Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 01:00 AM EST

PDB ID	:	1DLU
Title	:	UNLIGANDED BIOSYNTHETIC THIOLASE FROM ZOOGLOEA RAMIGERA
Authors	:	Modis, Y.; Wierenga, R.K.
Deposited on	:	1999-12-12
Resolution	:	2.25 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

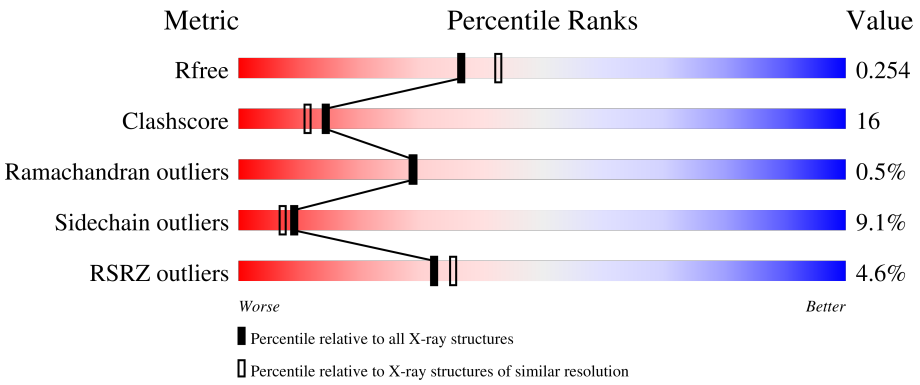
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (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 <=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	.% 46% 40% 13% •
1	B	389	2% 52% 35% 11% •
1	C	389	3% 61% 31% 7% •
1	D	389	12% 61% 33% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MPD	A	1001	-	-	X	-
3	MPD	B	1002	-	-	X	-
3	MPD	C	1003	-	-	X	-
3	MPD	D	1004	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12065 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.

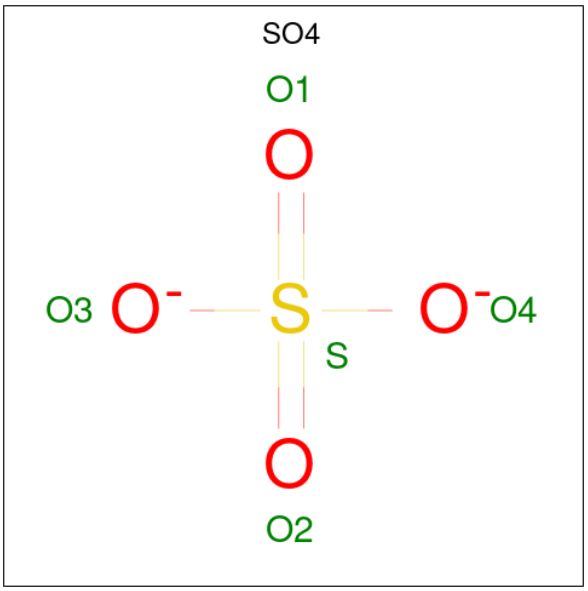
- Molecule 1 is a protein called BIOSYNTHETIC THIOLASE.

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

There are 8 discrepancies between the modelled and reference sequences:

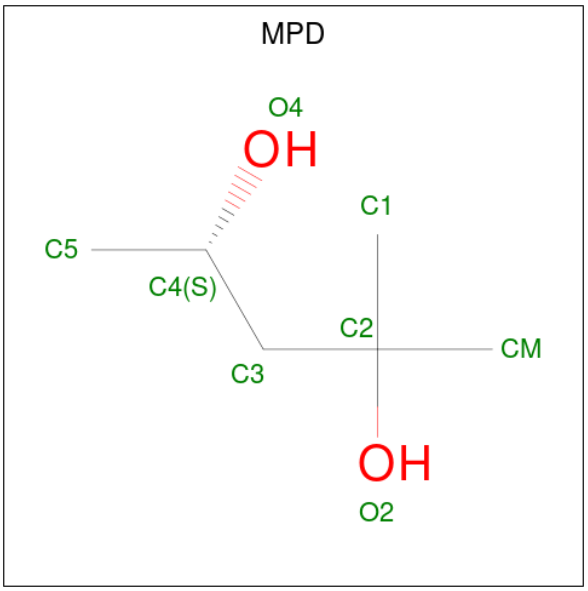
Chain	Residue	Modelled	Actual	Comment	Reference
A	11	ALA	-	insertion	UNP P07097
A	129	ARG	ALA	conflict	UNP P07097
B	11	ALA	-	insertion	UNP P07097
B	129	ARG	ALA	conflict	UNP P07097
C	11	ALA	-	insertion	UNP P07097
C	129	ARG	ALA	conflict	UNP P07097
D	11	ALA	-	insertion	UNP P07097
D	129	ARG	ALA	conflict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

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



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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	8	6	2	0	0
3	B	1	8	6	2	0	0
3	C	1	8	6	2	0	0
3	D	1	8	6	2	0	0

- Molecule 4 is water.

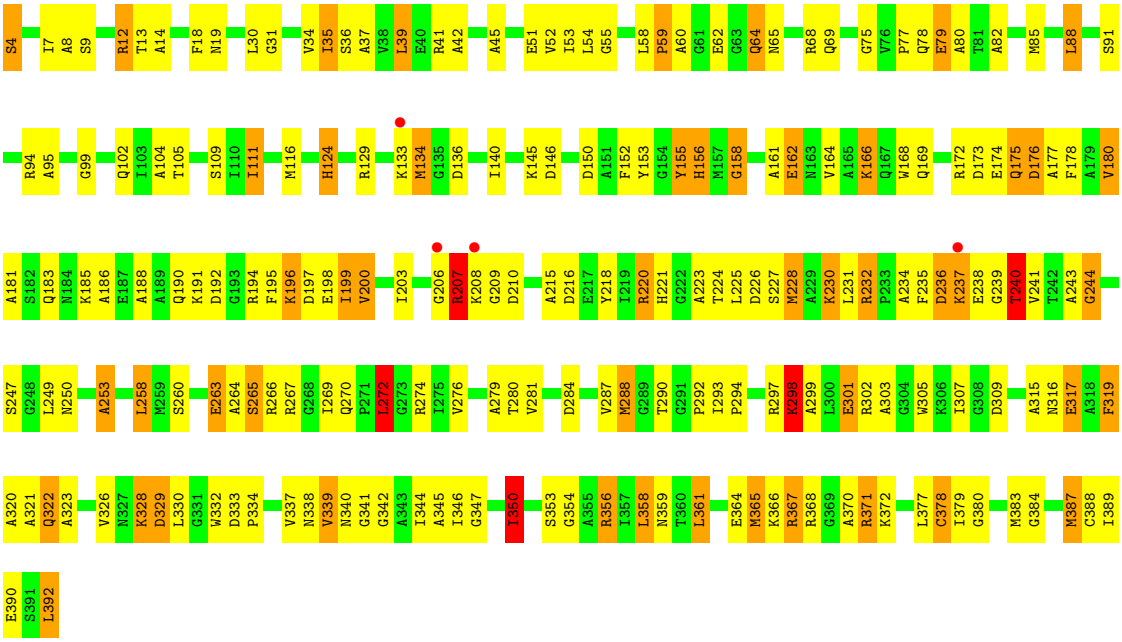
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	293	293	293	4	0
4	B	287	287	287	4	0
4	C	101	101	101	3	0
4	D	70	70	70	3	0

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.

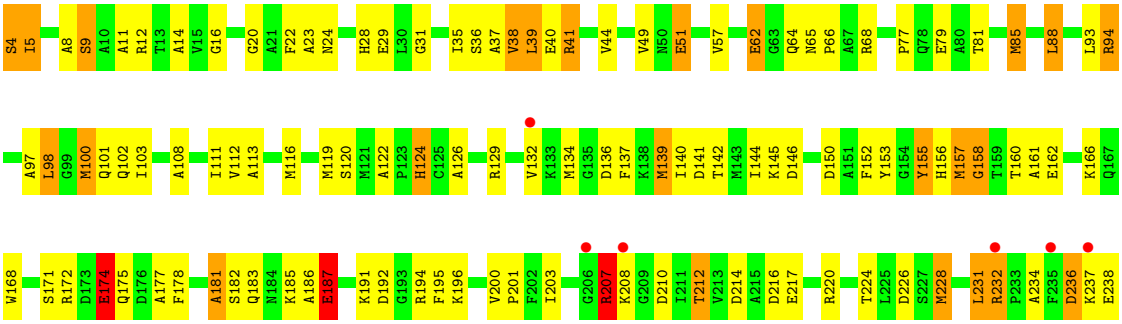
• Molecule 1: BIOSYNTHETIC THIOLASE

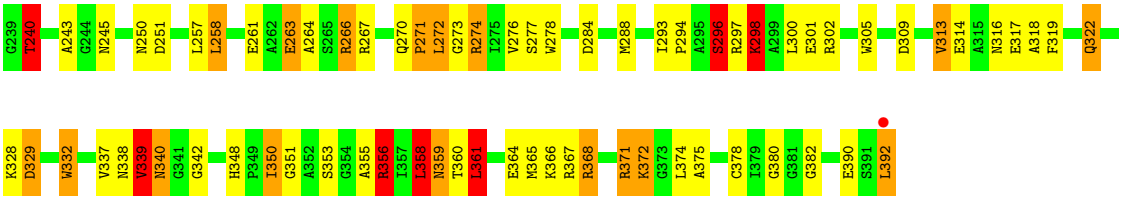
Chain A:



• Molecule 1: BIOSYNTHETIC THIOLASE

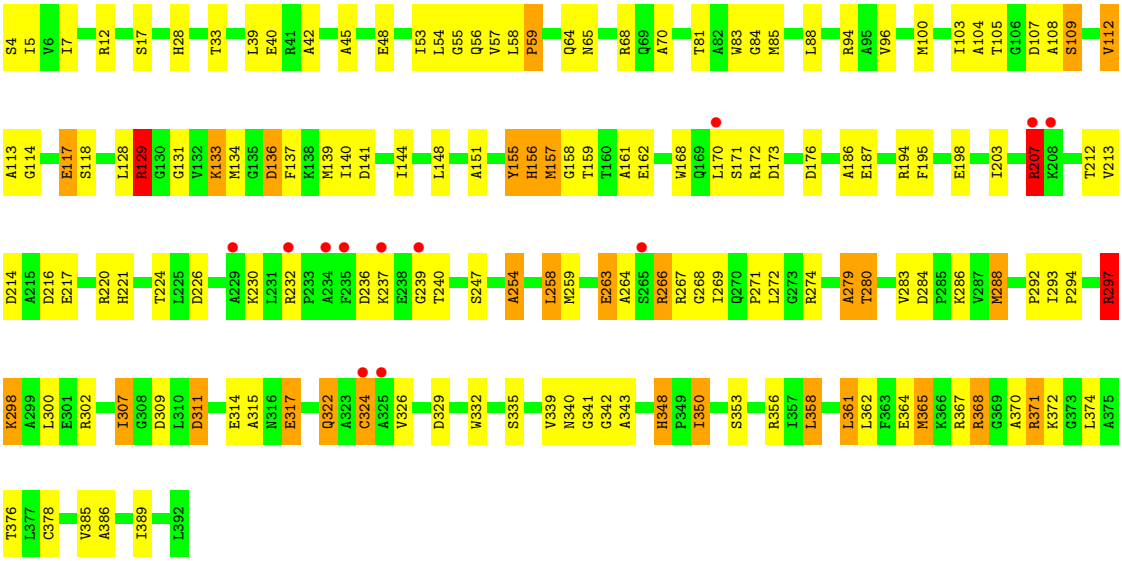
Chain B:





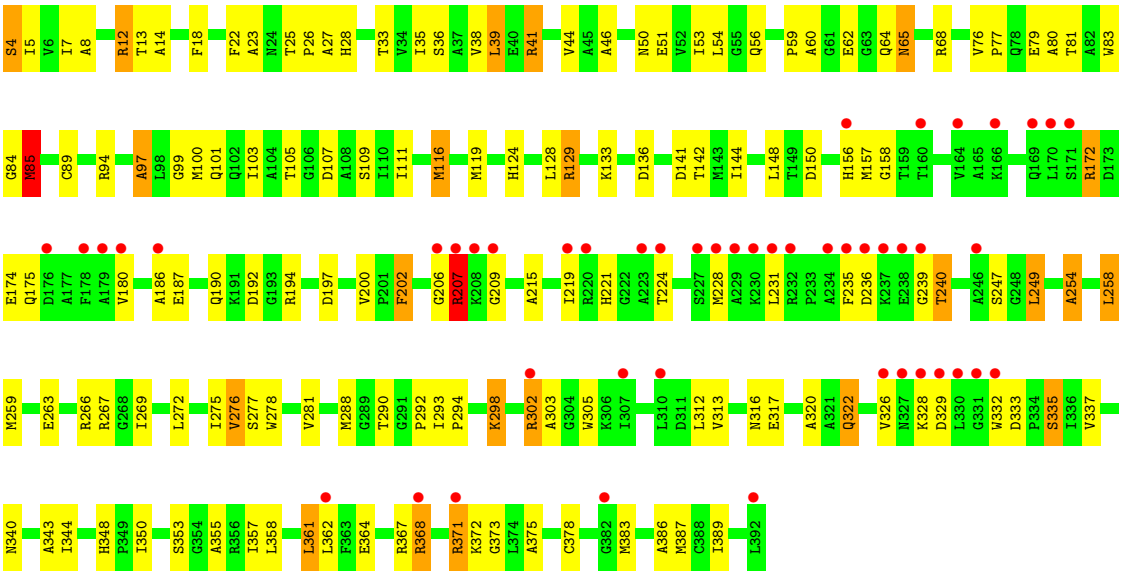
• Molecule 1: BIOSYNTHETIC THIOLASE

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	84.71Å 79.73Å 150.48Å 90.00° 93.07° 90.00°	Depositor
Resolution (Å)	20.00 – 2.25 39.86 – 2.21	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.25) 83.7 (39.86-2.21)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.263 0.209 , 0.254	Depositor DCC
R_{free} test set	4898 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	21.2	Xtriage
Anisotropy	0.985	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 55.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12065	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, 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	5/2854 (0.2%)	2.91	232/3853 (6.0%)
1	B	1.18	6/2854 (0.2%)	2.62	192/3853 (5.0%)
1	C	0.60	0/2854	1.90	82/3853 (2.1%)
1	D	0.59	0/2854	1.86	63/3853 (1.6%)
All	All	0.95	11/11416 (0.1%)	2.37	569/15412 (3.7%)

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	3
1	B	0	3
All	All	0	6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	ARG	NE-CZ	-7.43	1.23	1.33
1	A	79	GLU	CD-OE1	6.96	1.33	1.25
1	B	201	PRO	N-CD	6.05	1.56	1.47
1	B	353	SER	CA-CB	5.65	1.61	1.52
1	A	109	SER	CA-CB	5.63	1.61	1.52
1	B	317	GLU	CD-OE1	5.47	1.31	1.25
1	A	59	PRO	N-CD	5.24	1.55	1.47
1	A	190	GLN	N-CA	-5.20	1.35	1.46
1	B	314	GLU	CA-CB	5.18	1.65	1.53
1	B	88	LEU	C-O	5.15	1.33	1.23
1	A	359	ASN	CB-CG	5.07	1.62	1.51

All (569) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	194	ARG	NE-CZ-NH1	34.08	137.34	120.30
1	D	367	ARG	CD-NE-CZ	28.39	163.35	123.60
1	A	266	ARG	NE-CZ-NH2	-25.74	107.43	120.30
1	A	172	ARG	NE-CZ-NH1	-25.55	107.53	120.30
1	B	266	ARG	NE-CZ-NH2	-22.53	109.03	120.30
1	A	41	ARG	NE-CZ-NH1	21.77	131.19	120.30
1	B	266	ARG	NE-CZ-NH1	21.26	130.93	120.30
1	A	41	ARG	NE-CZ-NH2	-21.12	109.74	120.30
1	A	12	ARG	NE-CZ-NH1	20.63	130.61	120.30
1	A	371	ARG	NE-CZ-NH2	-19.73	110.44	120.30
1	A	68	ARG	NE-CZ-NH2	-19.45	110.58	120.30
1	D	41	ARG	NE-CZ-NH1	18.85	129.73	120.30
1	B	129	ARG	NE-CZ-NH1	-18.45	111.08	120.30
1	A	194	ARG	NE-CZ-NH2	-17.85	111.37	120.30
1	B	216	ASP	CB-CG-OD1	17.69	134.22	118.30
1	B	41	ARG	NE-CZ-NH1	17.57	129.09	120.30
1	A	371	ARG	NE-CZ-NH1	17.18	128.89	120.30
1	A	220	ARG	CD-NE-CZ	16.76	147.06	123.60
1	A	302	ARG	NE-CZ-NH2	-16.47	112.07	120.30
1	D	172	ARG	NE-CZ-NH1	16.31	128.45	120.30
1	B	220	ARG	NE-CZ-NH1	15.79	128.19	120.30
1	B	356	ARG	NE-CZ-NH1	-15.55	112.53	120.30
1	A	172	ARG	NH1-CZ-NH2	15.45	136.40	119.40
1	C	367	ARG	NE-CZ-NH2	-15.28	112.66	120.30
1	A	12	ARG	NE-CZ-NH2	-15.24	112.68	120.30
1	A	297	ARG	NE-CZ-NH2	-15.19	112.71	120.30
1	B	172	ARG	NE-CZ-NH1	-15.13	112.73	120.30
1	B	367	ARG	NE-CZ-NH1	14.78	127.69	120.30
1	A	173	ASP	CB-CG-OD1	14.46	131.31	118.30
1	B	267	ARG	NE-CZ-NH1	14.03	127.32	120.30
1	C	267	ARG	NE-CZ-NH1	13.91	127.25	120.30
1	C	68	ARG	NE-CZ-NH2	-13.69	113.46	120.30
1	A	220	ARG	NE-CZ-NH2	-13.62	113.49	120.30
1	B	367	ARG	NE-CZ-NH2	-13.44	113.58	120.30
1	A	367	ARG	NE-CZ-NH1	13.36	126.98	120.30
1	B	371	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	A	210	ASP	CB-CG-OD1	13.16	130.14	118.30
1	A	197	ASP	CB-CG-OD2	12.94	129.94	118.30
1	A	309	ASP	CB-CG-OD2	12.89	129.90	118.30
1	A	274	ARG	NE-CZ-NH1	12.78	126.69	120.30
1	A	356	ARG	NE-CZ-NH1	-12.70	113.95	120.30
1	D	68	ARG	NE-CZ-NH1	12.64	126.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	ASP	CB-CG-OD2	-12.58	106.98	118.30
1	A	228	MET	CA-CB-CG	12.40	134.38	113.30
1	A	266	ARG	NH1-CZ-NH2	12.37	133.01	119.40
1	B	267	ARG	NE-CZ-NH2	-12.30	114.15	120.30
1	B	41	ARG	CD-NE-CZ	12.24	140.74	123.60
1	B	220	ARG	CD-NE-CZ	12.14	140.60	123.60
1	B	194	ARG	NE-CZ-NH1	12.09	126.34	120.30
1	D	94	ARG	NE-CZ-NH2	12.02	126.31	120.30
1	C	368	ARG	NE-CZ-NH2	11.96	126.28	120.30
1	C	94	ARG	CD-NE-CZ	11.82	140.15	123.60
1	B	220	ARG	NE-CZ-NH2	-11.75	114.43	120.30
1	B	49	VAL	CG1-CB-CG2	-11.72	92.15	110.90
1	A	274	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	B	251	ASP	CB-CG-OD1	11.38	128.54	118.30
1	A	320	ALA	N-CA-CB	11.25	125.86	110.10
1	B	302	ARG	CD-NE-CZ	10.81	138.74	123.60
1	D	41	ARG	NH1-CZ-NH2	-10.69	107.64	119.40
1	A	356	ARG	NE-CZ-NH2	10.67	125.64	120.30
1	B	361	LEU	CB-CG-CD2	10.46	128.79	111.00
1	A	155	TYR	CB-CG-CD2	10.35	127.21	121.00
1	C	274	ARG	CD-NE-CZ	10.24	137.94	123.60
1	D	136	ASP	CB-CG-OD2	10.22	127.50	118.30
1	A	274	ARG	CD-NE-CZ	10.14	137.79	123.60
1	A	42	ALA	N-CA-CB	-10.13	95.91	110.10
1	B	207	ARG	NE-CZ-NH2	-10.07	115.26	120.30
1	B	375	ALA	N-CA-CB	-9.91	96.22	110.10
1	C	274	ARG	NE-CZ-NH2	-9.90	115.35	120.30
1	A	368	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	A	136	ASP	CB-CG-OD1	9.75	127.07	118.30
1	B	44	VAL	CG1-CB-CG2	-9.75	95.30	110.90
1	A	326	VAL	CA-CB-CG2	9.69	125.43	110.90
1	B	150	ASP	CB-CG-OD2	-9.67	109.60	118.30
1	B	68	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	A	231	LEU	CB-CG-CD1	-9.64	94.61	111.00
1	A	129	ARG	NE-CZ-NH1	-9.63	115.48	120.30
1	A	192	ASP	CB-CG-OD1	9.63	126.97	118.30
1	B	29	GLU	OE1-CD-OE2	-9.50	111.90	123.30
1	C	279	ALA	N-CA-CB	9.43	123.29	110.10
1	A	8	ALA	O-C-N	-9.40	107.66	122.70
1	A	156	HIS	CA-CB-CG	9.34	129.48	113.60
1	B	141	ASP	CB-CG-OD1	9.31	126.68	118.30
1	A	150	ASP	CB-CG-OD2	-9.31	109.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	318	ALA	N-CA-CB	9.25	123.05	110.10
1	C	302	ARG	NE-CZ-NH2	-9.23	115.69	120.30
1	C	263	GLU	OE1-CD-OE2	9.20	134.34	123.30
1	C	194	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	178	PHE	CB-CG-CD2	-9.06	114.45	120.80
1	B	274	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	D	302	ARG	NE-CZ-NH2	-9.01	115.79	120.30
1	B	172	ARG	NH1-CZ-NH2	8.93	129.22	119.40
1	B	297	ARG	NE-CZ-NH1	8.93	124.76	120.30
1	C	315	ALA	CB-CA-C	8.85	123.38	110.10
1	A	34	VAL	CA-CB-CG2	-8.82	97.67	110.90
1	B	236	ASP	CB-CG-OD1	8.82	126.24	118.30
1	B	364	GLU	OE1-CD-OE2	-8.81	112.73	123.30
1	D	254	ALA	CB-CA-C	8.79	123.29	110.10
1	B	4	SER	CA-C-O	-8.79	101.64	120.10
1	D	368	ARG	NE-CZ-NH2	8.79	124.69	120.30
1	D	371	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	D	68	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	A	240	THR	N-CA-CB	-8.73	93.71	110.30
1	C	367	ARG	CD-NE-CZ	8.71	135.80	123.60
1	A	207	ARG	CD-NE-CZ	8.65	135.71	123.60
1	B	231	LEU	CB-CG-CD1	-8.63	96.33	111.00
1	D	136	ASP	CB-CG-OD1	-8.62	110.54	118.30
1	A	220	ARG	NE-CZ-NH1	8.59	124.59	120.30
1	A	235	PHE	CB-CG-CD2	-8.55	114.81	120.80
1	D	14	ALA	N-CA-CB	-8.50	98.20	110.10
1	B	22	PHE	CB-CG-CD2	-8.48	114.86	120.80
1	A	172	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	C	129	ARG	NE-CZ-NH2	-8.43	116.09	120.30
1	A	94	ARG	O-C-N	8.41	136.15	122.70
1	B	339	VAL	CA-CB-CG2	8.40	123.50	110.90
1	B	146	ASP	CB-CG-OD1	8.34	125.80	118.30
1	A	299	ALA	O-C-N	-8.33	109.38	122.70
1	B	224	THR	CA-CB-CG2	-8.29	100.79	112.40
1	B	284	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	A	303	ALA	C-N-CA	8.27	139.67	122.30
1	B	129	ARG	NH1-CZ-NH2	8.22	128.45	119.40
1	A	155	TYR	CG-CD1-CE1	8.19	127.85	121.30
1	A	218	TYR	CG-CD2-CE2	8.18	127.85	121.30
1	B	296	SER	N-CA-CB	8.18	122.78	110.50
1	D	41	ARG	CD-NE-CZ	8.18	135.05	123.60
1	A	8	ALA	N-CA-CB	-8.16	98.68	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	5	ILE	CB-CG1-CD1	8.14	136.68	113.90
1	B	126	ALA	CB-CA-C	-8.13	97.90	110.10
1	A	339	VAL	N-CA-CB	-8.13	93.62	111.50
1	A	218	TYR	CB-CG-CD1	8.12	125.87	121.00
1	C	68	ARG	NH1-CZ-NH2	8.12	128.33	119.40
1	B	155	TYR	CA-CB-CG	8.10	128.79	113.40
1	D	200	VAL	CA-CB-CG1	8.09	123.04	110.90
1	B	309	ASP	CB-CG-OD2	8.08	125.58	118.30
1	A	368	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	B	68	ARG	NH1-CZ-NH2	-8.04	110.55	119.40
1	A	319	PHE	CB-CG-CD1	8.03	126.42	120.80
1	D	207	ARG	CD-NE-CZ	8.00	134.80	123.60
1	D	107	ASP	CB-CG-OD2	8.00	125.50	118.30
1	A	329	ASP	CB-CG-OD2	7.98	125.48	118.30
1	A	195	PHE	CG-CD1-CE1	7.97	129.56	120.80
1	B	113	ALA	O-C-N	-7.96	109.67	123.20
1	B	152	PHE	CB-CG-CD2	7.95	126.37	120.80
1	A	263	GLU	CG-CD-OE1	7.95	134.20	118.30
1	D	267	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	B	68	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	368	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	B	329	ASP	CB-CG-OD1	-7.88	111.21	118.30
1	A	228	MET	CG-SD-CE	-7.87	87.61	100.20
1	A	79	GLU	O-C-N	-7.79	110.23	122.70
1	A	228	MET	CB-CA-C	-7.78	94.85	110.40
1	B	302	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	C	207	ARG	CD-NE-CZ	7.77	134.47	123.60
1	A	42	ALA	C-N-CA	7.75	138.57	122.30
1	A	198	GLU	N-CA-CB	-7.74	96.66	110.60
1	A	265	SER	O-C-N	-7.73	110.34	122.70
1	B	367	ARG	CD-NE-CZ	7.72	134.41	123.60
1	B	178	PHE	CD1-CE1-CZ	7.69	129.33	120.10
1	D	329	ASP	CB-CG-OD2	7.69	125.22	118.30
1	C	214	ASP	CB-CG-OD1	7.65	125.19	118.30
1	D	172	ARG	NH1-CZ-NH2	-7.63	111.00	119.40
1	D	119	MET	CG-SD-CE	7.63	112.41	100.20
1	A	216	ASP	CB-CG-OD1	7.63	125.16	118.30
1	C	274	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	D	267	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	192	ASP	O-C-N	-7.55	110.37	123.20
1	A	253	ALA	N-CA-CB	7.53	120.65	110.10
1	D	142	THR	CA-CB-CG2	-7.53	101.85	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	200	VAL	CG1-CB-CG2	-7.53	98.85	110.90
1	D	12	ARG	NE-CZ-NH1	-7.52	116.54	120.30
1	B	358	LEU	CB-CA-C	-7.51	95.93	110.20
1	A	301	GLU	OE1-CD-OE2	-7.48	114.32	123.30
1	A	272	LEU	CA-CB-CG	7.47	132.48	115.30
1	B	62	GLU	OE1-CD-OE2	7.45	132.24	123.30
1	C	194	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	146	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	236	ASP	CB-CG-OD2	7.41	124.97	118.30
1	B	372	LYS	CD-CE-NZ	-7.39	94.69	111.70
1	A	194	ARG	NH1-CZ-NH2	-7.38	111.28	119.40
1	B	298	LYS	CA-CB-CG	7.37	129.62	113.40
1	A	199	ILE	CA-CB-CG2	7.31	125.52	110.90
1	B	322	GLN	CB-CG-CD	7.30	130.58	111.60
1	C	94	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	A	226	ASP	CB-CG-OD2	7.25	124.82	118.30
1	A	174	GLU	C-N-CA	7.23	139.78	121.70
1	A	198	GLU	OE1-CD-OE2	-7.22	114.64	123.30
1	B	228	MET	CA-CB-CG	7.21	125.56	113.30
1	C	314	GLU	N-CA-CB	7.19	123.54	110.60
1	C	311	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	B	319	PHE	CB-CG-CD2	7.15	125.81	120.80
1	B	16	GLY	O-C-N	-7.14	111.28	122.70
1	B	228	MET	CG-SD-CE	7.11	111.58	100.20
1	A	392	LEU	CA-CB-CG	7.09	131.62	115.30
1	B	152	PHE	CB-CG-CD1	-7.08	115.85	120.80
1	B	297	ARG	NH1-CZ-NH2	-7.07	111.62	119.40
1	B	214	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	243	ALA	N-CA-CB	-7.06	100.21	110.10
1	A	91	SER	C-N-CA	7.05	137.11	122.30
1	A	232	ARG	CA-CB-CG	7.05	128.90	113.40
1	A	129	ARG	NH1-CZ-NH2	7.02	127.12	119.40
1	A	244	GLY	O-C-N	-7.02	111.47	122.70
1	C	367	ARG	NE-CZ-NH1	7.01	123.81	120.30
1	B	332	TRP	CH2-CZ2-CE2	-7.00	110.40	117.40
1	C	4	SER	CA-C-N	6.98	132.56	117.20
1	A	68	ARG	NH1-CZ-NH2	6.98	127.08	119.40
1	A	339	VAL	CA-CB-CG2	6.96	121.34	110.90
1	B	187	GLU	CG-CD-OE1	-6.96	104.38	118.30
1	B	240	THR	N-CA-CB	-6.95	97.10	110.30
1	A	176	ASP	O-C-N	-6.95	111.59	122.70
1	B	261	GLU	OE1-CD-OE2	-6.94	114.97	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	29	GLU	CG-CD-OE1	6.93	132.16	118.30
1	A	155	TYR	O-C-N	6.90	133.75	122.70
1	B	187	GLU	OE1-CD-OE2	6.90	131.58	123.30
1	A	358	LEU	CB-CG-CD2	6.89	122.72	111.00
1	C	371	ARG	CD-NE-CZ	6.87	133.22	123.60
1	A	30	LEU	C-N-CA	-6.86	107.89	122.30
1	A	174	GLU	N-CA-CB	-6.84	98.28	110.60
1	A	153	TYR	CB-CG-CD1	-6.84	116.90	121.00
1	A	158	GLY	O-C-N	-6.83	111.77	122.70
1	B	85	MET	CA-CB-CG	6.82	124.90	113.30
1	A	226	ASP	O-C-N	-6.82	111.79	122.70
1	A	264	ALA	O-C-N	-6.81	111.80	122.70
1	A	12	ARG	CD-NE-CZ	6.81	133.13	123.60
1	A	42	ALA	CA-C-N	6.81	129.81	116.20
1	C	68	ARG	CD-NE-CZ	6.80	133.12	123.60
1	A	207	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	D	200	VAL	N-CA-CB	6.79	126.45	111.50
1	A	104	ALA	N-CA-CB	6.79	119.60	110.10
1	D	276	VAL	CB-CA-C	6.78	124.28	111.40
1	B	194	ARG	NH1-CZ-NH2	-6.76	111.97	119.40
1	D	94	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	B	210	ASP	CB-CG-OD1	6.74	124.37	118.30
1	C	317	GLU	OE1-CD-OE2	-6.74	115.21	123.30
1	A	243	ALA	N-CA-CB	-6.74	100.67	110.10
1	A	232	ARG	NE-CZ-NH1	-6.71	116.95	120.30
1	A	162	GLU	OE1-CD-OE2	-6.70	115.26	123.30
1	A	36	SER	O-C-N	-6.70	111.98	122.70
1	A	387	MET	CG-SD-CE	6.67	110.87	100.20
1	A	298	LYS	N-CA-CB	-6.66	98.61	110.60
1	A	18	PHE	CG-CD1-CE1	6.65	128.12	120.80
1	B	11	ALA	CB-CA-C	-6.63	100.16	110.10
1	B	192	ASP	CA-C-N	6.63	129.46	116.20
1	D	23	ALA	CB-CA-C	-6.62	100.18	110.10
1	A	150	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	94	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	C	176	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	178	PHE	CG-CD1-CE1	-6.56	113.59	120.80
1	C	4	SER	CA-C-O	-6.56	106.33	120.10
1	C	104	ALA	CB-CA-C	-6.55	100.27	110.10
1	D	107	ASP	CB-CG-OD1	-6.55	112.41	118.30
1	A	195	PHE	CB-CG-CD1	6.54	125.38	120.80
1	C	254	ALA	N-CA-CB	6.53	119.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	297	ARG	CD-NE-CZ	6.52	132.73	123.60
1	A	317	GLU	OE1-CD-OE2	6.51	131.11	123.30
1	B	297	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	D	12	ARG	CG-CD-NE	6.50	125.45	111.80
1	A	95	ALA	N-CA-CB	6.49	119.19	110.10
1	B	318	ALA	CB-CA-C	-6.46	100.41	110.10
1	A	223	ALA	CB-CA-C	6.45	119.77	110.10
1	A	263	GLU	OE1-CD-OE2	-6.45	115.56	123.30
1	C	302	ARG	NH1-CZ-NH2	6.44	126.48	119.40
1	C	371	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	111	ILE	CB-CG1-CD1	6.43	131.90	113.90
1	B	187	GLU	CB-CG-CD	-6.43	96.85	114.20
1	A	250	ASN	OD1-CG-ND2	-6.40	107.18	121.90
1	A	269	ILE	CB-CG1-CD1	-6.40	95.98	113.90
1	B	119	MET	CG-SD-CE	-6.40	89.97	100.20
1	C	104	ALA	N-CA-CB	6.39	119.04	110.10
1	A	379	ILE	C-N-CA	6.38	135.70	122.30
1	B	378	CYS	O-C-N	-6.37	112.51	122.70
1	A	364	GLU	OE1-CD-OE2	-6.37	115.66	123.30
1	B	137	PHE	CB-CG-CD2	6.36	125.25	120.80
1	A	236	ASP	OD1-CG-OD2	-6.36	111.22	123.30
1	B	250	ASN	CB-CG-ND2	6.36	131.95	116.70
1	D	207	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	C	236	ASP	CB-CG-OD1	6.34	124.01	118.30
1	B	183	GLN	CG-CD-OE1	6.34	134.28	121.60
1	B	98	LEU	CB-CG-CD2	-6.34	100.23	111.00
1	B	302	ARG	CG-CD-NE	6.34	125.11	111.80
1	B	41	ARG	NH1-CZ-NH2	-6.33	112.43	119.40
1	B	196	LYS	N-CA-CB	-6.32	99.22	110.60
1	B	108	ALA	N-CA-CB	6.31	118.93	110.10
1	B	328	LYS	N-CA-CB	6.29	121.92	110.60
1	B	11	ALA	N-CA-CB	6.28	118.89	110.10
1	B	314	GLU	CA-C-N	6.26	130.96	117.20
1	A	14	ALA	CB-CA-C	-6.22	100.77	110.10
1	D	202	PHE	CB-CG-CD1	-6.22	116.45	120.80
1	A	34	VAL	CG1-CB-CG2	-6.21	100.97	110.90
1	C	324	CYS	CA-CB-SG	-6.20	102.84	114.00
1	B	207	ARG	CD-NE-CZ	6.20	132.27	123.60
1	B	236	ASP	OD1-CG-OD2	-6.17	111.58	123.30
1	C	133	LYS	N-CA-CB	6.16	121.69	110.60
1	B	319	PHE	CG-CD2-CE2	6.16	127.58	120.80
1	C	348	HIS	N-CA-CB	-6.16	99.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	383	MET	C-N-CA	6.15	135.21	122.30
1	B	146	ASP	OD1-CG-OD2	-6.15	111.62	123.30
1	D	150	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	A	239	GLY	O-C-N	-6.13	112.90	122.70
1	A	365	MET	C-N-CA	6.12	137.00	121.70
1	A	321	ALA	O-C-N	-6.11	112.93	122.70
1	B	157	MET	CA-CB-CG	-6.11	102.92	113.30
1	D	85	MET	CA-CB-CG	6.10	123.67	113.30
1	A	309	ASP	OD1-CG-OD2	-6.10	111.72	123.30
1	B	359	ASN	CA-C-O	6.09	132.90	120.10
1	B	113	ALA	CA-C-N	6.09	128.38	116.20
1	D	231	LEU	CB-CG-CD1	-6.09	100.64	111.00
1	B	153	TYR	CA-CB-CG	-6.08	101.85	113.40
1	A	236	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	239	GLY	CA-C-O	6.08	131.54	120.60
1	A	284	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	20	GLY	O-C-N	-6.04	113.03	122.70
1	D	76	VAL	CA-CB-CG2	-6.04	101.84	110.90
1	A	287	VAL	CG1-CB-CG2	-6.04	101.24	110.90
1	A	359	ASN	CB-CG-OD1	-6.04	109.52	121.60
1	D	129	ARG	NE-CZ-NH2	6.03	123.32	120.30
1	A	299	ALA	C-N-CA	6.02	136.76	121.70
1	A	247	SER	CA-CB-OG	-6.01	94.96	111.20
1	A	350	ILE	CG1-CB-CG2	-6.01	98.17	111.40
1	B	392	LEU	N-CA-CB	6.00	122.41	110.40
1	A	350	ILE	CA-CB-CG1	6.00	122.40	111.00
1	B	112	VAL	CA-CB-CG1	-5.98	101.93	110.90
1	B	305	TRP	CE3-CZ3-CH2	5.98	127.78	121.20
1	A	270	GLN	CB-CA-C	5.97	122.35	110.40
1	C	371	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	364	GLU	O-C-N	-5.96	113.16	122.70
1	B	182	SER	CB-CA-C	-5.95	98.81	110.10
1	B	41	ARG	CG-CD-NE	5.94	124.28	111.80
1	A	54	LEU	CB-CG-CD1	5.91	121.05	111.00
1	B	245	ASN	CB-CA-C	5.88	122.16	110.40
1	A	129	ARG	CG-CD-NE	-5.87	99.47	111.80
1	A	175	GLN	CA-C-O	-5.87	107.78	120.10
1	A	302	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	129	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	A	258	LEU	CB-CG-CD2	5.87	120.97	111.00
1	B	23	ALA	O-C-N	-5.86	113.32	122.70
1	B	339	VAL	CB-CA-C	5.86	122.53	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	339	VAL	N-CA-CB	-5.86	98.61	111.50
1	A	218	TYR	CZ-CE2-CD2	-5.85	114.53	119.80
1	A	232	ARG	CD-NE-CZ	5.85	131.79	123.60
1	B	116	MET	CG-SD-CE	5.84	109.55	100.20
1	D	231	LEU	CB-CG-CD2	-5.84	101.08	111.00
1	D	62	GLU	OE1-CD-OE2	5.83	130.29	123.30
1	A	79	GLU	CG-CD-OE2	5.81	129.92	118.30
1	D	13	THR	N-CA-CB	5.81	121.34	110.30
1	C	118	SER	N-CA-CB	5.81	119.21	110.50
1	D	133	LYS	CA-CB-CG	5.81	126.17	113.40
1	C	33	THR	CA-CB-CG2	5.80	120.52	112.40
1	B	166	LYS	N-CA-CB	5.80	121.03	110.60
1	B	216	ASP	OD1-CG-OD2	-5.79	112.30	123.30
1	B	278	TRP	CA-CB-CG	-5.78	102.71	113.70
1	C	356	ARG	CA-CB-CG	5.77	126.09	113.40
1	B	88	LEU	CB-CG-CD1	5.77	120.80	111.00
1	C	112	VAL	N-CA-CB	5.76	124.17	111.50
1	B	162	GLU	N-CA-CB	5.76	120.97	110.60
1	A	266	ARG	CD-NE-CZ	5.75	131.65	123.60
1	A	379	ILE	O-C-N	-5.75	113.42	123.20
1	B	313	VAL	CA-CB-CG1	5.73	119.49	110.90
1	A	197	ASP	CB-CG-OD1	-5.73	113.15	118.30
1	A	267	ARG	N-CA-CB	-5.72	100.30	110.60
1	C	267	ARG	CD-NE-CZ	5.72	131.60	123.60
1	A	297	ARG	NH1-CZ-NH2	5.71	125.68	119.40
1	A	199	ILE	CB-CA-C	-5.71	100.18	111.60
1	B	160	THR	N-CA-CB	5.70	121.14	110.30
1	A	365	MET	CG-SD-CE	5.70	109.32	100.20
1	B	340	ASN	CB-CG-OD1	-5.70	110.20	121.60
1	A	94	ARG	NE-CZ-NH2	5.70	123.15	120.30
1	B	353	SER	CA-CB-OG	-5.70	95.82	111.20
1	C	343	ALA	CB-CA-C	5.69	118.63	110.10
1	B	187	GLU	CA-CB-CG	-5.67	100.92	113.40
1	B	356	ARG	NH1-CZ-NH2	5.67	125.64	119.40
1	A	64	GLN	CA-C-O	-5.65	108.23	120.10
1	B	4	SER	CB-CA-C	5.65	120.84	110.10
1	A	13	THR	OG1-CB-CG2	-5.64	97.03	110.00
1	B	35	ILE	CB-CA-C	-5.64	100.33	111.60
1	B	234	ALA	N-CA-CB	-5.63	102.21	110.10
1	A	51	GLU	OE1-CD-OE2	5.63	130.06	123.30
1	A	342	GLY	O-C-N	5.63	131.71	122.70
1	A	388	CYS	CA-CB-SG	-5.63	103.87	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	234	ALA	N-CA-CB	-5.63	102.22	110.10
1	B	12	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	A	270	GLN	CG-CD-NE2	5.62	130.19	116.70
1	A	281	VAL	CG1-CB-CG2	-5.62	101.91	110.90
1	C	264	ALA	N-CA-CB	5.62	117.96	110.10
1	A	18	PHE	CB-CG-CD1	5.60	124.72	120.80
1	A	79	GLU	CA-C-O	5.60	131.86	120.10
1	A	195	PHE	CZ-CE2-CD2	5.60	126.82	120.10
1	B	158	GLY	O-C-N	-5.59	113.75	122.70
1	C	297	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	227	SER	O-C-N	-5.59	113.76	122.70
1	A	102	GLN	OE1-CD-NE2	5.58	134.74	121.90
1	C	266	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	166	LYS	CB-CG-CD	5.58	126.11	111.60
1	A	192	ASP	OD1-CG-OD2	-5.58	112.70	123.30
1	B	194	ARG	CB-CG-CD	5.57	126.08	111.60
1	C	96	VAL	CA-CB-CG1	5.57	119.25	110.90
1	A	230	LYS	N-CA-CB	-5.56	100.59	110.60
1	B	216	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	D	79	GLU	OE1-CD-OE2	5.55	129.96	123.30
1	B	79	GLU	OE1-CD-OE2	-5.55	116.64	123.30
1	B	145	LYS	CB-CG-CD	5.55	126.02	111.60
1	C	48	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	B	16	GLY	CA-C-O	5.54	130.58	120.60
1	B	195	PHE	CD1-CE1-CZ	-5.53	113.47	120.10
1	B	226	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	141	ASP	CA-C-O	-5.52	108.51	120.10
1	B	44	VAL	C-N-CA	-5.51	107.92	121.70
1	A	322	GLN	CA-CB-CG	5.51	125.52	113.40
1	A	347	GLY	O-C-N	-5.50	113.90	122.70
1	A	134	MET	CA-CB-CG	5.49	122.64	113.30
1	B	24	ASN	CA-CB-CG	-5.49	101.32	113.40
1	B	355	ALA	CB-CA-C	5.49	118.33	110.10
1	B	158	GLY	CA-C-O	5.49	130.47	120.60
1	A	290	THR	CA-CB-OG1	-5.48	97.50	109.00
1	D	361	LEU	CB-CA-C	-5.48	99.79	110.20
1	C	356	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	C	112	VAL	CA-CB-CG1	-5.47	102.69	110.90
1	A	177	ALA	O-C-N	-5.47	113.95	122.70
1	B	66	PRO	N-CD-CG	-5.47	95.00	103.20
1	A	350	ILE	CA-CB-CG2	-5.46	99.97	110.90
1	B	217	GLU	CG-CD-OE1	5.46	129.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	231	LEU	CD1-CG-CD2	5.46	126.88	110.50
1	B	195	PHE	O-C-N	-5.45	113.98	122.70
1	A	383	MET	O-C-N	-5.44	113.95	123.20
1	A	287	VAL	CA-CB-CG2	5.44	119.06	110.90
1	C	280	THR	CA-CB-OG1	-5.44	97.58	109.00
1	C	4	SER	CA-CB-OG	5.43	125.87	111.20
1	A	267	ARG	CG-CD-NE	-5.43	100.39	111.80
1	B	177	ALA	N-CA-CB	5.43	117.70	110.10
1	B	277	SER	O-C-N	5.43	131.39	122.70
1	A	194	ARG	CD-NE-CZ	5.42	131.19	123.60
1	B	5	ILE	CB-CA-C	-5.42	100.76	111.60
1	A	155	TYR	CD1-CE1-CZ	-5.41	114.93	119.80
1	B	137	PHE	CB-CG-CD1	-5.41	117.01	120.80
1	B	300	LEU	O-C-N	-5.41	114.05	122.70
1	B	274	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	B	338	ASN	O-C-N	-5.40	114.06	122.70
1	A	39	LEU	CB-CG-CD1	5.39	120.16	111.00
1	A	346	ILE	CA-C-O	5.38	131.40	120.10
1	A	88	LEU	O-C-N	-5.37	114.10	122.70
1	C	279	ALA	O-C-N	5.37	131.29	122.70
1	B	144	ILE	CB-CG1-CD1	5.37	128.94	113.90
1	B	113	ALA	C-N-CA	5.37	133.57	122.30
1	D	4	SER	CA-C-N	5.37	129.01	117.20
1	A	4	SER	CA-CB-OG	5.37	125.69	111.20
1	A	35	ILE	CA-C-O	5.36	131.37	120.10
1	A	62	GLU	O-C-N	-5.36	114.08	123.20
1	A	166	LYS	O-C-N	-5.36	114.12	122.70
1	D	355	ALA	CB-CA-C	5.36	118.14	110.10
1	B	212	THR	CA-CB-OG1	-5.35	97.76	109.00
1	C	109	SER	CB-CA-C	-5.35	99.93	110.10
1	B	351	GLY	O-C-N	-5.35	114.14	122.70
1	C	172	ARG	CD-NE-CZ	5.35	131.08	123.60
1	A	172	ARG	CG-CD-NE	-5.34	100.58	111.80
1	B	111	ILE	CB-CA-C	-5.34	100.91	111.60
1	B	122	ALA	CB-CA-C	5.34	118.11	110.10
1	B	22	PHE	CB-CG-CD1	5.34	124.54	120.80
1	D	362	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	80	ALA	CA-C-O	-5.32	108.92	120.10
1	C	314	GLU	OE1-CD-OE2	-5.32	116.92	123.30
1	C	129	ARG	NH1-CZ-NH2	5.32	125.25	119.40
1	A	94	ARG	CD-NE-CZ	5.32	131.04	123.60
1	A	367	ARG	CA-C-N	5.32	128.89	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	267	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
1	C	339	VAL	CB-CA-C	5.31	121.49	111.40
1	A	8	ALA	CA-C-O	5.30	131.23	120.10
1	B	367	ARG	O-C-N	-5.30	114.22	122.70
1	B	181	ALA	O-C-N	-5.29	114.23	122.70
1	C	151	ALA	CB-CA-C	-5.29	102.16	110.10
1	A	188	ALA	O-C-N	5.29	131.16	122.70
1	C	356	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	78	GLN	CA-CB-CG	-5.28	101.78	113.40
1	B	4	SER	CA-C-N	5.28	128.81	117.20
1	A	75	GLY	CA-C-O	-5.28	111.10	120.60
1	A	45	ALA	O-C-N	-5.28	114.26	122.70
1	D	97	ALA	CB-CA-C	5.27	118.01	110.10
1	B	124	HIS	O-C-N	-5.27	114.27	122.70
1	A	69	GLN	O-C-N	-5.26	114.28	122.70
1	C	114	GLY	C-N-CA	-5.26	111.25	122.30
1	A	152	PHE	CB-CG-CD1	-5.26	117.12	120.80
1	B	382	GLY	O-C-N	-5.26	114.29	122.70
1	B	120	SER	CB-CA-C	-5.25	100.13	110.10
1	B	77	PRO	N-CA-CB	5.24	109.59	103.30
1	D	124	HIS	N-CA-CB	5.24	120.03	110.60
1	A	326	VAL	CA-CB-CG1	-5.23	103.05	110.90
1	B	36	SER	CA-CB-OG	5.23	125.33	111.20
1	C	283	VAL	N-CA-CB	5.23	123.02	111.50
1	B	14	ALA	N-CA-CB	5.23	117.42	110.10
1	A	224	THR	OG1-CB-CG2	-5.23	97.97	110.00
1	C	131	GLY	CA-C-O	-5.23	111.19	120.60
1	A	60	ALA	CA-C-O	5.23	131.07	120.10
1	C	173	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	195	PHE	CD1-CE1-CZ	-5.22	113.83	120.10
1	C	216	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	100	MET	O-C-N	-5.22	114.35	122.70
1	A	288	MET	C-N-CA	5.21	133.24	122.30
1	A	297	ARG	C-N-CA	-5.21	108.68	121.70
1	D	22	PHE	C-N-CA	5.20	134.70	121.70
1	A	55	GLY	N-CA-C	-5.19	100.12	113.10
1	A	339	VAL	CB-CA-C	5.19	121.26	111.40
1	A	298	LYS	CA-CB-CG	5.18	124.81	113.40
1	C	55	GLY	N-CA-C	-5.18	100.14	113.10
1	B	358	LEU	O-C-N	-5.18	114.41	122.70
1	B	264	ALA	O-C-N	-5.18	114.42	122.70
1	D	259	MET	CA-CB-CG	5.18	122.10	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	164	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	B	139	MET	CA-CB-CG	-5.17	104.50	113.30
1	B	273	GLY	O-C-N	5.17	130.98	122.70
1	C	42	ALA	CB-CA-C	-5.17	102.34	110.10
1	C	365	MET	CA-CB-CG	5.17	122.08	113.30
1	A	65	ASN	N-CA-CB	-5.16	101.31	110.60
1	A	145	LYS	O-C-N	5.15	130.95	122.70
1	A	333	ASP	CB-CG-OD2	5.15	122.94	118.30
1	C	59	PRO	N-CA-CB	-5.15	96.94	102.60
1	A	334	PRO	O-C-N	-5.15	114.47	122.70
1	A	180	VAL	CA-C-O	-5.14	109.30	120.10
1	B	271	PRO	O-C-N	5.14	130.93	122.70
1	D	215	ALA	N-CA-CB	5.14	117.30	110.10
1	A	307	ILE	C-N-CA	5.14	133.09	122.30
1	A	19	ASN	O-C-N	-5.14	114.46	123.20
1	A	215	ALA	C-N-CA	5.14	134.54	121.70
1	D	79	GLU	CA-CB-CG	-5.13	102.10	113.40
1	A	317	GLU	CG-CD-OE2	-5.13	108.03	118.30
1	A	370	ALA	N-CA-CB	5.13	117.28	110.10
1	B	14	ALA	CB-CA-C	-5.13	102.41	110.10
1	B	94	ARG	NH1-CZ-NH2	5.12	125.03	119.40
1	A	124	HIS	N-CA-CB	-5.12	101.38	110.60
1	A	323	ALA	N-CA-CB	5.12	117.27	110.10
1	C	45	ALA	CB-CA-C	5.12	117.77	110.10
1	D	128	LEU	N-CA-CB	-5.12	100.17	110.40
1	A	36	SER	N-CA-CB	-5.11	102.84	110.50
1	A	378	CYS	N-CA-CB	5.10	119.77	110.60
1	A	224	THR	N-CA-CB	5.09	119.98	110.30
1	A	266	ARG	CG-CD-NE	-5.09	101.10	111.80
1	D	14	ALA	CB-CA-C	5.09	117.74	110.10
1	C	141	ASP	CA-C-O	-5.09	109.41	120.10
1	D	194	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	B	141	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	111	ILE	O-C-N	5.08	130.83	122.70
1	A	383	MET	CA-CB-CG	5.08	121.93	113.30
1	C	156	HIS	CA-CB-CG	5.08	122.23	113.60
1	A	218	TYR	N-CA-CB	-5.08	101.46	110.60
1	D	109	SER	N-CA-CB	5.08	118.11	110.50
1	A	4	SER	CA-C-N	5.07	128.36	117.20
1	A	155	TYR	CA-CB-CG	5.07	123.04	113.40
1	A	196	LYS	N-CA-CB	-5.07	101.47	110.60
1	A	228	MET	CA-C-O	5.07	130.74	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	9	SER	N-CA-CB	5.07	118.10	110.50
1	B	342	GLY	O-C-N	5.05	130.79	122.70
1	D	231	LEU	N-CA-CB	5.05	120.51	110.40
1	B	31	GLY	CA-C-O	-5.05	111.50	120.60
1	C	56	GLN	O-C-N	5.05	130.78	122.70
1	C	117	GLU	CB-CA-C	-5.05	100.31	110.40
1	B	195	PHE	CG-CD1-CE1	5.04	126.35	120.80
1	B	276	VAL	CA-CB-CG2	5.04	118.46	110.90
1	B	301	GLU	OE1-CD-OE2	5.04	129.34	123.30
1	D	231	LEU	CD1-CG-CD2	-5.03	95.40	110.50
1	C	258	LEU	CB-CG-CD2	5.03	119.55	111.00
1	A	302	ARG	N-CA-CB	-5.03	101.55	110.60
1	B	39	LEU	CA-C-O	5.03	130.65	120.10
1	B	174	GLU	CB-CA-C	5.02	120.45	110.40
1	B	142	THR	N-CA-CB	5.02	119.84	110.30
1	C	141	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	C	315	ALA	N-CA-CB	-5.01	103.08	110.10
1	D	281	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	A	265	SER	N-CA-CB	-5.01	102.98	110.50
1	C	157	MET	O-C-N	-5.01	114.68	123.20
1	D	60	ALA	N-CA-CB	5.01	117.11	110.10
1	A	241	VAL	O-C-N	5.01	130.71	122.70
1	C	136	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	200	VAL	Mainchain
1	A	203	ILE	Mainchain
1	A	315	ALA	Mainchain
1	B	358	LEU	Mainchain
1	B	51	GLU	Mainchain
1	B	93	LEU	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	2817	86	0
1	B	2813	0	2819	75	0
1	C	2813	0	2819	84	0
1	D	2813	0	2819	88	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
3	A	8	0	14	7	0
3	B	8	0	14	12	0
3	C	8	0	14	15	0
3	D	8	0	14	20	0
4	A	293	0	0	14	0
4	B	287	0	0	17	0
4	C	101	0	0	7	0
4	D	70	0	0	14	0
All	All	12065	0	11330	352	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 16.

All (352) 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)
3:D:1004:MPD:CM	3:D:1004:MPD:C2	1.79	1.59
3:B:1002:MPD:C2	3:B:1002:MPD:CM	1.79	1.58
3:A:1001:MPD:CM	3:A:1001:MPD:C2	1.79	1.58
3:C:1003:MPD:C2	3:C:1003:MPD:CM	1.81	1.57
3:C:1003:MPD:CM	3:C:1003:MPD:H4	1.67	1.24
3:C:1003:MPD:CM	3:C:1003:MPD:C4	2.15	1.23
1:A:258:LEU:HG	4:A:2051:HOH:O	1.40	1.22
3:D:1004:MPD:HM1	3:D:1004:MPD:H4	1.24	1.15
3:D:1004:MPD:CM	3:D:1004:MPD:H4	1.81	1.11
3:D:1004:MPD:CM	3:D:1004:MPD:C4	2.31	1.08
3:C:1003:MPD:CM	3:C:1003:MPD:C3	2.34	1.06
1:C:81:THR:HG22	1:D:383:MET:HG2	1.39	1.03
3:B:1002:MPD:CM	3:B:1002:MPD:C4	2.37	1.02
3:C:1003:MPD:C4	3:C:1003:MPD:HM1	1.82	1.02
3:B:1002:MPD:CM	3:B:1002:MPD:H4	1.90	1.02
3:B:1002:MPD:CM	3:B:1002:MPD:C3	2.38	1.01
3:C:1003:MPD:H4	3:C:1003:MPD:HM1	1.03	1.01
3:D:1004:MPD:CM	3:D:1004:MPD:C3	2.40	1.00
1:C:156:HIS:HE1	3:C:1003:MPD:HM3	1.28	0.96
3:B:1002:MPD:H4	3:B:1002:MPD:HM1	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:HIS:CE1	3:C:1003:MPD:HM3	2.03	0.92
3:A:1001:MPD:CM	3:A:1001:MPD:C3	2.48	0.91
1:B:4:SER:N	4:B:2282:HOH:O	2.04	0.90
1:D:156:HIS:HE1	3:D:1004:MPD:HM3	1.38	0.88
1:D:290:THR:HA	4:D:1056:HOH:O	1.74	0.87
1:C:203:ILE:HD13	1:C:212:THR:HG23	1.59	0.84
1:B:207:ARG:HG2	1:B:207:ARG:HH11	1.44	0.82
1:D:156:HIS:CE1	3:D:1004:MPD:HM3	2.15	0.82
1:A:175:GLN:HE22	1:A:240:THR:HG23	1.46	0.80
1:B:258:LEU:HG	4:B:2222:HOH:O	1.82	0.80
1:A:156:HIS:HB2	4:A:2232:HOH:O	1.82	0.80
1:B:156:HIS:CE1	3:B:1002:MPD:HM3	2.17	0.80
1:B:316:ASN:HB3	4:B:2027:HOH:O	1.81	0.80
3:C:1003:MPD:C4	3:C:1003:MPD:HM2	2.11	0.79
1:C:57:VAL:HG12	1:C:58:LEU:HG	1.64	0.78
3:B:1002:MPD:C4	3:B:1002:MPD:HM2	2.12	0.77
1:A:298:LYS:NZ	1:A:301:GLU:OE1	2.20	0.75
1:B:156:HIS:HE1	3:B:1002:MPD:HM3	1.50	0.75
1:C:7:ILE:HD13	1:C:362:LEU:HD11	1.68	0.74
1:C:168:TRP:CH2	1:C:329:ASP:HB2	2.25	0.72
1:A:206:GLY:HA3	1:A:209:GLY:O	1.88	0.72
1:A:175:GLN:HE22	1:A:240:THR:CG2	2.02	0.71
1:A:168:TRP:HH2	1:A:329:ASP:HB2	1.54	0.71
1:D:263:GLU:OE1	1:D:266:ARG:NH1	2.24	0.71
1:C:292:PRO:HB3	1:C:376:THR:OG1	1.91	0.70
1:D:317:GLU:HB3	1:D:344:ILE:HG13	1.74	0.70
1:C:268:GLY:HA2	4:C:1094:HOH:O	1.89	0.70
1:A:88:LEU:HD12	1:A:380:GLY:O	1.93	0.69
1:C:300:LEU:HD13	1:C:307:ILE:HG12	1.75	0.69
3:D:1004:MPD:O4	4:D:1042:HOH:O	2.10	0.69
1:A:387:MET:SD	4:A:2167:HOH:O	2.51	0.68
1:D:8:ALA:HB1	1:D:269:ILE:HG21	1.74	0.67
1:A:298:LYS:NZ	1:A:298:LYS:HA	2.09	0.67
3:D:1004:MPD:C4	3:D:1004:MPD:HM2	2.23	0.67
1:A:371:ARG:HG3	4:A:2211:HOH:O	1.95	0.67
1:C:358:LEU:HD22	1:C:362:LEU:HG	1.76	0.67
3:D:1004:MPD:HM1	3:D:1004:MPD:C4	2.05	0.67
1:B:171:SER:OG	4:B:2186:HOH:O	2.12	0.67
1:A:225:LEU:HG	4:A:2205:HOH:O	1.94	0.66
1:B:175:GLN:HE22	1:B:240:THR:HG23	1.60	0.66
1:C:361:LEU:O	1:C:365:MET:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:MET:HE2	4:B:2023:HOH:O	1.95	0.64
1:A:168:TRP:CH2	1:A:329:ASP:HB2	2.32	0.64
1:B:98:LEU:O	1:B:102:GLN:HG2	1.97	0.64
1:B:296:SER:HB3	1:B:374:LEU:HD11	1.78	0.64
1:B:5:ILE:HD12	1:B:103:ILE:CG2	2.28	0.63
1:C:133:LYS:HG2	4:C:1074:HOH:O	1.98	0.63
3:C:1003:MPD:HM2	3:C:1003:MPD:O4	1.96	0.63
1:B:191:LYS:NZ	1:B:191:LYS:HB3	2.13	0.63
1:D:207:ARG:HG2	1:D:207:ARG:HH11	1.63	0.63
1:C:293:ILE:HB	1:C:294:PRO:HD3	1.80	0.63
1:C:297:ARG:HG2	1:C:297:ARG:HH11	1.63	0.63
1:A:280:THR:HG23	1:B:81:THR:HG21	1.80	0.63
1:A:175:GLN:NE2	1:A:240:THR:HG23	2.14	0.63
1:D:258:LEU:HD22	1:D:258:LEU:N	2.14	0.62
1:B:156:HIS:HE1	3:B:1002:MPD:CM	2.12	0.62
1:A:176:ASP:O	1:A:180:VAL:HG23	2.00	0.62
1:D:27:ALA:HB1	1:D:116:MET:HB2	1.82	0.62
1:C:148:LEU:HD22	3:C:1003:MPD:HM2	1.82	0.61
1:D:316:ASN:HD21	1:D:348:HIS:CE1	2.18	0.61
1:C:207:ARG:HG2	1:C:207:ARG:HH11	1.63	0.61
1:A:298:LYS:O	1:A:298:LYS:HD3	2.01	0.61
1:A:133:LYS:HA	4:A:2258:HOH:O	2.01	0.61
1:B:187:GLU:HG2	4:B:2220:HOH:O	2.00	0.61
1:C:322:GLN:O	1:C:326:VAL:HG23	2.01	0.60
1:C:348:HIS:HD2	3:C:1003:MPD:H53	1.66	0.60
1:A:99:GLY:HA3	1:A:111:ILE:HG21	1.82	0.60
1:B:5:ILE:HD12	1:B:103:ILE:HG22	1.83	0.60
1:B:356:ARG:C	1:B:356:ARG:HD2	2.22	0.60
1:D:97:ALA:O	1:D:101:GLN:HG3	2.01	0.59
1:C:269:ILE:O	1:C:271:PRO:HD3	2.01	0.59
1:C:12:ARG:HB2	1:C:254:ALA:HB2	1.84	0.59
1:C:128:LEU:HD21	1:C:137:PHE:CE2	2.37	0.59
1:D:156:HIS:HE1	3:D:1004:MPD:CM	2.12	0.59
1:A:9:SER:HA	1:A:272:LEU:HD22	1.85	0.59
1:C:171:SER:OG	4:C:1027:HOH:O	2.15	0.59
1:B:175:GLN:HE22	1:B:240:THR:CG2	2.15	0.58
1:C:5:ILE:HG13	1:C:100:MET:HG2	1.84	0.58
1:D:175:GLN:HE22	1:D:240:THR:CG2	2.16	0.58
1:C:311:ASP:HB2	1:C:370:ALA:HB1	1.86	0.57
1:C:247:SER:OG	1:C:348:HIS:HB2	2.04	0.57
1:C:28:HIS:HB2	1:C:70:ALA:HB2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:GLU:OE2	4:A:2240:HOH:O	2.17	0.57
1:B:9:SER:HA	1:B:272:LEU:HD22	1.87	0.56
1:A:168:TRP:O	1:A:169:GLN:HB2	2.04	0.56
1:B:134:MET:HE2	1:C:144:ILE:HD11	1.88	0.56
1:B:156:HIS:ND1	1:B:157:MET:N	2.53	0.56
1:B:174:GLU:HB3	4:B:2186:HOH:O	2.06	0.56
1:A:316:ASN:HB3	4:A:2204:HOH:O	2.06	0.56
1:C:292:PRO:HD3	1:C:378:CYS:HB3	1.87	0.56
1:B:361:LEU:O	1:B:365:MET:HG3	2.06	0.55
1:C:361:LEU:HD13	1:C:365:MET:SD	2.47	0.55
1:C:300:LEU:CD1	1:C:307:ILE:HG12	2.35	0.55
1:A:12:ARG:O	1:A:199:ILE:HA	2.07	0.55
3:A:1001:MPD:CM	3:A:1001:MPD:O2	2.52	0.55
1:B:41:ARG:HD2	4:B:2190:HOH:O	2.06	0.54
1:C:364:GLU:O	1:C:368:ARG:HG2	2.06	0.54
1:B:191:LYS:HB3	1:B:191:LYS:HZ1	1.72	0.54
1:A:366:LYS:NZ	4:A:2094:HOH:O	2.40	0.54
1:B:158:GLY:O	1:B:161:ALA:HB3	2.08	0.54
1:B:232:ARG:O	4:B:2131:HOH:O	2.18	0.54
1:C:156:HIS:HE1	3:C:1003:MPD:CM	2.11	0.54
1:C:158:GLY:O	1:C:161:ALA:HB3	2.08	0.54
1:A:298:LYS:HA	1:A:298:LYS:HZ3	1.71	0.54
1:D:53:ILE:HD13	1:D:83:TRP:CZ2	2.42	0.54
1:B:38:VAL:HA	4:B:2190:HOH:O	2.07	0.54
1:D:298:LYS:HE2	1:D:302:ARG:HG3	1.88	0.54
1:B:41:ARG:CD	4:B:2190:HOH:O	2.56	0.53
1:B:339:VAL:HG11	1:B:368:ARG:NH2	2.23	0.53
1:C:280:THR:HG23	1:D:81:THR:HG21	1.90	0.53
1:A:116:MET:HA	1:A:253:ALA:HA	1.89	0.53
1:D:99:GLY:O	1:D:103:ILE:HD12	2.08	0.53
1:A:228:MET:HE3	1:A:244:GLY:HA3	1.91	0.53
1:D:206:GLY:HA3	1:D:209:GLY:O	2.08	0.53
1:C:64:GLN:HE22	1:D:157:MET:CE	2.21	0.53
1:C:239:GLY:HA3	4:C:1100:HOH:O	2.08	0.53
1:D:174:GLU:OE2	1:D:328:LYS:NZ	2.41	0.53
3:B:1002:MPD:H4	3:B:1002:MPD:HM2	1.80	0.52
1:D:5:ILE:HD12	1:D:103:ILE:CG2	2.39	0.52
3:D:1004:MPD:H51	4:D:1073:HOH:O	2.08	0.52
1:A:7:ILE:HG12	1:A:258:LEU:CD1	2.40	0.52
1:A:236:ASP:OD1	1:A:238:GLU:N	2.36	0.52
1:A:354:GLY:HA2	1:A:377:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:HD21	1:C:137:PHE:CZ	2.44	0.52
1:D:236:ASP:HB3	1:D:239:GLY:HA3	1.92	0.52
1:A:186:ALA:HB2	1:A:341:GLY:HA3	1.92	0.52
1:A:298:LYS:HD3	1:A:298:LYS:C	2.30	0.52
1:B:37:ALA:HB2	1:B:200:VAL:HG21	1.91	0.52
1:A:156:HIS:HE1	3:A:1001:MPD:HM2	1.75	0.52
1:C:53:ILE:HD13	1:C:83:TRP:CZ2	2.45	0.51
1:C:279:ALA:CB	1:C:298:LYS:HB3	2.40	0.51
1:D:99:GLY:HA3	4:D:1030:HOH:O	2.09	0.51
1:A:85:MET:HA	1:B:85:MET:HA	1.92	0.51
1:D:175:GLN:HE22	1:D:240:THR:HG21	1.75	0.51
1:A:236:ASP:O	1:A:237:LYS:C	2.49	0.51
1:D:148:LEU:HD22	3:D:1004:MPD:HM2	1.91	0.51
1:D:249:LEU:HD23	3:D:1004:MPD:H11	1.92	0.51
1:B:51:GLU:OE2	1:B:81:THR:OG1	2.25	0.51
1:D:207:ARG:N	1:D:207:ARG:HD3	2.25	0.51
1:D:278:TRP:HA	1:D:386:ALA:O	2.10	0.51
3:C:1003:MPD:CM	3:C:1003:MPD:C1	2.78	0.51
1:B:258:LEU:N	1:B:258:LEU:HD22	2.26	0.51
1:B:171:SER:HB2	4:B:2266:HOH:O	2.10	0.51
1:A:181:ALA:O	1:A:185:LYS:HG3	2.11	0.50
1:A:236:ASP:O	1:A:238:GLU:N	2.45	0.50
1:D:33:THR:HG1	1:D:202:PHE:HD1	1.58	0.50
1:D:258:LEU:HD23	4:D:1030:HOH:O	2.10	0.50
1:D:5:ILE:HG13	1:D:100:MET:HG2	1.92	0.50
1:D:266:ARG:NH2	4:D:1051:HOH:O	2.44	0.50
1:D:77:PRO:HA	4:D:1008:HOH:O	2.12	0.50
1:A:340:ASN:HB2	4:A:2047:HOH:O	2.12	0.50
1:B:186:ALA:HA	1:B:340:ASN:O	2.11	0.50
1:B:298:LYS:HE3	1:B:298:LYS:HA	1.93	0.50
1:C:213:VAL:HA	4:C:1098:HOH:O	2.10	0.50
1:B:274:ARG:HD2	4:B:2282:HOH:O	2.12	0.50
1:D:5:ILE:HD12	1:D:103:ILE:HG22	1.93	0.50
1:D:50:ASN:O	1:D:80:ALA:HB1	2.12	0.50
1:A:200:VAL:O	1:A:200:VAL:HG13	2.11	0.50
1:B:136:ASP:OD1	1:C:140:ILE:HA	2.12	0.50
1:B:191:LYS:NZ	1:B:191:LYS:CB	2.73	0.49
1:A:162:GLU:O	1:A:166:LYS:HG3	2.12	0.49
1:B:156:HIS:HB2	4:B:2287:HOH:O	2.13	0.49
1:B:28:HIS:ND1	1:B:62:GLU:OE2	2.28	0.49
1:D:275:ILE:HA	1:D:389:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ALA:O	1:B:185:LYS:HG3	2.12	0.49
1:B:191:LYS:HG3	4:B:2220:HOH:O	2.13	0.49
1:C:293:ILE:HB	1:C:294:PRO:CD	2.43	0.49
1:D:313:VAL:HG12	1:D:337:VAL:HG13	1.95	0.49
1:B:392:LEU:HD12	4:B:2137:HOH:O	2.12	0.49
1:D:357:ILE:CD1	1:D:375:ALA:HB1	2.43	0.49
1:A:207:ARG:HG2	1:A:208:LYS:H	1.77	0.48
1:B:168:TRP:CH2	1:B:329:ASP:HB2	2.48	0.48
1:D:156:HIS:ND1	1:D:157:MET:N	2.61	0.48
1:D:247:SER:OG	3:D:1004:MPD:H53	2.13	0.48
1:A:220:ARG:NH2	4:A:2097:HOH:O	2.46	0.48
1:C:112:VAL:HG12	1:C:113:ALA:N	2.28	0.48
1:A:158:GLY:O	1:A:161:ALA:HB3	2.13	0.48
1:B:372:LYS:HE3	4:B:2211:HOH:O	2.12	0.48
1:D:275:ILE:HG23	1:D:387:MET:SD	2.54	0.48
1:C:186:ALA:HA	1:C:340:ASN:O	2.14	0.48
1:C:385:VAL:HG22	1:C:386:ALA:N	2.29	0.47
1:D:101:GLN:O	1:D:105:THR:HG23	2.14	0.47
3:D:1004:MPD:O4	3:D:1004:MPD:HM2	2.13	0.47
1:A:58:LEU:HB3	4:A:2225:HOH:O	2.15	0.47
1:A:105:THR:HG21	1:B:101:GLN:HG2	1.97	0.47
1:C:155:TYR:CD2	1:C:159:THR:HG21	2.49	0.47
1:C:170:LEU:HD13	1:C:324:CYS:HB2	1.96	0.47
1:D:292:PRO:HD3	1:D:378:CYS:HA	1.96	0.47
1:D:322:GLN:O	1:D:326:VAL:HG23	2.15	0.47
1:D:333:ASP:OD1	1:D:335:SER:OG	2.31	0.47
1:B:132:VAL:O	1:D:129:ARG:HA	2.14	0.47
1:D:348:HIS:CD2	3:D:1004:MPD:H53	2.49	0.47
1:A:196:LYS:NZ	4:A:2224:HOH:O	2.47	0.47
1:C:105:THR:OG1	1:C:107:ASP:OD2	2.22	0.47
1:C:207:ARG:HD3	1:C:207:ARG:N	2.29	0.47
1:D:275:ILE:HD13	1:D:387:MET:HE1	1.96	0.47
1:C:129:ARG:HD3	1:D:18:PHE:CZ	2.50	0.47
1:A:279:ALA:HB1	1:A:298:LYS:HG3	1.95	0.47
1:A:236:ASP:OD1	1:A:236:ASP:C	2.53	0.47
1:A:237:LYS:HA	1:A:237:LYS:HD3	1.67	0.46
3:C:1003:MPD:CM	3:C:1003:MPD:O2	2.56	0.46
1:A:37:ALA:HB2	1:A:200:VAL:HG21	1.96	0.46
1:D:272:LEU:HD21	4:D:1040:HOH:O	2.15	0.46
1:A:124:HIS:HA	1:A:140:ILE:O	2.15	0.46
1:A:293:ILE:HB	1:A:294:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ILE:O	1:D:38:VAL:HG22	2.16	0.46
1:A:249:LEU:HD21	3:A:1001:MPD:C1	2.46	0.46
1:A:389:ILE:HG22	1:A:390:GLU:N	2.30	0.46
1:C:195:PHE:O	1:C:198:GLU:HG2	2.16	0.46
1:C:284:ASP:OD2	1:C:286:LYS:NZ	2.49	0.46
1:D:190:GLN:NE2	1:D:219:ILE:HD12	2.31	0.46
1:A:319:PHE:CE1	3:A:1001:MPD:HM1	2.52	0.45
1:B:64:GLN:O	1:B:65:ASN:C	2.55	0.45
1:A:361:LEU:O	1:A:365:MET:HG3	2.16	0.45
1:B:350:ILE:HD13	1:B:350:ILE:HG21	1.82	0.45
1:B:94:ARG:O	1:B:97:ALA:HB3	2.17	0.45
1:C:187:GLU:OE2	1:C:221:HIS:HA	2.17	0.45
1:D:51:GLU:HB3	1:D:111:ILE:HD12	1.99	0.45
1:A:317:GLU:OE1	1:A:344:ILE:HG13	2.17	0.45
1:C:7:ILE:HG21	1:C:362:LEU:CD1	2.47	0.45
1:C:85:MET:HA	1:D:85:MET:HA	1.99	0.45
1:D:298:LYS:HE2	1:D:302:ARG:CG	2.47	0.45
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.82	0.45
1:C:263:GLU:OE1	1:C:266:ARG:NH1	2.50	0.45
1:D:158:GLY:HA3	1:D:235:PHE:CD2	2.51	0.45
1:D:364:GLU:O	1:D:368:ARG:HG2	2.17	0.45
1:C:57:VAL:HB	1:C:117:GLU:OE1	2.17	0.44
1:B:348:HIS:CD2	3:B:1002:MPD:H53	2.52	0.44
1:D:46:ALA:HB3	4:D:1064:HOH:O	2.17	0.44
3:D:1004:MPD:CM	3:D:1004:MPD:O2	2.55	0.44
1:D:7:ILE:HG12	1:D:258:LEU:CD1	2.48	0.44
1:B:263:GLU:OE1	1:B:266:ARG:NH2	2.51	0.44
1:C:317:GLU:CD	1:C:342:GLY:HA3	2.38	0.44
1:A:196:LYS:O	1:A:196:LYS:HG2	2.16	0.44
1:A:305:TRP:CE2	1:A:372:LYS:HD3	2.53	0.44
1:C:7:ILE:HG21	1:C:362:LEU:HD13	1.98	0.44
1:D:305:TRP:CZ3	1:D:372:LYS:HB3	2.52	0.44
1:D:357:ILE:HD12	1:D:375:ALA:HB1	2.00	0.44
1:C:362:LEU:CD2	1:C:389:ILE:HG21	2.46	0.44
1:A:12:ARG:HD2	1:A:356:ARG:HG2	2.00	0.44
1:A:350:ILE:HD13	1:A:350:ILE:HG21	1.53	0.44
1:B:356:ARG:HD2	1:B:356:ARG:O	2.17	0.44
1:D:316:ASN:ND2	1:D:348:HIS:CE1	2.86	0.44
1:D:317:GLU:O	1:D:343:ALA:HB3	2.18	0.44
1:A:293:ILE:HG23	1:A:329:ASP:OD1	2.17	0.44
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:HIS:HA	1:B:140:ILE:O	2.18	0.43
1:C:54:LEU:O	1:C:84:GLY:HA2	2.18	0.43
1:D:12:ARG:HB2	1:D:254:ALA:HB2	2.01	0.43
1:D:39:LEU:HB3	1:D:44:VAL:O	2.18	0.43
1:C:293:ILE:CB	1:C:294:PRO:HD3	2.46	0.43
1:B:257:LEU:HD23	1:B:257:LEU:C	2.38	0.43
3:B:1002:MPD:HM2	3:B:1002:MPD:O4	2.18	0.43
1:C:57:VAL:CG2	1:C:88:LEU:HA	2.49	0.43
1:D:305:TRP:CE2	1:D:372:LYS:HD3	2.54	0.43
1:B:313:VAL:HB	1:B:337:VAL:HG22	1.99	0.43
1:A:183:GLN:HA	1:A:345:ALA:HB2	2.01	0.43
1:C:266:ARG:NH2	4:C:1053:HOH:O	2.42	0.43
1:A:225:LEU:O	1:A:228:MET:HB2	2.18	0.43
1:C:259:MET:HB3	1:C:259:MET:HE2	1.77	0.43
1:D:25:THR:HA	1:D:26:PRO:HD3	1.87	0.43
1:A:133:LYS:O	1:A:134:MET:HB2	2.19	0.42
1:B:57:VAL:HG21	1:B:350:ILE:HG22	2.01	0.42
1:C:288:MET:HG3	4:C:1009:HOH:O	2.19	0.42
1:B:5:ILE:HG13	1:B:100:MET:HG2	2.01	0.42
1:D:180:VAL:HG22	1:D:228:MET:HE3	2.02	0.42
1:A:260:SER:HB2	4:A:2135:HOH:O	2.19	0.42
1:A:31:GLY:O	1:A:35:ILE:HG13	2.19	0.42
1:B:175:GLN:NE2	1:B:240:THR:HG23	2.33	0.42
1:D:186:ALA:HA	1:D:340:ASN:O	2.20	0.42
1:D:249:LEU:CD2	3:D:1004:MPD:H11	2.49	0.42
1:A:52:VAL:O	1:A:82:ALA:HA	2.18	0.42
1:B:136:ASP:HA	1:C:139:MET:O	2.19	0.42
1:B:257:LEU:HD23	1:B:258:LEU:N	2.34	0.42
1:C:103:ILE:HA	1:C:108:ALA:O	2.19	0.42
1:C:226:ASP:O	1:C:230:LYS:HG3	2.19	0.42
1:C:358:LEU:O	1:C:362:LEU:HG	2.19	0.42
1:A:53:ILE:HD13	1:A:53:ILE:HG21	1.89	0.42
1:B:359:ASN:O	1:B:360:THR:C	2.57	0.42
1:C:156:HIS:ND1	1:C:157:MET:N	2.67	0.42
1:D:64:GLN:O	1:D:65:ASN:C	2.58	0.42
1:A:328:LYS:HB2	1:A:328:LYS:HE3	1.78	0.42
1:A:258:LEU:N	1:A:258:LEU:HD22	2.34	0.42
1:B:88:LEU:HD12	1:B:380:GLY:O	2.20	0.42
1:C:64:GLN:HE22	1:D:157:MET:HE2	1.83	0.42
1:C:297:ARG:HG2	1:C:297:ARG:NH1	2.33	0.42
1:D:28:HIS:HA	1:D:116:MET:SD	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLY:CA	1:A:111:ILE:HG21	2.48	0.41
1:A:361:LEU:HD22	1:A:365:MET:HG3	2.01	0.41
1:B:293:ILE:HB	1:B:294:PRO:CD	2.50	0.41
1:C:17:SER:HB2	1:C:217:GLU:OE2	2.19	0.41
1:C:155:TYR:CG	1:C:159:THR:HG21	2.55	0.41
1:C:279:ALA:HB3	1:C:298:LYS:HB3	2.02	0.41
1:C:186:ALA:HB2	1:C:341:GLY:HA3	2.01	0.41
1:D:111:ILE:HB	4:D:1030:HOH:O	2.20	0.41
1:D:172:ARG:NH1	4:D:1046:HOH:O	2.36	0.41
1:D:175:GLN:HE22	1:D:240:THR:HG23	1.85	0.41
1:A:280:THR:HA	1:A:384:GLY:O	2.20	0.41
1:D:56:GLN:HB3	4:D:1019:HOH:O	2.20	0.41
1:A:207:ARG:HH11	1:A:207:ARG:CG	2.34	0.41
1:C:162:GLU:OE1	1:C:240:THR:HG22	2.20	0.41
1:D:89:CYS:HB3	4:D:1031:HOH:O	2.20	0.41
1:D:293:ILE:HB	1:D:294:PRO:HD3	2.02	0.41
1:B:231:LEU:HD23	1:B:231:LEU:HA	1.86	0.41
1:A:298:LYS:HA	1:A:298:LYS:HZ2	1.81	0.41
1:A:337:VAL:O	1:A:338:ASN:C	2.59	0.41
1:B:8:ALA:HA	1:B:271:PRO:HB3	2.02	0.41
1:C:293:ILE:CB	1:C:294:PRO:CD	2.99	0.41
1:A:249:LEU:CD2	3:A:1001:MPD:H12	2.51	0.41
1:A:292:PRO:HD3	1:A:378:CYS:HA	2.01	0.41
1:B:207:ARG:HG2	1:B:208:LYS:H	1.85	0.41
1:D:348:HIS:CE1	1:D:353:SER:HG	2.38	0.41
3:D:1004:MPD:CM	3:D:1004:MPD:C1	2.81	0.41
1:A:168:TRP:CZ3	1:A:328:LYS:HB3	2.56	0.41
1:B:139:MET:O	1:C:136:ASP:HA	2.21	0.41
1:D:312:LEU:O	1:D:373:GLY:HA2	2.21	0.41
1:A:77:PRO:HB2	1:A:79:GLU:OE1	2.21	0.41
1:A:133:LYS:H	1:A:133:LYS:HG2	1.42	0.41
1:B:57:VAL:HG21	1:B:350:ILE:CG2	2.50	0.41
1:D:312:LEU:HD13	1:D:368:ARG:HD2	2.02	0.41
1:B:236:ASP:O	1:B:238:GLU:N	2.54	0.40
1:C:350:ILE:HD13	1:C:350:ILE:HG21	1.86	0.40
1:B:274:ARG:NH2	1:B:390:GLU:OE1	2.55	0.40
1:C:157:MET:O	1:C:158:GLY:C	2.60	0.40
1:D:46:ALA:N	4:D:1064:HOH:O	2.54	0.40
1:A:191:LYS:HB3	1:A:191:LYS:HE2	1.94	0.40
1:B:203:ILE:CD1	1:B:212:THR:OG1	2.70	0.40
1:D:41:ARG:NH1	1:D:197:ASP:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LEU:O	1:D:84:GLY:HA2	2.22	0.40
1:C:309:ASP:HB3	1:C:372:LYS:HD2	2.04	0.40
1:D:175:GLN:HB3	1:D:320:ALA:HB3	2.04	0.40
1:D:277:SER:OG	1:D:303:ALA:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	387/389 (100%)	363 (94%)	23 (6%)	1 (0%)	41	46
1	B	387/389 (100%)	366 (95%)	19 (5%)	2 (0%)	29	29
1	C	387/389 (100%)	364 (94%)	21 (5%)	2 (0%)	29	29
1	D	387/389 (100%)	367 (95%)	18 (5%)	2 (0%)	29	29
All	All	1548/1556 (100%)	1460 (94%)	81 (5%)	7 (0%)	29	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ILE
1	C	350	ILE
1	D	350	ILE
1	B	237	LYS
1	D	65	ASN
1	C	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%)	249 (90%)	27 (10%)	8 6
1	B	276/276 (100%)	252 (91%)	24 (9%)	10 8
1	C	276/276 (100%)	250 (91%)	26 (9%)	8 6
1	D	276/276 (100%)	252 (91%)	24 (9%)	10 8
All	All	1104/1104 (100%)	1003 (91%)	101 (9%)	9 7

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	39	LEU
1	A	59	PRO
1	A	64	GLN
1	A	155	TYR
1	A	207	ARG
1	A	221	HIS
1	A	230	LYS
1	A	232	ARG
1	A	237	LYS
1	A	240	THR
1	A	263	GLU
1	A	265	SER
1	A	272	LEU
1	A	276	VAL
1	A	288	MET
1	A	298	LYS
1	A	322	GLN
1	A	328	LYS
1	A	332	TRP
1	A	339	VAL
1	A	350	ILE
1	A	353	SER
1	A	358	LEU

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Mol	Chain	Res	Type
1	A	361	LEU
1	A	367	ARG
1	A	392	LEU
1	B	38	VAL
1	B	39	LEU
1	B	40	GLU
1	B	155	TYR
1	B	174	GLU
1	B	187	GLU
1	B	207	ARG
1	B	232	ARG
1	B	240	THR
1	B	258	LEU
1	B	263	GLU
1	B	270	GLN
1	B	272	LEU
1	B	288	MET
1	B	296	SER
1	B	298	LYS
1	B	322	GLN
1	B	332	TRP
1	B	339	VAL
1	B	356	ARG
1	B	358	LEU
1	B	361	LEU
1	B	366	LYS
1	B	371	ARG
1	C	39	LEU
1	C	40	GLU
1	C	59	PRO
1	C	109	SER
1	C	129	ARG
1	C	134	MET
1	C	155	TYR
1	C	207	ARG
1	C	220	ARG
1	C	224	THR
1	C	232	ARG
1	C	237	LYS
1	C	258	LEU
1	C	272	LEU
1	C	288	MET

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Mol	Chain	Res	Type
1	C	297	ARG
1	C	298	LYS
1	C	307	ILE
1	C	322	GLN
1	C	332	TRP
1	C	335	SER
1	C	353	SER
1	C	358	LEU
1	C	361	LEU
1	C	371	ARG
1	C	374	LEU
1	D	4	SER
1	D	36	SER
1	D	39	LEU
1	D	59	PRO
1	D	85	MET
1	D	116	MET
1	D	144	ILE
1	D	187	GLU
1	D	192	ASP
1	D	207	ARG
1	D	221	HIS
1	D	224	THR
1	D	240	THR
1	D	249	LEU
1	D	258	LEU
1	D	276	VAL
1	D	288	MET
1	D	298	LYS
1	D	322	GLN
1	D	332	TRP
1	D	335	SER
1	D	358	LEU
1	D	361	LEU
1	D	371	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	175	GLN
1	B	175	GLN

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Mol	Chain	Res	Type
1	B	184	ASN
1	C	78	GLN
1	C	184	ASN
1	C	316	ASN
1	D	175	GLN
1	D	184	ASN
1	D	190	GLN
1	D	316	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	A	2004	-	4,4,4	0.65	0	6,6,6	0.59	0
2	SO4	B	2001	-	4,4,4	0.73	0	6,6,6	0.44	0
2	SO4	A	2005	-	4,4,4	0.91	0	6,6,6	1.24	1 (16%)
2	SO4	B	2003	-	4,4,4	0.59	0	6,6,6	0.73	0
2	SO4	B	2006	-	4,4,4	0.72	0	6,6,6	0.81	0
2	SO4	A	2002	-	4,4,4	0.67	0	6,6,6	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MPD	A	1001	-	7,7,7	3.38	1 (14%)	9,10,10	2.90	5 (55%)
3	MPD	D	1004	-	7,7,7	3.41	1 (14%)	9,10,10	1.89	2 (22%)
3	MPD	C	1003	-	7,7,7	3.56	1 (14%)	9,10,10	2.26	3 (33%)
3	MPD	B	1002	-	7,7,7	3.35	1 (14%)	9,10,10	2.28	3 (33%)

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	MPD	D	1004	-	-	3/5/5/5	-
3	MPD	C	1003	-	-	3/5/5/5	-
3	MPD	A	1001	-	-	0/5/5/5	-
3	MPD	B	1002	-	-	2/5/5/5	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	MPD	CM-C2	9.27	1.81	1.52
3	D	1004	MPD	CM-C2	8.87	1.79	1.52
3	A	1001	MPD	CM-C2	8.71	1.79	1.52
3	B	1002	MPD	CM-C2	8.66	1.79	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	MPD	O4-C4-C3	4.70	130.34	111.36
3	A	1001	MPD	CM-C2-C1	4.65	120.27	110.57
3	B	1002	MPD	CM-C2-C1	4.56	120.07	110.57
3	C	1003	MPD	CM-C2-C3	-4.55	88.76	109.96
3	B	1002	MPD	CM-C2-C3	-4.04	91.14	109.96
3	D	1004	MPD	CM-C2-C3	-3.71	92.70	109.96
3	C	1003	MPD	C1-C2-C3	3.38	125.67	109.96
3	D	1004	MPD	CM-C2-C1	3.36	117.57	110.57
3	A	1001	MPD	O2-C2-C1	-3.00	98.45	108.08
3	A	1001	MPD	CM-C2-C3	-2.70	97.40	109.96
3	A	1001	MPD	O2-C2-C3	2.56	119.43	109.80
3	B	1002	MPD	C5-C4-C3	-2.43	100.22	111.69
3	C	1003	MPD	CM-C2-C1	2.26	115.28	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2005	SO4	O4-S-O1	2.02	119.83	109.31

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1002	MPD	O2-C2-C3-C4
3	B	1002	MPD	CM-C2-C3-C4
3	C	1003	MPD	O2-C2-C3-C4
3	C	1003	MPD	CM-C2-C3-C4
3	D	1004	MPD	O2-C2-C3-C4
3	D	1004	MPD	CM-C2-C3-C4
3	C	1003	MPD	C1-C2-C3-C4
3	D	1004	MPD	C1-C2-C3-C4

There are no ring outliers.

4 monomers are involved in 54 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	MPD	7	0
3	D	1004	MPD	20	0
3	C	1003	MPD	15	0
3	B	1002	MPD	12	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 (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	389/389 (100%)	-0.34	4 (1%)	82	84	12, 22, 51, 92	0
1	B	389/389 (100%)	-0.30	7 (1%)	68	71	14, 23, 50, 108	0
1	C	389/389 (100%)	0.28	12 (3%)	49	52	30, 52, 84, 122	0
1	D	389/389 (100%)	0.71	48 (12%)	4	3	30, 58, 109, 138	0
All	All	1556/1556 (100%)	0.09	71 (4%)	32	35	12, 44, 86, 138	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	331	GLY	6.4
1	D	223	ALA	5.9
1	D	232	ARG	5.8
1	D	170	LEU	5.5
1	B	208	LYS	5.0
1	D	330	LEU	4.8
1	C	207	ARG	4.7
1	D	392	LEU	4.7
1	D	208	LYS	4.6
1	C	237	LYS	4.6
1	D	235	PHE	4.5
1	D	186	ALA	4.5
1	D	230	LYS	4.3
1	D	224	THR	4.2
1	D	310	LEU	4.2
1	D	237	LYS	4.1
1	D	228	MET	3.5
1	D	307	ILE	3.4
1	D	180	VAL	3.3
1	C	208	LYS	3.3
1	A	237	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	206	GLY	3.2
1	C	324	CYS	3.2
1	C	235	PHE	3.2
1	D	209	GLY	3.2
1	C	232	ARG	3.2
1	D	234	ALA	3.1
1	B	232	ARG	3.0
1	D	220	ARG	3.0
1	D	231	LEU	2.9
1	D	164	VAL	2.9
1	D	206	GLY	2.9
1	D	178	PHE	2.9
1	D	166	LYS	2.9
1	D	302	ARG	2.8
1	C	229	ALA	2.7
1	C	170	LEU	2.7
1	D	207	ARG	2.6
1	C	239	GLY	2.6
1	D	382	GLY	2.6
1	A	208	LYS	2.6
1	D	227	SER	2.5
1	D	326	VAL	2.5
1	D	239	GLY	2.5
1	D	371	ARG	2.5
1	C	325	ALA	2.5
1	D	176	ASP	2.5
1	D	327	ASN	2.5
1	D	236	ASP	2.5
1	D	160	THR	2.5
1	D	332	TRP	2.4
1	D	219	ILE	2.4
1	D	171	SER	2.4
1	A	206	GLY	2.4
1	D	246	ALA	2.3
1	D	329	ASP	2.3
1	B	235	PHE	2.3
1	D	179	ALA	2.3
1	C	234	ALA	2.3
1	D	362	LEU	2.2
1	D	328	LYS	2.2
1	D	169	GLN	2.2
1	C	265	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	132	VAL	2.2
1	D	156	HIS	2.2
1	D	229	ALA	2.2
1	B	237	LYS	2.1
1	D	238	GLU	2.0
1	D	368	ARG	2.0
1	B	392	LEU	2.0
1	A	133	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MPD	C	1003	8/8	0.72	0.28	56,57,59,60	0
3	MPD	D	1004	8/8	0.75	0.32	60,61,64,64	0
3	MPD	A	1001	8/8	0.80	0.21	44,45,47,51	0
3	MPD	B	1002	8/8	0.86	0.17	36,38,39,39	0
2	SO4	A	2005	5/5	0.89	0.17	52,53,55,57	0
2	SO4	B	2001	5/5	0.93	0.14	74,75,76,76	0
2	SO4	A	2004	5/5	0.94	0.14	61,63,64,65	0
2	SO4	B	2006	5/5	0.95	0.10	39,41,45,45	0
2	SO4	B	2003	5/5	0.97	0.11	55,56,58,61	0
2	SO4	A	2002	5/5	0.97	0.11	54,56,56,57	0

6.5 Other polymers (i)

There are no such residues in this entry.