W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation 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 full wwPDB 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/ValidationPDFNotes.html

1 Overall quality at a glance ⓘ

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
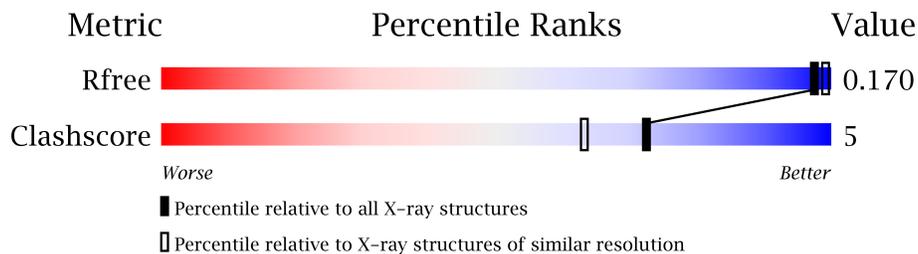
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	77520	3954 (1.80-1.80)
Clashscore	88313	4797 (1.80-1.80)

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PROTEIN DATA BANK

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 1352	C 854	N 230	O 259	S 9	0	0

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

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

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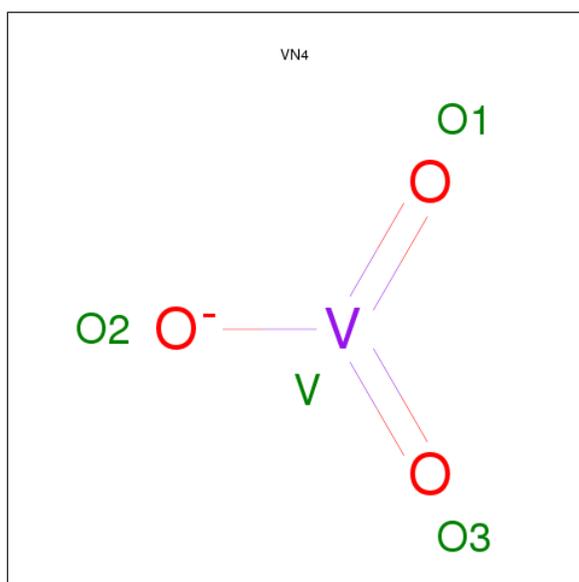
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	O 3	V 1	0	0

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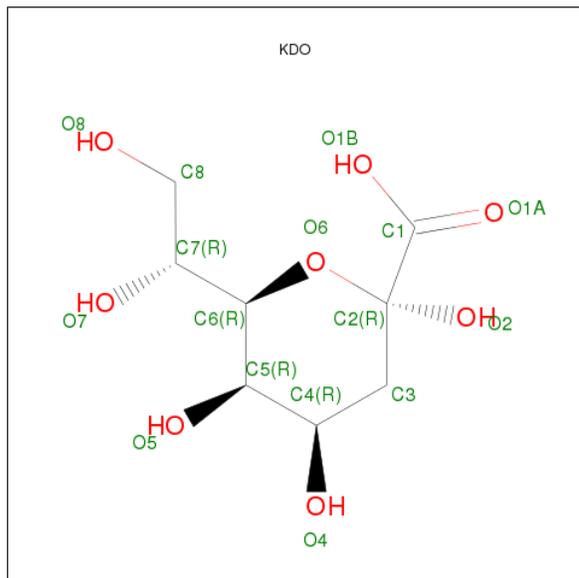
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 32	C 16	O 16	0	1

- Molecule 5 is water.

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

5.1   Standard geometry ⓘ

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 ⓘ

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.

All (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
1:A:90:ASP:OD2	5:A:416:HOH:O	2.19	0.52
4:A:203[B]:KDO:O7	4:A:203[B]:KDO:O5	2.24	0.51
1:A:84:LYS:NZ	3:A:202:VN4:O3	2.32	0.49
1:A:39:ARG:HG3	5:A:470:HOH:O	2.14	0.46
1:A:69:ILE:HG23	1:A:74:ILE:HB	1.98	0.45
1:A:75:LYS:HE2	1:A:76:LEU:HD23	2.00	0.43
1:A:37:HIS:CD2	1:A:39:ARG:H	2.37	0.42
1:A:37:HIS:HD2	1:A:39:ARG:H	1.68	0.40

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

Atom-1	Atom-2	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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
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%)
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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
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%)
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

All (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
1	A	100	GLU	CG-CD	5.87	1.53	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	ARG	CZ-NH1	-5.63	1.33	1.34
1	A	60	ARG	CZ-NH1	-5.28	1.33	1.34
1	A	113	PRO	CA-C	5.07	1.54	1.49
1	A	71	ASP	CB-CG	5.00	1.52	1.49
1	A	112	LEU	CA-C	4.89	1.54	1.49
1	A	149	ARG	CZ-NH1	-4.83	1.33	1.34
1	A	126	ASP	CB-CG	4.82	1.52	1.49
1	A	27	ASP	CB-CG	4.77	1.52	1.49
1	A	166	ASP	CA-C	4.70	1.54	1.49
1	A	175	VAL	CA-C	4.66	1.54	1.49
1	A	35	SER	CA-C	4.64	1.54	1.49
1	A	126	ASP	CA-C	4.57	1.54	1.49
1	A	83	GLU	CG-CD	4.54	1.52	1.49
1	A	107	ASP	CB-CG	4.45	1.52	1.49
1	A	14	ASP	CA-C	4.44	1.54	1.49
1	A	67	ARG	CA-C	4.44	1.54	1.49
1	A	51	ASP	CB-CG	4.43	1.52	1.49
1	A	105	ILE	CA-C	4.42	1.54	1.49
1	A	140	SER	CA-C	4.38	1.54	1.49
1	A	16	ASP	CB-CG	4.36	1.52	1.49
1	A	21	ASP	CB-CG	4.33	1.52	1.49
1	A	129	ILE	CA-C	4.32	1.54	1.49
1	A	38	VAL	CA-C	4.30	1.54	1.49
1	A	163	SER	CA-C	4.24	1.54	1.49
1	A	178	MET	CA-C	4.24	1.54	1.49
1	A	69	ILE	CA-C	4.21	1.53	1.49
1	A	94	GLN	CA-C	4.20	1.53	1.49
1	A	142	HIS	CA-C	4.19	1.53	1.49
1	A	37	HIS	CA-C	4.15	1.53	1.49
1	A	141	THR	CA-C	4.10	1.53	1.49
1	A	151	MET	CA-C	4.09	1.53	1.49
1	A	149	ARG	CA-C	4.07	1.53	1.49
1	A	111	ASP	CB-CG	4.06	1.52	1.49
1	A	4	LYS	CA-C	4.04	1.53	1.49
1	A	134	ALA	CA-C	4.03	1.53	1.49
1	A	137	HIS	CA-C	4.02	1.53	1.49
1	A	21	ASP	CA-C	4.01	1.53	1.49
1	A	125	ALA	CA-C	3.99	1.53	1.49
1	A	54	VAL	CA-C	3.99	1.53	1.49
1	A	78	PHE	CA-C	3.97	1.53	1.49
1	A	165	PHE	CA-C	3.97	1.53	1.49
1	A	109	SER	CA-C	3.95	1.53	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	PHE	CA-C	3.94	1.53	1.49
1	A	79	LEU	CA-C	3.91	1.53	1.49
1	A	71	ASP	CA-C	3.88	1.53	1.49
1	A	75	LYS	CA-C	3.87	1.53	1.49
1	A	162	SER	CA-C	3.86	1.53	1.49
1	A	87	ALA	CA-C	3.85	1.53	1.49
1	A	157	GLN	CA-C	3.85	1.53	1.49
1	A	49	ASP	CA-C	3.82	1.53	1.49
1	A	63	PRO	CA-C	3.81	1.53	1.49
1	A	91	LEU	CA-C	3.80	1.53	1.49
1	A	169	GLN	CA-C	3.80	1.53	1.49
1	A	74	ILE	CA-C	3.80	1.53	1.49
1	A	68	ARG	CA-C	3.80	1.53	1.49
1	A	66	ARG	CA-C	3.80	1.53	1.49
1	A	81	LYS	CA-C	3.78	1.53	1.49
1	A	177	SER	CA-C	3.78	1.53	1.49
1	A	145	LYS	CA-C	3.77	1.53	1.49
1	A	116	ALA	CA-C	3.74	1.53	1.49
1	A	153	ASP	CB-CG	3.74	1.52	1.49
1	A	90	ASP	CB-CG	3.74	1.52	1.49
1	A	2	GLN	CA-C	3.71	1.53	1.49
1	A	156	LEU	CA-C	3.70	1.53	1.49
1	A	28	ALA	CA-C	3.70	1.53	1.49
1	A	164	VAL	CA-C	3.67	1.53	1.49
1	A	100	GLU	CA-C	3.66	1.53	1.49
1	A	117	ALA	CA-C	3.66	1.53	1.49
1	A	110	VAL	CA-C	3.65	1.53	1.49
1	A	118	CYS	CA-C	3.65	1.53	1.49
1	A	101	GLN	CA-C	3.63	1.53	1.49
1	A	77	PHE	CA-C	3.63	1.53	1.49
1	A	49	ASP	CB-CG	3.59	1.51	1.49
1	A	102	THR	CA-C	3.59	1.53	1.49
1	A	27	ASP	CA-C	3.59	1.53	1.49
1	A	12	ILE	CA-C	3.57	1.53	1.49
1	A	108	ASP	CA-C	3.56	1.53	1.49
1	A	159	GLN	CA-C	3.55	1.53	1.49
1	A	138	VAL	CA-C	3.54	1.53	1.49
1	A	135	VAL	CA-C	3.53	1.53	1.49
1	A	103	ALA	CA-C	3.51	1.53	1.49
1	A	132	LYS	CA-C	3.49	1.53	1.49
1	A	167	THR	CA-C	3.48	1.53	1.49
1	A	174	SER	CA-C	3.47	1.53	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	THR	CA-C	3.45	1.53	1.49
1	A	114	ALA	CA-C	3.45	1.53	1.49
1	A	5	LEU	CA-C	3.44	1.53	1.49
1	A	8	ILE	CA-C	3.44	1.53	1.49
1	A	29	ASN	CA-C	3.41	1.53	1.49
1	A	152	SER	CA-C	3.40	1.53	1.49
1	A	176	LYS	CA-C	3.39	1.53	1.49
1	A	84	LYS	CA-C	3.39	1.53	1.49
1	A	52	ILE	CA-C	3.37	1.53	1.49
1	A	95	ALA	CA-C	3.36	1.53	1.49
1	A	65	LEU	CA-C	3.34	1.53	1.49
1	A	70	ALA	CA-C	3.34	1.53	1.49
1	A	40	ASP	CB-CG	3.33	1.51	1.49
1	A	51	ASP	CA-C	3.33	1.53	1.49
1	A	13	THR	CA-C	3.32	1.53	1.49
1	A	62	SER	CA-C	3.30	1.53	1.49
1	A	48	MET	CA-C	3.30	1.53	1.49
1	A	166	ASP	CB-CG	3.30	1.51	1.49
1	A	7	ASN	CA-C	3.30	1.53	1.49
1	A	24	LEU	CA-C	3.29	1.53	1.49
1	A	1	MET	CA-C	3.29	1.53	1.49
1	A	11	VAL	CA-C	3.28	1.53	1.49
1	A	50	ALA	CA-C	3.26	1.53	1.49
1	A	26	TYR	CA-C	3.25	1.53	1.49
1	A	40	ASP	CA-C	3.25	1.53	1.49
1	A	9	LYS	CA-C	3.25	1.53	1.49
1	A	57	LEU	CA-C	3.25	1.53	1.49
1	A	130	TYR	CA-C	3.23	1.53	1.49
1	A	90	ASP	CA-C	3.22	1.53	1.49
1	A	107	ASP	CA-C	3.19	1.52	1.49
1	A	76	LEU	CA-C	3.18	1.52	1.49
1	A	3	GLN	CA-C	3.18	1.52	1.49
1	A	47	LEU	CA-C	3.15	1.52	1.49
1	A	147	ALA	CA-C	3.14	1.52	1.49
1	A	158	ALA	CA-C	3.13	1.52	1.49
1	A	46	MET	CA-C	3.12	1.52	1.49
1	A	19	LEU	CA-C	3.12	1.52	1.49
1	A	20	THR	CA-C	3.12	1.52	1.49
1	A	124	VAL	CA-C	3.11	1.52	1.49
1	A	131	VAL	CA-C	3.11	1.52	1.49
1	A	44	ILE	CA-C	3.11	1.52	1.49
1	A	92	MET	CA-C	3.10	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	ILE	CA-C	3.10	1.52	1.49
1	A	122	PHE	CA-C	3.09	1.52	1.49
1	A	72	LEU	CA-C	3.08	1.52	1.49
1	A	172	LEU	CA-C	3.07	1.52	1.49
1	A	99	ALA	CA-C	3.07	1.52	1.49
1	A	58	SER	CA-C	3.05	1.52	1.49
1	A	36	PHE	CA-C	3.03	1.52	1.49
1	A	86	THR	CA-C	3.03	1.52	1.49
1	A	60	ARG	CA-C	3.01	1.52	1.49
1	A	121	SER	CA-C	3.00	1.52	1.49
1	A	82	LEU	CA-C	2.99	1.52	1.49
1	A	18	VAL	CA-C	2.99	1.52	1.49
1	A	139	LEU	CA-C	2.98	1.52	1.49
1	A	55	ALA	CA-C	2.98	1.52	1.49
1	A	89	PHE	CA-C	2.98	1.52	1.49
1	A	97	VAL	CA-C	2.97	1.52	1.49
1	A	32	ALA	CA-C	2.94	1.52	1.49
1	A	6	GLU	CG-CD	2.94	1.51	1.49
1	A	127	ALA	CA-C	2.92	1.52	1.49
1	A	6	GLU	CA-C	2.86	1.52	1.49
1	A	171	PHE	CA-C	2.86	1.52	1.49
1	A	88	CYS	CA-C	2.86	1.52	1.49
1	A	10	PHE	CA-C	2.85	1.52	1.49
1	A	53	GLN	CA-C	2.81	1.52	1.49
1	A	136	ASP	CA-C	2.81	1.52	1.49
1	A	111	ASP	CA-C	2.78	1.52	1.49
1	A	123	ALA	CA-C	2.75	1.52	1.49
1	A	39	ARG	CA-C	2.75	1.52	1.49
1	A	155	ILE	CA-C	2.74	1.52	1.49
1	A	133	ASN	CA-C	2.73	1.52	1.49
1	A	168	ALA	CA-C	2.69	1.52	1.49
1	A	83	GLU	CA-C	2.66	1.52	1.49
1	A	61	ASP	CA-C	2.63	1.52	1.49
1	A	153	ASP	CA-C	2.63	1.52	1.49
1	A	64	ILE	CA-C	2.62	1.52	1.49
1	A	31	GLU	CG-CD	2.59	1.51	1.49
1	A	85	GLU	CG-CD	2.56	1.51	1.49
1	A	56	VAL	CA-C	2.55	1.52	1.49
1	A	45	LYS	CA-C	2.55	1.52	1.49
1	A	34	LYS	CA-C	2.55	1.52	1.49
1	A	16	ASP	CA-C	2.54	1.52	1.49
1	A	115	PHE	CA-C	2.54	1.52	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	PRO	CA-C	2.51	1.52	1.49
1	A	31	GLU	CA-C	2.48	1.52	1.49
1	A	15	VAL	CA-C	2.42	1.52	1.49
1	A	161	LYS	CA-C	2.40	1.52	1.49
1	A	93	LYS	CA-C	2.37	1.52	1.49
1	A	42	LEU	CA-C	2.37	1.52	1.49
1	A	23	GLN	CA-C	2.31	1.52	1.49
1	A	104	TYR	CA-C	2.27	1.52	1.49
1	A	25	HIS	CE1-NE2	-2.23	1.32	1.34
1	A	120	THR	CA-C	2.20	1.52	1.49
1	A	37	HIS	CE1-ND1	-2.13	1.32	1.34
1	A	85	GLU	CA-C	2.12	1.51	1.49
1	A	150	GLU	CG-CD	2.07	1.51	1.49
1	A	25	HIS	CA-C	2.04	1.51	1.49
1	A	173	LYS	CA-C	2.04	1.51	1.49

All (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
1	A	167	THR	CB-CA-C	-4.12	108.47	112.70
1	A	20	THR	CB-CA-C	-3.80	108.79	112.70
1	A	97	VAL	CB-CA-C	-3.72	107.31	112.89
1	A	120	THR	CB-CA-C	-3.56	109.04	112.70
1	A	154	MET	CB-CA-C	-3.53	107.65	111.81
1	A	64	ILE	CB-CA-C	-3.50	106.92	112.72
1	A	141	THR	CB-CA-C	-3.48	109.12	112.70
1	A	11	VAL	CB-CA-C	-3.36	107.85	112.89
1	A	127	ALA	O-C-CA	-3.33	120.10	125.60
1	A	123	ALA	O-C-CA	-3.28	120.18	125.60
1	A	125	ALA	O-C-CA	-3.25	120.24	125.60
1	A	117	ALA	O-C-CA	-3.22	120.29	125.60
1	A	15	VAL	CB-CA-C	-3.16	108.14	112.89
1	A	134	ALA	O-C-CA	-3.15	120.39	125.60
1	A	107	ASP	C-CA-N	3.14	116.14	109.91
1	A	103	ALA	O-C-CA	-3.10	120.48	125.60
1	A	99	ALA	O-C-CA	-3.09	120.49	125.60
1	A	147	ALA	O-C-CA	-3.09	120.50	125.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	50	ALA	O-C-CA	-3.06	120.54	125.60
1	A	86	THR	CB-CA-C	-3.02	109.59	112.70
1	A	165	PHE	C-CA-N	3.01	115.88	109.91
1	A	84	LYS	C-CA-N	2.99	115.85	109.91
1	A	116	ALA	O-C-CA	-2.98	120.67	125.60
1	A	166	ASP	C-CA-N	2.96	115.79	109.91
1	A	158	ALA	O-C-CA	-2.96	120.71	125.60
1	A	32	ALA	O-C-CA	-2.96	120.71	125.60
1	A	114	ALA	O-C-CA	-2.95	120.72	125.60
1	A	168	ALA	O-C-CA	-2.94	120.75	125.60
1	A	162	SER	C-CA-N	2.94	115.74	109.91
1	A	87	ALA	O-C-CA	-2.91	120.79	125.60
1	A	28	ALA	O-C-CA	-2.91	120.79	125.60
1	A	6	GLU	CB-CA-C	-2.86	108.44	111.81
1	A	70	ALA	O-C-CA	-2.86	120.88	125.60
1	A	98	THR	CB-CA-C	-2.78	109.84	112.70
1	A	95	ALA	O-C-CA	-2.71	121.12	125.60
1	A	107	ASP	CB-CA-C	-2.70	106.82	111.50
1	A	86	THR	CB-CA-N	2.68	112.78	109.15
1	A	167	THR	CB-CA-N	2.65	112.74	109.15
1	A	133	ASN	CB-CA-C	-2.63	106.94	111.50
1	A	38	VAL	C-CA-N	2.58	115.23	109.79
1	A	31	GLU	CB-CA-C	-2.54	108.82	111.81
1	A	13	THR	CB-CA-C	-2.53	110.10	112.70
1	A	85	GLU	CB-CA-C	-2.51	108.85	111.81
1	A	128	PRO	O-C-CA	-2.48	119.13	125.60
1	A	173	LYS	C-CA-N	-2.46	105.02	109.91
1	A	55	ALA	O-C-CA	-2.46	121.53	125.60
1	A	112	LEU	O-C-CA	-2.45	119.40	125.62
1	A	142	HIS	CE1-ND1-CG	2.43	109.51	104.93
1	A	107	ASP	O-C-CA	-2.41	119.50	125.62
1	A	60	ARG	CB-CA-C	-2.39	109.00	111.81
1	A	122	PHE	CB-CA-C	-2.38	107.37	111.50
1	A	23	GLN	CB-CA-C	-2.36	109.03	111.81
1	A	37	HIS	CE1-ND1-CG	2.35	109.37	104.93
1	A	29	ASN	C-CA-N	2.35	114.57	109.91
1	A	25	HIS	CE1-ND1-CG	2.34	109.36	104.93
1	A	162	SER	O-C-CA	-2.34	119.68	125.62
1	A	137	HIS	CE1-ND1-CG	2.34	109.34	104.93
1	A	42	LEU	O-C-CA	-2.32	119.73	125.62
1	A	135	VAL	CB-CA-C	-2.30	109.43	112.89
1	A	92	MET	CB-CA-C	-2.29	109.11	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	76	LEU	O-C-CA	-2.30	119.79	125.62
1	A	47	LEU	CG-CB-CA	2.28	119.64	114.86
1	A	45	LYS	CB-CA-C	-2.26	109.15	111.81
1	A	20	THR	O-C-CA	-2.25	119.72	125.60
1	A	5	LEU	CG-CB-CA	2.23	119.55	114.86
1	A	125	ALA	C-CA-N	2.23	114.32	109.50
1	A	6	GLU	C-CA-N	2.21	114.30	109.91
1	A	124	VAL	CB-CA-C	-2.21	109.57	112.89
1	A	109	SER	O-C-CA	-2.20	120.02	125.62
1	A	166	ASP	O-C-CA	-2.20	120.03	125.62
1	A	84	LYS	O-C-CA	-2.20	120.03	125.62
1	A	177	SER	O-C-CA	-2.19	120.05	125.62
1	A	112	LEU	C-CA-N	2.19	114.26	109.91
1	A	113	PRO	O-C-CA	-2.19	119.90	125.60
1	A	1	MET	O-C-CA	-2.19	120.07	125.62
1	A	14	ASP	O-C-CA	-2.18	120.09	125.62
1	A	20	THR	CB-CA-N	2.17	112.09	109.15
1	A	109	SER	C-CA-N	2.17	114.21	109.91
1	A	140	SER	O-C-CA	-2.16	120.13	125.62
1	A	72	LEU	C-CA-N	2.15	114.18	109.91
1	A	75	LYS	CB-CA-C	-2.15	109.28	111.81
1	A	111	ASP	O-C-CA	-2.15	120.17	125.62
1	A	33	ILE	O-C-CA	-2.14	120.03	125.60
1	A	72	LEU	O-C-CA	-2.13	120.20	125.62
1	A	63	PRO	O-C-CA	-2.14	120.03	125.60
1	A	93	LYS	O-C-CA	-2.13	120.22	125.62
1	A	175	VAL	C-CA-N	2.13	114.27	109.79
1	A	130	TYR	O-C-CA	-2.12	120.23	125.62
1	A	85	GLU	O-C-CA	-2.12	120.23	125.62
1	A	38	VAL	O-C-CA	-2.12	120.06	125.60
1	A	178	MET	O-C-CA	-2.12	120.24	125.62
1	A	89	PHE	O-C-CA	-2.10	120.30	125.62
1	A	136	ASP	O-C-CA	-2.09	120.30	125.62
1	A	34	LYS	O-C-CA	-2.08	120.33	125.62
1	A	161	LYS	O-C-CA	-2.08	120.33	125.62
1	A	10	PHE	O-C-CA	-2.08	120.34	125.62
1	A	148	PHE	O-C-CA	-2.08	120.34	125.62
1	A	4	LYS	O-C-CA	-2.08	120.35	125.62
1	A	142	HIS	O-C-CA	-2.07	120.36	125.62
1	A	92	MET	O-C-CA	-2.07	120.36	125.62
1	A	159	GLN	O-C-CA	-2.06	120.38	125.62
1	A	2	GLN	O-C-CA	-2.06	120.38	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	MET	O-C-CA	-2.06	120.39	125.62
1	A	90	ASP	O-C-CA	-2.06	120.39	125.62
1	A	25	HIS	CD2-NE2-CE1	2.06	108.96	105.79
1	A	152	SER	O-C-CA	-2.06	120.40	125.62
1	A	165	PHE	O-C-CA	-2.06	120.40	125.62
1	A	62	SER	O-C-CA	-2.05	120.41	125.62
1	A	150	GLU	CB-CA-C	-2.05	109.39	111.81
1	A	102	THR	CB-CA-N	2.05	111.93	109.15
1	A	88	CYS	O-C-CA	-2.05	120.41	125.62
1	A	3	GLN	O-C-CA	-2.05	120.41	125.62
1	A	153	ASP	O-C-CA	-2.05	120.42	125.62
1	A	57	LEU	O-C-CA	-2.04	120.43	125.62
1	A	124	VAL	O-C-CA	-2.04	120.28	125.60
1	A	79	LEU	O-C-CA	-2.04	120.44	125.62
1	A	27	ASP	O-C-CA	-2.04	120.45	125.62
1	A	137	HIS	CD2-NE2-CE1	2.04	108.92	105.79
1	A	163	SER	C-CA-N	2.03	113.95	109.91
1	A	141	THR	CB-CA-N	2.03	111.90	109.15
1	A	174	SER	O-C-CA	-2.03	120.46	125.62
1	A	94	GLN	CB-CA-C	-2.03	109.42	111.81
1	A	142	HIS	CD2-NE2-CE1	2.03	108.91	105.79
1	A	1	MET	CB-CA-C	-2.03	109.42	111.81
1	A	12	ILE	CB-CA-C	-2.02	109.37	112.72
1	A	128	PRO	CB-CA-C	-2.02	110.00	112.76
1	A	157	GLN	O-C-CA	-2.02	120.49	125.62
1	A	37	HIS	CD2-NE2-CE1	2.02	108.89	105.79
1	A	45	LYS	O-C-CA	-2.02	120.50	125.62
1	A	112	LEU	CG-CB-CA	2.02	119.09	114.86
1	A	104	TYR	O-C-CA	-2.01	120.50	125.62
1	A	77	PHE	C-CA-N	2.01	113.91	109.91
1	A	52	ILE	CB-CA-C	-2.01	109.39	112.72
1	A	131	VAL	O-C-CA	-2.01	120.36	125.60
1	A	61	ASP	O-C-CA	-2.01	120.52	125.62
1	A	69	ILE	O-C-CA	-2.01	120.36	125.60
1	A	175	VAL	O-C-CA	-2.01	120.37	125.60
1	A	74	ILE	O-C-CA	-2.00	120.38	125.60
1	A	58	SER	O-C-CA	-2.00	120.54	125.62
1	A	66	ARG	O-C-CA	-2.00	120.54	125.62

There are no chirality outliers.

All (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
1	A	21	ASP	O-C-CA-CB
1	A	126	ASP	O-C-CA-CB
1	A	145	LYS	O-C-CA-CB
1	A	159	GLN	O-C-CA-CB

There are no ring outliers.

5.6 Ligand geometry (i)

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

All (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
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
4	A	203[B]	KDO	C7-C6	-10.42	1.29	1.52
4	A	203[A]	KDO	C7-C6	-10.32	1.29	1.52
4	A	203[B]	KDO	O6-C2	9.29	1.51	1.42
4	A	203[A]	KDO	O6-C6	8.15	1.57	1.44
4	A	203[B]	KDO	O6-C6	7.68	1.57	1.44
4	A	203[A]	KDO	O2-C2	7.67	1.49	1.40
4	A	203[B]	KDO	O2-C2	7.57	1.49	1.40
4	A	203[A]	KDO	O4-C4	4.24	1.53	1.43
4	A	203[B]	KDO	O4-C4	4.19	1.52	1.43
4	A	203[B]	KDO	C5-C6	3.67	1.62	1.52
4	A	203[A]	KDO	C5-C6	3.32	1.61	1.52
4	A	203[B]	KDO	O5-C5	-2.96	1.35	1.43
4	A	203[A]	KDO	C4-C5	-2.89	1.48	1.52
4	A	203[A]	KDO	O5-C5	-2.85	1.36	1.43
4	A	203[B]	KDO	C4-C5	-2.67	1.48	1.52
4	A	203[A]	KDO	C8-C7	2.14	1.58	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
4	A	203[A]	KDO	C3-C4-C5	5.43	115.69	110.80
4	A	203[B]	KDO	C4-C5-C6	5.38	121.62	110.51
4	A	203[A]	KDO	O6-C2-C3	4.89	113.10	110.22
4	A	203[A]	KDO	O8-C8-C7	4.47	120.85	111.06
4	A	203[B]	KDO	C2-C3-C4	4.15	118.72	110.76
4	A	203[A]	KDO	C2-C3-C4	3.97	118.38	110.76
4	A	203[B]	KDO	O6-C6-C7	3.87	113.55	106.69
4	A	203[B]	KDO	C7-C6-C5	3.56	119.91	114.14
4	A	203[A]	KDO	C2-O6-C6	3.56	119.56	113.91
4	A	203[A]	KDO	C4-C5-C6	3.47	117.69	110.51
4	A	203[B]	KDO	O4-C4-C5	-3.37	103.72	110.24
4	A	203[B]	KDO	O5-C5-C4	-3.15	104.27	110.00
4	A	203[B]	KDO	O8-C8-C7	3.00	117.62	111.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	203[B]	KDO	C3-C2-C1	-2.62	109.92	111.41
4	A	203[B]	KDO	O6-C2-C3	2.39	111.63	110.22

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 ⓘ

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(Å^2)	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(Å^2)	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(Å^2)	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 (i)

There are no such residues in this entry.