7.55	116.47	121.00
1	C	297	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	C	146	ASP	CB-CG-OD1	-7.45	111.60	118.30
1	C	368	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	B	186	ALA	CB-CA-C	7.42	121.23	110.10
1	A	251	ASP	CB-CG-OD2	-7.39	111.64	118.30
1	C	297	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	280	THR	CA-CB-CG2	-7.35	102.11	112.40
1	A	28	HIS	N-CA-CB	7.34	123.81	110.60
1	B	302	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	D	363	PHE	CD1-CG-CD2	-7.32	108.78	118.30
1	B	178	PHE	CD1-CG-CD2	-7.31	108.79	118.30
1	C	173	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	216	ASP	OD1-CG-OD2	-7.30	109.42	123.30
1	A	83	TRP	CG-CD2-CE3	7.30	140.47	133.90
1	A	329	ASP	CB-CG-OD1	7.26	124.83	118.30
1	A	49	VAL	CA-CB-CG1	7.24	121.77	110.90
1	A	129	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	339	VAL	N-CA-CB	-7.24	95.57	111.50
1	A	102	GLN	OE1-CD-NE2	7.19	138.43	121.90
1	A	29	GLU	N-CA-CB	7.17	123.50	110.60
1	D	207	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	D	12	ARG	CD-NE-CZ	7.12	133.57	123.60
1	B	368	ARG	NH1-CZ-NH2	7.08	127.19	119.40
1	A	278	TRP	CZ3-CH2-CZ2	7.07	130.08	121.60
1	D	297	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	D	367	ARG	CD-NE-CZ	7.05	133.47	123.60
1	A	85	MET	CB-CG-SD	7.04	133.53	112.40
1	B	87	GLN	N-CA-CB	7.04	123.26	110.60
1	C	266	ARG	CD-NE-CZ	7.04	133.45	123.60
1	B	192	ASP	CA-C-N	7.03	130.25	116.20
1	B	371	ARG	CG-CD-NE	7.01	126.53	111.80
1	B	280	THR	CA-CB-CG2	-7.00	102.60	112.40
1	B	202	PHE	CB-CG-CD1	-6.97	115.92	120.80
1	A	235	PHE	CB-CG-CD1	6.97	125.68	120.80
1	D	319	PHE	CB-CG-CD2	6.97	125.68	120.80
1	B	26	PRO	O-C-N	-6.96	111.57	122.70
1	B	38	VAL	CA-CB-CG2	6.94	121.31	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	358	LEU	CA-CB-CG	6.92	131.23	115.30
1	B	41	ARG	NH1-CZ-NH2	6.91	127.00	119.40
1	B	376	THR	CA-CB-CG2	-6.87	102.78	112.40
1	A	104	ALA	N-CA-CB	-6.86	100.50	110.10
1	B	12	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	C	356	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	C	12	ARG	CD-NE-CZ	6.78	133.10	123.60
1	A	194	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	88	LEU	O-C-N	-6.78	111.85	122.70
1	D	368	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	B	94	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	C	48	GLU	CG-CD-OE2	6.73	131.77	118.30
1	A	49	VAL	CA-C-O	-6.73	105.97	120.10
1	C	68	ARG	CD-NE-CZ	6.70	132.98	123.60
1	C	348	HIS	N-CA-CB	-6.69	98.56	110.60
1	A	89	CYS	C-N-CA	-6.68	108.27	122.30
1	A	216	ASP	OD1-CG-OD2	-6.68	110.61	123.30
1	A	155	TYR	CB-CG-CD2	6.66	125.00	121.00
1	A	239	GLY	CA-C-O	6.65	132.57	120.60
1	B	136	ASP	CB-CG-OD1	-6.65	112.32	118.30
1	D	194	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	A	157	MET	CG-SD-CE	6.62	110.79	100.20
1	B	339	VAL	N-CA-CB	-6.61	96.97	111.50
1	B	274	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	D	302	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	173	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	278	TRP	CE3-CZ3-CH2	-6.54	114.01	121.20
1	A	231	LEU	O-C-N	6.53	133.15	122.70
1	A	251	ASP	OD1-CG-OD2	-6.50	110.94	123.30
1	A	356	ARG	NH1-CZ-NH2	6.46	126.51	119.40
1	B	240	THR	N-CA-CB	-6.46	98.03	110.30
1	A	243	ALA	N-CA-CB	6.45	119.14	110.10
1	B	178	PHE	CE1-CZ-CE2	-6.45	108.38	120.00
1	A	68	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	A	230	LYS	N-CA-CB	-6.44	99.01	110.60
1	D	319	PHE	CD1-CG-CD2	-6.42	109.96	118.30
1	B	4	SER	N-CA-CB	6.41	120.12	110.50
1	B	197	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	40	GLU	CB-CG-CD	6.39	131.44	114.20
1	A	309	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	B	266	ARG	NE-CZ-NH1	6.37	123.49	120.30
1	A	343	ALA	N-CA-CB	6.36	119.01	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	88	LEU	O-C-N	-6.35	112.55	122.70
1	B	129	ARG	NH1-CZ-NH2	6.34	126.38	119.40
1	D	107	ASP	CB-CG-OD2	6.33	124.00	118.30
1	A	355	ALA	N-CA-CB	6.33	118.96	110.10
1	B	257	LEU	CB-CG-CD2	6.33	121.75	111.00
1	A	42	ALA	O-C-N	-6.31	112.47	123.20
1	A	191	LYS	CD-CE-NZ	6.30	126.20	111.70
1	A	89	CYS	O-C-N	6.29	133.89	123.20
1	C	214	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	366	LYS	CD-CE-NZ	-6.27	97.28	111.70
1	A	136	ASP	CB-CG-OD2	6.26	123.94	118.30
1	A	32	ALA	N-CA-CB	6.22	118.81	110.10
1	A	107	ASP	CB-CG-OD1	-6.20	112.72	118.30
1	D	68	ARG	NH1-CZ-NH2	-6.18	112.60	119.40
1	B	274	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	D	141	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	217	GLU	CG-CD-OE2	6.17	130.63	118.30
1	D	202	PHE	CB-CG-CD1	-6.17	116.48	120.80
1	A	266	ARG	CG-CD-NE	-6.17	98.85	111.80
1	A	38	VAL	CA-C-O	6.16	133.04	120.10
1	A	389	ILE	O-C-N	6.16	132.55	122.70
1	A	296	SER	N-CA-CB	6.14	119.70	110.50
1	B	6	VAL	O-C-N	6.13	132.51	122.70
1	A	228	MET	CG-SD-CE	-6.13	90.39	100.20
1	B	72	MET	CA-CB-CG	-6.12	102.90	113.30
1	B	319	PHE	CB-CG-CD2	6.11	125.08	120.80
1	B	4	SER	CA-C-N	6.10	130.63	117.20
1	B	261	GLU	OE1-CD-OE2	-6.10	115.98	123.30
1	B	284	ASP	CB-CG-OD1	6.09	123.79	118.30
1	B	370	ALA	N-CA-CB	6.09	118.63	110.10
1	A	274	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
1	B	29	GLU	N-CA-CB	6.04	121.48	110.60
1	A	68	ARG	O-C-N	-6.03	113.05	122.70
1	B	299	ALA	N-CA-CB	6.03	118.53	110.10
1	A	155	TYR	O-C-N	6.02	132.33	122.70
1	A	320	ALA	N-CA-CB	5.98	118.48	110.10
1	A	103	ILE	CA-C-O	-5.98	107.55	120.10
1	A	256	ALA	CB-CA-C	-5.97	101.14	110.10
1	A	367	ARG	NH1-CZ-NH2	-5.96	112.84	119.40
1	D	368	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	277	SER	N-CA-CB	5.94	119.42	110.50
1	C	274	ARG	NE-CZ-NH2	5.94	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	218	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	A	176	ASP	O-C-N	-5.93	113.20	122.70
1	A	152	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	C	139	MET	N-CA-C	-5.93	95.00	111.00
1	B	192	ASP	OD1-CG-OD2	-5.92	112.05	123.30
1	B	41	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	A	215	ALA	CB-CA-C	5.91	118.96	110.10
1	B	41	ARG	CG-CD-NE	5.88	124.15	111.80
1	A	202	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	A	361	LEU	CB-CG-CD2	5.85	120.94	111.00
1	A	51	GLU	CG-CD-OE2	-5.84	106.61	118.30
1	A	82	ALA	N-CA-CB	-5.84	101.92	110.10
1	A	283	VAL	CA-CB-CG1	5.83	119.65	110.90
1	B	210	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	A	65	ASN	CB-CG-ND2	5.83	130.69	116.70
1	D	276	VAL	CB-CA-C	5.80	122.42	111.40
1	C	276	VAL	CA-CB-CG2	5.80	119.60	110.90
1	A	164	VAL	CA-CB-CG2	-5.79	102.22	110.90
1	C	60	ALA	N-CA-CB	-5.78	102.00	110.10
1	A	347	GLY	C-N-CA	5.77	136.12	121.70
1	A	267	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	A	339	VAL	O-C-N	-5.74	113.52	122.70
1	D	12	ARG	CG-CD-NE	5.74	123.85	111.80
1	B	356	ARG	CB-CG-CD	-5.72	96.71	111.60
1	A	249	LEU	O-C-N	-5.72	113.54	122.70
1	A	198	GLU	O-C-N	-5.72	113.55	122.70
1	C	367	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	B	150	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	117	GLU	CG-CD-OE1	5.71	129.71	118.30
1	A	279	ALA	N-CA-CB	5.69	118.07	110.10
1	A	231	LEU	CA-C-O	-5.68	108.17	120.10
1	C	329	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	85	MET	CB-CA-C	5.67	121.75	110.40
1	D	85	MET	CA-CB-CG	5.67	122.94	113.30
1	A	114	GLY	CA-C-O	5.67	130.81	120.60
1	A	228	MET	N-CA-CB	-5.66	100.41	110.60
1	B	319	PHE	CG-CD2-CE2	5.66	127.03	120.80
1	B	383	MET	O-C-N	5.65	132.81	123.20
1	C	12	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	A	34	VAL	CA-CB-CG2	-5.64	102.44	110.90
1	C	368	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	D	129	ARG	CG-CD-NE	-5.64	99.95	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	281	VAL	CA-CB-CG2	5.62	119.33	110.90
1	D	136	ASP	OD1-CG-OD2	5.62	133.99	123.30
1	D	76	VAL	CG1-CB-CG2	-5.62	101.91	110.90
1	A	88	LEU	CA-C-N	5.61	129.54	117.20
1	C	274	ARG	CD-NE-CZ	5.60	131.44	123.60
1	A	325	ALA	N-CA-CB	-5.60	102.26	110.10
1	B	12	ARG	CG-CD-NE	5.60	123.55	111.80
1	B	129	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	94	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	A	195	PHE	O-C-N	-5.58	113.76	122.70
1	D	117	GLU	CG-CD-OE2	5.58	129.47	118.30
1	B	30	LEU	CB-CG-CD2	5.58	120.49	111.00
1	B	56	GLN	OE1-CD-NE2	5.58	134.74	121.90
1	A	336	ILE	O-C-N	-5.58	113.78	122.70
1	A	353	SER	CA-CB-OG	-5.57	96.17	111.20
1	D	60	ALA	CB-CA-C	5.56	118.44	110.10
1	A	191	LYS	N-CA-CB	5.55	120.59	110.60
1	A	98	LEU	O-C-N	-5.55	113.77	123.20
1	B	280	THR	OG1-CB-CG2	5.54	122.74	110.00
1	B	357	ILE	CA-C-N	5.54	129.38	117.20
1	A	220	ARG	N-CA-CB	5.53	120.56	110.60
1	B	153	TYR	CD1-CG-CD2	-5.53	111.82	117.90
1	B	298	LYS	CA-CB-CG	5.53	125.56	113.40
1	B	153	TYR	CG-CD2-CE2	5.53	125.72	121.30
1	B	12	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	C	295	ALA	CB-CA-C	5.52	118.38	110.10
1	D	363	PHE	CG-CD2-CE2	5.52	126.87	120.80
1	A	49	VAL	O-C-N	5.51	131.51	122.70
1	B	293	ILE	CG1-CB-CG2	-5.51	99.28	111.40
1	A	339	VAL	CA-CB-CG2	5.50	119.15	110.90
1	B	297	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	B	358	LEU	CB-CA-C	-5.50	99.75	110.20
1	C	172	ARG	CD-NE-CZ	5.49	131.29	123.60
1	B	155	TYR	CA-CB-CG	5.48	123.82	113.40
1	A	126	ALA	CB-CA-C	-5.47	101.89	110.10
1	D	251	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	49	VAL	CA-CB-CG1	5.47	119.10	110.90
1	A	302	ARG	CD-NE-CZ	5.47	131.25	123.60
1	A	27	ALA	N-CA-CB	-5.46	102.45	110.10
1	D	266	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
1	B	39	LEU	CA-C-O	5.45	131.55	120.10
1	C	36	SER	N-CA-CB	5.45	118.67	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	311	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	83	TRP	CE2-CD2-CG	-5.45	102.94	107.30
1	C	263	GLU	OE1-CD-OE2	5.44	129.83	123.30
1	C	194	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	284	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	54	LEU	C-N-CA	-5.43	110.89	122.30
1	D	23	ALA	CB-CA-C	-5.43	101.96	110.10
1	D	297	ARG	CD-NE-CZ	5.42	131.19	123.60
1	A	34	VAL	CA-C-O	-5.42	108.72	120.10
1	A	194	ARG	CG-CD-NE	5.42	123.18	111.80
1	B	362	LEU	O-C-N	5.42	131.38	122.70
1	D	85	MET	O-C-N	5.41	131.35	122.70
1	A	371	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	383	MET	CG-SD-CE	-5.40	91.56	100.20
1	B	107	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	78	GLN	CB-CG-CD	5.38	125.58	111.60
1	D	68	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	A	371	ARG	NH1-CZ-NH2	-5.37	113.49	119.40
1	A	123	PRO	N-CA-CB	-5.37	96.70	102.60
1	D	126	ALA	CB-CA-C	-5.35	102.07	110.10
1	B	62	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	A	337	VAL	CA-CB-CG1	5.34	118.91	110.90
1	A	172	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	13	THR	CA-CB-CG2	-5.30	104.98	112.40
1	B	250	ASN	CB-CG-ND2	5.30	129.43	116.70
1	A	187	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	B	117	GLU	CG-CD-OE2	5.29	128.87	118.30
1	C	297	ARG	CD-NE-CZ	5.29	131.00	123.60
1	B	4	SER	CA-C-O	-5.28	109.00	120.10
1	A	78	GLN	O-C-N	-5.27	114.27	122.70
1	B	385	VAL	CA-CB-CG1	5.27	118.80	110.90
1	A	352	ALA	CB-CA-C	-5.27	102.20	110.10
1	B	309	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	B	129	ARG	CD-NE-CZ	5.26	130.97	123.60
1	A	362	LEU	CB-CG-CD1	-5.26	102.05	111.00
1	A	286	LYS	N-CA-CB	5.25	120.06	110.60
1	B	322	GLN	CA-C-O	-5.25	109.07	120.10
1	A	187	GLU	CG-CD-OE1	5.24	128.79	118.30
1	A	102	GLN	CG-CD-NE2	-5.23	104.14	116.70
1	B	113	ALA	CA-C-O	-5.23	109.12	120.10
1	D	363	PHE	CE1-CZ-CE2	-5.22	110.61	120.00
1	A	219	ILE	CG1-CB-CG2	-5.21	99.94	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	172	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	113	ALA	N-CA-CB	5.20	117.38	110.10
1	A	137	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	B	114	GLY	O-C-N	-5.19	114.37	123.20
1	B	267	ARG	CD-NE-CZ	-5.19	116.34	123.60
1	A	333	ASP	OD1-CG-OD2	-5.18	113.45	123.30
1	A	183	GLN	O-C-N	-5.18	114.42	122.70
1	C	178	PHE	CB-CG-CD2	5.17	124.42	120.80
1	B	157	MET	CG-SD-CE	5.17	108.47	100.20
1	B	285	PRO	O-C-N	-5.16	114.44	122.70
1	D	81	THR	O-C-N	5.16	130.95	122.70
1	C	276	VAL	CB-CA-C	5.15	121.19	111.40
1	A	202	PHE	O-C-N	-5.14	114.47	122.70
1	A	80	ALA	CB-CA-C	5.14	117.81	110.10
1	A	298	LYS	CB-CA-C	5.13	120.66	110.40
1	B	276	VAL	CA-CB-CG2	5.13	118.59	110.90
1	A	311	ASP	CB-CG-OD1	5.13	122.92	118.30
1	C	283	VAL	CA-CB-CG1	5.13	118.59	110.90
1	A	87	GLN	N-CA-CB	5.13	119.83	110.60
1	A	13	THR	CA-CB-OG1	5.12	119.76	109.00
1	A	309	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	34	VAL	CA-CB-CG1	-5.12	103.22	110.90
1	A	141	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	217	GLU	CA-C-N	5.11	128.45	117.20
1	B	86	ASN	O-C-N	5.11	130.88	122.70
1	A	390	GLU	CG-CD-OE1	-5.11	108.08	118.30
1	D	14	ALA	CB-CA-C	5.11	117.76	110.10
1	A	166	LYS	O-C-N	-5.11	114.53	122.70
1	B	371	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	A	281	VAL	CA-CB-CG1	-5.08	103.28	110.90
1	A	71	ALA	N-CA-CB	-5.08	102.99	110.10
1	B	111	ILE	O-C-N	5.07	130.81	122.70
1	B	116	MET	CG-SD-CE	5.07	108.31	100.20
1	B	176	ASP	O-C-N	-5.07	114.59	122.70
1	B	94	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	367	ARG	O-C-N	-5.04	114.64	122.70
1	A	4	SER	CA-C-N	5.03	128.27	117.20
1	B	146	ASP	OD1-CG-OD2	-5.03	113.74	123.30
1	B	202	PHE	CB-CG-CD2	5.03	124.32	120.80
1	B	38	VAL	CG1-CB-CG2	-5.03	102.85	110.90
1	A	284	ASP	OD1-CG-OD2	-5.02	113.76	123.30
1	A	358	LEU	CB-CA-C	-5.02	100.66	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	243	ALA	CB-CA-C	-5.02	102.57	110.10
1	B	358	LEU	N-CA-CB	5.01	120.42	110.40
1	B	365	MET	CA-CB-CG	5.01	121.81	113.30
1	A	339	VAL	CG1-CB-CG2	5.00	118.91	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ILE	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2813	0	2818	68	0
1	B	2813	0	2819	72	0
1	C	2813	0	2819	64	0
1	D	2813	0	2819	70	0
2	A	15	0	0	0	0
2	B	15	0	0	1	0
3	A	48	0	32	4	0
3	B	48	0	31	2	0
3	C	48	0	31	0	0
3	D	48	0	31	2	0
4	A	287	0	0	13	2
4	B	276	0	0	17	1
4	C	96	0	0	14	0
4	D	59	0	0	10	0
All	All	12192	0	11400	269	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (269) 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:54:LEU:C	1:B:55:GLY:N	1.69	1.45
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.25	1.00
1:B:258:LEU:HG	4:B:5222:HOH:O	1.65	0.97
1:A:175:GLN:HE22	1:A:240:THR:CG2	1.79	0.95
1:B:356:ARG:HD2	1:B:356:ARG:C	1.92	0.89
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.38	0.86
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.12	0.84
1:D:326:VAL:HG22	4:D:4050:HOH:O	1.79	0.81
1:A:387:MET:SD	4:A:5168:HOH:O	2.37	0.80
1:A:247:SER:HB2	4:A:5232:HOH:O	1.83	0.79
1:A:225:LEU:HG	4:A:5206:HOH:O	1.81	0.79
1:B:54:LEU:C	1:B:55:GLY:CA	2.52	0.76
1:B:356:ARG:HD2	1:B:356:ARG:O	1.87	0.75
1:A:175:GLN:NE2	1:A:240:THR:HG23	1.99	0.75
1:B:5:ILE:HG13	1:B:100:MET:HG2	1.66	0.75
1:C:5:ILE:HG13	1:C:100:MET:HG2	1.66	0.74
1:A:12:ARG:HD2	1:A:356:ARG:HG2	1.70	0.73
1:B:186:ALA:HB2	1:B:341:GLY:HA3	1.71	0.72
1:C:175:GLN:HE22	1:C:240:THR:HG21	1.54	0.71
1:B:284:ASP:OD2	4:B:5117:HOH:O	2.09	0.71
1:C:175:GLN:HE22	1:C:240:THR:CG2	2.04	0.71
1:B:392:LEU:HD12	4:B:5137:HOH:O	1.89	0.71
1:C:238:GLU:O	4:C:3041:HOH:O	2.10	0.69
1:B:207:ARG:HH11	1:B:207:ARG:HG2	1.56	0.69
1:A:298:LYS:HA	1:A:298:LYS:NZ	2.07	0.69
1:B:134:MET:HG3	4:C:3009:HOH:O	1.92	0.69
1:A:298:LYS:HA	1:A:298:LYS:HZ2	1.57	0.69
1:D:272:LEU:HD21	4:D:4037:HOH:O	1.93	0.68
1:C:146:ASP:O	4:C:3025:HOH:O	2.11	0.67
1:D:258:LEU:HG	4:D:4027:HOH:O	1.94	0.67
1:D:290:THR:HA	4:D:4050:HOH:O	1.96	0.66
1:A:196:LYS:NZ	4:A:5227:HOH:O	2.29	0.65
1:A:279:ALA:HB1	1:A:298:LYS:HG3	1.78	0.65
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.32	0.64
1:C:107:ASP:OD2	4:C:3071:HOH:O	2.14	0.64
1:B:12:ARG:HD2	1:B:356:ARG:HG2	1.80	0.63
1:D:5:ILE:HG13	1:D:100:MET:HG2	1.80	0.63
1:B:372:LYS:HE3	4:B:5211:HOH:O	1.98	0.63
1:B:28:HIS:ND1	1:B:62:GLU:OE2	2.23	0.62
1:D:175:GLN:HE22	1:D:240:THR:CG2	2.13	0.62
1:C:268:GLY:HA2	4:C:3096:HOH:O	2.00	0.62
1:B:180:VAL:HG22	1:B:228:MET:HE3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:GLY:HA2	1:D:85:MET:O	1.99	0.62
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.13	0.61
1:A:348:HIS:HB3	4:A:5069:HOH:O	1.99	0.61
1:B:237:LYS:HB2	4:B:5138:HOH:O	2.01	0.61
1:A:281:VAL:HG12	1:A:282:GLY:N	2.15	0.60
1:D:207:ARG:HG2	1:D:207:ARG:HH11	1.63	0.60
1:A:101:GLN:O	1:A:105:THR:HG23	2.01	0.60
1:D:358:LEU:HD22	1:D:362:LEU:HG	1.84	0.59
1:D:258:LEU:N	1:D:258:LEU:HD22	2.17	0.59
1:A:228:MET:HE3	1:A:244:GLY:HA3	1.84	0.59
1:B:392:LEU:HB2	4:B:5137:HOH:O	2.02	0.59
1:B:88:LEU:HB2	1:B:379:ILE:HG23	1.85	0.58
1:A:343:ALA:O	4:A:5232:HOH:O	2.16	0.58
1:A:292:PRO:HG2	1:A:326:VAL:HG21	1.85	0.58
1:A:279:ALA:CB	1:A:298:LYS:HG3	2.33	0.58
1:C:207:ARG:HH11	1:C:207:ARG:HG2	1.69	0.58
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.70	0.57
1:C:266:ARG:NH2	4:C:3050:HOH:O	2.36	0.57
1:A:175:GLN:HE22	1:A:240:THR:HG21	1.65	0.57
1:B:55:GLY:HA3	1:B:91:SER:HB3	1.87	0.56
1:B:4:SER:N	4:B:5145:HOH:O	2.39	0.56
1:D:240:THR:HA	4:D:4043:HOH:O	2.06	0.56
1:C:41:ARG:NH1	1:C:197:ASP:O	2.39	0.56
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.70	0.55
1:D:322:GLN:O	1:D:326:VAL:HG23	2.06	0.55
1:C:124:HIS:HA	1:C:140:ILE:O	2.07	0.55
1:D:292:PRO:HD3	1:D:378:CYS:HA	1.89	0.55
1:B:191:LYS:HB3	1:B:191:LYS:NZ	2.22	0.54
1:D:9:SER:HA	1:D:272:LEU:HD22	1.89	0.54
1:C:37:ALA:HB2	1:C:200:VAL:HG21	1.89	0.54
1:C:297:ARG:HG2	1:C:297:ARG:HH11	1.73	0.54
1:C:180:VAL:HG22	1:C:228:MET:HE3	1.89	0.54
1:B:168:TRP:HH2	1:B:329:ASP:HB2	1.74	0.53
1:C:358:LEU:HD22	1:C:362:LEU:HG	1.91	0.53
1:C:236:ASP:HB3	1:C:239:GLY:HA3	1.90	0.53
1:D:88:LEU:HB2	1:D:379:ILE:HG23	1.90	0.53
1:B:4:SER:N	4:B:5282:HOH:O	2.41	0.52
1:C:189:ALA:CB	1:C:340:ASN:HB3	2.39	0.52
1:A:243:ALA:CB	3:A:1001:COA:H51A	2.39	0.52
1:D:236:ASP:HB3	1:D:239:GLY:HA3	1.91	0.52
1:A:105:THR:HG21	1:B:101:GLN:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:TRP:O	1:A:169:GLN:HB2	2.09	0.51
1:B:293:ILE:HB	1:B:294:PRO:CD	2.40	0.51
1:B:132:VAL:O	1:D:129:ARG:HA	2.10	0.51
1:B:326:VAL:HG13	1:B:330:LEU:HD12	1.91	0.51
1:A:276:VAL:HG22	1:A:388:CYS:O	2.10	0.51
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.45	0.51
1:D:203:ILE:HB	4:D:4054:HOH:O	2.10	0.51
1:C:293:ILE:HB	1:C:294:PRO:CD	2.41	0.51
1:B:374:LEU:HD23	1:B:374:LEU:C	2.31	0.51
1:C:8:ALA:HB1	1:C:269:ILE:HG21	1.93	0.50
1:C:143:MET:HG3	4:C:3030:HOH:O	2.11	0.50
1:C:258:LEU:N	1:C:258:LEU:HD22	2.26	0.50
1:C:125:CYS:HB2	1:D:123:PRO:HB2	1.94	0.50
1:B:158:GLY:O	1:B:161:ALA:HB3	2.11	0.50
1:A:354:GLY:HA2	1:A:377:LEU:HD11	1.94	0.50
3:B:2001:COA:H62	3:B:2001:COA:O9P	2.12	0.50
1:B:198:GLU:HB3	1:B:363:PHE:CD2	2.47	0.50
1:D:12:ARG:HD2	1:D:356:ARG:HG2	1.93	0.49
1:D:313:VAL:HG12	1:D:314:GLU:N	2.27	0.49
1:D:263:GLU:OE1	1:D:266:ARG:NH1	2.45	0.49
1:B:54:LEU:CA	1:B:55:GLY:N	2.69	0.49
1:A:168:TRP:CZ3	1:A:328:LYS:HB3	2.48	0.49
1:A:52:VAL:O	1:A:82:ALA:HA	2.13	0.48
1:A:247:SER:CB	4:A:5232:HOH:O	2.53	0.48
1:C:186:ALA:HA	1:C:340:ASN:O	2.14	0.48
1:B:38:VAL:HG23	1:B:257:LEU:HB2	1.96	0.48
1:B:298:LYS:HE2	2:B:5001:SO4:O1	2.13	0.48
1:D:136:ASP:OD2	4:D:4030:HOH:O	2.20	0.48
1:B:203:ILE:CD1	1:B:212:THR:OG1	2.61	0.48
1:C:54:LEU:HD13	1:C:116:MET:SD	2.54	0.48
1:B:191:LYS:HZ2	1:B:191:LYS:HB3	1.77	0.48
1:B:132:VAL:HA	4:B:5139:HOH:O	2.14	0.48
1:C:143:MET:CG	4:C:3030:HOH:O	2.61	0.48
1:A:88:LEU:HB2	1:A:379:ILE:HG23	1.95	0.48
1:B:9:SER:HA	1:B:272:LEU:HD22	1.95	0.48
1:A:191:LYS:NZ	4:A:5181:HOH:O	2.29	0.48
1:C:12:ARG:HD2	1:C:356:ARG:HG2	1.95	0.48
1:A:50:ASN:HB3	4:A:5212:HOH:O	2.13	0.48
1:B:207:ARG:HG2	1:B:208:LYS:H	1.78	0.47
1:D:18:PHE:HB2	1:D:249:LEU:O	2.14	0.47
1:A:133:LYS:HA	4:C:3074:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:HIS:HA	1:D:116:MET:SD	2.54	0.47
1:C:311:ASP:HB2	1:C:370:ALA:HB1	1.96	0.47
1:A:125:CYS:HB2	1:B:123:PRO:HB2	1.97	0.47
1:A:243:ALA:HB3	3:A:1001:COA:H51A	1.95	0.47
1:A:207:ARG:HG2	1:A:208:LYS:H	1.79	0.47
1:B:358:LEU:O	1:B:362:LEU:HG	2.14	0.47
1:C:364:GLU:O	1:C:368:ARG:HG2	2.14	0.47
1:B:186:ALA:HA	1:B:340:ASN:O	2.14	0.47
1:B:390:GLU:OE2	4:B:5243:HOH:O	2.20	0.47
1:D:228:MET:HE1	3:D:4001:COA:H61A	1.80	0.47
1:C:158:GLY:O	1:C:161:ALA:HB3	2.14	0.47
1:C:9:SER:HA	1:C:272:LEU:HD22	1.97	0.47
1:C:186:ALA:HB2	1:C:341:GLY:HA3	1.97	0.47
1:B:326:VAL:O	1:B:330:LEU:HB2	2.15	0.46
1:C:322:GLN:O	1:C:326:VAL:HG23	2.15	0.46
1:D:207:ARG:HD3	1:D:207:ARG:N	2.31	0.46
1:A:228:MET:HE2	4:A:5124:HOH:O	2.14	0.46
1:B:50:ASN:HB3	4:B:5235:HOH:O	2.16	0.46
1:B:281:VAL:HG12	1:B:282:GLY:N	2.29	0.46
1:D:293:ILE:HB	1:D:294:PRO:HD3	1.98	0.46
1:A:379:ILE:HB	1:A:383:MET:HB2	1.98	0.46
1:D:364:GLU:O	1:D:368:ARG:HG2	2.16	0.46
1:A:298:LYS:NZ	1:A:301:GLU:OE1	2.49	0.45
1:A:291:GLY:N	1:A:292:PRO:CD	2.78	0.45
1:C:207:ARG:HG2	1:C:208:LYS:H	1.82	0.45
1:B:350:ILE:HG21	1:B:350:ILE:HD13	1.65	0.45
1:D:167:GLN:HG2	4:D:4013:HOH:O	2.16	0.45
1:A:281:VAL:HG12	1:A:282:GLY:H	1.81	0.45
1:D:28:HIS:ND1	1:D:62:GLU:OE2	2.44	0.45
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.61	0.45
1:B:326:VAL:CG1	1:B:330:LEU:HD12	2.47	0.45
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.36	0.45
1:A:37:ALA:HB2	1:A:200:VAL:HG21	1.97	0.45
1:D:99:GLY:HA3	4:D:4027:HOH:O	2.16	0.45
1:D:206:GLY:HA3	1:D:209:GLY:O	2.17	0.45
1:D:54:LEU:O	1:D:84:GLY:HA2	2.17	0.45
1:C:168:TRP:CH2	1:C:329:ASP:HB2	2.51	0.45
1:C:288:MET:SD	1:C:288:MET:C	2.95	0.45
1:A:387:MET:HE3	1:A:389:ILE:HD11	1.99	0.45
1:A:274:ARG:CZ	1:A:276:VAL:HG12	2.47	0.45
1:C:60:ALA:HB3	4:C:3055:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:GLY:HA3	1:C:209:GLY:O	2.17	0.45
1:C:145:LYS:O	1:D:63:GLY:HA2	2.17	0.45
1:B:89:CYS:O	1:B:377:LEU:HD22	2.17	0.44
1:D:258:LEU:H	1:D:258:LEU:HD22	1.80	0.44
1:C:364:GLU:OE1	1:C:367:ARG:HD2	2.16	0.44
1:C:34:VAL:HG12	1:C:255:ALA:HB3	1.97	0.44
1:B:267:ARG:HH11	1:B:267:ARG:HD3	1.59	0.44
1:D:118:SER:OG	1:D:121:MET:HB2	2.16	0.44
1:B:175:GLN:HE22	1:B:240:THR:HG21	1.82	0.44
1:A:305:TRP:CZ3	1:A:388:CYS:HB3	2.52	0.44
1:A:153:TYR:CE2	1:A:286:LYS:HG2	2.52	0.44
1:D:356:ARG:NH2	1:D:357:ILE:HG22	2.33	0.44
1:A:101:GLN:HA	1:A:104:ALA:HB3	1.99	0.44
1:A:291:GLY:N	1:A:292:PRO:HD2	2.32	0.44
1:A:131:GLY:HA2	1:C:131:GLY:HA2	1.98	0.44
1:B:171:SER:HB2	4:B:5266:HOH:O	2.17	0.44
1:B:379:ILE:HB	1:B:383:MET:HB2	1.99	0.44
1:C:97:ALA:O	1:C:100:MET:HB3	2.18	0.44
1:D:89:CYS:SG	1:D:350:ILE:HG23	2.58	0.44
1:B:392:LEU:CG	4:B:5137:HOH:O	2.66	0.43
1:D:12:ARG:HA	1:D:254:ALA:HA	1.99	0.43
1:B:64:GLN:O	1:B:65:ASN:C	2.56	0.43
1:B:156:HIS:ND1	1:B:157:MET:N	2.66	0.43
1:B:180:VAL:CG2	1:B:228:MET:HE3	2.48	0.43
1:B:359:ASN:O	1:B:360:THR:C	2.55	0.43
1:C:312:LEU:HD23	1:C:365:MET:HG3	2.00	0.43
1:C:54:LEU:HD13	1:C:116:MET:CE	2.48	0.43
1:D:293:ILE:N	1:D:294:PRO:HD2	2.33	0.43
1:D:175:GLN:HB3	1:D:320:ALA:HB3	1.99	0.43
1:B:228:MET:HE2	4:B:5023:HOH:O	2.19	0.43
1:C:103:ILE:HA	1:C:108:ALA:O	2.17	0.43
1:B:247:SER:O	3:B:2001:COA:H72	2.18	0.43
1:B:368:ARG:NH2	4:B:5254:HOH:O	2.51	0.43
1:C:320:ALA:HB3	4:C:3063:HOH:O	2.18	0.43
1:A:9:SER:HA	1:A:272:LEU:HD22	2.01	0.43
1:A:330:LEU:HA	1:A:330:LEU:HD23	1.84	0.43
1:C:89:CYS:SG	1:C:350:ILE:HG23	2.59	0.43
1:C:12:ARG:HA	1:C:254:ALA:HA	2.00	0.43
1:A:374:LEU:HD21	1:A:376:THR:HB	2.01	0.43
1:D:49:VAL:HB	1:D:76:VAL:HG13	2.00	0.43
1:A:118:SER:HB2	4:A:5203:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:ARG:HD2	4:C:3034:HOH:O	2.19	0.42
1:A:286:LYS:HE3	4:A:5044:HOH:O	2.20	0.42
1:D:330:LEU:HD13	1:D:332:TRP:CH2	2.54	0.42
1:B:41:ARG:HG2	4:B:5039:HOH:O	2.19	0.42
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.38	0.42
1:C:330:LEU:HD13	1:C:332:TRP:CH2	2.54	0.42
1:A:12:ARG:HG3	1:A:13:THR:O	2.19	0.42
1:D:9:SER:HA	1:D:272:LEU:CD2	2.50	0.42
1:C:176:ASP:CG	1:C:228:MET:HG3	2.40	0.42
3:A:1001:COA:O5P	3:A:1001:COA:H21	2.18	0.42
1:A:200:VAL:HG13	1:A:200:VAL:O	2.18	0.42
1:D:195:PHE:O	1:D:198:GLU:HG2	2.19	0.42
1:C:309:ASP:HB3	1:C:372:LYS:HD2	2.02	0.42
1:D:51:GLU:HA	1:D:81:THR:O	2.19	0.42
1:D:247:SER:HB2	1:D:348:HIS:HB2	2.01	0.42
1:A:85:MET:HA	1:B:85:MET:HA	2.01	0.42
1:C:129:ARG:NH2	1:D:122:ALA:O	2.48	0.42
1:D:140:ILE:N	1:D:140:ILE:HD12	2.35	0.42
3:A:1001:COA:H52A	3:A:1001:COA:H2B	1.60	0.42
1:A:358:LEU:HD21	1:A:387:MET:HE3	2.01	0.42
1:D:291:GLY:O	1:D:294:PRO:HD2	2.20	0.42
1:C:305:TRP:CE2	1:C:372:LYS:HD3	2.55	0.42
1:B:12:ARG:HA	1:B:254:ALA:HA	2.02	0.42
1:A:387:MET:CE	1:A:389:ILE:HD11	2.50	0.42
1:A:298:LYS:C	1:A:298:LYS:HD3	2.41	0.42
3:D:4001:COA:H31	4:D:4039:HOH:O	2.19	0.42
1:D:158:GLY:O	1:D:161:ALA:HB3	2.20	0.42
1:A:54:LEU:O	1:A:84:GLY:HA2	2.20	0.42
1:A:361:LEU:O	1:A:365:MET:HG3	2.19	0.41
1:B:293:ILE:CB	1:B:294:PRO:CD	2.98	0.41
1:D:207:ARG:HG2	1:D:208:LYS:H	1.86	0.41
1:A:292:PRO:HD3	1:A:378:CYS:HA	2.01	0.41
1:C:293:ILE:HB	1:C:294:PRO:HD3	2.02	0.41
1:B:51:GLU:HA	1:B:81:THR:O	2.21	0.41
1:B:229:ALA:HB2	4:B:5136:HOH:O	2.21	0.41
1:A:247:SER:HB2	1:A:348:HIS:HB2	2.02	0.41
1:D:228:MET:HE2	1:D:228:MET:HB2	1.95	0.41
1:D:168:TRP:CH2	1:D:329:ASP:HB2	2.55	0.41
1:D:153:TYR:CE2	1:D:286:LYS:HD3	2.56	0.41
1:D:144:ILE:HD13	1:D:148:LEU:HD12	2.03	0.41
1:D:158:GLY:HA3	1:D:235:PHE:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LYS:O	4:A:5215:HOH:O	2.21	0.41
1:C:122:ALA:O	1:D:129:ARG:NH2	2.49	0.41
1:A:236:ASP:C	1:A:236:ASP:OD1	2.59	0.41
1:D:187:GLU:OE1	1:D:191:LYS:HE2	2.21	0.41
1:D:123:PRO:O	1:D:142:THR:HG23	2.20	0.41
1:D:314:GLU:OE2	1:D:338:ASN:HA	2.20	0.41
1:D:124:HIS:HA	1:D:140:ILE:O	2.20	0.41
1:B:25:THR:HA	1:B:26:PRO:HD3	1.90	0.41
1:B:37:ALA:HB2	1:B:200:VAL:HG21	2.02	0.41
1:C:276:VAL:HG11	1:C:390:GLU:HB2	2.03	0.41
1:D:313:VAL:CG1	1:D:314:GLU:N	2.84	0.40
1:C:60:ALA:CB	4:C:3055:HOH:O	2.69	0.40
1:C:175:GLN:HE22	1:C:240:THR:HG23	1.84	0.40
1:D:175:GLN:HE22	1:D:240:THR:HG23	1.82	0.40
1:D:183:GLN:OE1	1:D:220:ARG:HG2	2.22	0.40
1:B:98:LEU:O	1:B:102:GLN:HG2	2.21	0.40
1:C:153:TYR:CE2	1:C:286:LYS:HD3	2.56	0.40
1:C:363:PHE:HA	4:C:3040:HOH:O	2.22	0.40
1:D:354:GLY:HA2	1:D:377:LEU:HD11	2.03	0.40
1:A:328:LYS:HB2	1:A:328:LYS:HE3	1.83	0.40
1:D:186:ALA:HA	1:D:340:ASN:O	2.22	0.40
1:C:51:GLU:HA	1:C:81:THR:O	2.21	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:5238:HOH:O	4:A:5280:HOH:O[2_645]	1.94	0.26
4:A:5078:HOH:O	4:A:5084:HOH:O[2_655]	2.13	0.07
4:B:5202:HOH:O	4:B:5234:HOH:O[2_555]	2.16	0.04

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	387/389 (100%)	369 (95%)	17 (4%)	1 (0%)	46	57
1	B	387/389 (100%)	376 (97%)	10 (3%)	1 (0%)	46	57
1	C	387/389 (100%)	365 (94%)	21 (5%)	1 (0%)	46	57
1	D	387/389 (100%)	370 (96%)	14 (4%)	3 (1%)	24	27
All	All	1548/1556 (100%)	1480 (96%)	62 (4%)	6 (0%)	39	48

All (6) 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	65	ASN
1	A	350	ILE

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	276/276 (100%)	250 (91%)	26 (9%)	11	12
1	B	276/276 (100%)	255 (92%)	21 (8%)	16	20
1	C	276/276 (100%)	258 (94%)	18 (6%)	21	27
1	D	276/276 (100%)	258 (94%)	18 (6%)	21	27
All	All	1104/1104 (100%)	1021 (92%)	83 (8%)	17	21

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	85	MET
1	A	123	PRO

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Mol	Chain	Res	Type
1	A	133	LYS
1	A	155	TYR
1	A	207	ARG
1	A	220	ARG
1	A	221	HIS
1	A	225	LEU
1	A	230	LYS
1	A	237	LYS
1	A	240	THR
1	A	263	GLU
1	A	265	SER
1	A	272	LEU
1	A	286	LYS
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	332	TRP
1	A	339	VAL
1	A	348	HIS
1	A	353	SER
1	A	358	LEU
1	A	359	ASN
1	A	361	LEU
1	B	4	SER
1	B	39	LEU
1	B	133	LYS
1	B	134	MET
1	B	187	GLU
1	B	207	ARG
1	B	237	LYS
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	288	MET
1	B	298	LYS
1	B	322	GLN
1	B	328	LYS
1	B	332	TRP
1	B	339	VAL

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Mol	Chain	Res	Type
1	B	358	LEU
1	B	361	LEU
1	C	39	LEU
1	C	40	GLU
1	C	155	TYR
1	C	187	GLU
1	C	207	ARG
1	C	237	LYS
1	C	240	THR
1	C	258	LEU
1	C	272	LEU
1	C	288	MET
1	C	298	LYS
1	C	322	GLN
1	C	332	TRP
1	C	353	SER
1	C	357	ILE
1	C	358	LEU
1	C	361	LEU
1	C	371	ARG
1	D	39	LEU
1	D	155	TYR
1	D	187	GLU
1	D	207	ARG
1	D	237	LYS
1	D	240	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	322	GLN
1	D	332	TRP
1	D	353	SER
1	D	358	LEU
1	D	361	LEU
1	D	371	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	184	ASN
1	B	175	GLN
1	B	184	ASN
1	C	78	GLN
1	C	175	GLN
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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	COA	A	1001	-	40,50,50	2.07	12 (30%)	50,75,75	3.22	24 (48%)
2	SO4	A	5002	-	4,4,4	1.14	0	6,6,6	0.42	0
2	SO4	A	5004	-	4,4,4	1.00	0	6,6,6	0.67	0
2	SO4	A	5005	-	4,4,4	1.18	0	6,6,6	0.67	0
3	COA	B	2001	-	40,50,50	1.84	10 (25%)	50,75,75	2.65	16 (32%)
2	SO4	B	5001	-	4,4,4	1.13	0	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	B	5003	-	4,4,4	1.02	0	6,6,6	0.32	0
2	SO4	B	5006	-	4,4,4	1.01	0	6,6,6	0.56	0
3	COA	C	3001	-	40,50,50	1.91	8 (20%)	50,75,75	2.11	16 (32%)
3	COA	D	4001	-	40,50,50	1.92	11 (27%)	50,75,75	2.30	16 (32%)

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	A	1001	-	-	0/44/64/64	0/3/3/3
2	SO4	A	5002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	5004	-	-	0/0/0/0	0/0/0/0
2	SO4	A	5005	-	-	0/0/0/0	0/0/0/0
3	COA	B	2001	-	-	0/44/64/64	0/3/3/3
2	SO4	B	5001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	5003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	5006	-	-	0/0/0/0	0/0/0/0
3	COA	C	3001	-	-	0/44/64/64	0/3/3/3
3	COA	D	4001	-	-	0/44/64/64	0/3/3/3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	COA	O3B-C3B	-2.92	1.35	1.44
3	C	3001	COA	C9P-N8P	-2.57	1.28	1.33
3	B	2001	COA	C7P-C6P	-2.52	1.43	1.51
3	B	2001	COA	C9P-N8P	-2.51	1.28	1.33
3	A	1001	COA	C5A-N7A	-2.49	1.31	1.39
3	B	2001	COA	O3B-C3B	-2.47	1.36	1.44
3	A	1001	COA	C7P-C6P	-2.25	1.44	1.51
3	D	4001	COA	C9P-N8P	-2.20	1.29	1.33
3	B	2001	COA	C6P-C5P	-2.08	1.47	1.51
3	D	4001	COA	C7P-N8P	-2.07	1.41	1.46
3	A	1001	COA	O5P-C5P	2.18	1.27	1.23
3	A	1001	COA	P2A-O6A	2.19	1.69	1.59
3	D	4001	COA	O4B-C4B	2.22	1.50	1.45
3	D	4001	COA	OAP-CAP	2.28	1.46	1.42
3	A	1001	COA	O4B-C1B	2.32	1.44	1.41
3	A	1001	COA	P3B-O7A	2.45	1.59	1.51
3	D	4001	COA	C2A-N1A	2.46	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	COA	P3B-O7A	2.48	1.59	1.51
3	C	3001	COA	C2A-N1A	2.48	1.38	1.33
3	D	4001	COA	P3B-O3B	2.49	1.67	1.60
3	B	2001	COA	C2A-N1A	2.64	1.38	1.33
3	B	2001	COA	P3B-O3B	2.64	1.68	1.60
3	C	3001	COA	P3B-O3B	2.71	1.68	1.60
3	D	4001	COA	P3B-O7A	2.74	1.60	1.51
3	B	2001	COA	O4B-C1B	2.74	1.44	1.41
3	B	2001	COA	C2P-S1P	2.81	1.90	1.80
3	C	3001	COA	P3B-O7A	2.82	1.60	1.51
3	D	4001	COA	O5P-C5P	3.00	1.29	1.23
3	C	3001	COA	O4B-C1B	3.07	1.45	1.41
3	A	1001	COA	C3P-N4P	3.25	1.53	1.46
3	A	1001	COA	O4B-C4B	3.29	1.52	1.45
3	C	3001	COA	C3P-N4P	3.52	1.54	1.46
3	A	1001	COA	C2A-N1A	3.54	1.40	1.33
3	C	3001	COA	O5P-C5P	3.54	1.30	1.23
3	A	1001	COA	P3B-O3B	3.66	1.71	1.60
3	D	4001	COA	O4B-C1B	3.72	1.45	1.41
3	D	4001	COA	C3P-N4P	3.81	1.55	1.46
3	B	2001	COA	O9P-C9P	5.96	1.35	1.23
3	D	4001	COA	O9P-C9P	6.33	1.35	1.23
3	C	3001	COA	O9P-C9P	6.33	1.35	1.23
3	A	1001	COA	O9P-C9P	6.97	1.37	1.23

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	COA	C2P-C3P-N4P	-11.23	90.19	112.37
3	A	1001	COA	O6A-CCP-CBP	-6.70	99.78	110.55
3	D	4001	COA	C2P-C3P-N4P	-5.69	101.14	112.37
3	D	4001	COA	P3B-O3B-C3B	-5.53	108.30	121.56
3	A	1001	COA	C7P-N8P-C9P	-5.06	112.51	122.53
3	B	2001	COA	OAP-CAP-C9P	-5.05	98.79	110.38
3	B	2001	COA	C2P-C3P-N4P	-4.86	102.78	112.37
3	A	1001	COA	O3A-P2A-O6A	-4.65	90.60	102.94
3	D	4001	COA	CEP-CBP-CCP	-4.64	102.49	108.50
3	B	2001	COA	C6P-C5P-N4P	-4.57	108.53	116.46
3	A	1001	COA	C6P-C5P-N4P	-4.48	108.68	116.46
3	D	4001	COA	C4B-O4B-C1B	-4.41	104.87	109.72
3	B	2001	COA	O6A-CCP-CBP	-4.28	103.67	110.55
3	A	1001	COA	C2B-C3B-C4B	-4.15	95.49	103.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3001	COA	CEP-CBP-CCP	-4.09	103.20	108.50
3	C	3001	COA	C2P-C3P-N4P	-3.74	104.98	112.37
3	A	1001	COA	O4B-C4B-C5B	-3.68	96.16	109.32
3	C	3001	COA	P3B-O3B-C3B	-3.65	112.82	121.56
3	B	2001	COA	P3B-O3B-C3B	-3.46	113.28	121.56
3	A	1001	COA	C4B-O4B-C1B	-3.24	106.16	109.72
3	C	3001	COA	C4B-O4B-C1B	-3.23	106.17	109.72
3	A	1001	COA	CDP-CBP-CCP	-3.15	104.42	108.50
3	A	1001	COA	N3A-C2A-N1A	-3.06	126.55	128.89
3	A	1001	COA	P3B-O3B-C3B	-3.06	114.23	121.56
3	C	3001	COA	O3A-P2A-O6A	-2.96	95.08	102.94
3	A	1001	COA	O5B-C5B-C4B	-2.95	98.25	109.12
3	B	2001	COA	C4B-O4B-C1B	-2.76	106.69	109.72
3	C	3001	COA	O6A-CCP-CBP	-2.72	106.18	110.55
3	D	4001	COA	CAP-C9P-N8P	-2.52	110.89	116.47
3	A	1001	COA	C2B-C1B-N9A	-2.49	110.49	114.29
3	A	1001	COA	O2B-C2B-C3B	-2.47	104.04	111.16
3	B	2001	COA	O3A-P2A-O6A	-2.43	96.48	102.94
3	D	4001	COA	N3A-C2A-N1A	-2.36	127.08	128.89
3	C	3001	COA	C2B-C1B-N9A	-2.29	110.80	114.29
3	D	4001	COA	O3A-P2A-O6A	-2.27	96.92	102.94
3	D	4001	COA	OAP-CAP-C9P	-2.23	105.25	110.38
3	C	3001	COA	CAP-C9P-N8P	-2.18	111.63	116.47
3	C	3001	COA	O9A-P3B-O8A	2.05	115.19	107.38
3	C	3001	COA	C5B-C4B-C3B	2.08	121.81	114.31
3	C	3001	COA	O4B-C1B-N9A	2.09	112.48	108.10
3	D	4001	COA	C7P-C6P-C5P	2.10	115.78	112.31
3	D	4001	COA	C5B-C4B-C3B	2.11	121.90	114.31
3	B	2001	COA	O3B-C3B-C4B	2.11	118.26	109.99
3	D	4001	COA	O9A-P3B-O8A	2.15	115.58	107.38
3	C	3001	COA	C6P-C5P-N4P	2.16	120.21	116.46
3	B	2001	COA	O4B-C1B-N9A	2.38	113.08	108.10
3	A	1001	COA	C2A-N1A-C6A	2.40	123.06	118.77
3	D	4001	COA	C6P-C7P-N8P	2.53	117.42	111.88
3	B	2001	COA	C5B-C4B-C3B	2.59	123.66	114.31
3	A	1001	COA	O9A-P3B-O8A	2.64	117.45	107.38
3	B	2001	COA	O5P-C5P-C6P	2.81	126.84	121.98
3	A	1001	COA	C4A-C5A-N7A	2.83	112.08	109.48
3	A	1001	COA	O5P-C5P-C6P	2.83	126.86	121.98
3	D	4001	COA	C4A-C5A-N7A	2.90	112.15	109.48
3	A	1001	COA	C3P-N4P-C5P	2.92	128.53	122.79
3	A	1001	COA	N6A-C6A-N1A	2.93	125.49	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	3001	COA	C4A-C5A-N7A	3.00	112.23	109.48
3	A	1001	COA	O3B-C3B-C4B	3.01	121.79	109.99
3	D	4001	COA	C6P-C5P-N4P	3.05	121.75	116.46
3	B	2001	COA	N6A-C6A-N1A	3.09	125.84	119.20
3	A	1001	COA	CAP-C9P-N8P	3.19	123.54	116.47
3	B	2001	COA	CDP-CBP-CCP	3.35	112.84	108.50
3	B	2001	COA	C4A-C5A-N7A	3.66	112.85	109.48
3	C	3001	COA	C7P-C6P-C5P	3.75	118.49	112.31
3	C	3001	COA	CDP-CBP-CCP	3.96	113.64	108.50
3	D	4001	COA	CDP-CBP-CCP	4.04	113.74	108.50
3	B	2001	COA	C7P-N8P-C9P	5.98	134.36	122.53
3	A	1001	COA	CEP-CBP-CDP	6.66	122.64	109.28
3	A	1001	COA	C6P-C7P-N8P	6.67	126.51	111.88
3	D	4001	COA	C7P-N8P-C9P	6.78	135.95	122.53
3	C	3001	COA	C7P-N8P-C9P	7.20	136.78	122.53
3	B	2001	COA	C7P-C6P-C5P	10.63	129.83	112.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	COA	4	0
3	B	2001	COA	2	0
2	B	5001	SO4	1	0
3	D	4001	COA	2	0

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	389/389 (100%)	-0.16	4 (1%) 84 88	8, 17, 38, 83	0
1	B	389/389 (100%)	-0.10	5 (1%) 79 84	7, 18, 41, 95	0
1	C	389/389 (100%)	0.86	56 (14%) 3 5	16, 42, 74, 116	0
1	D	389/389 (100%)	1.38	108 (27%) 1 1	19, 48, 102, 127	0
All	All	1556/1556 (100%)	0.49	173 (11%) 7 11	7, 35, 75, 127	0

All (173) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	228	MET	8.2
1	D	307	ILE	7.2
1	D	330	LEU	6.9
1	D	164	VAL	6.4
1	D	169	GLN	6.1
1	D	206	GLY	6.1
1	D	392	LEU	6.0
1	C	207	ARG	6.0
1	D	310	LEU	5.5
1	D	224	THR	4.9
1	D	233	PRO	4.8
1	D	170	LEU	4.7
1	D	208	LYS	4.7
1	C	186	ALA	4.7
1	D	349	PRO	4.7
1	D	171	SER	4.5
1	D	289	GLY	4.5
1	D	308	GLY	4.5
1	D	367	ARG	4.4
1	B	208	LYS	4.3
1	C	179	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	240	THR	4.2
1	D	235	PHE	4.2
1	C	223	ALA	4.0
1	D	186	ALA	4.0
1	D	350	ILE	4.0
1	C	232	ARG	4.0
1	D	223	ALA	3.9
1	D	219	ILE	3.9
1	C	23	ALA	3.9
1	C	47	GLY	3.9
1	D	371	ARG	3.9
1	D	309	ASP	3.8
1	D	339	VAL	3.8
1	D	179	ALA	3.8
1	C	155	TYR	3.7
1	C	224	THR	3.7
1	C	262	ALA	3.7
1	C	297	ARG	3.7
1	D	285	PRO	3.6
1	D	189	ALA	3.6
1	D	238	GLU	3.5
1	C	370	ALA	3.5
1	D	288	MET	3.5
1	D	234	ALA	3.5
1	D	283	VAL	3.4
1	C	80	ALA	3.4
1	D	225	LEU	3.4
1	B	134	MET	3.3
1	C	280	THR	3.3
1	D	237	LYS	3.3
1	D	152	PHE	3.3
1	D	382	GLY	3.3
1	D	182	SER	3.3
1	D	231	LEU	3.3
1	D	194	ARG	3.2
1	B	4	SER	3.2
1	C	300	LEU	3.2
1	D	298	LYS	3.1
1	C	305	TRP	3.1
1	C	243	ALA	3.1
1	D	230	LYS	3.1
1	C	227	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	302	ARG	3.0
1	D	239	GLY	3.0
1	D	362	LEU	2.9
1	D	326	VAL	2.9
1	B	206	GLY	2.9
1	C	392	LEU	2.9
1	D	336	ILE	2.8
1	D	338	ASN	2.8
1	A	133	LYS	2.8
1	B	392	LEU	2.8
1	C	290	THR	2.8
1	C	208	LYS	2.8
1	D	227	SER	2.8
1	D	270	GLN	2.8
1	A	209	GLY	2.8
1	C	110	ILE	2.8
1	C	289	GLY	2.7
1	C	237	LYS	2.7
1	D	232	ARG	2.7
1	C	234	ALA	2.7
1	C	371	ARG	2.7
1	D	188	ALA	2.7
1	D	236	ASP	2.7
1	C	104	ALA	2.7
1	C	324	CYS	2.7
1	D	327	ASN	2.6
1	D	218	TYR	2.6
1	C	310	LEU	2.6
1	D	374	LEU	2.6
1	C	359	ASN	2.6
1	D	320	ALA	2.6
1	D	166	LYS	2.6
1	D	226	ASP	2.6
1	C	213	VAL	2.6
1	C	206	GLY	2.6
1	D	318	ALA	2.6
1	A	207	ARG	2.5
1	D	264	ALA	2.5
1	C	263	GLU	2.5
1	C	156	HIS	2.5
1	D	340	ASN	2.5
1	D	165	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	180	VAL	2.5
1	D	295	ALA	2.5
1	D	370	ALA	2.5
1	D	323	ALA	2.5
1	D	388	CYS	2.5
1	C	311	ASP	2.5
1	C	382	GLY	2.4
1	D	163	ASN	2.4
1	C	183	GLN	2.4
1	C	383	MET	2.4
1	D	88	LEU	2.4
1	C	42	ALA	2.4
1	C	202	PHE	2.4
1	D	18	PHE	2.4
1	D	11	ALA	2.4
1	C	90	GLY	2.4
1	D	244	GLY	2.4
1	D	195	PHE	2.4
1	C	67	ALA	2.4
1	D	325	ALA	2.4
1	D	191	LYS	2.4
1	A	208	LYS	2.3
1	D	246	ALA	2.3
1	D	286	LYS	2.3
1	C	57	VAL	2.3
1	D	42	ALA	2.3
1	D	168	TRP	2.3
1	D	174	GLU	2.3
1	D	347	GLY	2.2
1	C	269	ILE	2.2
1	D	287	VAL	2.2
1	D	175	GLN	2.2
1	C	45	ALA	2.2
1	D	269	ILE	2.2
1	D	178	PHE	2.2
1	D	92	GLY	2.2
1	D	99	GLY	2.2
1	D	222	GLY	2.2
1	D	36	SER	2.2
1	D	296	SER	2.2
1	D	108	ALA	2.2
1	D	207	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	275	ILE	2.1
1	D	276	VAL	2.1
1	D	160	THR	2.1
1	D	203	ILE	2.1
1	D	241	VAL	2.1
1	C	233	PRO	2.1
1	D	361	LEU	2.1
1	D	197	ASP	2.1
1	C	325	ALA	2.1
1	C	191	LYS	2.1
1	C	105	THR	2.1
1	C	229	ALA	2.1
1	C	231	LEU	2.1
1	D	305	TRP	2.1
1	C	153	TYR	2.1
1	C	170	LEU	2.1
1	D	290	THR	2.1
1	D	332	TRP	2.1
1	D	66	PRO	2.1
1	D	389	ILE	2.1
1	C	363	PHE	2.0
1	D	33	THR	2.0
1	C	108	ALA	2.0
1	D	229	ALA	2.0
1	D	344	ILE	2.0
1	D	176	ASP	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	5006	5/5	0.93	0.16	1.82	39,41,43,43	0
3	COA	D	4001	48/48	0.69	0.28	0.47	79,112,123,124	0
3	COA	B	2001	48/48	0.93	0.13	-0.04	15,29,52,57	0
3	COA	A	1001	48/48	0.93	0.13	-0.09	12,29,45,47	0
3	COA	C	3001	48/48	0.80	0.20	-0.17	56,78,93,95	0
2	SO4	A	5004	5/5	0.96	0.10	-1.23	47,49,51,54	0
2	SO4	B	5001	5/5	0.90	0.14	-	56,56,58,58	0
2	SO4	A	5005	5/5	0.86	0.20	-	48,50,51,54	0
2	SO4	A	5002	5/5	0.95	0.13	-	58,60,61,62	0
2	SO4	B	5003	5/5	0.97	0.13	-	50,52,54,57	0

6.5 Other polymers

There are no such residues in this entry.