



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:52 am GMT

PDB ID : 1OJD  
Title : HUMAN MONOAMINE OXIDASE B IN COMPLEX WITH LAURYLDIM  
ETHYLAMINE-N-OXIDE (LDAO)  
Authors : Binda, C.; Edmondson, D.E.; Mattevi, A.  
Deposited on : 2003-07-08  
Resolution : 3.10 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

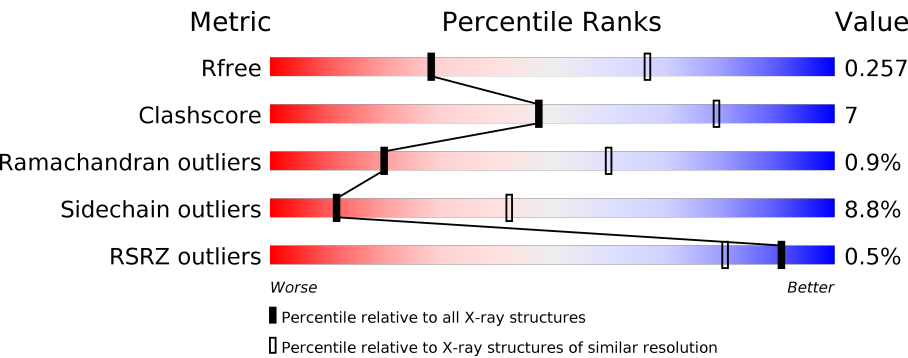
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

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	520	
1	B	520	
1	C	520	
1	D	520	
1	E	520	
1	F	520	

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Mol	Chain	Length	Quality of chain
1	G	520	 75% 18% • 5%
1	H	520	 75% 18% • •
1	I	520	 75% 18% • • •
1	L	520	 2% 73% 20% • • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LDA	A	601	-	-	-	X
3	LDA	B	601	-	-	-	X
3	LDA	C	601	-	-	-	X
3	LDA	D	601	-	-	-	X
3	LDA	E	601	-	-	-	X
3	LDA	F	601	-	-	-	X
3	LDA	G	601	-	-	-	X
3	LDA	H	601	-	-	-	X
3	LDA	I	601	-	-	-	X
3	LDA	L	601	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 40219 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 AMINE OXIDASE [FLAVIN-CONTAINING] B.

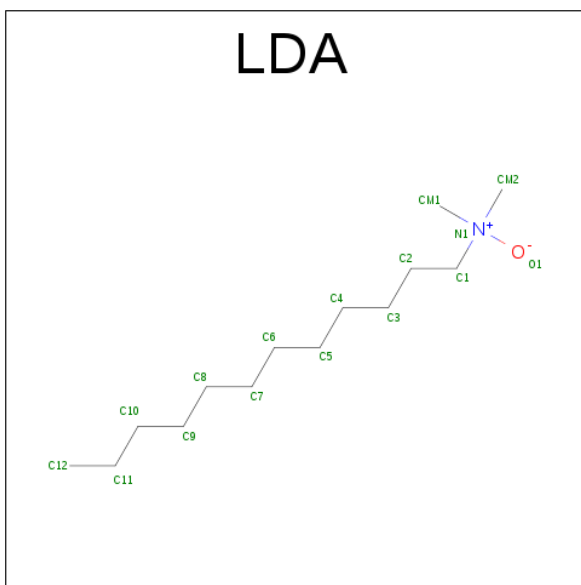
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	497	Total	C	N	O	S	0	0	0
			3958	2531	678	725	24			
1	B	494	Total	C	N	O	S	0	0	0
			3936	2517	675	720	24			
1	C	498	Total	C	N	O	S	0	0	0
			3963	2534	679	726	24			
1	D	494	Total	C	N	O	S	0	0	0
			3936	2517	675	720	24			
1	E	498	Total	C	N	O	S	0	0	0
			3963	2534	679	726	24			
1	F	497	Total	C	N	O	S	0	0	0
			3958	2531	678	725	24			
1	G	494	Total	C	N	O	S	0	0	0
			3936	2517	675	720	24			
1	H	498	Total	C	N	O	S	0	0	0
			3963	2534	679	726	24			
1	I	497	Total	C	N	O	S	0	0	0
			3958	2531	678	725	24			
1	L	497	Total	C	N	O	S	0	0	0
			3958	2531	678	725	24			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	L	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: C<sub>14</sub>H<sub>31</sub>NO).

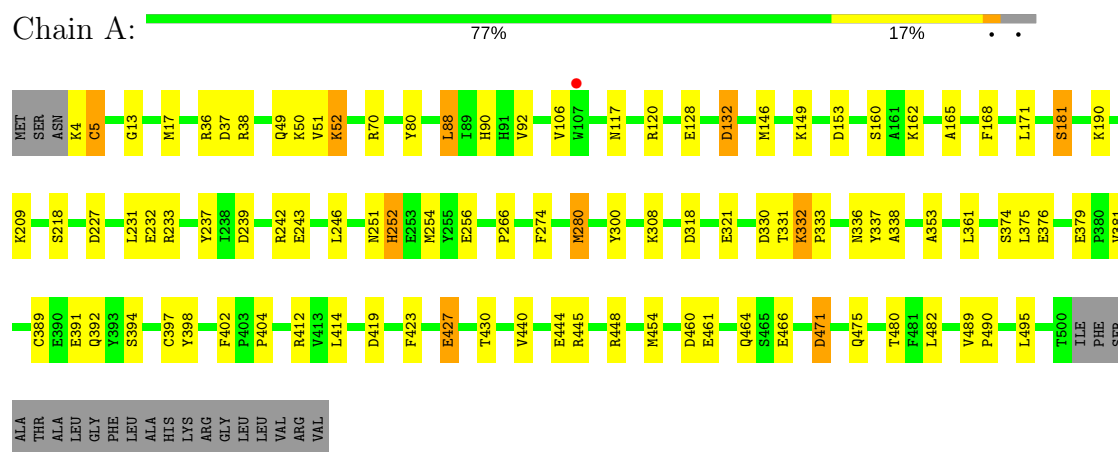


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 16	C 14	N 1	O 1	0	0
3	B	1	Total 16	C 14	N 1	O 1	0	0
3	C	1	Total 16	C 14	N 1	O 1	0	0
3	D	1	Total 16	C 14	N 1	O 1	0	0
3	E	1	Total 16	C 14	N 1	O 1	0	0
3	F	1	Total 16	C 14	N 1	O 1	0	0
3	G	1	Total 16	C 14	N 1	O 1	0	0
3	H	1	Total 16	C 14	N 1	O 1	0	0
3	I	1	Total 16	C 14	N 1	O 1	0	0
3	L	1	Total 16	C 14	N 1	O 1	0	0

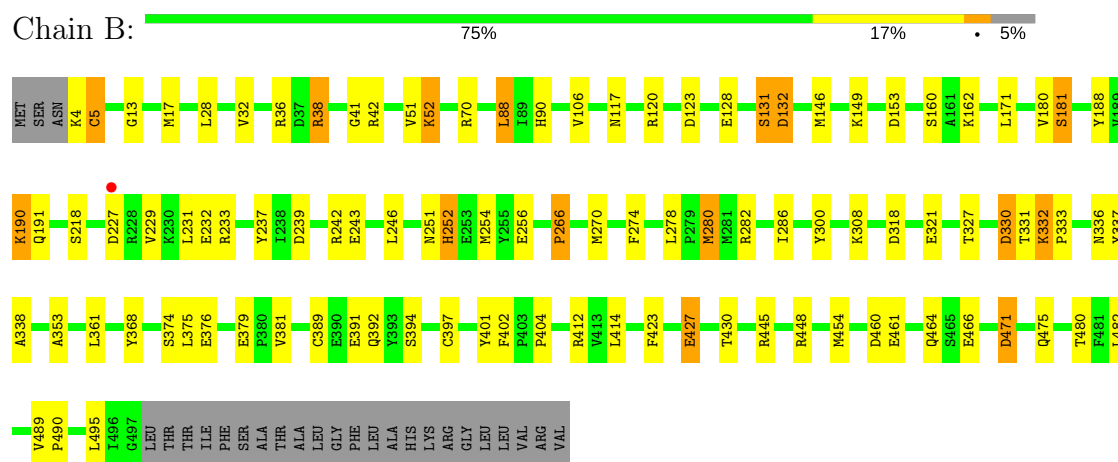
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

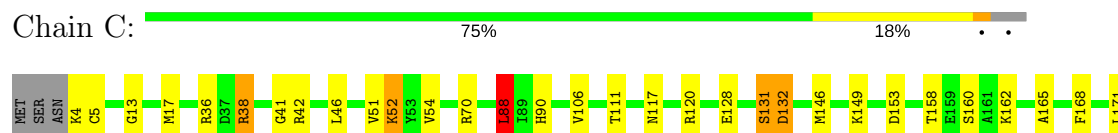
#### • Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B

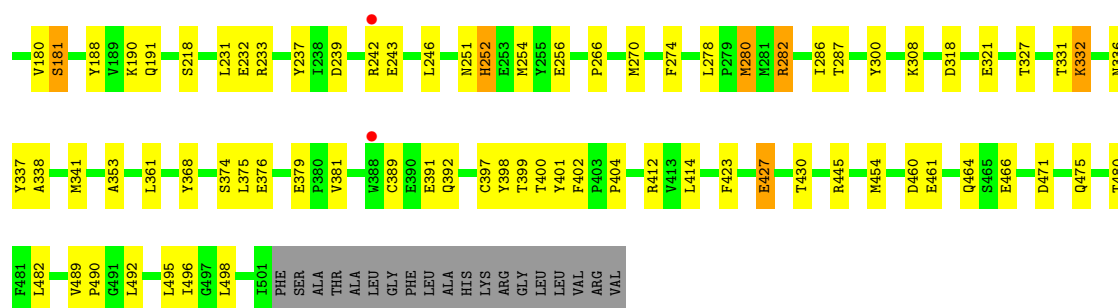


#### • Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B



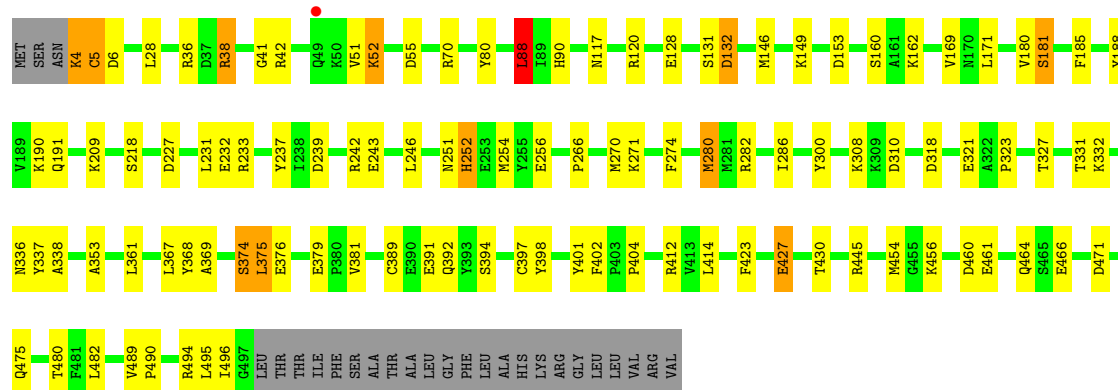
#### • Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B





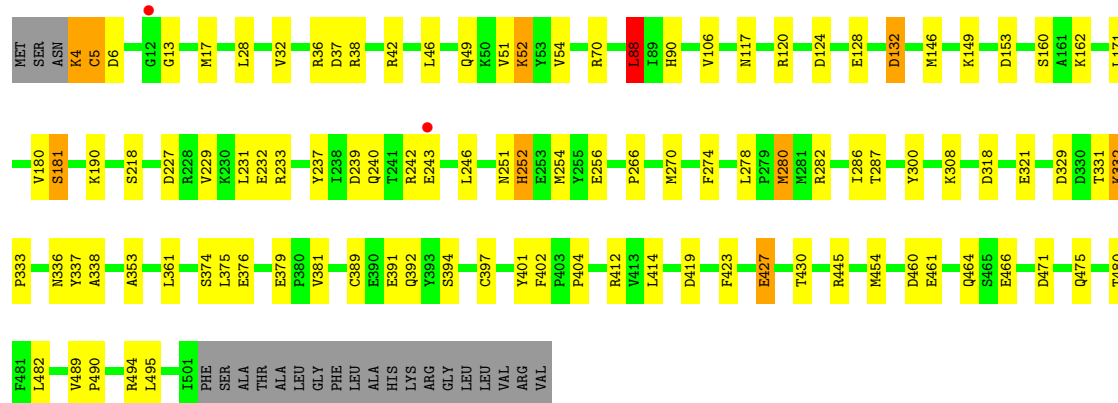
• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B

Chain D: 74% 18% 5%



• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B

Chain E: 76% 18% 5%

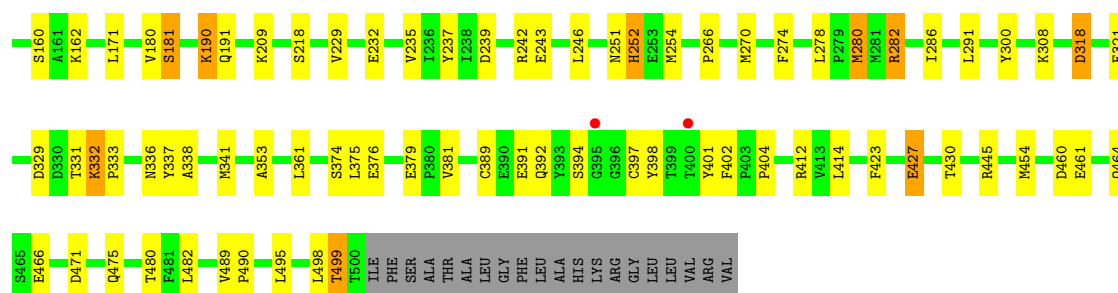


• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B

Chain F: 75% 18% 5%

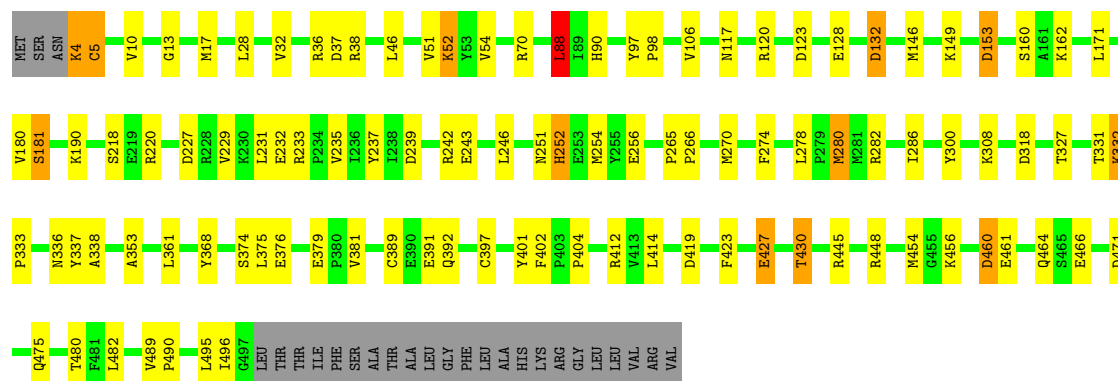






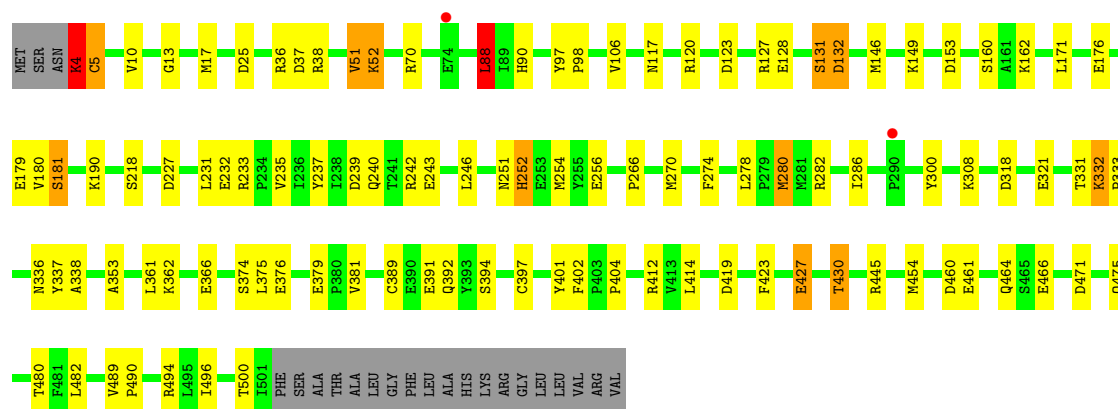
• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B

Chain G: 75% 18% 5%



• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B

Chain H: 75% 18%



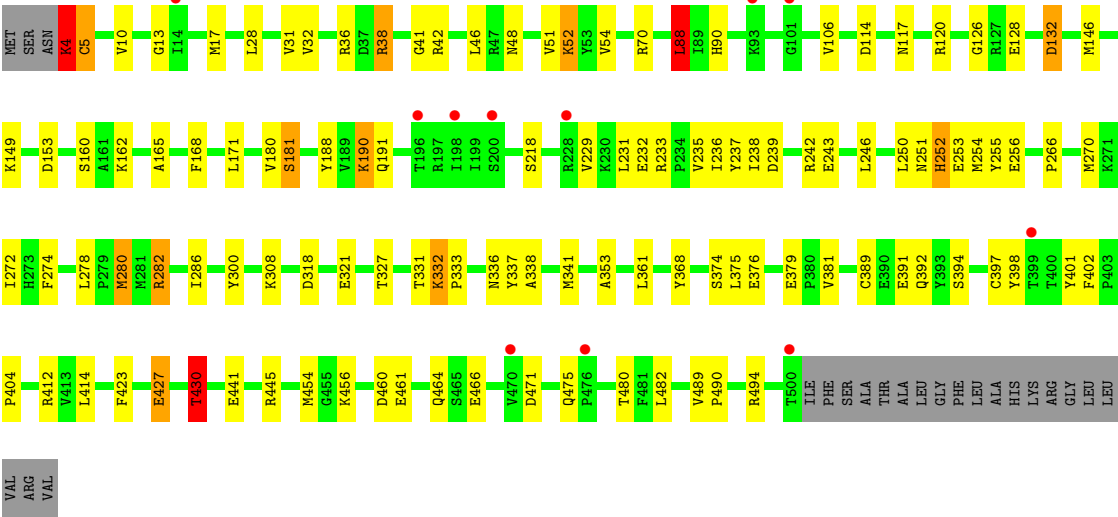
• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B

Chain I: 75% 18%





• Molecule 1: AMINE OXIDASE [FLAVIN-CONTAINING] B



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.41Å 132.43Å 154.84Å 90.14° 90.45° 114.02°	Depositor
Resolution (Å)	40.00 – 3.10 51.61 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.00-3.10) 95.8 (51.61-3.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 3.13Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.252 , 0.260 0.245 , 0.257	Depositor DCC
$R_{free}$ test set	1408 reflections (1.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.1	Xtriage
Anisotropy	0.881	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 0.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.186 for h,-h-k,-l 0.047 for -h,-k,l 0.046 for -h,h+k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	40219	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<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, 0.333 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: LDA, FAD

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	0.75	1/4055 (0.0%)	0.84	7/5504 (0.1%)
1	B	0.76	1/4033 (0.0%)	0.84	7/5473 (0.1%)
1	C	0.73	1/4060 (0.0%)	0.82	4/5511 (0.1%)
1	D	0.74	1/4033 (0.0%)	0.83	8/5473 (0.1%)
1	E	0.73	1/4060 (0.0%)	0.84	8/5511 (0.1%)
1	F	0.74	1/4055 (0.0%)	0.84	7/5504 (0.1%)
1	G	0.74	1/4033 (0.0%)	0.84	10/5473 (0.2%)
1	H	0.76	1/4060 (0.0%)	0.85	6/5511 (0.1%)
1	I	0.76	1/4055 (0.0%)	0.83	4/5504 (0.1%)
1	L	0.76	1/4055 (0.0%)	0.84	4/5504 (0.1%)
All	All	0.75	10/40499 (0.0%)	0.84	65/54968 (0.1%)

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	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	G	0	1
1	H	0	2
1	I	0	1
1	L	0	1
All	All	0	9

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	430	THR	CB-CG2	-9.03	1.22	1.52
1	G	430	THR	CB-CG2	-8.87	1.23	1.52
1	L	430	THR	CB-CG2	-8.51	1.24	1.52
1	I	430	THR	CB-CG2	-8.21	1.25	1.52
1	B	430	THR	CB-CG2	-7.28	1.28	1.52
1	F	430	THR	CB-CG2	-7.09	1.28	1.52
1	C	430	THR	CB-CG2	-7.03	1.29	1.52
1	E	430	THR	CB-CG2	-6.88	1.29	1.52
1	A	430	THR	CB-CG2	-6.82	1.29	1.52
1	D	430	THR	CB-CG2	-6.16	1.32	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	430	THR	OG1-CB-CG2	-10.92	84.89	110.00
1	H	430	THR	OG1-CB-CG2	-10.75	85.28	110.00
1	I	430	THR	OG1-CB-CG2	-10.02	86.97	110.00
1	G	430	THR	OG1-CB-CG2	-9.62	87.88	110.00
1	C	430	THR	OG1-CB-CG2	-7.74	92.19	110.00
1	A	430	THR	OG1-CB-CG2	-7.66	92.39	110.00
1	D	430	THR	OG1-CB-CG2	-7.58	92.58	110.00
1	F	430	THR	OG1-CB-CG2	-7.53	92.68	110.00
1	B	430	THR	OG1-CB-CG2	-7.47	92.81	110.00
1	H	123	ASP	CB-CG-OD2	7.23	124.80	118.30
1	E	430	THR	OG1-CB-CG2	-7.14	93.58	110.00
1	G	123	ASP	CB-CG-OD2	6.75	124.38	118.30
1	I	227	ASP	CB-CG-OD2	6.37	124.03	118.30
1	F	124	ASP	CB-CG-OD2	6.35	124.02	118.30
1	F	114	ASP	CB-CG-OD2	6.18	123.86	118.30
1	G	227	ASP	CB-CG-OD2	6.14	123.83	118.30
1	G	153	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	42	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	L	42	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	F	25	ASP	CB-CG-OD2	5.96	123.67	118.30
1	E	329	ASP	CB-CG-OD2	5.95	123.66	118.30
1	H	37	ASP	CB-CG-OD2	5.80	123.52	118.30
1	E	124	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	448	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	F	318	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	419	ASP	CB-CG-OD2	5.66	123.39	118.30
1	B	123	ASP	CB-CG-OD2	5.65	123.39	118.30
1	G	419	ASP	CB-CG-OD2	5.63	123.36	118.30
1	G	88	LEU	CA-CB-CG	5.62	128.23	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	471	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	88	LEU	CA-CB-CG	5.50	127.96	115.30
1	B	471	ASP	CB-CG-OD2	5.47	123.22	118.30
1	E	37	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	330	ASP	CB-CG-OD2	5.46	123.21	118.30
1	H	88	LEU	CA-CB-CG	5.46	127.86	115.30
1	L	114	ASP	CB-CG-OD2	5.44	123.20	118.30
1	I	37	ASP	CB-CG-OD2	5.42	123.18	118.30
1	F	329	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	132	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	42	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	448	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	D	227	ASP	CB-CG-OD2	5.34	123.11	118.30
1	H	25	ASP	CB-CG-OD2	5.32	123.09	118.30
1	I	124	ASP	CB-CG-OD2	5.31	123.08	118.30
1	D	310	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	227	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	42	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	G	37	ASP	CB-CG-OD2	5.25	123.03	118.30
1	E	6	ASP	CB-CG-OD2	5.24	123.01	118.30
1	A	37	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	42	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	88	LEU	CA-CB-CG	5.12	127.09	115.30
1	A	227	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	227	ASP	CB-CG-OD2	5.12	122.91	118.30
1	L	88	LEU	CA-CB-CG	5.11	127.06	115.30
1	A	330	ASP	CB-CG-OD2	5.08	122.88	118.30
1	C	42	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	H	227	ASP	CB-CG-OD2	5.07	122.86	118.30
1	G	448	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	D	6	ASP	CB-CG-OD2	5.06	122.86	118.30
1	E	88	LEU	CA-CB-CG	5.06	126.94	115.30
1	G	430	THR	N-CA-CB	-5.06	100.69	110.30
1	G	460	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	55	ASP	CB-CG-OD2	5.02	122.82	118.30
1	F	495	LEU	CA-CB-CG	5.02	126.84	115.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	131	SER	Peptide
1	D	4	LYS	Peptide
1	E	4	LYS	Peptide
1	G	4	LYS	Peptide
1	H	131	SER	Peptide
1	H	4	LYS	Peptide
1	I	4	LYS	Peptide
1	L	4	LYS	Peptide

## 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	3958	0	3959	60	0
1	B	3936	0	3934	63	0
1	C	3963	0	3961	60	0
1	D	3936	0	3934	65	0
1	E	3963	0	3961	56	1
1	F	3958	0	3959	59	0
1	G	3936	0	3934	62	1
1	H	3963	0	3961	66	0
1	I	3958	0	3959	69	0
1	L	3958	0	3959	69	0
2	A	53	0	29	0	0
2	B	53	0	29	0	0
2	C	53	0	29	0	0
2	D	53	0	29	0	0
2	E	53	0	29	0	0
2	F	53	0	29	0	0
2	G	53	0	29	0	0
2	H	53	0	29	0	0
2	I	53	0	29	0	0
2	L	53	0	29	0	0
3	A	16	0	31	3	0
3	B	16	0	31	3	0
3	C	16	0	31	2	0
3	D	16	0	31	3	0
3	E	16	0	31	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	16	0	31	2	0
3	G	16	0	31	3	0
3	H	16	0	31	3	0
3	I	16	0	31	3	0
3	L	16	0	31	3	0
All	All	40219	0	40121	561	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 7.

All (561) 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:G:4:LYS:HA	1:G:5:CYS:SG	1.59	1.39
1:A:49:GLN:OE1	1:H:362:LYS:HA	1.11	1.27
1:H:4:LYS:C	1:H:5:CYS:SG	2.14	1.25
1:A:49:GLN:OE1	1:H:362:LYS:CA	1.88	1.21
1:G:4:LYS:CA	1:G:5:CYS:SG	2.36	1.14
1:I:4:LYS:C	1:I:5:CYS:SG	2.34	1.05
1:H:4:LYS:CA	1:H:5:CYS:SG	2.45	1.03
1:E:4:LYS:N	1:E:5:CYS:HG	1.58	1.01
1:D:375:LEU:HD21	1:I:130:PRO:HG3	1.41	0.99
1:G:171:LEU:HD23	3:G:601:LDA:H61	1.43	0.99
1:F:4:LYS:C	1:F:5:CYS:SG	2.42	0.97
1:I:280:MET:HG3	1:L:389:CYS:HB3	1.45	0.97
1:E:4:LYS:N	1:E:5:CYS:SG	2.38	0.96
1:D:171:LEU:HD23	3:D:601:LDA:H61	1.47	0.96
1:C:171:LEU:HD23	3:C:601:LDA:H61	1.48	0.94
1:C:392:GLN:HE22	1:D:274:PHE:H	1.14	0.94
1:I:274:PHE:H	1:L:392:GLN:HE22	1.13	0.93
1:A:392:GLN:HE22	1:B:274:PHE:H	1.12	0.93
1:G:266:PRO:HD3	1:G:427:GLU:HG3	1.50	0.91
1:F:171:LEU:HD23	3:F:601:LDA:H61	1.52	0.91
1:I:171:LEU:HD23	3:I:601:LDA:H61	1.52	0.91
1:E:392:GLN:HE22	1:F:274:PHE:H	1.19	0.90
1:L:171:LEU:HD23	3:L:601:LDA:H61	1.51	0.90
1:G:392:GLN:HE22	1:H:274:PHE:H	1.20	0.89
1:H:266:PRO:HD3	1:H:427:GLU:HG3	1.54	0.89
1:E:171:LEU:HD23	3:E:601:LDA:H61	1.55	0.86
1:A:266:PRO:HD3	1:A:427:GLU:HG3	1.57	0.86
1:F:336:ASN:HB3	1:F:337:TYR:HD1	1.41	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HD23	3:A:601:LDA:H61	1.57	0.85
1:I:280:MET:HG3	1:L:389:CYS:CB	2.06	0.85
1:I:266:PRO:HD3	1:I:427:GLU:HG3	1.60	0.84
1:C:266:PRO:HD3	1:C:427:GLU:HG3	1.60	0.84
1:L:4:LYS:N	1:L:5:CYS:SG	2.51	0.83
1:D:375:LEU:HD21	1:I:130:PRO:CG	2.08	0.83
1:G:4:LYS:C	1:G:5:CYS:SG	2.56	0.83
1:H:4:LYS:C	1:H:5:CYS:HG	1.77	0.83
1:L:4:LYS:N	1:L:5:CYS:HG	1.77	0.83
1:E:266:PRO:HD3	1:E:427:GLU:HG3	1.59	0.82
1:E:274:PHE:H	1:F:392:GLN:HE22	1.23	0.82
1:C:336:ASN:HB3	1:C:337:TYR:HD1	1.43	0.82
1:B:331:THR:HG23	1:B:338:ALA:HA	1.62	0.82
1:F:266:PRO:HD3	1:F:427:GLU:HG3	1.61	0.81
1:D:331:THR:HG23	1:D:338:ALA:HA	1.62	0.81
1:D:4:LYS:C	1:D:5:CYS:SG	2.59	0.81
1:I:4:LYS:CA	1:I:5:CYS:SG	2.68	0.81
1:B:171:LEU:HD23	3:B:601:LDA:H61	1.62	0.81
1:C:389:CYS:HB3	1:D:280:MET:HG3	1.62	0.81
1:L:266:PRO:HD3	1:L:427:GLU:HG3	1.61	0.81
1:A:274:PHE:H	1:B:392:GLN:HE22	1.30	0.80
1:C:280:MET:HG3	1:D:389:CYS:HB3	1.63	0.80
1:I:392:GLN:HE22	1:L:274:PHE:H	1.29	0.80
1:H:336:ASN:HB3	1:H:337:TYR:HD1	1.47	0.80
1:H:171:LEU:HD23	3:H:601:LDA:H61	1.64	0.79
1:I:4:LYS:C	1:I:5:CYS:HG	1.86	0.79
1:D:375:LEU:CD2	1:I:130:PRO:HG3	2.12	0.78
1:E:280:MET:HE1	1:F:353:ALA:HB1	1.66	0.78
1:A:353:ALA:HB1	1:B:280:MET:HE1	1.65	0.78
1:L:336:ASN:HB3	1:L:337:TYR:HD1	1.49	0.77
1:A:336:ASN:HB3	1:A:337:TYR:HD1	1.49	0.77
1:B:336:ASN:HB3	1:B:337:TYR:HD1	1.48	0.77
1:I:336:ASN:HB3	1:I:337:TYR:HD1	1.47	0.77
1:B:266:PRO:HD3	1:B:427:GLU:HG3	1.67	0.77
1:G:336:ASN:HB3	1:G:337:TYR:HD1	1.49	0.77
1:E:353:ALA:HB1	1:F:280:MET:HE1	1.66	0.77
1:G:331:THR:HG23	1:G:338:ALA:HA	1.64	0.77
1:G:274:PHE:H	1:H:392:GLN:HE22	1.32	0.77
1:G:171:LEU:CD2	3:G:601:LDA:H61	2.15	0.77
1:C:274:PHE:H	1:D:392:GLN:HE22	1.31	0.77
1:D:171:LEU:CD2	3:D:601:LDA:H61	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:4:LYS:O	1:F:5:CYS:SG	2.43	0.76
1:A:280:MET:HG3	1:B:389:CYS:HB3	1.68	0.76
1:E:266:PRO:CD	1:E:427:GLU:HG3	2.17	0.75
1:A:171:LEU:CD2	3:A:601:LDA:H61	2.15	0.75
1:D:336:ASN:HB3	1:D:337:TYR:HD1	1.52	0.75
1:D:266:PRO:HD3	1:D:427:GLU:HG3	1.66	0.75
1:L:171:LEU:CD2	3:L:601:LDA:H61	2.16	0.75
1:D:4:LYS:N	1:D:5:CYS:SG	2.59	0.75
1:F:266:PRO:CD	1:F:427:GLU:HG3	2.16	0.75
1:C:171:LEU:CD2	3:C:601:LDA:H61	2.16	0.74
1:I:280:MET:HE1	1:L:353:ALA:HB1	1.69	0.74
1:H:480:THR:HG22	1:H:482:LEU:H	1.51	0.74
1:C:336:ASN:HB3	1:C:337:TYR:CD1	2.22	0.74
1:I:4:LYS:N	1:I:5:CYS:SG	2.60	0.74
1:E:480:THR:HG22	1:E:482:LEU:H	1.53	0.74
1:F:336:ASN:HB3	1:F:337:TYR:CD1	2.21	0.74
1:I:266:PRO:CD	1:I:427:GLU:HG3	2.17	0.74
1:B:171:LEU:CD2	3:B:601:LDA:H61	2.17	0.74
1:I:171:LEU:CD2	3:I:601:LDA:H61	2.17	0.74
1:L:266:PRO:CD	1:L:427:GLU:HG3	2.18	0.74
1:B:266:PRO:CD	1:B:427:GLU:HG3	2.17	0.73
1:F:171:LEU:CD2	3:F:601:LDA:H61	2.19	0.73
1:C:353:ALA:HB1	1:D:280:MET:HE1	1.69	0.73
1:E:336:ASN:HB3	1:E:337:TYR:HD1	1.53	0.73
1:G:389:CYS:HB3	1:H:280:MET:HG3	1.70	0.73
1:G:480:THR:HG22	1:G:482:LEU:H	1.53	0.73
1:C:331:THR:HG23	1:C:338:ALA:HA	1.70	0.73
1:G:4:LYS:CA	1:G:5:CYS:HG	2.00	0.72
1:C:266:PRO:CD	1:C:427:GLU:HG3	2.20	0.72
1:H:266:PRO:CD	1:H:427:GLU:HG3	2.20	0.72
1:A:389:CYS:HB3	1:B:280:MET:HG3	1.72	0.72
1:A:480:THR:HG22	1:A:482:LEU:H	1.54	0.72
1:G:266:PRO:CD	1:G:427:GLU:HG3	2.19	0.72
1:H:4:LYS:HA	1:H:5:CYS:SG	2.29	0.72
1:A:70:ARG:HD3	1:A:466:GLU:OE2	1.89	0.72
1:G:246:LEU:HD22	1:G:254:MET:HE2	1.70	0.71
1:A:331:THR:HG23	1:A:338:ALA:HA	1.70	0.71
1:A:336:ASN:HB3	1:A:337:TYR:CD1	2.25	0.71
1:H:171:LEU:CD2	3:H:601:LDA:H61	2.19	0.71
1:H:70:ARG:HD3	1:H:466:GLU:OE2	1.90	0.71
1:D:4:LYS:N	1:D:5:CYS:HG	1.88	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:336:ASN:HB3	1:E:337:TYR:CD1	2.25	0.71
1:E:171:LEU:CD2	3:E:601:LDA:H61	2.19	0.71
1:A:266:PRO:CD	1:A:427:GLU:HG3	2.20	0.71
1:D:246:LEU:HD22	1:D:254:MET:HE2	1.71	0.71
1:H:336:ASN:HB3	1:H:337:TYR:CD1	2.25	0.71
1:L:336:ASN:HB3	1:L:337:TYR:CD1	2.25	0.71
1:I:389:CYS:HB3	1:L:280:MET:HG3	1.73	0.71
1:B:336:ASN:HB3	1:B:337:TYR:CD1	2.26	0.70
1:H:331:THR:HG23	1:H:338:ALA:HA	1.72	0.70
1:A:49:GLN:OE1	1:H:362:LYS:CB	2.38	0.70
1:I:336:ASN:HB3	1:I:337:TYR:CD1	2.26	0.70
1:H:4:LYS:N	1:H:5:CYS:SG	2.64	0.70
1:F:70:ARG:HD3	1:F:466:GLU:OE2	1.91	0.70
1:L:70:ARG:HD3	1:L:466:GLU:OE2	1.91	0.70
1:B:480:THR:HG22	1:B:482:LEU:H	1.55	0.70
1:A:280:MET:HE1	1:B:353:ALA:HB1	1.72	0.70
1:E:280:MET:HG3	1:F:389:CYS:HB3	1.74	0.70
1:G:336:ASN:HB3	1:G:337:TYR:CD1	2.27	0.69
1:I:353:ALA:HB1	1:L:280:MET:HE1	1.72	0.69
1:I:480:THR:HG22	1:I:482:LEU:H	1.56	0.69
1:L:423:PHE:O	1:L:445:ARG:NH2	2.25	0.69
1:C:280:MET:HE1	1:D:353:ALA:HB1	1.73	0.69
1:D:237:TYR:CE2	1:D:239:ASP:HB2	2.28	0.69
1:F:480:THR:HG22	1:F:482:LEU:H	1.58	0.68
1:I:331:THR:HG23	1:I:338:ALA:HA	1.75	0.68
1:B:237:TYR:CE2	1:B:239:ASP:HB2	2.29	0.68
1:L:331:THR:HG23	1:L:338:ALA:HA	1.73	0.68
1:D:266:PRO:CD	1:D:427:GLU:HG3	2.23	0.68
1:E:389:CYS:HB3	1:F:280:MET:HG3	1.76	0.68
1:D:336:ASN:HB3	1:D:337:TYR:CD1	2.29	0.67
1:E:331:THR:HG23	1:E:338:ALA:HA	1.75	0.67
1:F:423:PHE:O	1:F:445:ARG:NH2	2.28	0.67
1:I:402:PHE:HZ	1:I:414:LEU:HD11	1.59	0.67
1:C:246:LEU:HD22	1:C:254:MET:HE2	1.76	0.66
1:F:237:TYR:CE2	1:F:239:ASP:HB2	2.31	0.66
1:A:389:CYS:CB	1:B:280:MET:HG3	2.26	0.66
1:F:331:THR:HG23	1:F:338:ALA:HA	1.77	0.66
1:D:402:PHE:HZ	1:D:414:LEU:HD11	1.61	0.66
1:D:480:THR:HG22	1:D:482:LEU:H	1.59	0.66
1:I:13:GLY:O	1:I:17:MET:HG2	1.95	0.66
1:I:246:LEU:HD22	1:I:254:MET:HE2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:402:PHE:HZ	1:E:414:LEU:HD11	1.61	0.66
1:G:389:CYS:CB	1:H:280:MET:HG3	2.26	0.65
1:A:423:PHE:O	1:A:445:ARG:NH2	2.28	0.65
1:L:237:TYR:CE2	1:L:239:ASP:HB2	2.32	0.65
1:D:375:LEU:HG	1:I:128:GLU:O	1.96	0.65
1:A:353:ALA:CB	1:B:280:MET:HE1	2.27	0.65
1:A:36:ARG:NH1	1:A:391:GLU:OE1	2.30	0.65
1:B:423:PHE:O	1:B:445:ARG:NH2	2.30	0.65
1:H:4:LYS:N	1:H:5:CYS:HG	1.95	0.64
1:A:4:LYS:C	1:A:5:CYS:SG	2.76	0.64
1:A:246:LEU:HD22	1:A:254:MET:HE2	1.79	0.64
1:C:181:SER:HB2	1:C:404:PRO:HA	1.79	0.64
1:E:353:ALA:CB	1:F:280:MET:HE1	2.28	0.64
1:C:237:TYR:CE2	1:C:239:ASP:HB2	2.31	0.64
1:B:246:LEU:HD22	1:B:254:MET:HE2	1.80	0.64
1:I:117:ASN:HD22	1:I:120:ARG:NH1	1.96	0.64
1:H:237:TYR:CE2	1:H:239:ASP:HB2	2.33	0.63
1:C:423:PHE:O	1:C:445:ARG:NH2	2.31	0.63
1:D:117:ASN:HD22	1:D:120:ARG:NH1	1.97	0.63
1:G:353:ALA:HB1	1:H:280:MET:HE1	1.79	0.63
1:H:51:VAL:HG22	1:H:300:TYR:CZ	2.34	0.63
1:I:70:ARG:HD3	1:I:466:GLU:OE2	1.99	0.63
1:E:36:ARG:NH1	1:E:391:GLU:OE1	2.32	0.63
1:C:402:PHE:HZ	1:C:414:LEU:HD11	1.64	0.62
1:E:252:HIS:CD2	1:F:252:HIS:CD2	2.86	0.62
1:A:402:PHE:HZ	1:A:414:LEU:HD11	1.64	0.62
1:F:246:LEU:HD22	1:F:254:MET:HE2	1.81	0.62
1:C:70:ARG:HD3	1:C:466:GLU:OE2	2.00	0.62
1:C:36:ARG:NH1	1:C:391:GLU:OE1	2.33	0.62
1:F:402:PHE:HZ	1:F:414:LEU:HD11	1.65	0.62
1:H:246:LEU:HD22	1:H:254:MET:HE2	1.80	0.62
1:G:280:MET:HE1	1:H:353:ALA:HB1	1.81	0.62
1:L:36:ARG:NH1	1:L:391:GLU:OE1	2.33	0.62
1:G:237:TYR:CE2	1:G:239:ASP:HB2	2.35	0.62
1:G:70:ARG:HD3	1:G:466:GLU:OE2	1.99	0.61
1:D:423:PHE:O	1:D:445:ARG:NH2	2.32	0.61
1:E:70:ARG:HD3	1:E:466:GLU:OE2	2.00	0.61
1:G:402:PHE:HZ	1:G:414:LEU:HD11	1.65	0.61
1:G:4:LYS:N	1:G:5:CYS:HG	1.99	0.61
1:A:237:TYR:CE2	1:A:239:ASP:HB2	2.35	0.61
1:A:181:SER:HB2	1:A:404:PRO:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:MET:HE1	1:F:353:ALA:CB	2.31	0.61
1:G:153:ASP:HA	1:G:162:LYS:HE2	1.83	0.61
1:B:88:LEU:N	1:B:88:LEU:HD23	2.16	0.61
1:C:389:CYS:CB	1:D:280:MET:HG3	2.30	0.61
1:I:280:MET:HE1	1:L:353:ALA:CB	2.30	0.60
1:L:480:THR:HG22	1:L:482:LEU:H	1.66	0.60
1:C:480:THR:HG22	1:C:482:LEU:H	1.65	0.60
1:B:402:PHE:HZ	1:B:414:LEU:HD11	1.67	0.60
1:B:70:ARG:HD3	1:B:466:GLU:OE2	2.00	0.60
1:H:423:PHE:O	1:H:445:ARG:NH2	2.34	0.60
1:L:402:PHE:HZ	1:L:414:LEU:HD11	1.66	0.60
1:H:36:ARG:NH1	1:H:391:GLU:OE1	2.34	0.60
1:A:252:HIS:CD2	1:B:252:HIS:CD2	2.90	0.60
1:A:280:MET:HE1	1:B:353:ALA:CB	2.32	0.59
1:B:117:ASN:HD22	1:B:120:ARG:NH1	2.00	0.59
1:I:181:SER:HB2	1:I:404:PRO:HA	1.83	0.59
1:I:353:ALA:CB	1:L:280:MET:HE1	2.32	0.59
1:G:117:ASN:HD22	1:G:120:ARG:NH1	2.00	0.59
1:I:423:PHE:O	1:I:445:ARG:NH2	2.36	0.59
1:F:36:ARG:NH1	1:F:391:GLU:OE1	2.35	0.59
1:E:237:TYR:CE2	1:E:239:ASP:HB2	2.38	0.58
1:A:4:LYS:N	1:A:5:CYS:HG	2.00	0.58
1:H:181:SER:HB2	1:H:404:PRO:HA	1.85	0.58
1:H:402:PHE:HZ	1:H:414:LEU:HD11	1.68	0.58
1:H:117:ASN:HD22	1:H:120:ARG:NH1	2.01	0.58
1:I:237:TYR:CE2	1:I:239:ASP:HB2	2.38	0.58
1:E:246:LEU:HD22	1:E:254:MET:HE2	1.84	0.58
1:E:423:PHE:O	1:E:445:ARG:NH2	2.36	0.58
1:D:36:ARG:NH1	1:D:391:GLU:OE1	2.37	0.58
1:D:70:ARG:HD3	1:D:466:GLU:OE2	2.04	0.58
1:E:181:SER:HB2	1:E:404:PRO:HA	1.84	0.58
1:G:36:ARG:NH1	1:G:391:GLU:OE1	2.36	0.58
1:D:374:SER:HA	1:I:128:GLU:OE2	2.04	0.58
1:L:246:LEU:HD22	1:L:254:MET:HE2	1.85	0.57
1:C:353:ALA:CB	1:D:280:MET:HE1	2.34	0.57
1:D:153:ASP:HA	1:D:162:LYS:HE2	1.86	0.57
1:F:117:ASN:HD22	1:F:120:ARG:NH1	2.02	0.57
1:F:181:SER:HB2	1:F:404:PRO:HA	1.85	0.57
1:G:51:VAL:HG22	1:G:300:TYR:CZ	2.39	0.57
1:L:51:VAL:HG22	1:L:300:TYR:CZ	2.39	0.57
1:A:251:ASN:O	1:A:252:HIS:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:VAL:HG22	1:C:300:TYR:CZ	2.40	0.57
1:E:117:ASN:HD22	1:E:120:ARG:NH1	2.01	0.57
1:H:278:LEU:HD13	1:H:282:ARG:HG2	1.86	0.57
1:B:51:VAL:HG22	1:B:300:TYR:CZ	2.40	0.57
1:F:51:VAL:HG22	1:F:300:TYR:CZ	2.39	0.57
1:I:389:CYS:CB	1:L:280:MET:HG3	2.35	0.57
1:G:280:MET:HG3	1:H:389:CYS:HB3	1.86	0.56
1:C:270:MET:HG2	1:C:286:ILE:HD12	1.87	0.56
1:B:4:LYS:C	1:B:5:CYS:SG	2.83	0.56
1:E:51:VAL:HG22	1:E:300:TYR:CZ	2.41	0.56
1:B:36:ARG:NH1	1:B:391:GLU:OE1	2.39	0.56
1:I:51:VAL:HG22	1:I:300:TYR:CZ	2.40	0.56
1:B:4:LYS:N	1:B:5:CYS:HG	2.04	0.56
1:E:4:LYS:C	1:E:5:CYS:SG	2.84	0.56
1:C:88:LEU:N	1:C:88:LEU:HD23	2.21	0.56
1:B:153:ASP:HA	1:B:162:LYS:HE2	1.88	0.56
1:F:251:ASN:O	1:F:252:HIS:HB2	2.05	0.55
1:L:153:ASP:HA	1:L:162:LYS:HE2	1.88	0.55
1:B:270:MET:HG2	1:B:286:ILE:HD12	1.87	0.55
1:B:181:SER:HB2	1:B:404:PRO:HA	1.89	0.55
1:A:153:ASP:HA	1:A:162:LYS:HE2	1.89	0.55
1:G:13:GLY:O	1:G:17:MET:HG2	2.05	0.55
1:I:36:ARG:NH1	1:I:391:GLU:OE1	2.40	0.55
1:H:153:ASP:HA	1:H:162:LYS:HE2	1.88	0.55
1:E:231:LEU:O	1:E:233:ARG:HD3	2.07	0.55
1:G:423:PHE:O	1:G:445:ARG:NH2	2.38	0.54
1:G:4:LYS:N	1:G:5:CYS:SG	2.80	0.54
1:A:117:ASN:HD22	1:A:120:ARG:NH1	2.05	0.54
1:E:88:LEU:N	1:E:88:LEU:HD23	2.23	0.54
1:D:231:LEU:O	1:D:233:ARG:HD3	2.08	0.54
1:G:270:MET:HG2	1:G:286:ILE:HD12	1.88	0.54
1:G:180:VAL:HG12	1:G:401:TYR:CD1	2.43	0.54
1:A:50:LYS:HE3	1:H:366:GLU:OE2	2.08	0.53
1:L:181:SER:HB2	1:L:404:PRO:HA	1.89	0.53
1:L:332:LYS:HB3	1:L:333:PRO:HD2	1.90	0.53
1:I:246:LEU:HD23	1:I:256:GLU:HG3	1.89	0.53
1:E:153:ASP:HA	1:E:162:LYS:HE2	1.89	0.53
1:E:246:LEU:HD23	1:E:256:GLU:HG3	1.90	0.53
1:G:181:SER:HB2	1:G:404:PRO:HA	1.91	0.53
1:A:51:VAL:HG22	1:A:300:TYR:CZ	2.43	0.53
1:A:252:HIS:CD2	1:B:252:HIS:HD2	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:LEU:HB3	1:C:254:MET:HE1	1.90	0.52
1:L:117:ASN:HD22	1:L:120:ARG:NH1	2.07	0.52
1:L:13:GLY:O	1:L:17:MET:HG2	2.08	0.52
1:F:153:ASP:HA	1:F:162:LYS:HE2	1.89	0.52
1:F:88:LEU:HD23	1:F:88:LEU:N	2.24	0.52
1:I:153:ASP:HA	1:I:162:LYS:HE2	1.91	0.52
1:G:90:HIS:HE1	1:G:318:ASP:OD2	1.92	0.52
1:A:280:MET:HG3	1:B:389:CYS:CB	2.39	0.52
1:H:231:LEU:O	1:H:233:ARG:HD3	2.09	0.52
1:L:48:ASN:OD1	1:L:51:VAL:HB	2.09	0.52
1:D:51:VAL:HG22	1:D:300:TYR:CZ	2.44	0.52
1:E:252:HIS:HD2	1:F:252:HIS:CD2	2.27	0.52
1:I:246:LEU:HB3	1:I:254:MET:HE1	1.92	0.51
1:G:231:LEU:O	1:G:233:ARG:HD3	2.10	0.51
1:I:88:LEU:HD23	1:I:88:LEU:N	2.25	0.51
1:L:278:LEU:HD13	1:L:282:ARG:HG2	1.92	0.51
1:F:246:LEU:HB3	1:F:254:MET:HE1	1.91	0.51
1:C:492:LEU:O	1:C:496:ILE:HD12	2.11	0.51
1:H:246:LEU:HB3	1:H:254:MET:HE1	1.91	0.51
1:A:90:HIS:HE1	1:A:318:ASP:OD2	1.93	0.51
1:C:251:ASN:O	1:C:252:HIS:HB2	2.11	0.51
1:F:251:ASN:O	1:F:252:HIS:CB	2.59	0.50
1:G:353:ALA:CB	1:H:280:MET:HE1	2.41	0.50
1:H:13:GLY:O	1:H:17:MET:HG2	2.11	0.50
1:I:280:MET:CG	1:L:389:CYS:HB3	2.31	0.50
1:C:280:MET:HG3	1:D:389:CYS:CB	2.37	0.50
1:F:4:LYS:C	1:F:5:CYS:HG	2.03	0.50
1:L:270:MET:HG2	1:L:286:ILE:HD12	1.94	0.50
1:A:489:VAL:N	1:A:490:PRO:HD2	2.27	0.50
1:A:252:HIS:HD2	1:B:252:HIS:CD2	2.29	0.50
1:I:231:LEU:O	1:I:233:ARG:HD3	2.12	0.50
1:D:181:SER:HB2	1:D:404:PRO:HA	1.92	0.50
1:D:28:LEU:HD11	1:D:454:MET:HE1	1.93	0.50
1:A:251:ASN:O	1:A:252:HIS:CB	2.59	0.50
1:B:332:LYS:HB3	1:B:333:PRO:HD2	1.94	0.50
1:C:88:LEU:H	1:C:88:LEU:HD23	1.77	0.49
1:I:278:LEU:HD13	1:I:282:ARG:HG2	1.94	0.49
1:I:430:THR:HB	1:I:441:GLU:OE1	2.12	0.49
1:H:4:LYS:CA	1:H:5:CYS:HG	2.12	0.49
1:A:246:LEU:HD23	1:A:256:GLU:HG3	1.95	0.49
1:E:251:ASN:O	1:E:252:HIS:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:LYS:C	1:E:5:CYS:HG	2.15	0.49
1:G:480:THR:HG22	1:G:482:LEU:N	2.26	0.49
1:E:90:HIS:HE1	1:E:318:ASP:OD2	1.95	0.49
1:C:392:GLN:NE2	1:D:274:PHE:H	1.96	0.49
1:D:246:LEU:HB3	1:D:254:MET:HE1	1.95	0.49
1:E:180:VAL:HG12	1:E:401:TYR:CD1	2.48	0.49
1:H:270:MET:HG2	1:H:286:ILE:HD12	1.94	0.49
1:L:38:ARG:NH2	1:L:41:GLY:O	2.46	0.49
1:L:4:LYS:C	1:L:5:CYS:SG	2.91	0.49
1:E:13:GLY:O	1:E:17:MET:HG2	2.12	0.49
1:F:51:VAL:O	1:F:332:LYS:NZ	2.46	0.49
1:C:51:VAL:O	1:C:332:LYS:NZ	2.46	0.48
1:E:252:HIS:CD2	1:F:252:HIS:HD2	2.31	0.48
3:E:601:LDA:H112	3:E:601:LDA:H82	1.46	0.48
1:B:51:VAL:O	1:B:332:LYS:NZ	2.46	0.48
1:G:251:ASN:O	1:G:252:HIS:HB2	2.13	0.48
1:D:270:MET:HG2	1:D:286:ILE:HD12	1.95	0.48
1:L:28:LEU:HD11	1:L:454:MET:HE1	1.95	0.48
1:A:246:LEU:HB3	1:A:254:MET:HE1	1.95	0.48
1:A:280:MET:HE3	1:A:280:MET:HB3	1.77	0.48
1:G:32:VAL:HB	1:G:229:VAL:HG22	1.95	0.48
1:C:278:LEU:HD13	1:C:282:ARG:HG2	1.95	0.48
1:H:180:VAL:HG12	1:H:401:TYR:CD1	2.48	0.48
1:H:500:THR:HG22	1:H:500:THR:O	2.13	0.48
1:A:13:GLY:O	1:A:17:MET:HG2	2.14	0.48
1:F:190:LYS:HG3	1:F:191:GLN:N	2.27	0.48
1:L:90:HIS:HE1	1:L:318:ASP:OD2	1.96	0.48
1:L:180:VAL:HG12	1:L:401:TYR:CD1	2.49	0.48
1:L:251:ASN:O	1:L:252:HIS:HB2	2.14	0.48
1:A:88:LEU:HD23	1:A:88:LEU:N	2.29	0.48
1:L:280:MET:HB3	1:L:280:MET:HE3	1.72	0.48
1:I:180:VAL:HG12	1:I:401:TYR:CD1	2.49	0.47
1:L:427:GLU:H	1:L:427:GLU:HG2	1.37	0.47
1:A:332:LYS:HB3	1:A:333:PRO:HD2	1.96	0.47
1:C:246:LEU:HD23	1:C:256:GLU:HG3	1.96	0.47
1:G:51:VAL:O	1:G:332:LYS:NZ	2.47	0.47
1:D:427:GLU:H	1:D:427:GLU:HG2	1.33	0.47
1:E:46:LEU:HB3	1:E:54:VAL:HG12	1.95	0.47
1:L:489:VAL:N	1:L:490:PRO:HD2	2.29	0.47
1:B:32:VAL:HB	1:B:229:VAL:HG22	1.97	0.47
1:L:231:LEU:O	1:L:233:ARG:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:LEU:HD13	1:F:282:ARG:HG2	1.96	0.47
1:G:489:VAL:N	1:G:490:PRO:HD2	2.29	0.47
1:I:489:VAL:N	1:I:490:PRO:HD2	2.30	0.47
1:E:489:VAL:N	1:E:490:PRO:HD2	2.29	0.47
1:E:389:CYS:CB	1:F:280:MET:HG3	2.42	0.47
1:F:321:GLU:CD	1:F:321:GLU:H	2.18	0.47
1:H:88:LEU:HD23	1:H:88:LEU:N	2.30	0.47
1:C:180:VAL:HG12	1:C:401:TYR:CD1	2.50	0.46
1:C:38:ARG:NH2	1:C:41:GLY:O	2.46	0.46
1:L:321:GLU:CD	1:L:321:GLU:H	2.19	0.46
3:B:601:LDA:H112	3:B:601:LDA:H82	1.48	0.46
1:E:278:LEU:HD13	1:E:282:ARG:HG2	1.97	0.46
1:G:246:LEU:HB3	1:G:254:MET:HE1	1.98	0.46
1:A:80:TYR:OH	1:A:209:LYS:HE2	2.15	0.46
1:C:117:ASN:HD22	1:C:120:ARG:NH1	2.13	0.46
1:D:489:VAL:N	1:D:490:PRO:HD2	2.30	0.46
1:F:489:VAL:N	1:F:490:PRO:HD2	2.30	0.46
1:B:38:ARG:NH2	1:B:41:GLY:O	2.47	0.46
1:B:489:VAL:N	1:B:490:PRO:HD2	2.31	0.46
1:G:392:GLN:NE2	1:H:274:PHE:H	2.00	0.46
1:L:246:LEU:HB3	1:L:254:MET:HE1	1.97	0.46
1:B:190:LYS:HG3	1:B:191:GLN:N	2.30	0.46
1:B:246:LEU:HB3	1:B:254:MET:HE1	1.97	0.46
1:B:28:LEU:HD11	1:B:454:MET:HE1	1.97	0.46
1:B:88:LEU:HD23	1:B:88:LEU:H	1.80	0.46
1:C:153:ASP:HA	1:C:162:LYS:HE2	1.98	0.46
3:G:601:LDA:H112	3:G:601:LDA:H82	1.57	0.46
1:H:51:VAL:O	1:H:332:LYS:NZ	2.49	0.46
1:A:480:THR:HG22	1:A:482:LEU:N	2.26	0.46
1:B:278:LEU:HD13	1:B:282:ARG:HG2	1.97	0.46
1:C:321:GLU:H	1:C:321:GLU:CD	2.19	0.46
1:D:321:GLU:H	1:D:321:GLU:CD	2.19	0.46
1:I:252:HIS:CD2	1:L:252:HIS:CD2	3.04	0.46
1:C:13:GLY:O	1:C:17:MET:HG2	2.16	0.46
1:I:251:ASN:O	1:I:252:HIS:HB2	2.16	0.45
1:D:90:HIS:HE1	1:D:318:ASP:OD2	1.98	0.45
1:E:270:MET:HG2	1:E:286:ILE:HD12	1.98	0.45
1:E:28:LEU:HD11	1:E:454:MET:HE1	1.99	0.45
1:F:270:MET:HG2	1:F:286:ILE:HD12	1.98	0.45
1:I:274:PHE:H	1:L:392:GLN:NE2	1.97	0.45
1:D:188:TYR:O	1:D:191:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:332:LYS:HB3	1:G:333:PRO:HD2	1.99	0.45
1:H:90:HIS:HE1	1:H:318:ASP:OD2	2.00	0.45
1:L:430:THR:HB	1:L:441:GLU:OE1	2.16	0.45
1:G:28:LEU:HD11	1:G:454:MET:HE1	1.99	0.45
1:H:489:VAL:N	1:H:490:PRO:HD2	2.31	0.45
1:C:327:THR:HG21	1:C:368:TYR:CE2	2.51	0.45
1:E:321:GLU:CD	1:E:321:GLU:H	2.19	0.45
1:I:117:ASN:HD22	1:I:120:ARG:HH11	1.65	0.45
1:I:427:GLU:HG2	1:I:427:GLU:H	1.29	0.45
1:B:90:HIS:HE1	1:B:318:ASP:OD2	2.00	0.45
1:F:13:GLY:O	1:F:17:MET:HG2	2.16	0.45
1:G:278:LEU:HD13	1:G:282:ARG:HG2	1.99	0.45
1:H:251:ASN:O	1:H:252:HIS:HB2	2.16	0.45
1:B:246:LEU:HD22	1:B:254:MET:CE	2.45	0.45
1:D:246:LEU:HD22	1:D:254:MET:CE	2.44	0.45
1:D:251:ASN:O	1:D:252:HIS:HB2	2.16	0.45
1:G:280:MET:HE1	1:H:353:ALA:CB	2.47	0.45
1:H:454:MET:HE3	1:H:454:MET:HB2	1.68	0.45
1:B:231:LEU:O	1:B:233:ARG:HD3	2.17	0.45
1:G:246:LEU:HD23	1:G:256:GLU:HG3	1.99	0.45
1:I:90:HIS:HE1	1:I:318:ASP:OD2	2.00	0.45
1:L:238:ILE:HD12	1:L:272:ILE:HG21	1.98	0.45
1:B:321:GLU:CD	1:B:321:GLU:H	2.20	0.45
1:C:165:ALA:O	1:C:168:PHE:HB3	2.17	0.45
1:D:4:LYS:CA	1:D:5:CYS:SG	3.04	0.45
1:F:38:ARG:NH2	1:F:41:GLY:O	2.49	0.45
1:G:246:LEU:HD22	1:G:254:MET:CE	2.44	0.45
1:B:4:LYS:N	1:B:5:CYS:SG	2.90	0.44
1:C:280:MET:HB3	1:C:280:MET:HE3	1.82	0.44
1:A:389:CYS:HB2	1:B:280:MET:HG3	1.99	0.44
1:C:327:THR:HA	1:C:341:MET:O	2.18	0.44
1:C:252:HIS:CD2	1:D:252:HIS:CD2	3.05	0.44
1:F:180:VAL:HG12	1:F:401:TYR:CD1	2.52	0.44
1:D:4:LYS:CA	1:D:5:CYS:HG	2.30	0.44
1:F:427:GLU:H	1:F:427:GLU:HG2	1.35	0.44
1:L:88:LEU:N	1:L:88:LEU:HD23	2.32	0.44
1:A:321:GLU:CD	1:A:321:GLU:H	2.21	0.44
1:B:427:GLU:HG2	1:B:427:GLU:H	1.37	0.44
1:C:188:TYR:O	1:C:191:GLN:HG3	2.17	0.44
1:A:4:LYS:C	1:A:5:CYS:HG	2.21	0.44
1:C:251:ASN:O	1:C:252:HIS:CB	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:280:MET:HE3	1:H:280:MET:HB3	1.72	0.44
1:D:454:MET:HE3	1:D:456:LYS:HE2	2.00	0.44
1:A:50:LYS:HE3	1:H:366:GLU:CD	2.38	0.44
1:H:480:THR:HG22	1:H:482:LEU:N	2.25	0.44
1:L:327:THR:HA	1:L:341:MET:O	2.17	0.44
1:L:246:LEU:HD23	1:L:256:GLU:HG3	2.00	0.44
1:C:90:HIS:HE1	1:C:318:ASP:OD2	2.01	0.44
1:C:427:GLU:H	1:C:427:GLU:HG2	1.32	0.44
1:E:251:ASN:O	1:E:252:HIS:CB	2.66	0.44
3:H:601:LDA:H22	3:H:601:LDA:HM13	1.81	0.44
3:D:601:LDA:H82	3:D:601:LDA:H112	1.53	0.43
1:H:246:LEU:HD22	1:H:254:MET:CE	2.47	0.43
1:C:336:ASN:O	1:C:337:TYR:C	2.55	0.43
1:F:246:LEU:HB3	1:F:254:MET:CE	2.47	0.43
1:H:240:GLN:OE1	1:H:419:ASP:HB3	2.19	0.43
1:H:494:ARG:HD3	1:H:494:ARG:HA	1.90	0.43
1:A:165:ALA:O	1:A:168:PHE:HB3	2.19	0.43
3:A:601:LDA:H112	3:A:601:LDA:H82	1.49	0.43
1:C:399:THR:OG1	1:C:400:THR:N	2.50	0.43
1:E:246:LEU:HD22	1:E:254:MET:CE	2.49	0.43
3:I:601:LDA:H82	3:I:601:LDA:H112	1.58	0.43
1:L:188:TYR:O	1:L:191:GLN:HG3	2.17	0.43
1:C:489:VAL:N	1:C:490:PRO:HD2	2.33	0.43
1:F:254:MET:HB3	1:F:254:MET:HE2	1.90	0.43
1:H:332:LYS:HB3	1:H:333:PRO:HD2	1.99	0.43
1:F:32:VAL:HB	1:F:229:VAL:HG22	2.00	0.43
1:G:454:MET:HE3	1:G:456:LYS:HE2	2.01	0.43
1:I:46:LEU:HB3	1:I:54:VAL:HG12	2.01	0.43
1:E:270:MET:HE1	1:E:287:THR:HG22	2.01	0.43
1:L:10:VAL:HG22	1:L:235:VAL:HG21	2.01	0.43
1:L:32:VAL:HB	1:L:229:VAL:HG22	2.00	0.43
1:F:341:MET:HB3	1:F:341:MET:HE2	1.88	0.43
1:A:454:MET:HE3	1:A:454:MET:HB2	1.82	0.43
1:D:38:ARG:NH2	1:D:41:GLY:O	2.50	0.43
1:L:253:GLU:OE1	1:L:255:TYR:OH	2.21	0.43
1:B:280:MET:HB3	1:B:280:MET:HE3	1.71	0.42
1:C:270:MET:O	1:D:271:LYS:HG2	2.19	0.42
1:E:32:VAL:HB	1:E:229:VAL:HG22	2.01	0.42
1:G:10:VAL:HG22	1:G:235:VAL:HG21	2.00	0.42
1:G:251:ASN:O	1:G:252:HIS:CB	2.67	0.42
1:I:321:GLU:CD	1:I:321:GLU:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:38:ARG:NH2	1:I:41:GLY:O	2.48	0.42
1:I:454:MET:HB2	1:I:454:MET:HE3	1.74	0.42
1:A:231:LEU:O	1:A:233:ARG:HD3	2.19	0.42
1:B:254:MET:HE2	1:B:254:MET:HB3	1.85	0.42
1:C:231:LEU:O	1:C:233:ARG:HD3	2.19	0.42
1:D:80:TYR:OH	1:D:209:LYS:HE2	2.19	0.42
1:E:246:LEU:HB3	1:E:254:MET:HE1	2.01	0.42
1:H:97:TYR:HA	1:H:98:PRO:HD3	1.85	0.42
1:I:51:VAL:O	1:I:332:LYS:NZ	2.52	0.42
1:A:51:VAL:O	1:A:332:LYS:NZ	2.52	0.42
1:B:327:THR:HG21	1:B:368:TYR:CE2	2.54	0.42
1:B:480:THR:HG22	1:B:482:LEU:N	2.29	0.42
1:F:90:HIS:HE1	1:F:318:ASP:OD2	2.02	0.42
1:H:321:GLU:CD	1:H:321:GLU:H	2.23	0.42
1:I:270:MET:HG2	1:I:286:ILE:HD12	2.00	0.42
1:I:480:THR:HG22	1:I:482:LEU:N	2.30	0.42
1:G:46:LEU:HB3	1:G:54:VAL:HG12	2.01	0.42
1:H:176:GLU:HB2	1:H:179:GLU:HG3	2.01	0.42
1:E:480:THR:HG22	1:E:482:LEU:N	2.27	0.42
1:I:165:ALA:O	1:I:168:PHE:HB3	2.20	0.42
1:I:280:MET:HG3	1:L:389:CYS:HB2	1.93	0.42
1:D:323:PRO:HD2	1:D:367:LEU:HD22	2.01	0.42
1:G:97:TYR:HA	1:G:98:PRO:HD3	1.88	0.42
1:D:51:VAL:O	1:D:332:LYS:NZ	2.52	0.42
1:F:246:LEU:HD22	1:F:254:MET:CE	2.49	0.42
1:G:327:THR:HG21	1:G:368:TYR:CE2	2.55	0.42
1:F:332:LYS:HB3	1:F:333:PRO:HD2	2.02	0.42
1:H:246:LEU:HD23	1:H:256:GLU:HG3	2.01	0.42
1:L:51:VAL:O	1:L:332:LYS:NZ	2.53	0.42
1:B:246:LEU:HD23	1:B:256:GLU:HG3	2.01	0.42
1:G:90:HIS:CE1	1:G:318:ASP:OD2	2.73	0.42
1:I:251:ASN:O	1:I:252:HIS:CB	2.68	0.42
1:A:90:HIS:CE1	1:A:318:ASP:OD2	2.72	0.41
1:C:270:MET:HE1	1:C:287:THR:HG22	2.02	0.41
1:D:246:LEU:HD23	1:D:256:GLU:HG3	2.01	0.41
3:L:601:LDA:H112	3:L:601:LDA:H82	1.52	0.41
1:B:188:TYR:O	1:B:191:GLN:HG3	2.20	0.41
1:C:280:MET:HE1	1:D:353:ALA:CB	2.44	0.41
1:F:454:MET:HE3	1:F:454:MET:HB2	1.72	0.41
1:L:251:ASN:O	1:L:252:HIS:CB	2.68	0.41
1:B:180:VAL:HG12	1:B:401:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:N	1:B:88:LEU:CD2	2.83	0.41
1:C:454:MET:HB2	1:C:454:MET:HE3	1.80	0.41
1:D:251:ASN:O	1:D:252:HIS:CB	2.68	0.41
1:D:180:VAL:HG12	1:D:401:TYR:CD1	2.55	0.41
1:D:369:ALA:O	1:I:138:PRO:HB3	2.21	0.41
1:I:280:MET:HE3	1:I:280:MET:HB3	1.75	0.41
1:L:327:THR:HG21	1:L:368:TYR:CE2	2.55	0.41
1:B:117:ASN:HD22	1:B:120:ARG:HH11	1.69	0.41
1:F:10:VAL:HG22	1:F:235:VAL:HG21	2.03	0.41
1:F:80:TYR:OH	1:F:209:LYS:HE2	2.20	0.41
1:H:10:VAL:HG22	1:H:235:VAL:HG21	2.02	0.41
1:E:332:LYS:HB3	1:E:333:PRO:HD2	2.02	0.41
1:I:332:LYS:HB3	1:I:333:PRO:HD2	2.03	0.41
1:I:97:TYR:HA	1:I:98:PRO:HD3	1.85	0.41
1:I:253:GLU:OE1	1:I:255:TYR:OH	2.27	0.41
1:G:88:LEU:HD23	1:G:88:LEU:N	2.36	0.41
1:C:111:THR:HA	1:C:158:THR:HG21	2.03	0.41
1:E:240:GLN:OE1	1:E:419:ASP:HB3	2.21	0.41
1:G:427:GLU:H	1:G:427:GLU:HG2	1.40	0.41
1:L:46:LEU:HB3	1:L:54:VAL:HG12	2.02	0.41
1:A:440:VAL:O	1:A:444:GLU:HG3	2.20	0.41
1:F:97:TYR:HA	1:F:98:PRO:HD3	1.88	0.41
1:G:88:LEU:O	1:G:98:PRO:HA	2.20	0.41
1:D:169:VAL:HG22	1:D:185:PHE:CZ	2.55	0.40
1:F:46:LEU:HB3	1:F:54:VAL:HG12	2.03	0.40
1:G:252:HIS:CD2	1:H:252:HIS:CD2	3.09	0.40
1:L:165:ALA:O	1:L:168:PHE:HB3	2.20	0.40
1:L:236:ILE:HG21	1:L:250:LEU:HD13	2.03	0.40
1:B:13:GLY:O	1:B:17:MET:HG2	2.21	0.40
1:B:251:ASN:O	1:B:252:HIS:HB2	2.20	0.40
1:D:375:LEU:HD21	1:I:130:PRO:CD	2.49	0.40
1:H:127:ARG:HD2	1:H:127:ARG:HH11	1.72	0.40
1:L:90:HIS:CE1	1:L:318:ASP:OD2	2.74	0.40
1:L:454:MET:HE3	1:L:456:LYS:HE2	2.02	0.40
1:D:88:LEU:N	1:D:88:LEU:HD23	2.36	0.40
1:C:46:LEU:HB3	1:C:54:VAL:HG12	2.03	0.40
1:E:51:VAL:O	1:E:332:LYS:NZ	2.54	0.40
1:G:265:PRO:O	1:G:266:PRO:C	2.60	0.40
1:L:126:GLY:O	1:L:190:LYS:HD3	2.21	0.40
1:A:92:VAL:HG23	1:A:318:ASP:HB2	2.03	0.40
1:D:327:THR:HG21	1:D:368:TYR:CE2	2.55	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:GLN:NE2	1:G:220:ARG:NE[1_545]	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	495/520 (95%)	470 (95%)	21 (4%)	4 (1%)	22	62
1	B	492/520 (95%)	464 (94%)	24 (5%)	4 (1%)	22	62
1	C	496/520 (95%)	469 (95%)	23 (5%)	4 (1%)	22	62
1	D	492/520 (95%)	464 (94%)	24 (5%)	4 (1%)	22	62
1	E	496/520 (95%)	473 (95%)	19 (4%)	4 (1%)	22	62
1	F	495/520 (95%)	467 (94%)	22 (4%)	6 (1%)	15	51
1	G	492/520 (95%)	466 (95%)	22 (4%)	4 (1%)	22	62
1	H	496/520 (95%)	468 (94%)	24 (5%)	4 (1%)	22	62
1	I	495/520 (95%)	466 (94%)	23 (5%)	6 (1%)	15	51
1	L	495/520 (95%)	468 (94%)	23 (5%)	4 (1%)	22	62
All	All	4944/5200 (95%)	4675 (95%)	225 (5%)	44 (1%)	20	60

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	A	460	ASP
1	B	132	ASP
1	B	460	ASP
1	C	132	ASP
1	C	460	ASP
1	D	132	ASP

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Mol	Chain	Res	Type
1	D	460	ASP
1	E	132	ASP
1	E	460	ASP
1	F	460	ASP
1	G	132	ASP
1	G	460	ASP
1	H	132	ASP
1	H	460	ASP
1	I	132	ASP
1	I	460	ASP
1	L	132	ASP
1	L	460	ASP
1	A	252	HIS
1	F	132	ASP
1	F	252	HIS
1	A	52	LYS
1	B	52	LYS
1	B	252	HIS
1	C	52	LYS
1	C	252	HIS
1	D	52	LYS
1	D	252	HIS
1	E	52	LYS
1	E	252	HIS
1	F	5	CYS
1	F	52	LYS
1	G	52	LYS
1	G	252	HIS
1	H	52	LYS
1	H	252	HIS
1	I	52	LYS
1	I	252	HIS
1	L	52	LYS
1	L	252	HIS
1	F	499	THR
1	I	5	CYS
1	I	419	ASP

### 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	426/444 (96%)	391 (92%)	35 (8%)	13	45
1	B	423/444 (95%)	386 (91%)	37 (9%)	12	43
1	C	426/444 (96%)	388 (91%)	38 (9%)	11	41
1	D	423/444 (95%)	387 (92%)	36 (8%)	12	44
1	E	426/444 (96%)	391 (92%)	35 (8%)	13	45
1	F	426/444 (96%)	387 (91%)	39 (9%)	11	39
1	G	423/444 (95%)	388 (92%)	35 (8%)	13	45
1	H	426/444 (96%)	388 (91%)	38 (9%)	11	41
1	I	426/444 (96%)	386 (91%)	40 (9%)	10	38
1	L	426/444 (96%)	387 (91%)	39 (9%)	11	39
All	All	4251/4440 (96%)	3879 (91%)	372 (9%)	12	42

All (372) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	CYS
1	A	38	ARG
1	A	52	LYS
1	A	88	LEU
1	A	106	VAL
1	A	128	GLU
1	A	132	ASP
1	A	146	MET
1	A	149	LYS
1	A	160	SER
1	A	181	SER
1	A	190	LYS
1	A	218	SER
1	A	232	GLU
1	A	242	ARG
1	A	243	GLU
1	A	280	MET
1	A	308	LYS
1	A	332	LYS
1	A	361	LEU

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Mol	Chain	Res	Type
1	A	374	SER
1	A	375	LEU
1	A	376	GLU
1	A	379	GLU
1	A	381	VAL
1	A	394	SER
1	A	397	CYS
1	A	398	TYR
1	A	412	ARG
1	A	427	GLU
1	A	461	GLU
1	A	464	GLN
1	A	471	ASP
1	A	475	GLN
1	A	495	LEU
1	B	5	CYS
1	B	38	ARG
1	B	52	LYS
1	B	88	LEU
1	B	106	VAL
1	B	128	GLU
1	B	131	SER
1	B	132	ASP
1	B	146	MET
1	B	149	LYS
1	B	160	SER
1	B	181	SER
1	B	190	LYS
1	B	218	SER
1	B	232	GLU
1	B	242	ARG
1	B	243	GLU
1	B	266	PRO
1	B	280	MET
1	B	308	LYS
1	B	330	ASP
1	B	332	LYS
1	B	361	LEU
1	B	374	SER
1	B	375	LEU
1	B	376	GLU
1	B	379	GLU

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Mol	Chain	Res	Type
1	B	381	VAL
1	B	394	SER
1	B	397	CYS
1	B	412	ARG
1	B	427	GLU
1	B	461	GLU
1	B	464	GLN
1	B	471	ASP
1	B	475	GLN
1	B	495	LEU
1	C	4	LYS
1	C	5	CYS
1	C	38	ARG
1	C	52	LYS
1	C	88	LEU
1	C	106	VAL
1	C	128	GLU
1	C	131	SER
1	C	132	ASP
1	C	146	MET
1	C	149	LYS
1	C	160	SER
1	C	181	SER
1	C	190	LYS
1	C	218	SER
1	C	232	GLU
1	C	242	ARG
1	C	243	GLU
1	C	280	MET
1	C	282	ARG
1	C	308	LYS
1	C	332	LYS
1	C	361	LEU
1	C	374	SER
1	C	375	LEU
1	C	376	GLU
1	C	379	GLU
1	C	381	VAL
1	C	397	CYS
1	C	398	TYR
1	C	412	ARG
1	C	427	GLU

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Mol	Chain	Res	Type
1	C	461	GLU
1	C	464	GLN
1	C	471	ASP
1	C	475	GLN
1	C	495	LEU
1	C	498	LEU
1	D	5	CYS
1	D	38	ARG
1	D	52	LYS
1	D	88	LEU
1	D	128	GLU
1	D	131	SER
1	D	146	MET
1	D	149	LYS
1	D	160	SER
1	D	181	SER
1	D	190	LYS
1	D	218	SER
1	D	232	GLU
1	D	242	ARG
1	D	243	GLU
1	D	280	MET
1	D	282	ARG
1	D	308	LYS
1	D	361	LEU
1	D	374	SER
1	D	375	LEU
1	D	376	GLU
1	D	379	GLU
1	D	381	VAL
1	D	394	SER
1	D	397	CYS
1	D	398	TYR
1	D	412	ARG
1	D	427	GLU
1	D	461	GLU
1	D	464	GLN
1	D	471	ASP
1	D	475	GLN
1	D	494	ARG
1	D	495	LEU
1	D	496	ILE

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Mol	Chain	Res	Type
1	E	5	CYS
1	E	38	ARG
1	E	52	LYS
1	E	88	LEU
1	E	106	VAL
1	E	128	GLU
1	E	132	ASP
1	E	146	MET
1	E	149	LYS
1	E	160	SER
1	E	181	SER
1	E	190	LYS
1	E	218	SER
1	E	232	GLU
1	E	242	ARG
1	E	243	GLU
1	E	280	MET
1	E	308	LYS
1	E	332	LYS
1	E	361	LEU
1	E	374	SER
1	E	375	LEU
1	E	376	GLU
1	E	379	GLU
1	E	381	VAL
1	E	394	SER
1	E	397	CYS
1	E	412	ARG
1	E	427	GLU
1	E	461	GLU
1	E	464	GLN
1	E	471	ASP
1	E	475	GLN
1	E	494	ARG
1	E	495	LEU
1	F	5	CYS
1	F	38	ARG
1	F	52	LYS
1	F	88	LEU
1	F	106	VAL
1	F	128	GLU
1	F	131	SER

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Mol	Chain	Res	Type
1	F	132	ASP
1	F	146	MET
1	F	149	LYS
1	F	160	SER
1	F	181	SER
1	F	190	LYS
1	F	218	SER
1	F	232	GLU
1	F	242	ARG
1	F	243	GLU
1	F	280	MET
1	F	282	ARG
1	F	291	LEU
1	F	308	LYS
1	F	332	LYS
1	F	361	LEU
1	F	374	SER
1	F	375	LEU
1	F	376	GLU
1	F	379	GLU
1	F	381	VAL
1	F	394	SER
1	F	397	CYS
1	F	398	TYR
1	F	412	ARG
1	F	427	GLU
1	F	461	GLU
1	F	464	GLN
1	F	471	ASP
1	F	475	GLN
1	F	498	LEU
1	F	499	THR
1	G	5	CYS
1	G	38	ARG
1	G	52	LYS
1	G	88	LEU
1	G	106	VAL
1	G	128	GLU
1	G	132	ASP
1	G	146	MET
1	G	149	LYS
1	G	160	SER

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Mol	Chain	Res	Type
1	G	181	SER
1	G	190	LYS
1	G	218	SER
1	G	232	GLU
1	G	242	ARG
1	G	243	GLU
1	G	280	MET
1	G	308	LYS
1	G	332	LYS
1	G	361	LEU
1	G	374	SER
1	G	375	LEU
1	G	376	GLU
1	G	379	GLU
1	G	381	VAL
1	G	397	CYS
1	G	412	ARG
1	G	427	GLU
1	G	430	THR
1	G	461	GLU
1	G	464	GLN
1	G	471	ASP
1	G	475	GLN
1	G	495	LEU
1	G	496	ILE
1	H	4	LYS
1	H	5	CYS
1	H	38	ARG
1	H	51	VAL
1	H	52	LYS
1	H	88	LEU
1	H	106	VAL
1	H	128	GLU
1	H	131	SER
1	H	132	ASP
1	H	146	MET
1	H	149	LYS
1	H	160	SER
1	H	181	SER
1	H	190	LYS
1	H	218	SER
1	H	232	GLU

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Mol	Chain	Res	Type
1	H	242	ARG
1	H	243	GLU
1	H	280	MET
1	H	308	LYS
1	H	332	LYS
1	H	361	LEU
1	H	374	SER
1	H	375	LEU
1	H	376	GLU
1	H	379	GLU
1	H	381	VAL
1	H	394	SER
1	H	397	CYS
1	H	412	ARG
1	H	427	GLU
1	H	430	THR
1	H	461	GLU
1	H	464	GLN
1	H	471	ASP
1	H	475	GLN
1	H	496	ILE
1	I	4	LYS
1	I	5	CYS
1	I	38	ARG
1	I	52	LYS
1	I	88	LEU
1	I	106	VAL
1	I	128	GLU
1	I	131	SER
1	I	132	ASP
1	I	146	MET
1	I	149	LYS
1	I	160	SER
1	I	181	SER
1	I	190	LYS
1	I	218	SER
1	I	232	GLU
1	I	242	ARG
1	I	243	GLU
1	I	280	MET
1	I	282	ARG
1	I	308	LYS

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Mol	Chain	Res	Type
1	I	332	LYS
1	I	361	LEU
1	I	374	SER
1	I	375	LEU
1	I	376	GLU
1	I	379	GLU
1	I	381	VAL
1	I	394	SER
1	I	397	CYS
1	I	398	TYR
1	I	412	ARG
1	I	427	GLU
1	I	430	THR
1	I	461	GLU
1	I	464	GLN
1	I	471	ASP
1	I	475	GLN
1	I	495	LEU
1	I	500	THR
1	L	4	LYS
1	L	5	CYS
1	L	31	VAL
1	L	38	ARG
1	L	52	LYS
1	L	88	LEU
1	L	106	VAL
1	L	128	GLU
1	L	132	ASP
1	L	146	MET
1	L	149	LYS
1	L	160	SER
1	L	181	SER
1	L	190	LYS
1	L	218	SER
1	L	232	GLU
1	L	242	ARG
1	L	243	GLU
1	L	280	MET
1	L	282	ARG
1	L	308	LYS
1	L	332	LYS
1	L	361	LEU

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Mol	Chain	Res	Type
1	L	374	SER
1	L	375	LEU
1	L	376	GLU
1	L	379	GLU
1	L	381	VAL
1	L	394	SER
1	L	397	CYS
1	L	398	TYR
1	L	412	ARG
1	L	427	GLU
1	L	430	THR
1	L	461	GLU
1	L	464	GLN
1	L	471	ASP
1	L	475	GLN
1	L	494	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	HIS
1	A	117	ASN
1	A	252	HIS
1	A	382	HIS
1	A	392	GLN
1	B	90	HIS
1	B	117	ASN
1	B	252	HIS
1	B	392	GLN
1	C	90	HIS
1	C	117	ASN
1	C	170	ASN
1	C	382	HIS
1	C	392	GLN
1	D	90	HIS
1	D	117	ASN
1	D	170	ASN
1	D	382	HIS
1	D	392	GLN
1	E	90	HIS
1	E	117	ASN
1	E	252	HIS

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Mol	Chain	Res	Type
1	E	382	HIS
1	E	392	GLN
1	F	90	HIS
1	F	117	ASN
1	F	252	HIS
1	F	382	HIS
1	F	392	GLN
1	G	90	HIS
1	G	117	ASN
1	G	170	ASN
1	G	252	HIS
1	G	382	HIS
1	G	392	GLN
1	H	90	HIS
1	H	117	ASN
1	H	382	HIS
1	H	392	GLN
1	I	90	HIS
1	I	117	ASN
1	I	170	ASN
1	I	252	HIS
1	I	392	GLN
1	L	90	HIS
1	L	117	ASN
1	L	382	HIS
1	L	392	GLN

### 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

20 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	FAD	A	600	1	51,58,58	1.34	8 (15%)	54,89,89	2.02	8 (14%)
3	LDA	A	601	-	13,15,15	2.35	2 (15%)	14,17,17	1.17	1 (7%)
2	FAD	B	600	1	51,58,58	1.32	9 (17%)	54,89,89	1.91	7 (12%)
3	LDA	B	601	-	13,15,15	2.13	2 (15%)	14,17,17	1.00	0
2	FAD	C	600	1	51,58,58	1.35	7 (13%)	54,89,89	2.02	6 (11%)
3	LDA	C	601	-	13,15,15	2.16	2 (15%)	14,17,17	1.01	1 (7%)
2	FAD	D	600	1	51,58,58	1.39	7 (13%)	54,89,89	2.10	7 (12%)
3	LDA	D	601	-	13,15,15	2.05	1 (7%)	14,17,17	0.97	0
2	FAD	E	600	1	51,58,58	1.45	9 (17%)	54,89,89	2.03	9 (16%)
3	LDA	E	601	-	13,15,15	2.19	2 (15%)	14,17,17	1.36	1 (7%)
2	FAD	F	600	1	51,58,58	1.32	7 (13%)	54,89,89	2.01	8 (14%)
3	LDA	F	601	-	13,15,15	2.07	2 (15%)	14,17,17	1.07	1 (7%)
2	FAD	G	600	1	51,58,58	1.37	7 (13%)	54,89,89	1.94	8 (14%)
3	LDA	G	601	-	13,15,15	2.31	2 (15%)	14,17,17	1.28	1 (7%)
2	FAD	H	600	1	51,58,58	1.36	6 (11%)	54,89,89	1.90	7 (12%)
3	LDA	H	601	-	13,15,15	2.22	2 (15%)	14,17,17	1.12	1 (7%)
2	FAD	I	600	1	51,58,58	1.35	9 (17%)	54,89,89	1.86	6 (11%)
3	LDA	I	601	-	13,15,15	2.11	1 (7%)	14,17,17	1.18	1 (7%)
2	FAD	L	600	1	51,58,58	1.38	6 (11%)	54,89,89	2.00	7 (12%)
3	LDA	L	601	-	13,15,15	2.36	2 (15%)	14,17,17	1.42	1 (7%)

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	FAD	A	600	1	-	0/28/50/50	0/6/6/6
3	LDA	A	601	-	-	0/13/13/13	0/0/0/0
2	FAD	B	600	1	-	0/28/50/50	0/6/6/6
3	LDA	B	601	-	-	0/13/13/13	0/0/0/0
2	FAD	C	600	1	-	0/28/50/50	0/6/6/6
3	LDA	C	601	-	-	0/13/13/13	0/0/0/0
2	FAD	D	600	1	-	0/28/50/50	0/6/6/6
3	LDA	D	601	-	-	0/13/13/13	0/0/0/0
2	FAD	E	600	1	-	0/28/50/50	0/6/6/6
3	LDA	E	601	-	-	0/13/13/13	0/0/0/0
2	FAD	F	600	1	-	0/28/50/50	0/6/6/6
3	LDA	F	601	-	-	0/13/13/13	0/0/0/0
2	FAD	G	600	1	-	0/28/50/50	0/6/6/6
3	LDA	G	601	-	-	0/13/13/13	0/0/0/0
2	FAD	H	600	1	-	0/28/50/50	0/6/6/6
3	LDA	H	601	-	-	0/13/13/13	0/0/0/0
2	FAD	I	600	1	-	0/28/50/50	0/6/6/6
3	LDA	I	601	-	-	0/13/13/13	0/0/0/0
2	FAD	L	600	1	-	0/28/50/50	0/6/6/6
3	LDA	L	601	-	-	0/13/13/13	0/0/0/0

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	LDA	O1-N1	-8.14	1.26	1.42
3	G	601	LDA	O1-N1	-8.03	1.26	1.42
3	L	601	LDA	O1-N1	-7.86	1.26	1.42
3	H	601	LDA	O1-N1	-7.68	1.27	1.42
3	E	601	LDA	O1-N1	-7.55	1.27	1.42
3	C	601	LDA	O1-N1	-7.49	1.27	1.42
3	I	601	LDA	O1-N1	-7.42	1.27	1.42
3	B	601	LDA	O1-N1	-7.24	1.27	1.42
3	D	601	LDA	O1-N1	-7.16	1.28	1.42
3	F	601	LDA	O1-N1	-7.12	1.28	1.42
3	L	601	LDA	C1-N1	-3.22	1.44	1.51
2	G	600	FAD	C4-C4X	-2.86	1.35	1.41
3	B	601	LDA	C1-N1	-2.52	1.45	1.51
2	E	600	FAD	C6-C5X	-2.48	1.38	1.41
2	G	600	FAD	C6-C5X	-2.45	1.38	1.41
2	B	600	FAD	C4-C4X	-2.42	1.36	1.41
2	F	600	FAD	C6-C5X	-2.40	1.38	1.41
3	A	601	LDA	C1-N1	-2.35	1.46	1.51
2	I	600	FAD	C9A-C5X	-2.35	1.37	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	600	FAD	C4-C4X	-2.34	1.36	1.41
2	D	600	FAD	C6-C5X	-2.34	1.38	1.41
2	H	600	FAD	C9A-C5X	-2.32	1.37	1.42
3	E	601	LDA	C1-N1	-2.32	1.46	1.51
2	B	600	FAD	C6-C5X	-2.29	1.38	1.41
2	E	600	FAD	C9A-C5X	-2.26	1.37	1.42
2	C	600	FAD	C6-C5X	-2.25	1.38	1.41
2	C	600	FAD	C9A-C5X	-2.25	1.37	1.42
3	H	601	LDA	C1-N1	-2.23	1.46	1.51
2	E	600	FAD	C4-C4X	-2.22	1.37	1.41
2	D	600	FAD	O4B-C4B	-2.22	1.40	1.45
2	A	600	FAD	C4X-C10	-2.20	1.37	1.41
2	E	600	FAD	C2B-C1B	-2.19	1.50	1.53
2	F	600	FAD	C4-C4X	-2.16	1.37	1.41
2	A	600	FAD	C6-C5X	-2.16	1.38	1.41
3	F	601	LDA	C1-N1	-2.16	1.46	1.51
3	G	601	LDA	C1-N1	-2.11	1.46	1.51
2	B	600	FAD	C9A-C5X	-2.04	1.38	1.42
2	A	600	FAD	C4-C4X	-2.04	1.37	1.41
2	I	600	FAD	C4X-C10	-2.04	1.37	1.41
2	B	600	FAD	O4B-C4B	-2.04	1.40	1.45
3	C	601	LDA	C1-N1	-2.02	1.46	1.51
2	I	600	FAD	C6-C5X	-2.01	1.38	1.41
2	L	600	FAD	C1'-N10	2.03	1.50	1.48
2	E	600	FAD	C4X-N5	2.11	1.36	1.33
2	H	600	FAD	C2A-N1A	2.36	1.38	1.33
2	F	600	FAD	C2A-N1A	2.39	1.38	1.33
2	L	600	FAD	C2A-N1A	2.44	1.38	1.33
2	I	600	FAD	C4-N3	2.45	1.37	1.33
2	A	600	FAD	C2A-N1A	2.52	1.38	1.33
2	E	600	FAD	C2A-N1A	2.53	1.38	1.33
2	C	600	FAD	C2A-N1A	2.54	1.38	1.33
2	A	600	FAD	C4X-N5	2.59	1.37	1.33
2	C	600	FAD	C4X-N5	2.59	1.37	1.33
2	I	600	FAD	C4X-N5	2.59	1.37	1.33
2	B	600	FAD	C2A-N1A	2.60	1.38	1.33
2	B	600	FAD	C4-N3	2.60	1.37	1.33
2	G	600	FAD	C4X-N5	2.66	1.37	1.33
2	B	600	FAD	C10-N1	2.69	1.37	1.33
2	D	600	FAD	C4X-N5	2.72	1.37	1.33
2	A	600	FAD	C4-N3	2.73	1.38	1.33
2	A	600	FAD	C10-N1	2.76	1.37	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	600	FAD	C4X-N5	2.79	1.37	1.33
2	G	600	FAD	C10-N1	2.80	1.37	1.33
2	G	600	FAD	C2A-N1A	2.80	1.39	1.33
2	H	600	FAD	C4X-N5	2.82	1.37	1.33
2	G	600	FAD	C4-N3	2.83	1.38	1.33
2	B	600	FAD	C2A-N3A	2.92	1.37	1.32
2	I	600	FAD	C2A-N1A	2.92	1.39	1.33
2	L	600	FAD	C4X-N5	2.99	1.37	1.33
2	H	600	FAD	C4-N3	3.00	1.38	1.33
2	B	600	FAD	C4X-N5	3.02	1.37	1.33
2	D	600	FAD	C4-N3	3.11	1.38	1.33
2	D	600	FAD	C2A-N1A	3.19	1.39	1.33
2	F	600	FAD	C4-N3	3.21	1.38	1.33
2	I	600	FAD	C10-N1	3.22	1.37	1.33
2	C	600	FAD	C4-N3	3.23	1.38	1.33
2	E	600	FAD	C10-N1	3.27	1.37	1.33
2	F	600	FAD	C10-N1	3.29	1.37	1.33
2	E	600	FAD	C4-N3	3.32	1.39	1.33
2	D	600	FAD	C10-N1	3.43	1.38	1.33
2	G	600	FAD	C2A-N3A	3.54	1.38	1.32
2	L	600	FAD	C4-N3	3.56	1.39	1.33
2	C	600	FAD	C2A-N3A	3.60	1.38	1.32
2	H	600	FAD	C2A-N3A	3.72	1.38	1.32
2	F	600	FAD	C2A-N3A	3.79	1.38	1.32
2	C	600	FAD	C10-N1	3.94	1.38	1.33
2	I	600	FAD	C2A-N3A	3.95	1.38	1.32
2	A	600	FAD	C2A-N3A	4.01	1.38	1.32
2	L	600	FAD	C10-N1	4.08	1.39	1.33
2	H	600	FAD	C10-N1	4.08	1.39	1.33
2	D	600	FAD	C2A-N3A	4.43	1.39	1.32
2	L	600	FAD	C2A-N3A	4.59	1.39	1.32
2	E	600	FAD	C2A-N3A	4.81	1.40	1.32

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	FAD	N3A-C2A-N1A	-9.93	120.21	128.86
2	A	600	FAD	N3A-C2A-N1A	-9.61	120.48	128.86
2	L	600	FAD	N3A-C2A-N1A	-9.50	120.58	128.86
2	B	600	FAD	N3A-C2A-N1A	-8.97	121.05	128.86
2	C	600	FAD	N3A-C2A-N1A	-8.70	121.28	128.86
2	G	600	FAD	N3A-C2A-N1A	-8.53	121.43	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	600	FAD	N3A-C2A-N1A	-8.50	121.46	128.86
2	E	600	FAD	N3A-C2A-N1A	-8.29	121.64	128.86
2	H	600	FAD	N3A-C2A-N1A	-7.77	122.09	128.86
2	I	600	FAD	N3A-C2A-N1A	-7.73	122.12	128.86
2	F	600	FAD	C1'-N10-C10	-4.18	114.21	118.50
3	L	601	LDA	CM2-N1-CM1	-3.84	103.64	110.99
2	E	600	FAD	C4X-C4-N3	-3.81	118.06	123.48
3	E	601	LDA	CM2-N1-CM1	-3.72	103.88	110.99
2	C	600	FAD	C4X-C4-N3	-3.54	118.44	123.48
2	H	600	FAD	C4X-C4-N3	-3.51	118.48	123.48
3	G	601	LDA	CM2-N1-CM1	-3.50	104.28	110.99
2	B	600	FAD	C1'-N10-C10	-3.43	114.98	118.50
2	G	600	FAD	C4X-C4-N3	-3.34	118.73	123.48
2	A	600	FAD	C4X-C4-N3	-3.30	118.79	123.48
3	I	601	LDA	CM2-N1-CM1	-3.21	104.85	110.99
2	F	600	FAD	C4X-C4-N3	-3.20	118.92	123.48
2	B	600	FAD	C4X-C4-N3	-3.18	118.96	123.48
2	E	600	FAD	C1'-N10-C10	-3.09	115.33	118.50
2	I	600	FAD	C4X-C4-N3	-3.08	119.10	123.48
2	D	600	FAD	C8M-C8-C9	-3.07	112.63	120.34
2	L	600	FAD	C8M-C8-C9	-3.03	112.75	120.34
2	D	600	FAD	C4X-C4-N3	-2.98	119.25	123.48
2	L	600	FAD	C4X-C4-N3	-2.98	119.25	123.48
2	L	600	FAD	C1'-N10-C10	-2.92	115.50	118.50
2	I	600	FAD	C1'-N10-C10	-2.85	115.58	118.50
2	F	600	FAD	C8M-C8-C9	-2.71	113.54	120.34
3	A	601	LDA	CM2-N1-CM1	-2.62	105.98	110.99
2	C	600	FAD	C8M-C8-C9	-2.52	114.01	120.34
3	H	601	LDA	CM2-N1-CM1	-2.52	106.17	110.99
2	H	600	FAD	C8M-C8-C9	-2.51	114.06	120.34
2	E	600	FAD	C8M-C8-C9	-2.46	114.17	120.34
2	A	600	FAD	C8M-C8-C9	-2.40	114.32	120.34
2	G	600	FAD	C8M-C8-C9	-2.36	114.43	120.34
2	A	600	FAD	C1'-N10-C10	-2.32	116.12	118.50
2	G	600	FAD	O3B-C3B-C2B	-2.28	104.51	111.83
2	A	600	FAD	O2'-C2'-C1'	-2.25	104.58	109.79
3	C	601	LDA	CM2-N1-CM1	-2.24	106.71	110.99
2	B	600	FAD	C8M-C8-C9	-2.12	115.03	120.34
3	F	601	LDA	CM2-N1-CM1	-2.12	106.94	110.99
2	G	600	FAD	C1'-N10-C10	-2.08	116.37	118.50
2	H	600	FAD	C1'-N10-C10	-2.03	116.42	118.50
2	E	600	FAD	C4B-O4B-C1B	2.10	112.00	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	FAD	C4X-N5-C5X	2.13	119.01	116.76
2	H	600	FAD	C4X-N5-C5X	2.16	119.04	116.76
2	D	600	FAD	C2B-C3B-C4B	2.22	106.95	102.62
2	G	600	FAD	C4X-N5-C5X	2.26	119.15	116.76
2	E	600	FAD	C4X-N5-C5X	2.28	119.17	116.76
2	E	600	FAD	C1'-N10-C9A	2.38	120.52	118.35
2	F	600	FAD	C1'-N10-C9A	2.45	120.59	118.35
2	C	600	FAD	C4X-N5-C5X	2.61	119.52	116.76
2	B	600	FAD	C4X-N5-C5X	2.63	119.54	116.76
2	L	600	FAD	C4X-N5-C5X	2.67	119.58	116.76
2	F	600	FAD	C4X-N5-C5X	2.71	119.63	116.76
2	F	600	FAD	C5X-C9A-N10	2.76	119.70	117.66
2	I	600	FAD	C4X-N5-C5X	2.81	119.73	116.76
2	A	600	FAD	C4X-N5-C5X	3.12	120.05	116.76
2	B	600	FAD	C5X-C9A-N10	3.20	120.03	117.66
2	C	600	FAD	C5X-C9A-N10	3.38	120.17	117.66
2	A	600	FAD	C5X-C9A-N10	3.44	120.21	117.66
2	L	600	FAD	C5X-C9A-N10	3.55	120.29	117.66
2	E	600	FAD	C5X-C9A-N10	3.55	120.30	117.66
2	I	600	FAD	C5X-C9A-N10	3.79	120.47	117.66
2	G	600	FAD	C5X-C9A-N10	4.17	120.75	117.66
2	D	600	FAD	C5X-C9A-N10	4.21	120.78	117.66
2	H	600	FAD	C5X-C9A-N10	4.36	120.90	117.66
2	B	600	FAD	C4-N3-C2	6.53	120.87	115.16
2	L	600	FAD	C4-N3-C2	6.88	121.17	115.16
2	I	600	FAD	C4-N3-C2	6.91	121.20	115.16
2	A	600	FAD	C4-N3-C2	7.19	121.44	115.16
2	D	600	FAD	C4-N3-C2	7.19	121.45	115.16
2	G	600	FAD	C4-N3-C2	7.28	121.53	115.16
2	H	600	FAD	C4-N3-C2	7.58	121.78	115.16
2	F	600	FAD	C4-N3-C2	7.69	121.89	115.16
2	C	600	FAD	C4-N3-C2	8.08	122.23	115.16
2	E	600	FAD	C4-N3-C2	8.47	122.57	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	LDA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	LDA	3	0
3	C	601	LDA	2	0
3	D	601	LDA	3	0
3	E	601	LDA	3	0
3	F	601	LDA	2	0
3	G	601	LDA	3	0
3	H	601	LDA	3	0
3	I	601	LDA	3	0
3	L	601	LDA	3	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	497/520 (95%)	-0.00	1 (0%) 94 89	26, 37, 56, 96	0
1	B	494/520 (95%)	0.01	1 (0%) 94 89	26, 37, 54, 78	0
1	C	498/520 (95%)	-0.07	2 (0%) 92 84	26, 37, 56, 99	0
1	D	494/520 (95%)	-0.06	1 (0%) 94 89	26, 37, 55, 80	0
1	E	498/520 (95%)	-0.01	2 (0%) 92 84	26, 37, 56, 100	0
1	F	497/520 (95%)	0.00	2 (0%) 92 84	26, 37, 56, 98	0
1	G	494/520 (95%)	-0.06	0 100 100	26, 37, 55, 83	0
1	H	498/520 (95%)	-0.03	2 (0%) 92 84	26, 37, 57, 100	0
1	I	497/520 (95%)	-0.01	1 (0%) 94 89	26, 37, 56, 100	0
1	L	497/520 (95%)	0.14	11 (2%) 62 41	27, 37, 56, 100	0
All	All	4964/5200 (95%)	-0.01	23 (0%) 90 80	26, 37, 56, 100	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	196	THR	3.2
1	L	476	PRO	3.1
1	F	395	GLY	3.0
1	L	399	THR	2.7
1	I	227	ASP	2.4
1	L	198	ILE	2.4
1	H	290	PRO	2.4
1	B	227	ASP	2.3
1	A	107	TRP	2.3
1	L	500	THR	2.3
1	E	12	GLY	2.2
1	E	243	GLU	2.2
1	H	74	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	101	GLY	2.2
1	C	242	ARG	2.2
1	L	200	SER	2.1
1	L	470	VAL	2.1
1	C	388	TRP	2.0
1	L	14	ILE	2.0
1	L	228	ARG	2.0
1	F	400	THR	2.0
1	L	93	LYS	2.0
1	D	49	GLN	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
3	LDA	C	601	16/16	0.91	0.57	7.46	31,33,38,39	0
3	LDA	G	601	16/16	0.92	0.60	5.89	31,34,38,39	0
3	LDA	I	601	16/16	0.90	0.65	5.78	31,34,38,39	0
3	LDA	E	601	16/16	0.95	0.43	5.68	31,33,38,39	0
3	LDA	F	601	16/16	0.92	0.53	4.26	31,34,38,40	0
3	LDA	D	601	16/16	0.90	0.42	3.82	31,33,38,39	0
3	LDA	H	601	16/16	0.92	0.51	3.46	31,34,39,39	0
3	LDA	L	601	16/16	0.92	0.59	3.22	31,34,39,39	0
3	LDA	A	601	16/16	0.94	0.47	3.20	31,33,38,39	0
3	LDA	B	601	16/16	0.94	0.39	2.35	31,33,38,39	0
2	FAD	G	600	53/53	0.95	0.25	-0.05	26,37,47,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FAD	B	600	53/53	0.96	0.25	-0.06	26,37,46,49	0
2	FAD	H	600	53/53	0.96	0.25	-0.07	25,36,47,49	0
2	FAD	E	600	53/53	0.95	0.23	-0.34	26,37,47,49	0
2	FAD	C	600	53/53	0.95	0.22	-0.38	26,37,47,49	0
2	FAD	I	600	53/53	0.96	0.21	-0.39	26,36,46,49	0
2	FAD	L	600	53/53	0.93	0.22	-0.55	26,37,47,49	0
2	FAD	D	600	53/53	0.94	0.21	-0.61	26,37,46,49	0
2	FAD	A	600	53/53	0.95	0.20	-0.69	26,36,46,49	0
2	FAD	F	600	53/53	0.94	0.23	-0.70	26,37,47,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.