



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2018 – 01:59 PM EDT

PDB ID : 6D6C  
Title : The structure of ligand binding domain of LasR in complex with TP-1 homolog, compound 12  
Authors : Dong, S.H.; Nair, S.K.  
Deposited on : 2018-04-20  
Resolution : 1.88 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

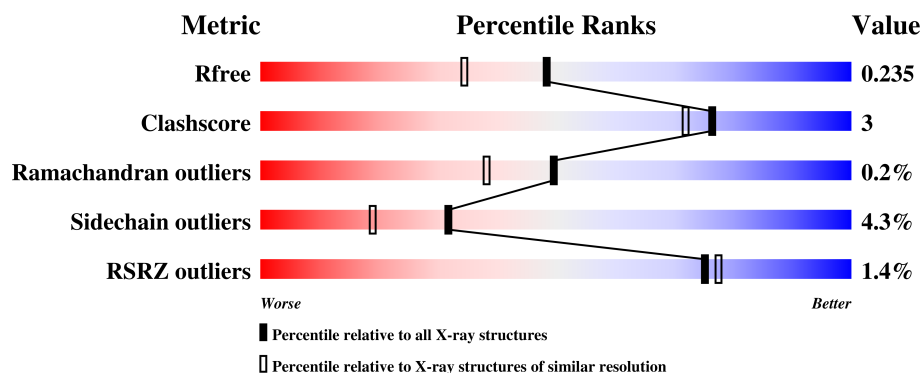
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.88 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))
$R_{free}$	111664	8255 (1.90-1.86)
Clashscore	122126	9028 (1.90-1.86)
Ramachandran outliers	120053	8930 (1.90-1.86)
Sidechain outliers	120020	8930 (1.90-1.86)
RSRZ outliers	108989	8087 (1.90-1.86)

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	170	<div> <div>88%</div> <div>7% ...</div> </div>
1	B	170	<div> <div>%</div> <div>91%</div> <div>6% ..</div> </div>
1	C	170	<div> <div>%</div> <div>89%</div> <div>5% ...</div> </div>
1	D	170	<div> <div>%</div> <div>91%</div> <div>6% .</div> </div>
1	E	170	<div> <div>2%</div> <div>85%</div> <div>12% ...</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	170	<div><div></div><div>%</div><div>91%</div><div>6% ..</div></div>
1	G	170	<div><div></div><div>2%</div><div>86%</div><div>8% • 5%</div></div>
1	H	170	<div><div></div><div>3%</div><div>78%</div><div>13% • 7%</div></div>
1	I	170	<div><div></div><div>2%</div><div>86%</div><div>9% • 5%</div></div>
1	J	170	<div><div></div><div>2%</div><div>82%</div><div>12% • 5%</div></div>
1	K	170	<div><div></div><div>3%</div><div>80%</div><div>13% • • •</div></div>
1	L	170	<div><div></div><div>%</div><div>88%</div><div>7% .. •</div></div>

## 2 Entry composition

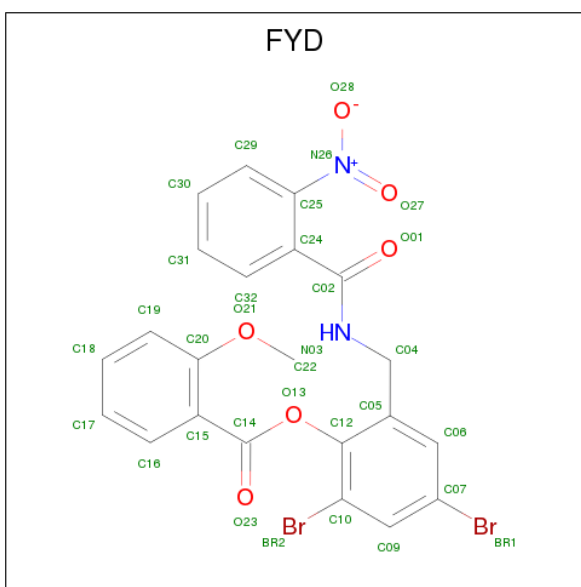
There are 4 unique types of molecules in this entry. The entry contains 17385 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transcriptional activator protein LasR.

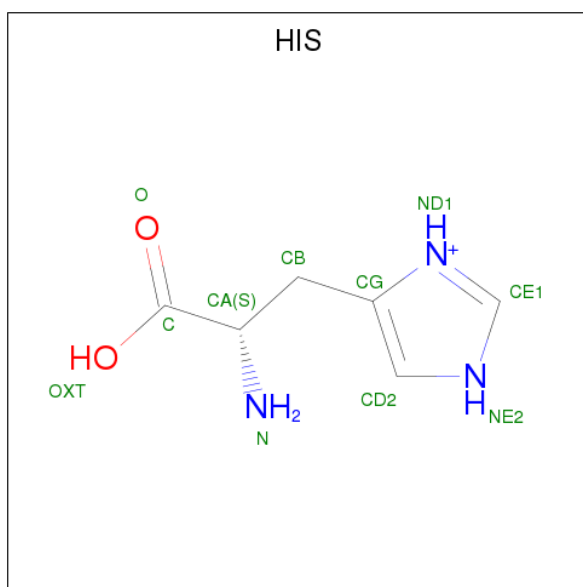
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	3	0
			1310	842	217	246	5			
1	B	166	Total	C	N	O	S	0	0	0
			1306	839	218	244	5			
1	C	164	Total	C	N	O	S	0	3	0
			1297	832	218	242	5			
1	D	166	Total	C	N	O	S	0	1	0
			1309	841	218	245	5			
1	E	165	Total	C	N	O	S	0	2	0
			1307	840	217	245	5			
1	F	167	Total	C	N	O	S	0	0	0
			1316	845	220	246	5			
1	G	162	Total	C	N	O	S	0	1	0
			1286	826	214	241	5			
1	H	158	Total	C	N	O	S	0	1	0
			1247	805	208	228	6			
1	I	162	Total	C	N	O	S	0	3	0
			1292	830	214	243	5			
1	J	162	Total	C	N	O	S	0	1	0
			1281	823	214	239	5			
1	K	164	Total	C	N	O	S	0	1	0
			1293	830	216	242	5			
1	L	164	Total	C	N	O	S	0	1	0
			1298	832	216	245	5			

- Molecule 2 is 2,4-dibromo-6-[[[(2-nitrobenzene-1-carbonyl)amino]methyl}phenyl 2-methoxybenzoate (three-letter code: FYD) (formula: C<sub>22</sub>H<sub>16</sub>Br<sub>2</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	B	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	C	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	D	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	E	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	F	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	G	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	H	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	I	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	J	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	K	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		
2	L	1	Total	Br	C	N	O	0	1
			64	4	44	4	12		

- Molecule 3 is HISTIDINE (three-letter code: HIS) (formula: C<sub>6</sub>H<sub>10</sub>N<sub>3</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	H	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	102	Total	O	0	0
			102	102		
4	B	77	Total	O	0	0
			77	77		
4	C	95	Total	O	0	0
			95	95		
4	D	117	Total	O	0	0
			117	117		
4	E	98	Total	O	0	0
			98	98		
4	F	65	Total	O	0	0
			65	65		
4	G	84	Total	O	0	0
			84	84		
4	H	58	Total	O	0	0
			58	58		
4	I	104	Total	O	0	0
			104	104		
4	J	67	Total	O	0	0
			67	67		
4	K	68	Total	O	0	0
			68	68		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	130	Total 130	O 130	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 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.

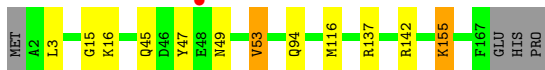
- Molecule 1: Transcriptional activator protein LasR

Chain A:  88% 7% ...




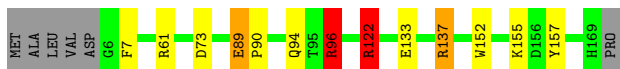
- Molecule 1: Transcriptional activator protein LasR

Chain B:  91% 6% ..

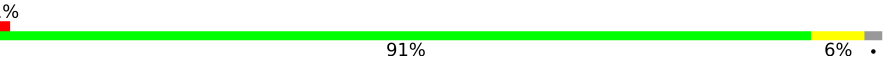


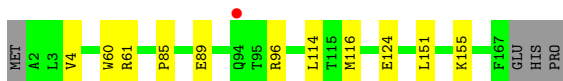
- Molecule 1: Transcriptional activator protein LasR

Chain C:  89% 5% ..




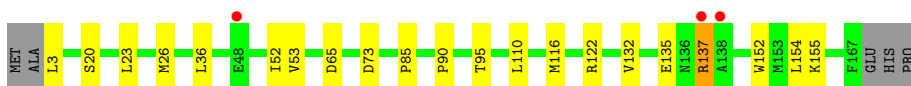
- Molecule 1: Transcriptional activator protein LasR

Chain D:  91% 6% ..

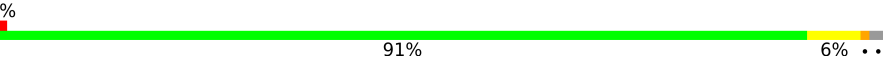


- Molecule 1: Transcriptional activator protein LasR

Chain E:  85% 12% ..



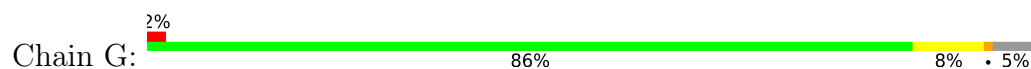
- Molecule 1: Transcriptional activator protein LasR

Chain F:  91% 6% ..

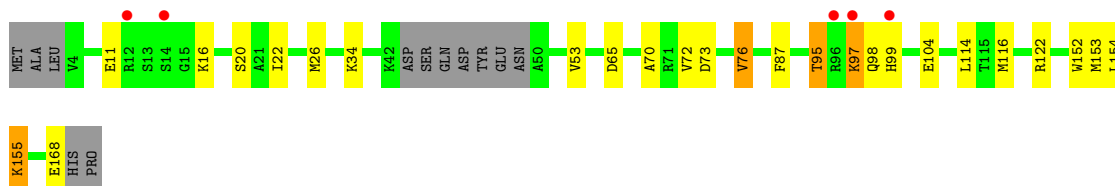
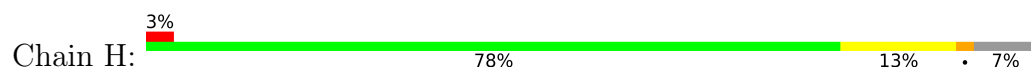




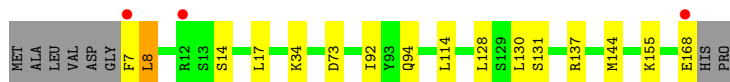
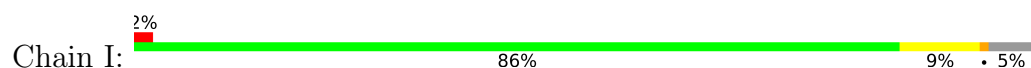
- Molecule 1: Transcriptional activator protein LasR



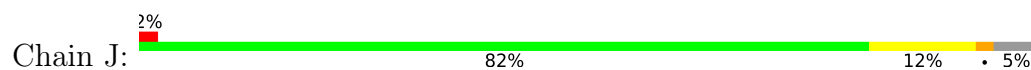
- Molecule 1: Transcriptional activator protein LasR



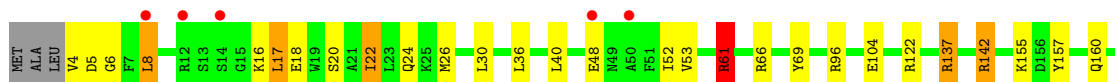
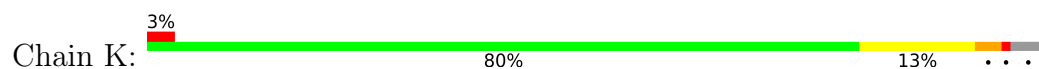
- Molecule 1: Transcriptional activator protein LasR



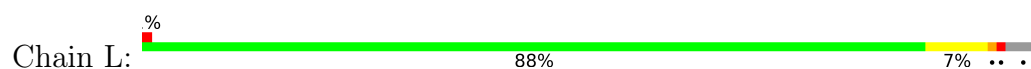
- Molecule 1: Transcriptional activator protein LasR



- Molecule 1: Transcriptional activator protein LasR



- Molecule 1: Transcriptional activator protein LasR





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.41Å 85.34Å 232.47Å 90.00° 96.57° 90.00°	Depositor
Resolution (Å)	230.94 – 1.88 37.71 – 1.88	Depositor EDS
% Data completeness (in resolution range)	87.5 (230.94-1.88) 87.6 (37.71-1.88)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.74 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, $R_{free}$	0.185 , 0.232 0.193 , 0.235	Depositor DCC
$R_{free}$ test set	7401 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.4	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	17385	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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 42.11 % 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 2.1405e-04. 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, 0.333 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: FYD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.04	1/1353 (0.1%)	1.02	7/1833 (0.4%)
1	B	0.88	0/1340	0.92	0/1816
1	C	0.98	0/1332	1.03	8/1804 (0.4%)
1	D	1.07	2/1346 (0.1%)	0.97	2/1824 (0.1%)
1	E	0.98	0/1347	0.93	6/1825 (0.3%)
1	F	0.90	0/1351	0.97	6/1831 (0.3%)
1	G	0.96	1/1323 (0.1%)	1.02	6/1792 (0.3%)
1	H	0.87	0/1282	0.93	2/1735 (0.1%)
1	I	0.94	0/1335	1.09	6/1808 (0.3%)
1	J	0.92	0/1318	0.94	4/1785 (0.2%)
1	K	0.90	0/1327	0.97	6/1798 (0.3%)
1	L	1.04	2/1335 (0.1%)	1.03	6/1808 (0.3%)
All	All	0.96	6/15989 (0.0%)	0.99	59/21659 (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	I	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	124	GLU	CD-OE1	6.15	1.32	1.25
1	G	89	GLU	CD-OE1	-5.92	1.19	1.25
1	L	61	ARG	CZ-NH1	5.22	1.39	1.33
1	D	60	TRP	CZ3-CH2	5.08	1.48	1.40
1	L	104	GLU	CD-OE1	5.02	1.31	1.25
1	A	56	TYR	CE1-CZ	5.00	1.45	1.38

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	137	ARG	NE-CZ-NH1	-18.10	111.25	120.30
1	I	137	ARG	NE-CZ-NH2	12.77	126.68	120.30
1	G	137	ARG	NE-CZ-NH1	-11.95	114.33	120.30
1	C	122	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	G	137	ARG	NE-CZ-NH2	10.01	125.30	120.30
1	L	61	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	C	122	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	L	61	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	F	96	ARG	CG-CD-NE	-8.13	94.73	111.80
1	C	61	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	G	73	ASP	CB-CG-OD1	7.11	124.70	118.30
1	E	73	ASP	CB-CG-OD1	6.86	124.47	118.30
1	A	142	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	H	73	ASP	CB-CG-OD1	6.75	124.38	118.30
1	D	96	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	K	137	ARG	NE-CZ-NH1	6.55	123.58	120.30
1	G	73	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	G	61	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	F	96	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	F	61	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	I	73	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	E	73	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	F	142	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	151	LEU	CB-CG-CD2	6.13	121.43	111.00
1	D	61	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	I	144	MET	CG-SD-CE	6.07	109.92	100.20
1	F	65	ASP	CB-CG-OD1	6.07	123.76	118.30
1	J	137	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	A	66	ARG	NE-CZ-NH2	5.97	123.28	120.30
1	G	61	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	L	156	ASP	CB-CG-OD1	5.80	123.52	118.30
1	F	61	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	61	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	E	122	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	L	5	ASP	CB-CG-OD1	5.75	123.48	118.30
1	C	122	ARG	CD-NE-CZ	5.67	131.54	123.60
1	K	142	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	65	ASP	CB-CG-OD1	5.63	123.37	118.30
1	J	151	LEU	CA-CB-CG	5.62	128.23	115.30
1	C	61	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	65	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	C	122	ARG	CG-CD-NE	5.44	123.23	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	MET	CG-SD-CE	5.35	108.75	100.20
1	A	73	ASP	CB-CG-OD1	5.34	123.11	118.30
1	L	5	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	H	122	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	E	137	ARG	CG-CD-NE	5.22	122.77	111.80
1	C	73	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	E	122	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	L	96	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	J	71	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	I	73	ASP	CB-CG-OD1	5.12	122.91	118.30
1	K	122	ARG	NE-CZ-NH1	5.11	122.85	120.30
1	I	137	ARG	CD-NE-CZ	5.09	130.73	123.60
1	K	61	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	C	96	ARG	CB-CG-CD	5.04	124.72	111.60
1	K	122	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	J	142	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	K	8	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	8	LEU	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	1310	0	1274	8	0
1	B	1306	0	1264	4	0
1	C	1297	0	1248	7	0
1	D	1309	0	1269	8	0
1	E	1307	0	1269	9	0
1	F	1316	0	1266	3	0
1	G	1286	0	1243	6	0
1	H	1247	0	1220	16	0
1	I	1292	0	1253	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1281	0	1240	11	0
1	K	1293	0	1248	21	0
1	L	1298	0	1250	8	0
2	A	64	0	0	1	0
2	B	64	0	0	0	0
2	C	64	0	0	0	0
2	D	64	0	0	0	0
2	E	64	0	0	1	0
2	F	64	0	0	0	0
2	G	64	0	0	1	0
2	H	64	0	0	1	0
2	I	64	0	0	1	0
2	J	64	0	0	0	0
2	K	64	0	0	0	0
2	L	64	0	0	1	0
3	H	10	0	6	1	0
4	A	102	0	0	0	0
4	B	77	0	0	1	0
4	C	95	0	0	1	0
4	D	117	0	0	4	0
4	E	98	0	0	2	0
4	F	65	0	0	2	0
4	G	84	0	0	2	0
4	H	58	0	0	1	0
4	I	104	0	0	1	0
4	J	67	0	0	0	0
4	K	68	0	0	10	1
4	L	130	0	0	3	1
All	All	17385	0	15050	104	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 (104) 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:K:24:GLN:NE2	4:K:301:HOH:O	1.82	1.13
1:K:66:ARG:HD2	4:K:351:HOH:O	1.66	0.93
1:K:36:LEU:HD21	1:K:52:ILE:HG23	1.58	0.84
1:F:84:LEU:HD11	4:K:348:HOH:O	1.83	0.79
1:L:96:ARG:NH2	4:L:301:HOH:O	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:4:VAL:HG11	4:K:366:HOH:O	1.82	0.79
1:C:7:PHE:HB2	1:C:157:TYR:CD1	2.28	0.68
1:H:168:GLU:O	3:H:201:HIS:N	2.25	0.68
1:D:116:MET:HG3	1:D:151:LEU:HD21	1.75	0.67
1:E:20:SER:HB2	1:E:53:VAL:HG13	1.76	0.67
1:E:137:ARG:NE	4:E:302:HOH:O	2.27	0.66
1:K:4:VAL:HG21	4:K:366:HOH:O	1.95	0.65
1:F:151:LEU:HB3	4:F:361:HOH:O	1.95	0.64
1:E:36:LEU:HD21	1:E:52:ILE:HG23	1.78	0.63
1:C:133:GLU:O	1:K:96:ARG:NH1	2.33	0.61
1:J:34:LYS:HB2	1:J:131[B]:SER:OG	2.02	0.60
1:J:132:VAL:HG11	1:J:143:PHE:CD2	2.37	0.60
1:L:108:ALA:O	4:L:302:HOH:O	2.17	0.58
1:K:157:TYR:HA	4:K:348:HOH:O	2.03	0.58
1:D:85:PRO:HB3	1:D:116:MET:SD	2.44	0.57
1:B:94:GLN:NE2	4:B:301:HOH:O	2.36	0.57
1:D:151:LEU:O	1:D:151:LEU:HD23	2.06	0.56
1:G:30:LEU:HD11	1:G:150:THR:HG21	1.88	0.56
1:K:61:ARG:NH2	4:K:302:HOH:O	2.16	0.55
1:H:70:ALA:O	1:H:76:VAL:HG21	2.06	0.55
1:E:137:ARG:NH2	4:E:304:HOH:O	2.38	0.55
1:I:92:ILE:O	4:I:301:HOH:O	2.19	0.54
1:E:85:PRO:HB3	1:E:116:MET:SD	2.49	0.52
1:H:26:MET:HE2	1:H:154:LEU:HD13	1.90	0.52
1:K:24:GLN:CD	4:K:301:HOH:O	2.31	0.52
1:B:45:GLN:NE2	1:B:47:TYR:OH	2.43	0.52
1:J:132:VAL:HG11	1:J:143:PHE:CE2	2.44	0.52
1:L:168:GLU:O	4:L:303:HOH:O	2.19	0.51
1:L:139:GLU:HG2	1:L:143:PHE:CE2	2.46	0.51
1:A:4:VAL:O	1:A:8:LEU:HD22	2.11	0.51
1:G:111:VAL:HG13	1:G:112:TYR:CD1	2.46	0.51
1:A:96:ARG:HG2	1:G:103:GLU:CD	2.32	0.50
1:J:116:MET:HG2	1:J:155:LYS:HG2	1.92	0.50
1:A:116:MET:HG2	1:A:155:LYS:HG2	1.92	0.50
1:H:20:SER:HB2	1:H:53:VAL:HG13	1.93	0.50
1:C:96:ARG:HB3	1:C:96:ARG:NH1	2.27	0.50
1:H:34:LYS:NZ	4:H:306:HOH:O	2.44	0.49
1:K:6:GLY:HA3	1:K:26:MET:CE	2.42	0.49
1:I:34:LYS:HB2	1:I:131[B]:SER:OG	2.13	0.49
1:C:89:GLU:HG3	1:C:90:PRO:HD2	1.93	0.49
1:G:119:HIS:HD2	4:G:359:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:MET:HG2	1:C:152:TRP:CD2	2.48	0.49
1:H:95:THR:HG22	1:H:98:GLN:CG	2.43	0.48
1:H:95:THR:HG21	1:H:97:LYS:NZ	2.28	0.48
1:K:16:LYS:NZ	4:K:307:HOH:O	2.45	0.48
1:D:89:GLU:HG2	4:D:381:HOH:O	2.14	0.47
1:A:116:MET:HG2	1:A:155:LYS:CG	2.44	0.47
1:F:116:MET:CG	4:F:361:HOH:O	2.63	0.47
1:D:4:VAL:HG23	4:D:367:HOH:O	2.14	0.46
1:B:116:MET:HE2	1:B:155:LYS:HG2	1.98	0.46
2:L:201[B]:FYD:BR2	2:L:201[B]:FYD:C14	3.18	0.46
2:A:201[B]:FYD:BR2	2:A:201[B]:FYD:C14	3.19	0.46
1:B:16:LYS:HE3	1:B:53:VAL:HG12	1.97	0.46
1:A:116:MET:HE3	1:A:151:LEU:HD22	1.99	0.45
1:H:153:MET:CE	1:J:148:LEU:HG	2.45	0.45
1:K:20:SER:HB2	1:K:53:VAL:HG13	1.97	0.45
1:H:72:VAL:HG22	1:H:97:LYS:HE3	1.98	0.45
1:H:22:ILE:O	1:H:26:MET:HG3	2.17	0.45
4:D:309:HOH:O	1:L:119:HIS:CE1	2.69	0.45
1:H:116[B]:MET:HG2	1:H:155:LYS:HG3	1.98	0.45
1:D:151:LEU:C	1:D:151:LEU:HD23	2.37	0.44
2:H:202[B]:FYD:C14	2:H:202[B]:FYD:BR2	3.21	0.44
4:D:309:HOH:O	1:L:119:HIS:HE1	2.00	0.44
1:K:18:GLU:O	1:K:22:ILE:HG23	2.18	0.44
1:A:151:LEU:O	1:A:151:LEU:HD23	2.18	0.44
1:K:17:LEU:HD12	1:K:17:LEU:H	1.82	0.44
1:J:32:PHE:CD1	1:J:132:VAL:HG13	2.53	0.43
1:K:160:GLN:HB3	4:K:348:HOH:O	2.16	0.43
1:G:10:LEU:HD22	1:G:19:TRP:CE2	2.53	0.43
1:H:20:SER:CB	1:H:53:VAL:HG13	2.48	0.43
1:J:116:MET:HG2	1:J:155:LYS:CG	2.49	0.43
1:K:36:LEU:CD2	1:K:52:ILE:HG23	2.39	0.43
1:J:16:LYS:HA	1:J:165:LEU:HD21	2.00	0.43
1:D:116:MET:HG3	1:D:151:LEU:CD2	2.48	0.42
1:A:34:LYS:HB2	1:A:131[A]:SER:OG	2.19	0.42
1:J:128:LEU:HG	1:J:130:LEU:HD11	2.01	0.42
1:K:30:LEU:HA	1:K:30:LEU:HD12	1.92	0.42
1:K:16:LYS:HE3	1:K:53:VAL:HG23	2.01	0.42
2:G:201[B]:FYD:C14	2:G:201[B]:FYD:BR2	3.23	0.42
1:E:23:LEU:HA	1:E:26:MET:HE2	2.00	0.42
1:K:4:VAL:O	1:K:8:LEU:HD13	2.20	0.42
1:G:111:VAL:HG13	1:G:112:TYR:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:94:GLN:HE21	1:L:94:GLN:HB3	1.66	0.42
1:H:11:GLU:HA	1:H:11:GLU:OE2	2.20	0.41
1:H:95:THR:HG22	1:H:98:GLN:HB2	2.01	0.41
1:E:95:THR:HA	1:L:146:SER:OG	2.20	0.41
2:I:201[B]:FYD:BR2	2:I:201[B]:FYD:C14	3.23	0.41
1:J:118:LEU:HB3	1:J:159:LEU:HD13	2.03	0.41
1:K:4:VAL:HG22	1:K:5:ASP:H	1.85	0.41
1:E:110:LEU:HD13	2:E:201[A]:FYD:O27	2.21	0.41
1:E:154:LEU:HD23	1:E:154:LEU:C	2.41	0.41
1:H:114:LEU:HD12	1:H:114:LEU:C	2.41	0.41
1:I:128:LEU:HG	1:I:130:LEU:HD11	2.03	0.41
4:G:307:HOH:O	1:J:139:GLU:HG3	2.21	0.41
1:H:87:PHE:CE2	1:H:114:LEU:HD23	2.56	0.41
1:C:137:ARG:HD2	4:C:364:HOH:O	2.21	0.40
1:D:114:LEU:HD21	1:D:151:LEU:HD11	2.03	0.40
1:K:69:TYR:OH	1:K:104:GLU:OE1	2.29	0.40
1:C:122:ARG:HA	1:C:122:ARG:HD3	1.84	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:K:363:HOH:O	4:L:407:HOH:O[1_465]	2.16	0.04

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	166/170 (98%)	165 (99%)	1 (1%)	0	100	100
1	B	164/170 (96%)	161 (98%)	2 (1%)	1 (1%)	27	15
1	C	162/170 (95%)	160 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	165/170 (97%)	165 (100%)	0	0	100	100
1	E	165/170 (97%)	161 (98%)	4 (2%)	0	100	100
1	F	165/170 (97%)	162 (98%)	3 (2%)	0	100	100
1	G	161/170 (95%)	156 (97%)	5 (3%)	0	100	100
1	H	155/170 (91%)	151 (97%)	4 (3%)	0	100	100
1	I	163/170 (96%)	159 (98%)	3 (2%)	1 (1%)	27	15
1	J	161/170 (95%)	157 (98%)	3 (2%)	1 (1%)	27	15
1	K	162/170 (95%)	158 (98%)	4 (2%)	0	100	100
1	L	163/170 (96%)	161 (99%)	2 (1%)	0	100	100
All	All	1952/2040 (96%)	1916 (98%)	33 (2%)	3 (0%)	49	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	GLY
1	I	14	SER
1	J	13	SER

### 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	137/138 (99%)	133 (97%)	4 (3%)	45	34
1	B	134/138 (97%)	128 (96%)	6 (4%)	30	17
1	C	133/138 (96%)	127 (96%)	6 (4%)	30	17
1	D	135/138 (98%)	134 (99%)	1 (1%)	85	84
1	E	136/138 (99%)	130 (96%)	6 (4%)	31	18
1	F	135/138 (98%)	129 (96%)	6 (4%)	31	18
1	G	133/138 (96%)	129 (97%)	4 (3%)	44	32
1	H	128/138 (93%)	119 (93%)	9 (7%)	16	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	135/138 (98%)	128 (95%)	7 (5%)	25	13
1	J	132/138 (96%)	126 (96%)	6 (4%)	30	17
1	K	133/138 (96%)	125 (94%)	8 (6%)	21	9
1	L	134/138 (97%)	130 (97%)	4 (3%)	44	32
All	All	1605/1656 (97%)	1538 (96%)	67 (4%)	32	20

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	30	LEU
1	A	151	LEU
1	A	155	LYS
1	B	3	LEU
1	B	49	ASN
1	B	53	VAL
1	B	137	ARG
1	B	142	ARG
1	B	155	LYS
1	C	89	GLU
1	C	94	GLN
1	C	96	ARG
1	C	122	ARG
1	C	137	ARG
1	C	155	LYS
1	D	155	LYS
1	E	3	LEU
1	E	90	PRO
1	E	132	VAL
1	E	135	GLU
1	E	152	TRP
1	E	155	LYS
1	F	3	LEU
1	F	25	LYS
1	F	53	VAL
1	F	96	ARG
1	F	155	LYS
1	F	168	GLU
1	G	30	LEU
1	G	85	PRO
1	G	135	GLU

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Mol	Chain	Res	Type
1	G	155	LYS
1	H	16	LYS
1	H	65	ASP
1	H	76	VAL
1	H	95	THR
1	H	97	LYS
1	H	99	HIS
1	H	104	GLU
1	H	152	TRP
1	H	155	LYS
1	I	7	PHE
1	I	8	LEU
1	I	17	LEU
1	I	94	GLN
1	I	114	LEU
1	I	155	LYS
1	I	168	GLU
1	J	17	LEU
1	J	122	ARG
1	J	137	ARG
1	J	151	LEU
1	J	152	TRP
1	J	155	LYS
1	K	17	LEU
1	K	22	ILE
1	K	40	LEU
1	K	48	GLU
1	K	61	ARG
1	K	137	ARG
1	K	142	ARG
1	K	155	LYS
1	L	94	GLN
1	L	96	ARG
1	L	151	LEU
1	L	155	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	136	ASN
1	B	45	GLN

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Mol	Chain	Res	Type
1	B	94	GLN
1	D	49	ASN
1	E	45	GLN
1	E	94	GLN
1	G	81	GLN
1	I	24	GLN
1	I	119	HIS
1	J	24	GLN
1	J	45	GLN
1	K	24	GLN
1	L	94	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

25 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	FYD	A	201[A]	-	33,34,34	2.09	3 (9%)	43,47,47	2.00	6 (13%)
2	FYD	A	201[B]	-	33,34,34	2.11	4 (12%)	43,47,47	1.42	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	FYD	B	201[A]	-	33,34,34	1.91	2 (6%)	43,47,47	1.39	4 (9%)
2	FYD	B	201[B]	-	33,34,34	1.98	3 (9%)	43,47,47	1.15	4 (9%)
2	FYD	C	201[A]	-	33,34,34	1.93	3 (9%)	43,47,47	1.40	5 (11%)
2	FYD	C	201[B]	-	33,34,34	1.95	4 (12%)	43,47,47	1.34	5 (11%)
2	FYD	D	201[A]	-	33,34,34	1.88	3 (9%)	43,47,47	1.58	6 (13%)
2	FYD	D	201[B]	-	33,34,34	2.00	4 (12%)	43,47,47	1.55	9 (20%)
2	FYD	E	201[A]	-	33,34,34	1.80	2 (6%)	43,47,47	1.63	7 (16%)
2	FYD	E	201[B]	-	33,34,34	1.84	3 (9%)	43,47,47	1.39	6 (13%)
2	FYD	F	201[A]	-	33,34,34	1.92	3 (9%)	43,47,47	1.75	5 (11%)
2	FYD	F	201[B]	-	33,34,34	1.93	3 (9%)	43,47,47	1.16	5 (11%)
2	FYD	G	201[A]	-	33,34,34	1.96	2 (6%)	43,47,47	1.43	7 (16%)
2	FYD	G	201[B]	-	33,34,34	2.01	4 (12%)	43,47,47	1.33	9 (20%)
3	HIS	H	201	-	6,10,11	1.25	1 (16%)	5,12,14	1.39	1 (20%)
2	FYD	H	202[A]	-	33,34,34	2.06	2 (6%)	43,47,47	1.33	7 (16%)
2	FYD	H	202[B]	-	33,34,34	2.10	4 (12%)	43,47,47	1.51	8 (18%)
2	FYD	I	201[A]	-	33,34,34	2.12	3 (9%)	43,47,47	1.91	7 (16%)
2	FYD	I	201[B]	-	33,34,34	2.12	3 (9%)	43,47,47	1.25	7 (16%)
2	FYD	J	201[A]	-	33,34,34	1.98	4 (12%)	43,47,47	1.55	4 (9%)
2	FYD	J	201[B]	-	33,34,34	2.03	6 (18%)	43,47,47	1.22	4 (9%)
2	FYD	K	201[A]	-	33,34,34	1.99	5 (15%)	43,47,47	1.63	7 (16%)
2	FYD	K	201[B]	-	33,34,34	1.96	5 (15%)	43,47,47	1.31	7 (16%)
2	FYD	L	201[A]	-	33,34,34	1.96	5 (15%)	43,47,47	1.86	9 (20%)
2	FYD	L	201[B]	-	33,34,34	2.01	6 (18%)	43,47,47	1.49	9 (20%)

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	FYD	A	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	A	201[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	B	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	B	201[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	C	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	C	201[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	D	201[A]	-	-	0/21/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FYD	D	201[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	E	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	E	201[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	F	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	F	201[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	G	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	G	201[B]	-	-	0/21/23/23	0/3/3/3
3	HIS	H	201	-	-	0/4/6/8	0/1/1/1
2	FYD	H	202[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	H	202[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	I	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	I	201[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	J	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	J	201[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	K	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	K	201[B]	-	-	0/21/23/23	0/3/3/3
2	FYD	L	201[A]	-	-	0/21/23/23	0/3/3/3
2	FYD	L	201[B]	-	-	0/21/23/23	0/3/3/3

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	201[B]	FYD	C15-C20	-2.58	1.35	1.40
2	D	201[B]	FYD	O01-C02	-2.54	1.18	1.23
2	D	201[A]	FYD	O01-C02	-2.53	1.18	1.23
2	C	201[A]	FYD	C15-C20	-2.44	1.36	1.40
2	F	201[A]	FYD	O01-C02	-2.41	1.18	1.23
2	F	201[B]	FYD	O01-C02	-2.39	1.18	1.23
2	H	202[B]	FYD	C15-C20	-2.31	1.36	1.40
2	L	201[A]	FYD	O13-C12	-2.27	1.36	1.40
2	I	201[B]	FYD	C24-C25	-2.23	1.36	1.41
2	I	201[A]	FYD	C24-C25	-2.23	1.36	1.41
2	L	201[A]	FYD	O01-C02	-2.20	1.18	1.23
2	K	201[B]	FYD	C24-C25	-2.18	1.36	1.41
2	L	201[B]	FYD	O01-C02	-2.15	1.18	1.23
2	K	201[A]	FYD	C24-C25	-2.15	1.36	1.41
2	L	201[B]	FYD	O13-C12	-2.11	1.37	1.40
2	J	201[A]	FYD	O01-C02	-2.10	1.19	1.23
2	J	201[B]	FYD	O01-C02	-2.09	1.19	1.23
2	C	201[B]	FYD	BR1-C07	2.00	1.94	1.90
2	G	201[B]	FYD	BR2-C10	2.01	1.94	1.89
2	J	201[A]	FYD	BR2-C10	2.05	1.94	1.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	201[B]	FYD	BR2-C10	2.11	1.94	1.89
2	K	201[B]	FYD	BR1-C07	2.13	1.94	1.90
3	H	201	HIS	CA-C	2.16	1.53	1.50
2	A	201[B]	FYD	O21-C20	2.21	1.40	1.37
2	K	201[B]	FYD	BR2-C10	2.46	1.95	1.89
2	K	201[A]	FYD	BR2-C10	2.47	1.95	1.89
2	K	201[A]	FYD	O21-C20	2.54	1.41	1.37
2	A	201[A]	FYD	BR2-C10	2.56	1.95	1.89
2	H	202[B]	FYD	O21-C20	2.62	1.41	1.37
2	A	201[B]	FYD	BR2-C10	2.67	1.96	1.89
2	J	201[B]	FYD	O21-C20	2.67	1.41	1.37
2	L	201[B]	FYD	BR2-C10	2.70	1.96	1.89
2	L	201[A]	FYD	BR2-C10	2.71	1.96	1.89
2	G	201[B]	FYD	O21-C20	2.73	1.41	1.37
2	C	201[B]	FYD	O21-C20	2.81	1.41	1.37
2	E	201[B]	FYD	O21-C20	2.94	1.41	1.37
2	L	201[B]	FYD	O21-C20	3.06	1.42	1.37
2	B	201[B]	FYD	O21-C20	3.10	1.42	1.37
2	E	201[A]	FYD	C02-N03	3.15	1.40	1.33
2	E	201[B]	FYD	C02-N03	3.19	1.40	1.33
2	G	201[B]	FYD	C02-N03	3.42	1.41	1.33
2	G	201[A]	FYD	C02-N03	3.47	1.41	1.33
2	D	201[B]	FYD	O21-C20	4.08	1.43	1.37
2	C	201[A]	FYD	C02-N03	4.09	1.42	1.33
2	C	201[B]	FYD	C02-N03	4.15	1.43	1.33
2	L	201[A]	FYD	C02-N03	4.26	1.43	1.33
2	L	201[B]	FYD	C02-N03	4.29	1.43	1.33
2	D	201[A]	FYD	C02-N03	4.39	1.43	1.33
2	F	201[A]	FYD	C02-N03	4.40	1.43	1.33
2	F	201[B]	FYD	C02-N03	4.41	1.43	1.33
2	D	201[B]	FYD	C02-N03	4.42	1.43	1.33
2	K	201[A]	FYD	C02-N03	4.51	1.43	1.33
2	K	201[B]	FYD	C02-N03	4.52	1.43	1.33
2	H	202[A]	FYD	C02-N03	4.70	1.44	1.33
2	B	201[A]	FYD	C02-N03	4.75	1.44	1.33
2	B	201[B]	FYD	C02-N03	4.77	1.44	1.33
2	H	202[B]	FYD	C02-N03	4.77	1.44	1.33
2	J	201[B]	FYD	C02-N03	4.80	1.44	1.33
2	J	201[A]	FYD	C02-N03	4.86	1.44	1.33
2	A	201[A]	FYD	C02-N03	5.08	1.45	1.33
2	A	201[B]	FYD	C02-N03	5.10	1.45	1.33
2	I	201[A]	FYD	C02-N03	5.22	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	201[B]	FYD	C02-N03	5.32	1.45	1.33
2	D	201[A]	FYD	O27-N26	8.03	1.37	1.22
2	D	201[B]	FYD	O27-N26	8.11	1.37	1.22
2	E	201[A]	FYD	O27-N26	8.14	1.37	1.22
2	E	201[B]	FYD	O27-N26	8.22	1.37	1.22
2	B	201[A]	FYD	O27-N26	8.33	1.37	1.22
2	L	201[B]	FYD	O27-N26	8.38	1.37	1.22
2	B	201[B]	FYD	O27-N26	8.40	1.37	1.22
2	K	201[B]	FYD	O27-N26	8.41	1.37	1.22
2	K	201[A]	FYD	O27-N26	8.46	1.37	1.22
2	L	201[A]	FYD	O27-N26	8.47	1.37	1.22
2	C	201[A]	FYD	O27-N26	8.50	1.38	1.22
2	C	201[B]	FYD	O27-N26	8.53	1.38	1.22
2	J	201[A]	FYD	O27-N26	8.56	1.38	1.22
2	J	201[B]	FYD	O27-N26	8.57	1.38	1.22
2	F	201[B]	FYD	O27-N26	8.75	1.38	1.22
2	F	201[A]	FYD	O27-N26	8.83	1.38	1.22
2	H	202[B]	FYD	O27-N26	9.01	1.38	1.22
2	H	202[A]	FYD	O27-N26	9.03	1.39	1.22
2	I	201[A]	FYD	O27-N26	9.09	1.39	1.22
2	I	201[B]	FYD	O27-N26	9.10	1.39	1.22
2	A	201[B]	FYD	O27-N26	9.19	1.39	1.22
2	A	201[A]	FYD	O27-N26	9.20	1.39	1.22
2	G	201[A]	FYD	O27-N26	9.28	1.39	1.22
2	G	201[B]	FYD	O27-N26	9.32	1.39	1.22

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201[A]	FYD	C22-O21-C20	-9.02	104.15	117.53
2	I	201[A]	FYD	C22-O21-C20	-8.13	105.47	117.53
2	F	201[A]	FYD	C22-O21-C20	-7.78	105.98	117.53
2	J	201[A]	FYD	C22-O21-C20	-6.69	107.60	117.53
2	L	201[A]	FYD	C22-O21-C20	-6.24	108.28	117.53
2	K	201[A]	FYD	C22-O21-C20	-5.99	108.64	117.53
2	E	201[A]	FYD	C22-O21-C20	-5.69	109.08	117.53
2	D	201[A]	FYD	C22-O21-C20	-5.63	109.17	117.53
2	B	201[A]	FYD	C22-O21-C20	-4.69	110.57	117.53
2	H	202[B]	FYD	C20-C15-C14	-4.58	112.44	123.35
2	G	201[A]	FYD	C22-O21-C20	-4.53	110.81	117.53
2	L	201[A]	FYD	O21-C20-C19	-4.29	117.14	124.36
2	I	201[A]	FYD	O21-C20-C19	-4.11	117.44	124.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201[A]	FYD	C22-O21-C20	-4.09	111.46	117.53
2	J	201[B]	FYD	C20-C15-C14	-4.04	113.72	123.35
2	D	201[B]	FYD	C22-O21-C20	-3.98	111.63	117.53
2	F	201[A]	FYD	O21-C20-C19	-3.98	117.67	124.36
2	A	201[A]	FYD	O21-C20-C19	-3.88	117.83	124.36
2	J	201[A]	FYD	O21-C20-C19	-3.87	117.85	124.36
2	K	201[B]	FYD	C20-C15-C14	-3.58	114.83	123.35
2	D	201[B]	FYD	C20-C15-C14	-3.43	115.18	123.35
2	H	202[A]	FYD	C22-O21-C20	-3.37	112.54	117.53
2	C	201[B]	FYD	C20-C15-C14	-3.30	115.48	123.35
2	D	201[A]	FYD	O21-C20-C19	-3.20	118.97	124.36
2	A	201[B]	FYD	C22-O21-C20	-3.08	112.96	117.53
2	F	201[B]	FYD	C20-C15-C14	-3.06	116.05	123.35
2	H	202[B]	FYD	C22-O21-C20	-2.96	113.14	117.53
2	E	201[B]	FYD	C20-C15-C14	-2.92	116.38	123.35
2	F	201[B]	FYD	O01-C02-C24	-2.81	115.74	120.98
2	G	201[A]	FYD	O21-C20-C19	-2.76	119.72	124.36
2	D	201[A]	FYD	C05-C06-C07	-2.74	115.61	119.94
2	L	201[A]	FYD	BR1-C07-C06	-2.71	115.49	119.27
2	A	201[B]	FYD	O01-C02-C24	-2.71	115.94	120.98
2	B	201[A]	FYD	O27-N26-C25	-2.68	114.11	118.92
2	B	201[A]	FYD	O21-C20-C19	-2.67	119.87	124.36
2	E	201[A]	FYD	O27-N26-C25	-2.63	114.19	118.92
2	A	201[A]	FYD	O01-C02-C24	-2.61	116.12	120.98
2	K	201[A]	FYD	O21-C20-C19	-2.59	120.00	124.36
2	L	201[B]	FYD	C20-C15-C14	-2.59	117.18	123.35
2	L	201[A]	FYD	C09-C10-C12	-2.58	117.77	122.54
2	E	201[A]	FYD	O21-C20-C19	-2.57	120.03	124.36
2	D	201[B]	FYD	C05-C06-C07	-2.57	115.88	119.94
2	H	202[B]	FYD	O01-C02-C24	-2.50	116.32	120.98
2	L	201[B]	FYD	BR1-C07-C06	-2.46	115.84	119.27
2	H	202[A]	FYD	O21-C20-C19	-2.46	120.23	124.36
2	E	201[B]	FYD	O27-N26-C25	-2.43	114.55	118.92
2	F	201[A]	FYD	O01-C02-C24	-2.43	116.45	120.98
2	C	201[B]	FYD	O01-C02-C24	-2.42	116.47	120.98
2	I	201[B]	FYD	C22-O21-C20	-2.41	113.95	117.53
2	G	201[B]	FYD	BR1-C07-C06	-2.38	115.95	119.27
2	B	201[B]	FYD	O27-N26-C25	-2.37	114.67	118.92
2	L	201[B]	FYD	C09-C10-C12	-2.37	118.15	122.54
2	E	201[A]	FYD	C05-C06-C07	-2.37	116.20	119.94
2	L	201[A]	FYD	C05-C06-C07	-2.36	116.21	119.94
2	C	201[A]	FYD	O21-C20-C19	-2.36	120.40	124.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201[B]	FYD	C22-O21-C20	-2.34	114.07	117.53
2	B	201[B]	FYD	C20-C15-C14	-2.33	117.80	123.35
2	K	201[A]	FYD	C09-C10-C12	-2.33	118.23	122.54
2	C	201[B]	FYD	O13-C14-O23	-2.31	118.02	123.10
2	K	201[A]	FYD	O27-N26-C25	-2.30	114.80	118.92
2	H	202[A]	FYD	O01-C02-C24	-2.26	116.77	120.98
2	E	201[B]	FYD	C05-C06-C07	-2.24	116.40	119.94
2	L	201[B]	FYD	C05-C06-C07	-2.22	116.42	119.94
2	G	201[B]	FYD	C20-C15-C14	-2.22	118.07	123.35
2	C	201[A]	FYD	O01-C02-C24	-2.20	116.89	120.98
2	G	201[B]	FYD	C09-C10-C12	-2.18	118.51	122.54
2	G	201[A]	FYD	C05-C06-C07	-2.17	116.50	119.94
2	G	201[B]	FYD	C05-C06-C07	-2.15	116.53	119.94
2	K	201[B]	FYD	C09-C10-C12	-2.13	118.59	122.54
2	G	201[B]	FYD	O21-C20-C19	-2.10	120.84	124.36
2	I	201[B]	FYD	C20-C15-C14	-2.09	118.36	123.35
2	K	201[B]	FYD	O27-N26-C25	-2.09	115.17	118.92
2	G	201[B]	FYD	O01-C02-N03	-2.04	118.48	122.60
2	G	201[A]	FYD	BR1-C07-C06	-2.03	116.44	119.27
2	I	201[A]	FYD	C20-C15-C14	-2.02	118.53	123.35
2	I	201[B]	FYD	O01-C02-C24	-2.02	117.22	120.98
2	D	201[B]	FYD	O01-C02-C24	-2.01	117.23	120.98
2	G	201[A]	FYD	C09-C10-C12	-2.00	118.83	122.54
2	H	202[A]	FYD	C24-C02-N03	2.01	121.34	117.42
2	I	201[A]	FYD	O13-C14-O23	2.03	127.55	123.10
2	D	201[A]	FYD	O21-C20-C15	2.04	119.09	116.49
2	D	201[B]	FYD	C16-C15-C14	2.05	122.87	118.67
2	H	202[A]	FYD	C29-C25-N26	2.06	118.89	116.50
2	F	201[B]	FYD	C05-C12-C10	2.07	119.80	116.95
2	D	201[A]	FYD	C06-C05-C12	2.09	121.77	118.61
2	K	201[B]	FYD	C16-C15-C20	2.10	120.94	118.21
2	E	201[A]	FYD	C12-O13-C14	2.11	122.87	117.48
2	G	201[B]	FYD	O21-C20-C15	2.11	119.18	116.49
2	B	201[B]	FYD	C05-C12-C10	2.12	119.87	116.95
2	F	201[B]	FYD	C24-C02-N03	2.13	121.58	117.42
2	A	201[A]	FYD	C24-C02-N03	2.16	121.63	117.42
2	B	201[A]	FYD	O21-C20-C15	2.18	119.26	116.49
3	H	201	HIS	CD2-NE2-CE1	2.21	109.22	105.78
2	K	201[B]	FYD	C29-C25-N26	2.22	119.08	116.50
2	L	201[A]	FYD	C29-C25-N26	2.24	119.11	116.50
2	F	201[A]	FYD	C05-C12-C10	2.28	120.09	116.95
2	L	201[B]	FYD	C16-C15-C20	2.28	121.18	118.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	201[B]	FYD	C06-C05-C12	2.29	122.07	118.61
2	I	201[B]	FYD	C24-C02-N03	2.31	121.91	117.42
2	D	201[B]	FYD	O21-C20-C15	2.32	119.43	116.49
2	A	201[B]	FYD	C24-C02-N03	2.32	121.94	117.42
2	G	201[A]	FYD	O21-C20-C15	2.34	119.46	116.49
2	F	201[B]	FYD	C16-C15-C14	2.34	123.47	118.67
2	L	201[B]	FYD	C29-C25-N26	2.34	119.23	116.50
2	H	202[B]	FYD	C29-C25-N26	2.35	119.24	116.50
2	G	201[A]	FYD	C05-C12-C10	2.36	120.20	116.95
2	E	201[B]	FYD	C16-C15-C20	2.36	121.28	118.21
2	I	201[B]	FYD	C05-C12-C10	2.38	120.23	116.95
2	A	201[B]	FYD	O21-C20-C15	2.38	119.52	116.49
2	I	201[B]	FYD	C16-C15-C20	2.41	121.34	118.21
2	J	201[A]	FYD	C05-C12-C10	2.41	120.27	116.95
2	K	201[A]	FYD	C16-C15-C20	2.42	121.35	118.21
2	G	201[B]	FYD	C05-C12-C10	2.43	120.30	116.95
2	B	201[B]	FYD	C16-C15-C20	2.44	121.38	118.21
2	D	201[B]	FYD	C05-C12-C10	2.45	120.33	116.95
2	H	202[B]	FYD	C16-C15-C20	2.47	121.42	118.21
2	H	202[B]	FYD	C24-C02-N03	2.52	122.34	117.42
2	J	201[B]	FYD	C05-C12-C10	2.59	120.53	116.95
2	A	201[A]	FYD	O21-C20-C15	2.59	119.79	116.49
2	C	201[B]	FYD	C16-C15-C14	2.61	124.02	118.67
2	J	201[B]	FYD	C16-C15-C14	2.69	124.18	118.67
2	H	202[B]	FYD	C05-C12-C10	2.69	120.66	116.95
2	I	201[B]	FYD	O21-C20-C15	2.71	119.93	116.49
2	K	201[B]	FYD	C16-C15-C14	2.71	124.22	118.67
2	L	201[A]	FYD	O21-C20-C15	2.76	120.00	116.49
2	L	201[B]	FYD	O21-C20-C15	2.79	120.03	116.49
2	E	201[A]	FYD	C29-C25-N26	2.81	119.77	116.50
2	I	201[A]	FYD	C16-C15-C20	2.81	121.87	118.21
2	H	202[A]	FYD	C05-C12-C10	2.82	120.83	116.95
2	D	201[B]	FYD	C16-C15-C20	2.86	121.93	118.21
2	L	201[A]	FYD	C32-C24-C25	2.91	122.33	118.35
2	D	201[A]	FYD	C05-C12-C10	2.92	120.97	116.95
2	L	201[B]	FYD	C32-C24-C25	2.93	122.35	118.35
2	H	202[A]	FYD	O21-C20-C15	2.93	120.22	116.49
2	C	201[A]	FYD	C05-C12-C10	2.95	121.02	116.95
2	K	201[B]	FYD	C05-C12-C10	2.99	121.08	116.95
2	J	201[B]	FYD	C16-C15-C20	3.00	122.11	118.21
2	E	201[B]	FYD	C29-C25-N26	3.02	120.02	116.50
2	E	201[B]	FYD	C05-C12-C10	3.04	121.14	116.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	201[A]	FYD	O21-C20-C15	3.04	120.36	116.49
2	C	201[A]	FYD	C29-C25-N26	3.07	120.07	116.50
2	E	201[A]	FYD	C05-C12-C10	3.12	121.25	116.95
2	C	201[B]	FYD	C29-C25-N26	3.24	120.27	116.50
2	I	201[A]	FYD	C05-C12-C10	3.32	121.52	116.95
2	K	201[A]	FYD	O21-C20-C15	3.33	120.72	116.49
2	A	201[B]	FYD	C05-C12-C10	3.35	121.57	116.95
2	A	201[A]	FYD	C05-C12-C10	3.38	121.61	116.95
2	K	201[A]	FYD	C05-C12-C10	3.57	121.87	116.95
2	H	202[B]	FYD	C16-C15-C14	3.63	126.11	118.67
2	L	201[B]	FYD	C05-C12-C10	3.65	121.98	116.95
2	L	201[A]	FYD	C05-C12-C10	3.85	122.26	116.95
2	F	201[A]	FYD	O21-C20-C15	3.88	121.43	116.49
2	I	201[A]	FYD	O21-C20-C15	3.90	121.45	116.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201[B]	FYD	1	0
2	E	201[A]	FYD	1	0
2	G	201[B]	FYD	1	0
3	H	201	HIS	1	0
2	H	202[B]	FYD	1	0
2	I	201[B]	FYD	1	0
2	L	201[B]	FYD	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	165/170 (97%)	-0.22	0 <span>100</span> <span>100</span>	8, 17, 35, 50	0
1	B	166/170 (97%)	-0.12	1 (0%) <span>89</span> <span>90</span>	12, 21, 39, 58	0
1	C	164/170 (96%)	-0.07	0 <span>100</span> <span>100</span>	9, 16, 38, 52	3 (1%)
1	D	166/170 (97%)	-0.28	1 (0%) <span>89</span> <span>90</span>	8, 15, 31, 42	0
1	E	165/170 (97%)	-0.18	3 (1%) <span>68</span> <span>70</span>	10, 18, 38, 54	0
1	F	167/170 (98%)	-0.03	1 (0%) <span>89</span> <span>90</span>	14, 24, 42, 56	0
1	G	162/170 (95%)	-0.19	3 (1%) <span>66</span> <span>69</span>	12, 21, 37, 60	0
1	H	158/170 (92%)	0.18	5 (3%) <span>47</span> <span>49</span>	15, 26, 50, 65	0
1	I	162/170 (95%)	-0.16	3 (1%) <span>66</span> <span>69</span>	11, 19, 38, 55	0
1	J	162/170 (95%)	-0.03	4 (2%) <span>57</span> <span>59</span>	15, 25, 45, 56	0
1	K	164/170 (96%)	-0.08	5 (3%) <span>50</span> <span>52</span>	14, 23, 43, 70	1 (0%)
1	L	164/170 (96%)	-0.11	2 (1%) <span>79</span> <span>81</span>	8, 15, 36, 60	0
All	All	1965/2040 (96%)	-0.11	28 (1%) <span>75</span> <span>77</span>	8, 21, 41, 70	4 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	99	HIS	3.6
1	H	96	ARG	3.4
1	K	48	GLU	3.4
1	L	14	SER	3.3
1	B	48	GLU	3.1
1	I	12	ARG	3.1
1	K	12	ARG	3.0
1	K	14	SER	2.8
1	J	50	ALA	2.8
1	E	137	ARG	2.7
1	J	48	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	H	14	SER	2.5
1	G	12	ARG	2.4
1	I	7	PHE	2.4
1	E	138	ALA	2.4
1	K	50	ALA	2.3
1	L	12	ARG	2.3
1	D	94	GLN	2.3
1	G	168	GLU	2.3
1	H	97	LYS	2.3
1	K	8	LEU	2.2
1	F	12	ARG	2.2
1	G	14	SER	2.2
1	J	167	PHE	2.2
1	H	12	ARG	2.1
1	E	48	GLU	2.1
1	J	43	ASP	2.0
1	I	168	GLU	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	HIS	H	201	10/11	0.75	0.24	45,55,64,65	0
2	FYD	F	201[A]	32/32	0.98	0.09	20,24,30,31	32
2	FYD	H	202[B]	32/32	0.98	0.09	23,26,30,40	32
2	FYD	E	201[A]	32/32	0.98	0.09	15,20,22,30	32
2	FYD	H	202[A]	32/32	0.98	0.09	21,25,30,40	32
2	FYD	K	201[B]	32/32	0.98	0.11	18,21,24,34	32

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	FYD	E	201[B]	32/32	0.98	0.09	13,16,20,30	32
2	FYD	K	201[A]	32/32	0.98	0.11	18,22,24,34	32
2	FYD	F	201[B]	32/32	0.98	0.09	18,20,24,30	32
2	FYD	B	201[B]	32/32	0.98	0.09	18,20,22,30	32
2	FYD	J	201[B]	32/32	0.98	0.11	20,23,27,36	32
2	FYD	B	201[A]	32/32	0.98	0.09	18,21,24,30	32
2	FYD	J	201[A]	32/32	0.98	0.11	22,26,34,37	32
2	FYD	C	201[B]	32/32	0.98	0.09	8,15,18,22	32
2	FYD	C	201[A]	32/32	0.98	0.09	15,17,22,22	32
2	FYD	L	201[A]	32/32	0.99	0.09	12,15,19,23	32
2	FYD	G	201[B]	32/32	0.99	0.09	15,18,21,28	32
2	FYD	G	201[A]	32/32	0.99	0.09	18,20,29,29	32
2	FYD	D	201[A]	32/32	0.99	0.08	13,16,22,23	32
2	FYD	L	201[B]	32/32	0.99	0.09	7,13,15,22	32
2	FYD	D	201[B]	32/32	0.99	0.08	8,13,16,22	32
2	FYD	A	201[A]	32/32	0.99	0.07	13,16,21,23	32
2	FYD	I	201[A]	32/32	0.99	0.08	14,19,24,27	32
2	FYD	A	201[B]	32/32	0.99	0.07	12,14,16,23	32
2	FYD	I	201[B]	32/32	0.99	0.08	13,15,20,26	32

## 6.5 Other polymers

There are no such residues in this entry.