



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:19 PM GMT

PDB ID : 1SZO  
Title : Crystal Structure Analysis of the 6-Oxo Camphor Hydrolase His122Ala Mutant Bound to Its Natural Product (2S,4S)-alpha-Campholinic Acid  
Authors : Leonard, P.M.; Grogan, G.  
Deposited on : 2004-04-06  
Resolution : 1.90 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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

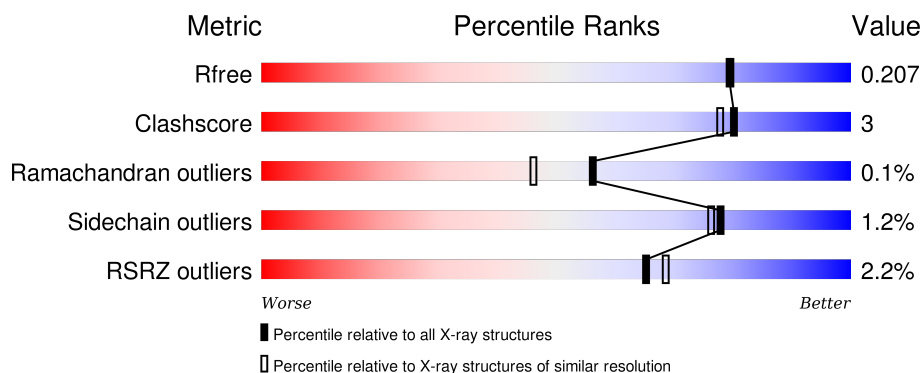
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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.

Mol	Chain	Length	Quality of chain
1	A	257	<div> <div>2%</div> <div>91%</div> <div>• • •</div> </div>
1	B	257	<div> <div>%</div> <div>87%</div> <div>9% • •</div> </div>
1	C	257	<div> <div>%</div> <div>86%</div> <div>10% •</div> </div>
1	D	257	<div> <div>2%</div> <div>88%</div> <div>9% • •</div> </div>
1	E	257	<div> <div>%</div> <div>88%</div> <div>7% • •</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	257	
1	G	257	
1	H	257	
1	I	257	
1	J	257	
1	K	257	
1	L	257	

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
2	CA	B	2001	-	-	-	X
2	CA	F	2002	-	-	-	X
2	CA	I	2003	-	-	-	X
2	CA	K	2004	-	-	-	X
3	CAX	B	5002	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25284 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 6-oxocamphor hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	6	0
			1944	1239	334	366	5			
1	B	248	Total	C	N	O	S	0	5	0
			1948	1237	336	370	5			
1	C	248	Total	C	N	O	S	0	4	0
			1941	1233	335	368	5			
1	D	251	Total	C	N	O	S	0	3	0
			1942	1234	336	367	5			
1	E	248	Total	C	N	O	S	0	1	0
			1927	1226	332	364	5			
1	F	248	Total	C	N	O	S	0	4	0
			1939	1230	334	370	5			
1	G	249	Total	C	N	O	S	0	1	0
			1928	1224	334	365	5			
1	H	248	Total	C	N	O	S	0	2	0
			1919	1224	329	361	5			
1	I	249	Total	C	N	O	S	0	4	0
			1941	1234	336	366	5			
1	J	249	Total	C	N	O	S	0	2	0
			1919	1222	327	365	5			
1	K	249	Total	C	N	O	S	0	2	0
			1925	1225	332	363	5			
1	L	248	Total	C	N	O	S	0	2	0
			1922	1221	333	363	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	ALA	HIS	ENGINEERED	UNP Q93TU6
B	122	ALA	HIS	ENGINEERED	UNP Q93TU6
C	122	ALA	HIS	ENGINEERED	UNP Q93TU6
D	122	ALA	HIS	ENGINEERED	UNP Q93TU6
E	122	ALA	HIS	ENGINEERED	UNP Q93TU6

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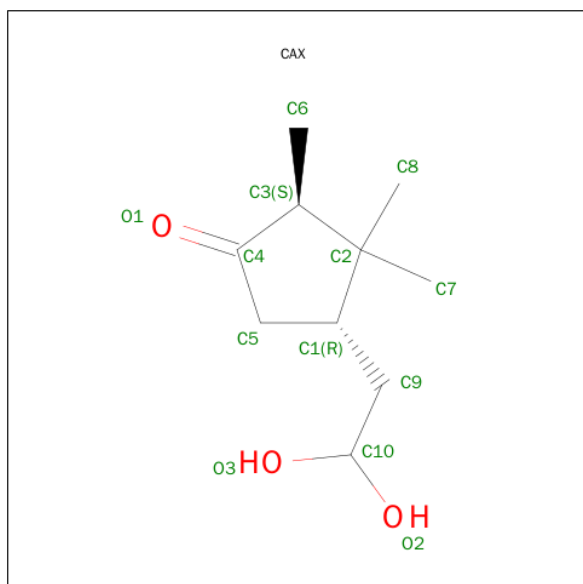
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Chain	Residue	Modelled	Actual	Comment	Reference
F	122	ALA	HIS	ENGINEERED	UNP Q93TU6
G	122	ALA	HIS	ENGINEERED	UNP Q93TU6
H	122	ALA	HIS	ENGINEERED	UNP Q93TU6
I	122	ALA	HIS	ENGINEERED	UNP Q93TU6
J	122	ALA	HIS	ENGINEERED	UNP Q93TU6
K	122	ALA	HIS	ENGINEERED	UNP Q93TU6
L	122	ALA	HIS	ENGINEERED	UNP Q93TU6

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	I	1	Total Ca 1 1	0	0
2	K	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- Molecule 3 is (2S,4S)-4-(2,2-DIHYDROXYETHYL)-2,3,3-TRIMETHYLCYCLOPENTANONE (three-letter code: CAX) (formula: C<sub>10</sub>H<sub>18</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 10 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	10	3		
3	C	1	Total	C	O	0	0
			13	10	3		
3	D	1	Total	C	O	0	0
			13	10	3		
3	E	1	Total	C	O	0	0
			13	10	3		
3	F	1	Total	C	O	0	0
			13	10	3		
3	G	1	Total	C	O	0	0
			13	10	3		
3	H	1	Total	C	O	0	0
			13	10	3		
3	I	1	Total	C	O	0	0
			13	10	3		
3	J	1	Total	C	O	0	0
			13	10	3		
3	K	1	Total	C	O	0	0
			13	10	3		
3	L	1	Total	C	O	0	0
			13	10	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	184	Total	O	0	0
			184	184		
4	C	194	Total	O	0	0
			194	194		
4	D	144	Total	O	0	0
			144	144		
4	E	167	Total	O	0	0
			167	167		
4	F	175	Total	O	0	0
			175	175		
4	G	161	Total	O	0	0
			161	161		
4	H	130	Total	O	0	0
			130	130		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	163	Total 163	O 163	0	0
4	J	135	Total 135	O 135	0	0
4	K	138	Total 138	O 138	0	0
4	L	132	Total 132	O 132	0	0

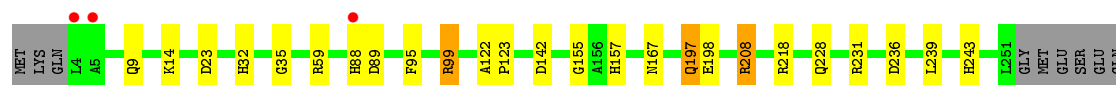
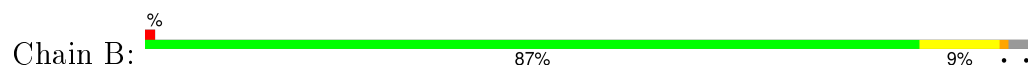
### 3 Residue-property plots [i](#)

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.

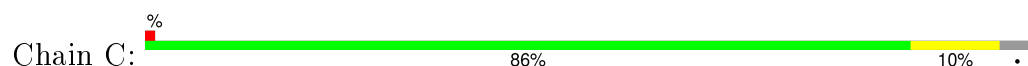
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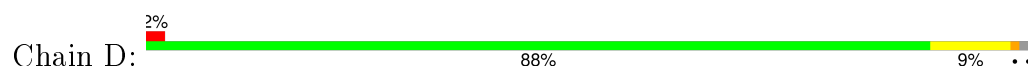
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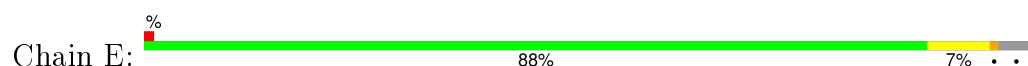
- Molecule 1: 6-oxocamphor hydrolase



- Molecule 1: 6-oxocamphor hydrolase



- Molecule 1: 6-oxocamphor hydrolase



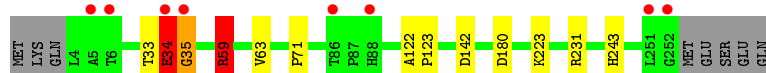




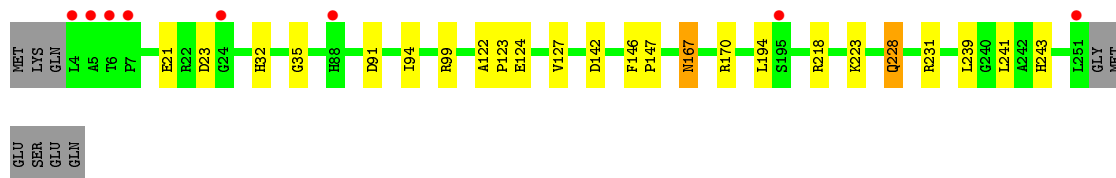
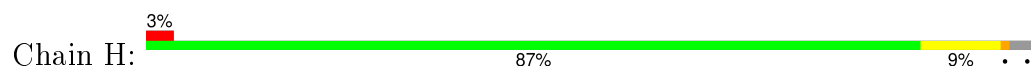
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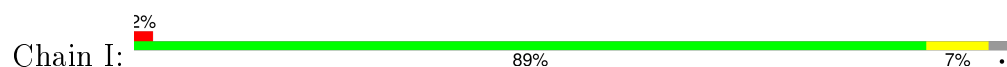
- Molecule 1: 6-oxocamphor hydrolase



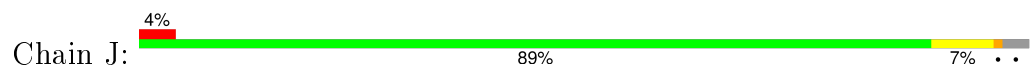
- Molecule 1: 6-oxocamphor hydrolase



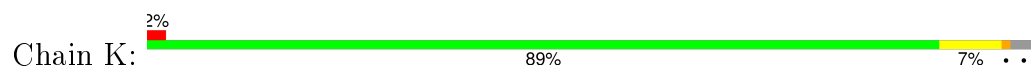
- Molecule 1: 6-oxocamphor hydrolase



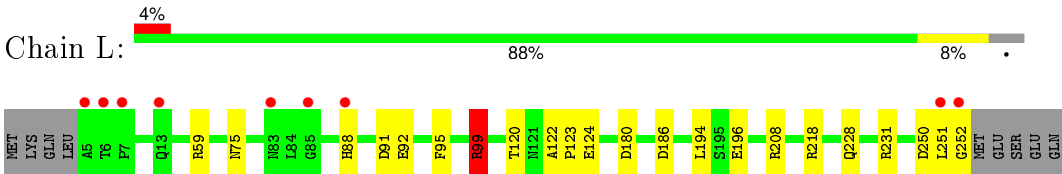
- Molecule 1: 6-oxocamphor hydrolase



- Molecule 1: 6-oxocamphor hydrolase



- Molecule 1: 6-oxocamphor hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.28Å 132.01Å 135.42Å 90.00° 94.11° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90 27.52 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-1.90) 99.8 (27.52-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.56 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.164 , 0.198 0.177 , 0.207	Depositor DCC
$R_{free}$ test set	11469 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 229538 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	25284	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 19.83 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.9393e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.85	0/2012	0.91	7/2745 (0.3%)
1	B	0.83	0/2012	0.90	6/2744 (0.2%)
1	C	0.84	0/2000	0.94	8/2728 (0.3%)
1	D	0.85	3/1997 (0.2%)	0.94	9/2725 (0.3%)
1	E	0.83	1/1973 (0.1%)	0.91	7/2692 (0.3%)
1	F	0.84	1/2000 (0.1%)	0.88	4/2727 (0.1%)
1	G	0.88	2/1976 (0.1%)	0.95	7/2696 (0.3%)
1	H	0.80	1/1971 (0.1%)	0.91	7/2690 (0.3%)
1	I	0.86	2/2000 (0.1%)	0.92	7/2728 (0.3%)
1	J	0.79	0/1970	0.97	11/2690 (0.4%)
1	K	0.84	1/1976 (0.1%)	0.92	7/2696 (0.3%)
1	L	0.82	2/1973 (0.1%)	1.00	13/2693 (0.5%)
All	All	0.84	13/23860 (0.1%)	0.93	93/32554 (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
1	F	1	0
1	G	0	1
All	All	1	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	34	GLU	C-O	-10.89	1.02	1.23
1	L	228	GLN	CB-CG	6.62	1.70	1.52
1	D	228	GLN	CB-CG	6.46	1.70	1.52
1	G	34	GLU	C-N	-6.28	1.21	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	228	GLN	CG-CD	6.06	1.65	1.51
1	E	127	VAL	CB-CG1	-5.92	1.40	1.52
1	I	228	GLN	CB-CG	5.80	1.68	1.52
1	D	29	VAL	CB-CG2	-5.74	1.40	1.52
1	D	228	GLN	CG-CD	5.67	1.64	1.51
1	I	228	GLN	CG-CD	5.41	1.63	1.51
1	H	228	GLN	CG-CD	5.29	1.63	1.51
1	F	120	THR	CB-CG2	-5.07	1.35	1.52
1	K	136	GLU	CD-OE2	-5.05	1.20	1.25

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	34	GLU	O-C-N	-14.59	98.41	123.20
1	G	34	GLU	CA-C-N	9.70	135.60	116.20
1	C	231	ARG	NE-CZ-NH2	-9.33	115.63	120.30
1	C	231	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	D	231	ARG	NE-CZ-NH2	-8.91	115.84	120.30
1	J	231	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	L	59	ARG	NE-CZ-NH1	-8.87	115.87	120.30
1	D	231	ARG	NE-CZ-NH1	8.83	124.72	120.30
1	J	208	ARG	NE-CZ-NH2	8.74	124.67	120.30
1	L	231	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	H	231	ARG	NE-CZ-NH1	8.33	124.47	120.30
1	I	231	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	L	231	ARG	NE-CZ-NH1	-8.06	116.27	120.30
1	K	231	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	L	208	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	A	231	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	G	231	ARG	NE-CZ-NH2	7.73	124.16	120.30
1	L	250	ASP	CB-CG-OD2	7.67	125.20	118.30
1	B	99	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	I	231	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	D	142	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	154	ASP	CB-CG-OD2	7.37	124.94	118.30
1	I	99	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	H	231	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	K	142	ASP	CB-CG-OD2	7.09	124.68	118.30
1	J	89	ASP	CB-CG-OD2	7.03	124.62	118.30
1	A	99	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	G	35	GLY	N-CA-C	6.97	130.53	113.10
1	L	218	ARG	NE-CZ-NH2	-6.95	116.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	180	ASP	CB-CG-OD1	6.90	124.51	118.30
1	I	99	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	K	91	ASP	CB-CG-OD2	6.82	124.43	118.30
1	J	231	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	L	186	ASP	CB-CG-OD2	6.72	124.35	118.30
1	A	231	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	C	99	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	D	23	ASP	CB-CG-OD2	6.58	124.23	118.30
1	K	231	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	J	78	ASP	CB-CG-OD2	6.48	124.13	118.30
1	H	91	ASP	CB-CG-OD2	6.45	124.11	118.30
1	G	59	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	B	99	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	L	59	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	E	250	ASP	CB-CG-OD2	6.40	124.06	118.30
1	E	142	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	236	ASP	CB-CG-OD2	6.32	123.98	118.30
1	C	142	ASP	CB-CG-OD2	6.31	123.98	118.30
1	C	91	ASP	CB-CG-OD2	6.29	123.96	118.30
1	C	54	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	142	ASP	CB-CG-OD2	6.27	123.94	118.30
1	C	99	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	D	91	ASP	CB-CG-OD2	6.13	123.81	118.30
1	H	142	ASP	CB-CG-OD2	6.12	123.80	118.30
1	B	208	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	D	89	ASP	CB-CG-OD2	6.10	123.79	118.30
1	F	23	ASP	CB-CG-OD2	6.07	123.77	118.30
1	D	186	ASP	CB-CG-OD2	6.04	123.73	118.30
1	F	120	THR	CA-CB-CG2	6.03	120.84	112.40
1	D	99	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	K	54	ASP	CB-CG-OD2	5.96	123.66	118.30
1	J	208	ARG	NE-CZ-NH1	-5.94	117.33	120.30
1	E	91	ASP	CB-CG-OD2	5.87	123.58	118.30
1	F	59	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	E	186	ASP	CB-CG-OD2	5.81	123.53	118.30
1	L	91	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	208	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	F	250	ASP	CB-CG-OD2	5.63	123.37	118.30
1	B	23	ASP	CB-CG-OD2	5.58	123.33	118.30
1	I	180	ASP	CB-CG-OD1	5.54	123.29	118.30
1	J	142	ASP	CB-CG-OD2	5.51	123.26	118.30
1	H	218	ARG	NE-CZ-NH1	5.51	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	23	ASP	CB-CG-OD1	5.51	123.25	118.30
1	A	186	ASP	CB-CG-OD2	5.48	123.23	118.30
1	L	99	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	J	250	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	99	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	L	180	ASP	CB-CG-OD1	5.40	123.16	118.30
1	J	99	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	K	180	ASP	CB-CG-OD1	5.34	123.11	118.30
1	L	194	LEU	CA-CB-CG	5.33	127.57	115.30
1	K	170	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	H	99	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	J	154	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	99	ARG	NE-CZ-NH2	5.23	122.92	120.30
1	C	23	ASP	CB-CG-OD1	5.22	123.00	118.30
1	G	142	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	136	GLU	CG-CD-OE2	5.19	128.69	118.30
1	E	4	LEU	CA-CB-CG	5.16	127.16	115.30
1	I	142	ASP	CB-CG-OD2	5.13	122.92	118.30
1	E	59	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	I	250	ASP	CB-CG-OD2	5.04	122.84	118.30
1	L	218	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	J	19	ARG	NE-CZ-NH2	-5.00	117.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	120	THR	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	34	GLU	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	1944	0	1910	16	0
1	B	1948	0	1911	23	0
1	C	1941	0	1906	20	0
1	D	1942	0	1899	15	0
1	E	1927	0	1888	11	0
1	F	1939	0	1899	3	0
1	G	1928	0	1888	12	0
1	H	1919	0	1881	16	0
1	I	1941	0	1908	15	0
1	J	1919	0	1863	12	0
1	K	1925	0	1880	15	0
1	L	1922	0	1877	7	0
2	B	1	0	0	0	0
2	F	1	0	0	0	0
2	I	1	0	0	0	0
2	K	1	0	0	0	0
3	A	13	0	15	0	0
3	B	13	0	15	2	0
3	C	13	0	15	2	0
3	D	13	0	15	0	0
3	E	13	0	15	1	0
3	F	13	0	15	1	0
3	G	13	0	15	0	0
3	H	13	0	15	0	0
3	I	13	0	15	1	0
3	J	13	0	15	2	0
3	K	13	0	15	3	0
3	L	13	0	15	1	0
4	A	206	0	0	5	0
4	B	184	0	0	8	1
4	C	194	0	0	8	0
4	D	144	0	0	3	0
4	E	167	0	0	0	0
4	F	175	0	0	1	1
4	G	161	0	0	3	0
4	H	130	0	0	2	0
4	I	163	0	0	2	0
4	J	135	0	0	3	0
4	K	138	0	0	3	0
4	L	132	0	0	2	0
All	All	25284	0	22890	157	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 3.



All (157) 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:A:228:GLN:NE2	1:A:231:ARG:NH1	2.05	1.05
1:A:228:GLN:HE22	1:A:231:ARG:NH1	1.56	1.02
1:A:228:GLN:NE2	1:A:231:ARG:HH11	1.67	0.89
1:H:32:HIS:HD2	1:H:35:GLY:H	1.21	0.88
1:F:75:ASN:HA	1:F:120:THR:HG22	1.54	0.88
1:D:132:VAL:H	1:D:191:ASN:HD22	1.25	0.84
1:J:7:PRO:HA	4:J:5070:HOH:O	1.77	0.82
1:H:243:HIS:HE1	1:I:223:LYS:HZ3	1.27	0.82
1:C:213:LYS:O	4:C:5031:HOH:O	1.99	0.81
1:G:223:LYS:HZ3	1:I:243:HIS:HE1	1.26	0.80
1:J:132:VAL:H	1:J:191:ASN:HD22	1.33	0.77
1:B:32:HIS:HD2	1:B:35:GLY:H	1.32	0.76
1:A:186:ASP:OD1	4:A:5038:HOH:O	2.01	0.76
1:B:197:GLN:HE21	1:B:197:GLN:H	1.34	0.76
1:L:124:GLU:OE1	4:L:5083:HOH:O	2.06	0.73
1:G:243:HIS:HE1	1:H:223:LYS:HZ3	1.34	0.72
1:D:223:LYS:HZ3	1:E:243:HIS:HE1	1.36	0.72
1:J:89:ASP:OD1	4:J:5079:HOH:O	2.13	0.67
1:A:228:GLN:HE22	1:A:231:ARG:HH12	1.42	0.67
1:A:148:SER:OG	4:A:5156:HOH:O	2.07	0.67
1:A:45:HIS:HE1	4:A:5007:HOH:O	1.78	0.67
1:G:33:THR:O	1:G:34:GLU:O	2.13	0.66
1:K:163[B]:VAL:HG13	4:K:5078:HOH:O	1.96	0.65
1:B:32:HIS:CD2	1:B:35:GLY:H	2.15	0.65
1:D:45:HIS:HE1	4:D:5021:HOH:O	1.79	0.65
1:B:243:HIS:HE1	1:C:223:LYS:NZ	1.94	0.65
1:G:33:THR:C	1:G:34:GLU:O	2.22	0.64
1:G:223:LYS:HZ3	1:I:243:HIS:CE1	2.12	0.64
1:H:32:HIS:CD2	1:H:35:GLY:H	2.08	0.64
1:K:142:ASP:OD1	1:K:145:HIS:HD2	1.81	0.64
1:K:162:HIS:HE1	4:L:5080:HOH:O	1.80	0.62
1:B:89:ASP:OD2	4:B:5182:HOH:O	2.16	0.62
1:I:59:ARG:HH21	1:L:92:GLU:HA	1.66	0.61
1:B:243:HIS:HE1	1:C:223:LYS:HZ3	1.48	0.61
4:H:5067:HOH:O	1:I:162:HIS:HE1	1.83	0.60
1:C:45:HIS:HE1	4:C:5034:HOH:O	1.84	0.60
1:J:45:HIS:HE1	4:J:5024:HOH:O	1.85	0.59
1:G:59:ARG:HD3	4:G:5120:HOH:O	2.02	0.59
1:D:132:VAL:H	1:D:191:ASN:ND2	1.95	0.59
1:H:243:HIS:HE1	1:I:223:LYS:NZ	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLN:NE2	1:A:231:ARG:HH12	1.97	0.59
1:J:45:HIS:HD2	1:J:46:ASP:OD1	1.86	0.58
4:B:5103:HOH:O	1:C:162:HIS:HE1	1.86	0.57
1:K:145:HIS:HE1	3:K:5011:CAX:O2	1.87	0.57
1:D:223:LYS:NZ	1:E:243:HIS:HE1	2.02	0.57
1:F:228:GLN:NE2	1:F:231:ARG:HH21	2.02	0.57
1:G:59:ARG:CD	4:G:5120:HOH:O	2.52	0.57
1:H:228:GLN:HG3	4:H:5051:HOH:O	2.04	0.56
1:I:239:LEU:O	1:I:243:HIS:HD2	1.88	0.56
1:A:45:HIS:HD2	1:A:46:ASP:OD1	1.88	0.56
1:B:197:GLN:H	1:B:197:GLN:NE2	2.01	0.56
1:A:10:GLU:O	4:A:5109:HOH:O	2.17	0.56
1:B:218:ARG:NH1	4:B:5180:HOH:O	2.35	0.55
1:E:228:GLN:NE2	1:E:231:ARG:HH21	2.05	0.54
1:B:218:ARG:NE	4:B:5180:HOH:O	2.17	0.54
1:I:148:SER:OG	4:I:5112:HOH:O	2.17	0.54
1:E:162:HIS:HE1	4:F:5092:HOH:O	1.90	0.54
1:H:167:ASN:HD22	1:H:167:ASN:N	2.06	0.53
1:J:132:VAL:H	1:J:191:ASN:ND2	2.02	0.53
1:C:124:GLU:OE2	4:C:5032:HOH:O	2.18	0.52
1:J:95:PHE:CE2	1:J:99:ARG:HD3	2.45	0.52
1:B:95:PHE:CE2	1:B:99:ARG:HD3	2.44	0.52
1:D:45:HIS:HD2	1:D:46:ASP:OD1	1.93	0.51
1:C:167:ASN:ND2	1:C:170:ARG:HH21	2.08	0.51
1:I:167:ASN:HD22	1:I:167:ASN:N	2.07	0.51
1:K:228[A]:GLN:NE2	1:K:231:ARG:HH21	2.08	0.51
1:C:95:PHE:CE2	1:C:99:ARG:HD3	2.45	0.51
1:B:197:GLN:HE21	1:B:197:GLN:N	2.06	0.51
1:D:95:PHE:CE2	1:D:99:ARG:HD3	2.46	0.50
1:C:45:HIS:HD2	1:C:46:ASP:OD1	1.95	0.50
1:G:243:HIS:HE1	1:H:223:LYS:NZ	2.08	0.50
1:G:243:HIS:CE1	1:H:223:LYS:HZ3	2.22	0.50
1:H:167:ASN:ND2	1:H:170:ARG:HH21	2.10	0.50
1:A:99:ARG:NH1	4:A:5183:HOH:O	2.43	0.49
1:B:239:LEU:HD23	1:B:239:LEU:C	2.32	0.49
1:A:161:PRO:HB2	1:B:228[B]:GLN:HE22	1.76	0.49
1:I:71:PRO:HG2	4:I:5167:HOH:O	2.12	0.49
1:B:239:LEU:O	1:B:243:HIS:HD2	1.96	0.48
1:J:157:HIS:HE1	1:J:236:ASP:O	1.96	0.48
1:C:167:ASN:HD22	1:C:167:ASN:N	2.11	0.48
1:I:157:HIS:HE1	1:I:236:ASP:O	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:157:HIS:HE1	1:K:236:ASP:O	1.97	0.48
1:J:155:GLY:H	1:J:157:HIS:CD2	2.32	0.47
1:A:157:HIS:HE1	1:A:236:ASP:O	1.97	0.47
3:F:5006:CAX:C4	3:F:5006:CAX:C10	2.92	0.47
1:J:223:LYS:HZ3	1:K:243:HIS:HE1	1.62	0.47
1:J:223:LYS:NZ	1:K:243:HIS:HE1	2.12	0.47
1:C:239:LEU:HD11	1:D:238[A]:SER:OG	2.16	0.46
1:B:167:ASN:HD22	1:B:167:ASN:N	2.13	0.46
1:D:223:LYS:HZ3	1:E:243:HIS:CE1	2.25	0.46
1:B:157:HIS:HE1	1:B:236:ASP:O	1.98	0.46
1:K:146:PHE:N	1:K:147:PRO:CD	2.79	0.46
1:K:142:ASP:OD1	1:K:145:HIS:CD2	2.67	0.46
1:C:157:HIS:HE1	1:C:236:ASP:O	1.97	0.46
1:D:239:LEU:C	1:D:239:LEU:HD23	2.35	0.46
3:B:5002:CAX:C4	3:B:5002:CAX:O3	2.64	0.46
1:I:167:ASN:ND2	1:I:170:ARG:HH21	2.14	0.45
1:C:13:GLN:NE2	4:C:5185:HOH:O	2.48	0.45
1:B:14:LYS:CE	4:B:5174:HOH:O	2.64	0.45
1:K:145:HIS:CE1	3:K:5011:CAX:O2	2.69	0.45
1:L:95:PHE:CE2	1:L:99:ARG:HD3	2.51	0.45
1:I:124:GLU:HA	1:I:127[A]:VAL:HG22	1.99	0.45
1:K:228[B]:GLN:NE2	4:K:5143:HOH:O	2.50	0.45
1:E:8:PHE:HA	1:E:11:TYR:CE2	2.51	0.45
1:E:239:LEU:O	1:E:243:HIS:HD2	1.99	0.45
1:K:212:GLU:HG2	4:K:5063:HOH:O	2.16	0.44
1:B:155:GLY:H	1:B:157:HIS:CD2	2.36	0.44
1:C:9:GLN:O	4:C:5160:HOH:O	2.20	0.44
1:C:5:ALA:O	1:C:7:PRO:HD3	2.17	0.44
1:C:62:LYS:O	1:C:218:ARG:HD2	2.17	0.44
3:B:5002:CAX:C4	3:B:5002:CAX:C10	2.96	0.44
1:J:208:ARG:HG2	1:J:208:ARG:HH21	1.82	0.43
1:H:239:LEU:O	1:H:243:HIS:HD2	2.01	0.43
3:K:5011:CAX:C10	3:K:5011:CAX:C4	2.96	0.43
4:C:5186:HOH:O	1:D:246:LEU:HD13	2.17	0.43
3:C:5003:CAX:O3	3:C:5003:CAX:C4	2.66	0.43
1:E:228:GLN:HE21	1:E:231:ARG:HH21	1.65	0.43
1:D:228:GLN:HG3	4:D:5061:HOH:O	2.19	0.43
1:B:59:ARG:HG2	4:B:5106:HOH:O	2.18	0.43
1:H:146:PHE:N	1:H:147:PRO:CD	2.81	0.43
1:L:122:ALA:N	1:L:123:PRO:CD	2.82	0.43
1:L:251:LEU:O	1:L:252:GLY:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:122:ALA:N	1:K:123:PRO:CD	2.81	0.43
3:J:5010:CAX:O3	3:J:5010:CAX:C4	2.66	0.43
1:B:32:HIS:HE1	4:B:5046:HOH:O	2.00	0.43
1:K:239:LEU:O	1:K:243:HIS:HD2	2.02	0.43
3:J:5010:CAX:C4	3:J:5010:CAX:C10	2.96	0.42
1:E:146:PHE:N	1:E:147:PRO:CD	2.82	0.42
1:D:62:LYS:O	1:D:218:ARG:HD2	2.19	0.42
1:C:218:ARG:NE	4:C:5031:HOH:O	2.36	0.42
1:B:122:ALA:N	1:B:123:PRO:CD	2.83	0.42
1:H:94:ILE:HG12	1:H:241:LEU:HB3	2.01	0.42
1:H:243:HIS:CE1	1:I:223:LYS:HZ3	2.18	0.42
1:E:204:TRP:O	1:E:208:ARG:HG2	2.20	0.42
3:C:5003:CAX:C10	3:C:5003:CAX:C4	2.98	0.42
1:I:155:GLY:H	1:I:157:HIS:HD2	1.68	0.41
1:A:228:GLN:HE22	1:A:231:ARG:HH11	1.28	0.41
1:L:75[B]:ASN:OD1	1:L:120:THR:HG21	2.20	0.41
1:G:33:THR:O	1:G:34:GLU:C	2.58	0.41
3:I:5009:CAX:C4	3:I:5009:CAX:C10	2.98	0.41
1:C:218:ARG:NH2	4:C:5031:HOH:O	2.48	0.41
1:A:155:GLY:H	1:A:157:HIS:CD2	2.38	0.41
1:B:231:ARG:HD3	4:B:5047:HOH:O	2.19	0.41
1:H:122:ALA:N	1:H:123:PRO:CD	2.84	0.41
1:C:94:ILE:HG12	1:C:241:LEU:HB3	2.02	0.41
4:D:5128:HOH:O	1:E:162:HIS:HD2	2.04	0.41
3:L:5012:CAX:C4	3:L:5012:CAX:O3	2.69	0.41
1:H:124:GLU:HA	1:H:127:VAL:HG22	2.03	0.41
1:G:122:ALA:N	1:G:123:PRO:CD	2.84	0.41
1:D:146:PHE:N	1:D:147:PRO:CD	2.84	0.41
1:F:146:PHE:N	1:F:147:PRO:CD	2.84	0.41
1:A:239:LEU:C	1:A:239:LEU:HD23	2.42	0.41
1:B:243:HIS:CE1	1:C:223:LYS:NZ	2.81	0.40
1:G:59:ARG:HD2	4:G:5120:HOH:O	2.19	0.40
1:D:182:ARG:HD2	1:D:182:ARG:HA	1.66	0.40
3:E:5005:CAX:C10	3:E:5005:CAX:C4	2.99	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)
4:B:5179:HOH:O	4:F:5165:HOH:O[1_655]	1.98	0.22

## 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	253/257 (98%)	248 (98%)	5 (2%)	0	100	100
1	B	251/257 (98%)	247 (98%)	4 (2%)	0	100	100
1	C	250/257 (97%)	247 (99%)	3 (1%)	0	100	100
1	D	252/257 (98%)	248 (98%)	4 (2%)	0	100	100
1	E	247/257 (96%)	243 (98%)	4 (2%)	0	100	100
1	F	250/257 (97%)	246 (98%)	4 (2%)	0	100	100
1	G	248/257 (96%)	242 (98%)	4 (2%)	2 (1%)	24	11
1	H	248/257 (96%)	245 (99%)	3 (1%)	0	100	100
1	I	251/257 (98%)	248 (99%)	3 (1%)	0	100	100
1	J	249/257 (97%)	245 (98%)	4 (2%)	0	100	100
1	K	249/257 (97%)	244 (98%)	5 (2%)	0	100	100
1	L	248/257 (96%)	244 (98%)	4 (2%)	0	100	100
All	All	2996/3084 (97%)	2947 (98%)	47 (2%)	2 (0%)	56	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	34	GLU
1	G	35	GLY

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/214 (97%)	207 (100%)	1 (0%)	92	92
1	B	210/214 (98%)	205 (98%)	5 (2%)	57	49
1	C	209/214 (98%)	209 (100%)	0	100	100
1	D	206/214 (96%)	202 (98%)	4 (2%)	65	59
1	E	204/214 (95%)	198 (97%)	6 (3%)	50	40
1	F	208/214 (97%)	207 (100%)	1 (0%)	92	92
1	G	204/214 (95%)	201 (98%)	3 (2%)	72	69
1	H	202/214 (94%)	199 (98%)	3 (2%)	72	69
1	I	208/214 (97%)	207 (100%)	1 (0%)	92	92
1	J	201/214 (94%)	199 (99%)	2 (1%)	82	81
1	K	203/214 (95%)	202 (100%)	1 (0%)	92	92
1	L	203/214 (95%)	200 (98%)	3 (2%)	72	69
All	All	2466/2568 (96%)	2436 (99%)	30 (1%)	78	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	228	GLN
1	B	9	GLN
1	B	88	HIS
1	B	197	GLN
1	B	198	GLU
1	B	208	ARG
1	D	4	LEU
1	D	14	LYS
1	D	182	ARG
1	D	194	LEU
1	E	4	LEU
1	E	14	LYS
1	E	20	LEU
1	E	59	ARG
1	E	88	HIS
1	E	231	ARG
1	F	197	GLN
1	G	59	ARG
1	G	63	VAL
1	G	71	PRO
1	H	21	GLU
1	H	167	ASN

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Mol	Chain	Res	Type
1	H	194	LEU
1	I	167	ASN
1	J	4	LEU
1	J	194	LEU
1	K	20	LEU
1	L	88	HIS
1	L	99	ARG
1	L	196	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	145	HIS
1	A	157	HIS
1	A	228	GLN
1	B	9	GLN
1	B	32	HIS
1	B	53	HIS
1	B	157	HIS
1	B	167	ASN
1	B	197	GLN
1	B	243	HIS
1	C	13	GLN
1	C	45	HIS
1	C	88	HIS
1	C	102	ASN
1	C	157	HIS
1	C	162	HIS
1	C	167	ASN
1	C	197	GLN
1	D	45	HIS
1	D	53	HIS
1	D	177	GLN
1	D	191	ASN
1	E	88	HIS
1	E	162	HIS
1	E	228	GLN
1	E	243	HIS
1	F	102	ASN
1	F	103	ASN
1	F	228	GLN

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Mol	Chain	Res	Type
1	G	53	HIS
1	G	243	HIS
1	H	32	HIS
1	H	53	HIS
1	H	167	ASN
1	H	228	GLN
1	H	243	HIS
1	I	9	GLN
1	I	102	ASN
1	I	157	HIS
1	I	162	HIS
1	I	167	ASN
1	I	243	HIS
1	J	45	HIS
1	J	53	HIS
1	J	157	HIS
1	J	177	GLN
1	J	191	ASN
1	K	83	ASN
1	K	145	HIS
1	K	157	HIS
1	K	162	HIS
1	K	243	HIS
1	L	102	ASN
1	L	103	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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$
3	CAX	A	5001	-	8,13,13	3.90	1 (12%)	13,20,20	3.16	4 (30%)
3	CAX	B	5002	-	8,13,13	3.92	1 (12%)	13,20,20	3.64	4 (30%)
3	CAX	C	5003	-	8,13,13	3.71	1 (12%)	13,20,20	3.76	5 (38%)
3	CAX	D	5004	-	8,13,13	3.79	1 (12%)	13,20,20	4.95	3 (23%)
3	CAX	E	5005	-	8,13,13	3.41	1 (12%)	13,20,20	4.55	3 (23%)
3	CAX	F	5006	-	8,13,13	4.04	1 (12%)	13,20,20	3.78	5 (38%)
3	CAX	G	5007	-	8,13,13	3.79	1 (12%)	13,20,20	3.66	2 (15%)
3	CAX	H	5008	-	8,13,13	3.71	1 (12%)	13,20,20	3.83	3 (23%)
3	CAX	I	5009	-	8,13,13	3.82	1 (12%)	13,20,20	4.75	3 (23%)
3	CAX	J	5010	-	8,13,13	3.76	1 (12%)	13,20,20	4.23	4 (30%)
3	CAX	K	5011	-	8,13,13	3.80	1 (12%)	13,20,20	4.71	4 (30%)
3	CAX	L	5012	-	8,13,13	3.51	1 (12%)	13,20,20	4.49	4 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAX	A	5001	-	-	0/2/24/24	0/1/1/1
3	CAX	B	5002	-	-	0/2/24/24	0/1/1/1
3	CAX	C	5003	-	-	0/2/24/24	0/1/1/1
3	CAX	D	5004	-	-	0/2/24/24	0/1/1/1
3	CAX	E	5005	-	-	0/2/24/24	0/1/1/1
3	CAX	F	5006	-	-	0/2/24/24	0/1/1/1
3	CAX	G	5007	-	-	0/2/24/24	0/1/1/1
3	CAX	H	5008	-	-	0/2/24/24	0/1/1/1
3	CAX	I	5009	-	-	0/2/24/24	0/1/1/1
3	CAX	J	5010	-	-	0/2/24/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAX	K	5011	-	-	0/2/24/24	0/1/1/1
3	CAX	L	5012	-	-	0/2/24/24	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	5005	CAX	O1-C4	9.56	1.38	1.21
3	L	5012	CAX	O1-C4	9.75	1.38	1.21
3	C	5003	CAX	O1-C4	10.28	1.39	1.21
3	H	5008	CAX	O1-C4	10.36	1.40	1.21
3	J	5010	CAX	O1-C4	10.45	1.40	1.21
3	G	5007	CAX	O1-C4	10.54	1.40	1.21
3	D	5004	CAX	O1-C4	10.59	1.40	1.21
3	K	5011	CAX	O1-C4	10.70	1.40	1.21
3	I	5009	CAX	O1-C4	10.76	1.40	1.21
3	A	5001	CAX	O1-C4	10.92	1.40	1.21
3	B	5002	CAX	O1-C4	10.98	1.41	1.21
3	F	5006	CAX	O1-C4	11.37	1.41	1.21

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5004	CAX	O1-C4-C5	-16.80	106.13	125.86
3	I	5009	CAX	O1-C4-C5	-15.71	107.41	125.86
3	K	5011	CAX	O1-C4-C5	-15.15	108.07	125.86
3	E	5005	CAX	O1-C4-C5	-15.10	108.13	125.86
3	L	5012	CAX	O1-C4-C5	-13.68	109.79	125.86
3	J	5010	CAX	O1-C4-C5	-13.08	110.50	125.86
3	H	5008	CAX	O1-C4-C5	-11.76	112.05	125.86
3	F	5006	CAX	O1-C4-C5	-11.19	112.72	125.86
3	C	5003	CAX	O1-C4-C5	-9.93	114.20	125.86
3	B	5002	CAX	O1-C4-C5	-9.73	114.44	125.86
3	A	5001	CAX	O1-C4-C5	-9.69	114.48	125.86
3	G	5007	CAX	O1-C4-C3	-9.62	115.58	125.53
3	G	5007	CAX	O1-C4-C5	-8.58	115.78	125.86
3	L	5012	CAX	O1-C4-C3	-7.16	118.12	125.53
3	C	5003	CAX	O1-C4-C3	-6.81	118.48	125.53
3	B	5002	CAX	O1-C4-C3	-6.66	118.64	125.53
3	H	5008	CAX	O1-C4-C3	-5.95	119.37	125.53
3	J	5010	CAX	O1-C4-C3	-5.90	119.43	125.53
3	K	5011	CAX	O1-C4-C3	-5.27	120.08	125.53
3	F	5006	CAX	C9-C1-C5	-4.72	105.36	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5003	CAX	C9-C1-C5	-4.48	105.80	113.83
3	B	5002	CAX	C9-C1-C5	-4.31	106.09	113.83
3	I	5009	CAX	O1-C4-C3	-4.24	121.15	125.53
3	D	5004	CAX	C9-C1-C5	-4.20	106.29	113.83
3	F	5006	CAX	O1-C4-C3	-4.16	121.22	125.53
3	K	5011	CAX	C9-C1-C5	-4.15	106.38	113.83
3	J	5010	CAX	C9-C1-C5	-4.14	106.39	113.83
3	E	5005	CAX	O1-C4-C3	-4.09	121.30	125.53
3	I	5009	CAX	C9-C1-C5	-3.97	106.70	113.83
3	A	5001	CAX	O1-C4-C3	-3.95	121.44	125.53
3	E	5005	CAX	C9-C1-C5	-3.88	106.87	113.83
3	L	5012	CAX	C9-C1-C5	-3.69	107.21	113.83
3	D	5004	CAX	O1-C4-C3	-3.25	122.17	125.53
3	A	5001	CAX	C9-C1-C5	-3.06	108.34	113.83
3	H	5008	CAX	C9-C1-C5	-2.82	108.77	113.83
3	F	5006	CAX	C1-C5-C4	-2.56	100.75	104.84
3	C	5003	CAX	C5-C4-C3	-2.03	107.08	109.36
3	A	5001	CAX	C9-C1-C2	2.07	119.12	115.16
3	K	5011	CAX	C2-C3-C4	2.13	106.00	103.04
3	J	5010	CAX	C9-C1-C2	2.18	119.34	115.16
3	L	5012	CAX	C9-C1-C2	2.47	119.90	115.16
3	C	5003	CAX	C2-C3-C4	2.58	106.63	103.04
3	F	5006	CAX	C9-C1-C2	2.91	120.75	115.16
3	B	5002	CAX	C9-C1-C2	3.02	120.95	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	5002	CAX	2	0
3	C	5003	CAX	2	0
3	E	5005	CAX	1	0
3	F	5006	CAX	1	0
3	I	5009	CAX	1	0
3	J	5010	CAX	2	0
3	K	5011	CAX	3	0
3	L	5012	CAX	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	249/257 (96%)	-0.03	5 (2%) 68 71	13, 18, 29, 45	0
1	B	248/257 (96%)	0.00	3 (1%) 81 83	13, 19, 29, 40	0
1	C	248/257 (96%)	-0.07	3 (1%) 81 83	13, 19, 29, 40	0
1	D	251/257 (97%)	-0.01	6 (2%) 62 66	14, 20, 30, 45	1 (0%)
1	E	248/257 (96%)	-0.08	3 (1%) 81 83	14, 19, 29, 42	0
1	F	248/257 (96%)	-0.02	3 (1%) 81 83	13, 19, 29, 45	0
1	G	249/257 (96%)	0.04	8 (3%) 51 54	14, 20, 30, 45	0
1	H	248/257 (96%)	-0.06	8 (3%) 51 54	14, 20, 30, 41	0
1	I	249/257 (96%)	-0.07	5 (2%) 68 71	13, 19, 29, 45	1 (0%)
1	J	249/257 (96%)	-0.02	9 (3%) 46 50	14, 20, 29, 44	2 (0%)
1	K	249/257 (96%)	-0.07	4 (1%) 74 78	14, 20, 30, 45	1 (0%)
1	L	248/257 (96%)	0.01	9 (3%) 46 50	14, 20, 30, 46	0
All	All	2984/3084 (96%)	-0.03	66 (2%) 65 68	13, 19, 30, 46	5 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	5	ALA	7.0
1	G	251	LEU	6.7
1	L	5	ALA	5.1
1	K	5	ALA	4.8
1	I	252	GLY	4.7
1	L	252	GLY	4.7
1	L	251	LEU	3.9
1	H	251	LEU	3.8
1	L	88	HIS	3.8
1	K	4	LEU	3.7
1	A	252	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	F	252	GLY	3.6
1	D	252	GLY	3.5
1	G	88	HIS	3.5
1	G	35	GLY	3.4
1	G	5	ALA	3.3
1	E	88	HIS	3.3
1	B	5	ALA	3.3
1	E	4	LEU	3.3
1	L	7	PRO	3.2
1	A	5	ALA	3.2
1	B	88	HIS	3.1
1	J	88	HIS	3.1
1	D	9	GLN	3.1
1	A	4	LEU	3.1
1	L	6	THR	3.0
1	G	252	GLY	3.0
1	F	7	PRO	2.9
1	K	252	GLY	2.9
1	I	66[A]	LEU	2.9
1	A	66[A]	LEU	2.8
1	H	5	ALA	2.8
1	K	7	PRO	2.8
1	B	4	LEU	2.7
1	E	5	ALA	2.7
1	I	251	LEU	2.7
1	L	85	GLY	2.7
1	I	5	ALA	2.7
1	C	4	LEU	2.7
1	J	6	THR	2.6
1	C	10	GLU	2.6
1	G	34	GLU	2.6
1	J	201	PRO	2.5
1	J	4	LEU	2.5
1	D	7	PRO	2.5
1	L	83	ASN	2.4
1	L	13	GLN	2.4
1	H	195	SER	2.4
1	J	7	PRO	2.3
1	J	10	GLU	2.3
1	J	251	LEU	2.3
1	C	5	ALA	2.2
1	H	4	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	127[A]	VAL	2.2
1	D	251	LEU	2.2
1	H	7	PRO	2.1
1	G	86	THR	2.1
1	D	2	LYS	2.1
1	G	6	THR	2.1
1	H	6	THR	2.1
1	I	88	HIS	2.1
1	J	24	GLY	2.1
1	D	5	ALA	2.0
1	H	24	GLY	2.0
1	F	88	HIS	2.0
1	H	88	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	CA	I	2003	1/1	0.98	0.29	12.62	33,33,33,33	0
2	CA	B	2001	1/1	0.99	0.26	8.61	27,27,27,27	0
2	CA	K	2004	1/1	0.92	0.24	4.83	33,33,33,33	0
2	CA	F	2002	1/1	0.97	0.19	2.88	37,37,37,37	0
3	CAX	B	5002	13/13	0.94	0.13	2.43	16,23,28,29	0
3	CAX	F	5006	13/13	0.95	0.12	1.59	17,23,25,25	0
3	CAX	G	5007	13/13	0.93	0.15	1.41	22,24,27,27	0
3	CAX	I	5009	13/13	0.94	0.12	1.04	16,25,28,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CAX	C	5003	13/13	0.95	0.11	0.88	17,21,24,27	0
3	CAX	D	5004	13/13	0.95	0.12	0.84	17,22,25,27	0
3	CAX	H	5008	13/13	0.95	0.10	0.82	17,23,25,27	0
3	CAX	K	5011	13/13	0.93	0.12	0.80	22,28,31,32	0
3	CAX	A	5001	13/13	0.95	0.11	0.40	15,18,21,23	0
3	CAX	L	5012	13/13	0.94	0.11	0.28	20,25,27,28	0
3	CAX	J	5010	13/13	0.96	0.10	0.28	19,25,28,31	0
3	CAX	E	5005	13/13	0.95	0.10	0.18	18,23,26,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.