



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:26 am BST

PDB ID : 6ISO  
Title : Human SIRT3 Recognizing H3K4cr  
Authors : Wang, Y.; Hao, Q.  
Deposited on : 2018-11-17  
Resolution : 2.95 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

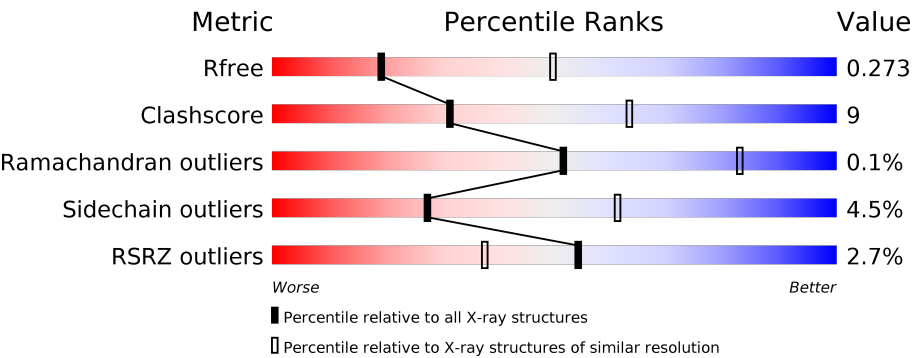
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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))
$R_{free}$	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 respectively. 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	275	<div><div>%</div><div><div></div><div>82%</div><div>15%</div><div>••</div></div></div>
1	B	275	<div><div></div><div>85%</div><div>9%</div><div>••</div></div>
1	E	275	<div><div></div><div>80%</div><div>13%</div><div>••</div></div>
1	G	275	<div><div>4%</div><div></div><div>75%</div><div>16%</div><div>•</div><div>7%</div></div>
1	I	275	<div><div>4%</div><div></div><div>68%</div><div>21%</div><div>•</div><div>10%</div></div>
1	K	275	<div><div>5%</div><div></div><div>52%</div><div>16%</div><div>•</div><div>29%</div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	C	7	 100%
2	D	7	 43% 57%
2	F	7	 14% 86% 14%
2	H	7	 57% 43%
2	J	7	 14% 57% 43%
2	L	7	 43% 43% 14%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CRD	L	101	-	-	-	X
5	GOL	E	401	-	-	-	X
5	GOL	K	401	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12241 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 NAD-dependent protein deacetylase sirtuin-3, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	1	1	0
			2127	1371	366	381	9			
1	B	264	Total	C	N	O	S	0	1	0
			2067	1335	354	369	9			
1	E	263	Total	C	N	O	S	1	1	0
			2059	1326	353	371	9			
1	G	255	Total	C	N	O	S	0	1	0
			1986	1281	342	355	8			
1	I	248	Total	C	N	O	S	0	0	0
			1924	1241	333	341	9			
1	K	194	Total	C	N	O	S	1	1	0
			1495	958	263	269	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	395	ALA	-	expression tag	UNP Q9NTG7
B	395	ALA	-	expression tag	UNP Q9NTG7
E	395	ALA	-	expression tag	UNP Q9NTG7
G	395	ALA	-	expression tag	UNP Q9NTG7
I	395	ALA	-	expression tag	UNP Q9NTG7
K	395	ALA	-	expression tag	UNP Q9NTG7

- Molecule 2 is a protein called ARG-THR-LYS-GLN-THR-ALA-ARG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			59	34	15	10			
2	D	7	Total	C	N	O	0	0	0
			59	34	15	10			
2	F	7	Total	C	N	O	0	0	0
			59	34	15	10			

*Continued on next page...*

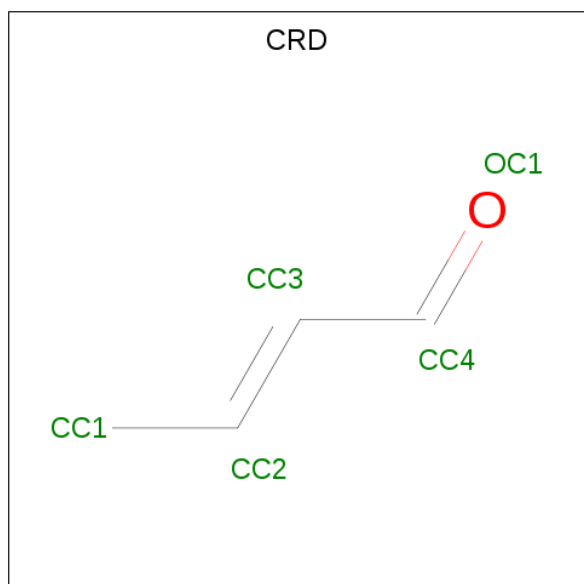
*Continued from previous page...*

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	H	7	Total	C	N	O	0	0	0
			59	34	15	10			
2	L	6	Total	C	N	O	0	0	0
			48	28	11	9			
2	J	7	Total	C	N	O	0	0	0
			59	34	15	10			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	I	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (2E)-BUT-2-ENAL (three-letter code: CRD) (formula: C<sub>4</sub>H<sub>6</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			5	4	1		

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			5	4	1		
4	F	1	Total	C	O	0	0
			5	4	1		
4	H	1	Total	C	O	0	0
			5	4	1		
4	L	1	Total	C	O	0	0
			5	4	1		
4	J	1	Total	C	O	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		
5	G	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		

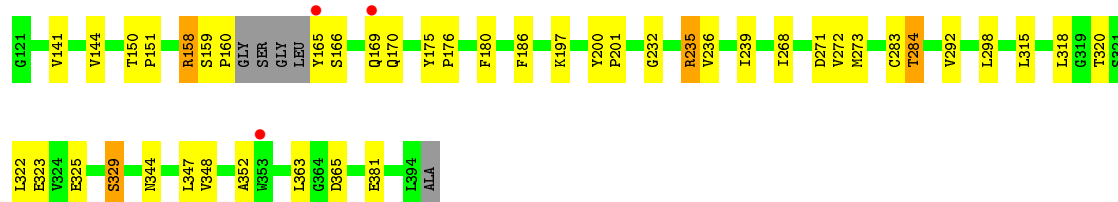
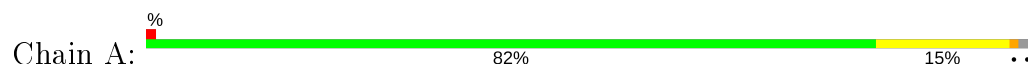
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	37	Total 37	O 37	0	0
6	B	30	Total 30	O 30	0	0
6	D	1	Total 1	O 1	0	0
6	E	24	Total 24	O 24	0	0
6	F	1	Total 1	O 1	0	0
6	H	2	Total 2	O 2	0	0
6	G	37	Total 37	O 37	0	0
6	L	2	Total 2	O 2	0	0
6	I	26	Total 26	O 26	0	0
6	J	1	Total 1	O 1	0	0
6	K	20	Total 20	O 20	0	0

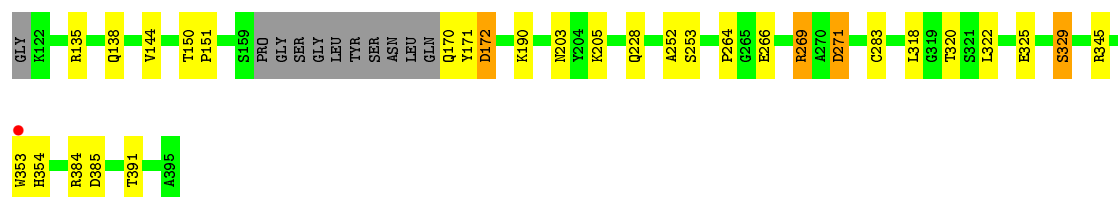
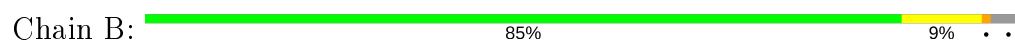
### 3 Residue-property plots [i](#)

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.

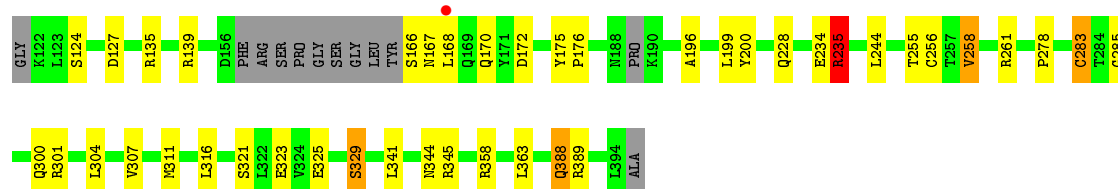
- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



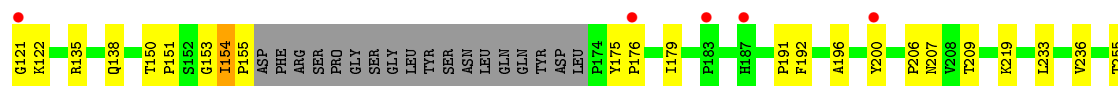
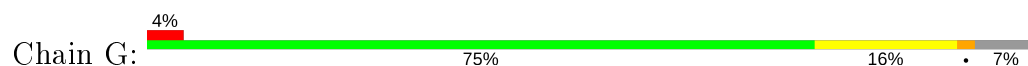
- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



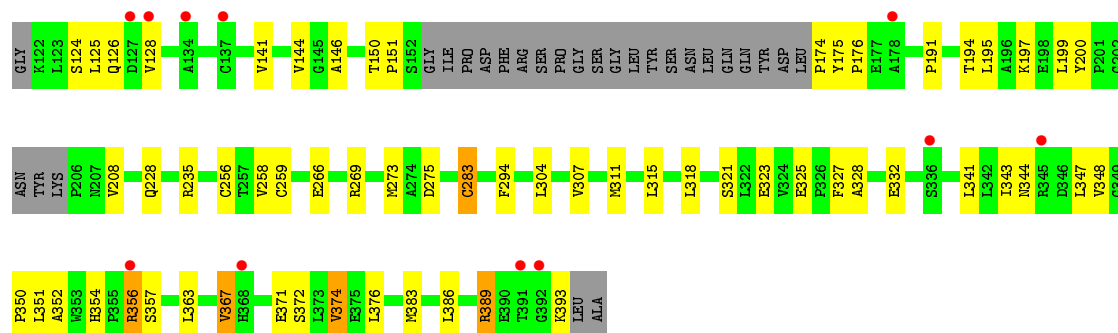
- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



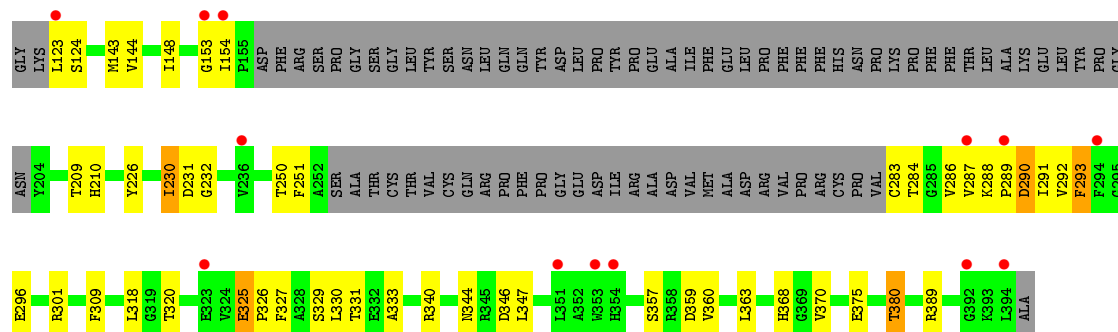




- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial



- Molecule 1: NAD-dependent protein deacetylase sirtuin-3, mitochondrial

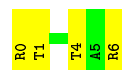


- Molecule 2: ARG-THR-LYS-GLN-THR-ALA-ARG

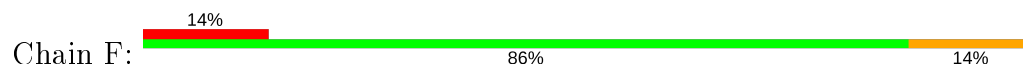


There are no outlier residues recorded for this chain.

- Molecule 2: ARG-THR-LYS-GLN-THR-ALA-ARG

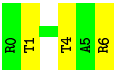


- Molecule 2: ARG-THR-LYS-GLN-THR-ALA-ARG





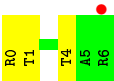
• Molecule 2: ARG-THR-LYS-GLN-THR-ALA-ARG



• Molecule 2: ARG-THR-LYS-GLN-THR-ALA-ARG



• Molecule 2: ARG-THR-LYS-GLN-THR-ALA-ARG



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.09Å 138.09Å 225.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.25 – 2.95 39.25 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.25-2.95) 98.0 (39.25-2.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 2.95Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.221 , 0.275 0.221 , 0.273	Depositor DCC
$R_{free}$ test set	2319 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	48.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12241	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, CRD

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	0.69	0/2186	0.84	3/2977 (0.1%)
1	B	0.66	0/2124	0.82	2/2894 (0.1%)
1	E	0.67	0/2112	0.89	5/2875 (0.2%)
1	G	0.65	0/2039	0.85	2/2776 (0.1%)
1	I	0.65	0/1970	0.80	0/2681
1	K	0.76	2/1528 (0.1%)	0.83	0/2078
2	C	0.76	0/58	1.04	0/75
2	D	0.65	0/58	1.02	0/75
2	F	0.68	0/58	0.98	0/75
2	H	0.65	0/58	0.91	0/75
2	J	0.72	0/58	0.94	0/75
2	L	0.71	0/47	1.02	0/61
All	All	0.68	2/12296 (0.0%)	0.84	12/16717 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	329[A]	SER	CB-OG	8.45	1.53	1.42
1	K	329[B]	SER	CB-OG	8.45	1.53	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	235	ARG	NE-CZ-NH2	-16.98	111.81	120.30
1	E	235	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	G	329[A]	SER	CA-CB-OG	-6.91	92.53	111.20
1	G	329[B]	SER	CA-CB-OG	-6.91	92.53	111.20
1	E	329[A]	SER	CA-CB-OG	-6.91	92.54	111.20
1	E	329[B]	SER	CA-CB-OG	-6.91	92.54	111.20
1	A	329[A]	SER	CA-CB-OG	-6.88	92.62	111.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329[B]	SER	CA-CB-OG	-6.88	92.62	111.20
1	B	329[A]	SER	CA-CB-OG	-6.79	92.87	111.20
1	B	329[B]	SER	CA-CB-OG	-6.79	92.87	111.20
1	E	235	ARG	CD-NE-CZ	6.61	132.85	123.60
1	A	365	ASP	CB-CG-OD1	-5.16	113.66	118.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2127	0	2141	35	0
1	B	2067	0	2077	14	1
1	E	2059	0	2071	28	0
1	G	1986	0	2013	50	1
1	I	1924	0	1935	50	0
1	K	1495	0	1527	38	0
2	C	59	0	65	0	0
2	D	59	0	65	3	0
2	F	59	0	66	1	0
2	H	59	0	66	3	0
2	J	59	0	66	1	0
2	L	48	0	52	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
4	C	5	0	5	1	0
4	D	5	0	5	0	0
4	F	5	0	5	0	0
4	H	5	0	5	0	0
4	J	5	0	5	0	0
4	L	5	0	5	0	0
5	B	6	0	8	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	6	0	8	1	0
5	G	6	0	8	0	0
5	K	6	0	8	0	0
6	A	37	0	0	4	0
6	B	30	0	0	1	0
6	D	1	0	0	1	0
6	E	24	0	0	2	0
6	F	1	0	0	0	0
6	G	37	0	0	5	0
6	H	2	0	0	0	0
6	I	26	0	0	5	0
6	J	1	0	0	0	0
6	K	20	0	0	2	0
6	L	2	0	0	0	0
All	All	12241	0	12206	218	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 9.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:NH1	1:A:239:ILE:O	1.61	1.28
1:A:166:SER:HB3	1:A:169:GLN:HG3	1.30	1.09
1:G:154:ILE:HG13	1:G:155:PRO:HD3	1.12	1.06
1:G:283:CYS:SG	6:G:533:HOH:O	2.01	1.05
1:E:258:VAL:HG13	1:E:283:CYS:SG	1.99	1.02
1:A:235:ARG:HH11	1:A:235:ARG:HG2	1.30	0.97
1:A:159:SER:HB3	1:A:160:PRO:HA	1.46	0.97
1:G:154:ILE:HG13	1:G:155:PRO:CD	1.96	0.95
1:I:347:LEU:HD12	1:I:348:VAL:N	1.80	0.95
1:A:158:ARG:NH1	1:A:323:GLU:OE1	1.99	0.94
1:G:280:CYS:SG	6:G:530:HOH:O	2.17	0.92
1:I:356:ARG:HD3	1:I:357:SER:H	1.37	0.90
1:I:347:LEU:HD12	1:I:348:VAL:H	1.34	0.88
1:K:288:LYS:HG2	1:K:289:PRO:HD2	1.54	0.88
1:G:256:CYS:O	1:G:257:THR:OG1	1.91	0.88
1:E:244:LEU:O	1:E:301:ARG:NH1	2.08	0.88
1:E:258:VAL:CG1	1:E:283:CYS:SG	2.62	0.86
1:G:154:ILE:CG1	1:G:155:PRO:HD3	2.03	0.84
1:G:200:TYR:CD2	1:G:269:ARG:HD3	2.14	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:TYR:O	1:A:170:GLN:NE2	2.13	0.82
1:G:280:CYS:HB3	1:G:283:CYS:O	1.82	0.80
1:I:374:VAL:HG21	1:I:383:MET:HG3	1.65	0.79
1:I:150:THR:OG1	1:I:151:PRO:HD3	1.84	0.77
1:E:321:SER:OG	1:E:323:GLU:HG2	1.84	0.77
1:E:323:GLU:OE1	5:E:401:GOL:O1	2.03	0.76
1:G:255:THR:HG22	1:G:260:GLN:HB3	1.66	0.75
1:A:200:TYR:O	6:A:501:HOH:O	2.04	0.74
1:I:356:ARG:HD3	1:I:357:SER:N	2.03	0.73
1:B:266:GLU:OE2	1:B:269:ARG:NH2	2.21	0.72
1:I:228:GLN:HG3	1:I:327:PHE:CE2	2.25	0.72
1:A:320:THR:HG22	1:A:322:LEU:H	1.54	0.72
1:I:256:CYS:HB3	1:I:259:CYS:O	1.88	0.72
1:K:250:THR:O	1:K:290:ASP:O	2.08	0.71
1:G:280:CYS:SG	6:G:532:HOH:O	2.50	0.70
1:G:179:ILE:HD11	1:G:192:PHE:N	2.07	0.70
1:B:320:THR:HG22	1:B:322:LEU:H	1.57	0.69
1:I:124:SER:HB2	6:I:524:HOH:O	1.91	0.69
1:A:283:CYS:O	1:A:284:THR:HG22	1.92	0.69
1:A:166:SER:HB3	1:A:169:GLN:CG	2.15	0.69
1:G:206:PRO:HG3	1:G:236:VAL:HG23	1.75	0.69
1:K:327:PHE:O	1:K:330:LEU:HG	1.93	0.69
1:K:288:LYS:HD2	1:K:289:PRO:O	1.93	0.68
1:K:288:LYS:CG	1:K:289:PRO:HD2	2.24	0.68
1:I:350:PRO:O	1:I:354:HIS:N	2.22	0.68
1:G:209:THR:HG22	1:G:370:VAL:HG21	1.76	0.67
1:G:233:LEU:HA	1:G:236:VAL:HG22	1.76	0.67
1:I:175:TYR:HB2	1:I:176:PRO:HD2	1.78	0.66
1:I:197:LYS:HE3	1:I:273:MET:O	1.97	0.64
1:I:347:LEU:HD11	1:I:352:ALA:CA	2.27	0.64
1:G:135:ARG:NH1	1:G:219:LYS:O	2.31	0.64
1:G:200:TYR:HD2	1:G:269:ARG:HD3	1.64	0.63
1:G:196:ALA:O	1:G:200:TYR:HD1	1.82	0.63
1:B:385:ASP:OD2	1:E:135:ARG:NH1	2.32	0.63
1:E:124:SER:OG	1:E:127:ASP:OD1	2.17	0.62
1:I:372:SER:O	1:I:376:LEU:HD13	1.98	0.61
1:K:231:ASP:OD1	1:K:232:GLY:N	2.33	0.61
1:G:256:CYS:HB3	1:G:260:GLN:HA	1.82	0.61
1:G:256:CYS:O	1:G:286:VAL:O	2.19	0.61
1:G:258:VAL:O	1:G:260:GLN:N	2.35	0.60
1:A:150:THR:OG1	1:A:151:PRO:HD3	2.02	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:TYR:CD2	1:G:269:ARG:CD	2.83	0.59
1:A:348:VAL:HG12	6:A:525:HOH:O	2.03	0.59
1:G:255:THR:CG2	1:G:260:GLN:HB3	2.33	0.58
1:I:228:GLN:CG	1:I:327:PHE:CD2	2.86	0.58
1:A:158:ARG:CG	1:A:158:ARG:HH11	2.16	0.58
1:A:235:ARG:HG2	1:A:235:ARG:NH1	2.06	0.58
2:F:6:ARG:O	2:F:6:ARG:HG2	2.03	0.58
1:A:159:SER:HB3	1:A:160:PRO:CA	2.25	0.58
1:A:347:LEU:CD2	1:A:352:ALA:HA	2.34	0.57
1:G:200:TYR:CE2	1:G:269:ARG:HD3	2.38	0.57
1:A:381:GLU:HG2	6:A:528:HOH:O	2.05	0.56
1:I:351:LEU:HA	1:I:354:HIS:O	2.05	0.56
2:L:1:THR:HG23	2:L:3:GLN:HE21	1.70	0.56
1:G:264:PRO:HD2	1:G:267:ASP:OD2	2.05	0.56
1:K:289:PRO:O	1:K:291:ILE:HG13	2.05	0.56
1:G:207:ASN:OD1	1:G:209:THR:OG1	2.16	0.56
1:I:347:LEU:HD11	1:I:352:ALA:HA	1.85	0.56
1:K:291:ILE:HG22	1:K:292:VAL:H	1.71	0.56
1:I:347:LEU:CD1	1:I:352:ALA:HB2	2.36	0.56
2:D:0:ARG:HG3	2:D:1:THR:N	2.22	0.55
1:I:311:MET:HG3	6:I:501:HOH:O	2.06	0.55
1:A:284:THR:HG23	6:A:527:HOH:O	2.05	0.55
1:E:258:VAL:HG11	1:E:283:CYS:SG	2.43	0.55
1:E:255:THR:OG1	6:E:501:HOH:O	2.16	0.55
1:A:232:GLY:O	1:A:236:VAL:HG23	2.07	0.55
1:G:150:THR:O	1:G:153:GLY:HA3	2.07	0.55
1:A:166:SER:CB	1:A:169:GLN:HG3	2.21	0.54
1:G:280:CYS:O	1:G:283:CYS:O	2.24	0.54
1:A:141:VAL:HG23	1:A:315:LEU:HD13	1.90	0.54
1:I:141:VAL:HG23	1:I:315:LEU:HD13	1.89	0.54
1:B:172:ASP:N	1:B:172:ASP:OD1	2.30	0.54
1:G:258:VAL:HB	6:G:533:HOH:O	2.07	0.54
1:I:208:VAL:HG21	1:I:367:VAL:HG23	1.90	0.54
1:K:340:ARG:HD3	1:K:359:ASP:OD1	2.06	0.54
1:I:325:GLU:OE1	1:I:328:ALA:HB3	2.08	0.54
1:E:166:SER:OG	1:E:167:ASN:N	2.41	0.53
1:E:316:LEU:CD2	1:E:341:LEU:HD23	2.38	0.53
2:L:1:THR:CG2	2:L:3:GLN:HE21	2.22	0.53
1:A:347:LEU:HD23	1:A:352:ALA:HB2	1.90	0.53
1:E:388:GLN:HG3	1:E:389:ARG:N	2.24	0.52
1:I:269:ARG:HD3	6:I:526:HOH:O	2.08	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ASP:OD1	1:B:271:ASP:N	2.43	0.52
1:E:235:ARG:HE	1:E:235:ARG:HA	1.73	0.52
1:G:257:THR:OG1	1:G:286:VAL:O	2.28	0.52
1:G:179:ILE:CD1	1:G:191:PRO:HB2	2.40	0.51
1:I:191:PRO:O	1:I:194:THR:OG1	2.27	0.51
1:G:277:VAL:HG12	1:G:286:VAL:HG12	1.93	0.51
1:B:353:TRP:HB2	1:B:354:HIS:ND1	2.25	0.51
1:I:195:LEU:O	1:I:199:LEU:HD13	2.11	0.51
1:K:143:MET:HA	1:K:226:TYR:O	2.10	0.51
1:K:144:VAL:HG12	1:K:318:LEU:HB2	1.93	0.50
1:G:175:TYR:HB2	1:G:176:PRO:HD2	1.94	0.50
1:G:179:ILE:HD11	1:G:191:PRO:C	2.32	0.50
1:A:186:PHE:CD2	1:E:300:GLN:HG3	2.47	0.50
1:I:228:GLN:CD	1:I:327:PHE:CD2	2.85	0.50
1:K:144:VAL:HB	1:K:148:ILE:HG12	1.93	0.50
1:K:289:PRO:HB2	1:K:291:ILE:HD11	1.94	0.50
1:I:125:LEU:O	1:I:128:VAL:HG22	2.11	0.50
1:G:200:TYR:HD2	1:G:269:ARG:CD	2.25	0.49
1:A:325:GLU:OE1	1:A:329[B]:SER:HB3	2.12	0.49
1:E:196:ALA:O	1:E:200:TYR:HD1	1.95	0.49
1:I:200:TYR:HB2	1:I:273:MET:HE1	1.95	0.49
1:B:325:GLU:OE1	1:B:329[B]:SER:HB3	2.13	0.49
1:K:344:ASN:O	1:K:363:LEU:HA	2.13	0.49
2:H:6:ARG:HG3	1:G:353:TRP:CH2	2.47	0.48
1:K:368:HIS:HB2	6:K:517:HOH:O	2.12	0.48
1:E:258:VAL:CG1	1:E:285:GLY:HA3	2.43	0.48
1:G:381:GLU:HG3	1:G:384:ARG:NH1	2.29	0.48
1:I:341:LEU:HD22	1:I:343:ILE:HG13	1.94	0.48
1:K:153:GLY:O	1:K:154:ILE:HG13	2.14	0.48
1:K:330:LEU:O	1:K:331:THR:C	2.52	0.48
1:E:234:GLU:HB2	1:E:244:LEU:HD21	1.94	0.48
1:E:325:GLU:OE1	1:E:329[B]:SER:HB3	2.13	0.48
1:G:325:GLU:OE1	1:G:329[B]:SER:HB3	2.14	0.48
1:G:283:CYS:SG	1:G:285:GLY:N	2.85	0.47
1:I:199:LEU:N	1:I:199:LEU:HD12	2.29	0.47
1:K:325:GLU:CG	1:K:326:PRO:HA	2.44	0.47
1:G:257:THR:C	1:G:260:GLN:HG3	2.34	0.47
1:K:250:THR:HG23	1:K:251:PHE:N	2.29	0.47
1:G:280:CYS:CB	6:G:530:HOH:O	2.59	0.47
2:H:4:THR:HG22	1:G:294:PHE:CE1	2.50	0.47
1:I:386:LEU:HA	1:I:389:ARG:HD3	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:309:PHE:HB3	1:K:333:ALA:O	2.14	0.46
1:A:165:TYR:C	1:A:170:GLN:HE21	2.16	0.46
1:I:197:LYS:CE	1:I:273:MET:O	2.63	0.46
2:D:6:ARG:NH2	6:D:201:HOH:O	2.48	0.46
2:L:1:THR:CG2	2:L:3:GLN:NE2	2.79	0.46
1:A:235:ARG:NH1	1:A:235:ARG:CG	2.73	0.46
1:E:168:LEU:O	1:E:172:ASP:N	2.49	0.46
1:E:175:TYR:HB2	1:E:176:PRO:HD2	1.98	0.46
1:G:150:THR:O	1:G:153:GLY:CA	2.64	0.46
1:A:292:VAL:HG11	1:A:298:LEU:CD2	2.45	0.46
1:K:347:LEU:HD23	1:K:347:LEU:C	2.37	0.45
1:I:208:VAL:CG2	1:I:367:VAL:HG23	2.47	0.45
1:K:320:THR:O	1:K:344:ASN:ND2	2.49	0.45
1:K:287:VAL:CG1	1:K:288:LYS:N	2.79	0.45
1:K:290:ASP:N	1:K:290:ASP:OD1	2.46	0.45
1:B:150:THR:HB	1:B:151:PRO:HD3	1.98	0.45
1:B:320:THR:HG23	5:B:401:GOL:C1	2.47	0.45
1:E:358:ARG:NH2	6:E:502:HOH:O	2.50	0.45
1:G:150:THR:HB	1:G:151:PRO:HD3	1.99	0.45
1:B:252:ALA:O	1:B:264:PRO:O	2.35	0.45
1:G:121:GLY:HA2	1:G:122:LYS:HA	1.74	0.45
1:K:123:LEU:N	6:K:501:HOH:O	2.49	0.45
1:K:123:LEU:O	1:K:360:VAL:HG22	2.16	0.44
1:A:197:LYS:HE3	1:A:273:MET:O	2.17	0.44
1:K:148:ILE:HD12	1:K:210:HIS:NE2	2.33	0.44
1:A:180:PHE:CZ	4:C:101:CRD:HC12	2.53	0.44
1:G:280:CYS:CB	1:G:283:CYS:O	2.60	0.44
1:K:148:ILE:HD12	1:K:210:HIS:CE1	2.53	0.43
1:I:321:SER:HB2	1:I:323:GLU:HG2	2.00	0.43
1:A:158:ARG:CG	1:A:158:ARG:NH1	2.81	0.43
1:K:290:ASP:O	1:K:291:ILE:HG12	2.18	0.43
1:G:179:ILE:HA	1:G:179:ILE:HD12	1.80	0.43
1:I:126:GLN:HA	1:I:376:LEU:HD23	1.99	0.43
1:I:126:GLN:CD	6:I:508:HOH:O	2.57	0.43
1:I:150:THR:N	1:I:151:PRO:CD	2.82	0.43
1:E:258:VAL:O	1:K:301:ARG:NH2	2.50	0.43
1:B:345:ARG:HG3	6:B:515:HOH:O	2.19	0.43
1:E:258:VAL:HG12	1:E:285:GLY:HA3	1.99	0.43
1:I:347:LEU:HD11	1:I:352:ALA:HB2	2.01	0.43
1:E:196:ALA:O	1:E:200:TYR:CD1	2.71	0.42
1:G:276:ARG:HH12	1:I:393:LYS:C	2.23	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:LEU:HD12	1:G:298:LEU:N	2.33	0.42
1:I:258:VAL:HB	1:I:283:CYS:SG	2.59	0.42
1:B:228:GLN:HB3	5:B:401:GOL:H32	2.00	0.42
1:A:200:TYR:CB	1:A:201:PRO:CD	2.97	0.42
1:I:124:SER:CB	6:I:524:HOH:O	2.57	0.42
1:E:256:CYS:SG	1:E:258:VAL:HG13	2.60	0.42
1:K:209:THR:HG22	1:K:370:VAL:HG21	2.00	0.42
1:A:175:TYR:HB2	1:A:176:PRO:HD2	2.02	0.42
1:G:304:LEU:O	1:G:307:VAL:HG22	2.20	0.42
1:E:304:LEU:O	1:E:307:VAL:HG12	2.20	0.41
1:I:175:TYR:HB2	1:I:176:PRO:CD	2.48	0.41
1:B:144:VAL:HA	1:B:318:LEU:O	2.20	0.41
1:I:294:PHE:CE1	2:J:4:THR:HG23	2.55	0.41
1:I:125:LEU:O	1:I:128:VAL:CG2	2.68	0.41
1:I:371:GLU:O	1:I:374:VAL:HG12	2.20	0.41
2:D:0:ARG:HG3	2:D:1:THR:H	1.83	0.41
2:H:1:THR:HG22	1:G:297:PRO:CA	2.50	0.41
1:E:199:LEU:HA	1:E:199:LEU:HD23	1.84	0.41
1:I:304:LEU:O	1:I:307:VAL:HG12	2.21	0.41
1:K:375:GLU:HG2	1:K:380:THR:OG1	2.21	0.41
1:E:344:ASN:O	1:E:363:LEU:HA	2.21	0.41
1:A:144:VAL:HA	1:A:318:LEU:O	2.20	0.41
1:I:144:VAL:HA	1:I:318:LEU:O	2.21	0.41
1:K:287:VAL:HG12	1:K:288:LYS:N	2.36	0.41
1:K:230:ILE:HD12	1:K:251:PHE:CZ	2.57	0.40
1:A:268:ILE:O	1:A:272:VAL:HG23	2.21	0.40
1:I:146:ALA:O	1:I:150:THR:HG23	2.22	0.40
1:B:135:ARG:HD2	1:B:138:GLN:HE21	1.86	0.40
1:I:228:GLN:HG3	1:I:327:PHE:CD2	2.50	0.40
1:K:293:PHE:O	1:K:296:GLU:HB2	2.21	0.40
1:K:309:PHE:CZ	1:K:330:LEU:HB3	2.57	0.40
1:A:344:ASN:O	1:A:363:LEU:HA	2.22	0.40
1:I:344:ASN:O	1:I:363:LEU:HA	2.21	0.40
1:K:288:LYS:CD	1:K:289:PRO:HD2	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:LYS:NZ	1:G:267:ASP:OD1[3_454]	2.10	0.10

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/275 (97%)	259 (97%)	8 (3%)	0	100	100
1	B	261/275 (95%)	257 (98%)	4 (2%)	0	100	100
1	E	258/275 (94%)	255 (99%)	3 (1%)	0	100	100
1	G	250/275 (91%)	242 (97%)	6 (2%)	2 (1%)	19	53
1	I	242/275 (88%)	235 (97%)	7 (3%)	0	100	100
1	K	189/275 (69%)	176 (93%)	13 (7%)	0	100	100
2	C	5/7 (71%)	5 (100%)	0	0	100	100
2	D	5/7 (71%)	5 (100%)	0	0	100	100
2	F	5/7 (71%)	5 (100%)	0	0	100	100
2	H	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
2	J	5/7 (71%)	4 (80%)	1 (20%)	0	100	100
2	L	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
All	All	1496/1692 (88%)	1450 (97%)	44 (3%)	2 (0%)	51	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	154	ILE
1	G	282	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	236/237 (100%)	232 (98%)	4 (2%)	60	83
1	B	227/237 (96%)	216 (95%)	11 (5%)	25	59
1	E	228/237 (96%)	217 (95%)	11 (5%)	25	59
1	G	219/237 (92%)	213 (97%)	6 (3%)	44	74
1	I	210/237 (89%)	200 (95%)	10 (5%)	25	59
1	K	164/237 (69%)	152 (93%)	12 (7%)	14	41
2	C	6/6 (100%)	6 (100%)	0	100	100
2	D	6/6 (100%)	5 (83%)	1 (17%)	2	9
2	F	6/6 (100%)	5 (83%)	1 (17%)	2	9
2	H	6/6 (100%)	6 (100%)	0	100	100
2	J	6/6 (100%)	4 (67%)	2 (33%)	0	1
2	L	5/6 (83%)	4 (80%)	1 (20%)	1	5
All	All	1319/1458 (90%)	1260 (96%)	59 (4%)	27	61

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	ARG
1	A	235	ARG
1	A	271	ASP
1	A	284	THR
1	B	170	GLN
1	B	171	TYR
1	B	172	ASP
1	B	203	ASN
1	B	205	LYS
1	B	253	SER
1	B	269	ARG
1	B	271	ASP
1	B	283	CYS
1	B	384	ARG
1	B	391	THR
2	D	4	THR
1	E	139	ARG
1	E	170	GLN
1	E	228	GLN
1	E	235	ARG
1	E	258	VAL
1	E	261	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	278	PRO
1	E	283	CYS
1	E	311	MET
1	E	345	ARG
1	E	388	GLN
2	F	6	ARG
1	G	138	GLN
1	G	266	GLU
1	G	269	ARG
1	G	279	ARG
1	G	283	CYS
1	G	286	VAL
2	L	0	ARG
1	I	174	PRO
1	I	235	ARG
1	I	266	GLU
1	I	275	ASP
1	I	283	CYS
1	I	332	GLU
1	I	356	ARG
1	I	367	VAL
1	I	374	VAL
1	I	389	ARG
2	J	0	ARG
2	J	1	THR
1	K	124	SER
1	K	230	ILE
1	K	283	CYS
1	K	284	THR
1	K	286	VAL
1	K	290	ASP
1	K	293	PHE
1	K	325	GLU
1	K	346	ASP
1	K	357	SER
1	K	380	THR
1	K	389	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	170	GLN
1	B	138	GLN
1	B	203	ASN
2	D	3	GLN
1	E	138	GLN
1	E	228	GLN
2	F	3	GLN
2	L	3	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](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	CRD	D	101	2	4,4,4	0.89	0	2,3,3	1.40	0
4	CRD	F	101	2	4,4,4	1.07	0	2,3,3	1.10	0
5	GOL	K	401	-	5,5,5	0.19	0	5,5,5	0.41	0
5	GOL	G	401	-	5,5,5	0.13	0	5,5,5	0.36	0
4	CRD	L	101	2	4,4,4	0.97	0	2,3,3	3.07	2 (100%)
5	GOL	E	401	-	5,5,5	0.18	0	5,5,5	0.43	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CRD	H	101	2	4,4,4	1.20	0	2,3,3	2.35	1 (50%)
4	CRD	J	101	2	4,4,4	0.70	0	2,3,3	1.82	1 (50%)
4	CRD	C	101	2	4,4,4	0.82	0	2,3,3	0.81	0
5	GOL	B	401	-	5,5,5	0.16	0	5,5,5	0.49	0

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
4	CRD	D	101	2	-	1/2/2/2	-
4	CRD	F	101	2	-	1/2/2/2	-
5	GOL	K	401	-	-	2/4/4/4	-
5	GOL	G	401	-	-	4/4/4/4	-
4	CRD	L	101	2	-	0/2/2/2	-
5	GOL	E	401	-	-	2/4/4/4	-
4	CRD	H	101	2	-	1/2/2/2	-
4	CRD	J	101	2	-	1/2/2/2	-
4	CRD	C	101	2	-	1/2/2/2	-
5	GOL	B	401	-	-	1/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	101	CRD	CC1-CC2-CC3	-3.28	117.32	125.55
4	L	101	CRD	CC1-CC2-CC3	-3.22	117.46	125.55
4	L	101	CRD	OC1-CC4-CC3	-2.91	115.74	125.67
4	J	101	CRD	CC1-CC2-CC3	-2.16	120.13	125.55

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	401	GOL	O1-C1-C2-O2
4	D	101	CRD	CC2-CC3-CC4-OC1
4	F	101	CRD	CC2-CC3-CC4-OC1
4	H	101	CRD	CC2-CC3-CC4-OC1
5	E	401	GOL	O1-C1-C2-C3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
4	J	101	CRD	CC2-CC3-CC4-OC1
4	C	101	CRD	CC2-CC3-CC4-OC1
5	K	401	GOL	C1-C2-C3-O3
5	E	401	GOL	O1-C1-C2-O2
5	G	401	GOL	O1-C1-C2-C3
5	G	401	GOL	C1-C2-C3-O3
5	K	401	GOL	O2-C2-C3-O3
5	G	401	GOL	O2-C2-C3-O3
5	B	401	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	401	GOL	1	0
4	C	101	CRD	1	0
5	B	401	GOL	2	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	270/275 (98%)	-0.17	3 (1%) 80 65	20, 35, 70, 98	1 (0%)
1	B	264/275 (96%)	-0.10	1 (0%) 92 84	18, 38, 78, 109	0
1	E	263/275 (95%)	-0.11	1 (0%) 92 84	25, 42, 76, 98	1 (0%)
1	G	255/275 (92%)	0.16	10 (3%) 39 25	24, 48, 89, 109	0
1	I	248/275 (90%)	0.28	11 (4%) 34 21	31, 61, 94, 120	0
1	K	194/275 (70%)	0.23	13 (6%) 17 10	29, 63, 96, 132	0
2	C	7/7 (100%)	-0.18	0 100 100	32, 35, 65, 76	0
2	D	7/7 (100%)	0.03	0 100 100	42, 49, 67, 86	0
2	F	7/7 (100%)	0.36	1 (14%) 2 1	40, 52, 84, 99	0
2	H	7/7 (100%)	0.06	0 100 100	52, 60, 85, 95	0
2	J	7/7 (100%)	0.50	1 (14%) 2 1	55, 72, 116, 126	0
2	L	6/7 (85%)	0.89	0 100 100	79, 89, 95, 103	0
All	All	1535/1692 (90%)	0.04	41 (2%) 54 38	18, 47, 89, 132	2 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	282	VAL	7.0
1	K	287	VAL	5.6
1	I	368	HIS	5.3
1	K	353	TRP	4.4
1	K	294	PHE	4.4
1	K	394	LEU	3.9
1	G	121	GLY	3.8
1	A	165	TYR	3.6
1	I	391	THR	3.2
1	I	128	VAL	3.2
1	G	176	PRO	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	I	356	ARG	2.8
1	G	283	CYS	2.7
1	I	134	ALA	2.7
1	E	168	LEU	2.7
1	K	354	HIS	2.6
1	K	154	ILE	2.6
1	I	392	GLY	2.6
1	K	153	GLY	2.6
1	I	336	SER	2.6
1	K	323	GLU	2.5
1	G	281	PRO	2.5
1	G	187	HIS	2.5
1	G	277	VAL	2.4
1	I	137	CYS	2.4
2	F	6	ARG	2.4
1	K	236	VAL	2.3
1	I	178	ALA	2.3
1	K	289	PRO	2.3
1	G	200	TYR	2.3
1	I	127	ASP	2.3
1	G	354	HIS	2.2
1	K	392	GLY	2.2
1	G	183	PRO	2.2
1	A	353	TRP	2.2
1	K	351	LEU	2.1
1	K	123	LEU	2.1
2	J	6	ARG	2.1
1	B	353	TRP	2.0
1	I	345	ARG	2.0
1	A	169	GLN	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
5	GOL	E	401	6/6	0.36	0.54	89,103,114,118	0
4	CRD	L	101	5/5	0.77	0.42	46,54,65,73	0
5	GOL	K	401	6/6	0.80	0.66	81,90,91,93	0
5	GOL	G	401	6/6	0.93	0.23	64,70,71,75	0
4	CRD	J	101	5/5	0.94	0.20	47,48,53,54	0
5	GOL	B	401	6/6	0.94	0.18	45,49,51,51	0
4	CRD	C	101	5/5	0.96	0.30	29,30,33,33	0
4	CRD	H	101	5/5	0.96	0.18	41,42,46,49	0
4	CRD	F	101	5/5	0.96	0.16	38,38,40,41	0
4	CRD	D	101	5/5	0.98	0.24	28,29,30,31	0
3	ZN	B	402	1/1	0.98	0.04	55,55,55,55	0
3	ZN	I	401	1/1	0.99	0.09	32,32,32,32	0
3	ZN	G	402	1/1	0.99	0.06	98,98,98,98	0
3	ZN	A	401	1/1	0.99	0.08	41,41,41,41	0
3	ZN	E	402	1/1	1.00	0.10	33,33,33,33	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.