



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:43 PM GMT

PDB ID : 1GTZ  
Title : STRUCTURE OF STREPTOMYCES COELICOLOR TYPE II DEHYDRO-  
QUINASE R23A MUTANT IN COMPLEX WITH DEHYDROSHIKIMATE  
Authors : Roszak, A.W.; Krell, T.; Robinson, D.A.; Hunter, I.S.; Coggins, J.R.;  
Lapthorn, A.J.  
Deposited on : 2002-01-22  
Resolution : 1.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

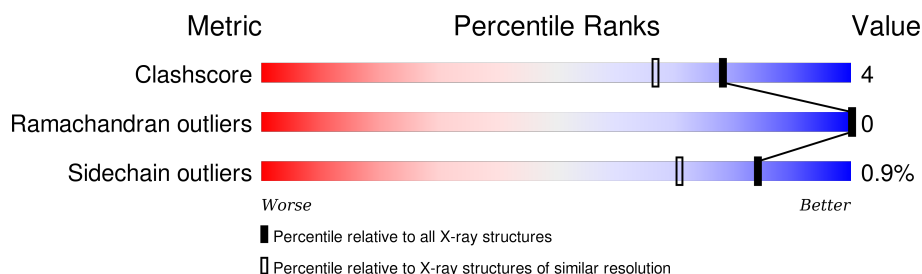
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	 85%      8%    . .
1	B	156	 79%      14%    . .
1	C	156	 74%      19%    . .
1	D	156	 79%      15%    . .
1	E	156	 83%      11%    . .
1	F	156	 81%      12%    . .
1	G	156	 81%      13%    . .

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Mol	Chain	Length	Quality of chain
1	H	156	<div><div></div><div>74%</div><div>19%</div><div>..</div></div>
1	I	156	<div><div></div><div>83%</div><div>12%</div><div>.</div></div>
1	J	156	<div><div></div><div>74%</div><div>19%</div><div>..</div></div>
1	K	156	<div><div></div><div>81%</div><div>13%</div><div>..</div></div>
1	L	156	<div><div></div><div>80%</div><div>14%</div><div>.</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15328 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 3-DEHYDROQUINATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	B	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	C	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	D	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	E	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	F	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	G	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	H	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	I	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	J	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	K	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			
1	L	149	Total	C	N	O	S	0	6	0
			1131	704	206	215	6			

There are 12 discrepancies between the modelled and reference sequences:

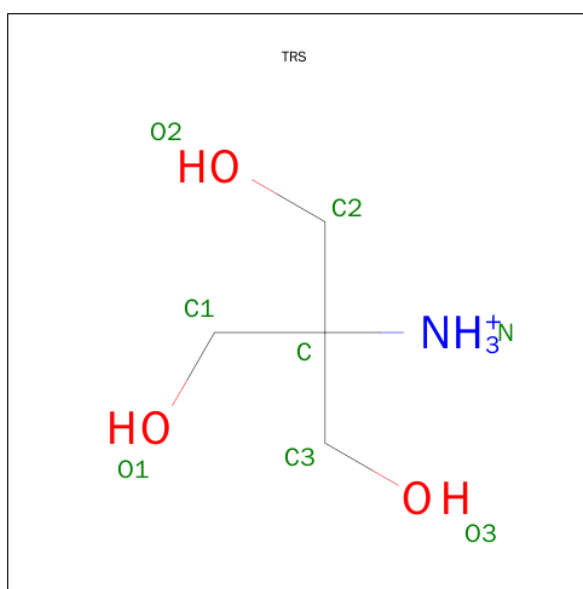
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
B	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
C	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
D	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
E	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474

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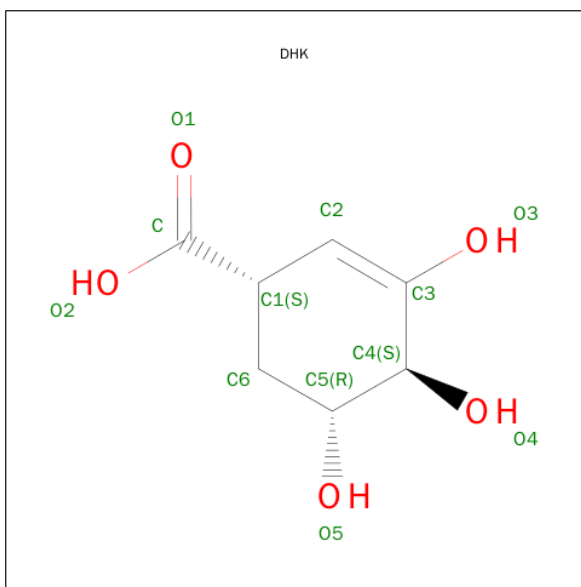
Chain	Residue	Modelled	Actual	Comment	Reference
F	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
G	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
H	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
I	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
J	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
K	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474
L	23	ALA	ARG	ENGINEERED MUTATION	UNP P15474

- Molecule 2 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	4	1	3		
2	D	1	Total	C	N	O	0	0
			8	4	1	3		
2	G	1	Total	C	N	O	0	0
			8	4	1	3		
2	J	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 3 is 3-DEHYDROSHIKIMATE (three-letter code: DHK) (formula:  $C_7H_{10}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	7	5		
3	B	1	Total	C	O	0	0
			12	7	5		
3	C	1	Total	C	O	0	0
			12	7	5		
3	D	1	Total	C	O	0	0
			12	7	5		
3	E	1	Total	C	O	0	0
			12	7	5		
3	F	1	Total	C	O	0	0
			12	7	5		
3	G	1	Total	C	O	0	0
			12	7	5		
3	H	1	Total	C	O	0	0
			12	7	5		
3	I	1	Total	C	O	0	0
			12	7	5		
3	J	1	Total	C	O	0	0
			12	7	5		
3	K	1	Total	C	O	0	0
			12	7	5		
3	L	1	Total	C	O	0	0
			12	7	5		

- Molecule 4 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	140	Total 140	O 140	0	0
4	B	116	Total 116	O 116	0	0
4	C	93	Total 93	O 93	0	0
4	D	137	Total 137	O 137	0	0
4	E	163	Total 163	O 163	0	0
4	F	135	Total 135	O 135	0	0
4	G	154	Total 154	O 154	0	0
4	H	140	Total 140	O 140	0	0
4	I	153	Total 153	O 153	0	0
4	J	109	Total 109	O 109	0	0
4	K	134	Total 134	O 134	0	0
4	L	106	Total 106	O 106	0	0

### 3 Residue-property plots [i](#)

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


Note EDS was not executed.

#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain A: 



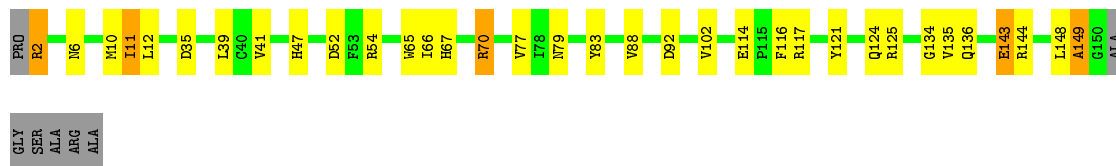
#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain B: 




#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain C: 




#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain D: 


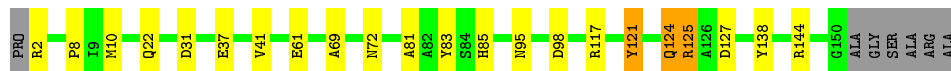


#### • Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE


Chain E: 



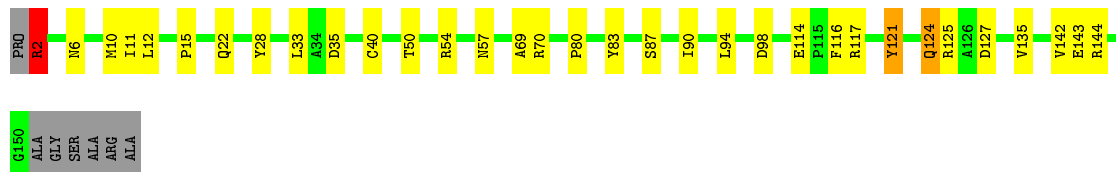
## ● Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain F:  81% 12% . .


## ● Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain G:  81% 13% . .

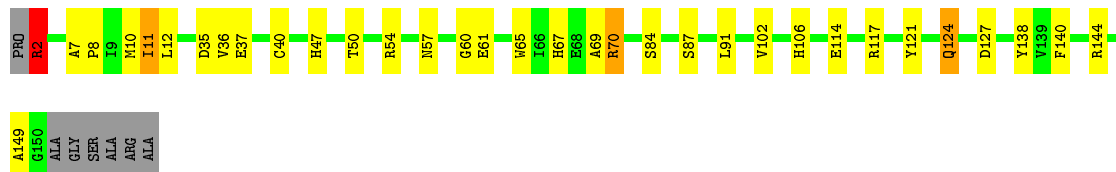
## ● Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain H:  74% 19% . .


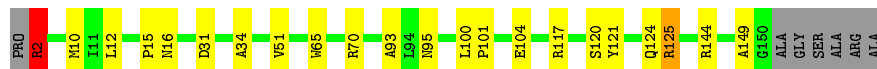
## ● Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain I:  83% 12% . .

## ● Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain J:  74% 19% . .

## ● Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain K:  81% 13% . .

## ● Molecule 1: 3-DEHYDROQUINATE DEHYDRATASE

Chain L:  80% 14% . .



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.10 Å   136.20 Å   96.70 Å 90.00°   101.28°   90.00°	Depositor
Resolution (Å)	45.00 – 1.60	Depositor
% Data completeness (in resolution range)	73.8 (45.00-1.60)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.179 , 0.221	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15328	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, DHK

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	1.08	1/1184 (0.1%)	1.76	19/1613 (1.2%)
1	B	1.07	1/1184 (0.1%)	1.68	22/1613 (1.4%)
1	C	1.23	1/1184 (0.1%)	1.94	34/1613 (2.1%)
1	D	1.08	0/1184	1.66	16/1613 (1.0%)
1	E	1.12	0/1184	1.70	20/1613 (1.2%)
1	F	1.05	0/1184	1.72	18/1613 (1.1%)
1	G	1.07	0/1184	1.69	15/1613 (0.9%)
1	H	1.06	1/1184 (0.1%)	1.79	29/1613 (1.8%)
1	I	1.06	0/1184	1.82	20/1613 (1.2%)
1	J	1.19	3/1184 (0.3%)	1.95	33/1613 (2.0%)
1	K	1.11	0/1184	1.63	14/1613 (0.9%)
1	L	1.02	0/1184	1.74	21/1613 (1.3%)
All	All	1.10	7/14208 (0.0%)	1.76	261/19356 (1.3%)

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
1	A	0	1
1	C	0	2
1	D	0	1
1	F	0	2
1	H	0	1
1	L	0	1
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	60	GLY	CA-C	5.57	1.60	1.51
1	A	114	GLU	CD-OE1	5.39	1.31	1.25
1	C	136	GLN	C-N	5.20	1.42	1.33
1	B	59	GLU	CD-OE1	5.19	1.31	1.25
1	H	87	SER	CB-OG	-5.16	1.35	1.42
1	J	87	SER	N-CA	-5.08	1.36	1.46
1	J	84	SER	CB-OG	5.05	1.48	1.42

All (261) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	144	ARG	NE-CZ-NH1	-25.52	107.54	120.30
1	A	2	ARG	CD-NE-CZ	19.50	150.91	123.60
1	I	2	ARG	NE-CZ-NH1	-17.70	111.45	120.30
1	A	2	ARG	NE-CZ-NH1	16.64	128.62	120.30
1	J	117	ARG	NE-CZ-NH2	-16.13	112.23	120.30
1	I	144	ARG	NE-CZ-NH2	13.93	127.27	120.30
1	K	144	ARG	NE-CZ-NH1	-12.89	113.86	120.30
1	L	144	ARG	NE-CZ-NH2	12.76	126.68	120.30
1	H	117	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	F	144	ARG	NE-CZ-NH2	11.93	126.26	120.30
1	E	127	ASP	CB-CG-OD2	11.85	128.97	118.30
1	G	113	ARG	NE-CZ-NH2	11.68	126.14	120.30
1	F	117	ARG	NE-CZ-NH2	-11.56	114.52	120.30
1	H	144	ARG	NE-CZ-NH2	11.51	126.06	120.30
1	J	54	ARG	NE-CZ-NH1	11.25	125.92	120.30
1	E	144	ARG	NE-CZ-NH2	11.20	125.90	120.30
1	B	54	ARG	NE-CZ-NH2	11.19	125.89	120.30
1	A	144	ARG	NE-CZ-NH2	11.01	125.81	120.30
1	I	54	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	B	54	ARG	NE-CZ-NH1	-10.96	114.82	120.30
1	C	144	ARG	NE-CZ-NH2	10.95	125.77	120.30
1	D	144	ARG	NE-CZ-NH2	10.73	125.66	120.30
1	E	117	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	G	144	ARG	NE-CZ-NH2	10.49	125.54	120.30
1	E	125	ARG	NE-CZ-NH1	10.45	125.53	120.30
1	L	127	ASP	CB-CG-OD2	10.32	127.59	118.30
1	C	70	ARG	NE-CZ-NH2	10.29	125.44	120.30
1	D	70	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	H	2	ARG	CD-NE-CZ	9.55	136.97	123.60
1	K	2	ARG	NE-CZ-NH2	9.31	124.96	120.30
1	H	54	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	G	37	GLU	OE1-CD-OE2	-9.11	112.37	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	2	ARG	CD-NE-CZ	9.08	136.31	123.60
1	L	117	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	K	144	ARG	NE-CZ-NH2	9.05	124.83	120.30
1	C	54	ARG	NE-CZ-NH2	8.99	124.80	120.30
1	A	2	ARG	NE-CZ-NH2	-8.98	115.81	120.30
1	L	113	ARG	NE-CZ-NH2	-8.92	115.84	120.30
1	D	117	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	114	GLU	OE1-CD-OE2	-8.80	112.73	123.30
1	G	127	ASP	CB-CG-OD1	8.71	126.14	118.30
1	J	70	ARG	NE-CZ-NH2	8.69	124.64	120.30
1	J	2	ARG	NE-CZ-NH1	8.47	124.53	120.30
1	C	149	ALA	CB-CA-C	8.47	122.80	110.10
1	H	127	ASP	CB-CG-OD2	8.43	125.89	118.30
1	K	31	ASP	CB-CG-OD2	8.42	125.88	118.30
1	J	144	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	B	2	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	D	31	ASP	CB-CG-OD2	8.26	125.73	118.30
1	D	113	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	L	92	ASP	CB-CG-OD1	8.15	125.64	118.30
1	I	113	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	J	2	ARG	CD-NE-CZ	8.13	134.99	123.60
1	F	127	ASP	CB-CG-OD2	8.11	125.59	118.30
1	I	2	ARG	NH1-CZ-NH2	7.99	128.19	119.40
1	F	61	GLU	OE1-CD-OE2	-7.96	113.75	123.30
1	A	124[A]	GLN	CA-CB-CG	7.95	130.89	113.40
1	A	124[B]	GLN	CA-CB-CG	7.95	130.89	113.40
1	A	54	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	C	144	ARG	NH1-CZ-NH2	-7.82	110.80	119.40
1	K	117	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	H	125	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	J	8	PRO	O-C-N	7.65	134.95	122.70
1	B	83	TYR	CB-CG-CD2	7.64	125.58	121.00
1	B	125	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	C	54	ARG	CD-NE-CZ	7.57	134.20	123.60
1	G	125	ARG	CD-NE-CZ	7.54	134.16	123.60
1	J	138	TYR	CG-CD1-CE1	-7.51	115.29	121.30
1	H	124[A]	GLN	CA-CB-CG	7.25	129.34	113.40
1	H	124[B]	GLN	CA-CB-CG	7.25	129.34	113.40
1	B	111	HIS	O-C-N	-7.19	111.20	122.70
1	J	35	ASP	CB-CG-OD2	7.11	124.70	118.30
1	G	114	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	J	149	ALA	CB-CA-C	7.06	120.70	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	117	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	C	114	GLU	OE1-CD-OE2	-7.03	114.87	123.30
1	F	125	ARG	CD-NE-CZ	7.01	133.41	123.60
1	A	121	TYR	CB-CG-CD1	7.00	125.20	121.00
1	G	121	TYR	CG-CD1-CE1	-7.00	115.70	121.30
1	H	83	TYR	CB-CG-CD1	7.00	125.20	121.00
1	J	50	THR	O-C-N	6.88	133.72	122.70
1	L	70	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	L	53	PHE	CB-CG-CD1	6.87	125.61	120.80
1	C	83	TYR	CD1-CE1-CZ	6.85	125.96	119.80
1	I	35	ASP	CB-CG-OD2	6.84	124.45	118.30
1	F	121	TYR	CB-CG-CD1	-6.81	116.92	121.00
1	H	114	GLU	OE1-CD-OE2	-6.78	115.17	123.30
1	K	125	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	G	2	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	E	83	TYR	CD1-CE1-CZ	6.63	125.77	119.80
1	J	124[A]	GLN	CA-CB-CG	6.63	127.99	113.40
1	J	124[B]	GLN	CA-CB-CG	6.63	127.99	113.40
1	F	31	ASP	CB-CG-OD2	6.63	124.27	118.30
1	C	66	ILE	O-C-N	-6.61	112.12	122.70
1	A	83	TYR	CB-CG-CD2	6.61	124.97	121.00
1	B	138	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	L	2	ARG	CD-NE-CZ	6.53	132.74	123.60
1	E	117	ARG	CD-NE-CZ	6.52	132.72	123.60
1	G	92	ASP	CB-CG-OD1	6.49	124.14	118.30
1	C	116	PHE	CB-CG-CD2	6.48	125.33	120.80
1	J	91	LEU	O-C-N	-6.42	112.43	122.70
1	J	106	HIS	N-CA-CB	6.41	122.13	110.60
1	J	138	TYR	O-C-N	6.40	132.94	122.70
1	I	121	TYR	CZ-CE2-CD2	-6.40	114.04	119.80
1	D	68	GLU	OE1-CD-OE2	6.37	130.94	123.30
1	H	98	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	B	149	ALA	CB-CA-C	6.31	119.57	110.10
1	C	2	ARG	CD-NE-CZ	6.30	132.42	123.60
1	D	59	GLU	OE1-CD-OE2	-6.29	115.75	123.30
1	B	92	ASP	CB-CG-OD1	6.29	123.96	118.30
1	I	113	ARG	NH1-CZ-NH2	6.29	126.32	119.40
1	A	127	ASP	CB-CG-OD2	6.27	123.94	118.30
1	J	61	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	C	144	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	L	2	ARG	NE-CZ-NH2	6.21	123.41	120.30
1	J	138	TYR	CB-CG-CD1	-6.18	117.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	J	37	GLU	OE1-CD-OE2	-6.13	115.95	123.30
1	H	83	TYR	CD1-CG-CD2	-6.11	111.18	117.90
1	A	114	GLU	CG-CD-OE2	6.10	130.51	118.30
1	H	83	TYR	CD1-CE1-CZ	6.10	125.29	119.80
1	J	140	PHE	CG-CD1-CE1	6.08	127.49	120.80
1	J	36	VAL	CG1-CB-CG2	6.08	120.63	110.90
1	E	37	GLU	OE1-CD-OE2	-6.06	116.02	123.30
1	I	125	ARG	CD-NE-CZ	6.05	132.07	123.60
1	G	113	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	83	TYR	CG-CD2-CE2	6.01	126.11	121.30
1	F	8	PRO	O-C-N	5.99	132.28	122.70
1	D	108	SER	N-CA-CB	-5.98	101.53	110.50
1	C	143[A]	GLU	O-C-N	-5.94	113.20	122.70
1	C	143[B]	GLU	O-C-N	-5.94	113.20	122.70
1	I	150	GLY	CA-C-O	5.91	131.24	120.60
1	I	92	ASP	CB-CG-OD1	5.88	123.60	118.30
1	H	94	LEU	CB-CG-CD1	5.88	121.00	111.00
1	I	113	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	F	98	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	98	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	D	144	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	11[A]	ILE	N-CA-CB	5.82	124.19	110.80
1	C	11[B]	ILE	N-CA-CB	5.82	124.19	110.80
1	F	124[A]	GLN	CA-CB-CG	5.82	126.19	113.40
1	F	124[B]	GLN	CA-CB-CG	5.82	126.19	113.40
1	B	127	ASP	CB-CG-OD2	5.80	123.52	118.30
1	F	138	TYR	CB-CG-CD1	5.80	124.48	121.00
1	H	121	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	L	44	ALA	N-CA-CB	5.79	118.20	110.10
1	B	92	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	C	117	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	G	2	ARG	CD-NE-CZ	-5.72	115.59	123.60
1	E	83	TYR	CG-CD2-CE2	5.71	125.87	121.30
1	D	114	GLU	OE1-CD-OE2	-5.71	116.45	123.30
1	I	140	PHE	CB-CG-CD2	5.70	124.79	120.80
1	L	80	PRO	N-CA-CB	5.70	110.14	103.30
1	J	102	VAL	O-C-N	-5.70	113.59	122.70
1	A	70	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	D	124[A]	GLN	CA-CB-CG	5.61	125.73	113.40
1	D	124[B]	GLN	CA-CB-CG	5.61	125.73	113.40
1	H	124[A]	GLN	OE1-CD-NE2	5.60	134.78	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	124[B]	GLN	OE1-CD-NE2	5.60	134.78	121.90
1	D	92	ASP	CB-CG-OD1	5.59	123.33	118.30
1	D	54	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	L	114	GLU	OE1-CD-OE2	-5.56	116.62	123.30
1	C	70	ARG	NH1-CZ-NH2	-5.56	113.29	119.40
1	B	144	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	C	134	GLY	O-C-N	-5.55	113.81	122.70
1	H	142	VAL	O-C-N	-5.55	113.83	122.70
1	K	149	ALA	CB-CA-C	5.54	118.41	110.10
1	C	79	ASN	N-CA-CB	5.54	120.57	110.60
1	C	125	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	D	138	TYR	CZ-CE2-CD2	-5.50	114.85	119.80
1	E	64	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	J	70	ARG	NH1-CZ-NH2	-5.50	113.36	119.40
1	L	35	ASP	CB-CG-OD1	-5.48	113.36	118.30
1	H	50	THR	O-C-N	5.48	131.47	122.70
1	H	144	ARG	NH1-CZ-NH2	-5.48	113.38	119.40
1	L	113	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	121	TYR	CB-CG-CD1	5.46	124.28	121.00
1	C	54	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	K	104	GLU	O-C-N	5.44	131.41	122.70
1	E	64	ASP	CA-CB-CG	5.44	125.36	113.40
1	K	51	VAL	O-C-N	-5.43	114.00	122.70
1	C	41	VAL	CG1-CB-CG2	-5.41	102.24	110.90
1	K	70	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	C	35	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	4	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	F	81	ALA	CA-C-O	-5.39	108.79	120.10
1	G	64	ASP	CB-CG-OD2	5.38	123.14	118.30
1	F	72	ASN	O-C-N	-5.38	114.09	122.70
1	C	102	VAL	C-N-CA	5.38	135.15	121.70
1	B	64	ASP	CB-CG-OD1	5.38	123.14	118.30
1	J	36	VAL	CA-CB-CG2	-5.38	102.83	110.90
1	E	18	ASN	O-C-N	-5.38	114.10	122.70
1	A	64	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	104	GLU	OE1-CD-OE2	5.36	129.73	123.30
1	H	90	ILE	O-C-N	-5.36	114.12	122.70
1	C	65	TRP	CE3-CZ3-CH2	-5.35	115.32	121.20
1	H	121	TYR	CG-CD2-CE2	-5.33	117.03	121.30
1	J	47	HIS	O-C-N	-5.33	114.13	123.20
1	K	93	ALA	O-C-N	-5.32	114.19	122.70
1	I	143[A]	GLU	OE1-CD-OE2	5.30	129.66	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	143[B]	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	A	125	ARG	NE-CZ-NH2	5.30	122.95	120.30
1	G	35	ASP	CB-CG-OD2	5.29	123.06	118.30
1	J	114	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	K	65	TRP	O-C-N	-5.28	114.25	122.70
1	A	35	ASP	CB-CG-OD2	5.27	123.04	118.30
1	J	117	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	92	ASP	CB-CA-C	5.26	120.92	110.40
1	C	92	ASP	CB-CG-OD2	5.25	123.03	118.30
1	G	91	LEU	CB-CG-CD2	-5.25	102.07	111.00
1	B	124[A]	GLN	CA-CB-CG	5.25	124.96	113.40
1	B	124[B]	GLN	CA-CB-CG	5.25	124.96	113.40
1	L	83	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	H	83	TYR	CG-CD2-CE2	5.24	125.50	121.30
1	C	83	TYR	CG-CD2-CE2	5.24	125.49	121.30
1	I	54	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
1	I	144	ARG	NH1-CZ-NH2	5.23	125.15	119.40
1	J	7	ALA	N-CA-CB	-5.23	102.78	110.10
1	C	2	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	K	125	ARG	CD-NE-CZ	5.21	130.90	123.60
1	L	2	ARG	O-C-N	-5.21	114.36	122.70
1	H	70	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	J	144	ARG	NH1-CZ-NH2	-5.19	113.70	119.40
1	C	52	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	E	92	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	121	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	J	127	ASP	O-C-N	-5.17	114.41	123.20
1	E	64	ASP	CB-CG-OD2	5.16	122.94	118.30
1	F	117	ARG	NH1-CZ-NH2	5.16	125.07	119.40
1	I	116	PHE	CB-CG-CD1	5.16	124.41	120.80
1	B	4	LEU	CB-CA-C	-5.14	100.42	110.20
1	J	57	ASN	N-CA-CB	-5.14	101.34	110.60
1	L	124[A]	GLN	CG-CD-OE1	-5.14	111.33	121.60
1	L	124[B]	GLN	CG-CD-OE1	-5.14	111.33	121.60
1	J	114	GLU	CA-CB-CG	5.13	124.69	113.40
1	L	97	CYS	CA-CB-SG	5.12	123.21	114.00
1	E	143[A]	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	E	143[B]	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	H	116	PHE	CB-CG-CD2	5.10	124.37	120.80
1	C	83	TYR	CB-CG-CD1	5.09	124.06	121.00
1	H	35	ASP	CB-CG-OD1	-5.09	113.72	118.30
1	C	88	VAL	CA-CB-CG2	-5.09	103.27	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	54	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	E	125	ARG	CD-NE-CZ	5.08	130.71	123.60
1	K	51	VAL	C-N-CA	5.08	134.40	121.70
1	D	114	GLU	CG-CD-OE2	5.08	128.45	118.30
1	B	2	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	H	117	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	E	124[A]	GLN	CA-CB-CG	5.05	124.51	113.40
1	E	124[B]	GLN	CA-CB-CG	5.05	124.51	113.40
1	H	28	TYR	CB-CG-CD1	5.05	124.03	121.00
1	F	61	GLU	CG-CD-OE1	5.04	128.39	118.30
1	H	2	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	J	2	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	L	4	LEU	CB-CG-CD1	-5.03	102.46	111.00
1	F	124[A]	GLN	OE1-CD-NE2	5.02	133.46	121.90
1	F	124[B]	GLN	OE1-CD-NE2	5.02	133.46	121.90
1	C	39	LEU	C-N-CA	5.01	134.22	121.70
1	C	92	ASP	OD1-CG-OD2	-5.01	113.79	123.30
1	I	26	GLU	CG-CD-OE1	5.01	128.31	118.30
1	B	141	GLY	O-C-N	-5.00	114.70	122.70

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	SER	Mainchain
1	C	135	VAL	Mainchain
1	C	149	ALA	Mainchain
1	D	89	ALA	Mainchain
1	F	83	TYR	Mainchain
1	F	85	HIS	Mainchain
1	H	135	VAL	Mainchain
1	L	39	LEU	Mainchain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1131	0	1101	4	0
1	B	1131	0	1101	10	0
1	C	1131	0	1101	8	0
1	D	1131	0	1101	8	0
1	E	1131	0	1101	11	0
1	F	1131	0	1101	7	1
1	G	1131	0	1101	8	0
1	H	1131	0	1101	13	1
1	I	1131	0	1101	6	1
1	J	1131	0	1100	9	0
1	K	1131	0	1101	9	0
1	L	1131	0	1101	4	1
2	A	8	0	12	0	0
2	D	8	0	12	0	0
2	G	8	0	12	0	0
2	J	8	0	12	0	0
3	A	12	0	6	0	0
3	B	12	0	6	0	0
3	C	12	0	7	0	0
3	D	12	0	7	0	0
3	E	12	0	6	0	0
3	F	12	0	6	0	0
3	G	12	0	7	0	0
3	H	12	0	8	0	0
3	I	12	0	6	0	0
3	J	12	0	7	0	0
3	K	12	0	6	0	0
3	L	12	0	5	0	0
4	A	140	0	0	0	2
4	B	116	0	0	2	0
4	C	93	0	0	0	0
4	D	137	0	0	2	0
4	E	163	0	0	1	3
4	F	135	0	0	2	2
4	G	154	0	0	2	2
4	H	140	0	0	2	0
4	I	153	0	0	2	2
4	J	109	0	0	0	0
4	K	134	0	0	2	3
4	L	106	0	0	0	0
All	All	15328	0	13336	97	9

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 4.

All (97) 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:H:22:GLN:NE2	4:H:2027:HOH:O	1.98	0.94
1:J:10[B]:MET:SD	1:J:12:LEU:HD21	2.18	0.83
1:D:143[B]:GLU:OE1	4:D:2133:HOH:O	1.99	0.80
1:A:10[B]:MET:SD	1:A:69:ALA:HB2	2.22	0.80
1:H:2:ARG:HH21	1:H:2:ARG:HG2	1.49	0.75
1:E:2:ARG:HB2	1:E:2:ARG:NH2	2.02	0.75
1:H:143[B]:GLU:OE1	4:H:2133:HOH:O	2.07	0.72
1:F:37:GLU:OE1	4:F:2050:HOH:O	2.07	0.71
1:G:121:TYR:O	1:G:124[B]:GLN:HG2	1.93	0.69
1:J:10[B]:MET:HE3	1:J:69:ALA:HB2	1.75	0.68
1:B:120:SER:O	1:B:124[B]:GLN:NE2	2.28	0.67
1:K:2:ARG:HD3	4:K:2090:HOH:O	1.95	0.66
1:E:2:ARG:HB2	1:E:2:ARG:HH21	1.61	0.65
1:I:10[B]:MET:SD	1:I:12:LEU:HD21	2.37	0.64
1:K:121:TYR:O	1:K:124[B]:GLN:HG2	1.99	0.63
1:L:10[B]:MET:SD	1:L:12:LEU:HD21	2.38	0.63
1:E:3:SER:CB	4:E:2004:HOH:O	2.46	0.62
1:L:120:SER:O	1:L:124[A]:GLN:NE2	2.32	0.62
1:G:121:TYR:O	1:G:124[A]:GLN:HG2	2.00	0.61
1:C:10[B]:MET:SD	1:C:12:LEU:HD21	2.40	0.61
1:F:121:TYR:O	1:F:124[B]:GLN:HG2	2.02	0.59
1:F:10[B]:MET:CE	1:F:69:ALA:HB2	2.32	0.59
1:A:121:TYR:O	1:A:124[B]:GLN:HG2	2.03	0.58
1:A:121:TYR:O	1:A:124[A]:GLN:HG2	2.05	0.57
1:B:2:ARG:NH1	1:B:71:LEU:O	2.37	0.57
1:K:121:TYR:O	1:K:124[A]:GLN:HG2	2.05	0.56
1:D:121:TYR:O	1:D:124[A]:GLN:HG2	2.05	0.56
1:I:8:PRO:HB3	4:I:2063:HOH:O	2.06	0.56
1:D:22:GLN:NE2	4:D:2026:HOH:O	2.39	0.55
1:B:121:TYR:O	1:B:124[A]:GLN:HG2	2.06	0.55
1:F:95:ASN:HD22	1:F:125:ARG:HD3	1.71	0.54
1:K:120:SER:O	1:K:124[B]:GLN:NE2	2.41	0.54
1:H:121:TYR:O	1:H:124[B]:GLN:HG2	2.08	0.54
1:L:11[B]:ILE:HG12	1:L:77:VAL:HB	1.90	0.54
1:J:121:TYR:O	1:J:124[A]:GLN:HG2	2.08	0.53
1:G:120:SER:O	1:G:124[A]:GLN:NE2	2.42	0.53
1:E:95:ASN:HD22	1:E:125:ARG:HD3	1.74	0.52
1:H:2:ARG:NH2	1:H:2:ARG:HG2	2.19	0.52
1:J:10[B]:MET:CE	1:J:69:ALA:HB2	2.39	0.52
1:E:121:TYR:O	1:E:124[B]:GLN:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ASN:ND2	4:G:2009:HOH:O	1.84	0.51
1:C:121:TYR:O	1:C:124[A]:GLN:HG2	2.10	0.51
1:H:121:TYR:O	1:H:124[A]:GLN:HG2	2.11	0.51
1:L:121:TYR:O	1:L:124[B]:GLN:HG2	2.11	0.51
1:E:121:TYR:O	1:E:124[A]:GLN:HG2	2.10	0.51
1:H:10[B]:MET:SD	1:H:69:ALA:HB2	2.51	0.51
1:C:11[B]:ILE:HG12	1:C:77:VAL:HB	1.94	0.50
1:J:10[B]:MET:HE3	1:J:65:TRP:O	2.12	0.50
1:F:121:TYR:O	1:F:124[A]:GLN:HG2	2.12	0.49
1:K:95:ASN:HD22	1:K:125:ARG:HD3	1.76	0.49
1:E:10[B]:MET:SD	1:E:12:LEU:HD21	2.52	0.49
1:B:2:ARG:HD3	4:B:2068:HOH:O	2.12	0.49
1:K:10[B]:MET:SD	1:K:12:LEU:HD21	2.53	0.48
1:C:67:HIS:O	1:C:70:ARG:HB3	2.13	0.48
1:C:47:HIS:NE2	1:C:143[A]:GLU:OE1	2.45	0.47
1:I:121:TYR:O	1:I:124[B]:GLN:HG2	2.15	0.47
1:E:67:HIS:O	1:E:70:ARG:HB3	2.14	0.47
1:H:10[B]:MET:CE	1:H:69:ALA:HB2	2.44	0.47
1:E:2:ARG:CZ	1:E:2:ARG:HB2	2.45	0.46
1:B:67:HIS:O	1:B:70:ARG:HB3	2.15	0.46
1:C:2:ARG:HH11	1:C:6:ASN:HB3	1.80	0.46
1:G:95:ASN:HD22	1:G:125:ARG:HD3	1.80	0.46
1:D:10[B]:MET:HG2	1:D:12:LEU:HG	1.97	0.46
1:G:45:ALA:HB2	4:G:2065:HOH:O	2.15	0.45
1:D:33:LEU:HA	1:D:33:LEU:HD12	1.87	0.45
1:I:8:PRO:CB	4:I:2063:HOH:O	2.64	0.45
1:G:10[B]:MET:SD	1:G:12:LEU:HD21	2.57	0.45
1:B:10[B]:MET:SD	1:B:12:LEU:HD21	2.57	0.45
1:H:10[B]:MET:HE1	1:H:69:ALA:HB2	1.99	0.45
1:D:10[B]:MET:SD	1:D:12:LEU:HD21	2.56	0.45
1:A:67:HIS:O	1:A:70:ARG:HB3	2.17	0.45
1:J:11[B]:ILE:HD13	1:J:40:CYS:SG	2.57	0.44
1:C:121:TYR:O	1:C:124[B]:GLN:HG2	2.18	0.44
1:J:2:ARG:HH11	1:J:2:ARG:HB3	1.81	0.43
1:H:33:LEU:HA	1:H:33:LEU:HD12	1.90	0.43
1:J:10[B]:MET:SD	1:J:12:LEU:CD2	3.00	0.43
1:B:121:TYR:O	1:B:124[B]:GLN:HG2	2.17	0.43
1:F:10[B]:MET:SD	1:F:69:ALA:HB2	2.59	0.43
1:F:41:VAL:HG11	4:F:2004:HOH:O	2.18	0.42
1:I:10[B]:MET:CG	1:I:12:LEU:HG	2.48	0.42
1:K:34:ALA:HA	4:K:2041:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ARG:CB	1:E:2:ARG:HH21	2.29	0.42
1:B:2:ARG:HB3	1:B:2:ARG:HE	1.58	0.42
1:J:67:HIS:O	1:J:70:ARG:HB3	2.20	0.42
1:H:10[B]:MET:SD	1:H:12:LEU:HD21	2.60	0.41
1:H:15:PRO:HA	1:H:57:ASN:OD1	2.20	0.41
1:K:100:LEU:HD12	1:K:101:PRO:HD2	2.03	0.41
1:D:71:LEU:HB2	1:D:72:ASN:ND2	2.36	0.41
1:D:100:LEU:HD12	1:D:101:PRO:HD2	2.01	0.41
1:K:15:PRO:O	1:K:16:ASN:HB2	2.19	0.41
1:B:10[B]:MET:HG2	1:B:12:LEU:HG	2.02	0.41
1:B:150:GLY:HA3	4:B:2114:HOH:O	2.21	0.41
1:H:11[B]:ILE:HD13	1:H:40:CYS:SG	2.61	0.41
1:E:120:SER:O	1:E:124[B]:GLN:NE2	2.55	0.40
1:I:67:HIS:O	1:I:70:ARG:HB3	2.21	0.40
1:G:67:HIS:O	1:G:70:ARG:HB3	2.20	0.40
1:C:148:LEU:HA	1:C:148:LEU:HD23	1.85	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2027:HOH:O	4:K:2066:HOH:O[2_645]	1.43	0.77
4:F:2047:HOH:O	4:I:2053:HOH:O[2_545]	1.69	0.51
4:E:2012:HOH:O	4:K:2023:HOH:O[2_645]	1.74	0.46
1:F:22:GLN:NE2	1:I:6:ASN:O[2_545]	1.84	0.36
4:F:2048:HOH:O	4:I:2025:HOH:O[2_545]	2.03	0.17
4:A:2058:HOH:O	4:G:2004:HOH:O[2_546]	2.09	0.11
4:E:2006:HOH:O	4:K:2042:HOH:O[2_645]	2.17	0.03
4:A:2065:HOH:O	4:G:2067:HOH:O[2_546]	2.17	0.03
1:H:6:ASN:OD1	1:L:68:GLU:OE2[1_455]	2.18	0.02

## 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	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	B	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
1	C	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	D	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	E	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	F	153/156 (98%)	150 (98%)	3 (2%)	0	100	100
1	G	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	H	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	I	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	J	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	K	153/156 (98%)	149 (97%)	4 (3%)	0	100	100
1	L	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
All	All	1836/1872 (98%)	1790 (98%)	46 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	122/119 (102%)	121 (99%)	1 (1%)	86	75
1	B	122/119 (102%)	120 (98%)	2 (2%)	70	47
1	C	122/119 (102%)	122 (100%)	0	100	100
1	D	122/119 (102%)	121 (99%)	1 (1%)	86	75
1	E	122/119 (102%)	121 (99%)	1 (1%)	86	75
1	F	122/119 (102%)	121 (99%)	1 (1%)	86	75
1	G	122/119 (102%)	122 (100%)	0	100	100
1	H	122/119 (102%)	120 (98%)	2 (2%)	70	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	122/119 (102%)	122 (100%)	0	100	100
1	J	122/119 (102%)	119 (98%)	3 (2%)	55	26
1	K	122/119 (102%)	121 (99%)	1 (1%)	86	75
1	L	122/119 (102%)	121 (99%)	1 (1%)	86	75
All	All	1464/1428 (102%)	1451 (99%)	13 (1%)	84	71

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	B	2	ARG
1	B	80	PRO
1	D	2	ARG
1	E	2	ARG
1	F	2	ARG
1	H	2	ARG
1	H	80	PRO
1	J	2	ARG
1	J	11[A]	ILE
1	J	11[B]	ILE
1	K	2	ARG
1	L	2	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	106	HIS
1	B	6	ASN
1	B	95	ASN
1	B	106	HIS
1	C	95	ASN
1	C	106	HIS
1	D	6	ASN
1	D	95	ASN
1	D	106	HIS
1	E	6	ASN
1	E	95	ASN
1	E	106	HIS
1	F	6	ASN

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Mol	Chain	Res	Type
1	F	24	GLN
1	F	95	ASN
1	F	106	HIS
1	G	95	ASN
1	G	106	HIS
1	H	6	ASN
1	H	95	ASN
1	H	106	HIS
1	I	6	ASN
1	I	95	ASN
1	I	106	HIS
1	J	6	ASN
1	J	95	ASN
1	J	106	HIS
1	K	6	ASN
1	K	24	GLN
1	K	95	ASN
1	K	106	HIS
1	L	6	ASN
1	L	95	ASN
1	L	106	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

16 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	TRS	A	1152	-	7,7,7	1.27	1 (14%)	9,9,9	2.29	4 (44%)
3	DHK	A	1162	-	7,12,12	5.51	5 (71%)	6,17,17	3.44	4 (66%)
3	DHK	B	1162	-	7,12,12	5.20	6 (85%)	6,17,17	2.45	4 (66%)
3	DHK	C	1162	-	7,12,12	4.27	5 (71%)	6,17,17	2.62	4 (66%)
2	TRS	D	1152	-	7,7,7	1.80	2 (28%)	9,9,9	1.88	3 (33%)
3	DHK	D	1162	-	7,12,12	5.53	5 (71%)	6,17,17	1.58	2 (33%)
3	DHK	E	1162	-	7,12,12	5.12	6 (85%)	6,17,17	2.00	2 (33%)
3	DHK	F	1162	-	7,12,12	4.89	6 (85%)	6,17,17	3.14	3 (50%)
2	TRS	G	1153	-	7,7,7	1.80	3 (42%)	9,9,9	2.18	3 (33%)
3	DHK	G	1162	-	7,12,12	4.34	6 (85%)	6,17,17	1.73	2 (33%)
3	DHK	H	1162	-	7,12,12	4.72	5 (71%)	6,17,17	2.30	4 (66%)
3	DHK	I	1162	-	7,12,12	4.64	5 (71%)	6,17,17	3.00	3 (50%)
2	TRS	J	1152	-	7,7,7	1.61	2 (28%)	9,9,9	1.74	3 (33%)
3	DHK	J	1162	-	7,12,12	3.89	6 (85%)	6,17,17	2.82	3 (50%)
3	DHK	K	1162	-	7,12,12	5.72	6 (85%)	6,17,17	3.11	5 (83%)
3	DHK	L	1162	-	7,12,12	5.18	6 (85%)	6,17,17	2.51	2 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRS	A	1152	-	-	0/9/9/9	0/0/0/0
3	DHK	A	1162	-	-	0/0/20/20	0/1/1/1
3	DHK	B	1162	-	-	0/0/20/20	0/1/1/1
3	DHK	C	1162	-	-	0/0/20/20	0/1/1/1
2	TRS	D	1152	-	-	0/9/9/9	0/0/0/0
3	DHK	D	1162	-	-	0/0/20/20	0/1/1/1
3	DHK	E	1162	-	-	0/0/20/20	0/1/1/1
3	DHK	F	1162	-	-	0/0/20/20	0/1/1/1
2	TRS	G	1153	-	-	0/9/9/9	0/0/0/0
3	DHK	G	1162	-	-	0/0/20/20	0/1/1/1
3	DHK	H	1162	-	-	0/0/20/20	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DHK	I	1162	-	-	0/0/20/20	0/1/1/1
2	TRS	J	1152	-	-	0/9/9/9	0/0/0/0
3	DHK	J	1162	-	-	0/0/20/20	0/1/1/1
3	DHK	K	1162	-	-	0/0/20/20	0/1/1/1
3	DHK	L	1162	-	-	0/0/20/20	0/1/1/1

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1162	DHK	C1-C2	-8.03	1.39	1.50
3	L	1162	DHK	C1-C2	-7.89	1.40	1.50
3	K	1162	DHK	C1-C2	-7.64	1.40	1.50
3	E	1162	DHK	C1-C2	-7.23	1.41	1.50
3	K	1162	DHK	C6-C1	-7.12	1.39	1.53
3	K	1162	DHK	C6-C5	-7.06	1.41	1.52
3	A	1162	DHK	C1-C2	-7.02	1.41	1.50
3	A	1162	DHK	C6-C1	-7.00	1.40	1.53
3	B	1162	DHK	C6-C1	-6.77	1.40	1.53
3	D	1162	DHK	C6-C5	-6.66	1.42	1.52
3	D	1162	DHK	C1-C2	-6.14	1.42	1.50
3	F	1162	DHK	C1-C2	-6.11	1.42	1.50
3	G	1162	DHK	C6-C5	-5.96	1.43	1.52
3	A	1162	DHK	C6-C5	-5.85	1.43	1.52
3	F	1162	DHK	O4-C4	-5.85	1.30	1.42
3	D	1162	DHK	C6-C1	-5.84	1.42	1.53
3	I	1162	DHK	C1-C2	-5.83	1.42	1.50
3	I	1162	DHK	C6-C1	-5.67	1.42	1.53
3	H	1162	DHK	C1-C2	-5.53	1.43	1.50
3	H	1162	DHK	C6-C5	-5.53	1.43	1.52
3	E	1162	DHK	C6-C1	-5.49	1.43	1.53
3	I	1162	DHK	C6-C5	-5.17	1.44	1.52
3	J	1162	DHK	C6-C5	-5.07	1.44	1.52
3	E	1162	DHK	C6-C5	-4.92	1.44	1.52
3	C	1162	DHK	C1-C2	-4.82	1.44	1.50
3	F	1162	DHK	C6-C5	-4.82	1.45	1.52
3	F	1162	DHK	C6-C1	-4.74	1.44	1.53
3	G	1162	DHK	C1-C2	-4.71	1.44	1.50
3	G	1162	DHK	O4-C4	-4.70	1.33	1.42
3	A	1162	DHK	O4-C4	-4.69	1.33	1.42
3	L	1162	DHK	C6-C1	-4.65	1.44	1.53
3	L	1162	DHK	C6-C5	-4.60	1.45	1.52
3	H	1162	DHK	O4-C4	-4.58	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	1162	DHK	C1-C2	-4.54	1.44	1.50
3	H	1162	DHK	C6-C1	-4.52	1.45	1.53
3	L	1162	DHK	O4-C4	-4.42	1.33	1.42
3	I	1162	DHK	O4-C4	-4.18	1.34	1.42
3	C	1162	DHK	C6-C1	-4.13	1.45	1.53
3	E	1162	DHK	O4-C4	-4.07	1.34	1.42
3	J	1162	DHK	C6-C1	-3.94	1.46	1.53
3	G	1162	DHK	C6-C1	-3.48	1.47	1.53
3	F	1162	DHK	O5-C5	-3.28	1.36	1.43
3	B	1162	DHK	O4-C4	-3.14	1.36	1.42
3	D	1162	DHK	O4-C4	-3.09	1.36	1.42
3	C	1162	DHK	O5-C5	-3.00	1.36	1.43
3	L	1162	DHK	O5-C5	-2.91	1.36	1.43
3	K	1162	DHK	O4-C4	-2.87	1.36	1.42
3	J	1162	DHK	O4-C4	-2.83	1.36	1.42
3	K	1162	DHK	O5-C5	-2.67	1.37	1.43
3	B	1162	DHK	C6-C5	-2.65	1.48	1.52
3	G	1162	DHK	O5-C5	-2.54	1.37	1.43
3	B	1162	DHK	O5-C5	-2.47	1.37	1.43
3	J	1162	DHK	O5-C5	-2.46	1.37	1.43
3	C	1162	DHK	O4-C4	-2.21	1.37	1.42
3	E	1162	DHK	O5-C5	-2.05	1.38	1.43
2	G	1153	TRS	O2-C2	2.16	1.49	1.42
2	A	1152	TRS	O1-C1	2.21	1.49	1.42
2	D	1152	TRS	O3-C3	2.27	1.49	1.42
2	J	1152	TRS	C3-C	2.66	1.58	1.53
2	G	1153	TRS	C1-C	2.76	1.58	1.53
2	G	1153	TRS	C2-C	2.87	1.58	1.53
2	J	1152	TRS	C2-C	2.97	1.58	1.53
2	D	1152	TRS	C2-C	3.89	1.60	1.53
3	J	1162	DHK	C2-C3	5.40	1.38	1.32
3	G	1162	DHK	C2-C3	5.73	1.39	1.32
3	I	1162	DHK	C2-C3	6.00	1.39	1.32
3	F	1162	DHK	C2-C3	6.21	1.39	1.32
3	H	1162	DHK	C2-C3	7.03	1.40	1.32
3	K	1162	DHK	C2-C3	7.39	1.40	1.32
3	L	1162	DHK	C2-C3	7.42	1.41	1.32
3	A	1162	DHK	C2-C3	7.43	1.41	1.32
3	B	1162	DHK	C2-C3	7.44	1.41	1.32
3	E	1162	DHK	C2-C3	7.51	1.41	1.32
3	C	1162	DHK	C2-C3	8.48	1.42	1.32
3	D	1162	DHK	C2-C3	9.25	1.43	1.32

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1162	DHK	O4-C4-C3	-4.15	100.34	111.21
3	C	1162	DHK	O4-C4-C3	-3.49	102.08	111.21
2	D	1152	TRS	C3-C-C2	-3.30	103.63	110.78
2	A	1152	TRS	C3-C-N	-3.09	102.47	108.09
3	F	1162	DHK	O3-C3-C2	-2.90	110.18	121.50
3	G	1162	DHK	O4-C4-C3	-2.81	103.87	111.21
2	J	1152	TRS	C3-C-C1	-2.78	104.75	110.78
3	H	1162	DHK	O4-C4-C3	-2.67	104.23	111.21
3	C	1162	DHK	O3-C3-C2	-2.50	111.74	121.50
2	G	1153	TRS	C2-C-C1	-2.50	105.37	110.78
3	I	1162	DHK	O3-C3-C2	-2.48	111.84	121.50
3	K	1162	DHK	O3-C3-C2	-2.43	112.03	121.50
3	B	1162	DHK	O5-C5-C6	-2.40	104.17	110.06
3	A	1162	DHK	O3-C3-C2	-2.32	112.46	121.50
3	B	1162	DHK	O3-C3-C2	-2.32	112.47	121.50
3	J	1162	DHK	O3-C3-C2	-2.28	112.63	121.50
3	H	1162	DHK	O3-C3-C2	-2.25	112.75	121.50
3	K	1162	DHK	O4-C4-C3	-2.20	105.46	111.21
2	J	1152	TRS	O1-C1-C	-2.08	106.97	111.18
2	A	1152	TRS	O1-C1-C	2.01	115.25	111.18
2	D	1152	TRS	O1-C1-C	2.07	115.37	111.18
3	H	1162	DHK	C6-C1-C2	2.15	115.20	108.65
2	G	1153	TRS	O3-C3-C	2.18	115.59	111.18
3	G	1162	DHK	C6-C1-C	2.20	115.80	111.59
3	D	1162	DHK	C6-C1-C	2.26	115.93	111.59
3	C	1162	DHK	C6-C1-C2	2.37	115.87	108.65
3	A	1162	DHK	C6-C1-C2	2.48	116.21	108.65
3	E	1162	DHK	C6-C1-C2	2.54	116.38	108.65
3	D	1162	DHK	C6-C1-C2	2.67	116.79	108.65
2	J	1152	TRS	O3-C3-C	2.82	116.88	111.18
3	F	1162	DHK	C6-C1-C2	2.91	117.50	108.65
3	K	1162	DHK	C6-C1-C2	3.08	118.04	108.65
3	I	1162	DHK	C5-C6-C1	3.23	117.04	109.91
2	D	1152	TRS	C3-C-N	3.28	114.06	108.09
3	B	1162	DHK	C6-C1-C2	3.37	118.92	108.65
3	B	1162	DHK	C6-C1-C	3.46	118.22	111.59
2	A	1152	TRS	O2-C2-C	3.54	118.35	111.18
2	A	1152	TRS	C2-C-C1	3.56	118.50	110.78
3	E	1162	DHK	C6-C1-C	3.78	118.83	111.59
3	H	1162	DHK	C6-C1-C	3.82	118.90	111.59
3	C	1162	DHK	C6-C1-C	3.85	118.97	111.59
3	K	1162	DHK	C5-C6-C1	3.87	118.45	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1162	DHK	C6-C1-C	3.98	119.21	111.59
3	L	1162	DHK	C6-C1-C2	4.27	121.67	108.65
3	A	1162	DHK	C5-C6-C1	4.36	119.53	109.91
3	J	1162	DHK	C6-C1-C	4.65	120.50	111.59
3	K	1162	DHK	C6-C1-C	4.76	120.70	111.59
2	G	1153	TRS	C2-C-N	4.86	116.94	108.09
3	I	1162	DHK	C6-C1-C	5.78	122.65	111.59
3	A	1162	DHK	C6-C1-C	6.20	123.46	111.59
3	F	1162	DHK	C6-C1-C	6.48	124.01	111.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.