



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 03:58 AM GMT

PDB ID : 1L6L
Title : Structures of Apolipoprotein A-II and a Lipid Surrogate Complex Provide Insights into Apolipoprotein-Lipid Interactions
Authors : Kumar, M.S.; Carson, M.; Hussain, M.M.; Murthy, H.M.K.
Deposited on : 2002-03-11
Resolution : 2.30 Å(reported)

This is a wwPDB validation summary 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/ValidationPDFNotes.html>

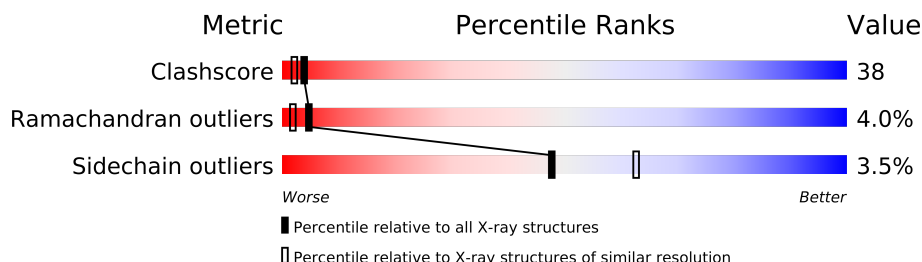
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 Å.









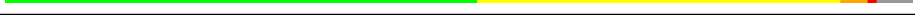

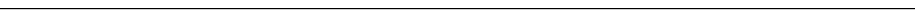
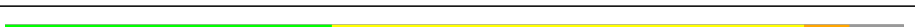



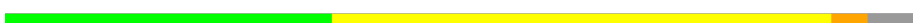

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	77	
1	2	77	
1	3	77	
1	4	77	
1	5	77	
1	6	77	
1	7	77	
1	8	77	
1	A	77	
1	B	77	
1	C	77	
1	D	77	
1	E	77	
1	F	77	
1	G	77	
1	H	77	
1	I	77	

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Mol	Chain	Length	Quality of chain
1	J	77	
1	K	77	
1	L	77	
1	M	77	
1	N	77	
1	P	77	
1	Q	77	
1	S	77	
1	T	77	
1	U	77	
1	V	77	
1	W	77	
1	X	77	
1	Y	77	
1	Z	77	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21106 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Apolipoprotein A-II.

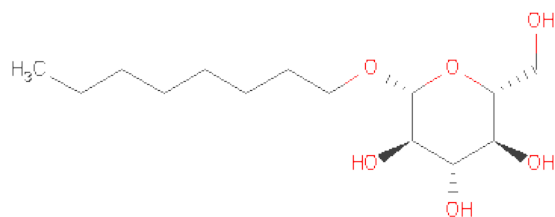
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	B	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	C	76	Total	C	N	O	S	0	0	0
			604	388	92	122	2			
1	D	74	Total	C	N	O	S	0	0	0
			590	380	90	118	2			
1	E	72	Total	C	N	O	S	0	0	0
			578	372	88	116	2			
1	F	75	Total	C	N	O	S	0	0	0
			595	383	91	119	2			
1	G	74	Total	C	N	O	S	0	0	0
			587	379	89	117	2			
1	H	74	Total	C	N	O	S	0	0	0
			587	379	89	117	2			
1	I	73	Total	C	N	O	S	0	0	0
			583	374	88	119	2			
1	J	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	K	74	Total	C	N	O	S	0	0	0
			590	380	90	118	2			
1	L	74	Total	C	N	O	S	0	0	0
			589	377	90	120	2			
1	M	76	Total	C	N	O	S	0	0	0
			604	388	92	122	2			
1	N	76	Total	C	N	O	S	0	0	0
			604	388	92	122	2			
1	P	73	Total	C	N	O	S	0	0	0
			582	376	88	116	2			
1	Q	73	Total	C	N	O	S	0	0	0
			576	370	88	116	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	S	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	T	74	Total	C	N	O	S	0	0	0
			590	379	89	120	2			
1	U	76	Total	C	N	O	S	0	0	0
			604	388	92	122	2			
1	V	75	Total	C	N	O	S	0	0	0
			595	383	91	119	2			
1	W	73	Total	C	N	O	S	0	0	0
			587	377	89	119	2			
1	X	75	Total	C	N	O	S	0	0	0
			595	383	91	119	2			
1	Y	74	Total	C	N	O	S	0	0	0
			587	379	89	117	2			
1	Z	72	Total	C	N	O	S	0	0	0
			573	371	87	113	2			
1	1	73	Total	C	N	O	S	0	0	0
			583	374	88	119	2			
1	2	73	Total	C	N	O	S	0	0	0
			581	374	88	117	2			
1	3	73	Total	C	N	O	S	0	0	0
			585	377	89	117	2			
1	4	74	Total	C	N	O	S	0	0	0
			586	378	90	116	2			
1	5	75	Total	C	N	O	S	0	0	0
			597	384	91	120	2			
1	6	75	Total	C	N	O	S	0	0	0
			597	384	91	120	2			
1	7	70	Total	C	N	O	S	0	0	0
			559	362	84	111	2			
1	8	74	Total	C	N	O	S	0	0	0
			587	379	89	117	2			

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total 10	C 9	O 1	0	0
2	B	1	Total 20	C 14	O 6	0	0
2	A	1	Total 20	C 14	O 6	0	0
2	A	1	Total 20	C 14	O 6	0	0
2	I	1	Total 20	C 14	O 6	0	0
2	B	1	Total 20	C 14	O 6	0	0
2	J	1	Total 20	C 14	O 6	0	0
2	J	1	Total 20	C 14	O 6	0	0
2	B	1	Total 20	C 14	O 6	0	0
2	K	1	Total 20	C 14	O 6	0	0
2	D	1	Total 20	C 14	O 6	0	0
2	D	1	Total 10	C 9	O 1	0	0
2	C	1	Total 20	C 14	O 6	0	0
2	L	1	Total 20	C 14	O 6	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	K	1	Total	C	O	0	0
			20	14	6		
2	N	1	Total	C	O	0	0
			20	14	6		
2	N	1	Total	C	O	0	0
			20	14	6		
2	F	1	Total	C	O	0	0
			20	14	6		
2	M	1	Total	C	O	0	0
			20	14	6		
2	M	1	Total	C	O	0	0
			20	14	6		
2	N	1	Total	C	O	0	0
			20	14	6		
2	E	1	Total	C	O	0	0
			20	14	6		
2	N	1	Total	C	O	0	0
			20	14	6		
2	M	1	Total	C	O	0	0
			20	14	6		
2	H	1	Total	C	O	0	0
			20	14	6		
2	Q	1	Total	C	O	0	0
			20	14	6		
2	Q	1	Total	C	O	0	0
			20	14	6		
2	H	1	Total	C	O	0	0
			20	14	6		
2	Q	1	Total	C	O	0	0
			20	14	6		
2	H	1	Total	C	O	0	0
			20	14	6		
2	P	1	Total	C	O	0	0
			20	14	6		
2	G	1	Total	C	O	0	0
			20	14	6		
2	G	1	Total	C	O	0	0
			20	14	6		
2	T	1	Total	C	O	0	0
			20	14	6		
2	2	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	S	1	Total	C	O	0	0
			20	14	6		
2	1	1	Total	C	O	0	0
			20	14	6		
2	T	1	Total	C	O	0	0
			20	14	6		
2	1	1	Total	C	O	0	0
			20	14	6		
2	2	1	Total	C	O	0	0
			20	14	6		
2	1	1	Total	C	O	0	0
			20	14	6		
2	U	1	Total	C	O	0	0
			20	14	6		
2	3	1	Total	C	O	0	0
			20	14	6		
2	4	1	Total	C	O	0	0
			20	14	6		
2	U	1	Total	C	O	0	0
			20	14	6		
2	3	1	Total	C	O	0	0
			20	14	6		
2	6	1	Total	C	O	0	0
			20	14	6		
2	W	1	Total	C	O	0	0
			20	14	6		
2	5	1	Total	C	O	0	0
			20	14	6		
2	5	1	Total	C	O	0	0
			20	14	6		
2	5	1	Total	C	O	0	0
			20	14	6		
2	6	1	Total	C	O	0	0
			20	14	6		
2	W	1	Total	C	O	0	0
			20	14	6		
2	5	1	Total	C	O	0	0
			20	14	6		
2	X	1	Total	C	O	0	0
			20	14	6		
2	7	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	8	1	Total	C	O	0	0
			20	14	6		
2	8	1	Total	C	O	0	0
			20	14	6		
2	Z	1	Total	C	O	0	0
			20	14	6		
2	Y	1	Total	C	O	0	0
			20	14	6		
2	Z	1	Total	C	O	0	0
			20	14	6		
2	Z	1	Total	C	O	0	0
			20	14	6		
2	Y	1	Total	C	O	0	0
			20	14	6		
2	Y	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	19	Total	O	0	0
			19	19		
3	2	27	Total	O	0	0
			27	27		
3	3	31	Total	O	0	0
			31	31		
3	4	28	Total	O	0	0
			28	28		
3	5	21	Total	O	0	0
			21	21		
3	6	23	Total	O	0	0
			23	23		
3	7	42	Total	O	0	0
			42	42		
3	8	65	Total	O	0	0
			65	65		
3	A	36	Total	O	0	0
			36	36		
3	B	30	Total	O	0	0
			30	30		
3	C	16	Total	O	0	0
			16	16		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	19	Total 19	O 19	0	0
3	E	46	Total 46	O 46	0	0
3	F	26	Total 26	O 26	0	0
3	G	70	Total 70	O 70	0	0
3	H	20	Total 20	O 20	0	0
3	I	38	Total 38	O 38	0	0
3	J	32	Total 32	O 32	0	0
3	K	32	Total 32	O 32	0	0
3	L	26	Total 26	O 26	0	0
3	M	31	Total 31	O 31	0	0
3	N	56	Total 56	O 56	0	0
3	P	34	Total 34	O 34	0	0
3	Q	39	Total 39	O 39	0	0
3	S	28	Total 28	O 28	0	0
3	T	22	Total 22	O 22	0	0
3	U	27	Total 27	O 27	0	0
3	V	23	Total 23	O 23	0	0
3	W	23	Total 23	O 23	0	0
3	X	20	Total 20	O 20	0	0
3	Y	38	Total 38	O 38	0	0
3	Z	23	Total 23	O 23	0	0

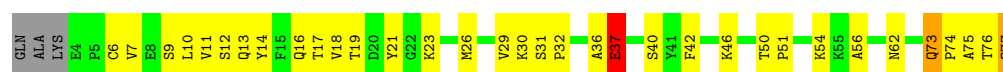
3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: Apolipoprotein A-II

Chain A: 



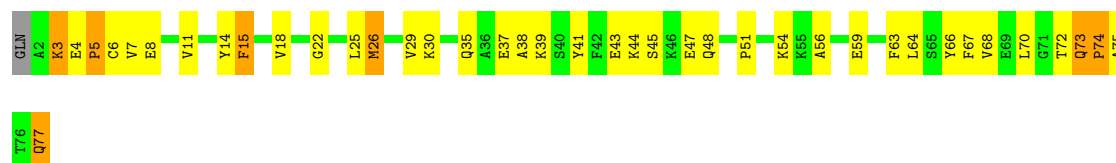
- Molecule 1: Apolipoprotein A-II

Chain B: 



- Molecule 1: Apolipoprotein A-II

Chain C: 



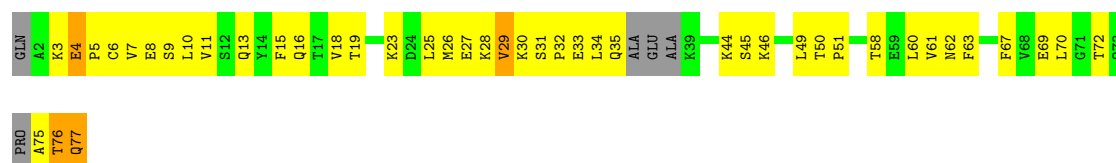
- Molecule 1: Apolipoprotein A-II

Chain D: 



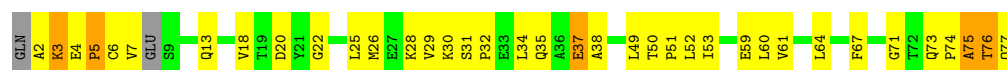
- Molecule 1: Apolipoprotein A-II

Chain E: 



- Molecule 1: Apolipoprotein A-II

Chain F: 



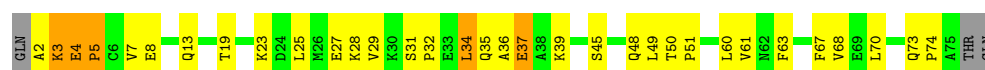
- Molecule 1: Apolipoprotein A-II

Chain G: 



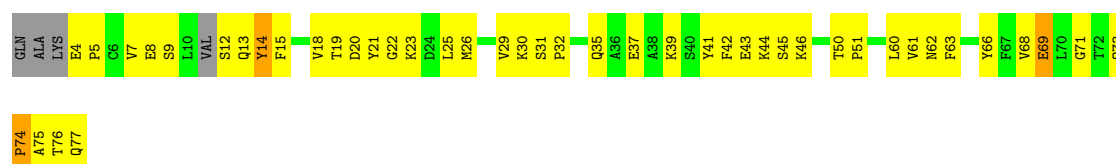
- Molecule 1: Apolipoprotein A-II

Chain H: 



- Molecule 1: Apolipoprotein A-II

Chain I: 



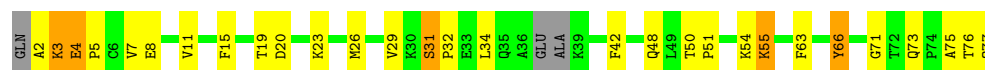
- Molecule 1: Apolipoprotein A-II

Chain J: 



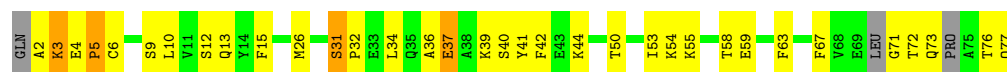
- Molecule 1: Apolipoprotein A-II

Chain K: 



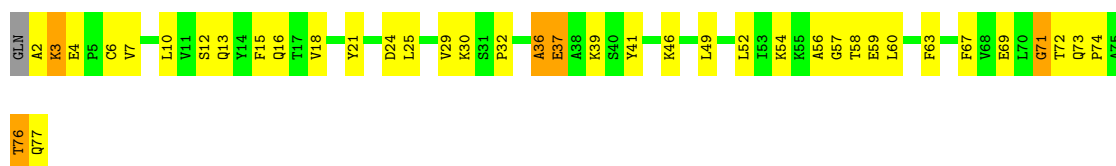
- Molecule 1: Apolipoprotein A-II

Chain L: 



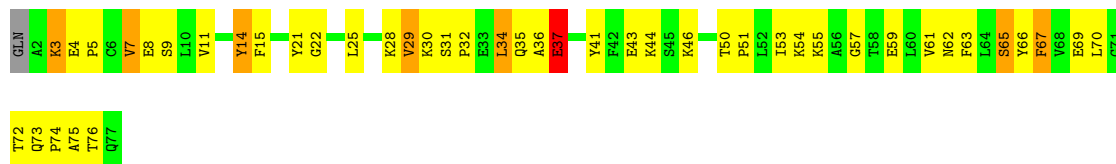
- Molecule 1: Apolipoprotein A-II

Chain M: 



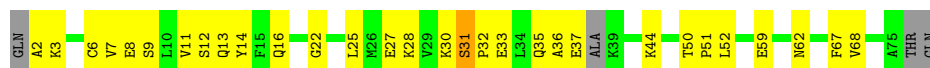
- Molecule 1: Apolipoprotein A-II

Chain N: 



- Molecule 1: Apolipoprotein A-II

Chain P: 



- Molecule 1: Apolipoprotein A-II

Chain Q: 



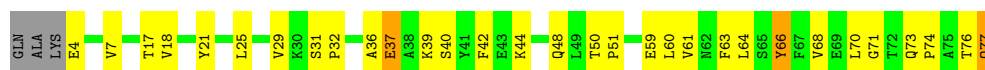
- Molecule 1: Apolipoprotein A-II

Chain S: 



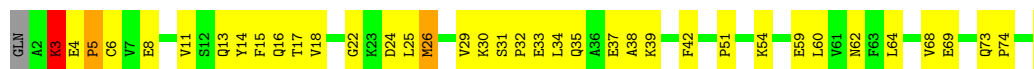
- Molecule 1: Apolipoprotein A-II

Chain T: 



- Molecule 1: Apolipoprotein A-II

Chain U: 



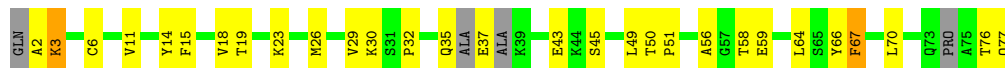
- Molecule 1: Apolipoprotein A-II

Chain V: 



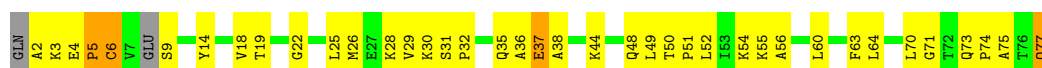
- Molecule 1: Apolipoprotein A-II

Chain W:



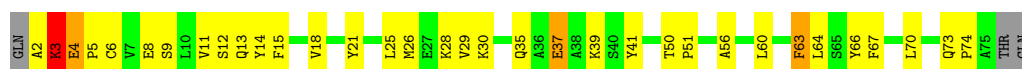
- Molecule 1: Apolipoprotein A-II

Chain X:



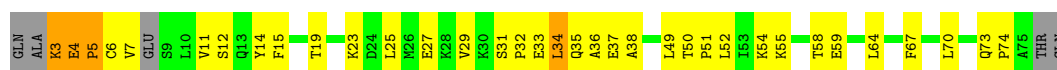
- Molecule 1: Apolipoprotein A-II

Chain Y:



- Molecule 1: Apolipoprotein A-II

Chain Z:



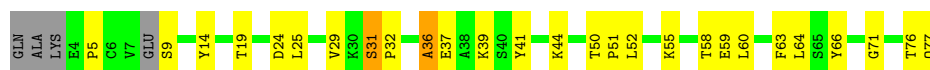
- Molecule 1: Apolipoprotein A-II

Chain 1:



- Molecule 1: Apolipoprotein A-II

Chain 2:



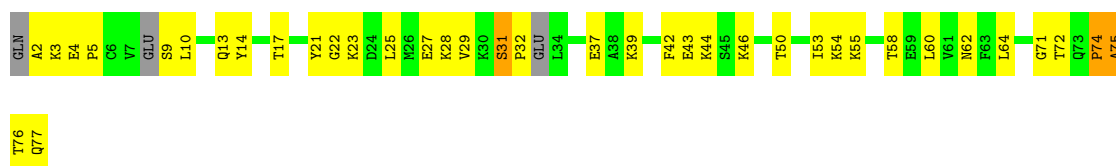
- Molecule 1: Apolipoprotein A-II

Chain 3:



- Molecule 1: Apolipoprotein A-II

Chain 4:



- Molecule 1: Apolipoprotein A-II

Chain 5:



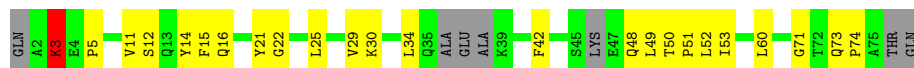
- Molecule 1: Apolipoprotein A-II

Chain 6:



- Molecule 1: Apolipoprotein A-II

Chain 7:



- Molecule 1: Apolipoprotein A-II

Chain 8:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	114.40Å 115.90Å 126.60Å 90.70° 96.20° 93.50°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	88.0 (8.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	21106	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	1	0.41	1/593 (0.2%)	0.49	0/797
1	2	0.41	1/591 (0.2%)	0.45	0/795
1	3	4.18	6/595 (1.0%)	0.53	0/799
1	4	0.42	1/595 (0.2%)	0.45	0/798
1	5	0.41	1/607 (0.2%)	0.49	0/815
1	6	0.41	1/607 (0.2%)	0.46	0/815
1	7	0.28	0/568	0.45	0/763
1	8	0.41	1/598 (0.2%)	0.46	0/806
1	A	0.40	1/601 (0.2%)	0.47	0/810
1	B	0.41	1/601 (0.2%)	0.48	0/810
1	C	0.40	1/615 (0.2%)	0.45	0/828
1	D	0.30	0/600	0.47	0/806
1	E	0.29	0/586	0.45	0/784
1	F	0.41	1/605 (0.2%)	0.51	0/813
1	G	0.41	1/598 (0.2%)	0.49	0/806
1	H	0.42	1/598 (0.2%)	0.47	0/806
1	I	0.41	1/593 (0.2%)	0.51	0/797
1	J	0.41	1/601 (0.2%)	0.45	0/810
1	K	4.11	6/600 (1.0%)	0.54	0/806
1	L	0.43	1/597 (0.2%)	0.45	0/799
1	M	0.42	1/615 (0.2%)	0.51	0/828
1	N	3.43	7/615 (1.1%)	0.63	2/828 (0.2%)
1	P	0.41	1/592 (0.2%)	0.47	0/796
1	Q	0.41	1/585 (0.2%)	0.49	0/787
1	S	0.41	1/601 (0.2%)	0.53	0/810
1	T	0.40	1/601 (0.2%)	0.47	0/810
1	U	0.41	1/615 (0.2%)	0.45	0/828
1	V	0.29	0/605	0.47	0/813
1	W	0.40	1/594 (0.2%)	0.44	0/793
1	X	0.41	1/605 (0.2%)	0.48	0/813
1	Y	0.40	1/598 (0.2%)	0.44	0/806
1	Z	0.42	1/583 (0.2%)	0.49	0/784

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	1.26	44/19158 (0.2%)	0.48	2/25759 (0.0%)

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	3	66	TYR	CD1-CE1	55.43	2.22	1.39
1	3	66	TYR	CD2-CE2	53.00	2.18	1.39
1	K	66	TYR	CD2-CE2	52.73	2.18	1.39
1	K	66	TYR	CD1-CE1	52.49	2.18	1.39
1	K	66	TYR	CE2-CZ	39.00	1.89	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	67	PHE	CD1-CG-CD2	5.09	124.92	118.30
1	N	67	PHE	CB-CG-CD2	-5.05	117.27	120.80

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	583	0	576	27	9
1	2	581	0	579	22	0
1	3	585	0	587	93	0
1	4	586	0	590	41	0
1	5	597	0	596	27	0
1	6	597	0	596	34	2
1	7	559	0	558	33	0
1	8	587	0	589	69	2
1	A	590	0	586	51	0
1	B	590	0	586	45	0
1	C	604	0	604	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	590	0	590	45	0
1	E	578	0	579	72	9
1	F	595	0	597	39	0
1	G	587	0	589	67	0
1	H	587	0	589	48	0
1	I	583	0	576	51	0
1	J	590	0	586	59	0
1	K	590	0	591	75	0
1	L	589	0	584	46	0
1	M	604	0	604	56	0
1	N	604	0	604	111	0
1	P	582	0	583	35	0
1	Q	576	0	579	40	0
1	S	590	0	586	35	0
1	T	590	0	586	63	0
1	U	604	0	604	49	0
1	V	595	0	597	63	0
1	W	587	0	584	30	0
1	X	595	0	597	51	0
1	Y	587	0	589	51	0
1	Z	573	0	577	45	0
2	1	60	0	84	7	0
2	2	40	0	56	2	0
2	3	40	0	56	34	0
2	4	20	0	28	0	0
2	5	80	0	112	13	0
2	6	40	0	56	3	0
2	7	20	0	28	3	0
2	8	40	0	56	4	0
2	A	40	0	56	3	0
2	B	60	0	84	8	0
2	C	20	0	28	3	0
2	D	30	0	45	5	0
2	E	20	0	28	7	0
2	F	20	0	28	9	0
2	G	40	0	56	17	0
2	H	60	0	84	7	0
2	I	30	0	43	7	0
2	J	40	0	56	1	0
2	K	40	0	56	38	0
2	L	20	0	28	4	0
2	M	60	0	84	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	80	0	112	52	0
2	P	20	0	28	1	0
2	Q	60	0	84	11	0
2	S	20	0	28	1	0
2	T	40	0	56	6	0
2	U	40	0	56	6	0
2	W	40	0	56	3	0
2	X	20	0	28	5	0
2	Y	60	0	84	6	0
2	Z	60	0	84	9	0
3	1	19	0	0	6	0
3	2	27	0	0	11	0
3	3	31	0	0	39	0
3	4	28	0	0	17	0
3	5	21	0	0	10	0
3	6	23	0	0	9	0
3	7	42	0	0	17	0
3	8	65	0	0	54	0
3	A	36	0	0	33	0
3	B	30	0	0	23	0
3	C	16	0	0	5	0
3	D	19	0	0	15	0
3	E	46	0	0	27	0
3	F	26	0	0	20	0
3	G	70	0	0	43	0
3	H	20	0	0	11	0
3	I	38	0	0	30	0
3	J	32	0	0	25	0
3	K	32	0	0	25	0
3	L	26	0	0	19	0
3	M	31	0	0	19	0
3	N	56	0	0	45	0
3	P	34	0	0	14	0
3	Q	39	0	0	20	0
3	S	28	0	0	20	0
3	T	22	0	0	12	0
3	U	27	0	0	21	0
3	V	23	0	0	12	0
3	W	23	0	0	15	0
3	X	20	0	0	23	0
3	Y	38	0	0	32	0
3	Z	23	0	0	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	21106	0	20586	1535	11

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 38.

The worst 5 of 1535 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:3:66:TYR:CD2	1:3:66:TYR:CG	1.77	1.70
1:3:66:TYR:CG	1:3:66:TYR:CD1	1.77	1.68
1:K:66:TYR:CD1	1:K:66:TYR:CG	1.76	1.68
1:N:67:PHE:CG	1:N:67:PHE:CD2	1.75	1.68
1:K:66:TYR:CD2	1:K:66:TYR:CG	1.77	1.67

The worst 5 of 11 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	Distance(Å)	Clash(Å)
1:E:28:LYS:CE	1:1:73:GLN:CD[1_455]	0.76	1.44
1:E:28:LYS:CE	1:1:73:GLN:OE1[1_455]	1.14	1.06
1:E:28:LYS:NZ	1:1:73:GLN:CG[1_455]	1.17	1.03
1:E:28:LYS:NZ	1:1:73:GLN:CB[1_455]	1.18	1.02
1:E:28:LYS:CE	1:1:73:GLN:CG[1_455]	1.26	0.94

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	1	69/77 (90%)	63 (91%)	5 (7%)	1 (1%)	16	15
1	2	69/77 (90%)	57 (83%)	9 (13%)	3 (4%)	4	2
1	3	69/77 (90%)	55 (80%)	11 (16%)	3 (4%)	4	2
1	4	68/77 (88%)	59 (87%)	6 (9%)	3 (4%)	4	1
1	5	71/77 (92%)	55 (78%)	14 (20%)	2 (3%)	8	4
1	6	72/77 (94%)	59 (82%)	8 (11%)	5 (7%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	7	64/77 (83%)	58 (91%)	4 (6%)	2 (3%)	7	3
1	8	72/77 (94%)	63 (88%)	6 (8%)	3 (4%)	4	2
1	A	72/77 (94%)	62 (86%)	8 (11%)	2 (3%)	8	4
1	B	72/77 (94%)	64 (89%)	6 (8%)	2 (3%)	8	4
1	C	74/77 (96%)	63 (85%)	8 (11%)	3 (4%)	4	2
1	D	70/77 (91%)	61 (87%)	3 (4%)	6 (9%)	1	0
1	E	66/77 (86%)	60 (91%)	3 (4%)	3 (4%)	4	1
1	F	71/77 (92%)	58 (82%)	8 (11%)	5 (7%)	2	0
1	G	72/77 (94%)	66 (92%)	6 (8%)	0	100	100
1	H	72/77 (94%)	62 (86%)	7 (10%)	3 (4%)	4	2
1	I	69/77 (90%)	59 (86%)	8 (12%)	2 (3%)	7	4
1	J	72/77 (94%)	59 (82%)	7 (10%)	6 (8%)	1	0
1	K	70/77 (91%)	58 (83%)	9 (13%)	3 (4%)	4	2
1	L	68/77 (88%)	54 (79%)	10 (15%)	4 (6%)	2	1
1	M	74/77 (96%)	54 (73%)	16 (22%)	4 (5%)	3	1
1	N	74/77 (96%)	59 (80%)	11 (15%)	4 (5%)	3	1
1	P	69/77 (90%)	61 (88%)	6 (9%)	2 (3%)	7	4
1	Q	69/77 (90%)	63 (91%)	6 (9%)	0	100	100
1	S	72/77 (94%)	61 (85%)	8 (11%)	3 (4%)	4	2
1	T	72/77 (94%)	67 (93%)	3 (4%)	2 (3%)	8	4
1	U	74/77 (96%)	65 (88%)	7 (10%)	2 (3%)	8	5
1	V	71/77 (92%)	60 (84%)	7 (10%)	4 (6%)	3	1
1	W	66/77 (86%)	56 (85%)	10 (15%)	0	100	100
1	X	71/77 (92%)	56 (79%)	9 (13%)	6 (8%)	1	0
1	Y	72/77 (94%)	69 (96%)	2 (3%)	1 (1%)	16	15
1	Z	68/77 (88%)	59 (87%)	7 (10%)	2 (3%)	7	4
All	All	2254/2464 (92%)	1925 (85%)	238 (11%)	91 (4%)	5	2

5 of 91 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	VAL
1	C	73	GLN

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Mol	Chain	Res	Type
1	D	4	GLU
1	E	4	GLU
1	E	76	THR

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	1	66/69 (96%)	63 (96%)	3 (4%)	38	50
1	2	66/69 (96%)	64 (97%)	2 (3%)	53	70
1	3	67/69 (97%)	63 (94%)	4 (6%)	27	35
1	4	66/69 (96%)	66 (100%)	0	100	100
1	5	67/69 (97%)	66 (98%)	1 (2%)	76	89
1	6	67/69 (97%)	65 (97%)	2 (3%)	53	70
1	7	64/69 (93%)	63 (98%)	1 (2%)	75	88
1	8	66/69 (96%)	63 (96%)	3 (4%)	38	50
1	A	67/69 (97%)	65 (97%)	2 (3%)	53	70
1	B	67/69 (97%)	65 (97%)	2 (3%)	53	70
1	C	68/69 (99%)	64 (94%)	4 (6%)	28	35
1	D	67/69 (97%)	65 (97%)	2 (3%)	53	70
1	E	66/69 (96%)	64 (97%)	2 (3%)	53	70
1	F	67/69 (97%)	63 (94%)	4 (6%)	27	35
1	G	66/69 (96%)	64 (97%)	2 (3%)	53	70
1	H	66/69 (96%)	64 (97%)	2 (3%)	53	70
1	I	66/69 (96%)	64 (97%)	2 (3%)	53	70
1	J	67/69 (97%)	67 (100%)	0	100	100
1	K	67/69 (97%)	64 (96%)	3 (4%)	38	50
1	L	66/69 (96%)	64 (97%)	2 (3%)	53	70
1	M	68/69 (99%)	65 (96%)	3 (4%)	39	51
1	N	68/69 (99%)	63 (93%)	5 (7%)	20	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	66/69 (96%)	66 (100%)	0	100	100
1	Q	65/69 (94%)	62 (95%)	3 (5%)	37	48
1	S	67/69 (97%)	65 (97%)	2 (3%)	53	70
1	T	67/69 (97%)	65 (97%)	2 (3%)	53	70
1	U	68/69 (99%)	65 (96%)	3 (4%)	39	51
1	V	67/69 (97%)	65 (97%)	2 (3%)	53	70
1	W	67/69 (97%)	65 (97%)	2 (3%)	53	70
1	X	67/69 (97%)	64 (96%)	3 (4%)	38	50
1	Y	66/69 (96%)	62 (94%)	4 (6%)	26	34
1	Z	65/69 (94%)	62 (95%)	3 (5%)	37	48
All	All	2130/2208 (96%)	2055 (96%)	75 (4%)	48	63

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	37	GLU
1	T	77	GLN
1	6	37	GLU
1	N	41	TYR
1	S	26	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	35	GLN
1	T	73	GLN
1	6	35	GLN
1	Q	73	GLN
1	T	77	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

64 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	BOG	1	1705	-	20,20,20	0.80	1 (5%)	25,25,25	0.65	0
2	BOG	1	1707	-	20,20,20	0.80	1 (5%)	25,25,25	0.65	0
2	BOG	1	1709	-	20,20,20	0.79	1 (5%)	25,25,25	0.66	0
2	BOG	2	1703	-	20,20,20	0.80	1 (5%)	25,25,25	0.64	0
2	BOG	2	1708	-	20,20,20	0.79	1 (5%)	25,25,25	0.65	0
2	BOG	3	1712	-	20,20,20	0.79	1 (5%)	25,25,25	0.63	0
2	BOG	3	1716	-	20,20,20	4.33	2 (10%)	25,25,25	1.03	2 (8%)
2	BOG	4	1714	-	20,20,20	0.81	1 (5%)	25,25,25	0.64	0
2	BOG	5	1719	-	20,20,20	0.79	1 (5%)	25,25,25	0.66	0
2	BOG	5	1720	-	20,20,20	0.78	1 (5%)	25,25,25	0.65	0
2	BOG	5	1721	-	20,20,20	0.83	1 (5%)	25,25,25	0.63	0
2	BOG	5	1724	-	20,20,20	0.78	1 (5%)	25,25,25	0.65	0
2	BOG	6	1717	-	20,20,20	0.80	1 (5%)	25,25,25	0.64	0
2	BOG	6	1722	-	20,20,20	0.80	1 (5%)	25,25,25	0.66	0
2	BOG	7	1726	-	20,20,20	0.80	1 (5%)	25,25,25	0.64	0
2	BOG	8	1727	-	20,20,20	0.79	1 (5%)	25,25,25	0.65	0
2	BOG	8	1728	-	20,20,20	0.79	1 (5%)	25,25,25	0.69	0
2	BOG	A	1603	-	20,20,20	0.78	1 (5%)	25,25,25	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BOG	A	1604	-	20,20,20	0.79	1 (5%)	25,25,25	0.64	0
2	BOG	B	1602	-	20,20,20	0.80	1 (5%)	25,25,25	0.65	0
2	BOG	B	1606	-	20,20,20	0.78	1 (5%)	25,25,25	0.67	0
2	BOG	B	1609	-	20,20,20	0.78	1 (5%)	25,25,25	0.67	0
2	BOG	C	1614	-	20,20,20	0.76	1 (5%)	25,25,25	0.66	0
2	BOG	D	1612	-	20,20,20	0.76	1 (5%)	25,25,25	0.68	0
2	BOG	D	1613	-	8,9,20	0.15	0	7,8,25	0.59	0
2	BOG	E	1623	-	20,20,20	0.81	1 (5%)	25,25,25	0.64	0
2	BOG	F	1619	-	20,20,20	0.77	1 (5%)	25,25,25	0.64	0
2	BOG	G	1633	-	20,20,20	0.79	1 (5%)	25,25,25	0.68	0
2	BOG	G	1634	-	20,20,20	0.79	1 (5%)	25,25,25	0.65	0
2	BOG	H	1626	-	20,20,20	0.79	1 (5%)	25,25,25	0.65	0
2	BOG	H	1629	-	20,20,20	0.78	1 (5%)	25,25,25	0.63	0
2	BOG	H	1631	-	20,20,20	0.79	1 (5%)	25,25,25	0.63	0
2	BOG	I	1601	-	7,8,20	3.85	1 (14%)	6,6,25	1.13	1 (16%)
2	BOG	I	1605	-	20,20,20	0.80	1 (5%)	25,25,25	0.65	0
2	BOG	J	1607	-	20,20,20	0.81	1 (5%)	25,25,25	0.65	0
2	BOG	J	1608	-	20,20,20	0.80	1 (5%)	25,25,25	0.65	0
2	BOG	K	1610	-	20,20,20	0.79	1 (5%)	25,25,25	0.66	0
2	BOG	K	1616	-	20,20,20	4.39	2 (10%)	25,25,25	1.09	2 (8%)
2	BOG	L	1615	-	20,20,20	0.79	1 (5%)	25,25,25	0.67	0
2	BOG	M	1620	-	20,20,20	0.77	1 (5%)	25,25,25	0.70	0
2	BOG	M	1621	-	20,20,20	0.87	1 (5%)	25,25,25	0.65	0
2	BOG	M	1625	-	20,20,20	0.83	1 (5%)	25,25,25	0.67	0
2	BOG	N	1617	-	20,20,20	0.80	1 (5%)	25,25,25	0.67	0
2	BOG	N	1618	-	20,20,20	0.87	1 (5%)	25,25,25	0.67	0
2	BOG	N	1622	-	20,20,20	0.81	1 (5%)	25,25,25	0.65	0
2	BOG	N	1624	-	20,20,20	3.85	2 (10%)	25,25,25	1.14	2 (8%)
2	BOG	P	1632	-	20,20,20	0.79	1 (5%)	25,25,25	0.65	0
2	BOG	Q	1627	-	20,20,20	0.79	1 (5%)	25,25,25	0.65	0
2	BOG	Q	1628	-	20,20,20	0.79	1 (5%)	25,25,25	0.69	0
2	BOG	Q	1630	-	20,20,20	0.78	1 (5%)	25,25,25	0.64	0
2	BOG	S	1704	-	20,20,20	0.78	1 (5%)	25,25,25	0.64	0
2	BOG	T	1702	-	20,20,20	0.80	1 (5%)	25,25,25	0.65	0
2	BOG	T	1706	-	20,20,20	0.78	1 (5%)	25,25,25	0.68	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	BOG	U	1710	-	20,20,20	0.78	1 (5%)	25,25,25	0.66	0
2	BOG	U	1715	-	20,20,20	0.78	1 (5%)	25,25,25	0.68	0
2	BOG	W	1718	-	20,20,20	0.81	1 (5%)	25,25,25	0.65	0
2	BOG	W	1723	-	20,20,20	0.79	1 (5%)	25,25,25	0.66	0
2	BOG	X	1725	-	20,20,20	0.81	1 (5%)	25,25,25	0.64	0
2	BOG	Y	1730	-	20,20,20	0.79	1 (5%)	25,25,25	0.65	0
2	BOG	Y	1733	-	20,20,20	0.78	1 (5%)	25,25,25	0.65	0
2	BOG	Y	1734	-	20,20,20	0.78	1 (5%)	25,25,25	0.67	0
2	BOG	Z	1729	-	20,20,20	0.79	1 (5%)	25,25,25	0.63	0
2	BOG	Z	1731	-	20,20,20	0.80	1 (5%)	25,25,25	0.63	0
2	BOG	Z	1732	-	20,20,20	0.79	1 (5%)	25,25,25	0.65	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	BOG	1	1705	-	-	0/11/31/31	0/1/1/1
2	BOG	1	1707	-	-	0/11/31/31	0/1/1/1
2	BOG	1	1709	-	-	0/11/31/31	0/1/1/1
2	BOG	2	1703	-	-	0/11/31/31	0/1/1/1
2	BOG	2	1708	-	-	0/11/31/31	0/1/1/1
2	BOG	3	1712	-	-	0/11/31/31	0/1/1/1
2	BOG	3	1716	-	-	0/11/31/31	0/1/1/1
2	BOG	4	1714	-	-	0/11/31/31	0/1/1/1
2	BOG	5	1719	-	-	0/11/31/31	0/1/1/1
2	BOG	5	1720	-	-	0/11/31/31	0/1/1/1
2	BOG	5	1721	-	-	0/11/31/31	0/1/1/1
2	BOG	5	1724	-	-	0/11/31/31	0/1/1/1
2	BOG	6	1717	-	-	0/11/31/31	0/1/1/1
2	BOG	6	1722	-	-	0/11/31/31	0/1/1/1
2	BOG	7	1726	-	-	0/11/31/31	0/1/1/1
2	BOG	8	1727	-	-	0/11/31/31	0/1/1/1
2	BOG	8	1728	-	-	0/11/31/31	0/1/1/1
2	BOG	A	1603	-	-	0/11/31/31	0/1/1/1
2	BOG	A	1604	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1602	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1606	-	-	0/11/31/31	0/1/1/1
2	BOG	B	1609	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	C	1614	-	-	0/11/31/31	0/1/1/1
2	BOG	D	1612	-	-	0/11/31/31	0/1/1/1
2	BOG	D	1613	-	-	0/7/7/31	0/0/0/1
2	BOG	E	1623	-	-	0/11/31/31	0/1/1/1
2	BOG	F	1619	-	-	0/11/31/31	0/1/1/1
2	BOG	G	1633	-	-	0/11/31/31	0/1/1/1
2	BOG	G	1634	-	-	0/11/31/31	0/1/1/1
2	BOG	H	1626	-	-	0/11/31/31	0/1/1/1
2	BOG	H	1629	-	-	0/11/31/31	0/1/1/1
2	BOG	H	1631	-	-	0/11/31/31	0/1/1/1
2	BOG	I	1601	-	-	0/5/5/31	0/0/0/1
2	BOG	I	1605	-	-	0/11/31/31	0/1/1/1
2	BOG	J	1607	-	-	0/11/31/31	0/1/1/1
2	BOG	J	1608	-	-	0/11/31/31	0/1/1/1
2	BOG	K	1610	-	-	0/11/31/31	0/1/1/1
2	BOG	K	1616	-	-	0/11/31/31	0/1/1/1
2	BOG	L	1615	-	-	0/11/31/31	0/1/1/1
2	BOG	M	1620	-	-	0/11/31/31	0/1/1/1
2	BOG	M	1621	-	-	0/11/31/31	0/1/1/1
2	BOG	M	1625	-	-	0/11/31/31	0/1/1/1
2	BOG	N	1617	-	-	0/11/31/31	0/1/1/1
2	BOG	N	1618	-	-	0/11/31/31	0/1/1/1
2	BOG	N	1622	-	-	0/11/31/31	0/1/1/1
2	BOG	N	1624	-	-	0/11/31/31	0/1/1/1
2	BOG	P	1632	-	-	0/11/31/31	0/1/1/1
2	BOG	Q	1627	-	-	0/11/31/31	0/1/1/1
2	BOG	Q	1628	-	-	0/11/31/31	0/1/1/1
2	BOG	Q	1630	-	-	0/11/31/31	0/1/1/1
2	BOG	S	1704	-	-	0/11/31/31	0/1/1/1
2	BOG	T	1702	-	-	0/11/31/31	0/1/1/1
2	BOG	T	1706	-	-	0/11/31/31	0/1/1/1
2	BOG	U	1710	-	-	0/11/31/31	0/1/1/1
2	BOG	U	1715	-	-	0/11/31/31	0/1/1/1
2	BOG	W	1718	-	-	0/11/31/31	0/1/1/1
2	BOG	W	1723	-	-	0/11/31/31	0/1/1/1
2	BOG	X	1725	-	-	0/11/31/31	0/1/1/1
2	BOG	Y	1730	-	-	0/11/31/31	0/1/1/1
2	BOG	Y	1733	-	-	0/11/31/31	0/1/1/1
2	BOG	Y	1734	-	-	0/11/31/31	0/1/1/1
2	BOG	Z	1729	-	-	0/11/31/31	0/1/1/1
2	BOG	Z	1731	-	-	0/11/31/31	0/1/1/1
2	BOG	Z	1732	-	-	0/11/31/31	0/1/1/1

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	1616	BOG	C5'-C4'	19.23	2.68	1.51
2	3	1716	BOG	C5'-C4'	18.96	2.67	1.51
2	N	1624	BOG	C3'-C2'	16.80	2.53	1.51
2	I	1601	BOG	C1'-C2'	-10.18	1.51	1.55
2	M	1621	BOG	O5-C1	2.51	1.48	1.41

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	1624	BOG	C3'-C2'-C1'	3.40	130.03	113.58
2	K	1616	BOG	C5'-C4'-C3'	3.17	131.79	114.61
2	N	1624	BOG	C4'-C3'-C2'	3.17	131.74	114.61
2	K	1616	BOG	C6'-C5'-C4'	3.17	131.74	114.61
2	3	1716	BOG	C5'-C4'-C3'	3.03	131.01	114.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.