W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Nov 7, 2014 – 06:44 PM EST

PDB ID   :   4HGP
Title   :   Crystal Structure of 2-keto-3-deoxyoctulosonate8-phosphate phosphohydrolase from Haemophilus influenzae in complex with transition state mimic
Authors   :   Daughtry, K.D.; Allen, K.N.
Deposited on   :   2012-10-08
Resolution   :   1.80 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

1 Overall quality at a glance (i)

The reported resolution of this entry is 1.80 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	Percentile Ranks	Value
Rfree		0.170
Clashscore		5

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
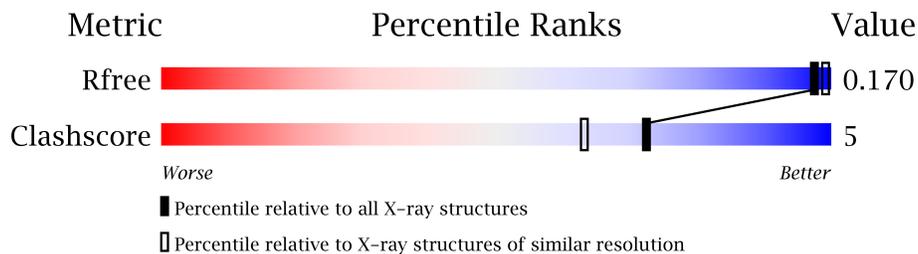
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	77520	3954 (1.80-1.80)
Clashscore	88313	4797 (1.80-1.80)

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 1566 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 polysaccharide(L) called 3-deoxy-D-manno-octulosonate8-phosphate phosphatase KdsC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
1	A	179	Total	C	N	O	S	0	0
			1352	854	230	259	9		

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is OXIDO(DIOXO)VANADIUM (three-letter code: VN4) (formula: O_3V).
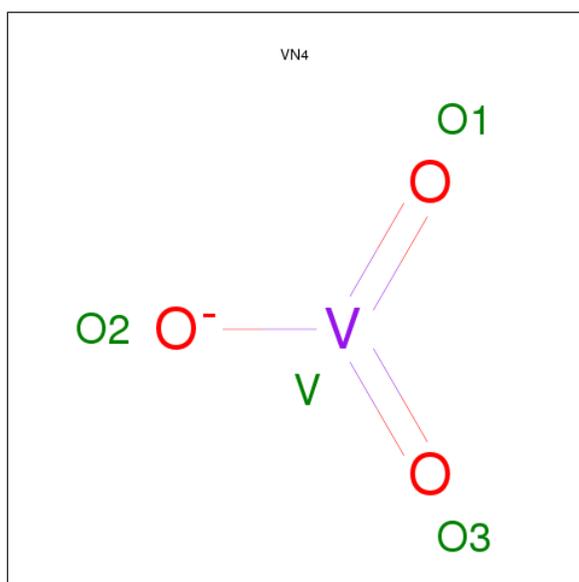
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	V	0	0
			4	3	1		

- Molecule 4 is SUGAR (3-DEOXY-D-MANNO-OCT-2-ULOSONICACID) (three-letter code: KDO) (formula: $C_8H_{14}O_8$).
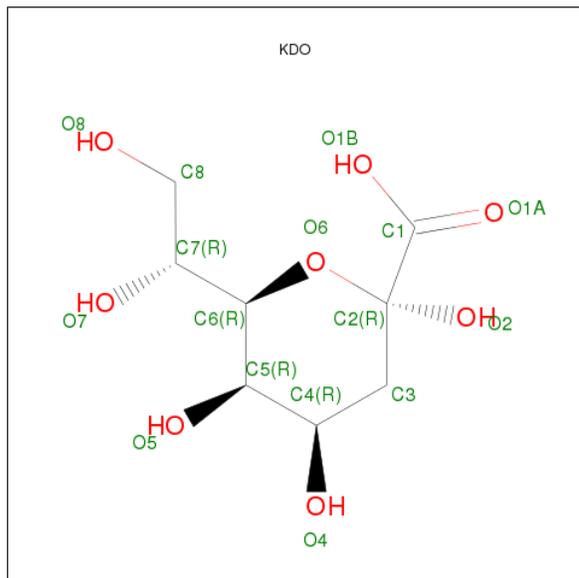
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	32	16	16	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	177	177	177	0	0

3 Residue-property plots (i)

There is no protein, DNA or RNA chain in this entry to show sequence plots.

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	79.85Å 79.85Å 52.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.46 – 1.80 29.46 – 1.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (29.46-1.80) 92.1 (29.46-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 1.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.147 , 0.173 0.143 , 0.170	Depositor DCC
R_{free} test set	715 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 25.4	EDS
Estimated twinning fraction	0.325 for -k,-h,-l	Xtriage
L-test for twinning [2]	$< |L| > = 0.38, < L^2 > = 0.21$	Xtriage
Outliers	0 of 14655 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	1566	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: KDO, MG, VN4

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	0.32	0/1371	0.49	0/1843

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts (i)

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	A	1352	0	1362	11	1
2	A	1	0	0	0	0
3	A	4	0	0	2	0
4	A	32	0	15	2	1
5	A	177	0	0	6	0
All	All	1566	0	1377	13	1

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 5.

The worst 5 of 13 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:173:LYS:NZ	5:A:455:HOH:O	2.15	0.80
1:A:37:HIS:NE2	5:A:470:HOH:O	2.20	0.74
1:A:133:ASN:ND2	5:A:430:HOH:O	2.25	0.70
1:A:132:LYS:NZ	5:A:454:HOH:O	2.28	0.65
3:A:202:VN4:O3	4:A:203[B]:KDO:O8	2.18	0.61

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	Distance(Å)	Clash(Å)
1:A:178:MET:O	4:A:203[A]:KDO:O4[3_555]	2.02	0.18

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

There are no protein chains in this entry.

5.3.2 Protein sidechains ⓘ

There are no protein chains in this entry.

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 ⓘ

179 carbohydrates 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
1	MET	A	1	-	7,7,8	1.28	1 (14%)	7,7,9	1.27	2 (28%)
1	PHE	A	10	-	11,11,12	0.92	1 (9%)	13,13,15	0.69	1 (7%)
1	GLU	A	100	-	6,8,9	2.85	2 (33%)	6,9,11	1.01	0
1	GLN	A	101	-	8,8,9	1.36	1 (12%)	9,9,11	0.92	0
1	THR	A	102	-	6,6,7	1.53	1 (16%)	7,7,9	2.09	2 (28%)
1	ALA	A	103	-	4,4,5	1.81	1 (25%)	4,4,6	1.65	1 (25%)
1	TYR	A	104	-	12,12,13	0.77	1 (8%)	15,15,17	0.66	1 (6%)
1	ILE	A	105	-	7,7,8	1.71	1 (14%)	8,8,10	0.71	0
1	GLY	A	106	-	3,3,4	0.62	0	1,2,4	1.01	0
1	ASP	A	107	2	5,7,8	2.47	2 (40%)	5,8,10	2.17	3 (60%)
1	ASP	A	108	-	5,7,8	3.12	2 (40%)	5,8,10	0.99	0
1	SER	A	109	-	5,5,6	1.81	1 (20%)	5,5,7	1.42	2 (40%)
1	VAL	A	11	-	6,6,7	1.40	1 (16%)	7,7,9	1.47	1 (14%)
1	VAL	A	110	-	6,6,7	1.55	1 (16%)	7,7,9	0.94	0
1	ASP	A	111	-	5,7,8	2.25	2 (40%)	5,8,10	1.26	1 (20%)
1	LEU	A	112	-	7,7,8	1.88	1 (14%)	8,8,10	1.42	3 (37%)
1	PRO	A	113	-	7,7,8	1.98	1 (14%)	8,8,10	1.16	1 (12%)
1	ALA	A	114	-	4,4,5	1.79	1 (25%)	4,4,6	1.55	1 (25%)
1	PHE	A	115	-	11,11,12	0.86	1 (9%)	13,13,15	0.64	0
1	ALA	A	116	-	4,4,5	1.93	1 (25%)	4,4,6	1.60	1 (25%)
1	ALA	A	117	-	4,4,5	1.88	1 (25%)	4,4,6	1.80	1 (25%)
1	CYS	A	118	-	5,5,6	1.68	1 (20%)	5,5,7	1.09	0
1	GLY	A	119	-	3,3,4	0.61	0	1,2,4	0.71	0
1	ILE	A	12	-	7,7,8	1.41	1 (14%)	8,8,10	1.01	1 (12%)
1	THR	A	120	-	6,6,7	0.97	1 (16%)	7,7,9	1.67	1 (14%)
1	SER	A	121	-	5,5,6	1.43	1 (20%)	5,5,7	1.00	0
1	PHE	A	122	-	11,11,12	1.01	1 (9%)	13,13,15	0.90	1 (7%)
1	ALA	A	123	-	4,4,5	1.45	1 (25%)	4,4,6	1.68	1 (25%)
1	VAL	A	124	-	6,6,7	1.32	1 (16%)	7,7,9	1.15	2 (28%)
1	ALA	A	125	-	4,4,5	2.03	1 (25%)	4,4,6	2.00	2 (50%)
1	ASP	A	126	-	5,7,8	3.00	2 (40%)	5,8,10	1.18	0
1	ALA	A	127	-	4,4,5	1.56	1 (25%)	4,4,6	1.72	1 (25%)
1	PRO	A	128	-	7,7,8	1.08	1 (14%)	8,8,10	1.36	2 (25%)
1	ILE	A	129	-	7,7,8	1.70	1 (14%)	8,8,10	0.79	0
1	THR	A	13	-	6,6,7	1.46	1 (16%)	7,7,9	1.50	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	TYR	A	130	-	12,12,13	0.99	1 (8%)	15,15,17	0.71	1 (6%)
1	VAL	A	131	-	6,6,7	1.33	1 (16%)	7,7,9	0.87	1 (14%)
1	LYS	A	132	-	8,8,9	1.30	1 (12%)	8,8,10	0.94	0
1	ASN	A	133	-	7,7,8	1.11	1 (14%)	8,8,10	1.30	1 (12%)
1	ALA	A	134	-	4,4,5	2.08	1 (25%)	4,4,6	1.82	1 (25%)
1	VAL	A	135	-	6,6,7	1.51	1 (16%)	7,7,9	1.15	1 (14%)
1	ASP	A	136	-	5,7,8	1.36	1 (20%)	5,8,10	1.27	1 (20%)
1	HIS	A	137	-	10,10,11	1.59	1 (10%)	12,12,14	4.14	3 (25%)
1	VAL	A	138	-	6,6,7	1.49	1 (16%)	7,7,9	0.90	0
1	LEU	A	139	-	7,7,8	1.19	1 (14%)	8,8,10	0.76	0
1	ASP	A	14	3,2	5,7,8	2.09	1 (20%)	5,8,10	1.20	1 (20%)
1	SER	A	140	-	5,5,6	2.02	1 (20%)	5,5,7	1.09	1 (20%)
1	THR	A	141	-	6,6,7	1.76	1 (16%)	7,7,9	1.79	2 (28%)
1	HIS	A	142	-	10,10,11	1.63	1 (10%)	12,12,14	4.18	4 (33%)
1	GLY	A	143	-	3,3,4	0.58	0	1,2,4	0.95	0
1	GLY	A	144	-	3,3,4	0.59	0	1,2,4	0.89	0
1	LYS	A	145	-	8,8,9	1.40	1 (12%)	8,8,10	0.98	0
1	GLY	A	146	-	3,3,4	0.58	0	1,2,4	0.88	0
1	ALA	A	147	-	4,4,5	1.62	1 (25%)	4,4,6	1.57	1 (25%)
1	PHE	A	148	-	11,11,12	1.23	1 (9%)	13,13,15	0.61	1 (7%)
1	ARG	A	149	-	8,10,11	2.26	2 (25%)	7,11,13	1.15	0
1	VAL	A	15	-	6,6,7	1.06	1 (16%)	7,7,9	1.55	1 (14%)
1	GLU	A	150	-	6,8,9	1.33	1 (16%)	6,9,11	1.15	1 (16%)
1	MET	A	151	-	7,7,8	1.63	1 (14%)	7,7,9	1.06	1 (14%)
1	SER	A	152	-	5,5,6	1.57	1 (20%)	5,5,7	1.11	1 (20%)
1	ASP	A	153	-	5,7,8	2.09	2 (40%)	5,8,10	1.06	1 (20%)
1	MET	A	154	-	7,7,8	1.00	0	7,7,9	1.63	1 (14%)
1	ILE	A	155	-	7,7,8	1.11	1 (14%)	8,8,10	0.94	0
1	LEU	A	156	-	7,7,8	1.44	1 (14%)	8,8,10	0.92	0
1	GLN	A	157	-	8,8,9	1.47	1 (12%)	9,9,11	1.04	1 (11%)
1	ALA	A	158	-	4,4,5	1.64	1 (25%)	4,4,6	1.53	1 (25%)
1	GLN	A	159	-	8,8,9	1.31	1 (12%)	9,9,11	0.95	1 (11%)
1	ASP	A	16	2	5,7,8	2.32	2 (40%)	5,8,10	0.89	0
1	GLY	A	160	-	3,3,4	0.63	0	1,2,4	0.87	0
1	LYS	A	161	-	8,8,9	0.97	1 (12%)	8,8,10	1.11	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	SER	A	162	-	5,5,6	1.78	1 (20%)	5,5,7	1.73	2 (40%)
1	SER	A	163	-	5,5,6	1.95	1 (20%)	5,5,7	1.32	1 (20%)
1	VAL	A	164	-	6,6,7	1.57	1 (16%)	7,7,9	1.01	0
1	PHE	A	165	-	11,11,12	1.24	1 (9%)	13,13,15	1.03	2 (15%)
1	ASP	A	166	-	5,7,8	2.60	2 (40%)	5,8,10	1.66	2 (40%)
1	THR	A	167	-	6,6,7	1.47	1 (16%)	7,7,9	2.04	2 (28%)
1	ALA	A	168	-	4,4,5	1.42	1 (25%)	4,4,6	1.52	1 (25%)
1	GLN	A	169	-	8,8,9	1.40	1 (12%)	9,9,11	0.91	0
1	GLY	A	17	-	3,3,4	0.65	0	1,2,4	0.81	0
1	GLY	A	170	-	3,3,4	0.57	0	1,2,4	0.79	0
1	PHE	A	171	-	11,11,12	0.96	1 (9%)	13,13,15	0.64	0
1	LEU	A	172	-	7,7,8	1.21	1 (14%)	8,8,10	0.95	0
1	LYS	A	173	-	8,8,9	0.87	1 (12%)	8,8,10	1.09	1 (12%)
1	SER	A	174	-	5,5,6	1.61	1 (20%)	5,5,7	1.06	1 (20%)
1	VAL	A	175	-	6,6,7	1.97	1 (16%)	7,7,9	1.23	2 (28%)
1	LYS	A	176	-	8,8,9	1.25	1 (12%)	8,8,10	0.89	0
1	SER	A	177	-	5,5,6	1.74	1 (20%)	5,5,7	1.17	1 (20%)
1	MET	A	178	-	7,7,8	1.64	1 (14%)	7,7,9	1.42	1 (14%)
1	GLY	A	179	-	3,3,4	0.67	0	1,2,4	0.74	0
1	VAL	A	18	-	6,6,7	1.29	1 (16%)	7,7,9	0.93	0
1	LEU	A	19	-	7,7,8	1.23	1 (14%)	8,8,10	0.78	0
1	GLN	A	2	-	8,8,9	1.35	1 (12%)	9,9,11	1.02	1 (11%)
1	THR	A	20	-	6,6,7	1.32	1 (16%)	7,7,9	1.91	3 (42%)
1	ASP	A	21	-	5,7,8	2.67	2 (40%)	5,8,10	1.16	0
1	GLY	A	22	-	3,3,4	0.64	0	1,2,4	0.93	0
1	GLN	A	23	-	8,8,9	0.94	1 (12%)	9,9,11	1.09	1 (11%)
1	LEU	A	24	-	7,7,8	1.33	1 (14%)	8,8,10	0.86	0
1	HIS	A	25	-	10,10,11	1.23	2 (20%)	12,12,14	4.10	3 (25%)
1	TYR	A	26	-	12,12,13	1.01	1 (8%)	15,15,17	0.84	0
1	ASP	A	27	-	5,7,8	2.70	2 (40%)	5,8,10	1.09	1 (20%)
1	ALA	A	28	-	4,4,5	1.90	1 (25%)	4,4,6	1.60	1 (25%)
1	ASN	A	29	-	7,7,8	1.36	1 (14%)	8,8,10	1.11	1 (12%)
1	GLN	A	3	-	8,8,9	1.20	1 (12%)	9,9,11	0.90	1 (11%)
1	GLY	A	30	-	3,3,4	0.61	0	1,2,4	1.02	0
1	GLU	A	31	-	6,8,9	1.54	2 (33%)	6,9,11	1.40	1 (16%)
1	ALA	A	32	-	4,4,5	1.55	1 (25%)	4,4,6	1.62	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	ILE	A	33	-	7,7,8	1.26	1 (14%)	8,8,10	0.95	1 (12%)
1	LYS	A	34	-	8,8,9	0.97	1 (12%)	8,8,10	1.16	1 (12%)
1	SER	A	35	-	5,5,6	2.12	1 (20%)	5,5,7	0.85	0
1	PHE	A	36	-	11,11,12	0.96	1 (9%)	13,13,15	0.61	0
1	HIS	A	37	-	10,10,11	1.66	2 (20%)	12,12,14	4.13	3 (25%)
1	VAL	A	38	-	6,6,7	1.84	1 (16%)	7,7,9	1.39	2 (28%)
1	ARG	A	39	-	8,10,11	2.51	2 (25%)	7,11,13	0.71	0
1	LYS	A	4	-	8,8,9	1.50	1 (12%)	8,8,10	0.94	1 (12%)
1	ASP	A	40	-	5,7,8	2.13	2 (40%)	5,8,10	0.90	0
1	GLY	A	41	-	3,3,4	0.54	0	1,2,4	0.84	0
1	LEU	A	42	-	7,7,8	0.96	1 (14%)	8,8,10	1.13	1 (12%)
1	GLY	A	43	-	3,3,4	0.63	0	1,2,4	0.81	0
1	ILE	A	44	-	7,7,8	1.23	1 (14%)	8,8,10	0.87	0
1	LYS	A	45	-	8,8,9	0.98	1 (12%)	8,8,10	1.18	2 (25%)
1	MET	A	46	-	7,7,8	1.23	1 (14%)	7,7,9	1.02	0
1	LEU	A	47	-	7,7,8	1.25	1 (14%)	8,8,10	1.22	1 (12%)
1	MET	A	48	-	7,7,8	1.36	1 (14%)	7,7,9	1.16	0
1	ASP	A	49	-	5,7,8	2.38	2 (40%)	5,8,10	1.04	0
1	LEU	A	5	-	7,7,8	1.33	1 (14%)	8,8,10	1.34	1 (12%)
1	ALA	A	50	-	4,4,5	1.70	1 (25%)	4,4,6	1.66	1 (25%)
1	ASP	A	51	-	5,7,8	2.51	2 (40%)	5,8,10	1.27	0
1	ILE	A	52	-	7,7,8	1.33	1 (14%)	8,8,10	1.16	1 (12%)
1	GLN	A	53	-	8,8,9	1.07	1 (12%)	9,9,11	0.78	0
1	VAL	A	54	-	6,6,7	1.68	1 (16%)	7,7,9	0.89	0
1	ALA	A	55	-	4,4,5	1.57	1 (25%)	4,4,6	1.39	1 (25%)
1	VAL	A	56	-	6,6,7	1.15	1 (16%)	7,7,9	0.97	0
1	LEU	A	57	-	7,7,8	1.29	1 (14%)	8,8,10	0.95	1 (12%)
1	SER	A	58	-	5,5,6	1.42	1 (20%)	5,5,7	1.23	1 (20%)
1	GLY	A	59	-	3,3,4	0.63	0	1,2,4	0.82	0
1	GLU	A	6	-	6,8,9	1.77	2 (33%)	6,9,11	1.68	2 (33%)
1	ARG	A	60	-	8,10,11	2.18	2 (25%)	7,11,13	1.19	1 (14%)
1	ASP	A	61	-	5,7,8	3.00	2 (40%)	5,8,10	1.13	1 (20%)
1	SER	A	62	-	5,5,6	1.53	1 (20%)	5,5,7	1.10	1 (20%)
1	PRO	A	63	-	7,7,8	1.50	1 (14%)	8,8,10	1.28	1 (12%)
1	ILE	A	64	-	7,7,8	1.04	1 (14%)	8,8,10	1.47	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	LEU	A	65	-	7,7,8	1.32	1 (14%)	8,8,10	0.87	0
1	ARG	A	66	-	8,10,11	2.42	2 (25%)	7,11,13	1.02	1 (14%)
1	ARG	A	67	-	8,10,11	3.24	2 (25%)	7,11,13	0.94	0
1	ARG	A	68	-	8,10,11	3.00	2 (25%)	7,11,13	0.76	0
1	ILE	A	69	-	7,7,8	1.64	1 (14%)	8,8,10	0.86	1 (12%)
1	ASN	A	7	-	7,7,8	1.31	1 (14%)	8,8,10	0.97	0
1	ALA	A	70	-	4,4,5	1.74	1 (25%)	4,4,6	1.63	1 (25%)
1	ASP	A	71	-	5,7,8	2.86	2 (40%)	5,8,10	0.97	0
1	LEU	A	72	-	7,7,8	1.22	1 (14%)	8,8,10	1.18	2 (25%)
1	GLY	A	73	-	3,3,4	0.60	0	1,2,4	0.82	0
1	ILE	A	74	-	7,7,8	1.48	1 (14%)	8,8,10	0.89	1 (12%)
1	LYS	A	75	-	8,8,9	1.42	1 (12%)	8,8,10	1.19	1 (12%)
1	LEU	A	76	-	7,7,8	1.26	1 (14%)	8,8,10	0.90	1 (12%)
1	PHE	A	77	-	11,11,12	1.13	1 (9%)	13,13,15	0.84	1 (7%)
1	PHE	A	78	-	11,11,12	1.24	1 (9%)	13,13,15	0.62	0
1	LEU	A	79	-	7,7,8	1.52	1 (14%)	8,8,10	0.82	1 (12%)
1	ILE	A	8	-	7,7,8	1.36	1 (14%)	8,8,10	0.91	0
1	GLY	A	80	-	3,3,4	0.63	0	1,2,4	0.78	0
1	LYS	A	81	-	8,8,9	1.39	1 (12%)	8,8,10	0.89	0
1	LEU	A	82	-	7,7,8	1.19	1 (14%)	8,8,10	1.06	0
1	GLU	A	83	-	6,8,9	2.20	2 (33%)	6,9,11	1.14	0
1	LYS	A	84	-	8,8,9	1.25	1 (12%)	8,8,10	1.45	2 (25%)
1	GLU	A	85	-	6,8,9	1.53	2 (33%)	6,9,11	1.46	2 (33%)
1	THR	A	86	-	6,6,7	1.31	1 (16%)	7,7,9	1.74	2 (28%)
1	ALA	A	87	-	4,4,5	1.97	1 (25%)	4,4,6	1.55	1 (25%)
1	CYS	A	88	-	5,5,6	1.34	1 (20%)	5,5,7	1.05	1 (20%)
1	PHE	A	89	-	11,11,12	0.96	1 (9%)	13,13,15	0.69	1 (7%)
1	LYS	A	9	-	8,8,9	1.21	1 (12%)	8,8,10	0.94	0
1	ASP	A	90	-	5,7,8	2.24	2 (40%)	5,8,10	1.10	1 (20%)
1	LEU	A	91	-	7,7,8	1.48	1 (14%)	8,8,10	0.84	0
1	MET	A	92	-	7,7,8	1.27	1 (14%)	7,7,9	1.34	2 (28%)
1	LYS	A	93	-	8,8,9	0.89	1 (12%)	8,8,10	1.08	1 (12%)
1	GLN	A	94	-	8,8,9	1.53	1 (12%)	9,9,11	1.06	1 (11%)
1	ALA	A	95	-	4,4,5	1.74	1 (25%)	4,4,6	1.52	1 (25%)
1	GLY	A	96	-	3,3,4	0.66	0	1,2,4	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	VAL	A	97	-	6,6,7	1.28	1 (16%)	7,7,9	1.55	1 (14%)
1	THR	A	98	-	6,6,7	1.47	1 (16%)	7,7,9	1.43	1 (14%)
1	ALA	A	99	-	4,4,5	1.59	1 (25%)	4,4,6	1.80	1 (25%)

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
1	MET	A	1	-	-	0/5/6/8	0/0/0/0
1	PHE	A	10	-	-	0/5/6/8	0/1/1/1
1	GLU	A	100	-	-	0/4/7/9	0/0/0/0
1	GLN	A	101	-	-	0/6/7/9	0/0/0/0
1	THR	A	102	-	-	0/5/6/8	0/0/0/0
1	ALA	A	103	-	-	0/1/2/4	0/0/0/0
1	TYR	A	104	-	-	0/5/6/8	0/1/1/1
1	ILE	A	105	-	-	0/7/8/10	0/0/0/0
1	GLY	A	106	-	-	0/0/1/2	0/0/0/0
1	ASP	A	107	2	-	0/3/6/8	0/0/0/0
1	ASP	A	108	-	-	0/3/6/8	0/0/0/0
1	SER	A	109	-	-	0/2/4/6	0/0/0/0
1	VAL	A	11	-	-	0/5/6/8	0/0/0/0
1	VAL	A	110	-	-	0/5/6/8	0/0/0/0
1	ASP	A	111	-	-	0/3/6/8	0/0/0/0
1	LEU	A	112	-	-	0/5/6/8	0/0/0/0
1	PRO	A	113	-	-	0/1/9/11	0/1/1/1
1	ALA	A	114	-	-	0/1/2/4	0/0/0/0
1	PHE	A	115	-	-	0/5/6/8	0/1/1/1
1	ALA	A	116	-	-	0/1/2/4	0/0/0/0
1	ALA	A	117	-	-	0/1/2/4	0/0/0/0
1	CYS	A	118	-	-	0/2/4/6	0/0/0/0
1	GLY	A	119	-	-	0/0/1/2	0/0/0/0
1	ILE	A	12	-	-	0/7/8/10	0/0/0/0
1	THR	A	120	-	-	0/5/6/8	0/0/0/0
1	SER	A	121	-	-	0/2/4/6	0/0/0/0
1	PHE	A	122	-	-	0/5/6/8	0/1/1/1
1	ALA	A	123	-	-	0/1/2/4	0/0/0/0
1	VAL	A	124	-	-	0/5/6/8	0/0/0/0
1	ALA	A	125	-	-	0/1/2/4	0/0/0/0
1	ASP	A	126	-	-	1/3/6/8	0/0/0/0
1	ALA	A	127	-	-	0/1/2/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PRO	A	128	-	-	0/1/9/11	0/1/1/1
1	ILE	A	129	-	-	0/7/8/10	0/0/0/0
1	THR	A	13	-	-	0/5/6/8	0/0/0/0
1	TYR	A	130	-	-	0/5/6/8	0/1/1/1
1	VAL	A	131	-	-	0/5/6/8	0/0/0/0
1	LYS	A	132	-	-	0/6/7/9	0/0/0/0
1	ASN	A	133	-	-	0/5/6/8	0/0/0/0
1	ALA	A	134	-	-	0/1/2/4	0/0/0/0
1	VAL	A	135	-	-	0/5/6/8	0/0/0/0
1	ASP	A	136	-	-	0/3/6/8	0/0/0/0
1	HIS	A	137	-	-	0/5/6/8	0/1/1/1
1	VAL	A	138	-	-	0/5/6/8	0/0/0/0
1	LEU	A	139	-	-	0/5/6/8	0/0/0/0
1	ASP	A	14	3,2	-	0/3/6/8	0/0/0/0
1	SER	A	140	-	-	0/2/4/6	0/0/0/0
1	THR	A	141	-	-	0/5/6/8	0/0/0/0
1	HIS	A	142	-	-	0/5/6/8	0/1/1/1
1	GLY	A	143	-	-	0/0/1/2	0/0/0/0
1	GLY	A	144	-	-	0/0/1/2	0/0/0/0
1	LYS	A	145	-	-	1/6/7/9	0/0/0/0
1	GLY	A	146	-	-	0/0/1/2	0/0/0/0
1	ALA	A	147	-	-	0/1/2/4	0/0/0/0
1	PHE	A	148	-	-	0/5/6/8	0/1/1/1
1	ARG	A	149	-	-	0/7/9/11	0/0/0/0
1	VAL	A	15	-	-	0/5/6/8	0/0/0/0
1	GLU	A	150	-	-	0/4/7/9	0/0/0/0
1	MET	A	151	-	-	0/5/6/8	0/0/0/0
1	SER	A	152	-	-	0/2/4/6	0/0/0/0
1	ASP	A	153	-	-	0/3/6/8	0/0/0/0
1	MET	A	154	-	-	0/5/6/8	0/0/0/0
1	ILE	A	155	-	-	0/7/8/10	0/0/0/0
1	LEU	A	156	-	-	0/5/6/8	0/0/0/0
1	GLN	A	157	-	-	0/6/7/9	0/0/0/0
1	ALA	A	158	-	-	0/1/2/4	0/0/0/0
1	GLN	A	159	-	-	1/6/7/9	0/0/0/0
1	ASP	A	16	2	-	0/3/6/8	0/0/0/0
1	GLY	A	160	-	-	0/0/1/2	0/0/0/0
1	LYS	A	161	-	-	1/6/7/9	0/0/0/0
1	SER	A	162	-	-	0/2/4/6	0/0/0/0
1	SER	A	163	-	-	0/2/4/6	0/0/0/0
1	VAL	A	164	-	-	0/5/6/8	0/0/0/0
1	PHE	A	165	-	-	0/5/6/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ASP	A	166	-	-	0/3/6/8	0/0/0/0
1	THR	A	167	-	-	0/5/6/8	0/0/0/0
1	ALA	A	168	-	-	0/1/2/4	0/0/0/0
1	GLN	A	169	-	-	0/6/7/9	0/0/0/0
1	GLY	A	17	-	-	0/0/1/2	0/0/0/0
1	GLY	A	170	-	-	0/0/1/2	0/0/0/0
1	PHE	A	171	-	-	0/5/6/8	0/1/1/1
1	LEU	A	172	-	-	1/5/6/8	0/0/0/0
1	LYS	A	173	-	-	0/6/7/9	0/0/0/0
1	SER	A	174	-	-	0/2/4/6	0/0/0/0
1	VAL	A	175	-	-	0/5/6/8	0/0/0/0
1	LYS	A	176	-	-	0/6/7/9	0/0/0/0
1	SER	A	177	-	-	0/2/4/6	0/0/0/0
1	MET	A	178	-	-	0/5/6/8	0/0/0/0
1	GLY	A	179	-	-	0/0/1/2	0/0/0/0
1	VAL	A	18	-	-	0/5/6/8	0/0/0/0
1	LEU	A	19	-	-	0/5/6/8	0/0/0/0
1	GLN	A	2	-	-	0/6/7/9	0/0/0/0
1	THR	A	20	-	-	0/5/6/8	0/0/0/0
1	ASP	A	21	-	-	1/3/6/8	0/0/0/0
1	GLY	A	22	-	-	0/0/1/2	0/0/0/0
1	GLN	A	23	-	-	0/6/7/9	0/0/0/0
1	LEU	A	24	-	-	0/5/6/8	0/0/0/0
1	HIS	A	25	-	-	1/5/6/8	0/1/1/1
1	TYR	A	26	-	-	0/5/6/8	0/1/1/1
1	ASP	A	27	-	-	0/3/6/8	0/0/0/0
1	ALA	A	28	-	-	0/1/2/4	0/0/0/0
1	ASN	A	29	-	-	0/5/6/8	0/0/0/0
1	GLN	A	3	-	-	0/6/7/9	0/0/0/0
1	GLY	A	30	-	-	0/0/1/2	0/0/0/0
1	GLU	A	31	-	-	0/4/7/9	0/0/0/0
1	ALA	A	32	-	-	0/1/2/4	0/0/0/0
1	ILE	A	33	-	-	0/7/8/10	0/0/0/0
1	LYS	A	34	-	-	0/6/7/9	0/0/0/0
1	SER	A	35	-	-	0/2/4/6	0/0/0/0
1	PHE	A	36	-	-	0/5/6/8	0/1/1/1
1	HIS	A	37	-	-	0/5/6/8	0/1/1/1
1	VAL	A	38	-	-	0/5/6/8	0/0/0/0
1	ARG	A	39	-	-	0/7/9/11	0/0/0/0
1	LYS	A	4	-	-	0/6/7/9	0/0/0/0
1	ASP	A	40	-	-	0/3/6/8	0/0/0/0
1	GLY	A	41	-	-	0/0/1/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LEU	A	42	-	-	0/5/6/8	0/0/0/0
1	GLY	A	43	-	-	0/0/1/2	0/0/0/0
1	ILE	A	44	-	-	0/7/8/10	0/0/0/0
1	LYS	A	45	-	-	0/6/7/9	0/0/0/0
1	MET	A	46	-	-	0/5/6/8	0/0/0/0
1	LEU	A	47	-	-	0/5/6/8	0/0/0/0
1	MET	A	48	-	-	0/5/6/8	0/0/0/0
1	ASP	A	49	-	-	0/3/6/8	0/0/0/0
1	LEU	A	5	-	-	0/5/6/8	0/0/0/0
1	ALA	A	50	-	-	0/1/2/4	0/0/0/0
1	ASP	A	51	-	-	1/3/6/8	0/0/0/0
1	ILE	A	52	-	-	0/7/8/10	0/0/0/0
1	GLN	A	53	-	-	0/6/7/9	0/0/0/0
1	VAL	A	54	-	-	0/5/6/8	0/0/0/0
1	ALA	A	55	-	-	0/1/2/4	0/0/0/0
1	VAL	A	56	-	-	0/5/6/8	0/0/0/0
1	LEU	A	57	-	-	0/5/6/8	0/0/0/0
1	SER	A	58	-	-	0/2/4/6	0/0/0/0
1	GLY	A	59	-	-	0/0/1/2	0/0/0/0
1	GLU	A	6	-	-	0/4/7/9	0/0/0/0
1	ARG	A	60	-	-	0/7/9/11	0/0/0/0
1	ASP	A	61	-	-	0/3/6/8	0/0/0/0
1	SER	A	62	-	-	0/2/4/6	0/0/0/0
1	PRO	A	63	-	-	0/1/9/11	0/1/1/1
1	ILE	A	64	-	-	0/7/8/10	0/0/0/0
1	LEU	A	65	-	-	0/5/6/8	0/0/0/0
1	ARG	A	66	-	-	0/7/9/11	0/0/0/0
1	ARG	A	67	-	-	0/7/9/11	0/0/0/0
1	ARG	A	68	-	-	0/7/9/11	0/0/0/0
1	ILE	A	69	-	-	0/7/8/10	0/0/0/0
1	ASN	A	7	-	-	1/5/6/8	0/0/0/0
1	ALA	A	70	-	-	0/1/2/4	0/0/0/0
1	ASP	A	71	-	-	0/3/6/8	0/0/0/0
1	LEU	A	72	-	-	0/5/6/8	0/0/0/0
1	GLY	A	73	-	-	0/0/1/2	0/0/0/0
1	ILE	A	74	-	-	0/7/8/10	0/0/0/0
1	LYS	A	75	-	-	0/6/7/9	0/0/0/0
1	LEU	A	76	-	-	0/5/6/8	0/0/0/0
1	PHE	A	77	-	-	0/5/6/8	0/1/1/1
1	PHE	A	78	-	-	0/5/6/8	0/1/1/1
1	LEU	A	79	-	-	0/5/6/8	0/0/0/0
1	ILE	A	8	-	-	0/7/8/10	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	GLY	A	80	-	-	0/0/1/2	0/0/0/0
1	LYS	A	81	-	-	0/6/7/9	0/0/0/0
1	LEU	A	82	-	-	0/5/6/8	0/0/0/0
1	GLU	A	83	-	-	0/4/7/9	0/0/0/0
1	LYS	A	84	-	-	0/6/7/9	0/0/0/0
1	GLU	A	85	-	-	0/4/7/9	0/0/0/0
1	THR	A	86	-	-	0/5/6/8	0/0/0/0
1	ALA	A	87	-	-	0/1/2/4	0/0/0/0
1	CYS	A	88	-	-	0/2/4/6	0/0/0/0
1	PHE	A	89	-	-	0/5/6/8	0/1/1/1
1	LYS	A	9	-	-	0/6/7/9	0/0/0/0
1	ASP	A	90	-	-	0/3/6/8	0/0/0/0
1	LEU	A	91	-	-	0/5/6/8	0/0/0/0
1	MET	A	92	-	-	0/5/6/8	0/0/0/0
1	LYS	A	93	-	-	0/6/7/9	0/0/0/0
1	GLN	A	94	-	-	0/6/7/9	0/0/0/0
1	ALA	A	95	-	-	0/1/2/4	0/0/0/0
1	GLY	A	96	-	-	0/0/1/2	0/0/0/0
1	VAL	A	97	-	-	0/5/6/8	0/0/0/0
1	THR	A	98	-	-	0/5/6/8	0/0/0/0
1	ALA	A	99	-	-	0/1/2/4	0/0/0/0

The worst 5 of 189 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ARG	CZ-NH1	-7.95	1.32	1.34
1	A	68	ARG	CZ-NH1	-7.50	1.32	1.34
1	A	39	ARG	CZ-NH1	-6.49	1.33	1.34
1	A	61	ASP	CB-CG	6.10	1.53	1.49
1	A	108	ASP	CB-CG	5.93	1.53	1.49

The worst 5 of 145 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	142	HIS	NE2-CE1-ND1	-13.77	108.35	115.81
1	A	37	HIS	NE2-CE1-ND1	-13.69	108.40	115.81
1	A	137	HIS	NE2-CE1-ND1	-13.68	108.40	115.81
1	A	25	HIS	NE2-CE1-ND1	-13.61	108.44	115.81
1	A	102	THR	CB-CA-C	-4.27	108.31	112.70

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	172	LEU	O-C-CA-CB
1	A	51	ASP	O-C-CA-CB
1	A	161	LYS	O-C-CA-CB
1	A	25	HIS	O-C-CA-CB
1	A	7	ASN	O-C-CA-CB

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	#$|Z| > 2$
3	VN4	A	202	1,4	0,3,3	0.00	-	0,3,3	0.00	-
4	KDO	A	203[A]	3	13,16,16	9.87	11 (84%)	19,24,24	5.02	9 (47%)
4	KDO	A	203[B]	-	13,16,16	9.74	10 (76%)	19,24,24	5.03	11 (57%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VN4	A	202	1,4	-	0/0/0/0	0/0/0/0
4	KDO	A	203[A]	3	-	0/6/30/30	0/1/1/1
4	KDO	A	203[B]	-	-	0/6/30/30	0/1/1/1

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203[B]	KDO	C3-C2	-25.17	1.18	1.51
4	A	203[A]	KDO	C3-C2	-25.02	1.18	1.51
4	A	203[A]	KDO	C3-C4	-15.71	1.27	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	203[B]	KDO	C3-C4	-15.37	1.28	1.53
4	A	203[A]	KDO	O6-C2	10.55	1.52	1.42

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	203[A]	KDO	O6-C6-C5	-16.58	84.57	108.69
4	A	203[B]	KDO	O6-C6-C5	-16.10	85.27	108.69
4	A	203[B]	KDO	C3-C4-C5	9.79	119.62	110.80
4	A	203[A]	KDO	C3-C2-C1	-6.32	107.80	111.41
4	A	203[A]	KDO	O6-C6-C7	6.15	117.61	106.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

There are no RSRZ outliers to report within protein, DNA, RNA chains in this entry.

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 ⓘ

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	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	VAL	A	15	7/8	0.09	-	12,13,14,15	0
1	VAL	A	110	7/8	0.10	-	13,14,17,18	0
1	MET	A	178	8/9	0.10	-	16,23,26,26	0
1	HIS	A	37	10/11	0.08	-	11,13,14,14	0
1	ASP	A	107	8/9	0.08	-	10,11,13,14	0
1	PHE	A	148	11/12	0.10	-	10,11,13,14	0
1	THR	A	120	7/8	0.10	-	14,17,18,18	0
1	LYS	A	132	9/10	0.14	-	13,16,17,17	0
1	ALA	A	55	5/6	0.09	-	15,16,18,18	0
1	ILE	A	105	8/9	0.10	-	9,10,12,12	0
1	LEU	A	82	8/9	0.21	-	18,18,22,24	0
1	VAL	A	11	7/8	0.11	-	12,14,15,16	0
1	LEU	A	112	8/9	0.10	-	13,14,16,17	0
1	LYS	A	93	9/10	0.11	-	17,18,23,24	0
1	GLN	A	159	9/10	0.10	-	15,16,19,20	0
1	SER	A	35	6/7	0.09	-	10,11,13,14	0
1	ALA	A	117	5/6	0.10	-	16,18,19,19	0
1	GLU	A	6	9/10	0.13	-	20,22,23,25	0
1	ASP	A	49	8/9	0.11	-	17,19,22,25	0
1	VAL	A	135	7/8	0.09	-	12,13,14,14	0
1	ILE	A	74	8/9	0.10	-	15,16,18,18	0
1	LEU	A	5	8/9	0.13	-	18,20,21,21	0
1	ILE	A	129	8/9	0.14	-	12,15,20,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	GLY	A	22	4/5	0.13	-	12,13,13,15	0
1	PHE	A	115	11/12	0.10	-	13,15,18,19	0
1	PRO	A	128	7/8	0.10	-	11,12,13,14	0
1	PHE	A	78	11/12	0.11	-	16,18,21,21	0
1	GLY	A	143	4/5	0.07	-	10,10,11,11	0
1	THR	A	102	7/8	0.11	-	15,16,19,20	0
1	PRO	A	113	7/8	0.07	-	15,16,17,18	0
1	PHE	A	171	11/12	0.11	-	18,20,23,24	0
1	TYR	A	130	12/13	0.09	-	13,14,16,19	0
1	ASN	A	133	8/9	0.10	-	16,17,20,21	0
1	ALA	A	32	5/6	0.10	-	14,15,15,18	0
1	ILE	A	8	8/9	0.12	-	14,17,19,20	0
1	GLN	A	53	9/10	0.09	-	15,17,19,19	0
1	VAL	A	164	7/8	0.09	-	15,17,18,18	0
1	MET	A	46	8/9	0.08	-	14,15,16,16	0
1	LYS	A	4	9/10	0.13	-	21,22,23,23	0
1	ASP	A	136	8/9	0.08	-	12,16,18,18	0
1	ASP	A	27	8/9	0.07	-	14,16,18,19	0
1	ASP	A	16	8/9	0.08	-	11,14,15,16	0
1	LEU	A	156	8/9	0.08	-	12,13,14,18	0
1	ALA	A	134	5/6	0.07	-	15,16,17,18	0
1	GLY	A	106	4/5	0.07	-	10,11,11,13	0
1	SER	A	62	6/7	0.10	-	16,17,18,19	0
1	PHE	A	77	11/12	0.10	-	17,18,20,21	0
1	ALA	A	87	5/6	0.12	-	15,17,17,18	0
1	ILE	A	33	8/9	0.12	-	10,12,15,19	0
1	LEU	A	72	8/9	0.09	-	15,18,19,20	0
1	VAL	A	54	7/8	0.09	-	15,16,18,19	0
1	GLY	A	146	4/5	0.07	-	11,11,12,12	0
1	ALA	A	28	5/6	0.09	-	15,16,17,18	0
1	THR	A	167	7/8	0.08	-	17,19,20,21	0
1	VAL	A	138	7/8	0.10	-	14,14,15,16	0
1	ASP	A	14	8/9	0.07	-	11,12,14,14	0
1	ASP	A	153	8/9	0.07	-	10,11,12,14	0
1	GLY	A	80	4/5	0.09	-	17,18,19,22	0
1	PHE	A	10	11/12	0.11	-	14,15,17,17	0
1	GLN	A	2	9/10	0.11	-	16,19,22,23	0
1	LYS	A	81	9/10	0.18	-	16,19,22,24	0
1	GLU	A	85	9/10	0.11	-	18,20,27,30	0
1	LYS	A	161	9/10	0.10	-	15,17,20,26	0
1	ASN	A	29	8/9	0.13	-	16,19,20,21	0
1	ASP	A	40	8/9	0.09	-	10,12,14,14	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	GLY	A	73	4/5	0.14	-	16,17,17,18	0
1	LYS	A	176	9/10	0.14	-	18,22,28,28	0
1	ASP	A	111	8/9	0.08	-	12,14,14,15	0
1	SER	A	109	6/7	0.08	-	12,13,13,15	0
1	LEU	A	79	8/9	0.10	-	16,17,18,18	0
1	LEU	A	19	8/9	0.09	-	11,12,14,15	0
1	PRO	A	63	7/8	0.08	-	14,16,19,19	0
1	ALA	A	70	5/6	0.09	-	17,18,18,18	0
1	MET	A	92	8/9	0.09	-	16,17,19,21	0
1	ILE	A	155	8/9	0.09	-	11,12,14,14	0
1	ASP	A	71	8/9	0.10	-	14,17,19,22	0
1	GLN	A	94	9/10	0.12	-	16,18,23,24	0
1	SER	A	121	6/7	0.10	-	12,13,14,14	0
1	LEU	A	91	8/9	0.11	-	14,16,17,18	0
1	ASP	A	21	8/9	0.09	-	11,13,13,16	0
1	ARG	A	66	11/12	0.10	-	14,18,22,22	0
1	CYS	A	88	6/7	0.08	-	16,18,19,20	0
1	ASN	A	7	8/9	0.12	-	20,23,29,30	0
1	VAL	A	124	7/8	0.10	-	9,11,11,12	0
1	ALA	A	147	5/6	0.08	-	10,10,11,12	0
1	SER	A	163	6/7	0.12	-	17,18,20,23	0
1	ARG	A	68	11/12	0.09	-	14,15,16,17	0
1	GLY	A	59	4/5	0.07	-	17,17,17,19	0
1	GLY	A	160	4/5	0.11	-	15,17,18,20	0
1	ARG	A	149	11/12	0.09	-	9,10,12,12	0
1	LEU	A	172	8/9	0.21	-	22,24,28,33	0
1	GLY	A	17	4/5	0.10	-	11,12,13,13	0
1	ASP	A	166	8/9	0.08	-	15,17,18,19	0
1	ALA	A	103	5/6	0.07	-	14,14,16,16	0
1	THR	A	13	7/8	0.08	-	12,13,14,15	0
1	GLU	A	83	9/10	0.12	-	16,19,22,23	0
1	GLY	A	179	4/5	0.22	-	27,29,36,36	0
1	PHE	A	165	11/12	0.10	-	12,13,15,15	0
1	GLY	A	30	4/5	0.10	-	13,13,15,16	0
1	ILE	A	64	8/9	0.10	-	13,15,16,16	0
1	SER	A	177	6/7	0.17	-	24,25,28,29	0
1	GLY	A	43	4/5	0.09	-	11,13,13,14	0
1	GLN	A	23	9/10	0.10	-	10,12,17,20	0
1	LYS	A	34	9/10	0.09	-	11,12,13,14	0
1	MET	A	151	8/9	0.09	-	8,11,13,14	0
1	ARG	A	60	11/12	0.10	-	16,17,19,20	0
1	LEU	A	47	8/9	0.09	-	14,16,16,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	LEU	A	76	8/9	0.09	-	15,16,17,18	0
1	ALA	A	168	5/6	0.09	-	18,20,22,22	0
1	ALA	A	95	5/6	0.09	-	16,16,19,21	0
1	LYS	A	84	9/10	0.11	-	14,15,17,18	0
1	SER	A	58	6/7	0.09	-	16,17,17,19	0
1	GLN	A	3	9/10	0.26	-	20,27,37,37	0
1	ALA	A	127	5/6	0.11	-	12,12,13,13	0
1	ALA	A	123	5/6	0.07	-	10,10,12,12	0
1	ARG	A	39	11/12	0.09	-	10,12,14,15	0
1	PHE	A	122	11/12	0.08	-	12,12,14,14	0
1	THR	A	98	7/8	0.08	-	19,21,22,24	0
1	ALA	A	50	5/6	0.11	-	17,17,17,20	0
1	LYS	A	173	9/10	0.25	-	25,28,35,35	0
1	VAL	A	38	7/8	0.12	-	12,14,15,16	0
1	ASP	A	90	8/9	0.10	-	18,20,24,24	0
1	MET	A	48	8/9	0.12	-	16,16,23,23	0
1	LEU	A	42	8/9	0.09	-	11,14,16,17	0
1	GLY	A	41	4/5	0.09	-	13,13,15,15	0
1	GLN	A	101	9/10	0.12	-	18,20,25,28	0
1	ILE	A	52	8/9	0.10	-	17,19,21,21	0
1	ASP	A	51	8/9	0.13	-	18,21,23,27	0
1	PHE	A	36	11/12	0.09	-	9,12,14,14	0
1	ILE	A	44	8/9	0.09	-	12,14,16,16	0
1	ALA	A	116	5/6	0.13	-	17,20,21,22	0
1	LYS	A	75	9/10	0.17	-	18,19,26,26	0
1	GLY	A	96	4/5	0.12	-	18,19,19,21	0
1	GLY	A	170	4/5	0.09	-	20,21,22,22	0
1	VAL	A	56	7/8	0.10	-	12,15,16,17	0
1	ALA	A	158	5/6	0.09	-	15,17,17,18	0
1	LEU	A	57	8/9	0.10	-	14,15,16,16	0
1	MET	A	154	8/9	0.08	-	11,12,14,18	0
1	GLN	A	169	9/10	0.18	-	23,25,28,29	0
1	ILE	A	69	8/9	0.11	-	16,17,18,19	0
1	LYS	A	45	9/10	0.10	-	15,16,20,22	0
1	ALA	A	114	5/6	0.09	-	15,16,16,16	0
1	GLU	A	31	9/10	0.10	-	13,14,16,18	0
1	GLY	A	119	4/5	0.11	-	15,17,18,18	0
1	TYR	A	104	12/13	0.09	-	13,13,15,15	0
1	PHE	A	89	11/12	0.09	-	16,18,20,22	0
1	VAL	A	18	7/8	0.08	-	10,11,12,13	0
1	CYS	A	118	6/7	0.10	-	18,19,19,19	0
1	ILE	A	12	8/9	0.09	-	11,13,15,16	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
1	THR	A	86	7/8	0.10	-	17,17,20,22	0
1	VAL	A	97	7/8	0.10	-	18,20,21,21	0
1	LEU	A	139	8/9	0.12	-	11,12,13,14	0
1	ALA	A	99	5/6	0.07	-	19,20,21,22	0
1	MET	A	1	8/9	0.11	-	16,20,21,23	0
1	ALA	A	125	5/6	0.09	-	11,13,14,14	0
1	GLY	A	144	4/5	0.06	-	10,12,14,14	0
1	SER	A	140	6/7	0.08	-	11,14,16,19	0
1	TYR	A	26	12/13	0.08	-	13,14,15,15	0
1	HIS	A	142	10/11	0.10	-	12,13,16,16	0
1	THR	A	20	7/8	0.09	-	11,11,14,14	0
1	VAL	A	131	7/8	0.09	-	10,13,14,14	0
1	LYS	A	9	9/10	0.11	-	17,18,23,26	0
1	VAL	A	175	7/8	0.14	-	24,25,28,28	0
1	HIS	A	137	10/11	0.09	-	12,14,16,16	0
1	ASP	A	61	8/9	0.09	-	17,20,21,23	0
1	LEU	A	65	8/9	0.10	-	14,15,16,17	0
1	THR	A	141	7/8	0.08	-	9,12,13,13	0
1	LEU	A	24	8/9	0.10	-	12,13,13,14	0
1	GLU	A	100	9/10	0.18	-	20,23,36,42	0
1	ARG	A	67	11/12	0.10	-	14,16,20,20	0
1	HIS	A	25	10/11	0.10	-	10,13,14,17	0
1	SER	A	162	6/7	0.07	-	13,15,17,17	0
1	SER	A	174	6/7	0.17	-	25,26,27,28	0
1	GLN	A	157	9/10	0.11	-	14,16,20,23	0
1	ASP	A	108	8/9	0.09	-	11,12,13,14	0
1	ASP	A	126	8/9	0.08	-	12,14,15,15	0
1	LYS	A	145	9/10	0.10	-	13,13,16,20	0
1	GLU	A	150	9/10	0.08	-	10,11,14,14	0
1	SER	A	152	6/7	0.06	-	10,10,11,12	0

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. 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	RSR	LLDF	B-factors(Å²)	Q<0.9
2	MG	A	201	1/1	0.05	-	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å²)	Q<0.9
4	KDO	A	203[B]	16/16	0.22	-	16,19,22,23	16
4	KDO	A	203[A]	16/16	0.22	-	16,19,22,23	16
3	VN4	A	202	4/4	0.12	-	13,15,18,18	0

6.5 Other polymers ⓘ

There are no such residues in this entry.