Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:45 PM GMT

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

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
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:

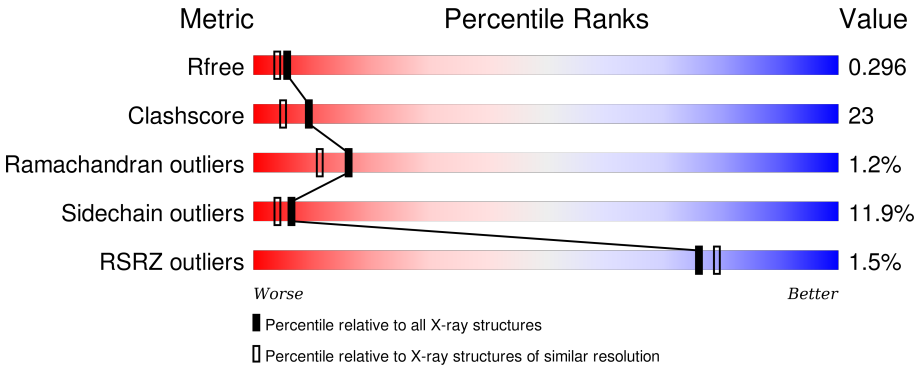
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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}	91344	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	353	56% 38% 5%
1	B	353	3% 49% 39% 10%
1	C	353	2% 52% 38% 9%
1	D	353	53% 36% 10%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLM	A	400	-	-	X	-
2	PLM	B	401	-	-	X	-
3	COA	B	402	-	-	-	X
3	COA	C	402	-	-	-	X

2 Entry composition

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

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

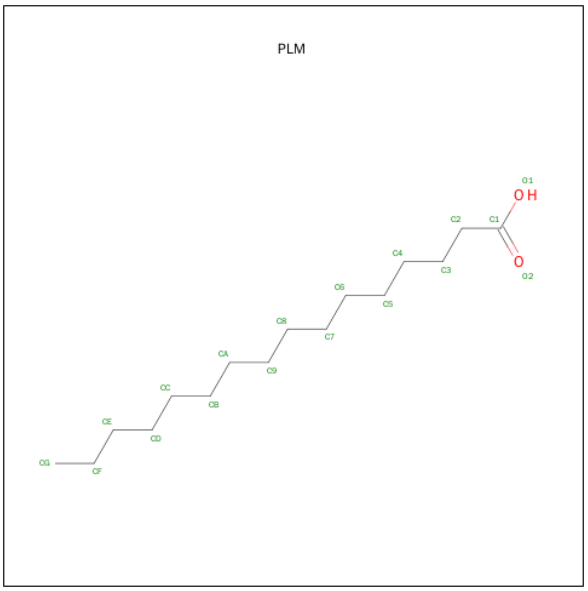
- Molecule 1 is a protein called Alpha-pyrone synthesis polyketide synthase-like Pks11.

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

There are 4 discrepancies between the modelled and reference sequences:

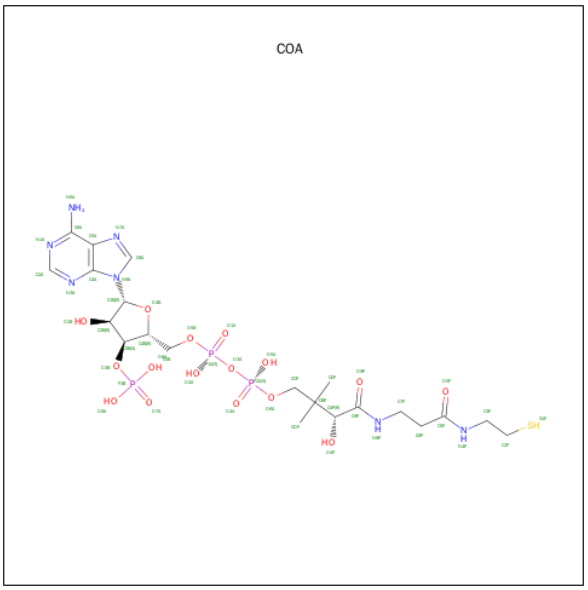
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	SER	CYS	ENGINEERED MUTATION	UNP O06587
C	138	SER	CYS	ENGINEERED MUTATION	UNP O06587
B	138	SER	CYS	ENGINEERED MUTATION	UNP O06587
D	138	SER	CYS	ENGINEERED MUTATION	UNP O06587

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



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

- Molecule 4 is water.

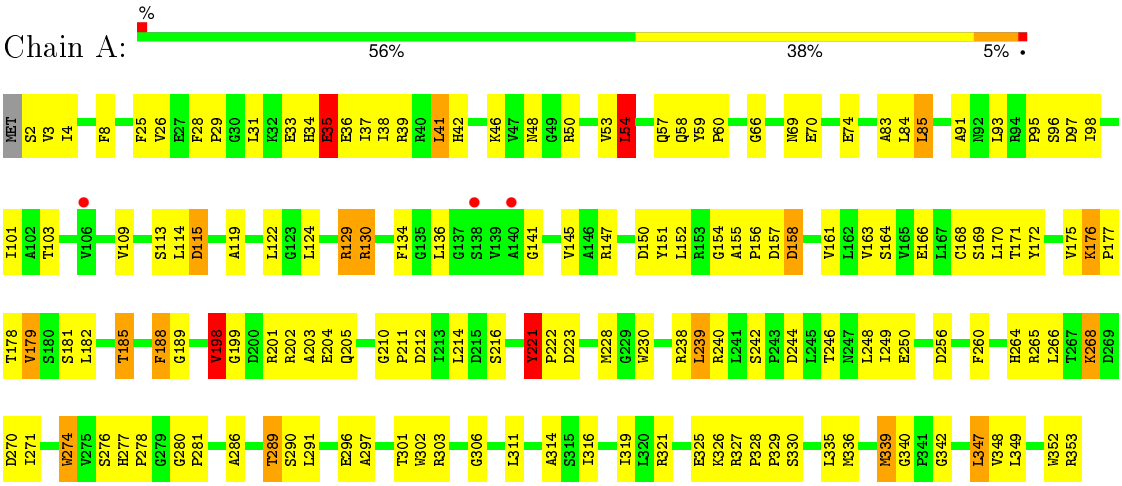
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	C	25	Total	O	0	0
			25	25		
4	B	30	Total	O	0	0
			30	30		
4	D	21	Total	O	0	0
			21	21		

3 Residue-property plots

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.

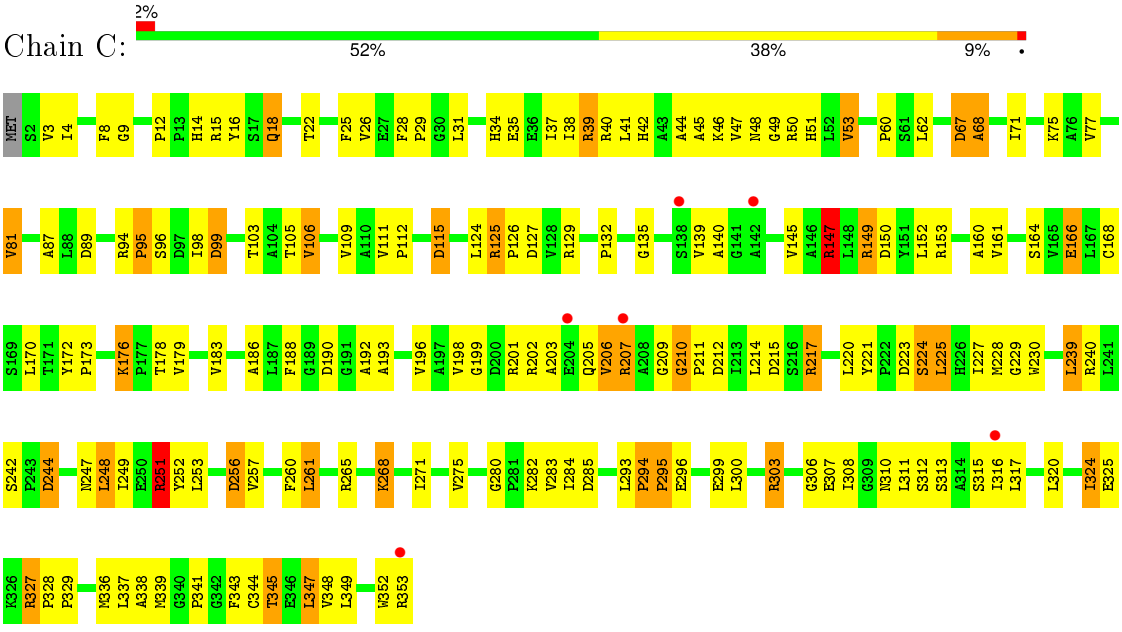
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain A:



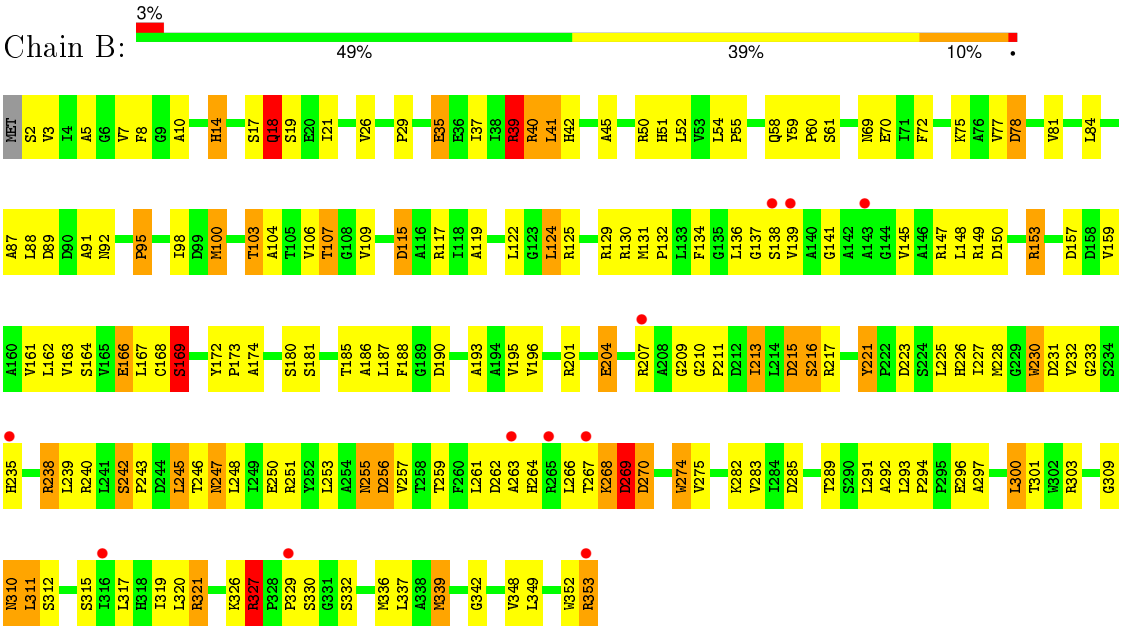
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain C:



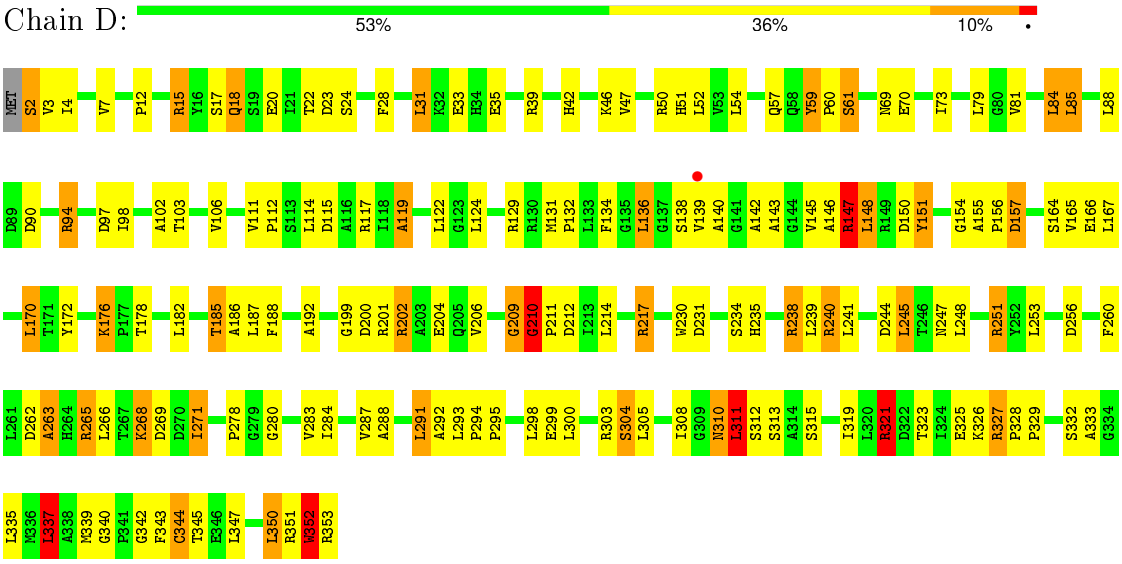
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain B:



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

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	72.17Å 48.86Å 194.47Å 90.00° 97.82° 90.00°	Depositor
Resolution (Å)	32.11 – 2.25 32.12 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (32.11-2.25) 68.6 (32.12-2.25)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.24Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.194 , 0.294 0.206 , 0.296	Depositor DCC
R_{free} test set	2255 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 25.4	EDS
Estimated twinning fraction	0.011 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 44351 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10842	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

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

[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, PLM

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	1.43	15/2695 (0.6%)	1.41	21/3671 (0.6%)
1	B	1.44	7/2706 (0.3%)	1.44	38/3686 (1.0%)
1	C	1.51	19/2695 (0.7%)	1.47	32/3671 (0.9%)
1	D	1.45	12/2695 (0.4%)	1.39	34/3671 (0.9%)
All	All	1.46	53/10791 (0.5%)	1.43	125/14699 (0.9%)

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

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

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	GLU	CD-OE2	-6.28	1.18	1.25
1	C	244	ASP	CB-CG	5.97	1.64	1.51
1	C	16	TYR	CE1-CZ	5.96	1.46	1.38
1	A	35	GLU	CG-CD	5.80	1.60	1.51
1	B	221	TYR	CE1-CZ	5.80	1.46	1.38
1	A	302	TRP	CE3-CZ3	5.79	1.48	1.38
1	A	260	PHE	CE1-CZ	5.76	1.48	1.37
1	A	25	PHE	CE2-CZ	5.73	1.48	1.37
1	C	168	CYS	CB-SG	5.72	1.92	1.82
1	C	53	VAL	CB-CG2	-5.69	1.41	1.52
1	C	41	LEU	C-O	5.68	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	204	GLU	CG-CD	5.61	1.60	1.51
1	C	295	PRO	N-CD	5.60	1.55	1.47
1	D	146	ALA	CA-CB	5.60	1.64	1.52
1	A	74	GLU	CD-OE2	5.55	1.31	1.25
1	B	159	VAL	CA-CB	5.54	1.66	1.54
1	D	240	ARG	CG-CD	5.51	1.65	1.51
1	D	70	GLU	CG-CD	5.48	1.60	1.51
1	C	173	PRO	N-CD	5.46	1.55	1.47
1	A	198	VAL	CB-CG2	-5.45	1.41	1.52
1	D	151	TYR	CE1-CZ	5.44	1.45	1.38
1	A	274	TRP	CE3-CZ3	5.37	1.47	1.38
1	C	203	ALA	CA-CB	-5.37	1.41	1.52
1	A	150	ASP	CB-CG	5.37	1.63	1.51
1	D	145	VAL	CA-CB	5.36	1.66	1.54
1	A	188	PHE	C-O	-5.36	1.13	1.23
1	C	68	ALA	CA-CB	5.31	1.63	1.52
1	B	18	GLN	CG-CD	5.30	1.63	1.51
1	C	251	ARG	CZ-NH2	5.28	1.40	1.33
1	C	106	VAL	CB-CG1	5.27	1.64	1.52
1	C	307	GLU	CD-OE1	5.25	1.31	1.25
1	D	142	ALA	CA-CB	5.22	1.63	1.52
1	B	274	TRP	CE3-CZ3	5.21	1.47	1.38
1	D	59	TYR	CD2-CE2	-5.18	1.31	1.39
1	D	102	ALA	CA-CB	5.17	1.63	1.52
1	C	25	PHE	CE1-CZ	5.17	1.47	1.37
1	C	325	GLU	CD-OE2	5.13	1.31	1.25
1	C	145	VAL	CB-CG2	-5.13	1.42	1.52
1	C	81	VAL	C-O	-5.09	1.13	1.23
1	B	70	GLU	CG-CD	5.09	1.59	1.51
1	A	260	PHE	CD1-CE1	-5.08	1.29	1.39
1	A	33	GLU	CD-OE1	5.07	1.31	1.25
1	A	221	TYR	CD1-CE1	5.06	1.47	1.39
1	B	166	GLU	CG-CD	5.05	1.59	1.51
1	D	321	ARG	CG-CD	5.05	1.64	1.51
1	C	294	PRO	N-CD	5.03	1.54	1.47
1	D	119	ALA	C-O	5.03	1.32	1.23
1	D	299	GLU	CD-OE2	5.03	1.31	1.25
1	D	202	ARG	CG-CD	5.03	1.64	1.51
1	A	188	PHE	C-N	5.02	1.42	1.33
1	A	33	GLU	CG-CD	5.01	1.59	1.51
1	C	260	PHE	CD2-CE2	5.01	1.49	1.39
1	A	151	TYR	CG-CD2	5.01	1.45	1.39

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	149	ARG	NE-CZ-NH1	-15.71	112.45	120.30
1	C	67	ASP	CB-CG-OD1	13.27	130.24	118.30
1	D	202	ARG	NE-CZ-NH1	-11.67	114.47	120.30
1	C	251	ARG	NE-CZ-NH1	-11.14	114.73	120.30
1	B	238	ARG	NE-CZ-NH1	10.65	125.62	120.30
1	C	201	ARG	NE-CZ-NH1	-9.89	115.36	120.30
1	C	149	ARG	NE-CZ-NH2	9.62	125.11	120.30
1	B	78	ASP	CB-CG-OD1	9.23	126.61	118.30
1	A	239	LEU	CA-CB-CG	-8.88	94.89	115.30
1	C	285	ASP	CB-CG-OD2	-8.83	110.35	118.30
1	B	89	ASP	CB-CG-OD1	-8.80	110.38	118.30
1	B	217	ARG	NE-CZ-NH2	8.58	124.59	120.30
1	A	85	LEU	CB-CG-CD2	-8.49	96.57	111.00
1	D	352	TRP	C-N-CA	8.45	142.82	121.70
1	C	251	ARG	NE-CZ-NH2	8.44	124.52	120.30
1	D	147	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	B	150	ASP	CB-CG-OD1	8.23	125.71	118.30
1	B	190	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	D	265	ARG	NE-CZ-NH2	8.03	124.31	120.30
1	D	212	ASP	CB-CG-OD1	8.01	125.50	118.30
1	C	99	ASP	CB-CG-OD1	-7.96	111.13	118.30
1	C	303	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	B	250	GLU	OE1-CD-OE2	7.76	132.62	123.30
1	B	78	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	C	67	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	A	130	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	A	129	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	D	202	ARG	NE-CZ-NH2	7.41	124.00	120.30
1	B	327	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	A	41	LEU	CA-CB-CG	7.20	131.85	115.30
1	D	150	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	339	MET	CG-SD-CE	7.04	111.46	100.20
1	D	23	ASP	CB-CG-OD1	7.01	124.61	118.30
1	B	150	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	B	117	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	C	256	ASP	CB-CG-OD2	-6.87	112.12	118.30
1	A	157	ASP	CB-CG-OD1	-6.83	112.15	118.30
1	B	256	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	40	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	240	ARG	NE-CZ-NH1	-6.72	116.94	120.30
1	C	240	ARG	NE-CZ-NH2	6.63	123.61	120.30
1	B	40	ARG	NE-CZ-NH1	6.55	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	201	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	D	238	ARG	NE-CZ-NH2	6.39	123.49	120.30
1	C	40	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	D	239	LEU	CB-CG-CD1	6.34	121.77	111.00
1	A	280	GLY	N-CA-C	-6.30	97.35	113.10
1	B	225	LEU	CA-CB-CG	6.25	129.68	115.30
1	D	352	TRP	O-C-N	-6.25	112.70	122.70
1	A	303	ARG	NE-CZ-NH2	6.21	123.41	120.30
1	B	240	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	B	303	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	A	303	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	A	270	ASP	CB-CG-OD1	-6.14	112.78	118.30
1	B	327	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	B	321	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	D	350	LEU	CB-CG-CD2	6.05	121.29	111.00
1	B	89	ASP	CB-CG-OD2	6.04	123.74	118.30
1	B	215	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	C	240	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	B	248	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	266	LEU	CB-CG-CD1	-5.92	100.93	111.00
1	A	158	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	149	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	C	129	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	A	256	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	C	347	LEU	CB-CG-CD1	5.84	120.92	111.00
1	C	230	TRP	CB-CA-C	-5.82	98.75	110.40
1	C	190	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	B	270	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	A	54	LEU	CA-CB-CG	5.76	128.54	115.30
1	D	148	LEU	CA-CB-CG	5.76	128.54	115.30
1	B	149	ARG	NE-CZ-NH2	5.75	123.17	120.30
1	D	85	LEU	CB-CG-CD1	-5.74	101.24	111.00
1	B	157	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	B	245	LEU	CA-CB-CG	5.73	128.49	115.30
1	C	39	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	172	TYR	C-N-CD	5.66	140.29	128.40
1	C	293	LEU	C-N-CD	5.65	140.26	128.40
1	D	155	ALA	C-N-CD	5.60	140.16	128.40
1	C	147	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	292	ALA	C-N-CA	5.57	135.62	121.70
1	D	269	ASP	CB-CG-OD1	-5.55	113.30	118.30
1	C	217	ARG	CG-CD-NE	-5.53	100.18	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	39	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	D	265	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	D	129	ARG	CG-CD-NE	-5.48	100.30	111.80
1	C	248	LEU	CB-CG-CD2	-5.46	101.71	111.00
1	C	89	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	266	LEU	CB-CG-CD2	-5.45	101.73	111.00
1	D	231	ASP	N-CA-CB	5.43	120.37	110.60
1	A	53	VAL	CB-CA-C	5.42	121.71	111.40
1	D	291	LEU	CB-CG-CD2	-5.42	101.78	111.00
1	A	319	ILE	CG1-CB-CG2	-5.42	99.48	111.40
1	C	176	LYS	C-N-CD	5.41	139.76	128.40
1	C	294	PRO	C-N-CD	5.41	139.75	128.40
1	C	225	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	170	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	166	GLU	OE1-CD-OE2	-5.33	116.90	123.30
1	D	157	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	D	344	CYS	CA-CB-SG	-5.32	104.43	114.00
1	D	303	ARG	NE-CZ-NH1	-5.29	117.66	120.30
1	D	337	LEU	CA-CB-CG	5.28	127.44	115.30
1	A	114	LEU	CA-CB-CG	5.27	127.42	115.30
1	B	231	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	349	LEU	CB-CG-CD1	-5.23	102.11	111.00
1	B	269	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	210	GLY	C-N-CD	5.20	139.32	128.40
1	C	153	ARG	NE-CZ-NH2	5.19	122.90	120.30
1	D	311	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	C	172	TYR	C-N-CD	5.18	139.28	128.40
1	C	125	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	B	256	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	D	311	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	179	VAL	CG1-CB-CG2	-5.13	102.69	110.90
1	D	136	LEU	CA-CB-CG	5.12	127.08	115.30
1	D	340	GLY	N-CA-C	-5.10	100.35	113.10
1	B	169	SER	CB-CA-C	-5.09	100.42	110.10
1	D	239	LEU	CA-CB-CG	-5.09	103.59	115.30
1	D	202	ARG	CD-NE-CZ	5.08	130.71	123.60
1	D	217	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	266	LEU	CA-CB-CG	5.07	126.96	115.30
1	C	256	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	230	TRP	CB-CA-C	-5.01	100.38	110.40
1	C	153	ARG	NE-CZ-NH1	-5.01	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2642	0	2675	112	0
1	B	2652	0	2681	142	0
1	C	2642	0	2675	134	0
1	D	2642	0	2673	126	1
2	A	18	0	31	11	0
2	B	18	0	31	9	0
2	C	18	0	31	3	0
2	D	18	0	31	5	0
3	B	48	0	32	4	0
3	C	48	0	32	5	1
4	A	20	0	0	0	0
4	B	30	0	0	5	0
4	C	25	0	0	3	0
4	D	21	0	0	2	0
All	All	10842	0	10892	490	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (490) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:SER:HB3	1:C:343:PHE:H	1.10	1.11
1:B:353:ARG:HH11	1:B:353:ARG:HG2	1.12	1.07
1:B:107:THR:HG21	1:B:167:LEU:H	1.00	1.06
1:C:106:VAL:HG11	2:C:401:PLM:H21	1.36	1.04
1:C:34:HIS:HB3	1:C:37:ILE:HD11	1.37	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:LEU:O	1:A:185:THR:HG22	1.61	1.00
1:D:17:SER:OG	1:D:20:GLU:HG3	1.66	0.95
1:B:107:THR:HG21	1:B:167:LEU:N	1.83	0.94
1:B:267:THR:HG22	1:B:269:ASP:H	1.32	0.93
1:D:94:ARG:HB3	1:D:94:ARG:CZ	1.94	0.93
1:C:217:ARG:HG2	1:C:217:ARG:NH2	1.83	0.92
1:B:257:VAL:O	1:B:261:LEU:HD12	1.70	0.91
1:D:15:ARG:CG	1:D:15:ARG:HH21	1.82	0.91
1:C:18:GLN:NE2	1:C:50:ARG:HH21	1.70	0.89
1:A:42:HIS:NE2	1:A:185:THR:HG23	1.87	0.89
1:B:84:LEU:HD23	1:B:122:LEU:HD12	1.54	0.89
1:B:230:TRP:HH2	2:B:401:PLM:H62	1.33	0.88
1:C:249:ILE:HD11	1:C:339:MET:HG3	1.52	0.87
1:A:178:THR:HG23	1:A:181:SER:H	1.37	0.86
1:B:268:LYS:HD2	1:B:291:LEU:O	1.76	0.85
3:C:402:COA:H52A	3:C:402:COA:H8A	1.58	0.84
1:D:308:ILE:HD12	1:D:311:LEU:HD21	1.62	0.82
1:C:140:ALA:HB3	1:C:313:SER:HB2	1.62	0.81
1:C:224:SER:HB3	1:C:343:PHE:N	1.93	0.80
1:C:166:GLU:HG3	1:C:312:SER:HB3	1.63	0.80
1:B:107:THR:CG2	1:B:167:LEU:H	1.91	0.80
1:B:103:THR:HG21	1:B:115:ASP:OD2	1.82	0.80
1:D:15:ARG:HG3	1:D:15:ARG:HH21	1.46	0.79
1:C:18:GLN:HE22	1:C:50:ARG:HH21	1.29	0.79
1:A:69:ASN:HD21	1:A:109:VAL:H	1.29	0.79
1:B:353:ARG:HG2	1:B:353:ARG:NH1	1.92	0.78
1:B:26:VAL:HG11	1:B:35:GLU:OE1	1.83	0.78
1:C:217:ARG:HG2	1:C:217:ARG:HH21	1.47	0.78
1:C:67:ASP:O	1:C:71:ILE:HG13	1.84	0.78
1:D:211:PRO:HG3	1:D:352:TRP:CE3	2.18	0.78
1:B:230:TRP:CH2	2:B:401:PLM:H62	2.19	0.77
1:B:141:GLY:O	1:B:145:VAL:HG23	1.83	0.77
1:B:201:ARG:HD2	1:D:353:ARG:HB2	1.67	0.77
1:C:198:VAL:HG13	1:C:202:ARG:HB3	1.67	0.76
1:C:183:VAL:HG13	3:C:402:COA:CDP	2.16	0.76
1:B:103:THR:HG22	1:B:132:PRO:HA	1.68	0.76
1:B:201:ARG:HE	1:D:353:ARG:HH11	1.33	0.76
1:C:106:VAL:CG1	2:C:401:PLM:H21	2.15	0.76
1:B:69:ASN:HD21	1:B:109:VAL:H	1.35	0.75
1:D:140:ALA:HB3	1:D:313:SER:HB3	1.69	0.74
1:C:337:LEU:HG	1:C:347:LEU:CD2	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:ILE:HD12	1:D:311:LEU:CD2	2.18	0.74
1:A:188:PHE:CZ	2:A:400:PLM:H62	2.23	0.73
1:C:294:PRO:HB2	1:C:295:PRO:HD2	1.71	0.73
1:A:188:PHE:CE1	2:A:400:PLM:H61	2.23	0.72
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.54	0.72
1:C:214:LEU:O	1:C:215:ASP:HB2	1.89	0.72
1:B:233:GLY:HA3	1:B:235[A]:HIS:CE1	2.25	0.72
1:D:310:ASN:HD22	1:D:312:SER:H	1.38	0.72
1:B:185:THR:HA	2:B:401:PLM:HB1	1.73	0.71
1:C:15:ARG:NH1	1:C:49:GLY:HA3	2.05	0.71
1:D:42:HIS:HD2	1:D:186:ALA:HB2	1.54	0.71
1:B:42:HIS:CD2	1:B:186:ALA:HB2	2.26	0.71
1:D:2:SER:N	1:D:200:ASP:OD1	2.23	0.71
1:C:135:GLY:HA2	1:D:111:VAL:HG22	1.71	0.70
1:C:28:PHE:HB2	1:C:31:LEU:HD12	1.73	0.70
1:D:119:ALA:HA	1:D:124:LEU:HG	1.72	0.70
1:A:274:TRP:CZ3	1:A:335:LEU:HD23	2.26	0.70
1:C:37:ILE:HG13	1:C:38:ILE:N	2.07	0.69
1:B:55:PRO:HD2	1:B:58:GLN:HE21	1.57	0.69
1:C:299:GLU:O	1:C:303:ARG:HG3	1.93	0.69
1:B:300:LEU:CD1	1:B:300:LEU:N	2.55	0.69
1:D:201:ARG:HH11	1:D:204:GLU:CD	1.96	0.69
1:B:209:GLY:O	1:B:353:ARG:HG3	1.93	0.69
1:D:178:THR:O	1:D:182:LEU:HG	1.92	0.69
1:D:271:ILE:N	1:D:271:ILE:HD13	2.06	0.69
1:A:3:VAL:HG22	1:A:212:ASP:OD1	1.94	0.68
1:B:211:PRO:HG3	1:B:352:TRP:CZ3	2.28	0.68
1:C:311:LEU:HD11	4:C:504:HOH:O	1.94	0.68
1:B:255:ASN:O	1:B:259:THR:HG23	1.93	0.68
1:A:29:PRO:HD2	1:A:60:PRO:HB3	1.75	0.68
1:C:15:ARG:HB2	1:C:51:HIS:CD2	2.29	0.68
1:B:72:PHE:HE1	1:B:107:THR:HG22	1.58	0.67
1:A:169:SER:HA	2:A:400:PLM:HF2	1.75	0.67
1:D:310:ASN:ND2	1:D:312:SER:H	1.91	0.67
1:B:283:VAL:HG23	3:B:402:COA:H61	1.76	0.67
1:B:300:LEU:HD13	1:B:300:LEU:H	1.59	0.67
1:C:336:MET:HB2	1:C:348:VAL:HB	1.77	0.67
1:D:342:GLY:N	1:D:343:PHE:HA	2.09	0.67
1:B:84:LEU:HD23	1:B:122:LEU:CD1	2.24	0.67
1:B:188:PHE:CD2	2:B:401:PLM:H72	2.30	0.67
1:C:280:GLY:O	1:C:284:ILE:HG13	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:PHE:CD1	1:D:60:PRO:HG3	2.30	0.67
1:D:217:ARG:HB2	1:D:260:PHE:CD1	2.30	0.66
1:D:15:ARG:HD3	1:D:51:HIS:CE1	2.30	0.66
1:B:300:LEU:HD13	1:B:300:LEU:N	2.09	0.66
1:A:28:PHE:HB2	1:A:31:LEU:HD12	1.77	0.66
1:A:188:PHE:CE1	2:A:400:PLM:C6	2.79	0.66
1:B:257:VAL:O	1:B:261:LEU:CD1	2.43	0.65
1:C:251:ARG:HG2	1:C:252:TYR:CE2	2.31	0.65
1:C:15:ARG:HD2	1:C:51:HIS:CE1	2.31	0.65
1:D:268:LYS:HE2	1:D:268:LYS:H	1.62	0.65
1:B:336:MET:HB2	1:B:348:VAL:HB	1.79	0.65
1:A:119:ALA:HA	1:A:124:LEU:HG	1.79	0.64
1:C:4:ILE:O	1:C:210:GLY:HA3	1.97	0.64
1:C:135:GLY:CA	1:D:111:VAL:HG22	2.27	0.64
1:B:153:ARG:HD2	4:B:525:HOH:O	1.97	0.64
1:C:257:VAL:HG13	1:C:261:LEU:HD22	1.78	0.64
1:A:155:ALA:N	1:A:156:PRO:HD3	2.12	0.64
1:C:308:ILE:HD12	1:C:311:LEU:HD22	1.80	0.64
1:D:202:ARG:HG3	1:D:202:ARG:O	1.98	0.64
1:A:3:VAL:HG13	1:A:353:ARG:HH22	1.62	0.64
1:C:42:HIS:CD2	1:C:186:ALA:HA	2.34	0.63
1:B:72:PHE:CE1	1:B:107:THR:HG22	2.33	0.63
1:D:94:ARG:CB	1:D:94:ARG:CZ	2.72	0.63
1:C:140:ALA:HB3	1:C:313:SER:CB	2.27	0.63
1:B:55:PRO:HD2	1:B:58:GLN:NE2	2.12	0.63
1:B:59:TYR:HE2	1:B:169:SER:HB3	1.63	0.63
1:D:28:PHE:HB2	1:D:31:LEU:HD23	1.81	0.63
1:C:99:ASP:OD1	1:C:125:ARG:NH1	2.31	0.63
1:C:209:GLY:O	1:C:210:GLY:O	2.16	0.63
1:B:193:ALA:HB3	1:B:317:LEU:HD12	1.80	0.63
1:A:311:LEU:HB3	1:A:314:ALA:HB3	1.81	0.62
1:B:274:TRP:CZ2	1:B:293:LEU:HD21	2.34	0.62
1:C:220:LEU:HB2	4:D:513:HOH:O	1.99	0.62
1:C:53:VAL:CG2	1:C:75:LYS:HD2	2.29	0.62
1:B:103:THR:CG2	1:B:115:ASP:OD2	2.47	0.62
1:C:244:ASP:HA	1:C:247:ASN:ND2	2.15	0.62
1:B:310:ASN:HD22	1:B:312:SER:H	1.48	0.62
1:A:329:PRO:CD	1:C:265:ARG:NH2	2.63	0.61
1:B:59:TYR:CE2	1:B:169:SER:HB3	2.35	0.61
1:B:294:PRO:HB2	1:B:296:GLU:OE2	2.01	0.61
1:B:29:PRO:HD2	1:B:60:PRO:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HB2	1:A:349:LEU:HD23	1.81	0.61
1:C:221:TYR:CD1	1:C:221:TYR:N	2.68	0.61
1:A:29:PRO:CD	1:A:60:PRO:HB3	2.30	0.61
1:C:239:LEU:HD13	2:C:401:PLM:H42	1.83	0.61
1:C:198:VAL:HG12	1:C:199:GLY:O	2.01	0.60
1:B:267:THR:N	1:B:270:ASP:OD2	2.32	0.60
1:C:18:GLN:HE22	1:C:50:ARG:NH2	1.97	0.60
1:D:278:PRO:HG3	1:D:319:ILE:HD11	1.83	0.60
1:A:265:ARG:HG3	1:D:154:GLY:HA2	1.84	0.60
1:D:15:ARG:CG	1:D:15:ARG:NH2	2.50	0.60
1:D:15:ARG:HG2	1:D:15:ARG:HH21	1.65	0.59
1:C:339:MET:HA	1:C:344:CYS:O	2.02	0.59
1:D:271:ILE:CD1	1:D:271:ILE:N	2.64	0.59
1:D:69:ASN:O	1:D:73:ILE:HG13	2.01	0.59
1:C:35:GLU:O	1:C:39:ARG:HG3	2.03	0.59
1:B:329:PRO:HD2	1:B:332:SER:OG	2.03	0.59
1:A:34:HIS:O	1:A:38:ILE:HG13	2.02	0.59
1:C:206:VAL:O	1:C:207:ARG:HB2	2.03	0.59
1:D:15:ARG:HG2	1:D:15:ARG:NH2	2.17	0.59
1:C:22:THR:O	1:C:26:VAL:HG13	2.03	0.59
1:A:188:PHE:CZ	2:A:400:PLM:C6	2.86	0.58
1:C:125:ARG:NH2	1:C:127:ASP:OD2	2.37	0.58
1:C:294:PRO:HB2	1:C:295:PRO:CD	2.34	0.58
1:B:326:LYS:O	1:B:326:LYS:HG2	2.03	0.58
1:C:198:VAL:CG1	1:C:202:ARG:HB3	2.33	0.58
1:C:77:VAL:O	1:C:81:VAL:HG23	2.03	0.58
1:C:251:ARG:HG2	1:C:252:TYR:CZ	2.39	0.57
1:A:321:ARG:O	1:A:325:GLU:HG3	2.05	0.57
1:C:308:ILE:O	1:C:311:LEU:HD13	2.04	0.57
1:D:333:ALA:HA	1:D:350:LEU:O	2.04	0.57
1:B:166:GLU:HG3	1:B:312:SER:HB3	1.87	0.57
1:D:42:HIS:CD2	1:D:186:ALA:HB2	2.38	0.57
1:C:95:PRO:HB3	1:C:124:LEU:HD12	1.86	0.57
1:B:193:ALA:HB3	1:B:317:LEU:CD1	2.34	0.57
1:C:221:TYR:O	1:C:224:SER:HB2	2.05	0.56
1:A:268:LYS:HB3	1:A:268:LYS:NZ	2.20	0.56
1:B:227:ILE:HA	1:B:242:SER:HB2	1.86	0.56
1:B:275:VAL:HG11	1:B:320:LEU:HB2	1.86	0.56
1:C:221:TYR:HD1	1:C:221:TYR:N	2.01	0.56
1:D:88:LEU:HD21	1:D:98:ILE:HD11	1.85	0.56
1:D:283:VAL:O	1:D:287:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:PRO:O	1:D:295:PRO:C	2.37	0.56
1:B:339:MET:HG2	1:B:339:MET:O	2.05	0.56
1:A:155:ALA:N	1:A:156:PRO:CD	2.68	0.56
1:B:119:ALA:HA	1:B:124:LEU:HG	1.87	0.56
1:B:283:VAL:CG2	3:B:402:COA:H61	2.34	0.56
1:A:26:VAL:HB	1:A:35:GLU:HB2	1.88	0.56
1:D:240:ARG:HG3	1:D:240:ARG:HH21	1.70	0.56
1:A:136:LEU:HG	1:B:132:PRO:HG2	1.88	0.56
1:D:35:GLU:O	1:D:39:ARG:HG3	2.05	0.56
1:B:106:VAL:CG1	2:B:401:PLM:H31	2.36	0.56
1:A:176:LYS:HD3	1:A:238:ARG:CZ	2.36	0.56
1:A:329:PRO:HG3	1:C:265:ARG:HH21	1.72	0.55
1:D:94:ARG:CB	1:D:94:ARG:NH1	2.69	0.55
1:D:111:VAL:HA	1:D:112:PRO:C	2.26	0.55
1:D:94:ARG:HB3	1:D:94:ARG:NH1	2.22	0.55
1:C:283:VAL:HG21	3:C:402:COA:H22	1.88	0.55
1:A:230:TRP:CH2	2:A:400:PLM:H72	2.42	0.55
1:D:28:PHE:CZ	1:D:60:PRO:HD3	2.41	0.55
1:B:87:ALA:HB1	1:B:196:VAL:HG23	1.88	0.54
1:A:28:PHE:O	1:A:29:PRO:C	2.42	0.54
1:C:111:VAL:HA	1:C:112:PRO:C	2.28	0.54
1:A:188:PHE:CD2	2:A:400:PLM:H92	2.43	0.54
1:B:2:SER:HB2	1:B:213:ILE:HD12	1.90	0.54
1:A:48:ASN:N	1:A:306:GLY:O	2.34	0.54
1:B:18:GLN:HE21	1:B:18:GLN:HA	1.72	0.54
1:C:229:GLY:HA2	1:D:111:VAL:HG12	1.90	0.54
1:C:4:ILE:O	1:C:210:GLY:CA	2.55	0.54
1:D:7:VAL:HG12	1:D:321:ARG:HB2	1.89	0.53
1:D:280:GLY:O	1:D:284:ILE:HG13	2.08	0.53
1:A:4:ILE:HB	1:A:211:PRO:HD2	1.89	0.53
1:D:85:LEU:HD21	1:D:122:LEU:HD22	1.89	0.53
1:B:227:ILE:O	1:B:228:MET:HB3	2.07	0.53
1:A:329:PRO:CD	1:C:265:ARG:HH22	2.22	0.53
1:D:140:ALA:HB3	1:D:313:SER:CB	2.37	0.53
1:A:59:TYR:CE1	1:A:169:SER:HB2	2.43	0.53
1:A:178:THR:O	1:A:182:LEU:HG	2.09	0.53
1:B:312:SER:OG	2:B:401:PLM:H21	2.09	0.53
1:B:59:TYR:N	1:B:60:PRO:CD	2.72	0.53
1:A:268:LYS:CB	1:A:268:LYS:NZ	2.71	0.53
1:B:14:HIS:HD2	1:B:52:LEU:O	1.91	0.53
1:C:337:LEU:HG	1:C:347:LEU:HD23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:SER:HA	1:A:347:LEU:O	2.08	0.53
1:C:320:LEU:O	1:C:324:ILE:HG13	2.09	0.52
1:B:35:GLU:O	1:B:39:ARG:HG3	2.09	0.52
1:C:295:PRO:HG2	1:C:296:GLU:H	1.74	0.52
1:B:247:ASN:HD21	1:B:251:ARG:HH21	1.57	0.52
1:B:353:ARG:HH11	1:B:353:ARG:CG	1.99	0.52
1:D:143:ALA:O	1:D:147:ARG:HG2	2.09	0.52
1:B:87:ALA:CB	1:B:196:VAL:HG23	2.40	0.52
1:A:221:TYR:CD1	1:A:221:TYR:N	2.78	0.52
1:A:188:PHE:CE2	2:A:400:PLM:H81	2.45	0.52
1:A:264:HIS:ND1	1:D:157:ASP:OD2	2.35	0.52
1:B:285:ASP:O	1:B:289:THR:N	2.39	0.52
1:A:178:THR:HG22	1:A:181:SER:HB2	1.91	0.51
1:D:265:ARG:O	1:D:266:LEU:HD23	2.11	0.51
1:B:216:SER:HB2	4:B:513:HOH:O	2.11	0.51
1:C:87:ALA:HB1	1:C:196:VAL:HG23	1.91	0.51
1:B:330:SER:HB2	1:B:353:ARG:OXT	2.10	0.51
1:D:352:TRP:O	1:D:353:ARG:HG2	2.11	0.51
1:B:301:THR:HA	1:B:319:ILE:HD13	1.93	0.51
1:D:3:VAL:HG12	1:D:4:ILE:O	2.11	0.51
1:A:221:TYR:HD1	1:A:221:TYR:N	2.08	0.51
1:D:188:PHE:CD2	2:D:400:PLM:H52	2.46	0.51
1:C:164:SER:O	1:C:192:ALA:HA	2.11	0.51
1:D:230:TRP:CH2	2:D:400:PLM:H42	2.45	0.51
1:A:154:GLY:O	1:B:153:ARG:HD3	2.11	0.51
1:B:268:LYS:NZ	1:B:268:LYS:HB3	2.25	0.51
1:D:81:VAL:HG13	1:D:122:LEU:HD21	1.93	0.50
1:C:228:MET:HG2	1:C:341:PRO:HG3	1.92	0.50
1:C:37:ILE:HG13	1:C:38:ILE:H	1.74	0.50
1:D:17:SER:HG	1:D:20:GLU:HG3	1.73	0.50
1:C:251:ARG:CG	1:C:252:TYR:CZ	2.94	0.50
1:D:323:THR:O	1:D:323:THR:HG22	2.10	0.50
1:B:201:ARG:HE	1:D:353:ARG:NH1	2.05	0.50
1:D:201:ARG:NE	1:D:201:ARG:HA	2.27	0.50
1:A:188:PHE:CG	2:A:400:PLM:H92	2.46	0.50
1:D:247:ASN:O	1:D:251:ARG:HB2	2.12	0.50
1:B:51:HIS:HE1	4:B:511:HOH:O	1.94	0.50
1:B:75:LYS:O	1:B:78:ASP:HB2	2.11	0.50
1:B:106:VAL:HG11	2:B:401:PLM:H31	1.93	0.50
1:C:179:VAL:O	1:C:183:VAL:HG23	2.11	0.50
1:A:274:TRP:CD1	1:A:297:ALA:HB1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:THR:HB	1:B:115:ASP:HB3	1.93	0.50
1:B:215:ASP:OD2	1:B:264:HIS:HE1	1.95	0.50
1:C:48:ASN:HB2	1:C:306:GLY:O	2.11	0.50
1:A:178:THR:CG2	1:A:181:SER:HB2	2.42	0.50
1:B:230:TRP:CH2	2:B:401:PLM:C6	2.94	0.50
1:A:182:LEU:O	1:A:185:THR:CG2	2.47	0.50
1:D:12:PRO:O	1:D:51:HIS:HD2	1.94	0.49
1:D:12:PRO:HG3	1:D:79:LEU:HD11	1.94	0.49
1:B:310:ASN:HD22	1:B:311:LEU:N	2.09	0.49
1:D:200:ASP:O	1:D:204:GLU:HG3	2.11	0.49
1:D:165:VAL:HG13	1:D:192:ALA:HB2	1.94	0.49
1:A:134:PHE:O	1:A:136:LEU:N	2.43	0.49
1:C:280:GLY:H	1:C:283:VAL:HB	1.78	0.49
1:B:26:VAL:O	1:B:26:VAL:CG1	2.59	0.49
1:C:14:HIS:O	1:C:51:HIS:HA	2.13	0.49
1:A:66:GLY:O	1:A:70:GLU:HG2	2.13	0.49
1:B:131:MET:O	1:B:131:MET:HG2	2.13	0.49
1:A:329:PRO:HD2	1:C:265:ARG:HH22	1.78	0.49
1:B:275:VAL:HG13	1:B:319:ILE:HG22	1.93	0.49
1:C:152:LEU:HD11	1:C:160:ALA:HB3	1.95	0.49
1:C:18:GLN:HA	1:C:18:GLN:HE21	1.77	0.48
1:D:230:TRP:HH2	2:D:400:PLM:H62	1.77	0.48
1:A:198:VAL:HG13	1:A:202:ARG:HB3	1.94	0.48
1:D:278:PRO:HG3	1:D:319:ILE:CD1	2.43	0.48
1:A:205:GLN:O	1:A:205:GLN:HG3	2.13	0.48
1:B:54:LEU:HB2	1:B:59:TYR:CZ	2.48	0.48
1:B:310:ASN:ND2	1:B:312:SER:H	2.10	0.48
1:B:221:TYR:N	1:B:221:TYR:CD1	2.82	0.48
1:A:98:ILE:CD1	1:A:161:VAL:HG11	2.43	0.48
1:B:243:PRO:HG3	3:B:402:COA:C2A	2.44	0.48
1:D:151:TYR:C	1:D:151:TYR:CD1	2.85	0.48
1:B:230:TRP:HZ3	1:B:239:LEU:HB2	1.78	0.48
1:A:59:TYR:N	1:A:60:PRO:CD	2.77	0.48
1:B:18:GLN:HE22	1:B:50:ARG:HH21	1.62	0.48
1:D:47:VAL:HG22	1:D:305:LEU:CD1	2.43	0.48
1:C:62:LEU:HD11	1:C:68:ALA:HA	1.95	0.48
1:A:155:ALA:O	1:A:158:ASP:HB2	2.14	0.47
1:A:329:PRO:CG	1:C:265:ARG:NH2	2.77	0.47
1:B:262:ASP:C	1:B:264:HIS:N	2.66	0.47
1:A:328:PRO:HB3	1:A:329:PRO:HD2	1.97	0.47
1:A:198:VAL:HG11	1:A:203:ALA:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:7:VAL:CG1	1:D:321:ARG:HB2	2.44	0.47
1:D:328:PRO:HG2	1:D:352:TRP:CD2	2.49	0.47
1:C:251:ARG:HG3	1:C:252:TYR:CE1	2.50	0.47
1:A:152:LEU:HD22	1:A:199:GLY:N	2.29	0.47
1:A:276:SER:O	1:A:301:THR:CG2	2.63	0.47
1:D:325:GLU:C	1:D:327:ARG:H	2.18	0.47
1:A:58:GLN:HG2	1:A:58:GLN:O	2.14	0.47
1:C:207:ARG:HH21	1:C:207:ARG:HG2	1.80	0.47
1:D:244:ASP:HA	1:D:247:ASN:HD22	1.80	0.47
1:C:328:PRO:HG2	1:C:352:TRP:CD2	2.50	0.47
1:B:7:VAL:HG12	1:B:8:PHE:N	2.29	0.47
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.28	0.47
1:D:59:TYR:C	1:D:61:SER:N	2.67	0.47
1:B:72:PHE:HE1	1:B:107:THR:CG2	2.28	0.47
1:D:166:GLU:HG3	1:D:312:SER:HB3	1.95	0.47
1:C:53:VAL:HG22	1:C:75:LYS:HD2	1.95	0.47
1:A:176:LYS:HB2	1:A:176:LYS:HE3	1.63	0.47
1:B:221:TYR:HD1	1:B:221:TYR:N	2.13	0.47
1:A:98:ILE:HG12	1:A:161:VAL:CG1	2.45	0.47
1:C:115:ASP:OD2	1:C:132:PRO:HB3	2.15	0.47
1:C:224:SER:OG	1:C:343:PHE:HB3	2.15	0.46
1:C:308:ILE:CD1	1:C:311:LEU:HD22	2.43	0.46
1:B:29:PRO:CD	1:B:60:PRO:HB3	2.45	0.46
1:B:294:PRO:HB2	1:B:296:GLU:CD	2.36	0.46
1:D:209:GLY:O	1:D:210:GLY:O	2.33	0.46
1:B:106:VAL:HB	1:B:137:GLY:HA2	1.97	0.46
1:A:328:PRO:CB	1:A:329:PRO:HD2	2.46	0.46
1:A:276:SER:O	1:A:301:THR:HG23	2.15	0.46
1:B:5:ALA:O	1:B:91:ALA:HA	2.15	0.46
1:C:214:LEU:HD12	1:C:349:LEU:HG	1.97	0.46
1:C:256:ASP:OD2	1:C:345:THR:HG21	2.14	0.46
1:C:188:PHE:HA	1:C:310:ASN:O	2.15	0.46
1:D:339:MET:HA	1:D:344:CYS:O	2.15	0.46
1:D:79:LEU:CD1	1:D:167:LEU:HD21	2.46	0.46
1:B:201:ARG:HD2	1:D:353:ARG:CB	2.41	0.46
1:B:40:ARG:HH22	3:B:402:COA:H52A	1.80	0.46
1:C:98:ILE:HD12	1:C:124:LEU:HD21	1.97	0.46
1:B:124:LEU:N	1:B:124:LEU:HD23	2.30	0.46
1:B:174:ALA:HB1	1:B:238:ARG:HB2	1.97	0.46
1:A:91:ALA:O	1:A:93:LEU:HG	2.14	0.46
1:B:77:VAL:O	1:B:81:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:GLU:CG	1:C:312:SER:HB3	2.41	0.46
1:B:296:GLU:O	1:B:297:ALA:C	2.54	0.46
1:D:103:THR:HG21	1:D:114:LEU:HB2	1.97	0.46
1:D:310:ASN:HD22	1:D:311:LEU:N	2.12	0.46
1:B:45:ALA:HB1	1:B:187:LEU:CD2	2.46	0.46
1:C:8:PHE:CE1	1:C:9:GLY:O	2.69	0.46
1:A:145:VAL:HG12	1:A:348:VAL:HG11	1.96	0.46
1:B:262:ASP:O	1:B:263:ALA:C	2.54	0.46
1:A:98:ILE:HG22	1:A:98:ILE:O	2.16	0.45
1:B:353:ARG:NH1	1:B:353:ARG:CG	2.69	0.45
1:C:217:ARG:HH21	1:C:217:ARG:CG	2.16	0.45
1:A:188:PHE:CE1	2:A:400:PLM:H62	2.47	0.45
1:A:329:PRO:HG3	1:C:265:ARG:NH2	2.30	0.45
1:A:168:CYS:HB2	1:A:189:GLY:O	2.16	0.45
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.74	0.45
1:D:248:LEU:HA	1:D:248:LEU:HD23	1.73	0.45
1:A:141:GLY:HA3	1:A:316:ILE:CG2	2.46	0.45
1:C:109:VAL:HG13	1:D:134:PHE:HE2	1.80	0.45
1:C:183:VAL:HG13	3:C:402:COA:H131	1.95	0.45
1:D:351:ARG:HD3	1:D:353:ARG:HE	1.82	0.45
1:C:225:LEU:HD11	1:D:117:ARG:HG2	1.99	0.45
1:C:225:LEU:HD13	1:D:117:ARG:NH1	2.32	0.45
1:D:234:SER:HB3	4:D:510:HOH:O	2.15	0.45
1:C:227:ILE:HD13	1:C:242:SER:CB	2.46	0.45
1:D:79:LEU:HD13	1:D:167:LEU:HD21	1.98	0.45
1:C:147:ARG:HD3	1:C:147:ARG:HA	1.78	0.45
1:B:98:ILE:HG12	1:B:161:VAL:HG13	1.99	0.45
1:B:37:ILE:HG12	1:B:41:LEU:HD22	1.99	0.45
1:D:241:LEU:HD11	1:D:245:LEU:CD1	2.47	0.45
1:B:130:ARG:NE	4:B:528:HOH:O	2.42	0.45
1:D:22:THR:HG23	1:D:42:HIS:ND1	2.32	0.45
1:D:304:SER:HB2	1:D:319:ILE:HG12	1.98	0.45
1:C:29:PRO:CD	1:C:60:PRO:HB3	2.46	0.45
1:D:337:LEU:C	1:D:337:LEU:HD12	2.37	0.45
1:A:109:VAL:CG1	1:B:232:VAL:HG21	2.47	0.45
1:A:39:ARG:NH1	1:A:39:ARG:HG2	2.26	0.45
1:C:139:VAL:HA	1:C:338:ALA:HB1	1.99	0.45
1:B:226:HIS:CD2	1:B:226:HIS:H	2.34	0.45
1:A:271:ILE:HG21	1:A:274:TRP:CE2	2.51	0.45
1:B:2:SER:C	1:B:3:VAL:HG23	2.37	0.45
1:C:327:ARG:HA	1:C:328:PRO:HD3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:VAL:HG13	1:D:134:PHE:CE2	2.52	0.45
1:A:171:THR:OG1	2:A:400:PLM:HA2	2.17	0.45
1:B:211:PRO:HG3	1:B:352:TRP:HZ3	1.78	0.45
1:D:18:GLN:HE22	1:D:50:ARG:NE	2.15	0.45
1:C:211:PRO:HD3	1:C:324:ILE:HD13	1.98	0.44
1:B:84:LEU:O	1:B:88:LEU:HG	2.17	0.44
1:A:95:PRO:O	1:A:96:SER:C	2.56	0.44
1:D:342:GLY:N	1:D:343:PHE:CA	2.79	0.44
1:D:85:LEU:HG	1:D:122:LEU:HD21	2.00	0.44
1:C:176:LYS:O	1:C:178:THR:N	2.46	0.44
1:D:201:ARG:NE	1:D:204:GLU:OE1	2.40	0.44
1:B:50:ARG:HG2	1:B:309:GLY:HA3	1.98	0.44
1:C:161:VAL:HG12	1:C:196:VAL:HG13	2.00	0.44
1:C:268:LYS:HE3	1:C:268:LYS:HB2	1.33	0.44
1:D:131:MET:HA	1:D:132:PRO:HD2	1.66	0.44
1:B:230:TRP:CZ3	1:B:239:LEU:HB2	2.52	0.44
1:B:2:SER:C	1:B:3:VAL:CG2	2.86	0.44
1:B:100:MET:HB2	1:B:129:ARG:HB2	1.98	0.44
1:D:214:LEU:HD11	1:D:351:ARG:HB2	2.00	0.44
1:D:166:GLU:HA	1:D:166:GLU:OE1	2.18	0.44
1:D:42:HIS:NE2	1:D:185:THR:CG2	2.81	0.43
1:C:45:ALA:O	1:C:46:LYS:HB2	2.18	0.43
1:D:94:ARG:O	1:D:97:ASP:HB2	2.18	0.43
1:C:4:ILE:O	1:C:210:GLY:N	2.51	0.43
1:A:289:THR:HG22	1:A:290:SER:N	2.32	0.43
1:C:253:LEU:HD11	1:C:337:LEU:HD21	1.99	0.43
1:D:111:VAL:CA	1:D:112:PRO:C	2.87	0.43
1:D:217:ARG:HH21	1:D:217:ARG:HD3	1.68	0.43
1:A:336:MET:HB2	1:A:348:VAL:HB	2.00	0.43
1:B:10:ALA:HA	4:B:522:HOH:O	2.18	0.43
1:B:72:PHE:CE1	1:B:107:THR:CG2	3.01	0.43
1:C:328:PRO:O	1:C:329:PRO:C	2.56	0.43
1:C:227:ILE:HD13	1:C:242:SER:HB3	1.99	0.43
1:C:147:ARG:HA	1:C:150:ASP:HB2	2.00	0.43
1:D:329:PRO:O	1:D:332:SER:OG	2.26	0.43
1:B:26:VAL:HG22	1:B:35:GLU:HA	2.00	0.43
1:D:230:TRP:CH2	2:D:400:PLM:H62	2.53	0.43
1:A:172:TYR:HA	1:A:175:VAL:HG23	2.01	0.43
1:A:274:TRP:CZ3	1:A:335:LEU:CD2	3.00	0.43
1:D:106:VAL:HG11	2:D:400:PLM:H22	2.01	0.43
1:B:88:LEU:O	1:B:92:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:HIS:HA	1:A:278:PRO:HD2	1.61	0.43
1:C:135:GLY:HA2	1:D:111:VAL:CG2	2.43	0.43
1:B:98:ILE:HG12	1:B:161:VAL:CG1	2.48	0.43
1:A:37:ILE:O	1:A:37:ILE:HG12	2.19	0.42
1:C:311:LEU:HB2	1:C:315:SER:OG	2.19	0.42
1:B:100:MET:CB	1:B:129:ARG:HB2	2.49	0.42
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.83	0.42
1:C:12:PRO:HD2	1:C:51:HIS:HB2	2.01	0.42
1:B:45:ALA:HB1	1:B:187:LEU:HD23	2.00	0.42
1:B:172:TYR:N	1:B:173:PRO:CD	2.83	0.42
1:C:3:VAL:HG22	1:C:212:ASP:OD1	2.19	0.42
1:A:3:VAL:HG11	1:A:353:ARG:HH12	1.84	0.42
1:D:291:LEU:O	1:D:292:ALA:HB3	2.18	0.42
1:A:109:VAL:HG13	1:B:134:PHE:HE2	1.85	0.42
1:A:54:LEU:HB2	1:A:59:TYR:CZ	2.55	0.42
1:C:44:ALA:HA	4:C:502:HOH:O	2.19	0.42
1:C:282:LYS:HD2	1:C:282:LYS:HA	1.78	0.42
1:A:103:THR:HA	1:A:163:VAL:O	2.19	0.42
1:D:124:LEU:N	1:D:124:LEU:HD23	2.34	0.42
1:C:152:LEU:O	4:C:518:HOH:O	2.22	0.42
1:C:29:PRO:HD3	1:C:60:PRO:HB3	2.02	0.42
1:C:45:ALA:HB1	1:C:47:VAL:HG23	2.00	0.42
1:D:136:LEU:O	1:D:139:VAL:HG12	2.20	0.42
1:D:31:LEU:HA	1:D:31:LEU:HD12	1.84	0.42
1:C:152:LEU:HA	1:C:152:LEU:HD23	1.85	0.42
1:A:57:GLN:CD	1:A:57:GLN:H	2.23	0.42
1:B:138:SER:N	2:B:401:PLM:O1	2.43	0.42
1:B:124:LEU:O	1:B:125:ARG:C	2.57	0.42
1:C:338:ALA:O	1:C:345:THR:HA	2.20	0.42
1:A:8:PHE:CD1	1:A:83:ALA:HA	2.55	0.42
1:D:262:ASP:O	1:D:263:ALA:C	2.58	0.42
1:A:228:MET:SD	1:A:340:GLY:HA2	2.60	0.42
1:A:95:PRO:O	1:A:97:ASP:N	2.53	0.41
1:A:46:LYS:HB2	1:A:281:PRO:HG3	2.02	0.41
1:A:50:ARG:NH1	1:A:188:PHE:O	2.36	0.41
1:B:21:ILE:HG21	1:B:21:ILE:HD13	1.67	0.41
1:B:294:PRO:CB	1:B:296:GLU:OE2	2.67	0.41
1:A:115:ASP:OD2	1:A:130:ARG:HB3	2.20	0.41
1:A:166:GLU:HA	1:A:166:GLU:OE1	2.19	0.41
1:A:250:GLU:HG2	1:A:286:ALA:HB1	2.03	0.41
1:B:162:LEU:HG	1:B:163:VAL:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:HD12	1:B:300:LEU:N	2.33	0.41
1:C:251:ARG:HG3	1:C:252:TYR:CD1	2.56	0.41
1:D:52:LEU:HD23	1:D:52:LEU:HA	1.80	0.41
1:A:248:LEU:O	1:A:249:ILE:C	2.57	0.41
1:A:211:PRO:HG3	1:A:352:TRP:CZ3	2.55	0.41
1:D:147:ARG:HA	1:D:147:ARG:HE	1.86	0.41
1:C:248:LEU:HA	1:C:248:LEU:HD23	1.47	0.41
1:C:337:LEU:HG	1:C:347:LEU:HD21	2.00	0.41
1:B:136:LEU:O	1:B:139:VAL:HG12	2.20	0.41
1:D:271:ILE:HA	1:D:271:ILE:HD12	1.68	0.41
1:A:330:SER:OG	1:A:353:ARG:OXT	2.29	0.41
1:D:156:PRO:O	1:D:199:GLY:HA3	2.21	0.41
1:B:311:LEU:HB2	1:B:315:SER:OG	2.21	0.41
1:A:54:LEU:HB2	1:A:59:TYR:OH	2.21	0.41
1:A:221:TYR:HA	1:A:222:PRO:HD3	1.89	0.41
1:A:58:GLN:O	1:A:58:GLN:CG	2.68	0.41
1:A:178:THR:OG1	1:A:179:VAL:N	2.53	0.40
1:C:251:ARG:CG	1:C:252:TYR:CE1	3.04	0.40
1:B:7:VAL:HG22	1:B:195:VAL:HG22	2.03	0.40
1:D:84:LEU:HA	1:D:84:LEU:HD23	1.84	0.40
1:D:288:ALA:HA	1:D:293:LEU:HD12	2.02	0.40
1:D:59:TYR:C	1:D:61:SER:H	2.23	0.40
1:B:168:CYS:SG	1:B:188:PHE:HB3	2.61	0.40
1:C:283:VAL:HG23	3:C:402:COA:C6P	2.51	0.40
1:B:253:LEU:O	1:B:256:ASP:HB2	2.21	0.40
1:A:239:LEU:HA	1:A:239:LEU:HD12	1.24	0.40
1:C:193:ALA:HB3	1:C:317:LEU:HD12	2.04	0.40
1:A:176:LYS:HB3	1:A:177:PRO:CD	2.51	0.40
1:D:310:ASN:HD22	1:D:312:SER:N	2.13	0.40
1:B:201:ARG:NE	1:D:353:ARG:HH11	2.08	0.40
1:D:119:ALA:HB1	1:D:124:LEU:HB2	2.04	0.40
1:A:250:GLU:HA	1:A:290:SER:OG	2.22	0.40
1:B:104:ALA:HB3	1:B:164:SER:HA	2.03	0.40
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.78	0.40

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

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	350/353 (99%)	320 (91%)	27 (8%)	3 (1%)	21 18
1	B	351/353 (99%)	317 (90%)	29 (8%)	5 (1%)	14 9
1	C	350/353 (99%)	313 (89%)	33 (9%)	4 (1%)	17 13
1	D	350/353 (99%)	314 (90%)	31 (9%)	5 (1%)	14 9
All	All	1401/1412 (99%)	1264 (90%)	120 (9%)	17 (1%)	16 11

All (17) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	280/281 (100%)	253 (90%)	27 (10%)	10 8
1	B	281/281 (100%)	241 (86%)	40 (14%)	4 2
1	C	280/281 (100%)	257 (92%)	23 (8%)	14 13
1	D	280/281 (100%)	237 (85%)	43 (15%)	3 1
All	All	1121/1124 (100%)	988 (88%)	133 (12%)	6 4

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	35	GLU
1	A	36	GLU
1	A	41	LEU
1	A	54	LEU
1	A	84	LEU
1	A	101	ILE
1	A	113	SER
1	A	115	ASP
1	A	129	ARG
1	A	147	ARG
1	A	164	SER
1	A	176	LYS
1	A	185	THR
1	A	198	VAL
1	A	204	GLU
1	A	221	TYR
1	A	223	ASP
1	A	242	SER
1	A	246	THR
1	A	268	LYS
1	A	289	THR
1	A	291	LEU
1	A	296	GLU
1	A	327	ARG
1	A	339	MET
1	A	347	LEU
1	C	18	GLN

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Mol	Chain	Res	Type
1	C	94	ARG
1	C	95	PRO
1	C	103	THR
1	C	105	THR
1	C	115	ASP
1	C	126	PRO
1	C	147	ARG
1	C	149	ARG
1	C	205	GLN
1	C	206	VAL
1	C	223	ASP
1	C	224	SER
1	C	251	ARG
1	C	261	LEU
1	C	268	LYS
1	C	271	ILE
1	C	275	VAL
1	C	300	LEU
1	C	316	ILE
1	C	324	ILE
1	C	345	THR
1	C	353	ARG
1	B	14	HIS
1	B	17	SER
1	B	18	GLN
1	B	19	SER
1	B	35	GLU
1	B	39	ARG
1	B	41	LEU
1	B	61	SER
1	B	95	PRO
1	B	100	MET
1	B	103	THR
1	B	107	THR
1	B	115	ASP
1	B	124	LEU
1	B	147	ARG
1	B	148	LEU
1	B	153	ARG
1	B	180	SER
1	B	181	SER
1	B	204	GLU

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Mol	Chain	Res	Type
1	B	207	ARG
1	B	213	ILE
1	B	216	SER
1	B	223	ASP
1	B	242	SER
1	B	245	LEU
1	B	246	THR
1	B	247	ASN
1	B	255	ASN
1	B	268	LYS
1	B	269	ASP
1	B	282	LYS
1	B	300	LEU
1	B	310	ASN
1	B	311	LEU
1	B	321	ARG
1	B	327	ARG
1	B	337	LEU
1	B	339	MET
1	B	353	ARG
1	D	2	SER
1	D	15	ARG
1	D	18	GLN
1	D	24	SER
1	D	31	LEU
1	D	33	GLU
1	D	46	LYS
1	D	54	LEU
1	D	57	GLN
1	D	61	SER
1	D	84	LEU
1	D	90	ASP
1	D	94	ARG
1	D	115	ASP
1	D	138	SER
1	D	147	ARG
1	D	148	LEU
1	D	164	SER
1	D	170	LEU
1	D	176	LYS
1	D	185	THR
1	D	187	LEU

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Mol	Chain	Res	Type
1	D	206	VAL
1	D	235	HIS
1	D	238	ARG
1	D	245	LEU
1	D	251	ARG
1	D	253	LEU
1	D	256	ASP
1	D	268	LYS
1	D	271	ILE
1	D	298	LEU
1	D	300	LEU
1	D	304	SER
1	D	310	ASN
1	D	311	LEU
1	D	315	SER
1	D	321	ARG
1	D	335	LEU
1	D	337	LEU
1	D	345	THR
1	D	347	LEU
1	D	352	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	B	264	HIS
1	B	310	ASN
1	D	18	GLN
1	D	51	HIS
1	D	247	ASN
1	D	310	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLM	A	400	-	14,17,17	0.42	0	14,17,17	0.73	0
2	PLM	B	401	-	14,17,17	0.76	0	14,17,17	1.68	3 (21%)
3	COA	B	402	-	40,50,50	1.13	3 (7%)	50,75,75	2.14	12 (24%)
2	PLM	C	401	-	14,17,17	0.53	0	14,17,17	1.80	3 (21%)
3	COA	C	402	-	40,50,50	1.15	4 (10%)	50,75,75	1.82	12 (24%)
2	PLM	D	400	-	14,17,17	0.62	0	14,17,17	1.86	4 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLM	A	400	-	-	0/13/15/15	0/0/0/0
2	PLM	B	401	-	-	0/13/15/15	0/0/0/0
3	COA	B	402	-	-	0/44/64/64	0/3/3/3
2	PLM	C	401	-	-	0/13/15/15	0/0/0/0
3	COA	C	402	-	-	0/44/64/64	0/3/3/3
2	PLM	D	400	-	-	0/13/15/15	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	COA	O5P-C5P	-2.78	1.17	1.23
3	B	402	COA	P3B-O8A	-2.42	1.46	1.54
3	C	402	COA	C5A-N7A	-2.36	1.31	1.39
3	C	402	COA	P3B-O9A	-2.19	1.46	1.54
3	C	402	COA	O9P-C9P	-2.08	1.19	1.23
3	B	402	COA	P3B-O9A	-2.04	1.47	1.54
3	C	402	COA	P1A-O2A	-2.02	1.46	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	402	COA	N3A-C2A-N1A	-8.52	122.37	128.89
3	C	402	COA	N3A-C2A-N1A	-5.67	124.55	128.89
3	B	402	COA	O3B-P3B-O7A	-4.29	96.41	107.11
2	D	400	PLM	C9-C8-C7	-4.20	92.85	114.53
2	C	401	PLM	C6-C5-C4	-3.96	94.08	114.53
2	D	400	PLM	CC-CB-CA	-3.28	97.60	114.53
3	C	402	COA	O3B-C3B-C4B	-3.21	97.39	109.99
3	B	402	COA	C2B-C1B-N9A	-3.17	109.45	114.29
2	B	401	PLM	C9-C8-C7	-3.03	98.88	114.53
2	D	400	PLM	C6-C5-C4	-2.77	100.24	114.53
3	B	402	COA	C1B-N9A-C4A	-2.71	122.85	126.94
3	B	402	COA	CDP-CBP-CAP	-2.43	104.92	109.34
2	C	401	PLM	C5-C4-C3	-2.25	102.90	114.53
2	B	401	PLM	C6-C5-C4	-2.23	102.99	114.53
3	C	402	COA	O8A-P3B-O7A	2.00	117.02	110.58
2	D	400	PLM	CD-CC-CB	2.01	124.90	114.53
3	C	402	COA	C3B-C2B-C1B	2.04	104.88	99.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	COA	C7P-N8P-C9P	2.07	126.62	122.53
3	C	402	COA	O2B-C2B-C3B	2.20	117.50	111.16
3	B	402	COA	N6A-C6A-N1A	2.31	124.17	119.20
3	C	402	COA	C1B-N9A-C4A	2.79	131.15	126.94
3	B	402	COA	C7P-C6P-C5P	2.92	117.12	112.31
3	B	402	COA	P3B-O3B-C3B	2.96	128.67	121.56
3	B	402	COA	C6P-C5P-N4P	3.04	121.74	116.46
3	C	402	COA	C4B-O4B-C1B	3.12	113.15	109.72
3	B	402	COA	O9A-P3B-O8A	3.14	119.35	107.38
3	C	402	COA	CEP-CBP-CCP	3.32	112.80	108.50
3	B	402	COA	C7P-N8P-C9P	3.39	129.25	122.53
3	C	402	COA	N6A-C6A-N1A	3.41	126.52	119.20
2	C	401	PLM	C4-C3-C2	3.54	128.86	113.90
2	B	401	PLM	C4-C3-C2	3.86	130.22	113.90
3	C	402	COA	P3B-O3B-C3B	3.91	130.94	121.56
3	B	402	COA	CDP-CBP-CCP	4.00	113.69	108.50
3	C	402	COA	O6A-CCP-CBP	4.06	117.08	110.55

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 38 short contacts:

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

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	352/353 (99%)	-0.09	3 (0%) 85 87	21, 36, 48, 61	0
1	B	352/353 (99%)	-0.09	11 (3%) 52 57	21, 35, 50, 66	0
1	C	352/353 (99%)	-0.15	6 (1%) 73 77	21, 34, 49, 70	0
1	D	352/353 (99%)	-0.13	1 (0%) 94 95	21, 35, 50, 65	0
All	All	1408/1412 (99%)	-0.11	21 (1%) 76 79	21, 35, 49, 70	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	267	THR	3.2
1	B	329	PRO	3.2
1	A	138	SER	3.2
1	C	207	ARG	3.1
1	B	265	ARG	3.0
1	B	316	ILE	2.6
1	C	204	GLU	2.5
1	B	263	ALA	2.5
1	C	142	ALA	2.5
1	C	353	ARG	2.4
1	A	140	ALA	2.4
1	A	106	VAL	2.3
1	B	353	ARG	2.3
1	D	139	VAL	2.2
1	B	139	VAL	2.2
1	B	207	ARG	2.2
1	B	143	ALA	2.1
1	C	138	SER	2.1
1	B	235[A]	HIS	2.1
1	B	138	SER	2.1
1	C	316	ILE	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
3	COA	B	402	48/48	0.90	0.26	2.99	24,37,50,56	0
3	COA	C	402	48/48	0.89	0.24	2.53	24,37,54,63	0
2	PLM	A	400	18/18	0.92	0.25	1.43	29,36,46,47	0
2	PLM	D	400	18/18	0.92	0.20	1.26	25,33,39,41	0
2	PLM	C	401	18/18	0.93	0.17	0.79	29,31,36,39	0
2	PLM	B	401	18/18	0.93	0.16	0.61	28,37,50,53	0

6.5 Other polymers (i)

There are no such residues in this entry.