



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:27 AM EDT

PDB ID : 1TQY / pdb_00001tqy
Title : The Actinorhodin Ketosynthase/Chain Length Factor
Authors : Keatinge-Clay, A.T.; Maltby, D.A.; Medzihradzsky, K.F.; Khosla, C.; Stroud, R.M.
Deposited on : 2004-06-18
Resolution : 2.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

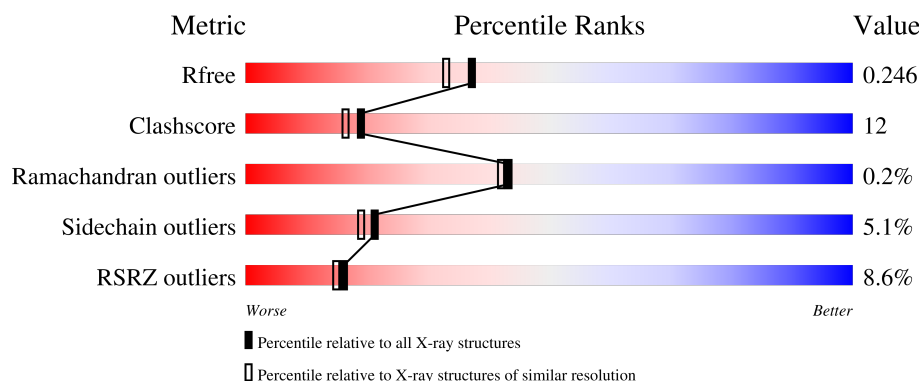
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	424	7% 72% 25% ..
1	C	424	11% 75% 22% ..
1	E	424	21% 73% 25% ..
1	G	424	7% 73% 22% ..
2	B	415	6% 71% 23% ..

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Mol	Chain	Length	Quality of chain
2	D	415	4% 75% 18% • •
2	F	415	6% 72% 22% • •
2	H	415	5% 74% 21% • •

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
4	ACE	E	633	-	-	X	-
4	ACE	G	633	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25535 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 Actinorhodin polyketide putative beta-ketoacyl synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3140	1936	570	618	16			
1	C	421	Total	C	N	O	S	0	0	0
			3140	1936	570	618	16			
1	E	421	Total	C	N	O	S	0	0	0
			3140	1936	570	618	16			
1	G	421	Total	C	N	O	S	0	0	0
			3140	1936	570	618	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q02059
C	1	MET	-	initiating methionine	UNP Q02059
E	1	MET	-	initiating methionine	UNP Q02059
G	1	MET	-	initiating methionine	UNP Q02059

- Molecule 2 is a protein called Actinorhodin polyketide putative beta-ketoacyl synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	402	Total	C	N	O	S	0	0	0
			2970	1863	537	565	5			
2	D	402	Total	C	N	O	S	0	0	0
			2970	1863	537	565	5			
2	F	402	Total	C	N	O	S	0	0	0
			2970	1863	537	565	5			
2	H	402	Total	C	N	O	S	0	0	0
			2970	1863	537	565	5			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q02062
B	-6	ASP	-	expression tag	UNP Q02062
B	-5	TYR	-	expression tag	UNP Q02062
B	-4	LYS	-	expression tag	UNP Q02062
B	-3	ASP	-	expression tag	UNP Q02062
B	-2	ASP	-	expression tag	UNP Q02062
B	-1	ASP	-	expression tag	UNP Q02062
B	0	ASP	-	expression tag	UNP Q02062
B	1	LYS	-	expression tag	UNP Q02062
D	-7	MET	-	initiating methionine	UNP Q02062
D	-6	ASP	-	expression tag	UNP Q02062
D	-5	TYR	-	expression tag	UNP Q02062
D	-4	LYS	-	expression tag	UNP Q02062
D	-3	ASP	-	expression tag	UNP Q02062
D	-2	ASP	-	expression tag	UNP Q02062
D	-1	ASP	-	expression tag	UNP Q02062
D	0	ASP	-	expression tag	UNP Q02062
D	1	LYS	-	expression tag	UNP Q02062
F	-7	MET	-	initiating methionine	UNP Q02062
F	-6	ASP	-	expression tag	UNP Q02062
F	-5	TYR	-	expression tag	UNP Q02062
F	-4	LYS	-	expression tag	UNP Q02062
F	-3	ASP	-	expression tag	UNP Q02062
F	-2	ASP	-	expression tag	UNP Q02062
F	-1	ASP	-	expression tag	UNP Q02062
F	0	ASP	-	expression tag	UNP Q02062
F	1	LYS	-	expression tag	UNP Q02062
H	-7	MET	-	initiating methionine	UNP Q02062
H	-6	ASP	-	expression tag	UNP Q02062
H	-5	TYR	-	expression tag	UNP Q02062
H	-4	LYS	-	expression tag	UNP Q02062
H	-3	ASP	-	expression tag	UNP Q02062
H	-2	ASP	-	expression tag	UNP Q02062
H	-1	ASP	-	expression tag	UNP Q02062
H	0	ASP	-	expression tag	UNP Q02062
H	1	LYS	-	expression tag	UNP Q02062

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

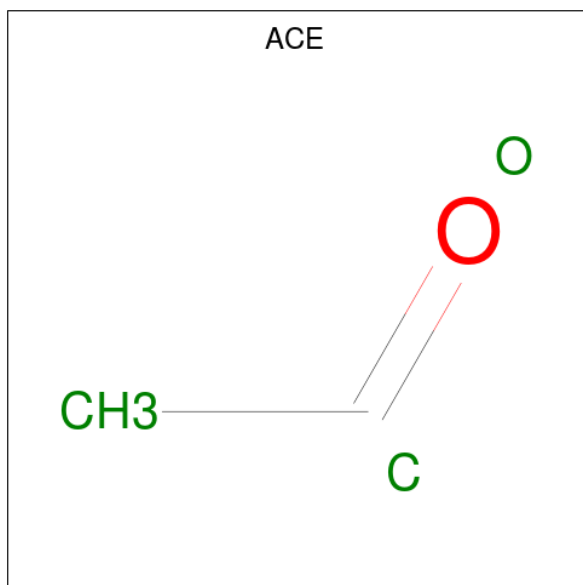
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ACETYL GROUP (CCD ID: ACE) (formula: C_2H_4O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			3	2	1		
4	C	1	Total	C	O	0	0
			3	2	1		
4	E	1	Total	C	O	0	0
			3	2	1		
4	G	1	Total	C	O	0	0
			3	2	1		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Na	0	0
			1	1		
5	D	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total 1	Na 1	0	0
5	H	1	Total 1	Na 1	0	0

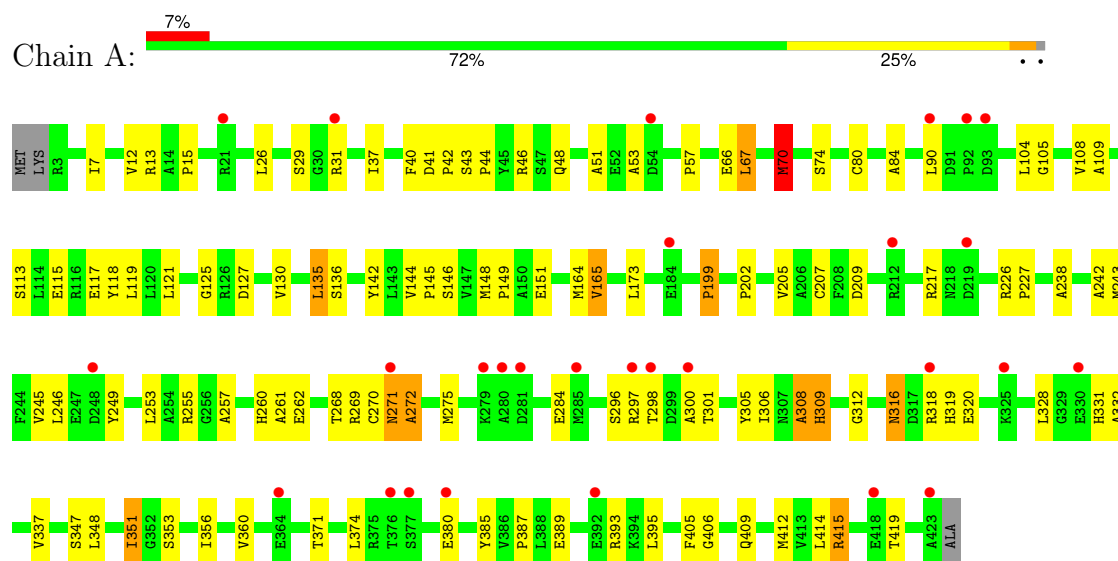
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total 99	O 99	0	0
6	B	144	Total 144	O 144	0	0
6	C	105	Total 105	O 105	0	0
6	D	187	Total 187	O 187	0	0
6	E	62	Total 62	O 62	0	0
6	F	157	Total 157	O 157	0	0
6	G	110	Total 110	O 110	0	0
6	H	211	Total 211	O 211	0	0

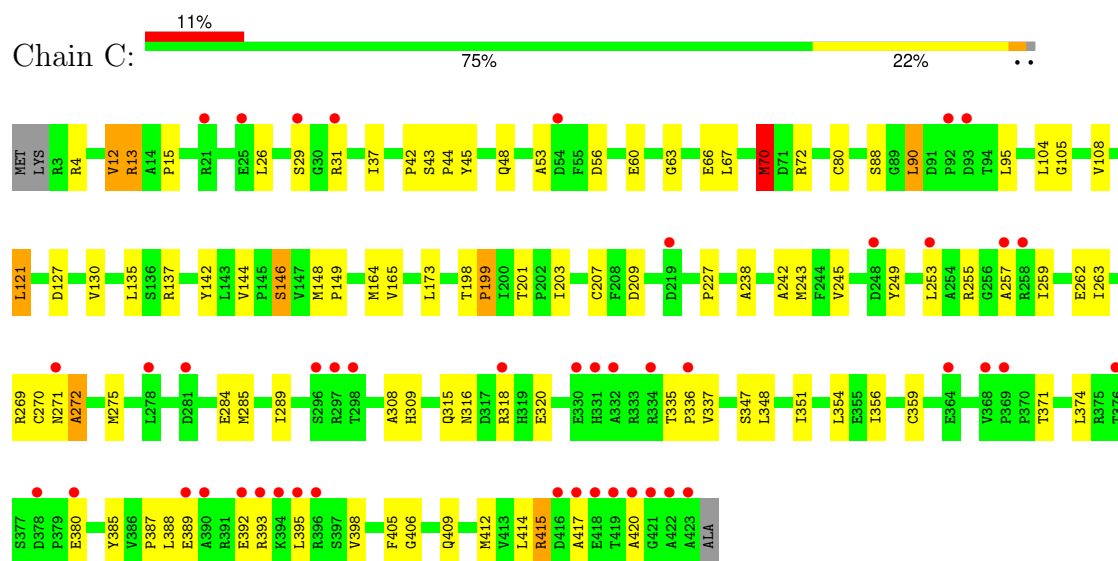
3 Residue-property plots

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

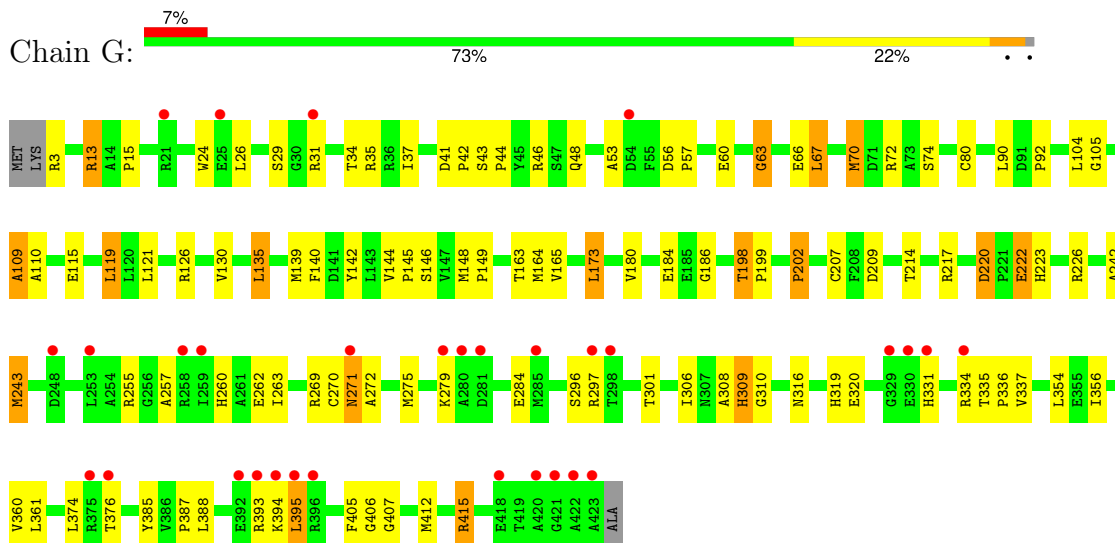
- Molecule 1: Actinorhodin polyketide putative beta-ketoacyl synthase 1



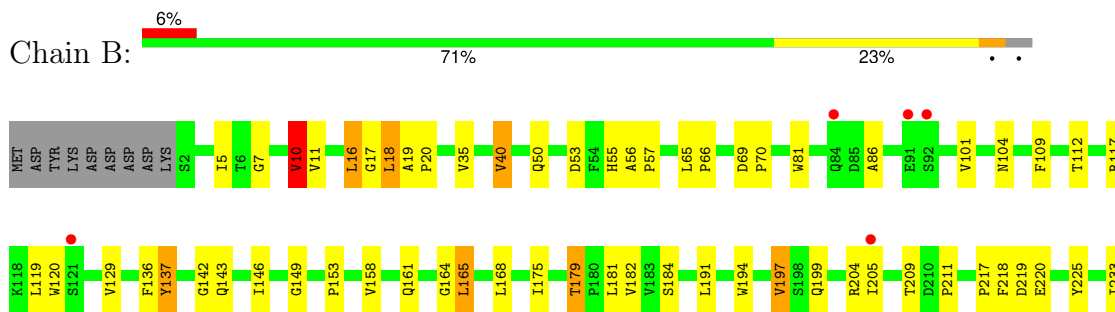
- Molecule 1: Actinorhodin polyketide putative beta-ketoacyl synthase 1

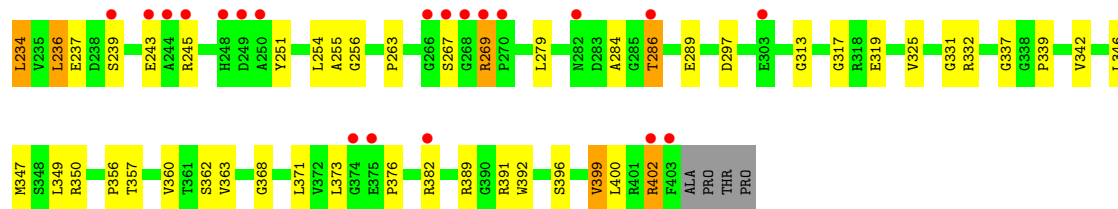


- Molecule 1: Actinorhodin polyketide putative beta-ketoacyl synthase 1

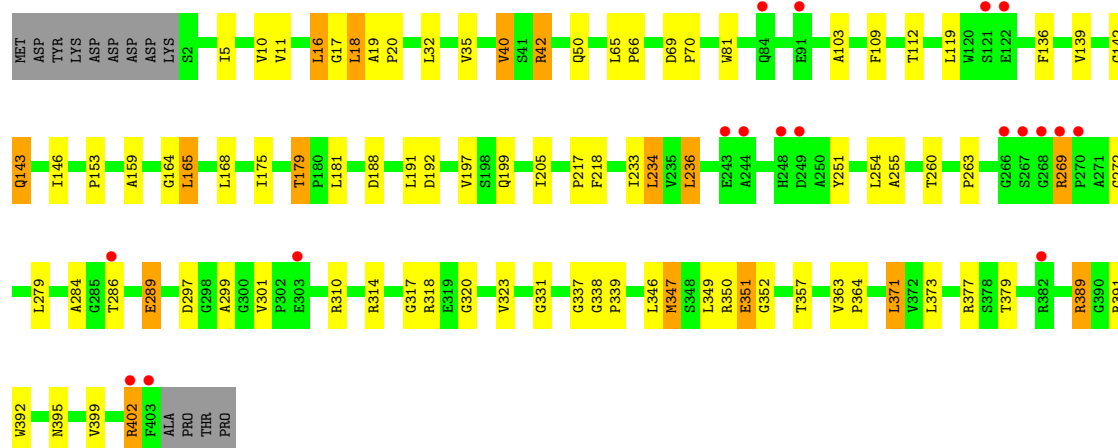
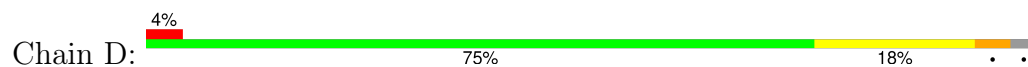


- Molecule 2: Actinorhodin polyketide putative beta-ketoacyl synthase 2

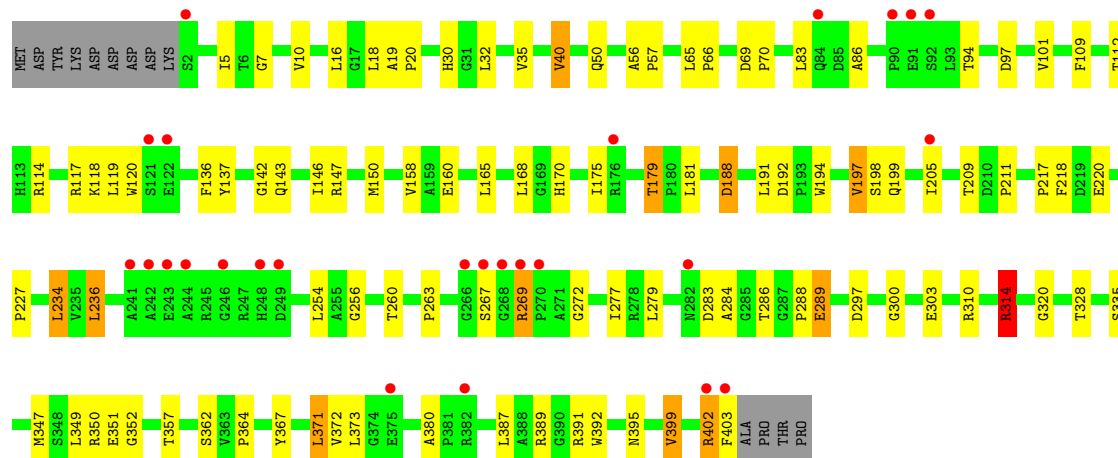




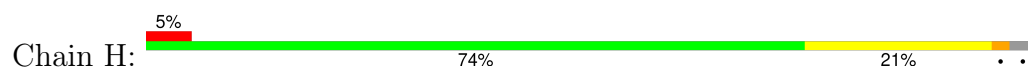
• Molecule 2: Actinorhodin polyketide putative beta-ketoacyl synthase 2

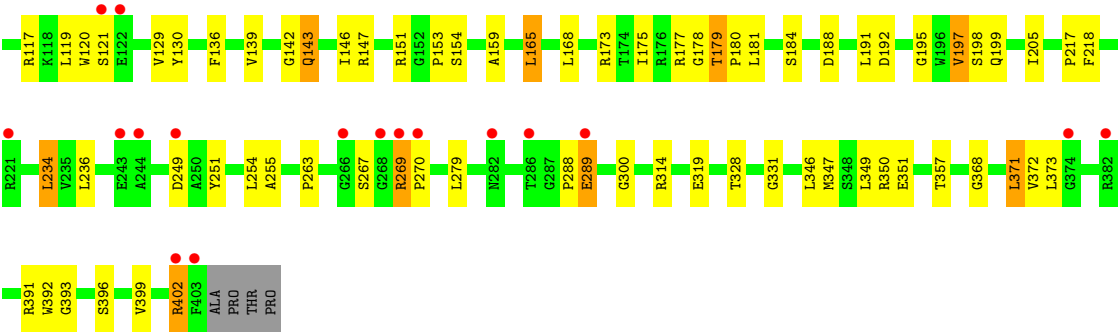


• Molecule 2: Actinorhodin polyketide putative beta-ketoacyl synthase 2



• Molecule 2: Actinorhodin polyketide putative beta-ketoacyl synthase 2





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	262.70Å 262.70Å 224.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.00) 98.7 (50.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.233 , 0.253 0.227 , 0.246	Depositor DCC
R_{free} test set	38543 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25535	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.06% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, NA, ACE

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	0.47	0/3199	1.00	16/4346 (0.4%)
1	C	0.48	0/3199	0.96	12/4346 (0.3%)
1	E	0.43	0/3199	0.92	14/4346 (0.3%)
1	G	0.47	0/3199	0.98	16/4346 (0.4%)
2	B	0.47	0/3041	0.96	6/4151 (0.1%)
2	D	0.52	0/3041	1.01	13/4151 (0.3%)
2	F	0.47	0/3041	1.01	9/4151 (0.2%)
2	H	0.51	0/3041	1.03	16/4151 (0.4%)
All	All	0.48	0/24960	0.98	102/33988 (0.3%)

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
2	B	0	1
2	F	0	2
All	All	0	3

There are no bond length outliers.

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	314	ARG	NE-CZ-NH2	-17.02	103.88	119.20
2	F	314	ARG	NE-CZ-NH1	14.05	135.55	121.50
2	H	314	ARG	NE-CZ-NH2	-14.01	106.59	119.20
2	H	314	ARG	NE-CZ-NH1	11.33	132.83	121.50
1	A	144	VAL	CA-C-N	8.98	128.62	119.82
1	A	144	VAL	C-N-CA	8.98	128.62	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	142	TYR	N-CA-C	-8.67	102.83	113.41
1	A	298	THR	CA-CB-OG1	-8.55	96.77	109.60
1	E	142	TYR	N-CA-C	-8.38	103.18	113.41
1	A	309	HIS	N-CA-C	-8.26	100.58	111.24
1	A	142	TYR	N-CA-C	-8.12	103.50	113.41
1	C	309	HIS	N-CA-C	-7.95	101.70	111.40
1	A	298	THR	CA-CB-CG2	7.94	123.99	110.50
1	C	142	TYR	N-CA-C	-7.86	103.30	113.12
1	C	144	VAL	CA-C-N	7.69	127.36	119.82
1	C	144	VAL	C-N-CA	7.69	127.36	119.82
2	D	192	ASP	N-CA-C	-7.68	98.83	110.50
2	H	314	ARG	CA-CB-CG	7.46	129.02	114.10
1	E	272	ALA	N-CA-C	-7.16	104.12	112.86
2	H	139	VAL	N-CA-C	7.13	118.75	110.62
2	D	139	VAL	N-CA-C	7.06	117.77	110.36
1	G	309	HIS	N-CA-C	-7.05	101.89	112.04
1	C	272	ALA	N-CA-C	-6.99	103.29	112.24
2	H	255	ALA	N-CA-C	6.74	118.70	111.36
2	H	109	PHE	N-CA-C	6.72	118.69	111.36
2	F	192	ASP	N-CA-C	-6.58	102.41	110.31
2	D	109	PHE	N-CA-C	6.58	118.53	111.36
2	H	314	ARG	CB-CG-CD	6.56	126.39	111.30
1	A	272	ALA	N-CA-C	-6.54	104.88	112.86
1	G	70	MET	N-CA-C	6.48	120.07	110.48
2	F	314	ARG	CG-CD-NE	6.45	126.18	112.00
2	F	314	ARG	CB-CG-CD	6.43	126.10	111.30
1	G	56	ASP	CA-C-N	6.41	125.91	119.24
1	G	56	ASP	C-N-CA	6.41	125.91	119.24
1	G	63	GLY	CA-C-N	6.41	125.90	119.24
1	G	63	GLY	C-N-CA	6.41	125.90	119.24
1	G	272	ALA	N-CA-C	-6.27	104.22	112.24
1	G	220	ASP	CA-C-N	6.18	125.67	119.24
1	G	220	ASP	C-N-CA	6.18	125.67	119.24
1	E	309	HIS	N-CA-C	-6.17	103.87	111.40
2	D	299	ALA	N-CA-C	6.16	118.00	111.28
2	B	331	GLY	N-CA-C	-5.95	103.85	112.17
1	E	45	TYR	N-CA-C	5.94	118.87	110.14
2	H	179	THR	CA-C-N	5.93	126.08	119.32
2	H	179	THR	C-N-CA	5.93	126.08	119.32
2	B	255	ALA	N-CA-C	5.77	117.37	111.14
1	E	144	VAL	CA-C-N	5.74	127.01	119.84
1	E	144	VAL	C-N-CA	5.74	127.01	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	MET	N-CA-C	5.72	119.23	110.20
1	C	121	LEU	N-CA-C	5.72	117.19	111.07
2	H	192	ASP	N-CA-C	-5.70	103.48	110.31
2	D	179	THR	CA-C-N	5.66	125.51	119.28
2	D	179	THR	C-N-CA	5.66	125.51	119.28
2	D	331	GLY	N-CA-C	-5.61	104.31	112.17
1	A	351	ILE	N-CA-C	5.58	116.98	110.62
1	E	70	MET	N-CA-C	5.54	118.96	110.20
1	A	316	ASN	N-CA-C	5.51	116.97	110.97
1	A	41	ASP	CA-C-N	5.46	125.54	119.87
1	A	41	ASP	C-N-CA	5.46	125.54	119.87
1	C	45	TYR	N-CA-C	5.45	118.87	110.42
2	H	331	GLY	N-CA-C	-5.44	104.75	112.81
1	A	127	ASP	N-CA-C	5.44	117.76	108.90
1	E	128	TRP	N-CA-C	-5.34	105.38	111.14
1	E	63	GLY	CA-C-N	5.33	124.78	119.24
1	E	63	GLY	C-N-CA	5.33	124.78	119.24
2	D	317	GLY	N-CA-C	-5.33	106.04	112.48
1	G	144	VAL	CA-C-N	5.31	125.03	119.82
1	G	144	VAL	C-N-CA	5.31	125.03	119.82
2	H	328	THR	N-CA-C	-5.29	105.92	112.38
1	C	70	MET	N-CA-C	5.29	118.55	110.20
2	H	165	LEU	N-CA-C	-5.25	105.64	111.36
2	B	337	GLY	N-CA-C	5.23	118.56	112.50
2	F	10	VAL	N-CA-C	5.22	115.99	108.48
2	D	103	ALA	N-CA-C	-5.21	101.66	109.95
2	B	10	VAL	N-CA-C	5.21	115.99	108.48
2	H	393	GLY	N-CA-C	5.17	122.44	115.00
1	A	165	VAL	N-CA-C	-5.15	100.95	108.17
2	B	179	THR	CA-C-N	5.15	124.77	119.05
2	B	179	THR	C-N-CA	5.15	124.77	119.05
1	G	198	THR	CA-C-N	5.15	127.12	120.89
1	G	198	THR	C-N-CA	5.15	127.12	120.89
1	C	127	ASP	N-CA-C	5.14	117.35	109.07
1	A	308	ALA	N-CA-C	5.14	116.74	110.41
2	H	43	TYR	CA-C-N	5.13	124.75	119.05
2	H	43	TYR	C-N-CA	5.13	124.75	119.05
2	D	255	ALA	N-CA-C	5.12	119.24	112.89
2	F	328	THR	N-CA-C	-5.12	106.29	112.54
1	C	63	GLY	CA-C-N	5.12	124.73	119.05
1	C	63	GLY	C-N-CA	5.12	124.73	119.05
1	C	388	LEU	N-CA-C	5.11	121.68	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	179	THR	CA-C-N	5.10	124.71	119.05
2	F	179	THR	C-N-CA	5.10	124.71	119.05
1	E	69	ARG	N-CA-C	5.08	117.80	111.24
1	A	12	VAL	N-CA-C	5.08	115.97	108.45
1	G	110	ALA	N-CA-C	5.07	118.61	112.93
1	G	163	THR	N-CA-C	5.03	115.94	108.60
2	D	301	VAL	CA-C-N	5.01	126.11	119.84
2	D	301	VAL	C-N-CA	5.01	126.11	119.84
1	E	281	ASP	N-CA-C	5.01	116.82	111.36
2	D	337	GLY	N-CA-C	5.01	118.31	112.50
1	E	198	THR	CA-C-N	5.01	126.95	120.89
1	E	198	THR	C-N-CA	5.01	126.95	120.89

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	137	TYR	Sidechain
2	F	137	TYR	Sidechain
2	F	314	ARG	Sidechain

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	3140	0	3032	84	0
1	C	3140	0	3032	76	0
1	E	3140	0	3032	79	0
1	G	3140	0	3032	83	0
2	B	2970	0	2903	79	0
2	D	2970	0	2903	67	0
2	F	2970	0	2903	78	0
2	H	2970	0	2903	69	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	3	1	0
4	C	3	0	3	1	0
4	E	3	0	3	2	0
4	G	3	0	3	2	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	H	1	0	0	0	0
6	A	99	0	0	1	0
6	B	144	0	0	2	1
6	C	105	0	0	9	0
6	D	187	0	0	11	0
6	E	62	0	0	1	0
6	F	157	0	0	7	1
6	G	110	0	0	6	0
6	H	211	0	0	4	0
All	All	25535	0	23752	570	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 12.

All (570) 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)
2:D:402:ARG:HG3	6:D:1237:HOH:O	1.39	1.21
1:G:376:THR:HG23	6:G:1143:HOH:O	1.47	1.13
1:C:392:GLU:HB2	6:C:1124:HOH:O	1.50	1.11
1:E:275:MET:HE3	2:F:146:ILE:HD12	1.36	1.07
1:C:146:SER:HB2	6:D:1189:HOH:O	1.54	1.05
1:G:275:MET:HE3	2:H:146:ILE:CD1	1.86	1.05
2:D:347:MET:HE2	2:D:347:MET:HA	1.38	1.05
1:G:275:MET:HE3	2:H:146:ILE:HD12	1.39	1.04
1:G:217:ARG:HD2	6:G:1200:HOH:O	1.63	0.99
1:A:412:MET:HE3	1:A:414:LEU:HD21	1.46	0.98
1:C:275:MET:HE3	2:D:146:ILE:HD12	1.43	0.97
1:C:412:MET:HE3	1:C:414:LEU:HD21	1.44	0.97
2:D:314:ARG:NH1	6:D:1103:HOH:O	2.02	0.93
2:H:347:MET:HE2	2:H:347:MET:HA	1.48	0.92
2:F:5:ILE:HD12	2:F:236:LEU:HD22	1.52	0.91
1:A:275:MET:HE3	2:B:146:ILE:CD1	2.02	0.90
2:H:35:VAL:HB	2:H:40:VAL:HG11	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:412:MET:HE3	1:E:414:LEU:HD21	1.53	0.88
1:E:275:MET:HE3	2:F:146:ILE:CD1	2.04	0.88
2:F:347:MET:HE2	2:F:347:MET:HA	1.55	0.86
1:G:275:MET:CE	1:G:406:GLY:HA2	2.07	0.85
1:C:308:ALA:HB1	1:C:320:GLU:OE2	1.76	0.85
1:C:275:MET:HE3	2:D:146:ILE:CD1	2.06	0.85
1:A:275:MET:HE3	2:B:146:ILE:HD12	1.58	0.84
1:E:146:SER:O	1:E:149:PRO:HD2	1.76	0.84
1:G:275:MET:HE2	1:G:275:MET:HA	1.60	0.83
2:F:5:ILE:CD1	2:F:236:LEU:HD22	2.08	0.83
2:D:199:GLN:HB3	2:D:205:ILE:HD11	1.62	0.82
2:H:269:ARG:HH11	2:H:269:ARG:HB3	1.43	0.81
1:A:146:SER:O	1:A:149:PRO:HD2	1.81	0.80
1:E:146:SER:HB2	6:F:1172:HOH:O	1.82	0.80
1:E:66:GLU:O	1:E:70:MET:HG2	1.82	0.79
2:D:351:GLU:HG2	6:D:1222:HOH:O	1.81	0.79
1:A:275:MET:HE2	1:A:275:MET:HA	1.66	0.78
2:B:347:MET:HA	2:B:347:MET:HE2	1.65	0.76
2:B:5:ILE:HD13	2:B:236:LEU:HD22	1.65	0.76
1:G:66:GLU:O	1:G:70:MET:HG2	1.86	0.76
1:G:275:MET:HE3	2:H:146:ILE:HD11	1.67	0.76
2:H:199:GLN:HB3	2:H:205:ILE:HD11	1.68	0.76
2:B:347:MET:HE1	2:B:350:ARG:CZ	2.16	0.75
1:G:269:ARG:NH1	2:H:153:PRO:HG3	2.01	0.75
1:E:57:PRO:HB3	1:E:67:LEU:HD11	1.68	0.75
2:D:402:ARG:HD2	6:D:1255:HOH:O	1.86	0.74
1:A:66:GLU:O	1:A:70:MET:HG3	1.88	0.74
2:H:402:ARG:HD2	6:H:1300:HOH:O	1.85	0.74
2:F:199:GLN:HB3	2:F:205:ILE:HD11	1.69	0.73
2:H:269:ARG:HB3	2:H:269:ARG:NH1	2.02	0.73
2:D:347:MET:HA	2:D:347:MET:CE	2.16	0.73
1:A:146:SER:HB2	6:B:1153:HOH:O	1.89	0.73
1:A:275:MET:CE	1:A:406:GLY:HA2	2.19	0.72
1:C:389:GLU:HG2	6:C:1197:HOH:O	1.89	0.72
2:F:347:MET:HE1	2:F:350:ARG:CZ	2.18	0.72
1:G:148:MET:HB2	1:G:149:PRO:HD3	1.72	0.72
1:E:37:ILE:HB	1:E:42:PRO:HG3	1.71	0.72
2:B:199:GLN:HB3	2:B:205:ILE:HD11	1.72	0.72
1:G:42:PRO:HB2	1:G:48:GLN:HB3	1.71	0.72
1:C:37:ILE:HB	1:C:42:PRO:HG3	1.71	0.71
2:D:19:ALA:HB3	2:D:20:PRO:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:MET:HE2	1:G:406:GLY:HA2	1.72	0.71
2:F:284:ALA:HB3	2:F:286:THR:HG22	1.73	0.71
2:D:402:ARG:CG	6:D:1237:HOH:O	2.10	0.71
1:A:148:MET:HB2	1:A:149:PRO:HD3	1.74	0.70
1:E:334:ARG:HH11	1:E:334:ARG:HG3	1.56	0.70
2:H:269:ARG:HH11	2:H:269:ARG:CB	2.03	0.70
2:D:371:LEU:HD13	2:D:373:LEU:HD21	1.74	0.69
1:E:405:PHE:CD2	4:E:633:ACE:H3	2.27	0.69
1:A:57:PRO:HB3	1:A:67:LEU:HD11	1.75	0.69
2:B:129:VAL:HG21	2:F:289:GLU:HG2	1.73	0.69
1:C:269:ARG:NH1	2:D:153:PRO:HG3	2.08	0.69
1:C:389:GLU:CG	6:C:1197:HOH:O	2.40	0.69
1:G:72:ARG:HG2	1:G:198:THR:HG21	1.74	0.69
2:D:35:VAL:HB	2:D:40:VAL:HG11	1.74	0.68
1:G:146:SER:HB2	6:H:1148:HOH:O	1.94	0.68
2:D:347:MET:HE1	2:D:350:ARG:CZ	2.24	0.68
2:B:204:ARG:NH1	6:B:1175:HOH:O	2.19	0.68
1:C:275:MET:CE	1:C:406:GLY:HA2	2.24	0.68
1:G:275:MET:HE1	1:G:406:GLY:HA2	1.74	0.67
1:E:275:MET:HA	1:E:275:MET:HE2	1.75	0.67
2:H:349:LEU:HB3	2:H:402:ARG:HG2	1.77	0.67
1:A:337:VAL:O	1:A:385:TYR:HA	1.95	0.67
1:G:308:ALA:HB1	1:G:320:GLU:OE2	1.95	0.66
2:D:5:ILE:CD1	2:D:236:LEU:HD22	2.26	0.66
2:F:69:ASP:CG	2:F:70:PRO:HD2	2.21	0.66
1:G:262:GLU:OE1	1:G:415:ARG:HD3	1.95	0.66
1:A:308:ALA:HB1	1:A:320:GLU:OE2	1.95	0.66
1:A:356:ILE:HG12	1:A:412:MET:HE2	1.78	0.65
2:H:391:ARG:HG2	2:H:391:ARG:HH11	1.61	0.65
1:E:66:GLU:HB3	1:E:70:MET:HE3	1.78	0.65
2:F:35:VAL:HB	2:F:40:VAL:HG11	1.79	0.65
1:A:135:LEU:HG	2:B:197:VAL:HG13	1.80	0.64
1:A:275:MET:HE3	2:B:146:ILE:HD11	1.78	0.64
1:E:293:LEU:HD21	1:E:303:ILE:HD11	1.79	0.64
2:F:297:ASP:OD2	2:F:389:ARG:HD3	1.98	0.64
2:B:19:ALA:HB3	2:B:20:PRO:HD3	1.80	0.64
1:E:115:GLU:OE1	1:E:202:PRO:HB2	1.98	0.63
1:C:275:MET:HA	1:C:275:MET:HE2	1.81	0.62
2:D:5:ILE:HG13	2:D:346:LEU:HD11	1.81	0.62
2:H:35:VAL:HB	2:H:40:VAL:CG1	2.27	0.62
2:D:351:GLU:CG	6:D:1222:HOH:O	2.44	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:135:LEU:HG	2:H:197:VAL:HG22	1.81	0.62
1:C:405:PHE:CD2	4:C:633:ACE:H3	2.36	0.61
1:C:359:CYS:HB3	1:C:398:VAL:HG21	1.82	0.61
1:E:17:GLY:HA2	1:E:22:GLN:HG2	1.82	0.61
1:E:42:PRO:HB2	1:E:48:GLN:HB3	1.81	0.61
2:H:52:ASP:OD1	6:H:1230:HOH:O	2.16	0.61
1:C:412:MET:CE	1:C:414:LEU:HD21	2.25	0.61
1:E:275:MET:HE1	2:F:142:GLY:HA3	1.83	0.61
2:H:263:PRO:HG3	2:H:269:ARG:HB2	1.81	0.61
1:E:29:SER:OG	1:E:31:ARG:HG2	2.01	0.61
1:A:29:SER:OG	1:A:31:ARG:HG2	2.00	0.60
2:D:35:VAL:HB	2:D:40:VAL:CG1	2.30	0.60
1:C:29:SER:OG	1:C:31:ARG:HG2	2.01	0.60
1:C:392:GLU:CB	6:C:1124:HOH:O	2.26	0.60
1:C:148:MET:HB2	1:C:149:PRO:HD3	1.83	0.60
1:A:70:MET:HE2	1:A:151:GLU:CD	2.27	0.60
2:F:263:PRO:HG3	2:F:269:ARG:HB2	1.83	0.60
1:C:392:GLU:CG	6:C:1124:HOH:O	2.50	0.60
1:C:417:ALA:O	1:C:420:ALA:HB3	2.01	0.60
1:E:164:MET:HE2	2:F:158:VAL:HG21	1.84	0.60
2:B:5:ILE:CD1	2:B:236:LEU:HD22	2.32	0.59
2:D:269:ARG:CB	2:D:269:ARG:HH11	2.15	0.59
2:F:19:ALA:HB3	2:F:20:PRO:HD3	1.83	0.59
1:A:108:VAL:HG21	1:A:199:PRO:HB3	1.83	0.59
2:F:234:LEU:N	2:F:234:LEU:HD23	2.18	0.59
2:D:10:VAL:HG22	2:D:18:LEU:N	2.18	0.59
1:E:275:MET:CE	1:E:406:GLY:HA2	2.33	0.59
2:H:347:MET:HA	2:H:347:MET:CE	2.30	0.59
1:C:43:SER:HB2	1:C:44:PRO:HD3	1.84	0.59
1:A:26:LEU:HD12	1:A:31:ARG:HG3	1.85	0.59
2:F:289:GLU:CD	2:F:289:GLU:H	2.10	0.59
1:C:146:SER:O	1:C:149:PRO:HD2	2.02	0.58
1:E:148:MET:HB2	1:E:149:PRO:HD3	1.85	0.58
1:E:262:GLU:OE1	1:E:415:ARG:HD3	2.03	0.58
1:C:104:LEU:HD23	1:C:243:MET:HE1	1.85	0.58
1:A:275:MET:HE2	1:A:406:GLY:HA2	1.83	0.58
1:G:37:ILE:HB	1:G:42:PRO:HG3	1.84	0.58
2:F:352:GLY:HA2	6:F:1212:HOH:O	2.01	0.58
1:E:37:ILE:HB	1:E:42:PRO:CG	2.33	0.58
2:H:119:LEU:C	2:H:119:LEU:HD23	2.28	0.58
2:B:269:ARG:HH11	2:B:269:ARG:CB	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:NH1	2:B:153:PRO:HG3	2.19	0.58
1:C:275:MET:HE2	1:C:406:GLY:HA2	1.84	0.58
1:G:57:PRO:HB3	1:G:67:LEU:HD11	1.84	0.58
1:C:392:GLU:HG3	6:C:1124:HOH:O	2.02	0.58
1:A:393:ARG:O	1:A:395:LEU:HD22	2.03	0.58
2:H:5:ILE:CD1	2:H:236:LEU:HD22	2.34	0.58
1:A:42:PRO:HB2	1:A:48:GLN:HB3	1.87	0.57
1:C:26:LEU:HD12	1:C:31:ARG:HG3	1.86	0.57
2:D:377:ARG:HG2	2:D:379:THR:HG23	1.87	0.57
1:A:318:ARG:HD3	1:A:380:GLU:CD	2.29	0.57
2:D:357:THR:HB	2:D:373:LEU:HD23	1.86	0.57
1:E:255:ARG:CZ	1:E:257:ALA:HB2	2.35	0.57
1:A:255:ARG:CZ	1:A:257:ALA:HB2	2.35	0.57
2:D:402:ARG:CD	6:D:1237:HOH:O	2.42	0.57
1:E:51:ALA:HB3	1:E:238:ALA:CB	2.35	0.57
2:D:69:ASP:CG	2:D:70:PRO:HD2	2.29	0.57
2:H:5:ILE:HD12	2:H:236:LEU:HD22	1.87	0.57
2:H:289:GLU:CD	2:H:289:GLU:H	2.10	0.57
1:C:15:PRO:HA	1:C:53:ALA:HA	1.85	0.57
1:A:275:MET:HE1	1:A:406:GLY:HA2	1.85	0.57
1:G:394:LYS:N	1:G:394:LYS:HD2	2.19	0.57
2:H:117:ARG:O	2:H:121:SER:HB2	2.05	0.57
2:B:17:GLY:O	2:B:20:PRO:HD2	2.05	0.56
1:E:315:GLN:HA	1:E:318:ARG:HH21	1.69	0.56
2:F:109:PHE:HA	2:F:112:THR:HG22	1.87	0.56
2:B:35:VAL:HB	2:B:40:VAL:HG11	1.87	0.56
2:D:310:ARG:HG2	2:D:314:ARG:NH2	2.20	0.56
2:H:5:ILE:HG13	2:H:346:LEU:HD11	1.86	0.56
2:B:117:ARG:HH21	2:F:314:ARG:CZ	2.18	0.56
2:B:263:PRO:HG3	2:B:269:ARG:HB2	1.87	0.56
1:C:66:GLU:O	1:C:70:MET:HG3	2.06	0.56
2:D:269:ARG:HH11	2:D:269:ARG:HB3	1.70	0.56
2:D:323:VAL:O	2:D:371:LEU:HD23	2.05	0.56
2:F:117:ARG:NH2	6:F:1230:HOH:O	2.38	0.56
1:G:149:PRO:HG2	1:G:164:MET:HB2	1.87	0.56
1:G:405:PHE:CD2	4:G:633:ACE:H3	2.41	0.56
2:H:69:ASP:CG	2:H:70:PRO:HD2	2.31	0.56
2:D:5:ILE:HD13	2:D:236:LEU:HD22	1.86	0.56
2:D:391:ARG:O	2:D:392:TRP:HB2	2.05	0.56
1:G:140:PHE:CE2	2:H:391:ARG:HD3	2.41	0.56
2:H:19:ALA:HB3	2:H:20:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:318:ARG:HD2	2:H:114:ARG:CZ	2.36	0.55
2:F:143:GLN:HE21	2:F:143:GLN:HA	1.71	0.55
1:E:24:TRP:HB2	1:E:361:LEU:HD13	1.86	0.55
2:B:56:ALA:HB3	2:B:57:PRO:HD3	1.88	0.55
1:C:227:PRO:HG2	1:C:371:THR:HG23	1.89	0.55
1:G:139:MET:HE3	1:G:139:MET:O	2.06	0.55
2:B:164:GLY:HA3	2:B:339:PRO:HD3	1.89	0.55
1:C:42:PRO:HB2	1:C:48:GLN:HB3	1.87	0.55
1:C:242:ALA:HB2	1:C:354:LEU:HD13	1.88	0.55
2:D:16:LEU:HD13	2:D:81:TRP:HH2	1.70	0.55
2:B:391:ARG:O	2:B:392:TRP:HB2	2.06	0.55
1:E:337:VAL:O	1:E:385:TYR:HA	2.07	0.55
1:G:139:MET:HE2	2:H:198:SER:OG	2.06	0.55
1:A:217:ARG:NH1	1:A:226:ARG:HD2	2.22	0.55
1:E:306:ILE:HB	1:E:337:VAL:HG22	1.88	0.55
1:G:217:ARG:CD	6:G:1200:HOH:O	2.38	0.55
1:G:255:ARG:CZ	1:G:257:ALA:HB2	2.37	0.55
2:D:251:TYR:HD1	2:D:347:MET:HE3	1.72	0.54
1:E:275:MET:CE	2:F:146:ILE:CD1	2.83	0.54
2:F:347:MET:HA	2:F:347:MET:CE	2.33	0.54
1:G:80:CYS:HB3	1:G:243:MET:HB2	1.89	0.54
1:E:301:THR:HA	1:E:331:HIS:CE1	2.42	0.54
2:F:114:ARG:O	2:F:118:LYS:HG3	2.07	0.54
1:G:29:SER:OG	1:G:31:ARG:HG2	2.07	0.54
1:C:337:VAL:O	1:C:385:TYR:HA	2.07	0.54
2:B:5:ILE:HG13	2:B:346:LEU:HD11	1.90	0.54
1:C:272:ALA:O	6:C:1179:HOH:O	2.18	0.54
2:D:234:LEU:HD23	2:D:234:LEU:N	2.21	0.54
2:D:263:PRO:HG3	2:D:269:ARG:HB2	1.89	0.54
1:E:43:SER:HB2	1:E:44:PRO:HD3	1.88	0.54
2:F:175:ILE:HA	2:F:179:THR:O	2.07	0.54
1:G:337:VAL:O	1:G:385:TYR:HA	2.07	0.54
2:B:297:ASP:OD2	2:B:389:ARG:HD3	2.08	0.54
2:D:284:ALA:HB3	2:D:286:THR:HG22	1.90	0.54
1:E:51:ALA:HB3	1:E:238:ALA:HB2	1.90	0.54
2:D:17:GLY:O	2:D:20:PRO:HD2	2.07	0.54
2:F:347:MET:HE1	2:F:350:ARG:NE	2.23	0.54
1:C:104:LEU:HD11	1:C:148:MET:HE2	1.90	0.54
2:F:181:LEU:C	2:F:181:LEU:HD23	2.33	0.54
1:G:66:GLU:HB3	1:G:70:MET:HE3	1.91	0.53
1:C:374:LEU:HD23	1:C:387:PRO:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:THR:HB	2:F:97:ASP:OD2	2.09	0.53
2:F:217:PRO:HA	2:F:300:GLY:HA2	1.90	0.53
2:F:209:THR:O	2:F:211:PRO:HD3	2.09	0.53
1:C:121:LEU:HB3	1:C:130:VAL:HB	1.91	0.53
2:F:391:ARG:O	2:F:392:TRP:HB2	2.08	0.53
1:C:270:CYS:O	1:C:284:GLU:HG2	2.09	0.53
2:F:284:ALA:HB2	2:F:399:VAL:HG11	1.91	0.53
1:A:275:MET:HE1	2:B:142:GLY:HA3	1.90	0.53
2:B:217:PRO:HG3	2:B:325:VAL:HG11	1.91	0.53
2:F:310:ARG:O	2:F:314:ARG:HG3	2.09	0.53
2:D:347:MET:HE1	2:D:350:ARG:NE	2.24	0.52
2:D:297:ASP:OD2	2:D:389:ARG:HD3	2.09	0.52
1:E:242:ALA:HB3	1:E:353:SER:HB3	1.91	0.52
1:E:121:LEU:HB3	1:E:130:VAL:HB	1.91	0.52
1:G:13:ARG:HB2	1:G:80:CYS:SG	2.50	0.52
2:B:55:HIS:HE1	6:F:1178:HOH:O	1.92	0.52
1:G:43:SER:HB2	1:G:44:PRO:HD3	1.91	0.52
2:H:347:MET:HE1	2:H:350:ARG:CZ	2.40	0.52
2:B:284:ALA:HB3	2:B:286:THR:HG22	1.91	0.52
2:D:289:GLU:H	2:D:289:GLU:CD	2.16	0.52
1:A:37:ILE:HB	1:A:42:PRO:HG3	1.92	0.52
1:A:262:GLU:OE1	1:A:415:ARG:HD3	2.11	0.51
2:B:256:GLY:N	2:B:399:VAL:HG13	2.26	0.51
2:H:56:ALA:CB	2:H:73:ARG:HD3	2.41	0.51
2:D:42:ARG:HG3	2:D:42:ARG:HH11	1.76	0.51
1:E:108:VAL:HG21	1:E:199:PRO:HB3	1.93	0.51
2:B:234:LEU:N	2:B:234:LEU:HD23	2.25	0.51
1:E:135:LEU:HG	2:F:197:VAL:HG13	1.91	0.51
2:B:165:LEU:HB3	2:B:396:SER:OG	2.10	0.51
1:A:249:TYR:CZ	1:A:253:LEU:HD11	2.45	0.51
2:B:357:THR:HB	2:B:373:LEU:HD23	1.91	0.51
1:C:249:TYR:HE1	1:C:259:ILE:HD13	1.76	0.51
1:E:275:MET:HE2	1:E:406:GLY:HA2	1.93	0.51
1:E:308:ALA:HB1	1:E:320:GLU:OE2	2.10	0.51
1:G:149:PRO:CG	1:G:164:MET:HB2	2.41	0.51
1:G:376:THR:CG2	6:G:1143:HOH:O	2.28	0.51
2:D:352:GLY:HA2	6:D:1157:HOH:O	2.11	0.51
2:H:181:LEU:C	2:H:181:LEU:HD23	2.36	0.51
1:A:118:TYR:HB2	2:B:194:TRP:CH2	2.46	0.51
1:A:260:HIS:HB3	1:A:360:VAL:CG1	2.41	0.51
1:A:316:ASN:O	1:A:319:HIS:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ARG:HB3	1:E:209:ASP:CG	2.35	0.51
1:C:4:ARG:HH22	1:C:420:ALA:C	2.19	0.50
2:F:35:VAL:HB	2:F:40:VAL:CG1	2.40	0.50
2:F:217:PRO:O	2:F:218:PHE:HB2	2.11	0.50
1:C:238:ALA:O	1:C:347:SER:HA	2.11	0.50
2:B:269:ARG:NH1	2:B:269:ARG:HB3	2.27	0.50
1:G:275:MET:HE1	2:H:142:GLY:HA3	1.92	0.50
2:B:269:ARG:HH11	2:B:269:ARG:HB3	1.75	0.50
2:B:175:ILE:HA	2:B:179:THR:O	2.11	0.50
2:B:251:TYR:CD1	2:B:347:MET:HE3	2.47	0.49
1:C:348:LEU:O	1:C:351:ILE:HG22	2.12	0.49
1:G:126:ARG:C	2:H:117:ARG:HH12	2.19	0.49
1:C:105:GLY:HA2	1:C:165:VAL:O	2.12	0.49
2:D:181:LEU:C	2:D:181:LEU:HD23	2.37	0.49
1:E:334:ARG:HG3	1:E:334:ARG:NH1	2.26	0.49
2:H:175:ILE:HA	2:H:179:THR:O	2.12	0.49
2:H:234:LEU:N	2:H:234:LEU:HD23	2.28	0.49
1:A:205:VAL:HG13	6:A:1131:HOH:O	2.12	0.49
2:H:50:GLN:HG2	2:H:191:LEU:HD13	1.94	0.49
1:G:309:HIS:HD2	1:G:316:ASN:HD21	1.60	0.49
2:F:69:ASP:CG	2:F:70:PRO:CD	2.86	0.49
2:F:272:GLY:HA2	6:F:1099:HOH:O	2.12	0.49
2:B:349:LEU:HB3	2:B:402:ARG:HG2	1.94	0.49
1:C:108:VAL:HG21	1:C:199:PRO:HB3	1.95	0.49
1:G:15:PRO:HA	1:G:53:ALA:HA	1.94	0.49
1:G:374:LEU:HD23	1:G:387:PRO:HB3	1.94	0.49
1:C:90:LEU:HD23	1:C:95:LEU:HD11	1.94	0.49
1:G:109:ALA:HB1	1:G:145:PRO:HB3	1.94	0.49
2:B:69:ASP:CG	2:B:70:PRO:HD2	2.38	0.49
1:C:149:PRO:HG2	1:C:164:MET:HB2	1.94	0.48
1:A:405:PHE:CD2	4:A:633:ACE:H3	2.48	0.48
1:C:37:ILE:HB	1:C:42:PRO:CG	2.41	0.48
2:F:56:ALA:HB3	2:F:57:PRO:HD3	1.95	0.48
2:B:66:PRO:HG3	2:F:320:GLY:O	2.14	0.48
2:D:251:TYR:CD1	2:D:347:MET:HE3	2.48	0.48
2:B:356:PRO:HD3	2:B:376:PRO:HG3	1.95	0.48
2:B:382:ARG:HG2	2:B:402:ARG:HB2	1.96	0.48
1:E:222:GLU:CD	1:E:222:GLU:H	2.21	0.48
1:G:35:ARG:NH1	1:G:222:GLU:HG3	2.29	0.48
1:A:270:CYS:O	1:A:284:GLU:HG2	2.13	0.48
2:B:104:ASN:O	2:B:158:VAL:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:275:MET:HE1	2:F:142:GLY:CA	2.44	0.48
2:B:109:PHE:HA	2:B:112:THR:HG22	1.96	0.48
1:C:262:GLU:OE1	1:C:415:ARG:HD3	2.14	0.48
2:D:350:ARG:NH1	6:D:1233:HOH:O	2.33	0.48
1:E:145:PRO:HG3	6:E:1099:HOH:O	2.12	0.48
1:G:271:ASN:HB2	1:G:407:GLY:HA3	1.95	0.48
1:A:356:ILE:HG12	1:A:412:MET:CE	2.41	0.48
1:A:15:PRO:HA	1:A:53:ALA:HA	1.96	0.48
2:B:11:VAL:HG23	2:B:11:VAL:O	2.12	0.48
1:G:63:GLY:O	1:G:67:LEU:HD22	2.14	0.48
1:C:12:VAL:O	1:C:13:ARG:HD3	2.13	0.47
2:F:83:LEU:HD21	2:F:150:MET:HE1	1.94	0.47
1:G:146:SER:O	1:G:149:PRO:HD2	2.14	0.47
1:G:220:ASP:OD2	1:G:223:HIS:HD2	1.97	0.47
1:G:260:HIS:HB3	1:G:360:VAL:CG1	2.44	0.47
2:B:233:ILE:C	2:B:234:LEU:HD23	2.39	0.47
2:D:50:GLN:HG2	2:D:191:LEU:HD13	1.96	0.47
1:E:80:CYS:HB3	1:E:243:MET:HB2	1.95	0.47
2:B:143:GLN:HE21	2:B:143:GLN:HA	1.79	0.47
2:D:11:VAL:HG23	2:D:11:VAL:O	2.14	0.47
2:D:175:ILE:HA	2:D:179:THR:O	2.14	0.47
1:G:37:ILE:HB	1:G:42:PRO:CG	2.43	0.47
2:H:195:GLY:O	2:H:199:GLN:HG3	2.14	0.47
2:D:289:GLU:HG2	2:H:129:VAL:HG21	1.95	0.47
2:D:349:LEU:HB3	2:D:402:ARG:HG2	1.96	0.47
2:F:30:HIS:ND1	2:F:32:LEU:HB2	2.29	0.47
2:H:67:GLN:HB3	2:H:130:TYR:CD1	2.49	0.47
2:B:267:SER:C	2:B:269:ARG:H	2.23	0.47
1:G:145:PRO:HG3	6:G:1106:HOH:O	2.15	0.47
2:H:100:VAL:O	2:H:154:SER:HB3	2.14	0.47
1:E:26:LEU:HD12	1:E:31:ARG:HG3	1.96	0.47
2:F:269:ARG:HH11	2:F:269:ARG:HB3	1.79	0.47
1:G:180:VAL:O	1:G:184:GLU:HG3	2.15	0.47
1:C:275:MET:HE1	2:D:142:GLY:HA3	1.97	0.47
2:H:199:GLN:HB3	2:H:205:ILE:CD1	2.44	0.46
1:C:271:ASN:HD21	1:C:409:GLN:NE2	2.14	0.46
1:C:393:ARG:O	1:C:395:LEU:HD22	2.14	0.46
2:B:10:VAL:HG22	2:B:18:LEU:N	2.30	0.46
2:B:219:ASP:HB2	2:B:360:VAL:HG13	1.96	0.46
1:C:104:LEU:O	1:C:164:MET:HA	2.15	0.46
2:B:284:ALA:HB2	2:B:399:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:ARG:HH21	1:G:60:GLU:CD	2.23	0.46
2:H:217:PRO:O	2:H:218:PHE:HB2	2.16	0.46
1:E:180:VAL:O	1:E:184:GLU:HG3	2.16	0.46
1:A:149:PRO:HG2	1:A:164:MET:HB2	1.98	0.46
2:B:35:VAL:HB	2:B:40:VAL:CG1	2.46	0.46
2:B:65:LEU:N	2:B:66:PRO:CD	2.79	0.46
1:G:275:MET:CE	1:G:275:MET:HA	2.41	0.46
2:H:35:VAL:CB	2:H:40:VAL:HG11	2.36	0.46
1:G:309:HIS:HD2	1:G:316:ASN:ND2	2.14	0.46
2:H:267:SER:C	2:H:269:ARG:H	2.23	0.46
1:A:296:SER:O	1:A:297:ARG:HB2	2.15	0.46
2:D:272:GLY:HA2	6:D:1118:HOH:O	2.16	0.46
1:E:118:TYR:HB2	2:F:194:TRP:CH2	2.51	0.46
2:F:269:ARG:HH11	2:F:269:ARG:CB	2.30	0.46
2:F:357:THR:HB	2:F:373:LEU:HD23	1.98	0.46
2:H:30:HIS:HB2	2:H:32:LEU:HD13	1.99	0.46
1:A:121:LEU:HB3	1:A:130:VAL:HB	1.98	0.45
1:G:115:GLU:OE1	1:G:202:PRO:HB2	2.15	0.45
1:A:328:LEU:HB2	1:A:332:ALA:HB2	1.98	0.45
1:E:363:LEU:HD21	1:E:398:VAL:HG13	1.97	0.45
2:H:391:ARG:HG2	2:H:391:ARG:NH1	2.28	0.45
1:G:301:THR:HA	1:G:331:HIS:CE1	2.51	0.45
2:H:173:ARG:O	2:H:177:ARG:HG3	2.15	0.45
1:G:405:PHE:N	4:G:633:ACE:O	2.38	0.45
2:H:357:THR:HB	2:H:373:LEU:HD23	1.97	0.45
2:B:256:GLY:H	2:B:399:VAL:HG13	1.81	0.45
2:F:349:LEU:HB3	2:F:402:ARG:HG2	1.99	0.45
1:A:125:GLY:O	2:B:117:ARG:NH1	2.50	0.45
2:D:217:PRO:O	2:D:218:PHE:HB2	2.16	0.45
2:F:284:ALA:HB2	2:F:399:VAL:CG1	2.46	0.45
1:A:356:ILE:HD13	1:A:412:MET:HE1	1.98	0.45
2:B:342:VAL:HG13	2:B:400:LEU:HD11	1.99	0.45
1:E:396:ARG:HA	1:E:416:ASP:OD2	2.15	0.45
2:F:371:LEU:HD23	2:F:372:VAL:N	2.32	0.45
1:G:104:LEU:HD23	1:G:243:MET:HE1	1.98	0.45
2:H:147:ARG:NH1	6:H:1196:HOH:O	2.45	0.45
1:A:51:ALA:HB3	1:A:238:ALA:CB	2.47	0.45
1:C:249:TYR:CZ	1:C:253:LEU:HD11	2.52	0.45
2:D:269:ARG:HB3	2:D:269:ARG:NH1	2.32	0.45
2:H:119:LEU:HD23	2:H:119:LEU:O	2.17	0.45
2:H:143:GLN:HE21	2:H:143:GLN:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:269:ARG:HB3	2:H:270:PRO:HD2	1.99	0.45
1:A:135:LEU:HD22	1:A:136:SER:O	2.17	0.45
1:C:88:SER:OG	1:C:90:LEU:HB2	2.17	0.45
1:C:275:MET:CE	2:D:146:ILE:CD1	2.87	0.45
1:E:46:ARG:HB3	1:E:209:ASP:OD1	2.17	0.45
2:F:50:GLN:HG2	2:F:191:LEU:HD13	1.98	0.45
2:F:260:THR:OG1	2:F:395:ASN:HB2	2.18	0.45
2:B:209:THR:O	2:B:211:PRO:HD3	2.17	0.44
1:C:66:GLU:HB3	1:C:70:MET:HE3	1.98	0.44
2:F:147:ARG:HD3	6:F:1200:HOH:O	2.16	0.44
2:F:199:GLN:HB3	2:F:205:ILE:CD1	2.42	0.44
2:B:181:LEU:HD23	2:B:181:LEU:C	2.42	0.44
2:D:310:ARG:O	2:D:314:ARG:HG3	2.16	0.44
2:F:188:ASP:OD1	2:F:335:SER:OG	2.35	0.44
1:E:275:MET:CE	2:F:146:ILE:HD12	2.26	0.44
1:C:201:THR:HG23	1:C:203:ILE:HG22	1.99	0.44
2:D:164:GLY:HA3	2:D:339:PRO:HD3	1.99	0.44
1:E:143:LEU:HD22	2:F:198:SER:HB3	1.99	0.44
1:E:260:HIS:O	1:E:261:ALA:HB2	2.17	0.44
2:F:267:SER:C	2:F:269:ARG:H	2.26	0.44
2:H:251:TYR:CD1	2:H:347:MET:HE3	2.53	0.44
2:F:288:PRO:HD2	2:F:289:GLU:OE2	2.18	0.44
2:H:288:PRO:HD2	2:H:289:GLU:OE2	2.18	0.44
1:C:149:PRO:CG	1:C:164:MET:HB2	2.47	0.44
2:F:364:PRO:HD2	2:F:367:TYR:CD2	2.53	0.44
1:G:209:ASP:HA	6:G:1113:HOH:O	2.18	0.44
1:G:334:ARG:HG3	1:G:334:ARG:HH11	1.82	0.44
1:A:46:ARG:HB3	1:A:209:ASP:CG	2.43	0.44
1:C:255:ARG:CZ	1:C:257:ALA:HB2	2.48	0.44
2:F:101:VAL:HG11	2:F:170:HIS:HB3	1.98	0.44
2:F:352:GLY:HA2	2:F:380:ALA:HA	1.98	0.44
1:A:374:LEU:HD23	1:A:387:PRO:HB3	2.00	0.44
2:B:181:LEU:HD23	2:B:182:VAL:N	2.33	0.44
1:A:272:ALA:HB1	2:B:149:GLY:HA2	2.00	0.44
2:B:363:VAL:HG21	2:B:371:LEU:HD12	2.00	0.44
2:F:65:LEU:HB2	2:F:66:PRO:HD3	2.00	0.44
2:F:143:GLN:HA	2:F:143:GLN:NE2	2.33	0.44
1:G:275:MET:CE	2:H:146:ILE:HD11	2.44	0.44
1:A:309:HIS:HD2	1:A:316:ASN:ND2	2.15	0.43
2:B:129:VAL:CG2	2:F:289:GLU:HG2	2.46	0.43
1:C:137:ARG:HD3	6:C:1131:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:MET:HE1	1:C:406:GLY:HA2	1.98	0.43
1:C:412:MET:HE3	1:C:414:LEU:CD2	2.31	0.43
1:E:405:PHE:CD2	4:E:633:ACE:CH3	3.01	0.43
1:G:41:ASP:HA	1:G:42:PRO:HD3	1.84	0.43
1:A:40:PHE:O	1:A:42:PRO:HD3	2.18	0.43
1:A:305:TYR:CD1	1:A:306:ILE:N	2.86	0.43
1:G:70:MET:HB2	1:G:74:SER:HB2	2.00	0.43
1:G:271:ASN:HB2	1:G:407:GLY:CA	2.48	0.43
1:G:393:ARG:O	1:G:395:LEU:HD22	2.18	0.43
2:B:284:ALA:CB	2:B:286:THR:HG22	2.48	0.43
1:G:121:LEU:HB3	1:G:130:VAL:HB	2.00	0.43
2:H:95:ASP:HB2	2:H:151:ARG:HG3	2.00	0.43
1:A:43:SER:HB2	1:A:44:PRO:HD3	2.00	0.43
1:A:115:GLU:OE1	1:A:202:PRO:HB2	2.18	0.43
1:G:119:LEU:HD11	2:H:120:TRP:CE2	2.54	0.43
1:A:301:THR:HA	1:A:331:HIS:CE1	2.54	0.43
1:E:72:ARG:HG2	1:E:198:THR:HG21	2.01	0.43
1:E:95:LEU:O	1:E:97:PRO:HD3	2.19	0.43
1:E:356:ILE:O	1:E:360:VAL:HG23	2.18	0.43
1:G:24:TRP:HB2	1:G:361:LEU:HD13	2.01	0.43
2:H:217:PRO:HA	2:H:300:GLY:HA2	2.00	0.43
2:H:391:ARG:O	2:H:392:TRP:HB2	2.19	0.43
1:A:242:ALA:HB3	1:A:353:SER:HB3	2.00	0.43
2:D:10:VAL:HG22	2:D:17:GLY:C	2.42	0.43
2:H:319:GLU:OE2	2:H:368:GLY:HA2	2.19	0.43
1:A:37:ILE:HB	1:A:42:PRO:CG	2.48	0.43
2:B:199:GLN:HB3	2:B:205:ILE:CD1	2.44	0.43
1:E:145:PRO:HB2	1:E:164:MET:HE1	2.00	0.43
1:G:26:LEU:HD12	1:G:31:ARG:NE	2.33	0.43
1:G:335:THR:HA	1:G:336:PRO:HD3	1.90	0.43
1:A:105:GLY:HA2	1:A:165:VAL:O	2.18	0.42
1:E:335:THR:HA	1:E:336:PRO:HD3	1.91	0.42
2:B:217:PRO:O	2:B:218:PHE:HB2	2.19	0.42
1:G:173:LEU:HD12	1:G:173:LEU:HA	1.91	0.42
1:A:271:ASN:HD22	1:A:271:ASN:HA	1.55	0.42
2:B:220:GLU:HG2	2:B:362:SER:OG	2.20	0.42
1:C:4:ARG:NH2	1:C:420:ALA:HB1	2.33	0.42
1:C:88:SER:HB3	1:C:245:VAL:HG21	2.01	0.42
2:D:165:LEU:HD13	2:D:338:GLY:HA3	2.00	0.42
1:E:334:ARG:HH11	1:E:334:ARG:CG	2.28	0.42
1:G:46:ARG:HB3	1:G:209:ASP:CG	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:ARG:HB2	1:C:80:CYS:SG	2.59	0.42
2:D:5:ILE:HD12	2:D:236:LEU:HD22	1.97	0.42
1:E:119:LEU:HD11	2:F:120:TRP:CE2	2.55	0.42
2:F:199:GLN:OE1	2:F:227:PRO:HB3	2.20	0.42
1:A:119:LEU:HD11	2:B:120:TRP:CE2	2.54	0.42
1:C:13:ARG:HH21	1:C:60:GLU:CD	2.26	0.42
2:H:42:ARG:HG3	2:H:42:ARG:HH11	1.83	0.42
1:A:145:PRO:HG2	2:B:137:TYR:CZ	2.55	0.42
1:A:268:THR:HA	1:A:409:GLN:O	2.20	0.42
1:E:104:LEU:HD23	1:E:243:MET:HE1	2.00	0.42
2:F:165:LEU:HD12	2:F:165:LEU:HA	1.83	0.42
1:A:374:LEU:CD2	1:A:385:TYR:HB2	2.49	0.42
2:D:233:ILE:C	2:D:234:LEU:HD23	2.45	0.42
1:E:351:ILE:O	1:E:355:GLU:HG3	2.18	0.42
2:F:303:GLU:HB2	6:F:1183:HOH:O	2.18	0.42
1:G:279:LYS:O	1:G:319:HIS:HD2	2.02	0.42
2:H:165:LEU:HB3	2:H:396:SER:OG	2.19	0.42
1:A:300:ALA:O	1:A:331:HIS:CD2	2.72	0.42
1:A:415:ARG:HG3	1:A:419:THR:HB	2.02	0.42
1:C:249:TYR:CE1	1:C:259:ILE:HD13	2.53	0.42
1:G:242:ALA:HB2	1:G:354:LEU:HD13	2.01	0.42
1:A:227:PRO:HG2	1:A:371:THR:HG23	2.02	0.42
1:C:318:ARG:HG3	1:C:380:GLU:HB3	2.02	0.42
2:F:7:GLY:HA3	2:F:86:ALA:HB2	2.02	0.42
1:G:105:GLY:HA2	1:G:165:VAL:O	2.20	0.42
1:A:146:SER:C	1:A:149:PRO:HD2	2.44	0.42
1:C:56:ASP:OD2	1:C:56:ASP:C	2.61	0.42
1:E:340:ILE:HD11	1:E:355:GLU:HG2	2.02	0.42
1:A:90:LEU:HD13	1:A:255:ARG:NE	2.34	0.41
2:B:237:GLU:OE2	2:B:245:ARG:NH2	2.45	0.41
2:D:260:THR:OG1	2:D:395:ASN:HB2	2.19	0.41
2:D:318:ARG:C	2:D:320:GLY:N	2.78	0.41
1:E:12:VAL:HG23	1:E:354:LEU:HD13	2.02	0.41
2:H:32:LEU:N	2:H:32:LEU:CD1	2.83	0.41
1:A:74:SER:OG	1:A:148:MET:HG2	2.20	0.41
2:B:7:GLY:HA3	2:B:86:ALA:HB2	2.02	0.41
1:C:72:ARG:HG2	1:C:198:THR:HG21	2.00	0.41
1:E:116:ARG:NH1	1:E:117:GLU:OE2	2.53	0.41
1:E:238:ALA:O	1:E:347:SER:HA	2.20	0.41
1:G:270:CYS:O	1:G:284:GLU:HG2	2.19	0.41
1:G:356:ILE:O	1:G:360:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ILE:HG12	1:A:246:LEU:CD2	2.51	0.41
1:C:209:ASP:HA	6:C:1105:HOH:O	2.20	0.41
1:C:356:ILE:HG12	1:C:412:MET:HE2	2.02	0.41
2:H:101:VAL:O	2:H:184:SER:HA	2.21	0.41
1:A:80:CYS:HB3	1:A:243:MET:HB2	2.01	0.41
1:E:118:TYR:OH	1:E:125:GLY:HA2	2.19	0.41
1:A:348:LEU:O	1:A:351:ILE:HG22	2.21	0.41
2:B:251:TYR:CE1	2:B:347:MET:HE3	2.56	0.41
1:C:315:GLN:HG3	1:C:316:ASN:N	2.36	0.41
1:G:306:ILE:HB	1:G:337:VAL:HG22	2.03	0.41
2:H:65:LEU:N	2:H:66:PRO:CD	2.84	0.41
2:B:161:GLN:HG3	2:B:161:GLN:O	2.20	0.41
1:C:263:ILE:HG12	1:C:412:MET:HE3	2.01	0.41
1:C:335:THR:HA	1:C:336:PRO:HD3	1.85	0.41
1:E:41:ASP:HA	1:E:42:PRO:HD3	1.81	0.41
1:A:51:ALA:HB3	1:A:238:ALA:HB2	2.03	0.41
2:B:313:GLY:O	2:B:317:GLY:N	2.53	0.41
1:E:249:TYR:CZ	1:E:253:LEU:HD11	2.56	0.41
2:F:220:GLU:HG2	2:F:362:SER:OG	2.21	0.41
1:G:263:ILE:HG12	1:G:412:MET:HE3	2.02	0.41
1:A:109:ALA:HB1	1:A:145:PRO:HB3	2.03	0.41
1:E:163:THR:OG1	1:E:164:MET:N	2.54	0.41
2:F:277:ILE:HG12	2:F:387:LEU:HD21	2.03	0.41
1:A:217:ARG:HH12	1:A:226:ARG:HD2	1.84	0.41
1:A:238:ALA:O	1:A:347:SER:HA	2.19	0.41
1:A:284:GLU:CD	1:A:284:GLU:H	2.29	0.41
2:B:16:LEU:HD22	2:B:81:TRP:CH2	2.56	0.41
2:B:53:ASP:OD2	2:B:53:ASP:N	2.52	0.41
2:D:65:LEU:N	2:D:66:PRO:CD	2.83	0.41
1:E:227:PRO:O	1:E:228:PHE:HB2	2.21	0.41
2:F:256:GLY:HA2	2:F:283:ASP:OD2	2.20	0.41
2:F:284:ALA:CB	2:F:399:VAL:HG11	2.51	0.41
1:G:34:THR:C	1:G:35:ARG:HG2	2.46	0.41
1:G:90:LEU:O	1:G:92:PRO:HD3	2.21	0.41
2:H:371:LEU:HD23	2:H:372:VAL:N	2.36	0.41
1:A:84:ALA:HB1	1:A:245:VAL:HG23	2.03	0.41
2:B:50:GLN:HG2	2:B:191:LEU:HD13	2.02	0.41
2:B:101:VAL:O	2:B:184:SER:HA	2.21	0.41
2:B:225:TYR:CG	2:B:332:ARG:HD3	2.56	0.41
2:D:143:GLN:HA	2:D:143:GLN:HE21	1.85	0.41
1:E:101:GLY:HA3	1:E:191:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:MET:HE2	1:A:151:GLU:OE2	2.19	0.40
2:B:65:LEU:HB2	2:B:66:PRO:HD3	2.03	0.40
1:E:199:PRO:O	1:E:201:THR:N	2.55	0.40
1:A:227:PRO:HA	1:A:312:GLY:HA2	2.03	0.40
2:B:319:GLU:OE2	2:B:368:GLY:HA2	2.20	0.40
2:H:32:LEU:N	2:H:32:LEU:HD12	2.37	0.40
1:E:3:ARG:HH21	1:E:186:GLY:HA2	1.87	0.40
1:E:270:CYS:O	1:E:284:GLU:HG2	2.21	0.40
2:H:178:GLY:O	2:H:180:PRO:HD3	2.21	0.40
1:A:260:HIS:HB3	1:A:360:VAL:HG11	2.03	0.40
1:C:285:MET:O	1:C:289:ILE:HG13	2.22	0.40
2:D:165:LEU:HD13	2:D:338:GLY:CA	2.51	0.40
2:D:363:VAL:HA	2:D:364:PRO:HD3	1.97	0.40
1:E:284:GLU:H	1:E:284:GLU:CD	2.29	0.40
2:F:402:ARG:NE	2:F:403:PHE:H	2.19	0.40
1:G:3:ARG:HH21	1:G:186:GLY:HA2	1.84	0.40
1:G:296:SER:O	1:G:297:ARG:HB2	2.22	0.40
1:A:113:SER:O	1:A:117:GLU:HG2	2.21	0.40
1:A:260:HIS:O	1:A:261:ALA:HB2	2.20	0.40
1:E:143:LEU:HD22	2:F:198:SER:CB	2.51	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)
6:B:1122:HOH:O	6:F:1120:HOH:O[9_554]	2.14	0.06

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	419/424 (99%)	397 (95%)	22 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	419/424 (99%)	393 (94%)	25 (6%)	1 (0%)	43	42
1	E	419/424 (99%)	394 (94%)	24 (6%)	1 (0%)	43	42
1	G	419/424 (99%)	399 (95%)	17 (4%)	3 (1%)	18	14
2	B	400/415 (96%)	379 (95%)	21 (5%)	0	100	100
2	D	400/415 (96%)	383 (96%)	16 (4%)	1 (0%)	36	35
2	F	400/415 (96%)	385 (96%)	15 (4%)	0	100	100
2	H	400/415 (96%)	381 (95%)	18 (4%)	1 (0%)	36	35
All	All	3276/3356 (98%)	3111 (95%)	158 (5%)	7 (0%)	43	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	310	GLY
1	G	388	LEU
1	E	388	LEU
1	G	109	ALA
1	C	146	SER
2	D	159	ALA
2	H	159	ALA

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	319/321 (99%)	308 (97%)	11 (3%)	32	33
1	C	319/321 (99%)	309 (97%)	10 (3%)	35	37
1	E	319/321 (99%)	312 (98%)	7 (2%)	45	50
1	G	319/321 (99%)	304 (95%)	15 (5%)	23	22
2	B	297/309 (96%)	277 (93%)	20 (7%)	15	11
2	D	297/309 (96%)	272 (92%)	25 (8%)	10	7
2	F	297/309 (96%)	278 (94%)	19 (6%)	16	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	297/309 (96%)	279 (94%)	18 (6%)	17	14
All	All	2464/2520 (98%)	2339 (95%)	125 (5%)	21	19

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	67	LEU
1	A	70	MET
1	A	104	LEU
1	A	135	LEU
1	A	173	LEU
1	A	199	PRO
1	A	207	CYS
1	A	271	ASN
1	A	389	GLU
1	A	415	ARG
2	B	10	VAL
2	B	16	LEU
2	B	18	LEU
2	B	40	VAL
2	B	119	LEU
2	B	136	PHE
2	B	165	LEU
2	B	168	LEU
2	B	197	VAL
2	B	234	LEU
2	B	236	LEU
2	B	239	SER
2	B	243	GLU
2	B	254	LEU
2	B	269	ARG
2	B	279	LEU
2	B	286	THR
2	B	289	GLU
2	B	399	VAL
2	B	402	ARG
1	C	12	VAL
1	C	13	ARG
1	C	67	LEU
1	C	70	MET
1	C	90	LEU

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Mol	Chain	Res	Type
1	C	135	LEU
1	C	173	LEU
1	C	199	PRO
1	C	207	CYS
1	C	415	ARG
2	D	16	LEU
2	D	18	LEU
2	D	32	LEU
2	D	40	VAL
2	D	42	ARG
2	D	112	THR
2	D	119	LEU
2	D	136	PHE
2	D	143	GLN
2	D	165	LEU
2	D	168	LEU
2	D	188	ASP
2	D	197	VAL
2	D	234	LEU
2	D	236	LEU
2	D	254	LEU
2	D	269	ARG
2	D	279	LEU
2	D	289	GLU
2	D	347	MET
2	D	351	GLU
2	D	371	LEU
2	D	389	ARG
2	D	399	VAL
2	D	402	ARG
1	E	13	ARG
1	E	67	LEU
1	E	119	LEU
1	E	135	LEU
1	E	199	PRO
1	E	389	GLU
1	E	415	ARG
2	F	16	LEU
2	F	18	LEU
2	F	40	VAL
2	F	119	LEU
2	F	136	PHE

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Mol	Chain	Res	Type
2	F	160	GLU
2	F	168	LEU
2	F	188	ASP
2	F	197	VAL
2	F	234	LEU
2	F	236	LEU
2	F	254	LEU
2	F	269	ARG
2	F	279	LEU
2	F	289	GLU
2	F	351	GLU
2	F	371	LEU
2	F	399	VAL
2	F	402	ARG
1	G	13	ARG
1	G	67	LEU
1	G	119	LEU
1	G	135	LEU
1	G	173	LEU
1	G	199	PRO
1	G	202	PRO
1	G	207	CYS
1	G	214	THR
1	G	222	GLU
1	G	226	ARG
1	G	243	MET
1	G	271	ASN
1	G	395	LEU
1	G	415	ARG
2	H	10	VAL
2	H	16	LEU
2	H	18	LEU
2	H	136	PHE
2	H	143	GLN
2	H	168	LEU
2	H	188	ASP
2	H	197	VAL
2	H	234	LEU
2	H	249	ASP
2	H	254	LEU
2	H	269	ARG
2	H	279	LEU

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Mol	Chain	Res	Type
2	H	289	GLU
2	H	351	GLU
2	H	371	LEU
2	H	399	VAL
2	H	402	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	A	365	HIS
2	B	55	HIS
2	B	67	GLN
2	B	143	GLN
1	C	75	GLN
1	C	260	HIS
1	C	271	ASN
1	C	316	ASN
1	C	365	HIS
1	C	409	GLN
2	D	67	GLN
2	D	143	GLN
2	D	248	HIS
2	D	395	ASN
1	E	316	ASN
2	F	55	HIS
2	F	248	HIS
2	F	395	ASN
1	G	316	ASN
2	H	55	HIS
2	H	395	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
4	ACE	C	633	1	1,2,2	1.05	0	0,1,1	-	-
4	ACE	E	633	1	1,2,2	1.04	0	0,1,1	-	-
4	ACE	G	633	1	1,2,2	1.07	0	0,1,1	-	-
4	ACE	A	633	1	1,2,2	1.06	0	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	633	ACE	1	0
4	E	633	ACE	2	0
4	G	633	ACE	2	0
4	A	633	ACE	1	0

5.7 Other polymers [i](#)

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, 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	421/424 (99%)	0.54	28 (6%) 24 22	20, 30, 45, 63	0
1	C	421/424 (99%)	0.68	45 (10%) 11 10	18, 29, 49, 79	0
1	E	421/424 (99%)	1.16	88 (20%) 2 2	20, 37, 56, 66	0
1	G	421/424 (99%)	0.47	31 (7%) 20 19	18, 28, 46, 62	0
2	B	402/415 (96%)	0.35	25 (6%) 26 25	18, 27, 43, 56	0
2	D	402/415 (96%)	0.07	18 (4%) 38 37	16, 23, 39, 56	0
2	F	402/415 (96%)	0.51	26 (6%) 25 23	19, 28, 45, 62	0
2	H	402/415 (96%)	0.17	21 (5%) 33 31	17, 24, 41, 59	0
All	All	3292/3356 (98%)	0.50	282 (8%) 16 15	16, 28, 48, 79	0

All (282) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	403	PHE	7.4
1	C	423	ALA	5.3
1	C	421	GLY	5.2
2	H	403	PHE	5.1
1	E	54	ASP	5.1
1	C	417	ALA	5.0
1	A	298	THR	5.0
1	G	423	ALA	5.0
1	E	376	THR	4.9
1	C	420	ALA	4.8
1	E	380	GLU	4.7
1	C	54	ASP	4.7
1	E	423	ALA	4.7
1	C	422	ALA	4.6
2	F	268	GLY	4.6
2	B	403	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	G	298	THR	4.6
2	F	244	ALA	4.5
2	D	403	PHE	4.4
1	E	298	THR	4.4
1	A	376	THR	4.3
1	G	394	LYS	4.3
1	E	422	ALA	4.2
2	F	402	ARG	4.2
1	C	380	GLU	4.2
1	E	390	ALA	4.1
1	G	271	ASN	4.1
2	H	269	ARG	4.1
2	B	268	GLY	4.1
2	B	249	ASP	4.1
1	C	297	ARG	4.0
1	A	297	ARG	4.0
1	G	297	ARG	4.0
2	F	269	ARG	4.0
1	E	421	GLY	4.0
2	F	248	HIS	3.9
1	E	375	ARG	3.9
1	E	396	ARG	3.9
2	D	402	ARG	3.9
2	B	266	GLY	3.8
2	F	243	GLU	3.8
1	E	21	ARG	3.8
2	D	269	ARG	3.8
2	D	268	GLY	3.8
2	F	382	ARG	3.8
1	C	298	THR	3.8
1	A	271	ASN	3.8
1	E	271	ASN	3.8
1	C	418	GLU	3.7
1	E	297	ARG	3.7
2	B	402	ARG	3.7
1	C	248	ASP	3.7
1	G	392	GLU	3.7
1	E	389	GLU	3.7
1	C	419	THR	3.7
1	G	21	ARG	3.7
2	B	269	ARG	3.7
1	C	330	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	271	ASN	3.6
1	C	296	SER	3.6
1	E	330	GLU	3.6
2	D	382	ARG	3.6
1	G	376	THR	3.6
1	C	392	GLU	3.6
2	H	266	GLY	3.5
1	E	328	LEU	3.5
1	E	388	LEU	3.5
1	C	416	ASP	3.5
2	D	249	ASP	3.5
1	E	367	VAL	3.5
1	A	90	LEU	3.4
2	B	244	ALA	3.4
2	H	268	GLY	3.4
2	F	249	ASP	3.4
1	E	257	ALA	3.4
1	G	418	GLU	3.4
2	D	270	PRO	3.4
1	C	394	LYS	3.4
2	F	176	ARG	3.3
1	A	219	ASP	3.3
1	E	417	ALA	3.3
1	E	31	ARG	3.3
1	C	376	THR	3.3
1	E	280	ALA	3.3
1	E	334	ARG	3.2
2	H	402	ARG	3.2
1	G	279	LYS	3.2
1	A	418	GLU	3.2
2	D	91	GLU	3.2
1	C	21	ARG	3.2
1	C	25	GLU	3.2
1	E	300	ALA	3.2
2	B	91	GLU	3.2
1	A	423	ALA	3.1
1	E	282	GLY	3.1
2	F	270	PRO	3.1
1	A	280	ALA	3.1
1	G	396	ARG	3.1
1	E	248	ASP	3.1
2	B	121	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	421	GLY	3.1
1	E	219	ASP	3.1
2	B	250	ALA	3.1
1	E	374	LEU	3.1
1	E	394	LYS	3.0
2	F	2	SER	3.0
1	A	21	ARG	3.0
2	B	382	ARG	3.0
1	A	380	GLU	3.0
1	E	25	GLU	3.0
1	G	54	ASP	3.0
1	E	418	GLU	3.0
1	G	334	ARG	3.0
1	E	293	LEU	3.0
1	A	248	ASP	3.0
2	B	84	GLN	2.9
1	E	295	GLU	2.9
1	A	31	ARG	2.9
1	E	30	GLY	2.9
1	E	279	LYS	2.9
1	E	281	ASP	2.9
2	H	270	PRO	2.9
1	C	281	ASP	2.8
1	A	364	GLU	2.8
1	A	279	LYS	2.8
2	H	84	GLN	2.8
1	G	248	ASP	2.8
1	C	389	GLU	2.8
2	H	244	ALA	2.8
1	E	318	ARG	2.8
2	H	382	ARG	2.8
2	B	243	GLU	2.8
2	B	270	PRO	2.8
1	C	390	ALA	2.7
1	E	419	THR	2.7
1	A	285	MET	2.7
2	F	91	GLU	2.7
2	B	303	GLU	2.7
1	E	377	SER	2.7
2	H	121	SER	2.7
1	E	93	ASP	2.7
1	G	31	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	420	ALA	2.7
1	E	383	LEU	2.7
2	H	91	GLU	2.7
1	E	294	ASP	2.7
1	E	381	CYS	2.7
1	C	393	ARG	2.7
1	E	301	THR	2.6
1	E	222	GLU	2.6
1	C	331	HIS	2.6
1	E	308	ALA	2.6
2	H	282	ASN	2.6
1	E	12	VAL	2.6
1	C	257	ALA	2.6
2	D	244	ALA	2.6
1	E	336	PRO	2.6
1	C	258	ARG	2.6
1	G	330	GLU	2.6
2	D	303	GLU	2.6
2	H	243	GLU	2.6
1	E	331	HIS	2.6
2	F	92	SER	2.6
1	A	54	ASP	2.5
1	E	332	ALA	2.5
1	C	395	LEU	2.5
1	E	395	LEU	2.5
1	E	185	GLU	2.5
2	B	375	GLU	2.5
2	F	266	GLY	2.5
1	C	318	ARG	2.5
2	D	121	SER	2.5
2	F	267	SER	2.5
1	E	26	LEU	2.5
1	E	90	LEU	2.5
1	G	285	MET	2.5
1	C	396	ARG	2.5
1	E	303	ILE	2.5
1	E	391	ARG	2.5
1	E	305	TYR	2.5
1	E	392	GLU	2.5
2	H	92	SER	2.5
1	E	420	ALA	2.5
1	A	212	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	212	ARG	2.5
1	G	393	ARG	2.5
2	D	266	GLY	2.5
2	B	239	SER	2.4
2	B	286	THR	2.4
1	A	92	PRO	2.4
1	C	93	ASP	2.4
1	A	377	SER	2.4
2	B	92	SER	2.4
1	G	280	ALA	2.4
2	D	248	HIS	2.4
2	H	122	GLU	2.4
2	H	289	GLU	2.4
1	A	281	ASP	2.4
1	E	378	ASP	2.4
2	F	205	ILE	2.4
2	B	267	SER	2.4
2	F	282	ASN	2.4
1	C	219	ASP	2.4
1	E	416	ASP	2.4
1	C	31	ARG	2.4
1	E	296	SER	2.4
1	A	184	GLU	2.3
1	G	395	LEU	2.3
2	D	84	GLN	2.3
1	C	378	ASP	2.3
1	E	91	ASP	2.3
1	G	281	ASP	2.3
1	C	364	GLU	2.3
1	C	253	LEU	2.3
1	C	334	ARG	2.3
2	F	121	SER	2.3
1	C	92	PRO	2.3
1	E	369	PRO	2.3
1	E	333	ARG	2.3
1	G	253	LEU	2.3
1	E	259	ILE	2.3
2	B	374	GLY	2.3
2	B	282	ASN	2.2
1	G	422	ALA	2.2
2	D	122	GLU	2.2
2	D	243	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	387	PRO	2.2
2	H	286	THR	2.2
1	A	93	ASP	2.2
1	A	300	ALA	2.2
1	E	184	GLU	2.2
2	F	242	ALA	2.2
2	F	84	GLN	2.2
2	D	267	SER	2.2
1	A	318	ARG	2.2
1	E	337	VAL	2.2
1	E	363	LEU	2.2
2	H	2	SER	2.2
1	E	24	TRP	2.2
2	B	205	ILE	2.1
1	E	277	GLY	2.1
2	F	246	GLY	2.1
1	E	278	LEU	2.1
2	F	122	GLU	2.1
2	H	249	ASP	2.1
1	E	92	PRO	2.1
1	E	379	PRO	2.1
2	B	248	HIS	2.1
1	G	258	ARG	2.1
1	E	327	ALA	2.1
2	F	241	ALA	2.1
1	A	325	LYS	2.1
1	E	414	LEU	2.1
1	A	330	GLU	2.1
1	A	392	GLU	2.1
2	F	375	GLU	2.1
1	E	258	ARG	2.1
1	E	329	GLY	2.1
1	G	259	ILE	2.1
2	H	221	ARG	2.1
1	E	85	PHE	2.1
1	C	29	SER	2.1
1	G	25	GLU	2.1
1	G	375	ARG	2.1
2	B	245	ARG	2.1
1	G	329	GLY	2.1
2	H	374	GLY	2.1
1	E	398	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	332	ALA	2.1
1	E	251	SER	2.1
1	C	369	PRO	2.0
1	E	335	THR	2.0
2	F	90	PRO	2.0
1	E	16	GLY	2.0
1	C	368	VAL	2.0
1	E	285	MET	2.0
1	C	278	LEU	2.0
1	E	250	ASP	2.0
1	E	302	ASP	2.0
1	G	331	HIS	2.0
1	C	336	PRO	2.0
2	D	286	THR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	ACE	G	633	3/3	0.70	0.28	46,46,47,47	0
3	MG	A	1095	1/1	0.71	0.23	51,51,51,51	0
4	ACE	E	633	3/3	0.73	0.25	47,47,48,48	0
4	ACE	A	633	3/3	0.76	0.26	52,52,52,52	0
4	ACE	C	633	3/3	0.79	0.22	52,52,53,53	0
5	NA	B	1091	1/1	0.83	0.12	39,39,39,39	0
3	MG	E	1097	1/1	0.87	0.20	47,47,47,47	0
3	MG	C	1096	1/1	0.87	0.14	39,39,39,39	0
5	NA	D	1092	1/1	0.92	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	G	1098	1/1	0.94	0.12	35,35,35,35	0
5	NA	H	1094	1/1	0.95	0.09	36,36,36,36	0
5	NA	F	1093	1/1	0.96	0.07	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.