



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:49 AM UTC

PDB ID : 5X1K / pdb_00005x1k
Title : Vanillate/3-O-methylgallate O-demethylase, LigM, 3-O-methylgallate complex form
Authors : Harada, A.; Senda, T.
Deposited on : 2017-01-26
Resolution : 2.15 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

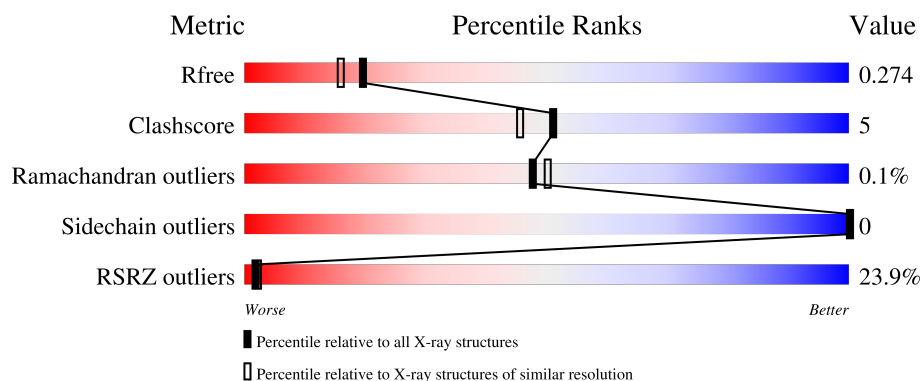
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	8% 90% 7% .
1	B	474	8% 85% 9% 5%
1	C	474	58% 74% 16% 9%

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
3	TRS	B	502	-	X	-	-
4	PEG	A	503	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10426 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.

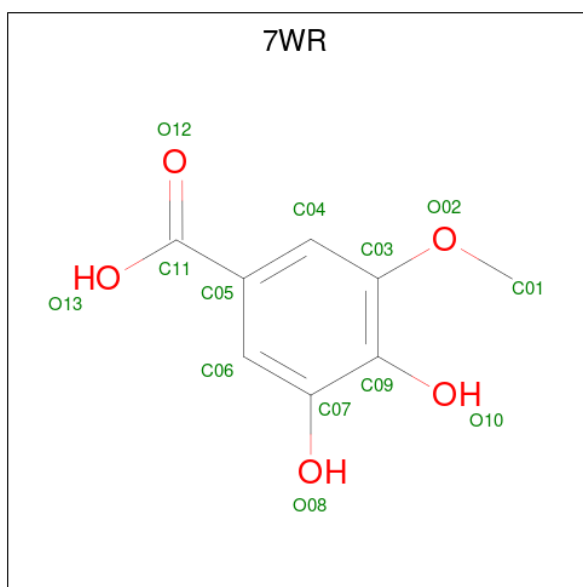
- Molecule 1 is a protein called Vanillate/3-O-methylgallate O-demethylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	457	Total	C	N	O	S	0	1	0
			3580	2291	608	668	13			
1	B	448	Total	C	N	O	S	0	1	0
			3478	2229	588	649	12			
1	C	430	Total	C	N	O	S	0	0	0
			3041	1922	532	576	11			

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 3-methoxy-4,5-bis(oxidanyl)benzoic acid (CCD ID: 7WR) (formula: C₈H₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



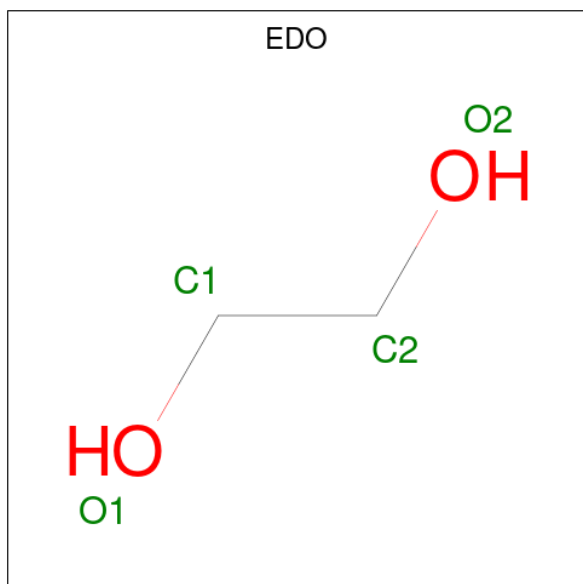
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

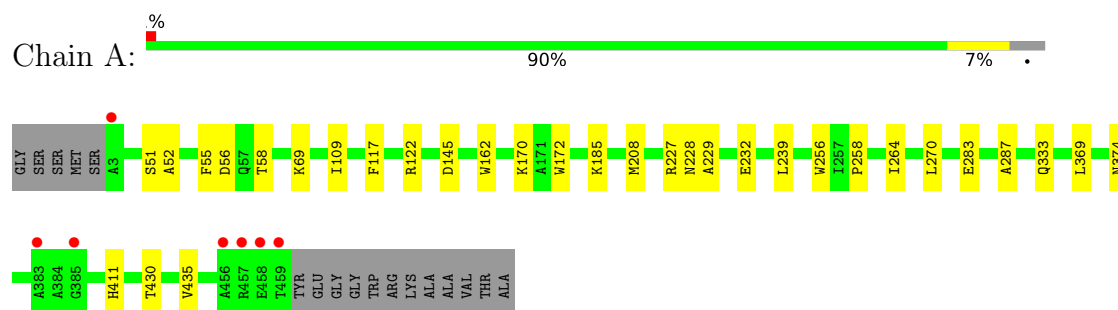
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	160	Total O 160 160	0	0
6	B	80	Total O 80 80	0	0
6	C	9	Total O 9 9	0	0

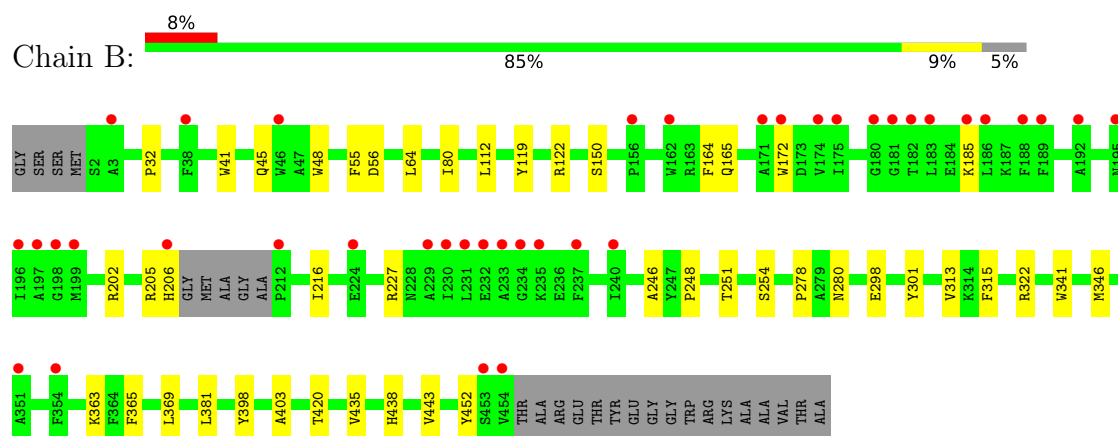
3 Residue-property plots [i](#)

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.

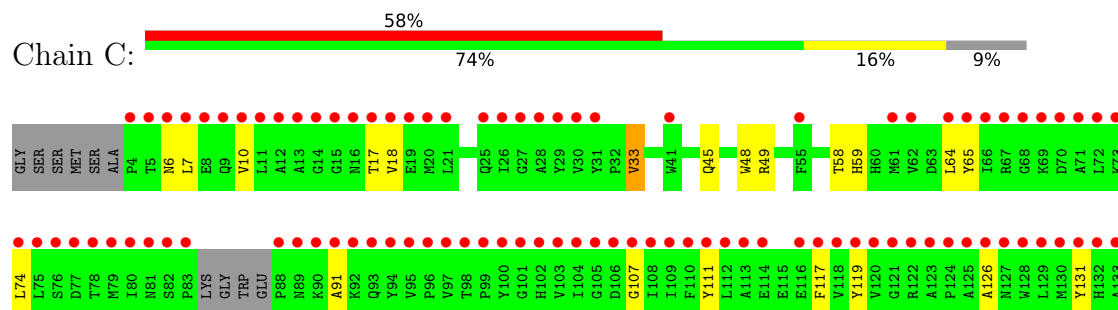
- Molecule 1: Vanillate/3-O-methylgallate O-demethylase

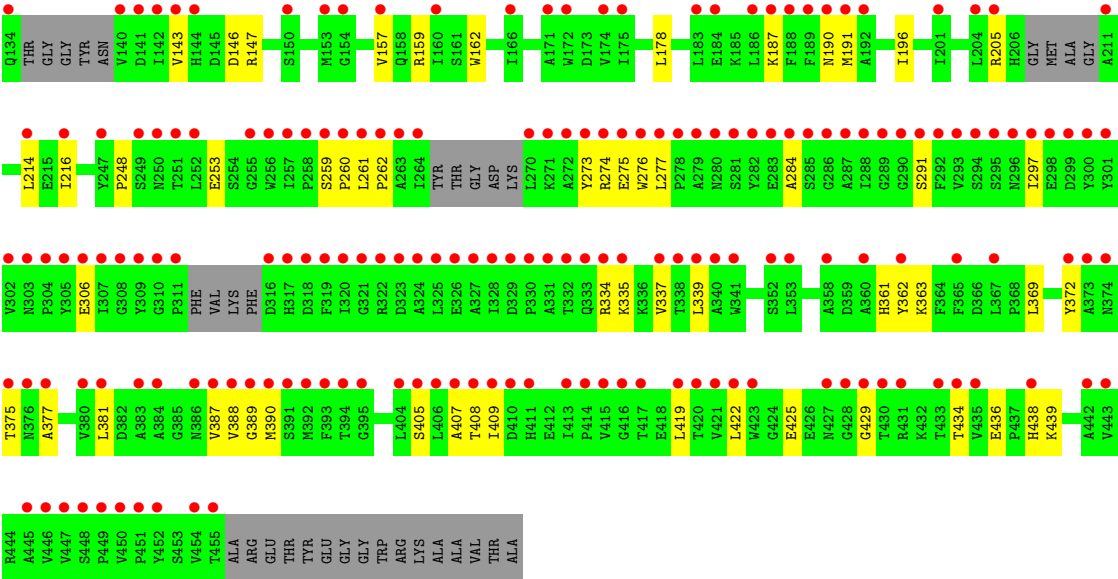


- Molecule 1: Vanillate/3-O-methylgallate O-demethylase



- 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	104.06Å 118.07Å 132.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.82 – 2.15 44.82 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.82-2.15) 90.2 (44.82-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.233 , 0.274 0.234 , 0.274	Depositor DCC
R_{free} test set	4524 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10426	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 7WR, TRS, PEG

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	0.39	0/3685	0.59	0/5023
1	B	0.32	0/3582	0.54	0/4890
1	C	0.26	0/3118	0.48	0/4265
All	All	0.33	0/10385	0.54	0/14178

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

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	3580	0	3447	24	0
1	B	3478	0	3294	26	0
1	C	3041	0	2571	52	0
2	A	13	0	0	1	0
2	B	13	0	0	1	0
2	C	13	0	0	0	0
3	A	8	0	12	2	0
3	B	8	0	12	1	0
4	A	7	0	10	4	0
5	A	12	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	6	0	0
6	A	160	0	0	1	0
6	B	80	0	0	1	0
6	C	9	0	0	2	0
All	All	10426	0	9370	101	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 5.

All (101) 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:C:143:VAL:O	6:C:601:HOH:O	1.84	0.95
1:A:56:ASP:OD2	1:A:227[B]:ARG:NH2	2.16	0.79
1:B:435:VAL:O	3:B:502:TRS:O2	2.01	0.77
1:C:389:GLY:HA3	1:C:409:ILE:HG22	1.68	0.75
1:A:55:PHE:HE2	1:A:208:MET:HE1	1.56	0.69
1:C:18:VAL:HG23	1:C:297:ILE:HG12	1.74	0.69
1:A:69:LYS:O	6:A:601:HOH:O	2.12	0.67
1:C:65:TYR:N	6:C:601:HOH:O	2.10	0.65
1:A:435:VAL:O	3:A:502:TRS:H31	1.98	0.63
1:C:119:TYR:HE2	1:C:126:ALA:HB2	1.64	0.63
1:C:17:THR:CB	1:C:297:ILE:HD11	2.31	0.60
1:C:162:TRP:HZ3	1:C:216:ILE:HG13	1.67	0.59
1:B:64:LEU:HB2	1:B:119:TYR:HB3	1.84	0.59
1:C:363:LYS:HB2	1:C:438:HIS:CD2	2.38	0.58
1:C:91:ALA:HB2	1:C:191:MET:HE2	1.84	0.58
1:C:363:LYS:NZ	1:C:436:GLU:OE1	2.34	0.58
1:C:372:TYR:O	1:C:434:THR:HG21	2.04	0.58
1:B:452:TYR:O	6:B:601:HOH:O	2.17	0.58
1:C:377:ALA:HB1	1:C:390:MET:HE2	1.86	0.58
1:A:232:GLU:OE1	4:A:503:PEG:O4	2.22	0.56
1:B:381:LEU:HB2	1:B:420:THR:HG23	1.88	0.56
1:A:172:TRP:CD1	1:A:185:LYS:HZ1	2.24	0.55
1:A:430:THR:O	3:A:502:TRS:H32	2.05	0.55
1:A:287:ALA:H	1:A:374:ASN:HD21	1.55	0.55
1:C:111:TYR:HA	1:C:117:PHE:CD1	2.42	0.55
1:B:122:ARG:HD2	2:B:501:7WR:O13	2.06	0.54
1:C:33:VAL:HG11	1:C:59:HIS:CE1	2.44	0.53
1:C:107:GLY:HA3	1:C:119:TYR:HE1	1.75	0.52
1:B:45:GLN:HG2	1:B:48:TRP:CH2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:HD12	1:C:262:PRO:HD2	1.92	0.51
1:A:122:ARG:HD2	2:A:501:7WR:O13	2.11	0.51
1:B:205:ARG:NH1	1:B:206:HIS:O	2.44	0.51
1:B:398:TYR:OH	1:C:361:HIS:NE2	2.30	0.50
1:C:58:THR:O	1:C:159:ARG:NH2	2.44	0.50
1:C:7:LEU:O	1:C:10:VAL:HG12	2.12	0.50
1:C:291:SER:HB2	1:C:422:LEU:HD23	1.92	0.50
1:C:45:GLN:HG2	1:C:48:TRP:CH2	2.47	0.50
1:C:306:GLU:HA	1:C:334:ARG:O	2.12	0.49
1:C:64:LEU:O	1:C:119:TYR:N	2.31	0.49
1:A:264:ILE:HA	1:A:270:LEU:HD13	1.94	0.48
1:B:341:TRP:HB2	1:B:403:ALA:HB3	1.95	0.48
1:A:55:PHE:CE2	1:A:208:MET:HE1	2.42	0.48
1:A:52:ALA:O	1:A:239:LEU:HA	2.14	0.47
1:C:58:THR:HG23	1:C:162:TRP:HA	1.96	0.47
1:C:107:GLY:HA3	1:C:119:TYR:CE1	2.49	0.47
1:A:229:ALA:HA	4:A:503:PEG:H21	1.97	0.47
1:B:298:GLU:HG2	1:B:301:TYR:CE2	2.49	0.47
1:C:7:LEU:HD13	1:C:284:ALA:HB2	1.96	0.47
1:C:362:TYR:CE1	1:C:439:LYS:HE3	2.50	0.47
1:C:131:TYR:HA	1:C:276:TRP:CZ3	2.51	0.46
1:A:51:SER:HA	1:A:170:LYS:HD2	1.98	0.46
1:B:248:PRO:HB2	1:B:369:LEU:HD22	1.96	0.46
1:C:33:VAL:HG21	1:C:157:VAL:HG11	1.97	0.46
1:B:341:TRP:CE3	1:B:443:VAL:HG11	2.51	0.46
1:C:273:TYR:O	1:C:277:LEU:HD13	2.15	0.46
1:C:248:PRO:HB2	1:C:369:LEU:HD22	1.97	0.46
1:C:388:VAL:HG11	1:C:419:LEU:HD11	1.97	0.46
1:B:164:PHE:HB2	1:B:216:ILE:HG13	1.98	0.46
1:C:178:LEU:HD13	1:C:196:ILE:HD12	1.98	0.45
1:B:56:ASP:OD2	1:B:227:ARG:NH2	2.49	0.45
1:C:187:LYS:O	1:C:190:ASN:HB2	2.16	0.45
1:C:335:LYS:O	1:C:408:THR:HA	2.16	0.45
1:B:32:PRO:HB3	1:B:150:SER:HA	1.98	0.45
1:B:55:PHE:HB2	1:B:165:GLN:HB2	1.98	0.45
1:C:111:TYR:N	1:C:191:MET:HE1	2.31	0.45
1:C:259:SER:N	1:C:260:PRO:HD3	2.32	0.45
1:B:278:PRO:HB2	1:B:280:ASN:OD1	2.17	0.44
1:C:74:LEU:HD12	1:C:74:LEU:O	2.17	0.44
1:C:131:TYR:HD1	1:C:276:TRP:CE3	2.36	0.44
1:B:363:LYS:HD3	1:B:438:HIS:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ASN:HD22	1:C:275:GLU:HA	1.83	0.43
1:C:205:ARG:HA	1:C:214:LEU:HD23	2.00	0.43
1:C:339:LEU:HB2	1:C:405:SER:OG	2.19	0.43
1:C:372:TYR:HB2	1:C:434:THR:OG1	2.19	0.42
1:C:261:LEU:HB2	1:C:375:THR:HG21	2.01	0.42
1:A:145:ASP:OD1	5:A:505:EDO:H11	2.19	0.42
1:C:111:TYR:HA	1:C:117:PHE:CE1	2.54	0.42
1:C:381:LEU:HD23	1:C:387:VAL:HA	2.02	0.42
1:B:45:GLN:HG2	1:B:48:TRP:CZ2	2.55	0.42
1:B:112:LEU:HD22	1:B:202:ARG:NH1	2.34	0.42
1:B:41:TRP:HB2	1:B:246:ALA:HB2	2.03	0.41
1:B:251:THR:HA	1:B:254:SER:OG	2.19	0.41
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.95	0.41
1:C:146:ASP:OD1	1:C:147:ARG:N	2.54	0.41
1:A:58:THR:HG23	1:A:162:TRP:HA	2.01	0.41
1:B:315:PHE:HB3	1:B:322:ARG:HH21	1.86	0.41
1:C:49:ARG:NH2	1:C:253:GLU:OE2	2.53	0.41
1:C:425:GLU:HB2	1:C:429:GLY:HA2	2.02	0.41
1:B:346:MET:HE1	1:B:365:PHE:CD2	2.55	0.41
1:C:7:LEU:HB3	1:C:274:ARG:O	2.21	0.41
1:C:337:VAL:N	1:C:407:ALA:O	2.48	0.41
1:A:256:TRP:CH2	1:A:258:PRO:HB3	2.56	0.41
1:A:228:ASN:HB3	4:A:503:PEG:O2	2.21	0.41
1:A:228:ASN:C	4:A:503:PEG:H21	2.47	0.40
1:A:333:GLN:O	1:A:411:HIS:HB3	2.20	0.40
1:A:283:GLU:OE1	1:A:283:GLU:N	2.44	0.40
1:B:172:TRP:CZ2	1:B:185:LYS:HG3	2.57	0.40
1:C:362:TYR:CZ	1:C:439:LYS:HE3	2.57	0.40
1:A:109:ILE:HD11	1:A:117:PHE:HB3	2.02	0.40
1:A:287:ALA:N	1:A:374:ASN:HD21	2.19	0.40
1:B:80:ILE:HD12	1:B:313:VAL:HG22	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/474 (96%)	444 (97%)	12 (3%)	0	100	100
1	B	445/474 (94%)	433 (97%)	12 (3%)	0	100	100
1	C	418/474 (88%)	398 (95%)	19 (4%)	1 (0%)	43	44
All	All	1319/1422 (93%)	1275 (97%)	43 (3%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	33	VAL

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	367/382 (96%)	367 (100%)	0	100	100
1	B	351/382 (92%)	351 (100%)	0	100	100
1	C	250/382 (65%)	250 (100%)	0	100	100
All	All	968/1146 (84%)	968 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	386	ASN
1	B	206	HIS
1	B	386	ASN
1	C	50	ASN
1	C	127	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
5	EDO	A	505	-	3,3,3	0.52	0	2,2,2	0.42	0
5	EDO	B	503	-	3,3,3	0.54	0	2,2,2	0.12	0
5	EDO	A	506	-	3,3,3	0.50	0	2,2,2	0.42	0
2	7WR	B	501	-	13,13,13	1.35	3 (23%)	18,18,18	1.55	3 (16%)
3	TRS	A	502	-	7,7,7	0.24	0	9,9,9	1.03	1 (11%)
2	7WR	A	501	-	13,13,13	1.42	2 (15%)	18,18,18	2.17	5 (27%)
3	TRS	B	502	-	7,7,7	0.37	0	9,9,9	1.28	2 (22%)
4	PEG	A	503	-	6,6,6	0.49	0	5,5,5	0.72	0
2	7WR	C	501	-	13,13,13	1.35	3 (23%)	18,18,18	1.67	2 (11%)
5	EDO	A	504	-	3,3,3	0.53	0	2,2,2	0.33	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
5	EDO	A	505	-	-	0/1/1/1	-
5	EDO	B	503	-	-	0/1/1/1	-
5	EDO	A	506	-	-	0/1/1/1	-
2	7WR	B	501	-	-	2/6/6/6	0/1/1/1
3	TRS	A	502	-	-	5/9/9/9	-
2	7WR	A	501	-	-	2/6/6/6	0/1/1/1
3	TRS	B	502	-	-	9/9/9/9	-
4	PEG	A	503	-	-	1/4/4/4	-
2	7WR	C	501	-	-	2/6/6/6	0/1/1/1
5	EDO	A	504	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	7WR	O02-C03	2.54	1.41	1.37
2	B	501	7WR	O02-C03	2.51	1.41	1.37
2	C	501	7WR	O02-C03	2.30	1.40	1.37
2	C	501	7WR	C05-C11	2.19	1.54	1.49
2	C	501	7WR	O08-C07	2.10	1.40	1.36
2	B	501	7WR	O10-C09	2.09	1.41	1.36
2	B	501	7WR	C05-C11	2.08	1.53	1.49
2	A	501	7WR	O08-C07	2.06	1.40	1.36

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	7WR	O02-C03-C09	6.65	121.49	114.53
2	C	501	7WR	O02-C03-C09	5.55	120.33	114.53
2	B	501	7WR	O02-C03-C09	5.14	119.90	114.53
2	A	501	7WR	C05-C06-C07	-2.91	117.55	120.09
3	A	502	TRS	C2-C-N	2.48	114.50	108.17
2	A	501	7WR	C04-C03-C09	-2.33	118.37	120.59
2	C	501	7WR	O02-C03-C04	-2.31	120.10	124.08
2	A	501	7WR	O02-C03-C04	-2.29	120.14	124.08
2	B	501	7WR	O13-C11-C05	2.21	120.52	114.84
3	B	502	TRS	O3-C3-C	-2.14	104.92	110.88
2	B	501	7WR	O02-C03-C04	-2.12	120.42	124.08
2	A	501	7WR	C04-C05-C11	-2.03	116.33	119.96
3	B	502	TRS	C3-C-C2	-2.03	105.26	110.66

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	7WR	C04-C03-O02-C01
2	A	501	7WR	C04-C03-O02-C01
2	C	501	7WR	C04-C03-O02-C01
2	B	501	7WR	C09-C03-O02-C01
3	B	502	TRS	C2-C-C1-O1
3	B	502	TRS	C2-C-C3-O3
2	A	501	7WR	C09-C03-O02-C01
2	C	501	7WR	C09-C03-O02-C01
4	A	503	PEG	C4-C3-O2-C2
3	B	502	TRS	N-C-C1-O1
3	B	502	TRS	C1-C-C2-O2
3	B	502	TRS	N-C-C2-O2
3	B	502	TRS	N-C-C3-O3
3	B	502	TRS	C1-C-C3-O3
3	A	502	TRS	C3-C-C2-O2
3	A	502	TRS	C2-C-C3-O3
3	B	502	TRS	C3-C-C1-O1
3	B	502	TRS	C3-C-C2-O2
3	A	502	TRS	C2-C-C1-O1
3	A	502	TRS	C1-C-C3-O3
3	A	502	TRS	N-C-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	EDO	1	0
2	B	501	7WR	1	0
3	A	502	TRS	2	0
2	A	501	7WR	1	0
3	B	502	TRS	1	0
4	A	503	PEG	4	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	457/474 (96%)	0.08	7 (1%) 72 76	10, 21, 35, 64	1 (0%)
1	B	448/474 (94%)	0.63	39 (8%) 16 17	11, 28, 49, 60	1 (0%)
1	C	430/474 (90%)	2.77	273 (63%) 0 0	27, 52, 73, 81	0
All	All	1335/1422 (93%)	1.13	319 (23%) 2 2	10, 30, 67, 81	2 (0%)

All (319) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	70	ASP	6.9
1	C	327	ALA	6.8
1	C	325	LEU	6.7
1	C	108	ILE	6.6
1	C	300	TYR	6.4
1	C	320	ILE	6.2
1	C	328	ILE	6.2
1	C	277	LEU	6.1
1	C	104	ILE	6.1
1	C	307	ILE	6.0
1	C	71	ALA	5.9
1	C	109	ILE	5.9
1	C	257	ILE	5.8
1	C	309	TYR	5.7
1	C	103	VAL	5.6
1	C	279	ALA	5.5
1	C	80	ILE	5.4
1	C	140	VAL	5.4
1	C	330	PRO	5.3
1	C	113	ALA	5.3
1	C	68	GLY	5.3
1	C	17	THR	5.2
1	C	293	VAL	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	66	ILE	5.2
1	C	132	HIS	5.2
1	C	131	TYR	5.1
1	C	304	PRO	5.1
1	C	118	VAL	5.1
1	C	83	PRO	5.0
1	C	273	TYR	5.0
1	C	324	ALA	5.0
1	C	331	ALA	4.9
1	C	455	THR	4.9
1	C	308	GLY	4.9
1	C	423	TRP	4.8
1	C	134	GLN	4.8
1	C	99	PRO	4.8
1	C	120	VAL	4.8
1	C	276	TRP	4.8
1	C	305	TYR	4.8
1	C	323	ASP	4.8
1	C	319	PHE	4.8
1	C	316	ASP	4.8
1	C	409	ILE	4.7
1	C	96	PRO	4.7
1	C	252	LEU	4.7
1	C	10	VAL	4.7
1	C	97	VAL	4.7
1	C	111	TYR	4.7
1	C	13	ALA	4.7
1	C	292	PHE	4.6
1	C	415	VAL	4.6
1	C	78	THR	4.6
1	C	81	ASN	4.6
1	C	31	TYR	4.6
1	C	7	LEU	4.6
1	C	318	ASP	4.6
1	C	98	THR	4.5
1	C	107	GLY	4.5
1	C	95	VAL	4.5
1	C	4	PRO	4.5
1	C	272	ALA	4.5
1	C	102	HIS	4.5
1	C	91	ALA	4.5
1	C	284	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	383	ALA	4.5
1	C	301	TYR	4.4
1	B	454	VAL	4.4
1	C	311	PRO	4.4
1	C	259	SER	4.4
1	C	264	ILE	4.4
1	C	189	PHE	4.4
1	C	62	VAL	4.4
1	C	11	LEU	4.4
1	C	321	GLY	4.4
1	C	101	GLY	4.3
1	C	332	THR	4.3
1	C	263	ALA	4.3
1	C	100	TYR	4.3
1	C	105	GLY	4.3
1	C	290	GLY	4.3
1	C	82	SER	4.3
1	C	126	ALA	4.3
1	C	407	ALA	4.3
1	C	14	GLY	4.3
1	C	282	TYR	4.3
1	C	450	VAL	4.2
1	C	416	GLY	4.2
1	C	124	PRO	4.2
1	B	186	LEU	4.2
1	C	74	LEU	4.2
1	C	413	ILE	4.2
1	C	79	MET	4.2
1	C	110	PHE	4.2
1	C	117	PHE	4.1
1	C	337	VAL	4.1
1	C	88	PRO	4.1
1	C	451	PRO	4.1
1	C	94	TYR	4.1
1	C	119	TYR	4.1
1	C	270	LEU	4.0
1	C	421	VAL	4.0
1	C	65	TYR	4.0
1	C	128	TRP	4.0
1	C	142	ILE	4.0
1	C	310	GLY	3.9
1	C	287	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	302	VAL	3.9
1	C	278	PRO	3.9
1	C	20	MET	3.9
1	C	26	ILE	3.9
1	C	141	ASP	3.9
1	C	12	ALA	3.9
1	C	76	SER	3.8
1	C	375	THR	3.8
1	C	125	ALA	3.8
1	C	75	LEU	3.8
1	C	275	GLU	3.8
1	C	335	LYS	3.8
1	C	288	ILE	3.8
1	C	16	ASN	3.8
1	C	388	VAL	3.8
1	C	256	TRP	3.7
1	C	338	THR	3.7
1	B	183	LEU	3.7
1	C	15	GLY	3.7
1	C	386	ASN	3.7
1	C	9	GLN	3.7
1	C	21	LEU	3.7
1	C	28	ALA	3.7
1	C	186	LEU	3.6
1	C	411	HIS	3.6
1	A	459	THR	3.6
1	C	262	PRO	3.6
1	C	374	ASN	3.6
1	C	121	GLY	3.6
1	C	143	VAL	3.6
1	C	390	MET	3.6
1	C	160	ILE	3.6
1	C	112	LEU	3.6
1	C	18	VAL	3.5
1	B	196	ILE	3.5
1	C	326	GLU	3.5
1	C	387	VAL	3.5
1	C	127	ASN	3.5
1	C	8	GLU	3.5
1	C	92	LYS	3.5
1	C	187	LYS	3.5
1	C	380	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	201	ILE	3.4
1	C	442	ALA	3.4
1	C	280	ASN	3.4
1	C	303	ASN	3.4
1	C	410	ASP	3.4
1	C	373	ALA	3.3
1	C	377	ALA	3.3
1	C	317	HIS	3.3
1	C	77	ASP	3.3
1	B	351	ALA	3.3
1	C	29	TYR	3.2
1	C	392	MET	3.2
1	C	408	THR	3.2
1	B	46	TRP	3.2
1	C	449	PRO	3.2
1	C	190	ASN	3.2
1	C	297	ILE	3.2
1	B	212	PRO	3.2
1	C	258	PRO	3.2
1	C	362	TYR	3.1
1	C	150	SER	3.1
1	C	420	THR	3.1
1	C	204	LEU	3.1
1	C	191	MET	3.1
1	C	428	GLY	3.1
1	A	456	ALA	3.1
1	C	447	VAL	3.1
1	C	454	VAL	3.1
1	B	453	SER	3.1
1	C	391	SER	3.1
1	C	89	ASN	3.0
1	C	372	TYR	3.0
1	C	214	LEU	3.0
1	C	422	LEU	3.0
1	C	27	GLY	3.0
1	C	417	THR	3.0
1	C	434	THR	3.0
1	C	188	PHE	3.0
1	C	133	ALA	3.0
1	C	211	ALA	3.0
1	C	129	LEU	3.0
1	B	175	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	232	GLU	2.9
1	C	73	LYS	2.9
1	B	182	THR	2.9
1	B	206	HIS	2.9
1	B	237	PHE	2.9
1	C	452	TYR	2.9
1	C	295	SER	2.9
1	C	90	LYS	2.9
1	C	69	LYS	2.9
1	C	431	ARG	2.9
1	C	340	ALA	2.9
1	C	72	LEU	2.8
1	C	393	PHE	2.8
1	B	192	ALA	2.8
1	C	283	GLU	2.8
1	B	189	PHE	2.8
1	A	458	GLU	2.8
1	C	261	LEU	2.8
1	C	381	LEU	2.8
1	C	446	VAL	2.8
1	C	291	SER	2.8
1	B	181	GLY	2.8
1	C	130	MET	2.7
1	C	114	GLU	2.7
1	C	406	LEU	2.7
1	C	260	PRO	2.7
1	C	25	GLN	2.7
1	B	354	PHE	2.7
1	C	394	THR	2.7
1	C	430	THR	2.7
1	C	294	SER	2.7
1	C	64	LEU	2.7
1	B	174	VAL	2.7
1	C	389	GLY	2.7
1	C	339	LEU	2.6
1	C	67	ARG	2.6
1	C	144	HIS	2.6
1	C	285	SER	2.6
1	C	205	ARG	2.6
1	C	30	VAL	2.6
1	B	229	ALA	2.6
1	C	192	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	188	PHE	2.6
1	C	405	SER	2.6
1	C	429	GLY	2.6
1	C	296	ASN	2.6
1	C	271	LYS	2.6
1	C	251	THR	2.6
1	C	298	GLU	2.5
1	C	286	GLY	2.5
1	A	3	ALA	2.5
1	B	171	ALA	2.5
1	C	414	PRO	2.5
1	C	93	GLN	2.5
1	C	353	LEU	2.5
1	B	180	GLY	2.5
1	C	174	VAL	2.5
1	C	19	GLU	2.5
1	C	395	GLY	2.5
1	B	240	ILE	2.5
1	C	6	ASN	2.5
1	C	116	GLU	2.5
1	C	123	ALA	2.5
1	C	404	LEU	2.5
1	C	322	ARG	2.5
1	C	166	ILE	2.5
1	C	435	VAL	2.4
1	C	61	MET	2.4
1	C	419	LEU	2.4
1	B	172	TRP	2.4
1	C	448	SER	2.4
1	C	274	ARG	2.4
1	C	172	TRP	2.4
1	C	122	ARG	2.4
1	C	334	ARG	2.4
1	C	306	GLU	2.3
1	C	333	GLN	2.3
1	C	41	TRP	2.3
1	B	195	ASN	2.3
1	C	154	GLY	2.3
1	C	329	ASP	2.3
1	C	433	THR	2.3
1	B	185	LYS	2.3
1	B	38	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	224	GLU	2.3
1	B	156	PRO	2.3
1	C	106	ASP	2.3
1	C	341	TRP	2.3
1	C	281	SER	2.2
1	B	235	LYS	2.2
1	C	299	ASP	2.2
1	B	3	ALA	2.2
1	C	255	GLY	2.2
1	C	358	ALA	2.2
1	C	384	ALA	2.2
1	A	457	ARG	2.2
1	C	376	ASN	2.2
1	C	153	MET	2.2
1	B	233	ALA	2.2
1	C	445	ALA	2.2
1	C	55	PHE	2.2
1	B	198	GLY	2.2
1	C	184	GLU	2.2
1	C	289	GLY	2.2
1	A	383	ALA	2.2
1	B	197	ALA	2.2
1	C	5	THR	2.2
1	C	175	ILE	2.1
1	C	443	VAL	2.1
1	C	360	ALA	2.1
1	C	352	SER	2.1
1	B	234	GLY	2.1
1	C	247	TYR	2.1
1	A	385	GLY	2.1
1	C	216	ILE	2.1
1	C	171	ALA	2.1
1	C	438	HIS	2.1
1	C	157	VAL	2.1
1	C	365	PHE	2.1
1	C	249	SER	2.1
1	B	199	MET	2.0
1	B	231	LEU	2.0
1	C	250	ASN	2.0
1	B	230	ILE	2.0
1	B	162	TRP	2.0
1	C	427	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	183	LEU	2.0
1	C	367	LEU	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(Å ²)	Q<0.9
2	7WR	C	501	13/13	0.80	0.15	44,49,58,59	0
3	TRS	B	502	8/8	0.81	0.16	33,36,39,40	0
3	TRS	A	502	8/8	0.83	0.12	14,24,29,31	0
4	PEG	A	503	7/7	0.87	0.17	22,25,29,33	0
5	EDO	A	505	4/4	0.87	0.12	27,30,32,37	0
2	7WR	B	501	13/13	0.89	0.10	22,27,35,35	0
5	EDO	A	506	4/4	0.94	0.09	16,21,23,25	0
5	EDO	B	503	4/4	0.95	0.08	21,21,22,22	0
2	7WR	A	501	13/13	0.96	0.07	14,17,22,23	0
5	EDO	A	504	4/4	0.97	0.06	18,18,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.