



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:44 AM UTC

PDB ID : 6QAP / pdb_00006qap
Title : Structure of the human aldehyde dehydrogenase 9A1 in C2 space group
Authors : Morera, S.; Vigouroux, A.
Deposited on : 2018-12-19
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

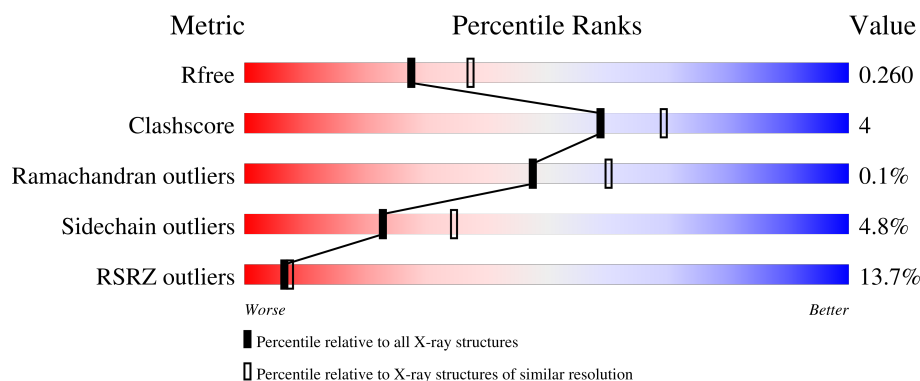
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	508	12% 78% 14% • 7%
1	B	508	13% 79% 12% • 7%
1	C	508	13% 79% 13% • 7%
1	D	508	13% 79% 13% • 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	505	-	-	X	-
2	EDO	D	507	-	-	X	-
3	PEG	B	504	-	-	X	-
3	PEG	C	506	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14878 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 4-trimethylaminobutyraldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3600	2279	615	678	28			
1	B	470	Total	C	N	O	S	0	0	0
			3600	2279	615	678	28			
1	C	471	Total	C	N	O	S	0	0	0
			3604	2281	616	679	28			
1	D	471	Total	C	N	O	S	0	2	0
			3620	2291	622	679	28			

There are 56 discrepancies between the modelled and reference sequences:

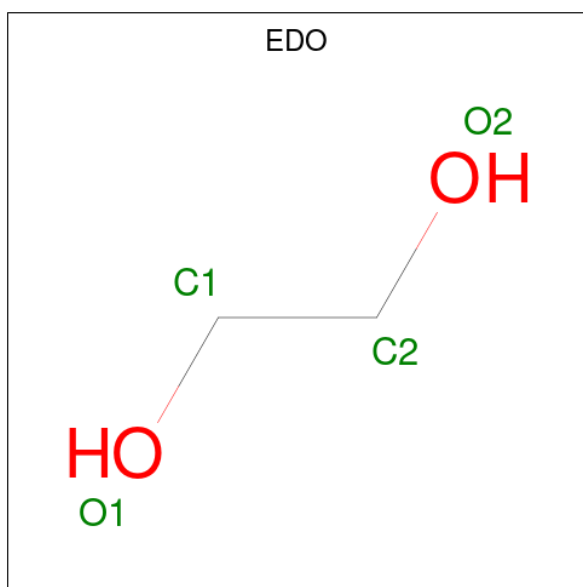
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P49189
A	-12	GLY	-	expression tag	UNP P49189
A	-11	SER	-	expression tag	UNP P49189
A	-10	SER	-	expression tag	UNP P49189
A	-9	HIS	-	expression tag	UNP P49189
A	-8	HIS	-	expression tag	UNP P49189
A	-7	HIS	-	expression tag	UNP P49189
A	-6	HIS	-	expression tag	UNP P49189
A	-5	HIS	-	expression tag	UNP P49189
A	-4	HIS	-	expression tag	UNP P49189
A	-3	SER	-	expression tag	UNP P49189
A	-2	GLN	-	expression tag	UNP P49189
A	-1	ASP	-	expression tag	UNP P49189
A	0	PRO	-	expression tag	UNP P49189
B	-13	MET	-	initiating methionine	UNP P49189
B	-12	GLY	-	expression tag	UNP P49189
B	-11	SER	-	expression tag	UNP P49189
B	-10	SER	-	expression tag	UNP P49189
B	-9	HIS	-	expression tag	UNP P49189
B	-8	HIS	-	expression tag	UNP P49189
B	-7	HIS	-	expression tag	UNP P49189

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP P49189
B	-5	HIS	-	expression tag	UNP P49189
B	-4	HIS	-	expression tag	UNP P49189
B	-3	SER	-	expression tag	UNP P49189
B	-2	GLN	-	expression tag	UNP P49189
B	-1	ASP	-	expression tag	UNP P49189
B	0	PRO	-	expression tag	UNP P49189
C	-13	MET	-	initiating methionine	UNP P49189
C	-12	GLY	-	expression tag	UNP P49189
C	-11	SER	-	expression tag	UNP P49189
C	-10	SER	-	expression tag	UNP P49189
C	-9	HIS	-	expression tag	UNP P49189
C	-8	HIS	-	expression tag	UNP P49189
C	-7	HIS	-	expression tag	UNP P49189
C	-6	HIS	-	expression tag	UNP P49189
C	-5	HIS	-	expression tag	UNP P49189
C	-4	HIS	-	expression tag	UNP P49189
C	-3	SER	-	expression tag	UNP P49189
C	-2	GLN	-	expression tag	UNP P49189
C	-1	ASP	-	expression tag	UNP P49189
C	0	PRO	-	expression tag	UNP P49189
D	-13	MET	-	initiating methionine	UNP P49189
D	-12	GLY	-	expression tag	UNP P49189
D	-11	SER	-	expression tag	UNP P49189
D	-10	SER	-	expression tag	UNP P49189
D	-9	HIS	-	expression tag	UNP P49189
D	-8	HIS	-	expression tag	UNP P49189
D	-7	HIS	-	expression tag	UNP P49189
D	-6	HIS	-	expression tag	UNP P49189
D	-5	HIS	-	expression tag	UNP P49189
D	-4	HIS	-	expression tag	UNP P49189
D	-3	SER	-	expression tag	UNP P49189
D	-2	GLN	-	expression tag	UNP P49189
D	-1	ASP	-	expression tag	UNP P49189
D	0	PRO	-	expression tag	UNP P49189

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



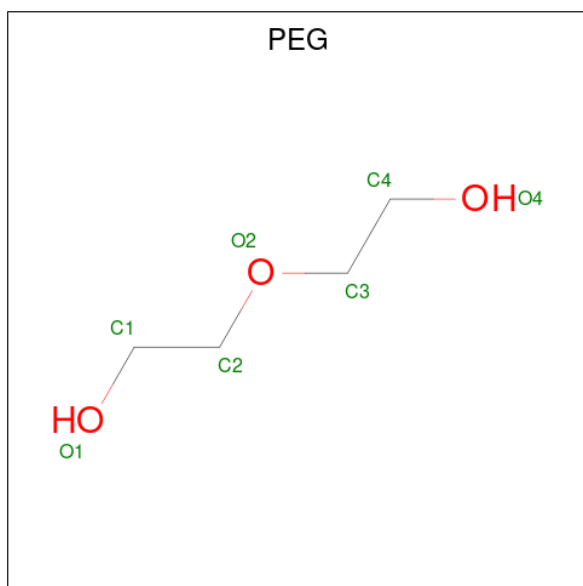
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total	Na	0	0
			3	3		
4	D	5	Total	Na	0	0
			5	5		

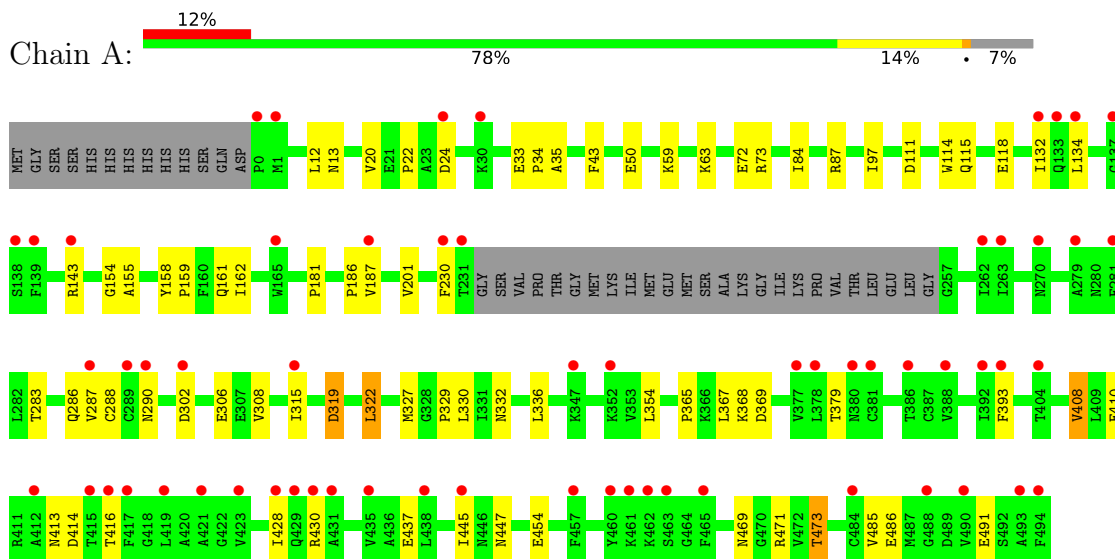
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	94	Total 94	O 94	0	0
5	B	85	Total 85	O 85	0	0
5	C	96	Total 96	O 96	0	0
5	D	83	Total 83	O 83	0	0

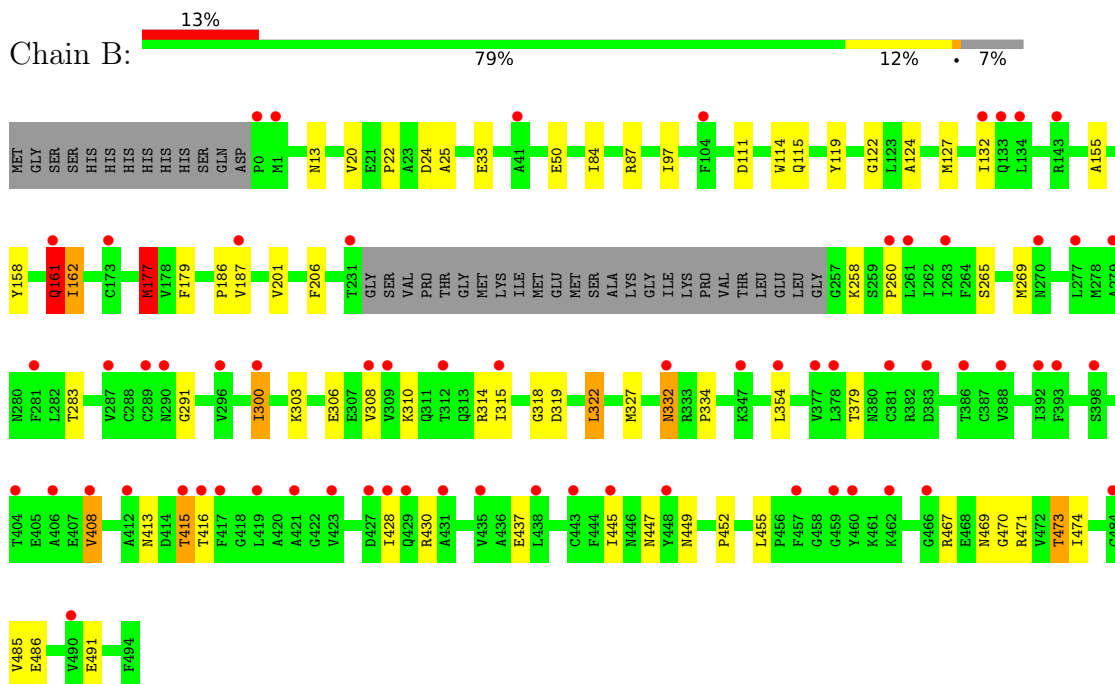
3 Residue-property plots [i](#)

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

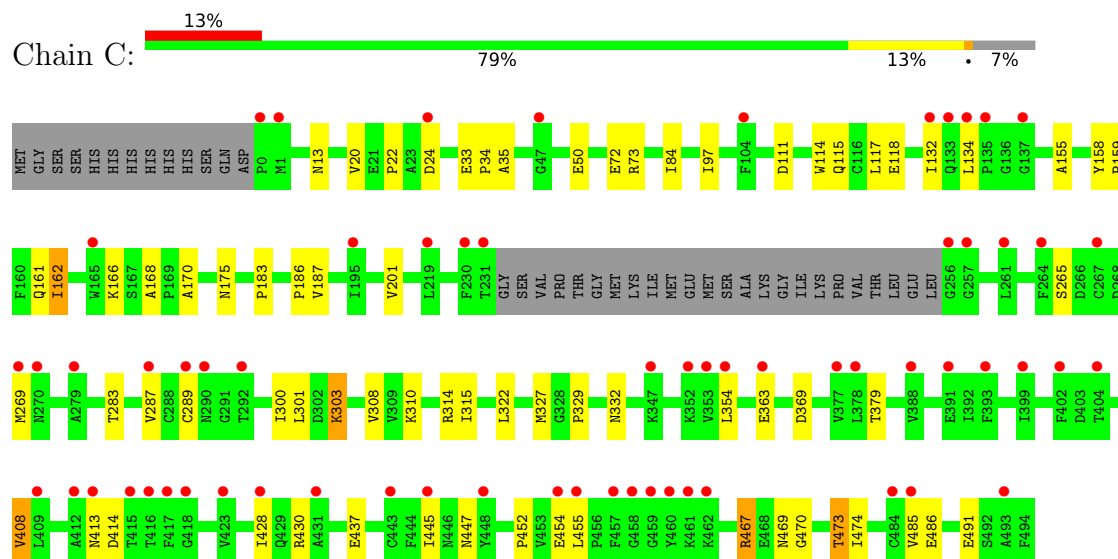
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



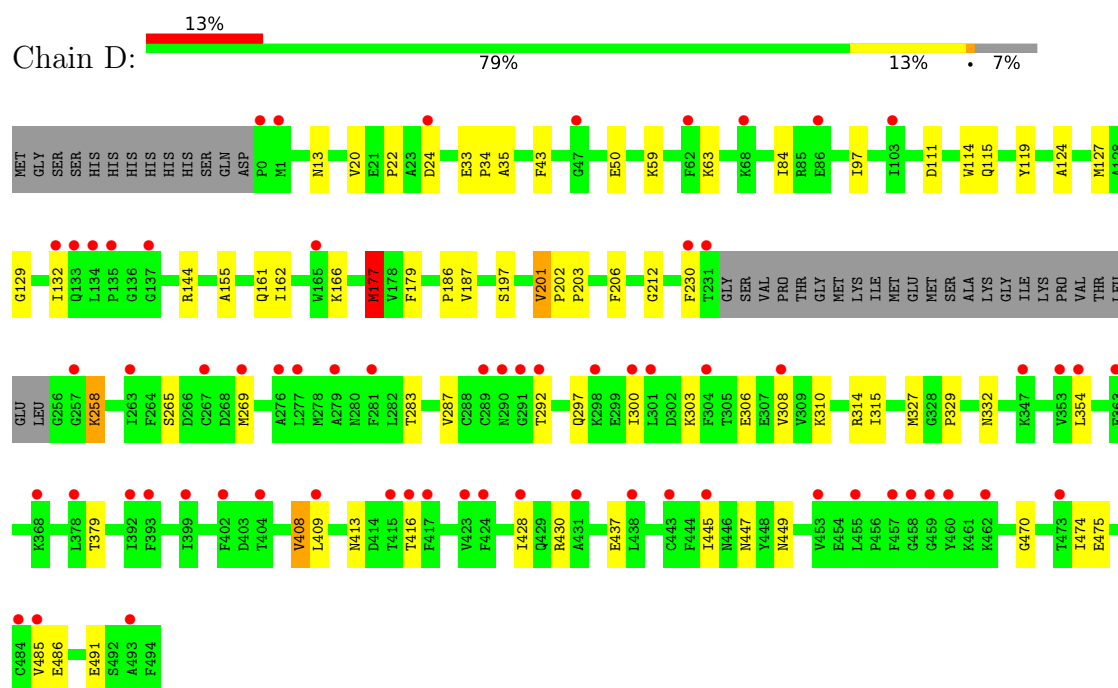
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



• Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



• Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	164.29Å 160.03Å 84.60Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	47.74 – 2.30 47.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.74-2.30) 99.9 (47.74-2.30)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.220 , 0.251 0.228 , 0.260	Depositor DCC
R_{free} test set	4843 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.008 for k,h,-l 0.006 for -k,-h,-l 0.289 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14878	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.86	0/3672	1.40	29/4966 (0.6%)
1	B	0.86	1/3672 (0.0%)	1.39	19/4966 (0.4%)
1	C	0.86	0/3676	1.40	22/4971 (0.4%)
1	D	0.86	1/3698 (0.0%)	1.38	18/4999 (0.4%)
All	All	0.86	2/14718 (0.0%)	1.39	88/19902 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	177	MET	SD-CE	-6.72	1.62	1.79
1	D	177	MET	SD-CE	-6.50	1.63	1.79

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	115	GLN	CA-C-N	8.07	130.94	120.44
1	D	115	GLN	C-N-CA	8.07	130.94	120.44
1	B	115	GLN	CA-C-N	7.95	130.77	120.44
1	B	115	GLN	C-N-CA	7.95	130.77	120.44
1	A	187	VAL	N-CA-C	7.85	117.80	110.42
1	B	187	VAL	N-CA-C	7.80	117.75	110.42
1	D	187	VAL	N-CA-C	7.71	117.67	110.42
1	A	115	GLN	CA-C-N	7.68	130.42	120.44
1	A	115	GLN	C-N-CA	7.68	130.42	120.44
1	C	201	VAL	N-CA-CB	7.62	117.84	109.99
1	C	115	GLN	CA-C-N	7.61	130.34	120.44
1	C	115	GLN	C-N-CA	7.61	130.34	120.44
1	B	201	VAL	N-CA-CB	7.50	117.71	109.99
1	A	201	VAL	N-CA-CB	7.48	117.69	109.99
1	C	187	VAL	N-CA-C	7.46	117.43	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	201	VAL	N-CA-CB	7.46	117.67	109.99
1	D	408	VAL	N-CA-CB	7.11	118.09	110.62
1	C	408	VAL	N-CA-CB	6.87	118.14	110.51
1	A	413	ASN	CA-C-N	6.85	130.73	120.17
1	A	413	ASN	C-N-CA	6.85	130.73	120.17
1	B	408	VAL	N-CA-CB	6.81	118.07	110.51
1	C	332	ASN	CA-C-N	6.79	129.35	120.26
1	C	332	ASN	C-N-CA	6.79	129.35	120.26
1	A	408	VAL	N-CA-CB	6.76	118.02	110.51
1	A	369	ASP	CA-C-N	6.64	126.65	120.34
1	A	369	ASP	C-N-CA	6.64	126.65	120.34
1	A	332	ASN	CA-C-N	6.33	128.74	120.26
1	A	332	ASN	C-N-CA	6.33	128.74	120.26
1	D	332	ASN	CA-C-N	6.05	128.37	120.26
1	D	332	ASN	C-N-CA	6.05	128.37	120.26
1	A	288	CYS	CA-C-N	6.04	128.29	120.44
1	A	288	CYS	C-N-CA	6.04	128.29	120.44
1	C	186	PRO	CA-C-N	5.63	127.59	120.72
1	C	186	PRO	C-N-CA	5.63	127.59	120.72
1	D	230	PHE	CA-C-N	5.59	131.76	121.70
1	D	230	PHE	C-N-CA	5.59	131.76	121.70
1	C	363	GLU	CB-CG-CD	5.57	122.07	112.60
1	B	413	ASN	CA-C-N	5.53	132.10	121.54
1	B	413	ASN	C-N-CA	5.53	132.10	121.54
1	A	414	ASP	N-CA-C	-5.51	104.40	113.50
1	A	302	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	291	GLY	CA-C-N	5.50	128.68	120.31
1	B	291	GLY	C-N-CA	5.50	128.68	120.31
1	C	369	ASP	CA-C-N	5.49	125.56	120.34
1	C	369	ASP	C-N-CA	5.49	125.56	120.34
1	C	414	ASP	N-CA-C	-5.49	104.44	113.50
1	D	212	GLY	CA-C-N	5.44	127.57	120.28
1	D	212	GLY	C-N-CA	5.44	127.57	120.28
1	A	186	PRO	CA-C-N	5.40	127.31	120.72
1	A	186	PRO	C-N-CA	5.40	127.31	120.72
1	D	24	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	301	LEU	CA-C-N	5.39	127.44	120.44
1	C	301	LEU	C-N-CA	5.39	127.44	120.44
1	A	319	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	73	ARG	CA-C-N	5.33	127.37	120.44
1	C	73	ARG	C-N-CA	5.33	127.37	120.44
1	C	24	ASP	CA-CB-CG	5.27	117.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	413	ASN	CA-C-N	5.24	128.23	120.17
1	C	413	ASN	C-N-CA	5.24	128.23	120.17
1	A	84	ILE	CA-C-N	5.23	127.29	120.28
1	A	84	ILE	C-N-CA	5.23	127.29	120.28
1	A	24	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	186	PRO	CA-C-N	5.18	127.05	120.72
1	B	186	PRO	C-N-CA	5.18	127.05	120.72
1	A	87	ARG	CA-C-N	5.17	128.58	120.82
1	A	87	ARG	C-N-CA	5.17	128.58	120.82
1	A	73	ARG	CA-C-N	5.16	127.15	120.44
1	A	73	ARG	C-N-CA	5.16	127.15	120.44
1	D	84	ILE	CA-C-N	5.12	127.14	120.28
1	D	84	ILE	C-N-CA	5.12	127.14	120.28
1	B	84	ILE	CA-C-N	5.12	127.14	120.28
1	B	84	ILE	C-N-CA	5.12	127.14	120.28
1	C	84	ILE	CA-C-N	5.12	127.14	120.28
1	C	84	ILE	C-N-CA	5.12	127.14	120.28
1	B	332	ASN	CA-CB-CG	5.10	117.70	112.60
1	D	186	PRO	CA-C-N	5.10	126.95	120.72
1	D	186	PRO	C-N-CA	5.10	126.95	120.72
1	B	161	GLN	CA-C-N	5.04	127.58	120.42
1	B	161	GLN	C-N-CA	5.04	127.58	120.42
1	D	297	GLN	CA-C-N	5.04	131.16	121.54
1	D	297	GLN	C-N-CA	5.04	131.16	121.54
1	B	87	ARG	CA-C-N	5.01	128.34	120.82
1	B	87	ARG	C-N-CA	5.01	128.34	120.82
1	A	230	PHE	CA-C-N	5.01	130.72	121.70
1	A	230	PHE	C-N-CA	5.01	130.72	121.70
1	A	367	LEU	CA-C-N	5.01	127.30	120.54
1	A	367	LEU	C-N-CA	5.01	127.30	120.54
1	B	318	GLY	N-CA-C	5.00	117.59	110.74

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3600	0	3574	32	0
1	B	3600	0	3574	35	0
1	C	3604	0	3577	32	0
1	D	3620	0	3603	36	0
2	A	20	0	30	8	0
2	B	12	0	18	3	0
2	C	4	0	6	0	0
2	D	24	0	35	12	0
3	B	7	0	10	4	0
3	C	21	0	30	6	0
4	C	3	0	0	0	0
4	D	5	0	0	0	0
5	A	94	0	0	0	0
5	B	85	0	0	2	0
5	C	96	0	0	1	0
5	D	83	0	0	0	0
All	All	14878	0	14457	127	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PRO:HA	2:A:505:EDO:H22	1.45	0.99
1:B:332:ASN:HB3	1:B:334:PRO:HD2	1.52	0.90
1:C:469:ASN:O	1:C:473:THR:HG23	1.72	0.87
1:B:24:ASP:HB2	3:B:504:PEG:H21	1.56	0.85
1:A:469:ASN:O	1:A:473:THR:HG23	1.78	0.83
1:D:144:ARG:HG3	2:D:511:EDO:H22	1.60	0.82
1:B:25:ALA:H	3:B:504:PEG:H41	1.44	0.80
1:B:122:GLY:HA2	3:C:506:PEG:H21	1.64	0.79
1:B:469:ASN:O	1:B:473:THR:HG23	1.84	0.76
1:D:43:PHE:HB2	2:D:508:EDO:H11	1.66	0.75
1:D:203:PRO:HA	2:D:507:EDO:H11	1.70	0.74
1:C:155:ALA:HB3	1:C:162:ILE:HD13	1.70	0.72
1:D:201:VAL:CG2	2:D:507:EDO:H21	2.19	0.71
1:A:159:PRO:CA	2:A:505:EDO:H22	2.19	0.70
1:D:201:VAL:HG23	2:D:507:EDO:H21	1.72	0.70
1:C:118:GLU:O	3:C:506:PEG:H12	1.92	0.68
2:B:502:EDO:H22	1:C:467:ARG:HH11	1.61	0.65
1:D:155:ALA:HB3	1:D:162:ILE:HD13	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:PHE:HB2	2:A:503:EDO:H11	1.80	0.63
1:C:118:GLU:OE1	3:C:506:PEG:H41	2.00	0.62
1:B:155:ALA:HB3	1:B:162:ILE:HD13	1.82	0.61
1:C:265:SER:HA	1:C:300:ILE:HG12	1.83	0.61
1:B:265:SER:HA	1:B:300:ILE:HG12	1.83	0.59
1:D:144:ARG:HG3	2:D:511:EDO:C2	2.31	0.59
1:B:124:ALA:HA	1:B:127:MET:HE3	1.85	0.58
1:D:124:ALA:HA	1:D:127:MET:HE3	1.86	0.57
1:D:265:SER:HA	1:D:300:ILE:HG12	1.86	0.57
1:A:486:GLU:HB2	1:B:447:ASN:HB2	1.85	0.57
5:B:610:HOH:O	3:C:506:PEG:H22	2.05	0.56
1:A:155:ALA:HB3	1:A:162:ILE:HD13	1.87	0.55
1:C:486:GLU:HB2	1:D:447:ASN:HB2	1.87	0.55
1:A:12:LEU:HB2	2:A:503:EDO:H21	1.89	0.55
1:A:181:PRO:HA	2:A:505:EDO:H11	1.89	0.55
1:A:447:ASN:HB2	1:B:486:GLU:HB2	1.88	0.54
1:A:319:ASP:HB3	1:A:322:LEU:HD22	1.88	0.53
1:A:471:ARG:HD2	5:B:601:HOH:O	2.08	0.53
1:B:354:LEU:HD11	1:B:379:THR:HB	1.91	0.53
1:A:365:PRO:O	1:A:368:LYS:HB2	2.09	0.53
1:D:258:LYS:HE2	1:D:292:THR:OG1	2.09	0.52
1:C:34:PRO:HB2	1:C:329:PRO:HG2	1.92	0.52
1:A:13:ASN:HB2	1:A:20:VAL:O	2.10	0.52
1:B:13:ASN:HB2	1:B:20:VAL:O	2.11	0.51
1:D:13:ASN:HB2	1:D:20:VAL:O	2.11	0.51
1:B:319:ASP:HB3	1:B:322:LEU:HD22	1.92	0.51
1:D:354:LEU:HD11	1:D:379:THR:HB	1.91	0.51
1:C:159:PRO:HG2	5:C:611:HOH:O	2.10	0.51
1:C:13:ASN:HB2	1:C:20:VAL:O	2.11	0.51
1:C:447:ASN:HB2	1:D:486:GLU:HB2	1.93	0.51
1:D:201:VAL:HG23	2:D:507:EDO:C2	2.40	0.51
1:C:287:VAL:HG12	1:C:289:CYS:H	1.77	0.50
1:C:35:ALA:HA	1:C:329:PRO:HG3	1.93	0.50
1:C:354:LEU:HD11	1:C:379:THR:HB	1.92	0.50
1:B:260:PRO:HD3	1:B:415:THR:HG21	1.94	0.50
1:B:24:ASP:HB2	3:B:504:PEG:H32	1.94	0.50
1:C:162:ILE:O	1:C:166:LYS:HG3	2.12	0.50
1:D:177:MET:HE2	1:D:206:PHE:HE1	1.76	0.49
1:D:33:GLU:HA	1:D:97:ILE:O	2.12	0.49
1:A:330:LEU:HD23	1:A:336:LEU:HA	1.93	0.49
1:C:485:VAL:HG22	1:D:445:ILE:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:PRO:HB2	1:A:329:PRO:HG2	1.95	0.48
1:B:452:PRO:HD2	1:B:455:LEU:HD22	1.96	0.48
1:D:177:MET:HE3	1:D:179:PHE:HD1	1.78	0.48
1:A:469:ASN:O	1:A:473:THR:CG2	2.56	0.48
1:A:33:GLU:HA	1:A:97:ILE:O	2.13	0.48
1:B:22:PRO:HB3	1:B:50:GLU:HG2	1.96	0.48
1:B:33:GLU:HA	1:B:97:ILE:O	2.13	0.48
1:B:469:ASN:O	1:B:473:THR:CG2	2.61	0.48
1:B:177:MET:HE3	1:B:179:PHE:HD1	1.79	0.47
1:C:269:MET:HE1	1:C:300:ILE:HB	1.97	0.47
1:D:111:ASP:HA	1:D:114:TRP:NE1	2.30	0.47
1:A:35:ALA:HA	1:A:329:PRO:HG3	1.95	0.47
1:D:129:GLY:HA2	2:D:511:EDO:H21	1.97	0.47
1:A:485:VAL:HG22	1:B:445:ILE:HD12	1.97	0.47
1:C:183:PRO:HD2	3:C:507:PEG:H21	1.95	0.47
1:A:154:GLY:HA3	2:A:505:EDO:H11	1.96	0.47
1:B:177:MET:HE2	1:B:206:PHE:HE1	1.78	0.46
1:A:111:ASP:HA	1:A:114:TRP:NE1	2.30	0.46
1:C:111:ASP:HA	1:C:114:TRP:NE1	2.30	0.46
1:C:452:PRO:HB2	1:C:455:LEU:HD13	1.96	0.46
1:B:161:GLN:HE22	1:B:452:PRO:HG2	1.80	0.46
1:D:269:MET:HE1	1:D:300:ILE:HB	1.98	0.46
1:C:33:GLU:HA	1:C:97:ILE:O	2.15	0.46
1:B:471:ARG:HH11	2:B:502:EDO:H12	1.81	0.46
1:A:22:PRO:HB3	1:A:50:GLU:HG2	1.99	0.45
1:B:111:ASP:HA	1:B:114:TRP:NE1	2.30	0.45
1:D:162:ILE:O	1:D:166:LYS:HG3	2.16	0.45
1:C:445:ILE:HD12	1:D:485:VAL:HG22	1.97	0.45
1:A:155:ALA:HB3	1:A:162:ILE:CD1	2.46	0.45
1:B:315:ILE:HG21	1:B:327:MET:HE3	1.98	0.45
1:D:202:PRO:O	2:D:507:EDO:H22	2.16	0.45
1:A:315:ILE:HG21	1:A:327:MET:HE3	1.98	0.45
1:D:22:PRO:HB3	1:D:50:GLU:HG2	1.99	0.45
1:D:203:PRO:HA	2:D:507:EDO:C1	2.43	0.45
1:C:22:PRO:HB3	1:C:50:GLU:HG2	1.99	0.45
1:D:34:PRO:HB2	1:D:329:PRO:HG2	1.98	0.45
1:D:315:ILE:HG21	1:D:327:MET:HE3	1.98	0.44
1:C:300:ILE:HA	1:C:303:LYS:HE2	2.00	0.44
1:A:158:TYR:HB3	1:A:161:GLN:HB3	2.00	0.44
1:C:158:TYR:HB2	1:C:162:ILE:HD12	1.99	0.44
1:C:315:ILE:HG21	1:C:327:MET:HE3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:O	2:A:505:EDO:H12	2.18	0.44
1:B:24:ASP:CB	3:B:504:PEG:H32	2.48	0.44
1:C:303:LYS:H	1:C:303:LYS:HG2	1.59	0.43
1:A:486:GLU:CB	1:B:447:ASN:HB2	2.48	0.43
1:B:470:GLY:O	1:B:474:ILE:HG12	2.18	0.43
1:A:118:GLU:HB3	2:A:504:EDO:H22	2.00	0.43
1:D:35:ALA:HA	1:D:329:PRO:HG3	1.99	0.43
1:C:170:ALA:O	1:C:175:ASN:HB2	2.19	0.42
1:D:409:LEU:O	1:D:413:ASN:HB2	2.18	0.42
1:B:119:TYR:HA	2:B:501:EDO:C2	2.49	0.42
1:A:354:LEU:HD11	1:A:379:THR:HB	2.02	0.42
1:B:122:GLY:HA2	3:C:506:PEG:C2	2.43	0.42
1:B:158:TYR:HB2	1:B:162:ILE:HD12	2.01	0.42
1:D:197:SER:OG	2:D:507:EDO:H12	2.20	0.42
1:C:117:LEU:HD12	1:C:168:ALA:HB2	2.01	0.42
1:D:470:GLY:O	1:D:474:ILE:HG12	2.20	0.42
1:A:286:GLN:O	1:A:393:PHE:HD1	2.02	0.41
1:A:445:ILE:HD12	1:B:485:VAL:HG22	2.02	0.41
1:D:119:TYR:HA	2:D:506:EDO:C1	2.51	0.41
1:C:469:ASN:O	1:C:473:THR:CG2	2.58	0.41
1:C:470:GLY:O	1:C:474:ILE:HG12	2.21	0.41
1:B:310:LYS:HE2	1:B:314:ARG:HH22	1.84	0.41
1:C:310:LYS:HE2	1:C:314:ARG:HH22	1.85	0.41
1:D:310:LYS:HE2	1:D:314:ARG:HH22	1.86	0.41
1:A:59:LYS:HG2	1:A:63:LYS:HE3	2.03	0.40
1:B:269:MET:HE1	1:B:300:ILE:HB	2.02	0.40
1:D:59:LYS:HG2	1:D:63:LYS:HE3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	466/508 (92%)	454 (97%)	11 (2%)	1 (0%)	43	55
1	B	466/508 (92%)	455 (98%)	11 (2%)	0	100	100
1	C	467/508 (92%)	454 (97%)	13 (3%)	0	100	100
1	D	469/508 (92%)	458 (98%)	11 (2%)	0	100	100
All	All	1868/2032 (92%)	1821 (98%)	46 (2%)	1 (0%)	48	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/416 (92%)	366 (95%)	18 (5%)	23	35
1	B	384/416 (92%)	363 (94%)	21 (6%)	19	28
1	C	384/416 (92%)	367 (96%)	17 (4%)	25	38
1	D	386/416 (93%)	369 (96%)	17 (4%)	25	38
All	All	1538/1664 (92%)	1465 (95%)	73 (5%)	23	35

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	132	ILE
1	A	134	LEU
1	A	143	ARG
1	A	283	THR
1	A	287	VAL
1	A	306	GLU
1	A	308	VAL
1	A	322	LEU
1	A	408	VAL

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Mol	Chain	Res	Type
1	A	410	GLU
1	A	416	THR
1	A	428	ILE
1	A	430	ARG
1	A	437	GLU
1	A	454	GLU
1	A	473	THR
1	A	491	GLU
1	B	132	ILE
1	B	161	GLN
1	B	162	ILE
1	B	177	MET
1	B	258	LYS
1	B	283	THR
1	B	300	ILE
1	B	303	LYS
1	B	306	GLU
1	B	308	VAL
1	B	322	LEU
1	B	408	VAL
1	B	415	THR
1	B	416	THR
1	B	428	ILE
1	B	430	ARG
1	B	437	GLU
1	B	449	ASN
1	B	467	ARG
1	B	473	THR
1	B	491	GLU
1	C	72	GLU
1	C	132	ILE
1	C	134	LEU
1	C	161	GLN
1	C	162	ILE
1	C	283	THR
1	C	303	LYS
1	C	308	VAL
1	C	322	LEU
1	C	408	VAL
1	C	428	ILE
1	C	430	ARG
1	C	437	GLU

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Mol	Chain	Res	Type
1	C	454	GLU
1	C	467	ARG
1	C	473	THR
1	C	491	GLU
1	D	132	ILE
1	D	161	GLN
1	D	177	MET
1	D	258	LYS
1	D	283	THR
1	D	287	VAL
1	D	303	LYS
1	D	306	GLU
1	D	308	VAL
1	D	408	VAL
1	D	416	THR
1	D	428	ILE
1	D	430	ARG
1	D	437	GLU
1	D	449	ASN
1	D	475	GLU
1	D	491	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	HIS
1	A	270	ASN
1	A	290	ASN
1	A	429	GLN
1	B	270	ASN
1	B	290	ASN
1	B	429	GLN
1	C	270	ASN
1	C	284	GLN
1	C	290	ASN
1	C	429	GLN
1	D	270	ASN
1	D	290	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 8 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	D	506	-	3,3,3	1.12	0	2,2,2	0.20	0
2	EDO	A	503	-	3,3,3	0.61	0	2,2,2	0.38	0
2	EDO	D	509	-	3,3,3	0.64	0	2,2,2	0.21	0
2	EDO	D	510	-	3,3,3	0.50	0	2,2,2	0.42	0
2	EDO	B	502	-	3,3,3	0.53	0	2,2,2	0.26	0
2	EDO	A	502	-	3,3,3	0.65	0	2,2,2	0.20	0
2	EDO	B	501	-	3,3,3	1.30	0	2,2,2	0.34	0
2	EDO	D	508	-	3,3,3	0.57	0	2,2,2	0.53	0
3	PEG	C	505	-	6,6,6	0.23	0	5,5,5	0.14	0
3	PEG	B	504	-	6,6,6	0.24	0	5,5,5	0.29	0
2	EDO	A	504	-	3,3,3	0.63	0	2,2,2	0.14	0
2	EDO	D	507	4	3,3,3	0.43	0	2,2,2	0.21	0
3	PEG	C	507	-	6,6,6	0.26	0	5,5,5	0.17	0
3	PEG	C	506	-	6,6,6	0.22	0	5,5,5	0.30	0
2	EDO	A	501	-	3,3,3	0.74	0	2,2,2	0.17	0
2	EDO	A	505	-	3,3,3	0.53	0	2,2,2	0.28	0
2	EDO	B	503	-	3,3,3	0.64	0	2,2,2	0.21	0
2	EDO	D	511	-	3,3,3	0.64	0	2,2,2	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	504	-	3,3,3	0.63	0	2,2,2	0.11	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	EDO	D	506	-	-	1/1/1/1	-
2	EDO	A	503	-	-	0/1/1/1	-
2	EDO	D	509	-	-	0/1/1/1	-
2	EDO	D	510	-	-	0/1/1/1	-
2	EDO	B	502	-	-	1/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	D	508	-	-	1/1/1/1	-
3	PEG	C	505	-	-	2/4/4/4	-
3	PEG	B	504	-	-	1/4/4/4	-
2	EDO	A	504	-	-	1/1/1/1	-
2	EDO	D	507	4	-	0/1/1/1	-
3	PEG	C	507	-	-	2/4/4/4	-
3	PEG	C	506	-	-	2/4/4/4	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	A	505	-	-	0/1/1/1	-
2	EDO	B	503	-	-	0/1/1/1	-
2	EDO	D	511	-	-	0/1/1/1	-
2	EDO	C	504	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	508	EDO	O1-C1-C2-O2
3	B	504	PEG	C1-C2-O2-C3
3	C	507	PEG	C1-C2-O2-C3
3	C	507	PEG	C4-C3-O2-C2
3	C	505	PEG	C1-C2-O2-C3
3	C	505	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
3	C	506	PEG	O2-C3-C4-O4
2	A	504	EDO	O1-C1-C2-O2
2	B	502	EDO	O1-C1-C2-O2
2	D	506	EDO	O1-C1-C2-O2
3	C	506	PEG	C1-C2-O2-C3
2	B	501	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	506	EDO	1	0
2	A	503	EDO	2	0
2	B	502	EDO	2	0
2	B	501	EDO	1	0
2	D	508	EDO	1	0
3	B	504	PEG	4	0
2	A	504	EDO	1	0
2	D	507	EDO	7	0
3	C	507	PEG	1	0
3	C	506	PEG	5	0
2	A	505	EDO	5	0
2	D	511	EDO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	470/508 (92%)	1.11	61 (12%) 7 8	32, 58, 95, 114	0
1	B	470/508 (92%)	1.16	66 (14%) 6 7	33, 61, 109, 134	0
1	C	471/508 (92%)	1.10	64 (13%) 7 7	34, 56, 102, 119	0
1	D	471/508 (92%)	1.09	66 (14%) 6 7	30, 55, 99, 116	2 (0%)
All	All	1882/2032 (92%)	1.11	257 (13%) 6 7	30, 57, 101, 134	2 (0%)

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	ILE	7.6
1	D	428	ILE	6.8
1	A	428	ILE	6.6
1	B	231	THR	5.2
1	A	132	ILE	4.9
1	C	0	PRO	4.5
1	A	231	THR	4.4
1	D	231	THR	4.4
1	C	47	GLY	4.4
1	D	0	PRO	4.3
1	A	431	ALA	4.3
1	B	460	TYR	4.1
1	C	137	GLY	4.0
1	D	460	TYR	4.0
1	C	428	ILE	4.0
1	D	431	ALA	4.0
1	A	133	GLN	4.0
1	B	412	ALA	3.8
1	C	134	LEU	3.8
1	B	1	MET	3.8
1	C	423	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	134	LEU	3.8
1	C	231	THR	3.7
1	A	460	TYR	3.7
1	C	165	TRP	3.6
1	D	457	PHE	3.6
1	B	431	ALA	3.6
1	C	457	PHE	3.6
1	C	135	PRO	3.5
1	C	460	TYR	3.5
1	A	415	THR	3.4
1	C	415	THR	3.4
1	D	423	VAL	3.4
1	C	484	CYS	3.4
1	D	462	LYS	3.4
1	A	134	LEU	3.3
1	A	187	VAL	3.2
1	C	132	ILE	3.2
1	B	457	PHE	3.1
1	D	415	THR	3.1
1	C	24	ASP	3.1
1	C	257	GLY	3.1
1	A	386	THR	3.1
1	D	289	CYS	3.1
1	D	47	GLY	3.1
1	D	132	ILE	3.1
1	D	133	GLN	3.1
1	D	347	LYS	3.1
1	D	354	LEU	3.1
1	C	416	THR	3.0
1	D	165	TRP	3.0
1	B	0	PRO	3.0
1	C	378	LEU	3.0
1	D	279	ALA	3.0
1	A	377	VAL	3.0
1	A	445	ILE	3.0
1	C	1	MET	3.0
1	C	264	PHE	3.0
1	D	455	LEU	3.0
1	B	392	ILE	3.0
1	A	270	ASN	3.0
1	A	490	VAL	2.9
1	B	490	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	2.9
1	C	289	CYS	2.9
1	D	257	GLY	2.9
1	D	368	LYS	2.9
1	A	423	VAL	2.9
1	C	391	GLU	2.9
1	B	332	ASN	2.9
1	A	493	ALA	2.8
1	A	484	CYS	2.8
1	B	132	ILE	2.8
1	B	415	THR	2.8
1	B	354	LEU	2.8
1	D	424	PHE	2.8
1	A	289	CYS	2.8
1	C	230	PHE	2.8
1	B	388	VAL	2.8
1	B	386	THR	2.8
1	D	290	ASN	2.8
1	B	133	GLN	2.8
1	D	135	PRO	2.8
1	D	378	LEU	2.8
1	C	462	LYS	2.8
1	A	279	ALA	2.8
1	B	308	VAL	2.8
1	A	404	THR	2.7
1	D	416	THR	2.7
1	A	412	ALA	2.7
1	C	445	ILE	2.7
1	B	459	GLY	2.7
1	C	404	THR	2.7
1	D	137	GLY	2.7
1	D	458	GLY	2.7
1	D	68	LYS	2.7
1	D	484	CYS	2.7
1	A	494	PHE	2.7
1	A	24	ASP	2.7
1	C	287	VAL	2.7
1	B	289	CYS	2.7
1	C	393	PHE	2.6
1	A	262	ILE	2.6
1	B	378	LEU	2.6
1	D	404	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	485	VAL	2.6
1	A	0	PRO	2.6
1	C	347	LYS	2.6
1	B	270	ASN	2.6
1	C	402	PHE	2.6
1	D	230	PHE	2.6
1	D	402	PHE	2.6
1	C	292	THR	2.6
1	D	1	MET	2.6
1	B	462	LYS	2.6
1	C	363	GLU	2.6
1	C	104	PHE	2.6
1	C	485	VAL	2.6
1	D	493	ALA	2.5
1	C	256	GLY	2.5
1	D	393	PHE	2.5
1	B	161	GLN	2.5
1	C	409	LEU	2.5
1	B	398	SER	2.5
1	C	133	GLN	2.5
1	C	354	LEU	2.5
1	A	462	LYS	2.5
1	C	418	GLY	2.5
1	B	279	ALA	2.5
1	C	412	ALA	2.5
1	B	423	VAL	2.4
1	A	143	ARG	2.4
1	A	263	ILE	2.4
1	B	445	ILE	2.4
1	D	409	LEU	2.4
1	C	290	ASN	2.4
1	A	421	ALA	2.4
1	B	421	ALA	2.4
1	A	461	LYS	2.4
1	C	443	CYS	2.4
1	B	417	PHE	2.4
1	B	287	VAL	2.4
1	B	408	VAL	2.4
1	C	267	CYS	2.4
1	D	304	PHE	2.4
1	C	454	GLU	2.4
1	A	165	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	388	VAL	2.3
1	B	296	VAL	2.3
1	B	393	PHE	2.3
1	A	419	LEU	2.3
1	B	438	LEU	2.3
1	B	383	ASP	2.3
1	D	445	ILE	2.3
1	C	377	VAL	2.3
1	D	86	GLU	2.3
1	D	308	VAL	2.3
1	B	261	LEU	2.3
1	A	315	ILE	2.3
1	B	435	VAL	2.3
1	B	347	LYS	2.3
1	C	352	LYS	2.3
1	A	137	GLY	2.3
1	B	312	THR	2.3
1	A	392	ILE	2.3
1	C	399	ILE	2.3
1	D	103	ILE	2.3
1	B	134	LEU	2.2
1	C	261	LEU	2.2
1	D	453	VAL	2.3
1	B	173	CYS	2.2
1	C	458	GLY	2.2
1	B	41	ALA	2.2
1	C	279	ALA	2.2
1	A	416	THR	2.2
1	A	417	PHE	2.2
1	D	62	PHE	2.2
1	D	353	VAL	2.2
1	D	24	ASP	2.2
1	B	143	ARG	2.2
1	B	443	CYS	2.2
1	B	484	CYS	2.2
1	D	443	CYS	2.2
1	D	291	GLY	2.2
1	D	292	THR	2.2
1	B	448	TYR	2.2
1	B	300	ILE	2.2
1	D	392	ILE	2.2
1	C	455	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	377	VAL	2.2
1	A	393	PHE	2.2
1	B	104	PHE	2.2
1	C	459	GLY	2.2
1	B	416	THR	2.2
1	D	276	ALA	2.2
1	A	435	VAL	2.2
1	B	309	VAL	2.2
1	B	263	ILE	2.1
1	D	399	ILE	2.1
1	D	438	LEU	2.1
1	B	290	ASN	2.1
1	B	427	ASP	2.1
1	C	353	VAL	2.1
1	C	413	ASN	2.1
1	D	269	MET	2.1
1	A	30	LYS	2.1
1	A	230	PHE	2.1
1	C	461	LYS	2.1
1	B	260	PRO	2.1
1	D	281	PHE	2.1
1	D	417	PHE	2.1
1	A	488	GLY	2.1
1	A	463	SER	2.1
1	C	493	ALA	2.1
1	A	378	LEU	2.1
1	B	315	ILE	2.1
1	C	388	VAL	2.1
1	A	457	PHE	2.1
1	B	281	PHE	2.1
1	A	430	ARG	2.1
1	B	404	THR	2.1
1	B	406	ALA	2.1
1	A	347	LYS	2.1
1	C	219	LEU	2.1
1	D	301	LEU	2.1
1	A	465	PHE	2.1
1	C	417	PHE	2.1
1	A	138	SER	2.1
1	A	381	CYS	2.1
1	B	381	CYS	2.1
1	C	269	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	277	LEU	2.1
1	B	419	LEU	2.1
1	A	290	ASN	2.1
1	C	195	ILE	2.1
1	C	270	ASN	2.1
1	D	300	ILE	2.1
1	A	287	VAL	2.1
1	A	139	PHE	2.1
1	A	281	PHE	2.1
1	D	298	LYS	2.0
1	D	473	THR	2.0
1	C	431	ALA	2.0
1	D	363	GLU	2.0
1	B	429	GLN	2.0
1	A	302	ASP	2.0
1	A	380	ASN	2.0
1	D	277	LEU	2.0
1	D	263	ILE	2.0
1	C	448	TYR	2.0
1	B	187	VAL	2.0
1	B	466	GLY	2.0
1	D	459	GLY	2.0
1	A	429	GLN	2.0
1	D	267	CYS	2.0
1	A	438	LEU	2.0
1	A	352	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	B	502	4/4	0.64	0.20	76,76,76,76	0
2	EDO	D	506	4/4	0.66	0.25	46,46,46,48	0
2	EDO	B	501	4/4	0.69	0.22	41,44,50,50	0
2	EDO	C	504	4/4	0.74	0.22	74,75,76,77	0
3	PEG	B	504	7/7	0.76	0.18	63,66,70,71	0
3	PEG	C	507	7/7	0.76	0.21	54,64,71,72	0
2	EDO	A	502	4/4	0.78	0.17	59,61,62,63	0
2	EDO	B	503	4/4	0.78	0.22	64,66,66,66	0
4	NA	D	502	1/1	0.78	0.30	65,65,65,65	0
2	EDO	D	509	4/4	0.79	0.14	69,70,72,72	0
4	NA	C	501	1/1	0.79	0.26	74,74,74,74	0
2	EDO	A	501	4/4	0.79	0.19	55,56,57,59	0
3	PEG	C	506	7/7	0.80	0.18	52,55,60,63	0
4	NA	D	501	1/1	0.81	0.14	47,47,47,47	0
3	PEG	C	505	7/7	0.81	0.16	72,74,75,76	0
2	EDO	A	504	4/4	0.83	0.21	55,57,59,60	0
2	EDO	D	510	4/4	0.83	0.15	68,70,70,72	0
2	EDO	D	508	4/4	0.83	0.23	50,56,59,62	0
2	EDO	D	507	4/4	0.87	0.24	48,51,51,53	0
2	EDO	A	503	4/4	0.88	0.19	39,50,55,57	0
2	EDO	D	511	4/4	0.88	0.13	44,45,46,46	0
2	EDO	A	505	4/4	0.88	0.19	41,44,46,47	0
4	NA	D	503	1/1	0.88	0.15	48,48,48,48	0
4	NA	C	502	1/1	0.89	0.26	71,71,71,71	0
4	NA	D	505	1/1	0.89	0.27	72,72,72,72	0
4	NA	C	503	1/1	0.91	0.20	60,60,60,60	0
4	NA	D	504	1/1	0.94	0.21	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.