



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:48 AM GMT

PDB ID : 2BL2
Title : THE MEMBRANE ROTOR OF THE V-TYPE ATPASE FROM ENTEROCOCCUS HIRAE
Authors : Murata, T.; Yamato, I.; Kakinuma, Y.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2005-02-25
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (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

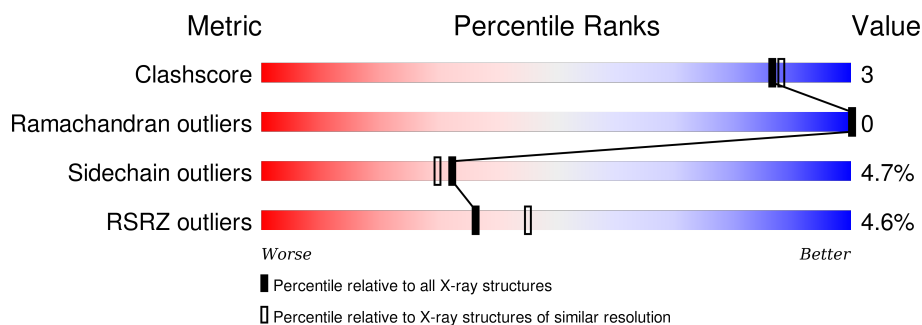
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 ≥ 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	156	<div> <div>4%</div> <div>94%</div> <div>• •</div> </div>
1	B	156	<div> <div>4%</div> <div>94%</div> <div>• •</div> </div>
1	C	156	<div> <div>6%</div> <div>94%</div> <div>• •</div> </div>
1	D	156	<div> <div>10%</div> <div>93%</div> <div>5% •</div> </div>
1	E	156	<div> <div>8%</div> <div>93%</div> <div>• •</div> </div>
1	F	156	<div> <div>5%</div> <div>94%</div> <div>• •</div> </div>
1	G	156	<div> <div>6%</div> <div>94%</div> <div>• •</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	156	
1	I	156	
1	J	156	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LHG	A	1158	-	-	-	X
2	LHG	A	1159	-	-	-	X
2	LHG	A	1164	-	-	-	X
2	LHG	B	1158	-	-	-	X
2	LHG	C	1158	-	-	-	X
2	LHG	C	1159	-	-	-	X
2	LHG	C	1163	-	-	-	X
2	LHG	D	1158	-	-	-	X
2	LHG	D	1162	-	-	-	X
2	LHG	E	1158	-	-	-	X
2	LHG	F	1158	-	-	-	X
2	LHG	F	1159	-	-	-	X
2	LHG	F	1164	-	-	-	X
2	LHG	F	1166	-	-	-	X
2	LHG	G	1158	-	-	-	X
2	LHG	H	1158	-	-	-	X
2	LHG	I	1158	-	-	-	X
2	LHG	I	1159	-	-	-	X
2	LHG	I	1165	-	-	-	X
2	LHG	J	1158	-	-	-	X
3	NA	A	1157	-	-	-	X
3	NA	B	1157	-	-	-	X
3	NA	C	1157	-	-	-	X
3	NA	D	1157	-	-	-	X
3	NA	E	1157	-	-	-	X
3	NA	F	1157	-	-	-	X
3	NA	G	1157	-	-	-	X
3	NA	H	1157	-	-	-	X
3	NA	J	1157	-	-	-	X
4	UMQ	A	1162	-	-	-	X
4	UMQ	A	1163	-	-	-	X
4	UMQ	B	1162	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UMQ	B	1163	-	-	-	X
4	UMQ	C	1161	-	-	-	X
4	UMQ	C	1162	-	-	-	X
4	UMQ	C	1164	X	-	-	X
4	UMQ	D	1161	-	-	-	X
4	UMQ	D	163	-	-	-	X
4	UMQ	E	1159	-	-	-	X
4	UMQ	E	1160	-	-	-	X
4	UMQ	F	1162	-	-	-	X
4	UMQ	F	1163	-	-	-	X
4	UMQ	F	1167	X	-	-	X
4	UMQ	G	1160	-	-	-	X
4	UMQ	H	1160	-	-	-	X
4	UMQ	I	1163	-	-	-	X
4	UMQ	I	1164	-	-	-	X
4	UMQ	J	1160	-	-	-	X

2 Entry composition

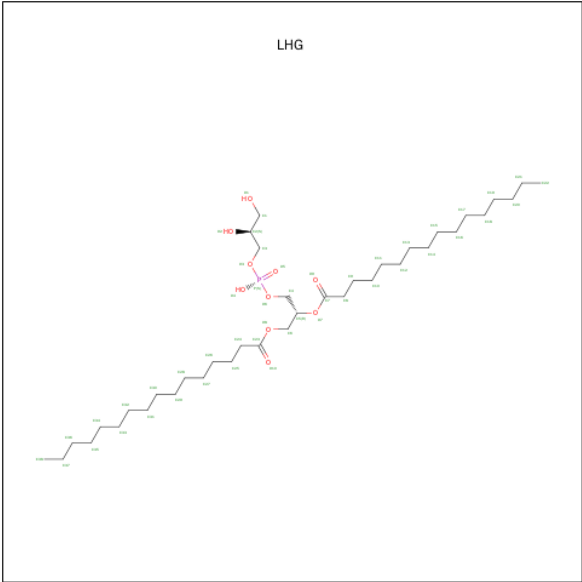
There are 5 unique types of molecules in this entry. The entry contains 13367 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 V-TYPE SODIUM ATP SYNTHASE SUBUNIT K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	B	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	C	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	D	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	E	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	F	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	G	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	H	156	Total	C	N	O	S	0	9	0
			1155	760	179	208	8			
1	I	156	Total	C	N	O	S	0	7	0
			1148	757	178	205	8			
1	J	156	Total	C	N	O	S	0	8	0
			1153	759	180	207	7			

- Molecule 2 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 10 10	0	0
2	A	1	Total C O P 49 38 10 1	0	0
2	A	1	Total C O 40 35 5	0	0
2	A	1	Total C 11 11	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C O 40 35 5	0	0
2	A	1	Total C 9 9	0	0
2	A	1	Total C 10 10	0	0
2	B	1	Total C O P 49 38 10 1	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 9 9	0	0
2	B	1	Total C 8 8	0	0
2	B	1	Total C 10 10	0	0
2	C	1	Total C 9 9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O P 49 38 10 1	0	0
2	C	1	Total C O 40 35 5	0	0
2	C	1	Total C 9 9	0	0
2	C	1	Total C O 40 35 5	0	0
2	D	1	Total C 5 5	0	0
2	D	1	Total C O P 49 38 10 1	0	0
2	D	1	Total C 9 9	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C O 40 35 5	0	0
2	D	1	Total C 9 9	0	0
2	D	1	Total C 8 8	0	0
2	D	1	Total C 8 8	0	0
2	E	1	Total C O P 49 38 10 1	0	0
2	F	1	Total C 10 10	0	0
2	F	1	Total C O P 49 38 10 1	0	0
2	F	1	Total C O 40 35 5	0	0
2	F	1	Total C 11 11	0	0
2	F	1	Total C 11 11	0	0
2	F	1	Total C O 40 35 5	0	0
2	F	1	Total C 7 7	0	0
2	F	1	Total C O 40 35 5	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C 9 9	0	0
2	G	1	Total C 10 10	0	0
2	G	1	Total C O P 49 38 10 1	0	0
2	H	1	Total C 9 9	0	0
2	H	1	Total C 10 10	0	0
2	H	1	Total C O P 49 38 10 1	0	0
2	H	1	Total C 9 9	0	0
2	I	1	Total C O P 49 38 10 1	0	0
2	I	1	Total C O 40 35 5	0	0
2	I	1	Total C 8 8	0	0
2	I	1	Total C 8 8	0	0
2	I	1	Total C 8 8	0	0
2	I	1	Total C O 40 35 5	0	0
2	J	1	Total C O P 49 38 10 1	0	0
2	J	1	Total C 11 11	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

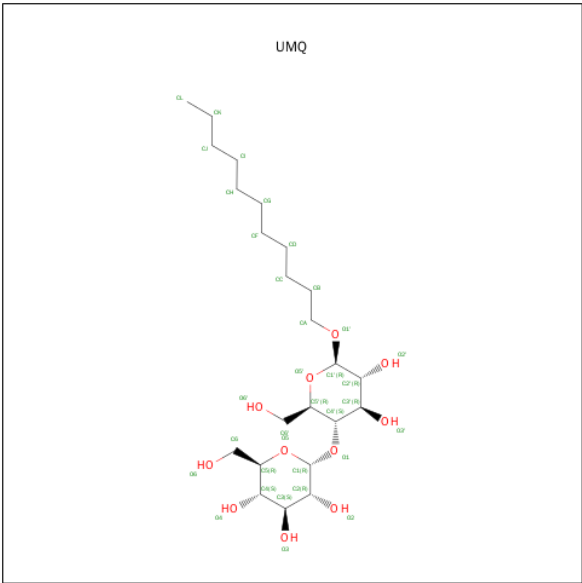
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Na 1 1	0	0
3	J	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0
3	E	1	Total Na 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	I	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		

- Molecule 4 is UNDECYL-MALTOSIDE (three-letter code: UMQ) (formula: C₂₃H₄₄O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			12	11	1		
4	A	1	Total	C	O	0	0
			12	11	1		
4	B	1	Total	C	O	0	0
			12	11	1		
4	B	1	Total	C	O	0	0
			12	11	1		
4	C	1	Total	C	O	0	0
			12	11	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			12	11	1		
4	C	1	Total	C	O	0	0
			34	23	11		
4	D	1	Total	C	O	0	0
			12	11	1		
4	D	1	Total	C	O	0	0
			12	11	1		
4	E	1	Total	C	O	0	0
			12	11	1		
4	E	1	Total	C	O	0	0
			12	11	1		
4	F	1	Total	C	O	0	0
			12	11	1		
4	F	1	Total	C	O	0	0
			12	11	1		
4	F	1	Total	C	O	0	0
			34	23	11		
4	G	1	Total	C	O	0	0
			12	11	1		
4	G	1	Total	C	O	0	0
			12	11	1		
4	H	1	Total	C	O	0	0
			12	11	1		
4	H	1	Total	C	O	0	0
			12	11	1		
4	I	1	Total	C	O	0	0
			12	11	1		
4	I	1	Total	C	O	0	0
			12	11	1		
4	J	1	Total	C	O	0	0
			12	11	1		
4	J	1	Total	C	O	0	0
			12	11	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	33	Total	O	0	0
			33	33		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	21	Total 21	O 21	0	0
5	D	26	Total 26	O 26	0	0
5	E	28	Total 28	O 28	0	0
5	F	34	Total 34	O 34	0	0
5	G	36	Total 36	O 36	0	0
5	H	44	Total 44	O 44	0	0
5	I	57	Total 57	O 57	0	0
5	J	37	Total 37	O 37	0	0

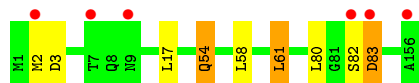
3 Residue-property plots [i](#)

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

- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K



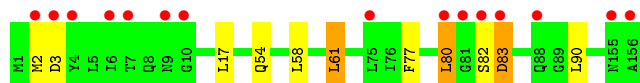
- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K



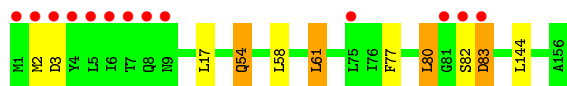
- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K



- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K



- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K

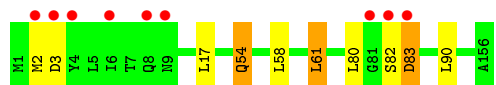


- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K

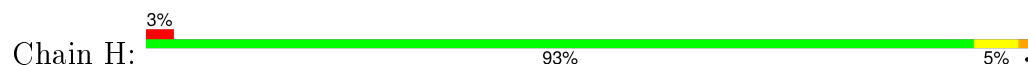




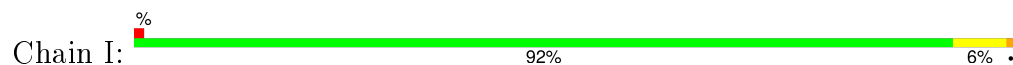
- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K



- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K



- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K



- Molecule 1: V-TYPE SODIUM ATP SYNTHASE SUBUNIT K



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.14Å 125.60Å 210.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.00 – 2.10 60.19 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (61.00-2.10) 99.3 (60.19-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.190 , 0.200 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 79.7	EDS
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	4 of 184566 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13367	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, NA, UMQ

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	0.42	0/1219	0.57	3/1649 (0.2%)
1	B	0.41	0/1219	0.57	3/1649 (0.2%)
1	C	0.40	0/1219	0.58	3/1649 (0.2%)
1	D	0.39	0/1219	0.57	3/1649 (0.2%)
1	E	0.39	0/1219	0.57	3/1649 (0.2%)
1	F	0.41	0/1219	0.57	2/1649 (0.1%)
1	G	0.43	0/1219	0.57	3/1649 (0.2%)
1	H	0.45	0/1219	0.57	3/1649 (0.2%)
1	I	0.48	0/1202	0.56	0/1626
1	J	0.47	0/1212	0.57	1/1640 (0.1%)
All	All	0.43	0/12166	0.57	24/16458 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	3	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	83[A]	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	83[B]	ASP	CB-CG-OD2	5.20	122.98	118.30
1	E	83[A]	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	83[B]	ASP	CB-CG-OD2	5.19	122.97	118.30
1	H	83[A]	ASP	CB-CG-OD2	5.16	122.95	118.30
1	H	83[B]	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	83[A]	ASP	CB-CG-OD2	5.15	122.93	118.30
1	C	83[B]	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	83[A]	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	83[B]	ASP	CB-CG-OD2	5.14	122.93	118.30
1	G	83[A]	ASP	CB-CG-OD2	5.14	122.92	118.30
1	G	83[B]	ASP	CB-CG-OD2	5.14	122.92	118.30
1	A	3	ASP	CB-CG-OD2	5.13	122.92	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	83[A]	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	83[B]	ASP	CB-CG-OD2	5.12	122.90	118.30
1	G	3	ASP	CB-CG-OD2	5.12	122.90	118.30
1	F	83[A]	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	83[B]	ASP	CB-CG-OD2	5.10	122.89	118.30
1	D	3	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	3	ASP	CB-CG-OD2	5.07	122.86	118.30
1	E	3	ASP	CB-CG-OD2	5.07	122.86	118.30
1	H	3	ASP	CB-CG-OD2	5.04	122.84	118.30
1	B	3	ASP	CB-CG-OD2	5.01	122.81	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	1155	0	1218	4	0
1	B	1155	0	1218	3	0
1	C	1155	0	1218	4	0
1	D	1155	0	1218	4	0
1	E	1155	0	1218	5	0
1	F	1155	0	1218	5	0
1	G	1155	0	1218	4	0
1	H	1155	0	1218	4	0
1	I	1148	0	1214	7	0
1	J	1153	0	1217	4	0
2	A	177	0	284	10	0
2	B	85	0	130	3	0
2	C	147	0	236	11	0
2	D	136	0	211	6	0
2	E	49	0	74	1	0
2	F	208	0	337	13	0
2	G	68	0	104	1	0
2	H	77	0	118	0	0
2	I	153	0	244	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	60	0	92	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	A	24	0	46	0	0
4	B	24	0	46	0	0
4	C	58	0	87	0	0
4	D	24	0	46	0	0
4	E	24	0	46	0	0
4	F	58	0	86	0	0
4	G	24	0	46	0	0
4	H	24	0	46	0	0
4	I	24	0	46	0	0
4	J	24	0	46	0	0
5	A	32	0	0	0	0
5	B	33	0	0	0	0
5	C	21	0	0	0	0
5	D	26	0	0	0	0
5	E	28	0	0	0	0
5	F	34	0	0	0	0
5	G	36	0	0	0	0
5	H	44	0	0	0	0
5	I	57	0	0	0	0
5	J	37	0	0	0	0
All	All	13367	0	14546	75	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 3.

All (75) 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)
2:A:1159:LHG:HC62	2:I:1165:LHG:HC81	1.73	0.69
1:I:10:GLY:O	1:I:13[A]:VAL:HG22	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1164:LHG:H192	1:B:17[B]:LEU:HD21	1.79	0.65
2:F:1166:LHG:H192	1:H:17[B]:LEU:HD21	1.79	0.64
2:F:1164:LHG:H192	1:G:17[B]:LEU:HD21	1.80	0.64
2:F:1164:LHG:HC81	2:F:1166:LHG:HC62	1.79	0.64
2:D:1162:LHG:H192	1:E:17[B]:LEU:HD21	1.80	0.63
2:C:1163:LHG:H192	1:D:17[B]:LEU:HD21	1.80	0.63
1:A:17[B]:LEU:HD21	2:A:1159:LHG:H192	1.81	0.63
1:C:17[B]:LEU:HD21	2:C:1159:LHG:H192	1.82	0.62
2:A:1159:LHG:C6	2:I:1165:LHG:HC81	2.30	0.62
1:I:17[B]:LEU:HD21	2:I:1159:LHG:H192	1.80	0.61
2:I:1165:LHG:H192	1:J:17[B]:LEU:HD21	1.82	0.61
2:F:1159:LHG:HC81	2:F:1164:LHG:HC62	1.80	0.61
1:F:17[B]:LEU:HD21	2:F:1159:LHG:H192	1.82	0.61
2:C:1159:LHG:HC81	2:C:1163:LHG:HC62	1.85	0.59
2:D:1162:LHG:HC81	2:F:1159:LHG:HC62	1.85	0.59
2:A:1159:LHG:HC81	2:A:1164:LHG:HC62	1.84	0.58
2:F:1164:LHG:HC81	2:F:1166:LHG:C6	2.34	0.57
2:A:1164:LHG:HC81	2:C:1159:LHG:HC62	1.87	0.55
2:C:1159:LHG:HC81	2:C:1163:LHG:C6	2.37	0.55
2:I:1159:LHG:HC81	2:I:1165:LHG:HC62	1.87	0.55
2:F:1159:LHG:HC81	2:F:1164:LHG:C6	2.37	0.55
1:I:9:ASN:HD21	1:I:84:MET:H	1.54	0.54
2:C:1163:LHG:HC81	2:D:1162:LHG:HC62	1.93	0.50
2:A:1159:LHG:HC81	2:A:1164:LHG:C6	2.41	0.50
2:E:1158:LHG:H342	2:F:1159:LHG:H331	1.94	0.49
1:I:9:ASN:HD21	1:I:83:ASP:HA	1.76	0.48
2:I:1158:LHG:H101	2:I:1160:LHG:HC92	1.95	0.48
2:B:1158:LHG:H342	2:C:1159:LHG:H331	1.95	0.48
2:C:1163:LHG:HC81	2:D:1162:LHG:C6	2.46	0.46
1:F:58:LEU:HA	1:F:61:LEU:HD22	1.98	0.46
2:B:1160:LHG:H112	2:B:1161:LHG:H111	1.99	0.45
2:F:1158:LHG:H342	2:F:1164:LHG:H331	1.99	0.45
2:F:1165:LHG:HC91	2:G:1158:LHG:H311	1.99	0.45
2:I:1158:LHG:H342	2:I:1165:LHG:H331	1.99	0.45
1:D:90:LEU:HD22	2:D:1162:LHG:H181	2.00	0.44
2:B:1159:LHG:HC92	2:B:1160:LHG:HC91	2.00	0.44
1:E:58:LEU:HA	1:E:61:LEU:HD22	1.99	0.44
1:H:58:LEU:HA	1:H:61:LEU:HD22	2.00	0.44
2:A:1159:LHG:H331	2:J:1158:LHG:H342	2.00	0.43
1:G:58:LEU:HA	1:G:61:LEU:HD22	2.01	0.43
1:D:58:LEU:HA	1:D:61:LEU:HD22	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1158:LHG:H101	2:C:1160:LHG:H102	2.01	0.43
1:A:58:LEU:HA	1:A:61:LEU:HD22	2.01	0.43
2:I:1160:LHG:H122	2:I:1161:LHG:H121	2.00	0.42
1:I:18:ALA:HB2	1:I:93:LEU:HA	2.01	0.42
1:B:58:LEU:HA	1:B:61:LEU:HD22	2.01	0.42
1:I:144:LEU:HD11	1:J:67:LEU:HD23	2.02	0.42
2:F:1166:LHG:H181	1:G:90:LEU:HD22	2.02	0.42
2:F:1166:LHG:HC81	2:I:1159:LHG:HC62	2.02	0.42
1:H:90:LEU:HD22	2:I:1159:LHG:H181	2.02	0.42
1:F:77:PHE:HA	1:F:80:LEU:HD22	2.02	0.41
1:I:58:LEU:HA	1:I:61:LEU:HD22	2.03	0.41
2:A:1158:LHG:H342	2:A:1164:LHG:H331	2.02	0.41
2:D:1160:LHG:HC82	2:D:1165:LHG:HC92	2.03	0.41
2:J:1158:LHG:H101	2:J:1159:LHG:H122	2.02	0.41
1:A:77:PHE:HA	1:A:80:LEU:HD22	2.03	0.41
1:C:90:LEU:HD22	2:C:1163:LHG:H181	2.03	0.41
1:E:144:LEU:HD11	1:F:67:LEU:HD23	2.03	0.41
1:C:58:LEU:HA	1:C:61:LEU:HD22	2.02	0.41
1:H:77:PHE:HA	1:H:80:LEU:HD22	2.03	0.41
2:C:1158:LHG:H182	2:C:1163:LHG:H361	2.03	0.40
2:A:1165:LHG:H132	2:A:1166:LHG:H151	2.03	0.40
1:E:77:PHE:HA	1:E:80:LEU:HD22	2.03	0.40
1:J:18:ALA:HB2	1:J:93:LEU:HA	2.03	0.40
2:I:1159:LHG:HC81	2:I:1165:LHG:C6	2.49	0.40
1:D:77:PHE:HA	1:D:80:LEU:HD22	2.03	0.40

There are no symmetry-related clashes.

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	163/156 (104%)	162 (99%)	1 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	163/156 (104%)	162 (99%)	1 (1%)	0	100	100
1	C	163/156 (104%)	162 (99%)	1 (1%)	0	100	100
1	D	163/156 (104%)	162 (99%)	1 (1%)	0	100	100
1	E	163/156 (104%)	162 (99%)	1 (1%)	0	100	100
1	F	163/156 (104%)	162 (99%)	1 (1%)	0	100	100
1	G	163/156 (104%)	162 (99%)	1 (1%)	0	100	100
1	H	163/156 (104%)	162 (99%)	1 (1%)	0	100	100
1	I	161/156 (103%)	161 (100%)	0	0	100	100
1	J	162/156 (104%)	162 (100%)	0	0	100	100
All	All	1627/1560 (104%)	1619 (100%)	8 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	122/113 (108%)	114 (93%)	8 (7%)	21	17
1	B	122/113 (108%)	114 (93%)	8 (7%)	21	17
1	C	122/113 (108%)	114 (93%)	8 (7%)	21	17
1	D	122/113 (108%)	114 (93%)	8 (7%)	21	17
1	E	122/113 (108%)	114 (93%)	8 (7%)	21	17
1	F	122/113 (108%)	114 (93%)	8 (7%)	21	17
1	G	122/113 (108%)	114 (93%)	8 (7%)	21	17
1	H	122/113 (108%)	114 (93%)	8 (7%)	21	17
1	I	120/113 (106%)	117 (98%)	3 (2%)	55	59
1	J	121/113 (107%)	118 (98%)	3 (2%)	55	59
All	All	1217/1130 (108%)	1147 (94%)	70 (6%)	32	21

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	54[A]	GLN
1	A	54[B]	GLN
1	A	61	LEU
1	A	80	LEU
1	A	82	SER
1	A	83[A]	ASP
1	A	83[B]	ASP
1	B	2	MET
1	B	54[A]	GLN
1	B	54[B]	GLN
1	B	61	LEU
1	B	80	LEU
1	B	82	SER
1	B	83[A]	ASP
1	B	83[B]	ASP
1	C	2	MET
1	C	54[A]	GLN
1	C	54[B]	GLN
1	C	61	LEU
1	C	80	LEU
1	C	82	SER
1	C	83[A]	ASP
1	C	83[B]	ASP
1	D	2	MET
1	D	54[A]	GLN
1	D	54[B]	GLN
1	D	61	LEU
1	D	80	LEU
1	D	82	SER
1	D	83[A]	ASP
1	D	83[B]	ASP
1	E	2	MET
1	E	54[A]	GLN
1	E	54[B]	GLN
1	E	61	LEU
1	E	80	LEU
1	E	82	SER
1	E	83[A]	ASP
1	E	83[B]	ASP
1	F	2	MET
1	F	54[A]	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	54[B]	GLN
1	F	61	LEU
1	F	80	LEU
1	F	82	SER
1	F	83[A]	ASP
1	F	83[B]	ASP
1	G	2	MET
1	G	54[A]	GLN
1	G	54[B]	GLN
1	G	61	LEU
1	G	80	LEU
1	G	82	SER
1	G	83[A]	ASP
1	G	83[B]	ASP
1	H	2	MET
1	H	54[A]	GLN
1	H	54[B]	GLN
1	H	61	LEU
1	H	80	LEU
1	H	82	SER
1	H	83[A]	ASP
1	H	83[B]	ASP
1	I	2	MET
1	I	61	LEU
1	I	83	ASP
1	J	54[A]	GLN
1	J	54[B]	GLN
1	J	61	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	9	ASN
1	I	79	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 82 ligands modelled in this entry, 10 are monoatomic - leaving 72 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$
2	LHG	A	1158	-	48,48,48	0.93	2 (4%)	49,54,54	1.01	2 (4%)
2	LHG	A	1159	-	39,39,48	0.99	2 (5%)	41,41,54	1.05	2 (4%)
2	LHG	A	1160	-	10,10,48	0.25	0	9,9,54	0.57	0
2	LHG	A	1161	-	7,7,48	0.26	0	6,6,54	0.50	0
4	UMQ	A	1162	-	11,11,35	0.24	0	10,10,46	0.58	0
4	UMQ	A	1163	-	11,11,35	0.24	0	10,10,46	0.58	0
2	LHG	A	1164	-	39,39,48	1.00	2 (5%)	41,41,54	1.06	2 (4%)
2	LHG	A	1165	-	8,8,48	0.26	0	7,7,54	0.53	0
2	LHG	A	1166	-	9,9,48	0.25	0	8,8,54	0.55	0
2	LHG	A	162	-	9,9,48	0.25	0	8,8,54	0.55	0
2	LHG	B	1158	-	48,48,48	0.94	2 (4%)	49,54,54	1.00	2 (4%)
2	LHG	B	1159	-	8,8,48	0.26	0	7,7,54	0.53	0
2	LHG	B	1160	-	8,8,48	0.26	0	7,7,54	0.53	0
2	LHG	B	1161	-	7,7,48	0.26	0	6,6,54	0.50	0
4	UMQ	B	1162	-	11,11,35	0.24	0	10,10,46	0.58	0
4	UMQ	B	1163	-	11,11,35	0.23	0	10,10,46	0.57	0
2	LHG	B	1164	-	9,9,48	0.25	0	8,8,54	0.54	0
2	LHG	C	1158	-	48,48,48	0.94	2 (4%)	49,54,54	1.00	2 (4%)
2	LHG	C	1159	-	39,39,48	1.00	2 (5%)	41,41,54	1.05	2 (4%)
2	LHG	C	1160	-	8,8,48	0.25	0	7,7,54	0.52	0
4	UMQ	C	1161	-	11,11,35	0.23	0	10,10,46	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	UMQ	C	1162	-	11,11,35	0.24	0	10,10,46	0.58	0
2	LHG	C	1163	-	39,39,48	1.00	2 (5%)	41,41,54	1.06	3 (7%)
4	UMQ	C	1164	-	35,35,35	1.06	2 (5%)	46,46,46	1.75	6 (13%)
2	LHG	C	161	-	8,8,48	0.25	0	7,7,54	0.53	0
2	LHG	D	1158	-	48,48,48	0.93	2 (4%)	49,54,54	1.00	2 (4%)
2	LHG	D	1159	-	8,8,48	0.26	0	7,7,54	0.53	0
2	LHG	D	1160	-	7,7,48	0.26	0	6,6,54	0.50	0
4	UMQ	D	1161	-	11,11,35	0.24	0	10,10,46	0.58	0
2	LHG	D	1162	-	39,39,48	1.00	2 (5%)	41,41,54	1.05	3 (7%)
2	LHG	D	1163	-	8,8,48	0.25	0	7,7,54	0.53	0
2	LHG	D	1164	-	7,7,48	0.26	0	6,6,54	0.50	0
2	LHG	D	1165	-	7,7,48	0.26	0	6,6,54	0.49	0
2	LHG	D	162	-	4,4,48	0.28	0	3,3,54	0.40	0
4	UMQ	D	163	-	11,11,35	0.23	0	10,10,46	0.58	0
2	LHG	E	1158	-	48,48,48	0.94	2 (4%)	49,54,54	1.00	2 (4%)
4	UMQ	E	1159	-	11,11,35	0.24	0	10,10,46	0.58	0
4	UMQ	E	1160	-	11,11,35	0.24	0	10,10,46	0.58	0
2	LHG	F	1158	-	48,48,48	0.94	2 (4%)	49,54,54	1.00	2 (4%)
2	LHG	F	1159	-	39,39,48	0.99	2 (5%)	41,41,54	1.05	3 (7%)
2	LHG	F	1160	-	10,10,48	0.25	0	9,9,54	0.57	0
2	LHG	F	1161	-	10,10,48	0.25	0	9,9,54	0.56	0
4	UMQ	F	1162	-	11,11,35	0.24	0	10,10,46	0.58	0
4	UMQ	F	1163	-	11,11,35	0.24	0	10,10,46	0.58	0
2	LHG	F	1164	-	39,39,48	1.00	2 (5%)	41,41,54	1.05	2 (4%)
2	LHG	F	1165	-	6,6,48	0.26	0	5,5,54	0.45	0
2	LHG	F	1166	-	39,39,48	1.00	2 (5%)	41,41,54	1.06	2 (4%)
4	UMQ	F	1167	-	35,35,35	1.07	2 (5%)	46,46,46	1.75	6 (13%)
2	LHG	F	162	-	9,9,48	0.25	0	8,8,54	0.54	0
2	LHG	G	1158	-	48,48,48	0.94	2 (4%)	49,54,54	1.01	2 (4%)
4	UMQ	G	1159	-	11,11,35	0.24	0	10,10,46	0.58	0
4	UMQ	G	1160	-	11,11,35	0.24	0	10,10,46	0.57	0
2	LHG	G	161	-	8,8,48	0.26	0	7,7,54	0.52	0
2	LHG	G	162	-	9,9,48	0.25	0	8,8,54	0.55	0
2	LHG	H	1158	-	48,48,48	0.93	2 (4%)	49,54,54	1.00	2 (4%)
2	LHG	H	1159	-	8,8,48	0.25	0	7,7,54	0.53	0
4	UMQ	H	1160	-	11,11,35	0.23	0	10,10,46	0.58	0
4	UMQ	H	1161	-	11,11,35	0.24	0	10,10,46	0.57	0
2	LHG	H	161	-	8,8,48	0.26	0	7,7,54	0.53	0
2	LHG	H	162	-	9,9,48	0.25	0	8,8,54	0.55	0
2	LHG	I	1158	-	48,48,48	0.94	2 (4%)	49,54,54	1.00	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LHG	I	1159	-	39,39,48	1.00	2 (5%)	41,41,54	1.06	2 (4%)
2	LHG	I	1160	-	7,7,48	0.26	0	6,6,54	0.50	0
2	LHG	I	1161	-	7,7,48	0.26	0	6,6,54	0.49	0
2	LHG	I	1162	-	7,7,48	0.26	0	6,6,54	0.49	0
4	UMQ	I	1163	-	11,11,35	0.24	0	10,10,46	0.57	0
4	UMQ	I	1164	-	11,11,35	0.24	0	10,10,46	0.57	0
2	LHG	I	1165	-	39,39,48	1.00	2 (5%)	41,41,54	1.03	2 (4%)
2	LHG	J	1158	-	48,48,48	0.94	2 (4%)	49,54,54	1.00	2 (4%)
2	LHG	J	1159	-	10,10,48	0.25	0	9,9,54	0.56	0
4	UMQ	J	1160	-	11,11,35	0.24	0	10,10,46	0.57	0
4	UMQ	J	1161	-	11,11,35	0.24	0	10,10,46	0.58	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
2	LHG	A	1158	-	-	0/53/53/53	0/0/0/0
2	LHG	A	1159	-	-	0/41/41/53	0/0/0/0
2	LHG	A	1160	-	-	0/8/8/53	0/0/0/0
2	LHG	A	1161	-	-	0/5/5/53	0/0/0/0
4	UMQ	A	1162	-	-	0/9/9/60	0/0/0/2
4	UMQ	A	1163	-	-	0/9/9/60	0/0/0/2
2	LHG	A	1164	-	-	0/41/41/53	0/0/0/0
2	LHG	A	1165	-	-	0/6/6/53	0/0/0/0
2	LHG	A	1166	-	-	0/7/7/53	0/0/0/0
2	LHG	A	162	-	-	0/7/7/53	0/0/0/0
2	LHG	B	1158	-	-	0/53/53/53	0/0/0/0
2	LHG	B	1159	-	-	0/6/6/53	0/0/0/0
2	LHG	B	1160	-	-	0/6/6/53	0/0/0/0
2	LHG	B	1161	-	-	0/5/5/53	0/0/0/0
4	UMQ	B	1162	-	-	0/9/9/60	0/0/0/2
4	UMQ	B	1163	-	-	0/9/9/60	0/0/0/2
2	LHG	B	1164	-	-	0/7/7/53	0/0/0/0
2	LHG	C	1158	-	-	0/53/53/53	0/0/0/0
2	LHG	C	1159	-	-	0/41/41/53	0/0/0/0
2	LHG	C	1160	-	-	0/6/6/53	0/0/0/0
4	UMQ	C	1161	-	-	0/9/9/60	0/0/0/2
4	UMQ	C	1162	-	-	0/9/9/60	0/0/0/2
2	LHG	C	1163	-	-	0/41/41/53	0/0/0/0
4	UMQ	C	1164	-	2/2/10/10	0/20/60/60	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LHG	C	161	-	-	0/6/6/53	0/0/0/0
2	LHG	D	1158	-	-	0/53/53/53	0/0/0/0
2	LHG	D	1159	-	-	0/6/6/53	0/0/0/0
2	LHG	D	1160	-	-	0/5/5/53	0/0/0/0
4	UMQ	D	1161	-	-	0/9/9/60	0/0/0/2
2	LHG	D	1162	-	-	0/41/41/53	0/0/0/0
2	LHG	D	1163	-	-	0/6/6/53	0/0/0/0
2	LHG	D	1164	-	-	0/5/5/53	0/0/0/0
2	LHG	D	1165	-	-	0/5/5/53	0/0/0/0
2	LHG	D	162	-	-	0/2/2/53	0/0/0/0
4	UMQ	D	163	-	-	0/9/9/60	0/0/0/2
2	LHG	E	1158	-	-	0/53/53/53	0/0/0/0
4	UMQ	E	1159	-	-	0/9/9/60	0/0/0/2
4	UMQ	E	1160	-	-	0/9/9/60	0/0/0/2
2	LHG	F	1158	-	-	0/53/53/53	0/0/0/0
2	LHG	F	1159	-	-	0/41/41/53	0/0/0/0
2	LHG	F	1160	-	-	0/8/8/53	0/0/0/0
2	LHG	F	1161	-	-	0/8/8/53	0/0/0/0
4	UMQ	F	1162	-	-	0/9/9/60	0/0/0/2
4	UMQ	F	1163	-	-	0/9/9/60	0/0/0/2
2	LHG	F	1164	-	-	0/41/41/53	0/0/0/0
2	LHG	F	1165	-	-	0/4/4/53	0/0/0/0
2	LHG	F	1166	-	-	0/41/41/53	0/0/0/0
4	UMQ	F	1167	-	2/2/10/10	0/20/60/60	0/2/2/2
2	LHG	F	162	-	-	0/7/7/53	0/0/0/0
2	LHG	G	1158	-	-	0/53/53/53	0/0/0/0
4	UMQ	G	1159	-	-	0/9/9/60	0/0/0/2
4	UMQ	G	1160	-	-	0/9/9/60	0/0/0/2
2	LHG	G	161	-	-	0/6/6/53	0/0/0/0
2	LHG	G	162	-	-	0/7/7/53	0/0/0/0
2	LHG	H	1158	-	-	0/53/53/53	0/0/0/0
2	LHG	H	1159	-	-	0/6/6/53	0/0/0/0
4	UMQ	H	1160	-	-	0/9/9/60	0/0/0/2
4	UMQ	H	1161	-	-	0/9/9/60	0/0/0/2
2	LHG	H	161	-	-	0/6/6/53	0/0/0/0
2	LHG	H	162	-	-	0/7/7/53	0/0/0/0
2	LHG	I	1158	-	-	0/53/53/53	0/0/0/0
2	LHG	I	1159	-	-	0/41/41/53	0/0/0/0
2	LHG	I	1160	-	-	0/5/5/53	0/0/0/0
2	LHG	I	1161	-	-	0/5/5/53	0/0/0/0
2	LHG	I	1162	-	-	0/5/5/53	0/0/0/0
4	UMQ	I	1163	-	-	0/9/9/60	0/0/0/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	UMQ	I	1164	-	-	0/9/9/60	0/0/0/2
2	LHG	I	1165	-	-	0/41/41/53	0/0/0/0
2	LHG	J	1158	-	-	0/53/53/53	0/0/0/0
2	LHG	J	1159	-	-	0/8/8/53	0/0/0/0
4	UMQ	J	1160	-	-	0/9/9/60	0/0/0/2
4	UMQ	J	1161	-	-	0/9/9/60	0/0/0/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1167	UMQ	O3-C3	-4.07	1.33	1.43
4	C	1164	UMQ	O3-C3	-4.04	1.33	1.43
4	F	1167	UMQ	O2-C2	-4.03	1.33	1.43
4	C	1164	UMQ	O2-C2	-3.97	1.33	1.43
2	F	1164	LHG	O7-C7	3.90	1.46	1.34
2	A	1159	LHG	O7-C7	3.90	1.46	1.34
2	A	1164	LHG	O7-C7	3.93	1.46	1.34
2	C	1163	LHG	O7-C7	3.93	1.46	1.34
2	D	1162	LHG	O7-C7	3.93	1.46	1.34
2	F	1159	LHG	O7-C7	3.93	1.46	1.34
2	I	1165	LHG	O7-C7	3.94	1.46	1.34
2	F	1166	LHG	O7-C7	3.96	1.46	1.34
2	C	1159	LHG	O7-C7	3.97	1.46	1.34
2	I	1159	LHG	O7-C7	3.97	1.46	1.34
2	B	1158	LHG	O7-C7	4.05	1.46	1.34
2	H	1158	LHG	O7-C7	4.06	1.46	1.34
2	D	1158	LHG	O7-C7	4.06	1.46	1.34
2	I	1158	LHG	O7-C7	4.07	1.46	1.34
2	J	1158	LHG	O7-C7	4.07	1.46	1.34
2	A	1158	LHG	O7-C7	4.08	1.46	1.34
2	C	1158	LHG	O7-C7	4.11	1.46	1.34
2	E	1158	LHG	O7-C7	4.12	1.46	1.34
2	F	1158	LHG	O7-C7	4.13	1.46	1.34
2	G	1158	LHG	O7-C7	4.15	1.46	1.34
2	F	1159	LHG	O8-C23	4.18	1.45	1.33
2	I	1159	LHG	O8-C23	4.20	1.46	1.33
2	C	1163	LHG	O8-C23	4.21	1.46	1.33
2	I	1165	LHG	O8-C23	4.21	1.46	1.33
2	A	1159	LHG	O8-C23	4.21	1.46	1.33
2	F	1164	LHG	O8-C23	4.22	1.46	1.33
2	C	1159	LHG	O8-C23	4.23	1.46	1.33
2	D	1162	LHG	O8-C23	4.24	1.46	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1164	LHG	O8-C23	4.24	1.46	1.33
2	F	1166	LHG	O8-C23	4.24	1.46	1.33
2	G	1158	LHG	O8-C23	4.25	1.46	1.33
2	A	1158	LHG	O8-C23	4.25	1.46	1.33
2	D	1158	LHG	O8-C23	4.25	1.46	1.33
2	H	1158	LHG	O8-C23	4.27	1.46	1.33
2	F	1158	LHG	O8-C23	4.27	1.46	1.33
2	E	1158	LHG	O8-C23	4.29	1.46	1.33
2	B	1158	LHG	O8-C23	4.30	1.46	1.33
2	J	1158	LHG	O8-C23	4.30	1.46	1.33
2	I	1158	LHG	O8-C23	4.30	1.46	1.33
2	C	1158	LHG	O8-C23	4.32	1.46	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1162	LHG	C5-O7-C7	-2.03	113.02	117.89
2	C	1163	LHG	C5-O7-C7	-2.01	113.06	117.89
2	F	1159	LHG	C5-O7-C7	-2.00	113.08	117.89
2	I	1165	LHG	O8-C23-C24	2.64	119.95	111.90
2	C	1158	LHG	O8-C23-C24	2.65	119.97	111.90
2	F	1158	LHG	O8-C23-C24	2.66	120.00	111.90
2	J	1158	LHG	O8-C23-C24	2.66	120.01	111.90
2	A	1158	LHG	O8-C23-C24	2.67	120.03	111.90
2	C	1159	LHG	O8-C23-C24	2.67	120.05	111.90
2	D	1162	LHG	O8-C23-C24	2.68	120.06	111.90
2	A	1159	LHG	O8-C23-C24	2.68	120.06	111.90
2	F	1159	LHG	O8-C23-C24	2.68	120.08	111.90
2	B	1158	LHG	O8-C23-C24	2.69	120.08	111.90
2	E	1158	LHG	O8-C23-C24	2.69	120.10	111.90
2	A	1164	LHG	O8-C23-C24	2.69	120.10	111.90
2	I	1159	LHG	O8-C23-C24	2.69	120.10	111.90
2	H	1158	LHG	O8-C23-C24	2.69	120.10	111.90
2	D	1158	LHG	O8-C23-C24	2.70	120.11	111.90
2	C	1163	LHG	O8-C23-C24	2.70	120.11	111.90
2	G	1158	LHG	O8-C23-C24	2.70	120.13	111.90
2	F	1164	LHG	O8-C23-C24	2.71	120.16	111.90
2	F	1166	LHG	O8-C23-C24	2.71	120.16	111.90
2	I	1158	LHG	O8-C23-C24	2.72	120.18	111.90
2	I	1165	LHG	O7-C7-C8	3.69	119.54	111.53
2	F	1159	LHG	O7-C7-C8	3.78	119.75	111.53
2	F	1164	LHG	O7-C7-C8	3.79	119.76	111.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1159	LHG	O7-C7-C8	3.79	119.76	111.53
2	A	1159	LHG	O7-C7-C8	3.80	119.78	111.53
2	D	1162	LHG	O7-C7-C8	3.80	119.79	111.53
2	I	1159	LHG	O7-C7-C8	3.83	119.86	111.53
2	C	1163	LHG	O7-C7-C8	3.85	119.89	111.53
2	A	1164	LHG	O7-C7-C8	3.85	119.89	111.53
2	F	1166	LHG	O7-C7-C8	3.87	119.95	111.53
4	F	1167	UMQ	O3-C3-C2	3.91	119.13	110.34
4	C	1164	UMQ	O3-C3-C2	3.94	119.21	110.34
2	C	1158	LHG	O7-C7-C8	4.08	120.39	111.53
2	D	1158	LHG	O7-C7-C8	4.09	120.41	111.53
4	C	1164	UMQ	O3-C3-C4	4.11	119.59	110.34
2	B	1158	LHG	O7-C7-C8	4.11	120.46	111.53
2	I	1158	LHG	O7-C7-C8	4.12	120.48	111.53
2	E	1158	LHG	O7-C7-C8	4.13	120.50	111.53
2	H	1158	LHG	O7-C7-C8	4.14	120.52	111.53
2	G	1158	LHG	O7-C7-C8	4.15	120.54	111.53
2	F	1158	LHG	O7-C7-C8	4.15	120.55	111.53
2	A	1158	LHG	O7-C7-C8	4.17	120.59	111.53
2	J	1158	LHG	O7-C7-C8	4.21	120.67	111.53
4	F	1167	UMQ	O3-C3-C4	4.24	119.88	110.34
4	C	1164	UMQ	O2-C2-C3	4.33	120.08	110.34
4	F	1167	UMQ	O2-C2-C3	4.43	120.32	110.34
4	F	1167	UMQ	C1-C2-C3	4.61	119.06	109.97
4	C	1164	UMQ	O2-C2-C1	4.62	120.15	110.02
4	F	1167	UMQ	O2-C2-C1	4.81	120.56	110.02
4	C	1164	UMQ	C1-C2-C3	4.84	119.50	109.97
4	F	1167	UMQ	C4-C3-C2	5.10	120.31	110.79
4	C	1164	UMQ	C4-C3-C2	5.24	120.56	110.79

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	C	1164	UMQ	C3
4	C	1164	UMQ	C2
4	F	1167	UMQ	C3
4	F	1167	UMQ	C2

There are no torsion outliers.

There are no ring outliers.

30 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1158	LHG	1	0
2	A	1159	LHG	6	0
2	A	1164	LHG	5	0
2	A	1165	LHG	1	0
2	A	1166	LHG	1	0
2	B	1158	LHG	1	0
2	B	1159	LHG	1	0
2	B	1160	LHG	2	0
2	B	1161	LHG	1	0
2	C	1158	LHG	2	0
2	C	1159	LHG	5	0
2	C	1160	LHG	1	0
2	C	1163	LHG	7	0
2	D	1160	LHG	1	0
2	D	1162	LHG	5	0
2	D	1165	LHG	1	0
2	E	1158	LHG	1	0
2	F	1158	LHG	1	0
2	F	1159	LHG	5	0
2	F	1164	LHG	6	0
2	F	1165	LHG	1	0
2	F	1166	LHG	5	0
2	G	1158	LHG	1	0
2	I	1158	LHG	2	0
2	I	1159	LHG	5	0
2	I	1160	LHG	2	0
2	I	1161	LHG	1	0
2	I	1165	LHG	6	0
2	J	1158	LHG	2	0
2	J	1159	LHG	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, 95th 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 ²)	Q<0.9
1	A	156/156 (100%)	0.09	6 (3%) 44 53	20, 24, 43, 54	0
1	B	156/156 (100%)	0.03	6 (3%) 44 53	19, 24, 43, 54	0
1	C	156/156 (100%)	0.14	9 (5%) 26 34	19, 24, 43, 55	0
1	D	156/156 (100%)	0.25	15 (9%) 10 14	20, 24, 43, 55	0
1	E	156/156 (100%)	0.34	13 (8%) 14 19	20, 24, 43, 55	0
1	F	156/156 (100%)	0.06	8 (5%) 32 40	19, 24, 42, 56	0
1	G	156/156 (100%)	0.05	9 (5%) 26 34	19, 24, 43, 56	0
1	H	156/156 (100%)	0.03	4 (2%) 59 66	19, 24, 43, 54	0
1	I	156/156 (100%)	-0.16	2 (1%) 79 84	20, 24, 39, 52	0
1	J	156/156 (100%)	-0.16	0 100 100	19, 24, 36, 52	0
All	All	1560/1560 (100%)	0.07	72 (4%) 36 45	19, 24, 43, 56	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	81	GLY	11.0
1	E	83[A]	ASP	9.5
1	E	82	SER	7.3
1	D	81	GLY	6.8
1	D	9	ASN	6.4
1	F	83[A]	ASP	6.0
1	E	7	THR	5.9
1	A	82	SER	5.8
1	G	82	SER	5.7
1	C	2	MET	5.6
1	C	82	SER	5.2
1	B	83[A]	ASP	5.1
1	E	9	ASN	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	83[A]	ASP	4.8
1	D	82	SER	4.8
1	B	82	SER	4.8
1	F	81	GLY	4.7
1	H	83[A]	ASP	4.6
1	A	83[A]	ASP	4.6
1	F	9	ASN	4.4
1	D	6	ILE	4.4
1	C	7	THR	4.4
1	E	5	LEU	4.4
1	C	3	ASP	4.3
1	E	6	ILE	4.3
1	H	82	SER	4.3
1	H	81	GLY	4.3
1	D	156	ALA	4.0
1	D	7	THR	4.0
1	G	2	MET	4.0
1	C	83[A]	ASP	4.0
1	F	6	ILE	3.9
1	E	1	MET	3.9
1	H	9	ASN	3.9
1	F	3	ASP	3.8
1	B	9	ASN	3.7
1	C	9	ASN	3.7
1	F	82	SER	3.6
1	E	2	MET	3.5
1	G	3	ASP	3.4
1	F	7	THR	3.4
1	B	2	MET	3.4
1	C	81	GLY	3.3
1	E	8	GLN	3.3
1	A	81	GLY	3.1
1	G	9	ASN	3.1
1	F	2	MET	3.1
1	G	83[A]	ASP	3.1
1	D	3	ASP	3.0
1	A	126	GLU	3.0
1	I	3	ASP	2.9
1	B	156	ALA	2.9
1	D	2	MET	2.9
1	G	4	TYR	2.9
1	D	4	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	4	TYR	2.7
1	D	155[A]	ASN	2.6
1	C	4	TYR	2.6
1	D	80	LEU	2.6
1	C	6	ILE	2.6
1	D	10	GLY	2.4
1	B	7	THR	2.3
1	E	3	ASP	2.3
1	I	9	ASN	2.3
1	A	3	ASP	2.3
1	D	88	GLN	2.2
1	G	8	GLN	2.2
1	A	6	ILE	2.2
1	D	75[A]	LEU	2.1
1	E	75[A]	LEU	2.1
1	G	6	ILE	2.0
1	G	81	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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(\AA^2)	Q<0.9
3	NA	F	1157	1/1	0.95	0.24	17.51	22,22,22,22	0
3	NA	G	1157	1/1	0.98	0.21	12.55	23,23,23,23	0
3	NA	A	1157	1/1	0.95	0.23	11.94	23,23,23,23	0
2	LHG	F	1158	49/49	0.56	0.25	11.58	70,82,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	LHG	I	1165	40/49	0.35	0.47	11.58	108,114,119,119	0
3	NA	E	1157	1/1	0.95	0.26	11.11	23,23,23,23	0
4	UMQ	I	1163	12/34	0.56	0.35	10.75	144,145,146,146	0
3	NA	B	1157	1/1	0.97	0.26	10.36	23,23,23,23	0
2	LHG	J	1158	49/49	0.55	0.34	9.54	68,83,94,95	0
3	NA	C	1157	1/1	0.96	0.23	9.29	22,22,22,22	0
4	UMQ	D	163	12/34	0.35	0.42	9.02	157,157,158,158	0
4	UMQ	J	1160	12/34	0.42	0.30	8.70	154,154,155,155	0
2	LHG	E	1158	49/49	0.54	0.27	8.54	69,83,93,95	0
2	LHG	A	1159	40/49	0.34	0.45	8.24	108,115,119,119	0
2	LHG	C	1158	49/49	0.62	0.26	7.80	71,83,94,95	0
2	LHG	A	1164	40/49	0.32	0.47	7.14	107,115,118,118	0
2	LHG	G	1158	49/49	0.59	0.26	6.91	68,83,94,95	0
4	UMQ	D	1161	12/34	0.74	0.28	6.85	154,154,154,154	0
2	LHG	B	1158	49/49	0.60	0.29	6.63	69,83,94,95	0
2	LHG	I	1158	49/49	0.56	0.33	6.35	69,83,95,95	0
2	LHG	D	1158	49/49	0.58	0.27	6.00	70,83,94,95	0
4	UMQ	F	1162	12/34	0.40	0.42	5.94	165,165,166,166	0
4	UMQ	C	1164	34/34	0.59	0.33	5.82	161,166,172,172	0
4	UMQ	I	1164	12/34	0.80	0.23	5.68	122,124,124,124	0
2	LHG	H	1158	49/49	0.51	0.32	5.33	69,83,94,95	0
2	LHG	I	1159	40/49	0.41	0.40	5.17	107,114,119,119	0
2	LHG	A	1158	49/49	0.61	0.28	4.86	69,83,94,95	0
3	NA	D	1157	1/1	0.96	0.17	4.72	24,24,24,24	0
3	NA	J	1157	1/1	0.98	0.14	4.43	22,22,22,22	0
4	UMQ	E	1160	12/34	0.63	0.31	4.41	152,153,153,153	0
4	UMQ	F	1167	34/34	0.56	0.34	4.40	153,159,169,169	0
4	UMQ	C	1161	12/34	0.45	0.26	4.28	162,162,162,162	0
3	NA	H	1157	1/1	0.99	0.13	4.03	23,23,23,23	0
4	UMQ	G	1160	12/34	0.54	0.32	3.99	143,143,143,143	0
2	LHG	F	1166	40/49	0.52	0.34	3.62	107,115,118,118	0
4	UMQ	F	1163	12/34	0.72	0.29	3.45	137,138,140,140	0
4	UMQ	B	1162	12/34	0.52	0.37	3.39	159,159,159,159	0
2	LHG	D	1162	40/49	0.34	0.43	3.16	108,115,118,118	0
4	UMQ	E	1159	12/34	0.64	0.28	3.14	159,160,160,160	0
4	UMQ	C	1162	12/34	0.53	0.25	3.02	150,151,151,151	0
4	UMQ	H	1160	12/34	0.51	0.32	3.01	157,157,158,158	0
2	LHG	F	1164	40/49	0.54	0.38	2.91	108,115,118,118	0
4	UMQ	B	1163	12/34	0.57	0.27	2.63	151,152,152,152	0
4	UMQ	A	1162	12/34	0.46	0.31	2.61	160,160,161,161	0
2	LHG	C	1163	40/49	0.46	0.38	2.61	108,115,118,118	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	LHG	F	1159	40/49	0.45	0.36	2.60	108,115,118,119	0
4	UMQ	A	1163	12/34	0.53	0.24	2.32	150,151,152,152	0
2	LHG	C	1159	40/49	0.45	0.37	2.02	108,115,119,119	0
4	UMQ	H	1161	12/34	0.68	0.20	0.83	137,138,139,139	0
3	NA	I	1157	1/1	0.99	0.10	0.39	21,21,21,21	0
2	LHG	F	1165	7/49	0.17	1.37	-	199,199,199,199	0
2	LHG	D	1163	9/49	0.54	1.61	-	195,196,196,196	0
4	UMQ	J	1161	12/34	0.70	0.27	-	153,153,153,153	0
2	LHG	F	162	10/49	0.46	1.61	-	196,196,196,196	0
2	LHG	I	1160	8/49	0.59	1.48	-	198,198,198,198	0
2	LHG	A	162	10/49	0.09	2.27	-	202,202,202,202	0
2	LHG	A	1160	11/49	0.70	1.61	-	197,197,197,197	0
2	LHG	D	1160	8/49	0.59	1.28	-	197,197,197,197	0
2	LHG	G	161	9/49	0.45	1.72	-	196,196,196,196	0
2	LHG	C	161	9/49	0.28	1.70	-	197,197,198,198	0
2	LHG	F	1161	11/49	0.29	1.35	-	196,196,196,196	0
2	LHG	B	1159	9/49	0.66	1.24	-	202,202,202,202	0
2	LHG	B	1160	9/49	0.65	1.37	-	198,198,198,198	0
2	LHG	D	1164	8/49	0.56	1.24	-	192,192,193,193	0
2	LHG	B	1161	8/49	0.26	1.84	-	196,196,197,197	0
2	LHG	B	1164	10/49	0.22	1.86	-	194,194,194,194	0
2	LHG	A	1161	8/49	0.45	1.33	-	199,199,199,199	0
2	LHG	D	1165	8/49	0.51	1.54	-	198,198,198,198	0
2	LHG	D	162	5/49	0.59	1.99	-	197,197,197,197	0
2	LHG	A	1165	9/49	0.48	2.01	-	198,198,198,198	0
4	UMQ	G	1159	12/34	0.59	0.35	-	159,159,159,159	0
2	LHG	C	1160	9/49	0.20	2.27	-	199,199,199,199	0
2	LHG	H	162	10/49	0.50	1.60	-	196,196,196,196	0
2	LHG	J	1159	11/49	0.62	1.94	-	197,198,198,198	0
2	LHG	I	1161	8/49	0.45	2.10	-	191,191,192,192	0
2	LHG	I	1162	8/49	0.22	2.01	-	196,196,196,196	0
2	LHG	F	1160	11/49	0.31	1.36	-	204,204,204,204	0
2	LHG	G	162	10/49	0.63	1.56	-	196,196,196,196	0
2	LHG	A	1166	10/49	0.58	1.74	-	197,197,197,198	0
2	LHG	D	1159	9/49	0.84	1.28	-	196,196,197,197	0
2	LHG	H	1159	9/49	0.44	1.15	-	196,196,196,196	0
2	LHG	H	161	9/49	-0.18	1.65	-	199,199,199,199	0

6.5 Other polymers ⓘ

There are no such residues in this entry.