



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:05 AM UTC

PDB ID : 5X1I / pdb_00005x1i
Title : Vanillate/3-O-methylgallate O-demethylase, LigM, substrate free form
Authors : Harada, A.; Senda, T.
Deposited on : 2017-01-26
Resolution : 1.90 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

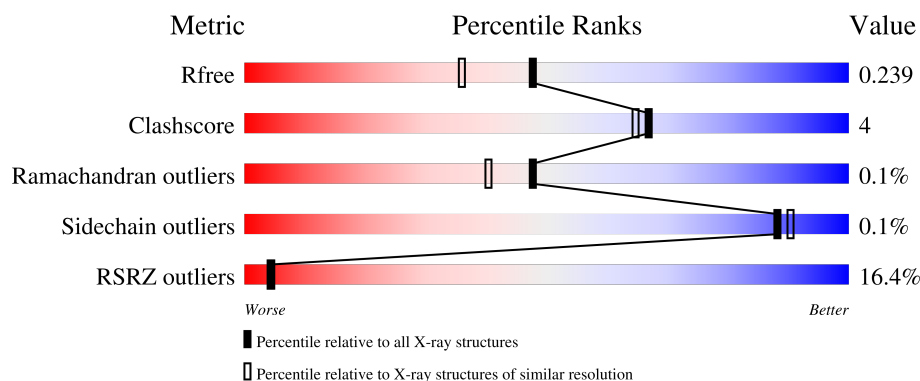
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	474	4% 87% 8% 5%
1	B	474	5% 91% • 5%
1	C	474	37% 82% 12% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10898 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 Vanillate/3-O-methylgallate O-demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	2	0
			3539	2269	595	661	14			
1	B	450	Total	C	N	O	S	0	1	0
			3512	2255	591	654	12			
1	C	448	Total	C	N	O	S	0	1	0
			3361	2154	572	623	12			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP G2IQS7
A	-1	SER	-	expression tag	UNP G2IQS7
A	0	SER	-	expression tag	UNP G2IQS7
B	-2	GLY	-	expression tag	UNP G2IQS7
B	-1	SER	-	expression tag	UNP G2IQS7
B	0	SER	-	expression tag	UNP G2IQS7
C	-2	GLY	-	expression tag	UNP G2IQS7
C	-1	SER	-	expression tag	UNP G2IQS7
C	0	SER	-	expression tag	UNP G2IQS7

- 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	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

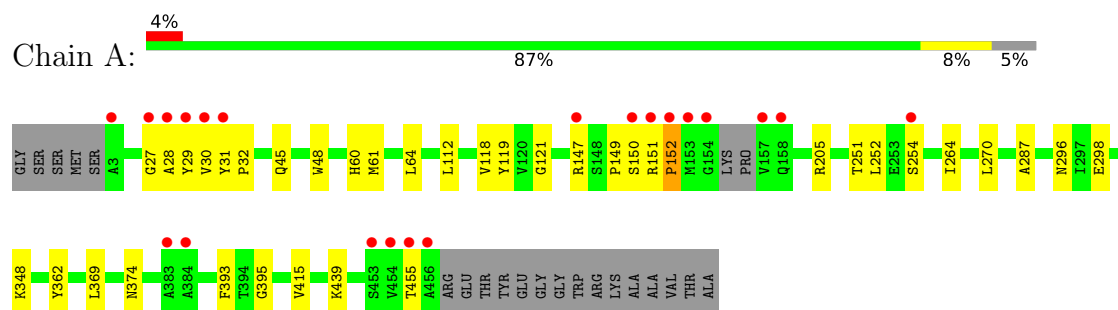
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	230	Total	O	0	0
			230	230		
3	B	184	Total	O	0	0
			184	184		
3	C	56	Total	O	0	0
			56	56		

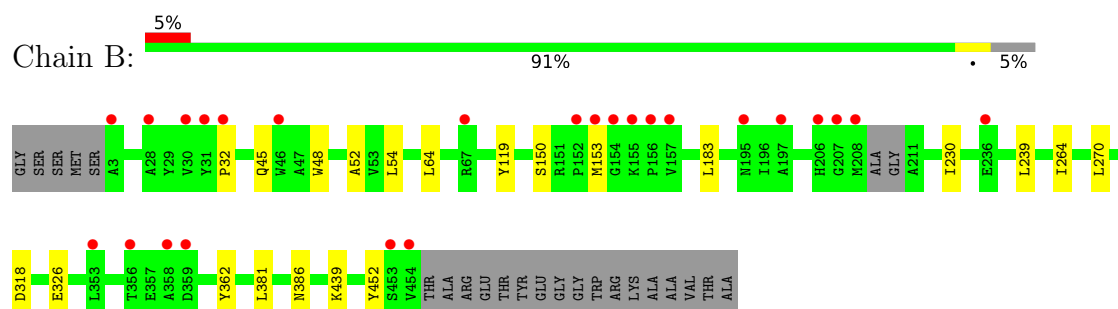
3 Residue-property plots [i](#)

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.

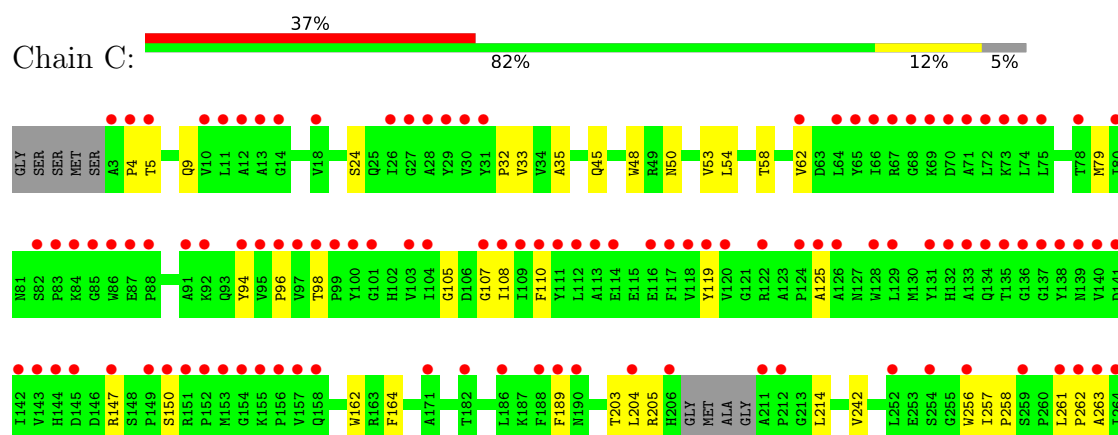
- Molecule 1: Vanillate/3-O-methylgallate O-demethylase

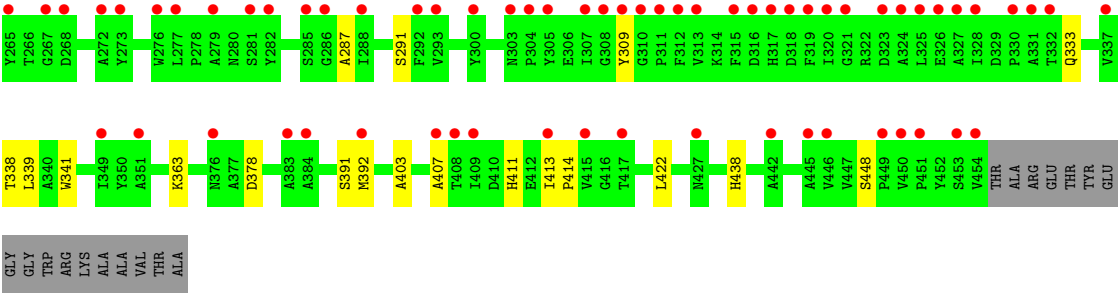


- Molecule 1: Vanillate/3-O-methylgallate O-demethylase



- Molecule 1: Vanillate/3-O-methylgallate O-demethylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	102.00Å 118.60Å 128.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.42 – 1.90 47.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.42-1.90) 93.8 (47.42-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.206 , 0.237 0.208 , 0.239	Depositor DCC
R_{free} test set	6188 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10898	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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

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	0.36	0/3639	0.56	0/4959
1	B	0.32	0/3613	0.54	0/4929
1	C	0.24	0/3460	0.43	0/4736
All	All	0.31	0/10712	0.52	0/14624

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	3539	0	3396	27	0
1	B	3512	0	3356	14	0
1	C	3361	0	3045	35	0
2	A	8	0	12	0	0
2	B	8	0	12	0	0
3	A	230	0	0	9	1
3	B	184	0	0	3	0
3	C	56	0	0	1	0
All	All	10898	0	9821	74	1

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 (74) 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:30:VAL:O	3:A:601:HOH:O	1.93	0.85
1:A:147:ARG:NH1	3:A:601:HOH:O	1.97	0.80
1:A:27:GLY:O	3:A:603:HOH:O	2.03	0.76
1:B:326:GLU:OE2	3:B:601:HOH:O	2.11	0.68
1:A:298:GLU:OE1	3:A:604:HOH:O	2.12	0.68
1:B:452:TYR:O	3:B:602:HOH:O	2.15	0.65
1:A:32:PRO:HB3	1:A:150:SER:HA	1.78	0.65
1:C:58:THR:HG23	1:C:162:TRP:HA	1.79	0.64
1:A:415:VAL:HG12	1:A:455:THR:HG21	1.82	0.61
1:C:203:THR:HB	1:C:214:LEU:HD22	1.82	0.61
1:C:261:LEU:HD12	1:C:262:PRO:HD2	1.81	0.61
1:A:254:SER:OG	3:A:602:HOH:O	1.93	0.59
1:C:205:ARG:HA	1:C:214:LEU:HD23	1.85	0.59
1:B:32:PRO:HB3	1:B:150:SER:HA	1.84	0.59
1:C:378:ASP:HB2	1:C:391:SER:HB3	1.86	0.58
1:B:153:MET:HE1	1:C:35:ALA:H	1.69	0.58
1:B:45:GLN:HG2	1:B:48:TRP:CH2	2.39	0.56
1:C:50:ASN:ND2	3:C:503:HOH:O	2.27	0.56
1:A:64:LEU:HB2	1:A:119:TYR:HB3	1.89	0.55
1:A:29:TYR:HB2	1:A:374:ASN:HD22	1.72	0.54
1:C:256:TRP:CD1	1:C:309:TYR:HH	2.26	0.53
1:C:4:PRO:HA	1:C:9:GLN:HE21	1.74	0.52
1:C:5:THR:H	1:C:9:GLN:NE2	2.06	0.52
1:C:45:GLN:HG2	1:C:48:TRP:CH2	2.46	0.52
1:C:107:GLY:HA3	1:C:119:TYR:CE1	2.45	0.51
1:A:61[B]:MET:HE2	1:A:121:GLY:HA2	1.92	0.51
1:A:287:ALA:N	1:A:374:ASN:OD1	2.41	0.50
1:A:147:ARG:NH2	3:A:607:HOH:O	2.34	0.50
1:C:24:SER:HB3	1:C:287:ALA:HB2	1.94	0.50
1:A:30:VAL:HB	1:A:150:SER:HB2	1.94	0.49
1:C:363:LYS:HB2	1:C:438:HIS:CD2	2.48	0.49
1:B:264:ILE:HA	1:B:270:LEU:HD13	1.95	0.48
1:A:60:HIS:CD2	1:A:61[A]:MET:HE2	2.47	0.48
1:A:251:THR:HA	1:A:254:SER:HB2	1.95	0.48
1:A:31:TYR:HA	3:A:601:HOH:O	2.14	0.48
1:A:112:LEU:HD11	1:A:118:VAL:HG23	1.96	0.47
1:C:98:THR:HG21	1:C:263:ALA:O	2.15	0.47
1:A:348:LYS:NZ	1:A:362:TYR:OH	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:PRO:HB3	1:C:150:SER:HA	1.97	0.47
1:A:369:LEU:HD11	1:A:393:PHE:CE2	2.49	0.46
1:A:296:ASN:HB3	3:A:604:HOH:O	2.15	0.46
1:C:79:MET:HB3	1:C:94:TYR:CE1	2.51	0.46
1:C:338:THR:OG1	1:C:448:SER:HB2	2.15	0.46
1:C:257:ILE:HD13	1:C:392:MET:HE3	1.98	0.46
1:B:318:ASP:OD2	3:B:603:HOH:O	2.21	0.45
1:B:362:TYR:CZ	1:B:439:LYS:HE3	2.51	0.45
1:A:28:ALA:O	1:A:30:VAL:HG23	2.17	0.45
1:C:333:GLN:O	1:C:411:HIS:HB3	2.17	0.44
1:C:256:TRP:CH2	1:C:258:PRO:HB3	2.53	0.44
1:C:108:ILE:HD12	1:C:189:PHE:CE2	2.52	0.44
1:C:110:PHE:CE2	1:C:204:LEU:HD22	2.53	0.43
1:B:153:MET:CE	1:C:35:ALA:H	2.30	0.43
1:C:108:ILE:HD12	1:C:189:PHE:HE2	1.84	0.43
1:A:151:ARG:NH2	3:A:605:HOH:O	2.15	0.43
1:C:119:TYR:OH	1:C:125:ALA:HB3	2.19	0.42
1:C:53:VAL:HB	1:C:242:VAL:HG23	2.00	0.42
1:C:62:VAL:HG22	1:C:147:ARG:H	1.84	0.42
1:C:291:SER:HB2	1:C:422:LEU:HD23	2.02	0.42
1:C:341:TRP:HB2	1:C:403:ALA:HB3	2.02	0.42
1:A:45:GLN:HG2	1:A:48:TRP:CH2	2.55	0.42
1:B:52:ALA:O	1:B:239:LEU:HA	2.19	0.42
1:B:54:LEU:HD13	1:B:230:ILE:HG21	2.02	0.42
1:A:362:TYR:CE1	1:A:439:LYS:HE3	2.55	0.41
1:B:183:LEU:HD12	1:B:183:LEU:HA	1.92	0.41
1:B:381:LEU:HA	1:B:386:ASN:O	2.21	0.41
1:C:413:ILE:HA	1:C:414:PRO:HD3	1.89	0.41
1:A:149:PRO:HG2	1:A:152:PRO:HB3	2.01	0.41
1:B:64:LEU:HB2	1:B:119:TYR:HB3	2.02	0.41
1:C:96:PRO:HD2	1:C:105:GLY:O	2.20	0.41
1:A:264:ILE:HA	1:A:270:LEU:HD13	2.03	0.41
1:C:54:LEU:HD11	1:C:164:PHE:HB3	2.01	0.41
1:C:339:LEU:CD2	1:C:407:ALA:HB3	2.51	0.40
1:A:252:LEU:HD11	1:A:395:GLY:HA3	2.03	0.40
1:C:32:PRO:HB2	1:C:33:VAL:HG23	2.03	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	Interatomic distance (Å)	Clash overlap (Å)
3:A:657:HOH:O	3:A:657:HOH:O[2_555]	2.06	0.14

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	450/474 (95%)	439 (98%)	10 (2%)	1 (0%)	43	36
1	B	447/474 (94%)	435 (97%)	12 (3%)	0	100	100
1	C	445/474 (94%)	435 (98%)	10 (2%)	0	100	100
All	All	1342/1422 (94%)	1309 (98%)	32 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	PRO

5.3.2 Protein sidechains [i](#)

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	361/382 (94%)	360 (100%)	1 (0%)	86	88
1	B	356/382 (93%)	356 (100%)	0	100	100
1	C	311/382 (81%)	311 (100%)	0	100	100
All	All	1028/1146 (90%)	1027 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	386	ASN
1	B	250	ASN
1	C	9	GLN
1	C	50	ASN
1	C	81	ASN
1	C	102	HIS
1	C	250	ASN
1	C	411	HIS

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 ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	501	-	3,3,3	0.57	0	2,2,2	0.24	0
2	EDO	B	502	-	3,3,3	0.43	0	2,2,2	0.53	0
2	EDO	A	502	-	3,3,3	0.40	0	2,2,2	0.81	0
2	EDO	B	501	-	3,3,3	0.45	0	2,2,2	0.30	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	A	501	-	-	0/1/1/1	-
2	EDO	B	502	-	-	0/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	B	501	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	452/474 (95%)	-0.05	21 (4%)	37 40	9, 21, 36, 54	2 (0%)
1	B	450/474 (94%)	0.26	25 (5%)	30 32	10, 26, 41, 60	1 (0%)
1	C	448/474 (94%)	1.75	176 (39%)	1 0	16, 42, 60, 77	1 (0%)
All	All	1350/1422 (94%)	0.65	222 (16%)	4 4	9, 28, 55, 77	4 (0%)

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	ALA	6.4
1	A	3	ALA	5.2
1	C	30	VAL	5.1
1	A	150	SER	4.8
1	A	31	TYR	4.8
1	C	109	ILE	4.8
1	A	28	ALA	4.8
1	C	140	VAL	4.7
1	B	208	MET	4.6
1	A	29	TYR	4.5
1	A	27	GLY	4.3
1	C	327	ALA	4.1
1	C	118	VAL	4.1
1	C	66	ILE	4.0
1	C	31	TYR	4.0
1	A	455	THR	4.0
1	A	154	GLY	4.0
1	A	30	VAL	4.0
1	C	309	TYR	3.9
1	C	64	LEU	3.9
1	C	74	LEU	3.9
1	C	65	TYR	3.8
1	C	85	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	30	VAL	3.8
1	C	384	ALA	3.7
1	C	256	TRP	3.7
1	C	3	ALA	3.7
1	C	408	THR	3.7
1	B	454	VAL	3.6
1	A	153	MET	3.6
1	C	313	VAL	3.6
1	C	29	TYR	3.5
1	C	131	TYR	3.5
1	C	155	LYS	3.5
1	C	133	ALA	3.5
1	C	86	TRP	3.5
1	C	112	LEU	3.5
1	C	318	ASP	3.5
1	C	150	SER	3.4
1	C	311	PRO	3.4
1	C	138	TYR	3.4
1	C	128	TRP	3.4
1	C	103	VAL	3.4
1	C	113	ALA	3.4
1	C	27	GLY	3.4
1	C	139	ASN	3.4
1	C	454	VAL	3.3
1	A	456	ALA	3.3
1	C	325	LEU	3.3
1	C	319	PHE	3.3
1	C	71	ALA	3.3
1	C	445	ALA	3.3
1	C	450	VAL	3.3
1	C	182	THR	3.3
1	C	72	LEU	3.2
1	C	312	PHE	3.2
1	C	126	ALA	3.2
1	C	134	GLN	3.2
1	C	143	VAL	3.2
1	C	137	GLY	3.2
1	C	142	ILE	3.1
1	C	157	VAL	3.1
1	C	292	PHE	3.1
1	C	78	THR	3.1
1	C	152	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	156	PRO	3.1
1	C	206	HIS	3.1
1	C	315	PHE	3.1
1	C	407	ALA	3.1
1	C	26	ILE	3.0
1	A	158	GLN	3.0
1	A	454	VAL	3.0
1	C	188	PHE	3.0
1	C	114	GLU	3.0
1	C	149	PRO	3.0
1	C	307	ILE	3.0
1	C	328	ILE	3.0
1	C	277	LEU	3.0
1	C	84	LYS	3.0
1	C	124	PRO	2.9
1	A	383	ALA	2.9
1	B	3	ALA	2.9
1	C	80	ILE	2.9
1	C	94	TYR	2.9
1	C	111	TYR	2.9
1	C	282	TYR	2.9
1	C	189	PHE	2.9
1	C	82	SER	2.9
1	A	157	VAL	2.8
1	B	153	MET	2.8
1	C	11	LEU	2.8
1	C	98	THR	2.8
1	C	279	ALA	2.8
1	C	383	ALA	2.8
1	C	83	PRO	2.8
1	C	330	PRO	2.8
1	C	332	THR	2.8
1	C	4	PRO	2.8
1	A	254	SER	2.7
1	C	91	ALA	2.7
1	C	97	VAL	2.7
1	C	427	ASN	2.7
1	C	116	GLU	2.7
1	C	107	GLY	2.7
1	C	110	PHE	2.7
1	C	117	PHE	2.7
1	C	264	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	320	ILE	2.7
1	C	87	GLU	2.7
1	C	95	VAL	2.7
1	C	272	ALA	2.7
1	C	100	TYR	2.7
1	C	212	PRO	2.7
1	C	413	ILE	2.7
1	C	68	GLY	2.6
1	C	122	ARG	2.6
1	C	5	THR	2.6
1	A	152	PRO	2.6
1	B	155	LYS	2.6
1	C	73	LYS	2.6
1	B	195	ASN	2.6
1	C	75	LEU	2.6
1	C	104	ILE	2.6
1	B	154	GLY	2.6
1	C	120	VAL	2.6
1	B	358	ALA	2.6
1	C	273	TYR	2.6
1	C	276	TRP	2.6
1	C	265	TYR	2.6
1	C	186	LEU	2.6
1	C	136	GLY	2.6
1	C	129	LEU	2.5
1	C	300	TYR	2.5
1	C	69	LYS	2.5
1	C	442	ALA	2.5
1	C	10	VAL	2.5
1	C	135	THR	2.5
1	C	337	VAL	2.5
1	B	152	PRO	2.5
1	C	141	ASP	2.5
1	C	268	ASP	2.5
1	C	67	ARG	2.5
1	C	211	ALA	2.5
1	C	304	PRO	2.5
1	A	384	ALA	2.4
1	C	262	PRO	2.4
1	B	31	TYR	2.4
1	C	409	ILE	2.4
1	C	331	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	415	VAL	2.4
1	C	153	MET	2.4
1	A	151	ARG	2.4
1	C	108	ILE	2.4
1	C	125	ALA	2.4
1	B	156	PRO	2.4
1	C	62	VAL	2.4
1	C	267	GLY	2.4
1	C	281	SER	2.4
1	B	206	HIS	2.3
1	C	303	ASN	2.3
1	B	28	ALA	2.3
1	C	310	GLY	2.3
1	B	453	SER	2.3
1	C	147	ARG	2.3
1	C	446	VAL	2.3
1	C	316	ASP	2.3
1	B	157	VAL	2.3
1	C	132	HIS	2.3
1	C	317	HIS	2.3
1	C	204	LEU	2.3
1	C	261	LEU	2.3
1	B	46	TRP	2.2
1	B	207	GLY	2.2
1	C	449	PRO	2.2
1	C	70	ASP	2.2
1	C	190	ASN	2.2
1	C	252	LEU	2.2
1	C	101	GLY	2.2
1	C	451	PRO	2.2
1	C	351	ALA	2.2
1	C	305	TYR	2.2
1	C	288	ILE	2.2
1	C	18	VAL	2.2
1	C	145	ASP	2.2
1	C	286	GLY	2.2
1	C	88	PRO	2.2
1	C	12	ALA	2.2
1	C	171	ALA	2.2
1	C	324	ALA	2.2
1	B	67	ARG	2.2
1	C	392	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	353	LEU	2.2
1	C	14	GLY	2.2
1	B	32	PRO	2.2
1	C	263	ALA	2.2
1	C	92	LYS	2.2
1	C	119	TYR	2.1
1	C	326	GLU	2.1
1	C	285	SER	2.1
1	C	154	GLY	2.1
1	C	321	GLY	2.1
1	C	144	HIS	2.1
1	C	376	ASN	2.1
1	C	349	ILE	2.1
1	C	96	PRO	2.1
1	C	13	ALA	2.1
1	C	158	GLN	2.1
1	B	359	ASP	2.1
1	A	147	ARG	2.1
1	C	151	ARG	2.1
1	A	453	SER	2.0
1	C	254	SER	2.0
1	C	259	SER	2.0
1	C	453	SER	2.0
1	B	356	THR	2.0
1	B	197	ALA	2.0
1	C	323	ASP	2.0
1	B	236	GLU	2.0
1	C	308	GLY	2.0
1	C	417	THR	2.0
1	C	99	PRO	2.0
1	C	293	VAL	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	A	502	4/4	0.84	0.14	28,31,32,33	0
2	EDO	B	502	4/4	0.94	0.10	24,26,34,39	0
2	EDO	B	501	4/4	0.98	0.08	20,21,22,23	0
2	EDO	A	501	4/4	0.98	0.06	16,18,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.