



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:29 AM GMT

PDB ID : 3AXY  
Title : Structure of Florigen Activation Complex Consisting of Rice Florigen Hd3a, 14-3-3 Protein GF14 and Rice FD Homolog OsFD1  
Authors : Ohki, I.; Furuita, K.; Hayashi, K.; Taoka, K.; Tsuji, H.; Nakagawa, A.; Shimamoto, K.; Kojima, C.  
Deposited on : 2011-04-19  
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

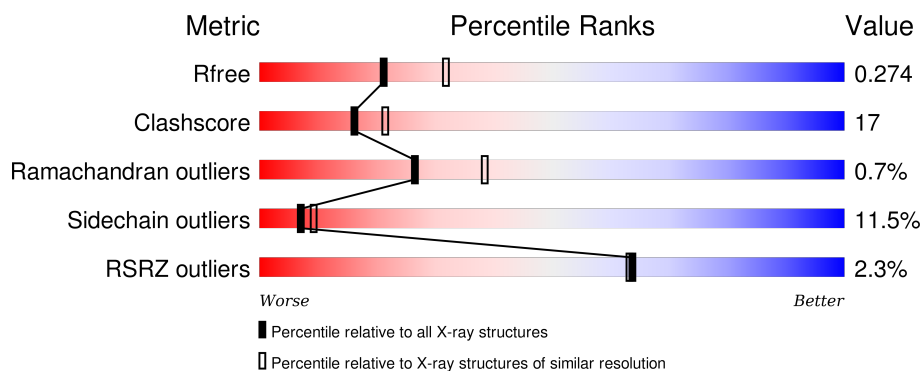
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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>3%</div> <div>74%</div> <div>19%</div> <div>• •</div> </div>
1	B	170	<div> <div>2%</div> <div>74%</div> <div>22%</div> <div>• •</div> </div>
1	G	170	<div> <div>%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	H	170	<div> <div>%</div> <div>70%</div> <div>24%</div> <div>• •</div> </div>
2	C	240	<div> <div>2%</div> <div>65%</div> <div>23%</div> <div>8%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	240	<div><div></div><div>3%</div><div>69%</div><div>24%</div><div>5%</div><div></div></div>
2	I	240	<div><div></div><div>3%</div><div>70%</div><div>21%</div><div>5%</div><div></div></div>
2	J	240	<div><div></div><div>3%</div><div>63%</div><div>27%</div><div>8%</div><div></div></div>
3	E	9	<div><div></div><div>33%</div><div>33%</div><div>11%</div><div>22%</div><div></div></div>
3	F	9	<div><div></div><div>33%</div><div>33%</div><div>11%</div><div>22%</div><div></div></div>
3	K	9	<div><div></div><div>33%</div><div>33%</div><div>11%</div><div>22%</div><div></div></div>
3	L	9	<div><div></div><div>11%</div><div>33%</div><div>22%</div><div>22%</div><div>22%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13751 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 Protein HEADING DATE 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1312	831	229	246	6			
1	B	166	Total	C	N	O	S	0	0	0
			1312	831	229	246	6			
1	G	165	Total	C	N	O	S	0	0	0
			1306	828	228	244	6			
1	H	166	Total	C	N	O	S	0	0	0
			1312	831	229	246	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP Q93WI9
A	2	PRO	-	EXPRESSION TAG	UNP Q93WI9
A	3	GLY	-	EXPRESSION TAG	UNP Q93WI9
A	4	HIS	-	EXPRESSION TAG	UNP Q93WI9
A	5	MET	-	EXPRESSION TAG	UNP Q93WI9
A	43	LEU	CYS	ENGINEERED MUTATION	UNP Q93WI9
A	109	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
A	166	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
B	1	GLY	-	EXPRESSION TAG	UNP Q93WI9
B	2	PRO	-	EXPRESSION TAG	UNP Q93WI9
B	3	GLY	-	EXPRESSION TAG	UNP Q93WI9
B	4	HIS	-	EXPRESSION TAG	UNP Q93WI9
B	5	MET	-	EXPRESSION TAG	UNP Q93WI9
B	43	LEU	CYS	ENGINEERED MUTATION	UNP Q93WI9
B	109	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
B	166	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
G	1	GLY	-	EXPRESSION TAG	UNP Q93WI9
G	2	PRO	-	EXPRESSION TAG	UNP Q93WI9
G	3	GLY	-	EXPRESSION TAG	UNP Q93WI9
G	4	HIS	-	EXPRESSION TAG	UNP Q93WI9
G	5	MET	-	EXPRESSION TAG	UNP Q93WI9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	43	LEU	CYS	ENGINEERED MUTATION	UNP Q93WI9
G	109	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
G	166	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
H	1	GLY	-	EXPRESSION TAG	UNP Q93WI9
H	2	PRO	-	EXPRESSION TAG	UNP Q93WI9
H	3	GLY	-	EXPRESSION TAG	UNP Q93WI9
H	4	HIS	-	EXPRESSION TAG	UNP Q93WI9
H	5	MET	-	EXPRESSION TAG	UNP Q93WI9
H	43	LEU	CYS	ENGINEERED MUTATION	UNP Q93WI9
H	109	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9
H	166	SER	CYS	ENGINEERED MUTATION	UNP Q93WI9

- Molecule 2 is a protein called 14-3-3-like protein GF14-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	235	Total	C	N	O	S	0	0	0
			1875	1181	312	373	9			
2	D	235	Total	C	N	O	S	0	0	0
			1875	1181	312	373	9			
2	I	235	Total	C	N	O	S	0	0	0
			1875	1181	312	373	9			
2	J	234	Total	C	N	O	S	0	0	0
			1867	1176	311	372	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
C	-3	PRO	-	EXPRESSION TAG	UNP Q6ZKC0
C	-2	LEU	-	EXPRESSION TAG	UNP Q6ZKC0
C	-1	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
C	0	SER	-	EXPRESSION TAG	UNP Q6ZKC0
D	-4	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
D	-3	PRO	-	EXPRESSION TAG	UNP Q6ZKC0
D	-2	LEU	-	EXPRESSION TAG	UNP Q6ZKC0
D	-1	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
D	0	SER	-	EXPRESSION TAG	UNP Q6ZKC0
I	-4	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
I	-3	PRO	-	EXPRESSION TAG	UNP Q6ZKC0
I	-2	LEU	-	EXPRESSION TAG	UNP Q6ZKC0
I	-1	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
I	0	SER	-	EXPRESSION TAG	UNP Q6ZKC0

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Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
J	-3	PRO	-	EXPRESSION TAG	UNP Q6ZKC0
J	-2	LEU	-	EXPRESSION TAG	UNP Q6ZKC0
J	-1	GLY	-	EXPRESSION TAG	UNP Q6ZKC0
J	0	SER	-	EXPRESSION TAG	UNP Q6ZKC0

- Molecule 3 is a protein called Rice FD homolog OsFD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	P	0	0	0
			60	37	10	12	1			
3	F	7	Total	C	N	O	P	0	0	0
			60	37	10	12	1			
3	K	7	Total	C	N	O	P	0	0	0
			60	37	10	12	1			
3	L	7	Total	C	N	O	P	0	0	0
			60	37	10	12	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	68	Total	O	0	0
			68	68		
4	C	118	Total	O	0	0
			118	118		
4	D	92	Total	O	0	0
			92	92		
4	E	9	Total	O	0	0
			9	9		
4	F	4	Total	O	0	0
			4	4		
4	G	120	Total	O	0	0
			120	120		
4	H	68	Total	O	0	0
			68	68		
4	I	104	Total	O	0	0
			104	104		
4	J	74	Total	O	0	0
			74	74		
4	K	8	Total	O	0	0
			8	8		

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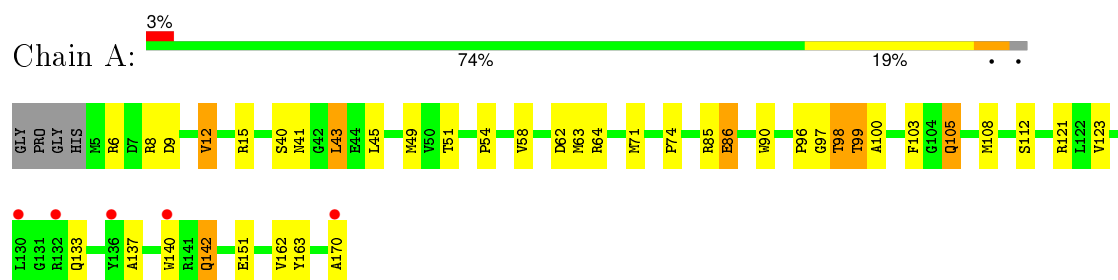
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	4	Total	O	0	0
			4	4		

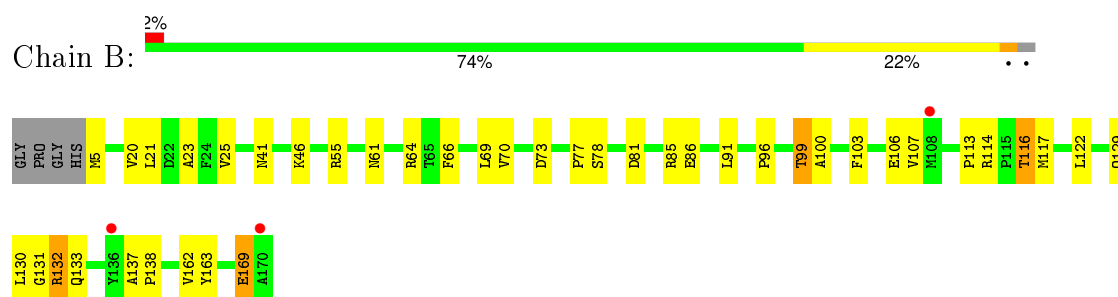
### 3 Residue-property plots [i](#)

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

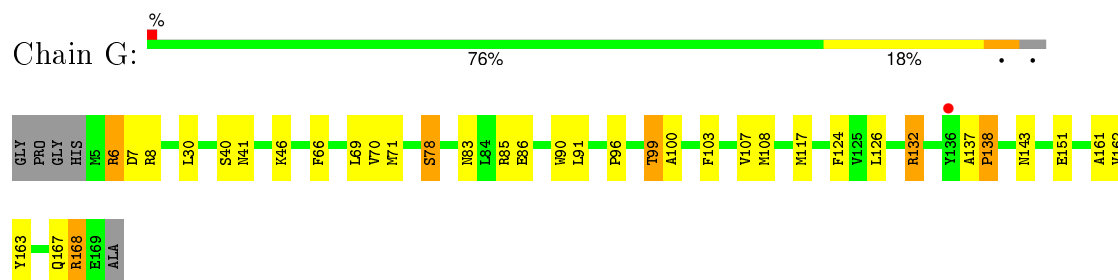
#### • Molecule 1: Protein HEADING DATE 3A



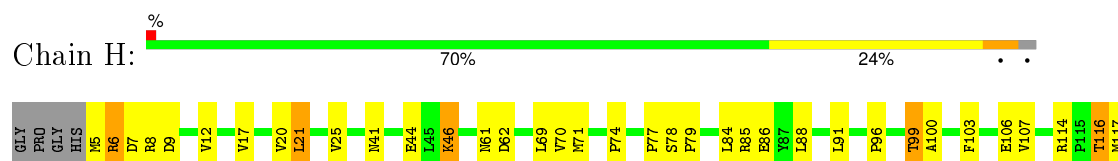
#### • Molecule 1: Protein HEADING DATE 3A



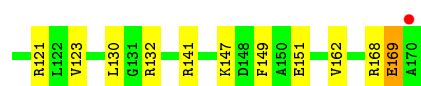
#### • Molecule 1: Protein HEADING DATE 3A



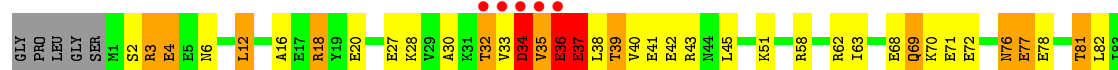
#### • Molecule 1: Protein HEADING DATE 3A







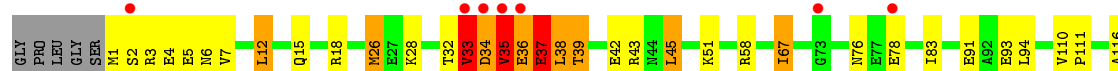
- Molecule 2: 14-3-3-like protein GF14-C



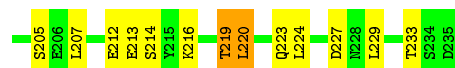
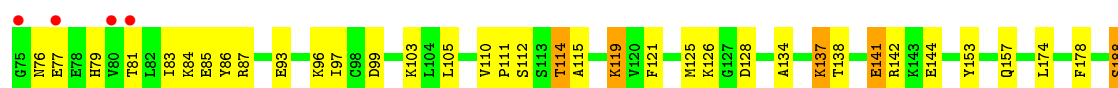
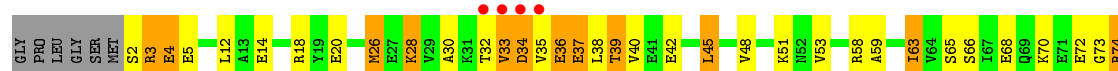
- Molecule 2: 14-3-3-like protein GF14-C



- Molecule 2: 14-3-3-like protein GF14-C

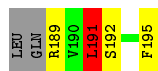


- Molecule 2: 14-3-3-like protein GF14-C

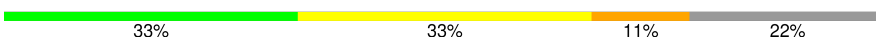


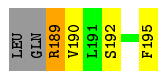
- Molecule 3: Rice FD homolog OsFD1

Chain E:  33% 33% 11% 22%



- Molecule 3: Rice FD homolog OsFD1

Chain F:  33% 33% 11% 22%

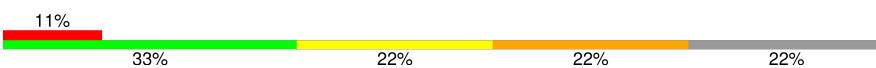


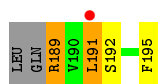
- Molecule 3: Rice FD homolog OsFD1

Chain K:  33% 33% 11% 22%



- Molecule 3: Rice FD homolog OsFD1

Chain L:  11% 33% 22% 22% 22%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.73Å 96.65Å 99.51Å 68.23° 87.90° 77.94°	Depositor
Resolution (Å)	50.00 – 2.40 37.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (50.00-2.40) 85.3 (37.86-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.73 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.227 , 0.276 0.227 , 0.274	Depositor DCC
$R_{free}$ test set	7276 reflections (7.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.2	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 99449 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13751	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	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 21.48 % 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 6.9501e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.39	0/1345	0.49	0/1831
1	B	0.33	0/1345	0.45	0/1831
1	G	0.37	0/1339	0.49	0/1824
1	H	0.34	0/1345	0.46	0/1831
2	C	0.38	0/1903	0.50	0/2563
2	D	0.35	0/1903	0.46	0/2563
2	I	0.37	0/1903	0.49	0/2563
2	J	0.34	0/1895	0.44	0/2553
3	E	0.43	0/50	0.92	1/64 (1.6%)
3	F	0.42	0/50	0.54	0/64
3	K	0.47	0/50	0.47	0/64
3	L	0.38	0/50	0.63	0/64
All	All	0.36	0/13178	0.48	1/17815 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
2	I	0	3
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	191	LEU	CA-CB-CG	5.19	127.23	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	129	TYR	Sidechain
2	C	36	GLU	Peptide
2	C	37	GLU	Peptide
2	I	33	VAL	Peptide
2	I	34	ASP	Peptide
2	I	37	GLU	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	1312	0	1283	36	0
1	B	1312	0	1283	39	0
1	G	1306	0	1278	33	0
1	H	1312	0	1283	44	0
2	C	1875	0	1868	76	0
2	D	1875	0	1868	54	0
2	I	1875	0	1868	79	0
2	J	1867	0	1856	87	0
3	E	60	0	56	5	0
3	F	60	0	56	6	0
3	K	60	0	56	9	0
3	L	60	0	56	6	0
4	A	108	0	0	7	0
4	B	68	0	0	2	0
4	C	118	0	0	10	0
4	D	92	0	0	3	0
4	E	9	0	0	0	0
4	F	4	0	0	2	0
4	G	120	0	0	4	0
4	H	68	0	0	4	0
4	I	104	0	0	7	0
4	J	74	0	0	8	0
4	K	8	0	0	2	0
4	L	4	0	0	0	0
All	All	13751	0	12811	434	0

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 17.

All (434) 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)
3:F:189:ARG:HG3	4:F:708:HOH:O	1.40	1.19
1:B:99:THR:CG2	1:B:100:ALA:H	1.54	1.17
1:G:6:ARG:HG2	1:G:6:ARG:HH11	1.13	1.13
2:I:39:THR:HG23	2:I:42:GLU:HG3	1.31	1.10
2:J:39:THR:HG21	4:J:574:HOH:O	1.50	1.09
1:H:99:THR:CG2	1:H:100:ALA:H	1.65	1.08
1:G:99:THR:HG23	1:G:100:ALA:H	1.11	1.07
1:B:99:THR:HG23	1:B:100:ALA:H	1.14	1.06
1:A:99:THR:HG23	1:A:100:ALA:H	1.22	1.02
2:I:26:MET:HE3	2:I:45:LEU:HB3	1.40	1.00
2:I:26:MET:CE	2:I:45:LEU:HB3	1.91	1.00
1:A:97:GLY:O	1:A:98:THR:HB	1.58	0.99
3:L:189:ARG:HG2	3:L:189:ARG:O	1.62	0.98
2:J:188:SER:HB3	4:J:598:HOH:O	1.61	0.98
1:A:98:THR:CG2	2:C:226:ARG:HH11	1.76	0.98
1:G:99:THR:CG2	1:G:100:ALA:H	1.76	0.97
1:A:99:THR:CG2	1:A:100:ALA:H	1.76	0.97
1:B:99:THR:CG2	1:B:100:ALA:N	2.21	0.96
2:J:33:VAL:HG13	2:J:36:GLU:H	1.28	0.95
2:J:110:VAL:CG1	2:J:111:PRO:HD3	1.97	0.93
2:J:110:VAL:HG12	2:J:111:PRO:HD3	1.50	0.93
2:I:39:THR:HG23	2:I:42:GLU:CG	2.00	0.92
1:H:99:THR:HG23	1:H:100:ALA:H	1.35	0.90
1:H:96:PRO:O	1:H:99:THR:HB	1.72	0.88
1:H:99:THR:CG2	1:H:100:ALA:N	2.33	0.88
2:I:26:MET:HE3	2:I:45:LEU:CB	2.03	0.88
1:B:99:THR:HG22	1:B:100:ALA:N	1.89	0.87
2:J:212:GLU:O	2:J:216:LYS:HG3	1.75	0.87
2:J:58:ARG:NH2	3:L:192:SEP:O1P	2.08	0.85
2:C:37:GLU:HA	4:C:262:HOH:O	1.74	0.85
1:G:99:THR:CG2	1:G:100:ALA:N	2.37	0.85
1:A:96:PRO:O	1:A:99:THR:HB	1.77	0.85
1:A:99:THR:CG2	1:A:100:ALA:N	2.35	0.85
2:J:39:THR:HG22	2:J:42:GLU:OE1	1.77	0.84
1:G:99:THR:HG23	1:G:100:ALA:N	1.92	0.84
1:H:99:THR:HG22	1:H:100:ALA:H	1.40	0.83
2:J:121:PHE:CE1	2:J:125:MET:CE	2.62	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:87:ARG:HG2	2:J:87:ARG:HH11	1.44	0.82
1:G:6:ARG:HG2	1:G:6:ARG:NH1	1.84	0.81
1:H:99:THR:HG22	1:H:100:ALA:N	1.95	0.81
2:J:121:PHE:HE1	2:J:125:MET:CE	1.94	0.81
2:J:20:GLU:HG2	4:J:240:HOH:O	1.80	0.80
3:K:189:ARG:HA	3:K:189:ARG:HH11	1.46	0.80
1:B:116:THR:HG23	1:B:117:MET:HG3	1.61	0.80
1:A:98:THR:HG21	2:C:226:ARG:HH11	1.46	0.80
1:A:62:ASP:OD2	1:A:64:ARG:HD3	1.82	0.79
2:D:233:THR:HG22	2:D:233:THR:O	1.80	0.79
1:A:98:THR:HG23	2:C:226:ARG:HH11	1.49	0.78
2:I:26:MET:CE	2:I:45:LEU:HD23	2.14	0.77
1:A:98:THR:HG23	2:C:226:ARG:NH1	1.98	0.77
1:B:96:PRO:O	1:B:99:THR:HB	1.84	0.77
1:A:98:THR:CG2	2:C:226:ARG:NH1	2.47	0.77
2:D:63:ILE:O	2:D:67:ILE:HD13	1.85	0.77
1:H:6:ARG:NH2	1:H:8:ARG:HH11	1.83	0.76
2:I:26:MET:CE	2:I:45:LEU:CB	2.61	0.75
2:I:154:LYS:HE2	4:I:488:HOH:O	1.87	0.74
2:C:28:LYS:HE3	4:C:566:HOH:O	1.86	0.74
1:B:55:ARG:NH1	2:D:233:THR:O	2.21	0.74
2:J:79:HIS:O	2:J:83:ILE:HG13	1.87	0.74
2:D:36:GLU:HG3	2:D:36:GLU:O	1.86	0.74
2:C:18:ARG:NH1	2:D:93:GLU:OE2	2.20	0.74
1:B:70:VAL:HG22	1:B:91:LEU:CD1	2.18	0.74
2:C:36:GLU:HG3	2:C:36:GLU:O	1.88	0.74
2:J:219:THR:O	2:J:223:GLN:HG3	1.88	0.74
1:B:66:PHE:CE1	1:B:132:ARG:HG2	2.22	0.74
1:G:96:PRO:O	1:G:99:THR:HB	1.88	0.73
2:J:33:VAL:HG22	2:J:36:GLU:CB	2.18	0.73
2:J:121:PHE:HE1	2:J:125:MET:HE1	1.51	0.73
2:C:233:THR:HG23	4:C:264:HOH:O	1.89	0.73
1:B:99:THR:HG22	1:B:100:ALA:H	1.43	0.73
2:J:233:THR:O	2:J:233:THR:HG22	1.89	0.73
2:D:34:ASP:HB2	4:D:664:HOH:O	1.88	0.73
2:C:16:ALA:HA	2:D:63:ILE:HD11	1.72	0.72
2:I:229:LEU:O	2:I:233:THR:HB	1.89	0.72
2:C:78:GLU:HG3	4:C:550:HOH:O	1.88	0.72
1:H:96:PRO:HD2	1:H:99:THR:HG21	1.71	0.72
1:B:116:THR:CG2	1:B:117:MET:HG3	2.19	0.72
4:G:171:HOH:O	2:I:233:THR:HG21	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:220:LEU:HD12	2:I:221:ILE:HD13	1.72	0.71
2:J:30:ALA:HA	2:J:38:LEU:HD21	1.73	0.71
2:I:224:LEU:HD23	3:K:191:LEU:HD13	1.73	0.71
2:I:233:THR:HG23	4:I:417:HOH:O	1.91	0.71
1:H:77:PRO:HD3	1:H:84:LEU:HG	1.73	0.71
1:G:6:ARG:CG	1:G:6:ARG:HH11	1.99	0.70
1:B:99:THR:HG23	1:B:100:ALA:N	1.93	0.70
2:D:227:ASP:HB3	3:F:189:ARG:NH2	2.06	0.70
2:C:12:LEU:HD13	2:D:86:TYR:CD2	2.26	0.70
2:I:26:MET:HE2	2:I:45:LEU:HB3	1.74	0.70
1:A:6:ARG:NH2	1:H:132:ARG:HH11	1.89	0.70
1:H:6:ARG:HH21	1:H:8:ARG:HH11	1.38	0.70
2:I:43:ARG:HD3	2:I:121:PHE:CZ	2.28	0.69
1:A:99:THR:HG22	1:A:100:ALA:N	2.07	0.69
2:J:33:VAL:CG1	2:J:36:GLU:H	2.04	0.69
1:A:64:ARG:HD2	2:C:215:TYR:CE1	2.27	0.69
1:H:168:ARG:CZ	4:H:730:HOH:O	2.39	0.69
2:I:58:ARG:NH2	3:K:192:SEP:O1P	2.23	0.69
2:J:37:GLU:OE1	2:J:114:THR:HB	1.93	0.69
1:H:6:ARG:HG3	4:H:564:HOH:O	1.92	0.68
2:C:32:THR:CG2	2:C:33:VAL:N	2.56	0.68
1:H:70:VAL:HG22	1:H:91:LEU:CD1	2.23	0.68
2:C:18:ARG:HH12	2:D:93:GLU:CD	1.97	0.68
1:H:5:MET:CE	1:H:12:VAL:HG12	2.23	0.68
2:J:33:VAL:HG22	2:J:36:GLU:HB2	1.75	0.68
1:G:78:SER:HB2	1:G:117:MET:HB2	1.76	0.68
2:C:224:LEU:HB3	3:E:191:LEU:HD21	1.74	0.67
1:H:91:LEU:HD23	1:H:107:VAL:HG11	1.76	0.67
2:C:3:ARG:HG2	2:C:32:THR:HG21	1.75	0.67
2:D:233:THR:O	2:D:233:THR:CG2	2.42	0.67
2:C:35:VAL:O	2:C:35:VAL:CG1	2.43	0.67
2:J:2:SER:HB3	2:J:5:GLU:HB2	1.78	0.66
1:H:6:ARG:HG2	1:H:8:ARG:HG2	1.77	0.66
2:C:58:ARG:NH2	3:E:192:SEP:O1P	2.23	0.66
1:B:41:ASN:HD21	1:B:162:VAL:HA	1.61	0.66
2:J:35:VAL:O	2:J:35:VAL:HG12	1.96	0.66
2:C:35:VAL:HA	2:C:112:SER:HB2	1.78	0.66
2:C:35:VAL:O	2:C:35:VAL:HG12	1.96	0.66
2:J:2:SER:N	4:J:600:HOH:O	2.29	0.66
2:J:105:LEU:O	2:J:110:VAL:HG12	1.96	0.65
2:I:36:GLU:O	2:I:37:GLU:C	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:189:ARG:HG2	3:E:189:ARG:O	1.96	0.65
2:J:33:VAL:HG13	2:J:36:GLU:N	2.06	0.65
1:B:131:GLY:O	1:B:133:GLN:HG2	1.97	0.65
2:I:227:ASP:HB3	4:I:258:HOH:O	1.97	0.65
1:A:99:THR:HG23	1:A:100:ALA:N	2.02	0.65
1:A:105:GLN:NE2	4:A:173:HOH:O	2.30	0.65
2:I:35:VAL:HG13	2:I:35:VAL:O	1.96	0.65
2:I:26:MET:HE1	2:I:45:LEU:HD23	1.79	0.64
2:J:26:MET:CE	2:J:45:LEU:HB3	2.27	0.64
2:J:3:ARG:HH12	2:J:33:VAL:HG23	1.63	0.64
2:J:76:ASN:HB3	4:J:670:HOH:O	1.95	0.64
2:D:233:THR:HG22	4:D:572:HOH:O	1.97	0.64
2:D:114:THR:HG22	2:D:115:ALA:N	2.13	0.64
2:D:58:ARG:NH2	3:F:192:SEP:O1P	2.31	0.64
2:D:87:ARG:HG2	2:D:87:ARG:HH11	1.63	0.64
2:I:18:ARG:HH12	2:J:93:GLU:CD	2.02	0.63
2:J:233:THR:CG2	2:J:233:THR:O	2.47	0.63
2:C:229:LEU:O	2:C:233:THR:HB	1.99	0.63
2:I:39:THR:HG23	2:I:42:GLU:CD	2.19	0.62
2:I:2:SER:OG	2:I:5:GLU:HG3	1.99	0.62
2:I:33:VAL:O	2:I:33:VAL:HG12	1.98	0.62
2:C:34:ASP:O	4:C:752:HOH:O	2.16	0.62
1:A:49:MET:HG3	4:A:194:HOH:O	1.99	0.61
2:J:39:THR:HG22	2:J:42:GLU:CD	2.19	0.61
1:G:41:ASN:HD21	1:G:162:VAL:HA	1.65	0.61
2:D:59:ALA:O	2:D:63:ILE:HD13	2.01	0.61
2:C:133:LEU:O	2:C:137:LYS:HG2	2.00	0.61
1:G:66:PHE:HE2	1:G:132:ARG:HE	1.47	0.60
2:I:154:LYS:CE	4:I:488:HOH:O	2.44	0.60
2:D:227:ASP:HB3	3:F:189:ARG:HH22	1.67	0.60
2:J:3:ARG:NH1	2:J:33:VAL:HG23	2.16	0.60
1:H:168:ARG:HD3	4:H:586:HOH:O	2.00	0.59
2:D:105:LEU:HD13	2:D:109:LEU:HD23	1.82	0.59
2:J:33:VAL:HG22	2:J:36:GLU:HB3	1.84	0.59
1:H:5:MET:CE	1:H:17:VAL:HG21	2.32	0.59
2:I:93:GLU:CD	2:J:18:ARG:HH12	2.06	0.59
2:J:110:VAL:HG13	2:J:111:PRO:HD3	1.82	0.59
3:L:189:ARG:CG	3:L:189:ARG:O	2.43	0.59
2:C:36:GLU:CG	2:C:36:GLU:O	2.50	0.59
2:J:224:LEU:HD22	3:L:191:LEU:HD21	1.83	0.59
1:B:99:THR:CG2	1:B:103:PHE:HB2	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:39:THR:OG1	2:J:40:VAL:N	2.35	0.59
2:J:114:THR:HG22	2:J:115:ALA:N	2.17	0.59
2:J:26:MET:HE3	2:J:45:LEU:CB	2.33	0.59
2:J:26:MET:CE	2:J:45:LEU:CB	2.80	0.58
1:H:91:LEU:HD23	1:H:107:VAL:CG1	2.33	0.58
1:H:41:ASN:HD21	1:H:162:VAL:HA	1.67	0.58
1:H:99:THR:CG2	1:H:103:PHE:HB2	2.34	0.58
2:J:77:GLU:O	2:J:81:THR:OG1	2.10	0.58
2:C:20:GLU:HG2	4:C:236:HOH:O	2.03	0.58
2:J:110:VAL:CG1	2:J:111:PRO:CD	2.77	0.58
2:C:32:THR:HG22	2:C:33:VAL:H	1.68	0.58
2:C:93:GLU:OE2	2:D:18:ARG:NH1	2.35	0.57
2:I:37:GLU:HG2	4:I:503:HOH:O	2.03	0.57
2:J:36:GLU:O	2:J:37:GLU:HB2	2.04	0.57
2:I:26:MET:HE2	2:I:45:LEU:HD23	1.85	0.57
1:H:9:ASP:HB3	1:H:12:VAL:HG13	1.86	0.57
2:I:6:ASN:OD1	2:I:28:LYS:HE2	2.04	0.57
2:J:110:VAL:HG13	2:J:111:PRO:CD	2.35	0.57
2:C:160:ALA:HB1	2:C:171:ARG:HG3	1.85	0.57
2:C:33:VAL:HB	2:C:36:GLU:HG3	1.85	0.57
2:C:215:TYR:CE1	2:C:219:THR:HG21	2.40	0.56
2:J:87:ARG:HG2	2:J:87:ARG:NH1	2.10	0.56
2:C:32:THR:HG23	2:C:33:VAL:N	2.20	0.56
1:H:5:MET:HE2	1:H:12:VAL:HG12	1.87	0.56
2:I:93:GLU:OE2	2:J:18:ARG:NH1	2.32	0.56
1:A:40:SER:HB3	1:A:43:LEU:HD22	1.87	0.56
2:D:114:THR:O	2:D:119:LYS:HE3	2.06	0.56
2:D:140:ALA:O	2:D:144:GLU:HG3	2.06	0.56
1:H:20:VAL:HG12	1:H:21:LEU:HD13	1.87	0.56
2:C:215:TYR:O	2:C:219:THR:HG23	2.05	0.55
1:B:5:MET:HB2	1:B:23:ALA:HB1	1.88	0.55
2:I:39:THR:CG2	2:I:42:GLU:HG3	2.22	0.55
2:J:26:MET:HE2	2:J:45:LEU:HB3	1.88	0.55
2:I:3:ARG:HD2	2:I:32:THR:OG1	2.07	0.55
2:C:93:GLU:CD	2:D:18:ARG:HH12	2.10	0.55
4:A:422:HOH:O	2:C:233:THR:HG21	2.06	0.55
2:I:32:THR:O	2:I:33:VAL:C	2.45	0.55
1:A:41:ASN:HD21	1:A:162:VAL:HA	1.72	0.55
1:B:106:GLU:OE1	4:B:344:HOH:O	2.18	0.55
1:B:70:VAL:HG22	1:B:91:LEU:HD13	1.87	0.54
1:H:99:THR:HG23	1:H:100:ALA:N	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:91:GLU:HA	2:I:94:LEU:HD12	1.88	0.54
2:I:67:ILE:HG22	2:I:83:ILE:HD13	1.89	0.54
2:C:176:LEU:HD13	2:C:225:LEU:HD13	1.89	0.54
2:C:3:ARG:CG	2:C:32:THR:HG21	2.38	0.54
2:C:143:LYS:O	2:C:147:GLU:HG2	2.07	0.54
2:I:184:GLU:OE1	3:K:190:VAL:HG11	2.07	0.54
1:H:78:SER:HB2	1:H:79:PRO:HD2	1.90	0.54
2:D:104:LEU:HG	2:D:109:LEU:HD22	1.89	0.54
2:C:3:ARG:HD3	2:C:6:ASN:HD22	1.71	0.53
1:A:99:THR:CG2	1:A:103:PHE:HB2	2.39	0.53
2:C:2:SER:OG	2:C:4:GLU:HG2	2.08	0.53
2:D:105:LEU:CD1	2:D:109:LEU:HD23	2.38	0.53
2:D:37:GLU:OE2	2:D:114:THR:HB	2.09	0.53
2:I:110:VAL:HB	2:I:111:PRO:HD3	1.89	0.53
2:J:39:THR:HG23	2:J:42:GLU:H	1.74	0.52
2:J:114:THR:O	2:J:119:LYS:HE2	2.09	0.52
2:J:72:GLU:OE1	4:J:747:HOH:O	2.19	0.52
2:D:69:GLN:HA	2:D:72:GLU:HB2	1.90	0.52
1:A:97:GLY:O	1:A:98:THR:CB	2.39	0.52
2:C:33:VAL:CG2	2:C:36:GLU:O	2.57	0.52
2:C:30:ALA:HA	2:C:38:LEU:HD21	1.90	0.52
3:F:189:ARG:N	4:F:708:HOH:O	2.42	0.52
1:A:98:THR:HG21	2:C:226:ARG:NH1	2.17	0.52
2:C:154:LYS:HD3	4:C:533:HOH:O	2.10	0.52
1:H:116:THR:HB	4:H:192:HOH:O	2.08	0.52
2:I:18:ARG:NH1	2:J:93:GLU:CD	2.63	0.52
2:J:128:ASP:OD1	2:J:153:TYR:OH	2.25	0.52
2:D:127:GLY:HA3	2:D:153:TYR:CE1	2.44	0.52
2:C:32:THR:CG2	2:C:33:VAL:H	2.20	0.51
3:E:191:LEU:C	3:E:191:LEU:HD23	2.30	0.51
2:C:195:LEU:O	2:C:195:LEU:HD23	2.10	0.51
2:I:18:ARG:NH1	2:J:93:GLU:OE2	2.42	0.51
1:G:99:THR:HG22	1:G:100:ALA:N	2.22	0.51
2:D:87:ARG:HG2	2:D:87:ARG:NH1	2.26	0.51
2:I:233:THR:HG22	4:I:573:HOH:O	2.09	0.51
1:A:140:TRP:HB2	1:A:142:GLN:OE1	2.10	0.51
4:A:328:HOH:O	2:C:204:ILE:HG21	2.10	0.51
2:I:133:LEU:O	2:I:137:LYS:HG2	2.10	0.51
1:A:49:MET:CG	4:A:194:HOH:O	2.55	0.51
2:C:198:GLN:NE2	2:C:202:GLU:OE1	2.44	0.51
2:I:39:THR:CG2	2:I:42:GLU:CD	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:104:LEU:HG	2:C:109:LEU:HD22	1.93	0.50
2:C:39:THR:HG23	2:C:42:GLU:CD	2.31	0.50
1:G:91:LEU:HD23	1:G:107:VAL:CG1	2.42	0.50
1:A:108:MET:SD	1:A:137:ALA:HB1	2.52	0.50
3:K:189:ARG:HA	3:K:189:ARG:NH1	2.22	0.50
1:G:41:ASN:HD22	1:G:163:TYR:H	1.59	0.50
1:B:99:THR:HG23	1:B:103:PHE:HB2	1.93	0.50
2:C:233:THR:HG23	2:C:233:THR:O	2.12	0.50
2:I:78:GLU:HA	2:I:78:GLU:OE1	2.11	0.50
2:C:43:ARG:HD3	2:C:121:PHE:CZ	2.47	0.50
2:I:233:THR:HG23	2:I:233:THR:O	2.11	0.50
2:I:220:LEU:HD11	4:I:400:HOH:O	2.11	0.50
2:D:114:THR:CG2	2:D:115:ALA:N	2.75	0.50
1:G:107:VAL:HG12	1:G:108:MET:HG2	1.92	0.50
2:D:33:VAL:HA	2:D:36:GLU:O	2.12	0.49
2:I:43:ARG:HD3	2:I:121:PHE:CE1	2.46	0.49
2:D:110:VAL:N	2:D:111:PRO:CD	2.75	0.49
2:J:26:MET:HE3	2:J:45:LEU:HB2	1.93	0.49
2:D:39:THR:OG1	2:D:42:GLU:HG3	2.12	0.49
1:A:6:ARG:HH22	1:H:132:ARG:HH11	1.60	0.49
2:D:231:LEU:O	2:D:234:SER:OG	2.23	0.49
2:J:33:VAL:HG13	2:J:36:GLU:HB2	1.93	0.49
1:B:91:LEU:HD23	1:B:107:VAL:HG11	1.94	0.49
2:C:174:LEU:C	2:C:174:LEU:HD13	2.33	0.49
2:I:116:ALA:O	2:I:120:VAL:HG23	2.12	0.49
2:I:220:LEU:CD1	2:I:221:ILE:HD13	2.40	0.49
2:I:136:PHE:CE2	2:I:137:LYS:HD3	2.48	0.49
2:J:72:GLU:C	2:J:74:ARG:H	2.16	0.49
1:B:77:PRO:HD2	1:B:81:ASP:O	2.13	0.49
2:D:213:GLU:H	2:D:213:GLU:CD	2.16	0.48
2:I:15:GLN:O	2:J:63:ILE:HD12	2.13	0.48
2:C:28:LYS:O	2:C:32:THR:HB	2.14	0.48
2:J:2:SER:OG	2:J:3:ARG:N	2.45	0.48
2:C:34:ASP:HB3	2:C:35:VAL:H	1.55	0.48
2:D:105:LEU:HA	2:D:109:LEU:HB2	1.95	0.48
2:I:174:LEU:C	2:I:174:LEU:HD13	2.33	0.48
1:A:71:MET:HA	1:A:123:VAL:O	2.14	0.48
1:G:138:PRO:HA	4:G:615:HOH:O	2.13	0.48
1:H:117:MET:H	1:H:168:ARG:NH1	2.11	0.48
2:J:188:SER:CB	4:J:598:HOH:O	2.37	0.48
3:K:189:ARG:N	4:K:713:HOH:O	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:43:ARG:HD3	2:I:121:PHE:CE2	2.49	0.48
2:I:34:ASP:C	2:I:36:GLU:H	2.15	0.48
2:C:124:LYS:HE3	3:E:195:PHE:CE1	2.48	0.48
1:H:132:ARG:NH2	2:J:205:SER:HA	2.29	0.48
1:G:99:THR:CG2	1:G:103:PHE:HB2	2.44	0.48
2:I:220:LEU:HD12	2:I:221:ILE:CD1	2.43	0.47
2:D:70:LYS:NZ	2:D:74:ARG:NH2	2.62	0.47
2:I:12:LEU:HD13	2:J:86:TYR:CD2	2.49	0.47
2:C:77:GLU:O	2:C:81:THR:HG22	2.14	0.47
2:D:32:THR:HG22	2:D:32:THR:O	2.14	0.47
2:J:3:ARG:HH12	2:J:33:VAL:CG2	2.27	0.47
2:C:195:LEU:C	2:C:195:LEU:HD23	2.35	0.47
2:D:47:SER:OG	3:F:195:PHE:OXT	2.31	0.47
2:D:34:ASP:O	2:D:35:VAL:HG22	2.15	0.47
2:J:35:VAL:HA	2:J:112:SER:HB2	1.96	0.47
2:J:26:MET:CE	2:J:45:LEU:HD23	2.44	0.47
1:A:85:ARG:HA	1:A:86:GLU:HA	1.65	0.47
1:A:74:PRO:HD2	1:A:121:ARG:O	2.14	0.47
2:D:22:MET:HG2	2:D:49:ALA:HB2	1.96	0.47
2:I:220:LEU:C	2:I:220:LEU:HD13	2.36	0.47
1:B:66:PHE:HE1	1:B:132:ARG:HG2	1.77	0.47
1:B:116:THR:HB	4:B:175:HOH:O	2.14	0.46
1:B:129:GLN:HB3	1:B:133:GLN:HE21	1.80	0.46
2:J:28:LYS:O	2:J:32:THR:HG23	2.15	0.46
1:H:99:THR:HG23	1:H:103:PHE:HB2	1.97	0.46
1:B:113:PRO:O	1:B:114:ARG:HD2	2.15	0.46
1:H:74:PRO:HD2	1:H:121:ARG:O	2.14	0.46
1:B:73:ASP:HB2	1:B:122:LEU:HD13	1.97	0.46
2:I:224:LEU:CD2	3:K:191:LEU:HD13	2.43	0.46
1:G:78:SER:HB2	1:G:117:MET:CB	2.43	0.46
2:J:157:GLN:HA	2:J:174:LEU:HD21	1.98	0.46
2:I:26:MET:CE	2:I:45:LEU:CD2	2.88	0.46
1:H:99:THR:HG23	1:H:103:PHE:CD1	2.50	0.46
2:J:59:ALA:O	2:J:63:ILE:HG12	2.16	0.46
2:I:26:MET:HE2	2:I:45:LEU:CB	2.41	0.46
2:I:26:MET:HE3	2:I:45:LEU:HB2	1.94	0.46
2:D:66:SER:HA	2:D:69:GLN:HG2	1.97	0.46
2:C:108:HIS:O	2:C:112:SER:HB3	2.17	0.46
2:J:26:MET:HE2	2:J:45:LEU:CB	2.45	0.46
2:C:62:ARG:NH2	4:C:304:HOH:O	2.48	0.46
2:D:50:TYR:CE1	2:D:101:ILE:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:99:THR:HG23	1:G:103:PHE:HB2	1.97	0.45
1:B:91:LEU:HD23	1:B:107:VAL:CG1	2.46	0.45
2:D:30:ALA:C	2:D:32:THR:H	2.20	0.45
1:A:51:THR:O	1:A:112:SER:HB3	2.17	0.45
1:G:108:MET:SD	1:G:137:ALA:HB1	2.57	0.45
2:C:172:LEU:HB3	2:C:221:ILE:HG21	1.98	0.45
2:I:161:LEU:O	2:I:161:LEU:HD22	2.16	0.45
2:I:76:ASN:HD22	2:I:76:ASN:N	2.15	0.45
1:B:64:ARG:HB2	1:H:6:ARG:HH22	1.82	0.45
1:H:91:LEU:HD21	1:H:149:PHE:CZ	2.52	0.45
2:C:20:GLU:H	2:C:20:GLU:CD	2.20	0.45
1:G:85:ARG:HA	1:G:86:GLU:HA	1.73	0.45
2:D:43:ARG:HD3	2:D:121:PHE:CZ	2.52	0.44
1:B:69:LEU:O	1:B:91:LEU:HD12	2.16	0.44
1:B:41:ASN:HD22	1:B:163:TYR:H	1.64	0.44
1:H:71:MET:HA	1:H:123:VAL:O	2.17	0.44
2:J:227:ASP:OD2	3:L:189:ARG:NH2	2.50	0.44
2:I:183:TYR:CE1	2:I:232:TRP:CD1	3.06	0.44
2:C:76:ASN:OD1	2:C:76:ASN:N	2.50	0.44
1:G:70:VAL:HG22	1:G:91:LEU:HD13	1.99	0.44
2:J:53:VAL:HG12	2:J:97:ILE:HD13	1.99	0.44
2:I:38:LEU:HA	2:I:42:GLU:OE1	2.18	0.44
2:C:28:LYS:CE	4:C:566:HOH:O	2.56	0.44
1:H:46:LYS:HG3	1:H:169:GLU:HG2	2.00	0.44
2:I:186:LEU:HD12	2:I:186:LEU:HA	1.81	0.44
2:J:26:MET:HE3	2:J:45:LEU:HB3	1.91	0.44
2:I:194:ASN:N	2:I:194:ASN:HD22	2.16	0.44
2:J:119:LYS:HE3	2:J:119:LYS:HB2	1.83	0.43
2:I:35:VAL:CG1	2:I:35:VAL:O	2.64	0.43
1:G:70:VAL:HG22	1:G:91:LEU:CD1	2.48	0.43
2:J:134:ALA:O	2:J:142:ARG:NH2	2.50	0.43
2:C:68:GLU:OE1	2:C:87:ARG:NE	2.35	0.43
2:D:60:SER:HA	2:D:63:ILE:HD11	1.99	0.43
1:H:117:MET:N	1:H:168:ARG:NH1	2.67	0.43
2:I:36:GLU:HB2	2:I:37:GLU:H	1.62	0.43
2:D:110:VAL:N	2:D:111:PRO:HD2	2.33	0.43
1:H:88:LEU:O	1:H:141:ARG:HD3	2.17	0.43
2:J:114:THR:CG2	2:J:115:ALA:N	2.81	0.43
1:A:41:ASN:HD22	1:A:163:TYR:H	1.67	0.43
2:I:172:LEU:HD21	2:I:203:ALA:HB2	2.01	0.43
3:L:195:PHE:CD1	3:L:195:PHE:C	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:33:VAL:HG12	2:J:34:ASP:N	2.34	0.43
1:A:170:ALA:HB2	4:A:705:HOH:O	2.18	0.43
1:A:54:PRO:HD2	1:A:90:TRP:CZ3	2.53	0.43
1:B:85:ARG:HA	1:B:86:GLU:HA	1.73	0.43
1:B:96:PRO:HD2	1:B:99:THR:HG21	2.00	0.43
2:J:121:PHE:CE1	2:J:125:MET:HE3	2.51	0.43
1:G:40:SER:O	1:G:41:ASN:C	2.57	0.43
2:C:77:GLU:O	2:C:81:THR:CG2	2.67	0.43
2:D:50:TYR:CZ	2:D:101:ILE:HB	2.53	0.43
2:C:69:GLN:HG2	2:C:69:GLN:H	1.67	0.43
1:H:85:ARG:HA	1:H:86:GLU:HA	1.75	0.43
2:C:154:LYS:HG2	4:C:619:HOH:O	2.18	0.43
1:B:46:LYS:HG2	1:B:169:GLU:CG	2.49	0.42
2:J:137:LYS:HA	2:J:137:LYS:HD2	1.51	0.42
1:B:20:VAL:HG12	1:B:21:LEU:HG	2.00	0.42
2:I:26:MET:HE2	2:I:45:LEU:CG	2.48	0.42
2:C:39:THR:HG23	2:C:42:GLU:OE1	2.19	0.42
1:B:55:ARG:HD3	4:D:572:HOH:O	2.19	0.42
2:I:35:VAL:C	2:I:36:GLU:HG3	2.39	0.42
2:I:1:MET:O	2:I:3:ARG:NH1	2.43	0.42
1:G:46:LYS:CE	4:G:330:HOH:O	2.67	0.42
2:J:220:LEU:O	2:J:220:LEU:HD22	2.18	0.42
1:G:71:MET:HB3	1:G:90:TRP:HB3	2.01	0.42
2:I:3:ARG:NE	2:I:6:ASN:ND2	2.67	0.42
2:D:27:GLU:OE1	2:D:104:LEU:HD22	2.20	0.42
1:A:99:THR:HG23	1:A:103:PHE:CD1	2.54	0.42
1:G:124:PHE:O	1:G:161:ALA:HA	2.20	0.42
2:I:33:VAL:O	2:I:33:VAL:CG1	2.68	0.42
2:I:3:ARG:O	2:I:7:VAL:HG23	2.20	0.42
1:A:63:MET:HE2	4:A:697:HOH:O	2.20	0.42
2:D:74:ARG:HB3	2:D:76:ASN:ND2	2.35	0.42
2:I:197:LYS:HE2	2:I:201:ASP:OD1	2.20	0.42
2:J:121:PHE:CE1	2:J:125:MET:HE2	2.52	0.42
1:H:69:LEU:O	1:H:91:LEU:HD12	2.19	0.42
2:C:72:GLU:OE2	2:C:84:LYS:NZ	2.53	0.42
2:J:137:LYS:HG3	2:J:141:GLU:HB2	2.02	0.41
1:B:132:ARG:HH21	1:G:6:ARG:NH2	2.18	0.41
2:D:63:ILE:HG12	2:D:64:VAL:N	2.34	0.41
2:C:172:LEU:HB3	2:C:221:ILE:CG2	2.49	0.41
1:B:137:ALA:C	1:B:138:PRO:O	2.57	0.41
2:J:126:LYS:HE3	4:J:238:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:168:HIS:HA	2:I:169:PRO:HD3	1.95	0.41
2:C:35:VAL:HG22	2:C:112:SER:HA	2.02	0.41
1:A:9:ASP:HB3	1:A:12:VAL:HG13	2.01	0.41
2:D:33:VAL:CG1	2:D:38:LEU:HG	2.51	0.41
1:B:41:ASN:ND2	1:B:162:VAL:HA	2.32	0.41
2:D:168:HIS:HE1	2:D:170:ILE:HD12	1.85	0.41
1:G:30:LEU:HD13	1:G:126:LEU:HD22	2.03	0.41
1:B:132:ARG:HG3	1:B:132:ARG:H	1.57	0.41
1:G:91:LEU:HD23	1:G:107:VAL:HG11	2.03	0.41
3:K:189:ARG:NH1	4:K:623:HOH:O	2.54	0.41
1:H:70:VAL:HG22	1:H:91:LEU:HD13	2.02	0.41
2:I:91:GLU:HG2	2:I:136:PHE:CD2	2.56	0.41
2:C:216:LYS:HE2	2:C:216:LYS:HB3	1.81	0.41
2:J:14:GLU:OE2	2:J:48:VAL:HG11	2.21	0.41
2:J:68:GLU:OE1	2:J:87:ARG:NE	2.53	0.41
1:H:99:THR:CG2	1:H:103:PHE:CB	2.99	0.40
2:C:35:VAL:HA	2:C:112:SER:CB	2.49	0.40
2:J:3:ARG:HG3	2:J:4:GLU:N	2.35	0.40
2:I:3:ARG:HE	2:I:6:ASN:ND2	2.20	0.40
1:G:143:ASN:ND2	4:G:221:HOH:O	2.51	0.40
2:D:98:CYS:O	2:D:102:LEU:HB2	2.22	0.40
2:C:39:THR:OG1	2:C:40:VAL:N	2.54	0.40
1:G:83:ASN:ND2	1:G:83:ASN:H	2.19	0.40
2:J:99:ASP:OD2	2:J:103:LYS:HE2	2.22	0.40
1:G:167:GLN:O	1:G:168:ARG:C	2.60	0.40
2:D:166:PRO:O	2:D:203:ALA:HB2	2.21	0.40
3:K:189:ARG:CZ	3:K:190:VAL:HG12	2.51	0.40
2:J:26:MET:HE2	2:J:45:LEU:HD23	2.02	0.40

There are no symmetry-related clashes.

## 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	164/170 (96%)	153 (93%)	11 (7%)	0	100	100
1	B	164/170 (96%)	159 (97%)	5 (3%)	0	100	100
1	G	163/170 (96%)	154 (94%)	7 (4%)	2 (1%)	16	23
1	H	164/170 (96%)	156 (95%)	8 (5%)	0	100	100
2	C	233/240 (97%)	224 (96%)	6 (3%)	3 (1%)	15	21
2	D	233/240 (97%)	221 (95%)	12 (5%)	0	100	100
2	I	233/240 (97%)	226 (97%)	3 (1%)	4 (2%)	11	14
2	J	232/240 (97%)	218 (94%)	12 (5%)	2 (1%)	21	30
3	E	4/9 (44%)	4 (100%)	0	0	100	100
3	F	4/9 (44%)	4 (100%)	0	0	100	100
3	K	4/9 (44%)	4 (100%)	0	0	100	100
3	L	4/9 (44%)	4 (100%)	0	0	100	100
All	All	1602/1676 (96%)	1527 (95%)	64 (4%)	11 (1%)	26	38

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	37	GLU
2	I	33	VAL
2	I	38	LEU
2	C	34	ASP
1	G	168	ARG
2	I	37	GLU
2	J	37	GLU
1	G	138	PRO
2	I	35	VAL
2	J	73	GLY
2	C	35	VAL

### 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	145/147 (99%)	132 (91%)	13 (9%)	12	17
1	B	145/147 (99%)	137 (94%)	8 (6%)	27	42
1	G	145/147 (99%)	137 (94%)	8 (6%)	27	42
1	H	145/147 (99%)	129 (89%)	16 (11%)	8	10
2	C	201/204 (98%)	166 (83%)	35 (17%)	2	2
2	D	201/204 (98%)	178 (89%)	23 (11%)	7	9
2	I	201/204 (98%)	182 (90%)	19 (10%)	11	15
2	J	200/204 (98%)	167 (84%)	33 (16%)	3	3
3	E	5/7 (71%)	4 (80%)	1 (20%)	1	1
3	F	5/7 (71%)	3 (60%)	2 (40%)	0	0
3	K	5/7 (71%)	4 (80%)	1 (20%)	1	1
3	L	5/7 (71%)	3 (60%)	2 (40%)	0	0
All	All	1403/1432 (98%)	1242 (88%)	161 (12%)	7	9

All (161) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	12	VAL
1	A	15	ARG
1	A	43	LEU
1	A	45	LEU
1	A	58	VAL
1	A	86	GLU
1	A	98	THR
1	A	99	THR
1	A	105	GLN
1	A	133	GLN
1	A	142	GLN
1	A	151	GLU
1	B	25	VAL
1	B	61	ASN
1	B	78	SER
1	B	99	THR
1	B	116	THR
1	B	130	LEU
1	B	132	ARG
1	B	169	GLU
2	C	3	ARG

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Mol	Chain	Res	Type
2	C	4	GLU
2	C	12	LEU
2	C	18	ARG
2	C	27	GLU
2	C	32	THR
2	C	34	ASP
2	C	36	GLU
2	C	39	THR
2	C	41	GLU
2	C	45	LEU
2	C	51	LYS
2	C	63	ILE
2	C	69	GLN
2	C	70	LYS
2	C	71	GLU
2	C	76	ASN
2	C	77	GLU
2	C	81	THR
2	C	82	LEU
2	C	84	LYS
2	C	96	LYS
2	C	102	LEU
2	C	109	LEU
2	C	143	LYS
2	C	154	LYS
2	C	172	LEU
2	C	178	PHE
2	C	186	LEU
2	C	198	GLN
2	C	207	LEU
2	C	220	LEU
2	C	225	LEU
2	C	231	LEU
2	C	233	THR
2	D	3	ARG
2	D	27	GLU
2	D	37	GLU
2	D	45	LEU
2	D	51	LYS
2	D	63	ILE
2	D	65	SER
2	D	72	GLU

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Mol	Chain	Res	Type
2	D	84	LYS
2	D	89	LYS
2	D	102	LEU
2	D	105	LEU
2	D	109	LEU
2	D	112	SER
2	D	114	THR
2	D	142	ARG
2	D	144	GLU
2	D	161	LEU
2	D	178	PHE
2	D	188	SER
2	D	207	LEU
2	D	213	GLU
2	D	231	LEU
3	E	191	LEU
3	F	189	ARG
3	F	190	VAL
1	G	6	ARG
1	G	7	ASP
1	G	8	ARG
1	G	69	LEU
1	G	78	SER
1	G	99	THR
1	G	132	ARG
1	G	151	GLU
1	H	6	ARG
1	H	7	ASP
1	H	21	LEU
1	H	25	VAL
1	H	44	GLU
1	H	46	LYS
1	H	61	ASN
1	H	62	ASP
1	H	99	THR
1	H	106	GLU
1	H	114	ARG
1	H	116	THR
1	H	130	LEU
1	H	147	LYS
1	H	151	GLU
1	H	169	GLU

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Mol	Chain	Res	Type
2	I	4	GLU
2	I	12	LEU
2	I	26	MET
2	I	35	VAL
2	I	36	GLU
2	I	39	THR
2	I	45	LEU
2	I	51	LYS
2	I	67	ILE
2	I	125	MET
2	I	138	THR
2	I	154	LYS
2	I	161	LEU
2	I	178	PHE
2	I	186	LEU
2	I	188	SER
2	I	213	GLU
2	I	231	LEU
2	I	233	THR
2	J	3	ARG
2	J	4	GLU
2	J	12	LEU
2	J	26	MET
2	J	28	LYS
2	J	33	VAL
2	J	34	ASP
2	J	36	GLU
2	J	39	THR
2	J	45	LEU
2	J	51	LYS
2	J	63	ILE
2	J	65	SER
2	J	66	SER
2	J	70	LYS
2	J	74	ARG
2	J	84	LYS
2	J	85	GLU
2	J	96	LYS
2	J	114	THR
2	J	119	LYS
2	J	137	LYS
2	J	138	THR

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Mol	Chain	Res	Type
2	J	141	GLU
2	J	144	GLU
2	J	178	PHE
2	J	188	SER
2	J	207	LEU
2	J	213	GLU
2	J	214	SER
2	J	219	THR
2	J	220	LEU
2	J	229	LEU
3	K	189	ARG
3	L	189	ARG
3	L	191	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	41	ASN
1	A	83	ASN
1	A	165	ASN
1	A	167	GLN
1	B	41	ASN
1	B	52	HIS
1	B	133	GLN
1	B	165	ASN
2	C	6	ASN
2	C	69	GLN
2	C	194	ASN
2	C	223	GLN
2	D	52	ASN
2	D	76	ASN
2	D	194	ASN
2	D	223	GLN
1	G	29	ASN
1	G	41	ASN
1	G	83	ASN
1	G	133	GLN
1	G	143	ASN
1	G	165	ASN
1	H	41	ASN
2	I	76	ASN

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Mol	Chain	Res	Type
2	I	194	ASN
2	I	198	GLN
2	J	52	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
3	SEP	E	192	3	8,9,10	1.40	1 (12%)	8,12,14	2.30	1 (12%)
3	SEP	F	192	3	8,9,10	1.55	1 (12%)	8,12,14	1.78	3 (37%)
3	SEP	K	192	3	8,9,10	1.53	1 (12%)	8,12,14	2.11	2 (25%)
3	SEP	L	192	3	8,9,10	1.47	1 (12%)	8,12,14	1.49	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SEP	E	192	3	-	0/6/8/10	0/0/0/0
3	SEP	F	192	3	-	0/6/8/10	0/0/0/0
3	SEP	K	192	3	-	0/6/8/10	0/0/0/0
3	SEP	L	192	3	-	0/6/8/10	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	192	SEP	P-O1P	2.83	1.60	1.51
3	L	192	SEP	P-O1P	2.92	1.60	1.51
3	K	192	SEP	P-O1P	3.18	1.61	1.51
3	F	192	SEP	P-O1P	3.40	1.62	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	192	SEP	O-C-CA	-2.01	120.25	125.49
3	F	192	SEP	O3P-P-OG	2.35	113.33	106.56
3	K	192	SEP	O3P-P-OG	2.40	113.47	106.56
3	L	192	SEP	OG-CB-CA	2.98	110.82	108.27
3	F	192	SEP	OG-CB-CA	3.74	111.46	108.27
3	K	192	SEP	OG-CB-CA	4.76	112.33	108.27
3	E	192	SEP	OG-CB-CA	5.45	112.93	108.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	192	SEP	1	0
3	F	192	SEP	1	0
3	K	192	SEP	1	0
3	L	192	SEP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	166/170 (97%)	-0.28	5 (3%) 54 53	12, 25, 44, 60	0
1	B	166/170 (97%)	-0.06	3 (1%) 71 71	17, 32, 56, 68	0
1	G	165/170 (97%)	-0.15	1 (0%) 90 90	13, 23, 44, 60	0
1	H	166/170 (97%)	-0.31	1 (0%) 90 90	17, 32, 48, 69	0
2	C	235/240 (97%)	-0.18	5 (2%) 67 66	15, 27, 58, 76	0
2	D	235/240 (97%)	-0.05	6 (2%) 59 58	18, 33, 64, 80	0
2	I	235/240 (97%)	-0.05	7 (2%) 54 53	14, 27, 60, 75	0
2	J	234/240 (97%)	-0.04	8 (3%) 49 49	19, 35, 69, 77	0
3	E	6/9 (66%)	0.28	0 100 100	25, 31, 43, 53	0
3	F	6/9 (66%)	0.47	0 100 100	30, 37, 44, 57	0
3	K	6/9 (66%)	-0.29	0 100 100	22, 30, 41, 52	0
3	L	6/9 (66%)	0.87	1 (16%) 2 2	35, 41, 49, 58	0
All	All	1626/1676 (97%)	-0.12	37 (2%) 64 63	12, 29, 57, 80	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	35	VAL	8.0
2	D	35	VAL	6.7
2	I	33	VAL	6.0
2	I	35	VAL	5.6
2	D	34	ASP	5.4
2	I	34	ASP	5.0
2	D	33	VAL	4.8
2	J	35	VAL	4.5
2	D	36	GLU	4.4
2	J	32	THR	4.3
1	B	170	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
2	I	73	GLY	3.9
2	C	32	THR	3.8
2	J	34	ASP	3.7
2	J	33	VAL	3.7
1	A	170	ALA	3.6
1	A	130	LEU	3.0
1	A	132	ARG	2.8
2	D	32	THR	2.8
1	H	170	ALA	2.8
2	C	34	ASP	2.7
3	L	191	LEU	2.7
2	J	75	GLY	2.7
2	C	33	VAL	2.6
2	C	36	GLU	2.6
2	D	235	ASP	2.4
2	J	77	GLU	2.4
1	B	136	TYR	2.2
2	I	78	GLU	2.2
1	A	140	TRP	2.2
2	I	36	GLU	2.2
2	J	81	THR	2.2
2	J	80	VAL	2.1
1	G	136	TYR	2.1
1	A	136	TYR	2.1
1	B	108	MET	2.0
2	I	2	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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	SEP	E	192	10/11	0.98	0.14	-	18,27,30,32	0
3	SEP	L	192	10/11	0.99	0.12	-	19,28,33,36	0
3	SEP	F	192	10/11	0.98	0.11	-	16,27,29,31	0
3	SEP	K	192	10/11	0.98	0.12	-	10,21,23,26	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.