



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 03:44 am GMT

PDB ID : 4U2K  
Title : X-ray structure uridine phosphorylase from *Vibrio cholerae* in complex with anticancer compound at 2.13 Å resolution  
Authors : Prokofev, I.I.; Lashkov, A.A.; Gabdoulkhakov, A.G.; Betzel, C.; Mikhailov, A.M.  
Deposited on : 2014-07-17  
Resolution : 2.13 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

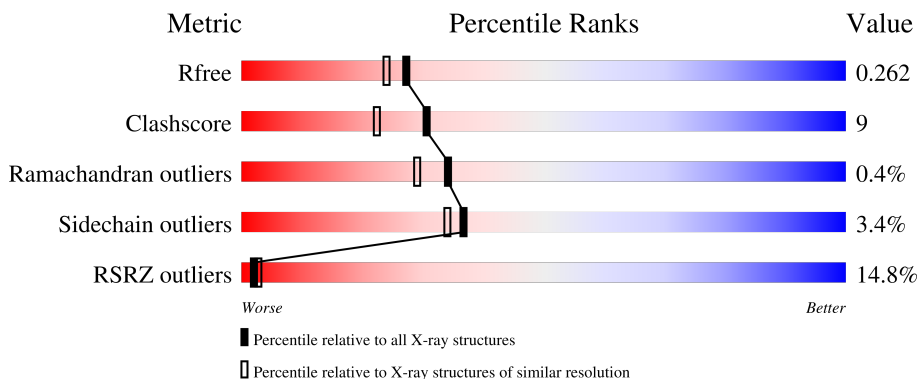
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.13 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))
$R_{free}$	130704	2523 (2.16-2.12)
Clashscore	141614	2653 (2.16-2.12)
Ramachandran outliers	138981	2618 (2.16-2.12)
Sidechain outliers	138945	2617 (2.16-2.12)
RSRZ outliers	127900	2485 (2.16-2.12)

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  $\geq 3$ , 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	253	
1	B	253	
1	C	253	
1	D	253	
1	E	253	

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Mol	Chain	Length	Quality of chain
1	F	253	

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
4	GOL	D	301	-	-	X	-
5	PEG	D	302	-	-	X	-
6	M5F	D	303[B]	-	X	-	-
6	M5F	F	302	-	X	-	-
7	TRS	F	301	-	-	-	X

## 2 Entry composition [i](#)

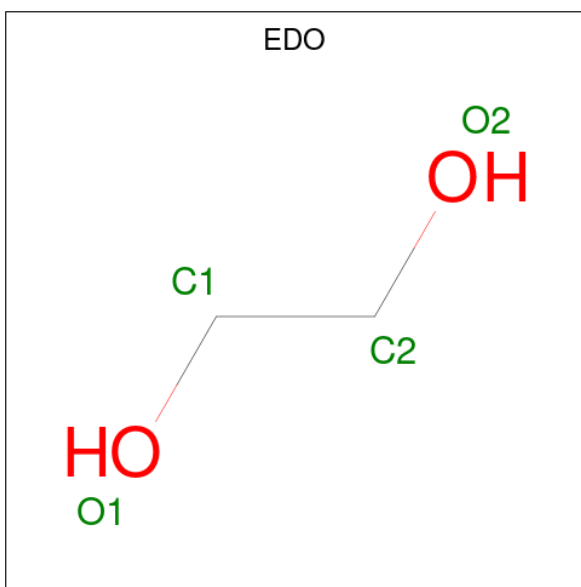
There are 8 unique types of molecules in this entry. The entry contains 11998 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Uridine phosphorylase.

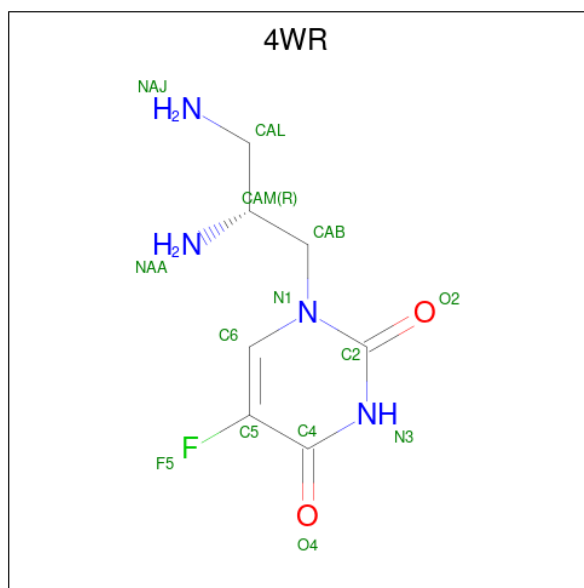
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	Total 1840	C 1154	N 321	O 352	S 13	0	2	0
1	B	245	Total 1848	C 1158	N 318	O 357	S 15	0	4	0
1	C	251	Total 1920	C 1204	N 336	O 366	S 14	0	6	0
1	D	242	Total 1866	C 1169	N 330	O 354	S 13	0	8	0
1	E	246	Total 1865	C 1170	N 328	O 353	S 14	0	4	0
1	F	251	Total 1918	C 1207	N 330	O 366	S 15	0	7	0

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

- Molecule 3 is 1-[(2R)-2,3-diaminopropyl]-5-fluoropyrimidine-2,4(1H,3H)-dione (three-letter code: 4WR) (formula: C<sub>7</sub>H<sub>11</sub>FN<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C F N O 14 7 1 4 2	0	0
3	D	1	Total C F N O 14 7 1 4 2	0	1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		

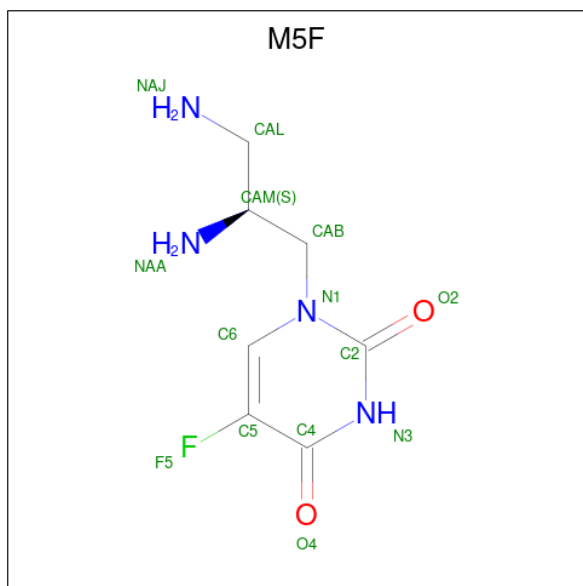
- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

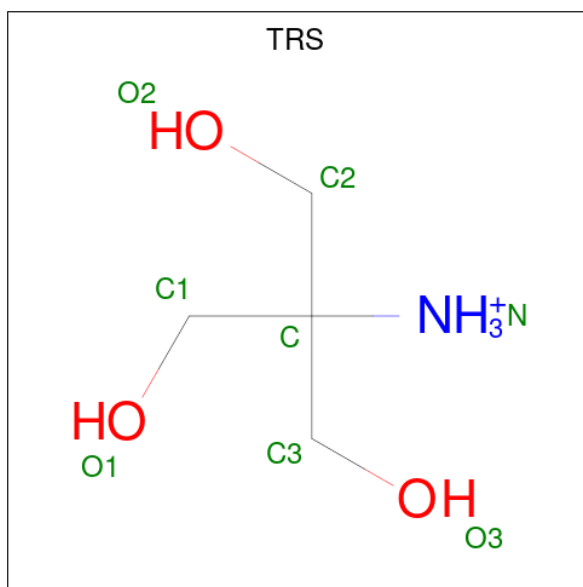
- Molecule 6 is 1-[(2S)-2,3-diaminopropyl]-5-fluoropyrimidine-2,4(1H,3H)-dione (three-letter

code: M5F) (formula: C<sub>7</sub>H<sub>11</sub>FN<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
6	D	1	14	7	1	4	2	0	1
6	F	1	14	7	1	4	2	0	0

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	F	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is water.

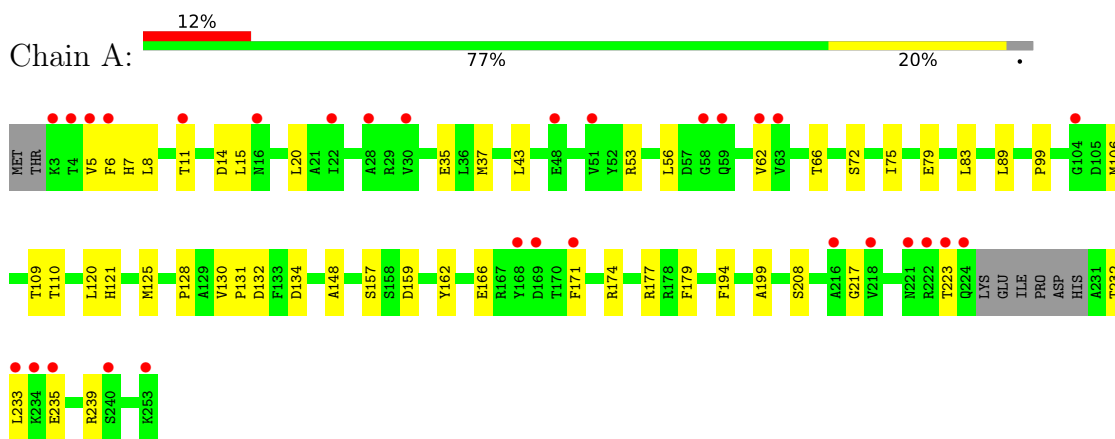
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	110	Total	O	0	8
			118	118		
8	B	86	Total	O	0	4
			90	90		
8	C	111	Total	O	0	6
			117	117		
8	D	85	Total	O	0	8
			93	93		
8	E	115	Total	O	0	6
			121	121		
8	F	85	Total	O	0	6
			91	91		



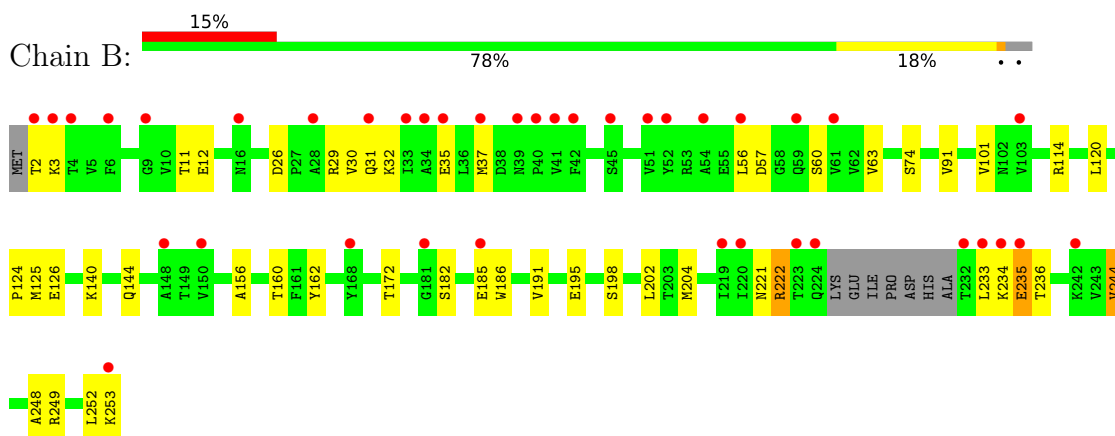
### 3 Residue-property plots [i](#)

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.

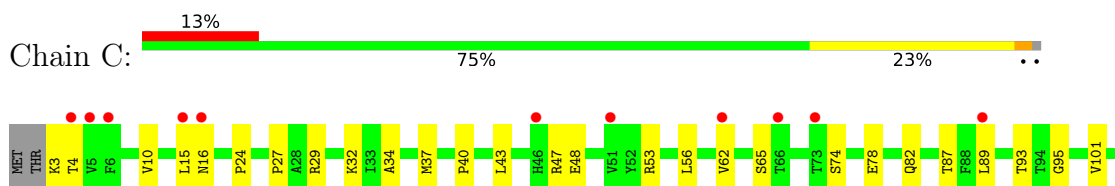
- Molecule 1: Uridine phosphorylase

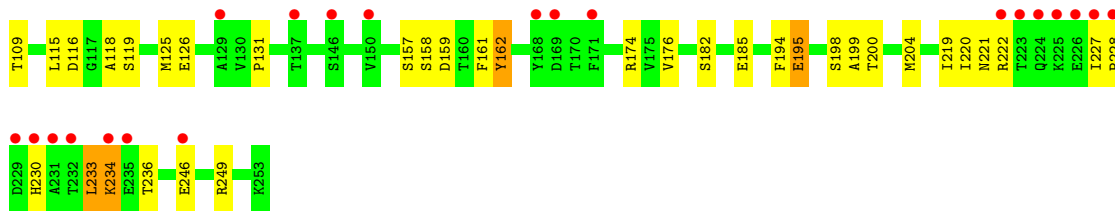


- Molecule 1: Uridine phosphorylase

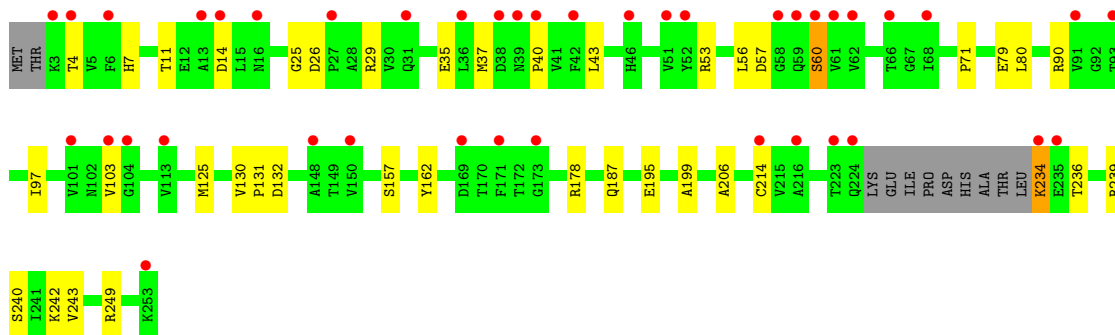
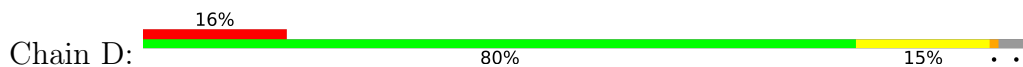


- Molecule 1: Uridine phosphorylase

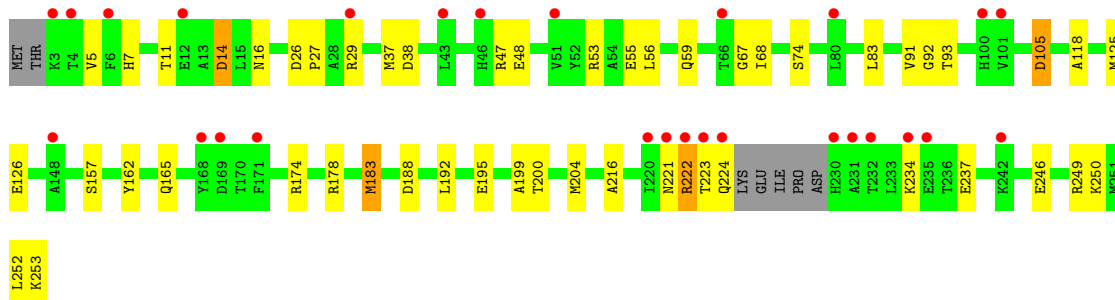
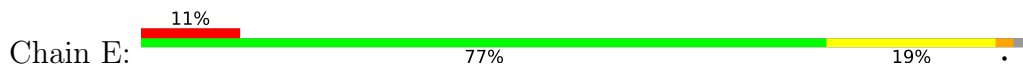




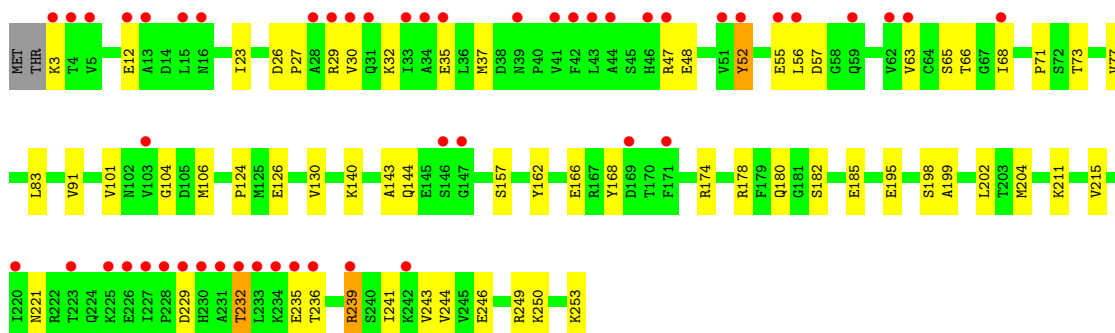
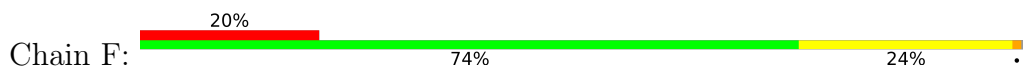
● Molecule 1: Uridine phosphorylase



● Molecule 1: Uridine phosphorylase



● Molecule 1: Uridine phosphorylase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.28Å 91.28Å 137.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.77 – 2.13 19.77 – 2.13	Depositor EDS
% Data completeness (in resolution range)	99.7 (19.77-2.13) 100.0 (19.77-2.13)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.81 (at 2.13Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.208 , 0.262 0.209 , 0.262	Depositor DCC
$R_{free}$ test set	2160 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.2	Xtrriage
Anisotropy	0.745	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11998	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.88 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.5209e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: TRS, PEG, EDO, GOL, M5F, 4WR

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	0.45	0/1874	0.61	0/2539
1	B	0.44	0/1888	0.59	0/2555
1	C	0.45	0/1969	0.58	0/2665
1	D	0.44	0/1916	0.59	0/2591
1	E	0.43	0/1906	0.61	0/2578
1	F	0.44	0/1971	0.62	0/2670
All	All	0.44	0/11524	0.60	0/15598

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	1840	0	1856	30	0
1	B	1848	0	1861	29	0
1	C	1920	0	1943	47	0
1	D	1866	0	1888	33	0
1	E	1865	0	1889	37	0
1	F	1918	0	1941	41	0
2	A	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	6	0	0
2	C	8	0	12	3	0
2	E	8	0	12	2	0
3	B	14	0	11	2	0
3	D	14	0	11	1	0
4	D	6	0	8	4	0
4	E	6	0	8	0	0
5	D	7	0	10	5	0
6	D	14	0	11	2	0
6	F	14	0	11	2	0
7	F	8	0	12	0	0
8	A	118	0	0	2	0
8	B	90	0	0	5	0
8	C	117	0	0	3	0
8	D	93	0	0	5	0
8	E	121	0	0	3	0
8	F	91	0	0	4	0
All	All	11998	0	11502	211	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 9.

All (211) 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:D:26:ASP:HB3	1:D:29[A]:ARG:HG2	1.63	0.80
1:C:174[B]:ARG:NH1	8:C:402:HOH:O	2.17	0.78
1:D:132:ASP:HB2	5:D:302:PEG:H41	1.66	0.77
1:C:29:ARG:HH11	1:C:32:LYS:HZ2	1.36	0.73
3:B:302:4WR:O4	8:B:401:HOH:O	2.06	0.73
1:C:15:LEU:HG	1:C:62:VAL:HG21	1.71	0.73
1:E:37:MET:HG2	1:E:56:LEU:HD13	1.71	0.72
1:E:47:ARG:HD3	1:F:68:ILE:HD11	1.74	0.70
1:F:180:GLN:NE2	8:F:401:HOH:O	2.24	0.69
1:C:37:MET:HG2	1:C:56:LEU:HD13	1.77	0.67
1:A:171:PHE:O	8:A:401:HOH:O	2.12	0.67
1:C:195:GLU:OE2	8:C:401:HOH:O	2.14	0.66
1:B:37:MET:HG2	1:B:56:LEU:HD13	1.79	0.65
1:F:3:LYS:HD3	1:F:12:GLU:HB2	1.79	0.65
1:F:3:LYS:HE2	1:F:83:LEU:HD23	1.78	0.65
1:D:29[B]:ARG:HA	1:D:29[B]:ARG:HH11	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:178:ARG:NH1	8:F:402[A]:HOH:O	2.29	0.64
1:B:12:GLU:OE2	8:B:402:HOH:O	2.15	0.64
1:C:246[A]:GLU:OE2	1:C:249:ARG:NH2	2.30	0.64
1:C:29:ARG:HD2	1:C:32:LYS:HZ2	1.62	0.64
8:B:468[B]:HOH:O	1:C:126[B]:GLU:OE2	2.13	0.64
1:B:26:ASP:HB3	1:B:29:ARG:HG2	1.78	0.64
1:F:29[B]:ARG:NH2	1:F:91:VAL:HG13	2.13	0.63
1:A:6:PHE:HD1	1:A:7:HIS:CE1	2.18	0.62
1:E:11:THR:OG1	1:E:14:ASP:OD1	2.16	0.62
1:D:60:SER:O	8:D:401:HOH:O	2.16	0.61
1:F:37:MET:HG2	1:F:56[B]:LEU:HD23	1.82	0.61
1:F:104:GLY:HA2	1:F:236:THR:HG21	1.83	0.61
1:C:78:GLU:OE2	1:C:82:GLN:NE2	2.26	0.60
1:C:194:PHE:HB2	1:C:222[B]:ARG:NH2	2.17	0.60
1:F:29[B]:ARG:HH22	1:F:91:VAL:HG13	1.67	0.59
1:D:132:ASP:CB	5:D:302:PEG:H41	2.31	0.59
1:F:232:THR:HA	1:F:235:GLU:HB3	1.84	0.59
1:C:115:LEU:HB2	1:C:158:SER:HA	1.84	0.59
1:A:174:ARG:NH1	8:A:405:HOH:O	2.34	0.59
1:B:222:ARG:HD3	8:B:401:HOH:O	2.03	0.59
1:D:37:MET:HG2	1:D:56:LEU:HD13	1.85	0.58
1:D:132:ASP:CA	5:D:302:PEG:H41	2.33	0.58
1:E:253:LYS:HA	1:E:253:LYS:NZ	2.19	0.58
6:F:302:M5F:H5	6:F:302:M5F:C6	2.34	0.58
1:A:106:MET:HE2	1:A:217:GLY:HA2	1.86	0.57
1:D:97:ILE:HD12	1:D:187:GLN:HG3	1.87	0.57
1:E:178:ARG:NH1	8:E:447[B]:HOH:O	2.38	0.57
1:F:157:SER:HB3	1:F:199:ALA:HB2	1.86	0.57
1:E:157:SER:HB3	1:E:199:ALA:HB2	1.87	0.57
1:C:47:ARG:HH22	4:D:301:GOL:H32	1.68	0.56
1:D:25:GLY:HA3	4:D:301:GOL:H12	1.88	0.56
1:E:216:ALA:HB2	2:E:303:EDO:H22	1.86	0.56
1:E:183:MET:HE1	1:E:222[B]:ARG:HG2	1.88	0.56
3:D:304[A]:4WR:H3	8:D:405:HOH:O	2.05	0.55
1:F:30:VAL:HG12	1:F:52[A]:TYR:HD2	1.71	0.54
6:D:303[B]:M5F:H5	6:D:303[B]:M5F:C6	2.38	0.54
1:E:14:ASP:O	1:E:53:ARG:HD3	2.08	0.54
1:A:5:VAL:HG11	1:A:8:LEU:HB2	1.89	0.54
1:D:35[B]:GLU:OE2	1:D:40:PRO:HG2	2.07	0.54
1:A:5:VAL:HG13	1:A:79:GLU:HB3	1.90	0.54
1:E:222[A]:ARG:NH1	8:E:407:HOH:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:SER:HB3	1:A:199:ALA:HB2	1.89	0.53
1:C:43:LEU:HD11	1:C:53:ARG:HB2	1.91	0.53
1:C:162:TYR:OH	1:D:79:GLU:OE2	2.24	0.53
1:A:148:ALA:HB2	1:A:239:ARG:HD3	1.91	0.53
1:A:11:THR:OG1	1:A:14:ASP:OD1	2.27	0.52
1:E:48:GLU:HG3	1:E:67:GLY:HA3	1.91	0.52
1:E:14:ASP:OD1	1:E:14:ASP:N	2.43	0.52
1:D:206:ALA:HA	5:D:302:PEG:H32	1.92	0.52
1:B:140:LYS:O	1:B:144:GLN:HG3	2.10	0.52
1:E:246:GLU:O	1:E:250:LYS:HG3	2.09	0.51
1:A:177:ARG:NH2	1:C:185:GLU:OE1	2.36	0.51
1:C:157:SER:OG	1:C:195:GLU:OE1	2.21	0.51
1:D:157:SER:HB3	1:D:199:ALA:HB2	1.92	0.51
1:F:26:ASP:HB3	1:F:29[A]:ARG:HG2	1.91	0.51
1:B:101:VAL:O	1:B:221:ASN:ND2	2.42	0.51
1:E:16:ASN:HB2	1:E:53:ARG:HD2	1.92	0.50
2:A:302:EDO:H12	1:B:120:LEU:HD22	1.93	0.50
1:C:74:SER:HA	1:C:204[B]:MET:SD	2.52	0.50
1:D:103:VAL:O	8:D:402:HOH:O	2.20	0.50
1:C:29:ARG:HD2	1:C:32:LYS:NZ	2.26	0.49
1:E:105:ASP:N	1:E:105:ASP:OD1	2.43	0.49
1:E:68:ILE:HD11	1:F:47:ARG:HD3	1.95	0.49
1:F:178:ARG:NH2	8:F:413:HOH:O	2.43	0.48
1:A:99:PRO:HD3	1:A:223:THR:HG21	1.95	0.48
1:E:5:VAL:HG13	1:E:83:LEU:HD21	1.94	0.48
1:F:91:VAL:HB	1:F:244:VAL:HG21	1.95	0.48
1:F:57:ASP:OD1	1:F:249:ARG:NH1	2.46	0.48
1:A:128:PRO:HB2	1:A:130[B]:VAL:HG23	1.95	0.48
1:F:101:VAL:O	1:F:221:ASN:ND2	2.41	0.48
1:B:120:LEU:HD21	1:B:125:MET:CE	2.43	0.48
1:B:2:THR:N	8:B:414:HOH:O	2.47	0.48
1:A:5:VAL:HG13	1:A:79:GLU:OE1	2.14	0.47
1:A:66:THR:O	1:A:72:SER:OG	2.19	0.47
1:A:120:LEU:HD21	1:A:125:MET:CE	2.44	0.47
1:F:106[A]:MET:HE1	1:F:243:VAL:HG21	1.95	0.47
1:A:121:HIS:ND1	1:B:160:THR:OG1	2.39	0.47
1:A:43:LEU:HD11	1:A:53:ARG:HB2	1.96	0.47
1:C:157:SER:HB3	1:C:199:ALA:HB2	1.96	0.47
1:F:198:SER:O	1:F:202:LEU:HG	2.15	0.47
1:B:29:ARG:CZ	1:B:32:LYS:HD2	2.44	0.47
1:C:161:PHE:CD1	2:C:301:EDO:H11	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ARG:HB3	1:D:214:CYS:HA	1.96	0.47
1:A:37:MET:HG2	1:A:56:LEU:HD13	1.97	0.47
1:A:110:THR:O	1:F:130:VAL:HG21	2.14	0.47
1:A:75:ILE:O	1:A:79:GLU:HG3	2.15	0.47
1:D:90:ARG:NH2	4:D:301:GOL:O1	2.48	0.46
1:F:140:LYS:O	1:F:144:GLN:HG3	2.15	0.46
1:D:234:LYS:HD3	1:D:236:THR:H	1.80	0.46
1:E:221:ASN:OD1	1:E:223:THR:N	2.35	0.46
1:E:252:LEU:O	1:E:253:LYS:HB2	2.15	0.46
1:F:73:THR:O	1:F:77:VAL:HG23	2.15	0.46
1:F:246:GLU:O	1:F:250:LYS:HG3	2.16	0.46
3:B:302:4WR:O2	3:B:302:4WR:H5	2.15	0.46
1:C:109:THR:O	1:C:131:PRO:HG3	2.16	0.46
1:A:15:LEU:HG	1:A:62:VAL:HG21	1.97	0.46
1:C:230:HIS:ND1	1:C:233:LEU:HD12	2.30	0.46
1:A:20:LEU:HD21	1:A:89:LEU:HD13	1.99	0.45
1:C:4:THR:OG1	1:C:10:VAL:N	2.49	0.45
1:E:7:HIS:NE2	6:F:302:M5F:NAJ	2.64	0.45
1:F:106[A]:MET:HE3	1:F:143:ALA:HB1	1.98	0.45
1:F:71:PRO:HD3	8:F:407:HOH:O	2.16	0.45
1:E:29[A]:ARG:NH2	1:E:92:GLY:HA2	2.32	0.45
1:B:57:ASP:CG	1:B:249:ARG:HE	2.20	0.45
1:C:101:VAL:O	1:C:221:ASN:ND2	2.49	0.45
1:C:118:ALA:HB3	1:C:200:THR:OG1	2.17	0.45
1:D:57:ASP:OD1	1:D:249:ARG:NH2	2.48	0.45
1:E:29[A]:ARG:NH2	1:E:91:VAL:HG13	2.32	0.45
1:C:29:ARG:NH1	1:C:32:LYS:HZ2	2.11	0.45
1:B:124:PRO:HB2	1:B:126:GLU:OE1	2.17	0.44
1:B:114:ARG:O	1:C:126[B]:GLU:HG2	2.17	0.44
1:C:29:ARG:HH11	1:C:32:LYS:NZ	2.11	0.44
1:C:219:ILE:O	1:C:228:PRO:HG2	2.18	0.44
1:A:5:VAL:HG21	1:A:83:LEU:HG	2.00	0.44
1:A:166:GLU:HG3	1:A:179:PHE:O	2.18	0.44
1:A:15:LEU:HG	1:A:62:VAL:CG2	2.47	0.44
1:B:3:LYS:O	1:B:11:THR:HG22	2.18	0.44
1:E:38:ASP:O	1:E:55:GLU:N	2.48	0.44
1:F:37:MET:HE3	1:F:37:MET:HB2	1.70	0.44
1:F:29[A]:ARG:NH2	1:F:241:ILE:HD13	2.33	0.44
1:A:208:SER:HB3	1:B:172:THR:HG21	2.00	0.43
1:B:126:GLU:HG3	1:C:125:MET:SD	2.58	0.43
1:F:3:LYS:HD3	1:F:12:GLU:CB	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:ASP:OD1	1:C:119:SER:OG	2.34	0.43
1:D:43:LEU:HD11	1:D:53[A]:ARG:HB2	2.00	0.43
1:E:93:THR:HG21	1:E:237:GLU:HG2	2.01	0.43
1:A:109:THR:O	1:A:131:PRO:HG3	2.17	0.43
1:C:174[B]:ARG:HD2	1:E:188:ASP:HB3	2.00	0.43
1:C:194:PHE:HB2	1:C:222[B]:ARG:HH22	1.81	0.43
1:B:235:GLU:H	1:B:235:GLU:HG2	1.46	0.43
1:F:124:PRO:HB2	1:F:126:GLU:OE1	2.19	0.43
1:E:74:SER:HA	1:E:204[B]:MET:HE1	2.00	0.43
1:C:236:THR:OG1	8:C:403:HOH:O	2.21	0.43
1:C:87:THR:HG22	1:C:89:LEU:CD1	2.49	0.43
1:C:233:LEU:HB3	1:C:234:LYS:NZ	2.34	0.43
1:B:198:SER:O	1:B:202:LEU:HG	2.19	0.43
1:C:234:LYS:H	1:C:234:LYS:HG2	1.51	0.43
1:B:182:SER:HA	1:B:185:GLU:OE1	2.19	0.43
1:C:16:ASN:O	1:C:16:ASN:ND2	2.51	0.43
1:D:130:VAL:HG23	1:D:131:PRO:HD2	2.00	0.42
6:D:303[B]:M5F:H2	8:D:405:HOH:O	2.19	0.42
1:C:27:PRO:HG3	1:C:48:GLU:O	2.19	0.42
1:C:182:SER:HA	1:C:185:GLU:OE1	2.19	0.42
1:E:26:ASP:HA	1:E:27:PRO:HD2	1.81	0.42
1:B:31:GLN:NE2	1:B:35:GLU:OE1	2.52	0.42
1:B:186:TRP:HB3	1:B:191:VAL:HG21	2.00	0.42
1:B:248:ALA:O	1:B:252:LEU:HG	2.20	0.42
1:C:24:PRO:O	1:C:65:SER:HA	2.20	0.42
1:F:91:VAL:HA	1:F:215:VAL:O	2.20	0.42
1:E:174:ARG:NH1	8:E:410:HOH:O	2.43	0.42
1:E:216:ALA:HB2	2:E:303:EDO:C2	2.49	0.42
1:B:233:LEU:HB3	1:B:236:THR:HG23	2.02	0.42
1:B:252:LEU:O	1:B:253:LYS:HB2	2.18	0.42
1:D:239:ARG:HE	1:D:239:ARG:HB3	1.69	0.42
1:E:59:GLN:HB2	1:E:252:LEU:HD13	2.00	0.42
1:F:30:VAL:HG13	1:F:63:VAL:HG12	2.00	0.42
1:D:239:ARG:O	1:D:243:VAL:HG23	2.20	0.42
1:F:26:ASP:HA	1:F:27:PRO:HD2	1.83	0.42
1:F:166:GLU:HG2	1:F:168:TYR:CE2	2.54	0.42
1:C:161:PHE:CE1	2:C:301:EDO:H11	2.54	0.42
1:C:34:ALA:HB1	1:C:40:PRO:HB3	2.02	0.41
1:D:80:LEU:HD23	1:D:80:LEU:HA	1.94	0.41
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.88	0.41
1:C:95:GLY:HA2	1:C:220:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:VAL:HB	1:B:244:VAL:HG21	2.03	0.41
1:E:118:ALA:HB3	1:E:200:THR:OG1	2.20	0.41
1:D:11:THR:O	1:D:14:ASP:HB2	2.21	0.41
1:D:57:ASP:OD2	1:D:249:ARG:NE	2.53	0.41
1:C:3:LYS:HB2	1:C:3:LYS:HE3	1.66	0.41
1:A:132:ASP:OD2	1:A:134:ASP:HB2	2.21	0.41
1:C:227:ILE:HA	1:C:228:PRO:HD3	1.90	0.41
1:D:178[B]:ARG:HH22	1:E:126:GLU:CD	2.24	0.41
1:F:211:LYS:HE3	1:F:211:LYS:HB3	1.83	0.41
1:F:229:ASP:OD1	1:F:229:ASP:N	2.54	0.41
1:E:192:LEU:HA	1:E:192:LEU:HD23	1.83	0.41
1:E:246:GLU:OE2	1:E:249:ARG:NH2	2.54	0.41
1:C:74:SER:HA	1:C:204[A]:MET:HE1	2.03	0.41
1:D:25:GLY:HA3	4:D:301:GOL:C1	2.50	0.41
1:D:71:PRO:HD3	8:D:418:HOH:O	2.21	0.41
1:D:234:LYS:CD	1:D:236:THR:H	2.34	0.41
1:D:43:LEU:HD11	1:D:53[B]:ARG:HB2	2.02	0.41
1:D:125:MET:HG3	1:E:125:MET:HG3	2.03	0.41
1:F:23:ILE:HB	1:F:66:THR:CG2	2.51	0.41
2:C:301:EDO:O1	1:D:7:HIS:NE2	2.34	0.40
1:F:30:VAL:HG21	1:F:65:SER:HB3	2.03	0.40
1:F:32:LYS:O	1:F:35[A]:GLU:HG2	2.20	0.40
1:A:128:PRO:HB2	1:A:130[B]:VAL:CG2	2.52	0.40
1:B:30:VAL:HG13	1:B:63:VAL:HG12	2.04	0.40
1:D:132:ASP:HA	5:D:302:PEG:H41	2.03	0.40
1:F:182:SER:HA	1:F:185:GLU:OE1	2.21	0.40
1:B:74:SER:HA	1:B:204[B]:MET:HE1	2.03	0.40
1:B:156:ALA:HB2	1:B:191:VAL:HG11	2.03	0.40
1:E:165:GLN:HB3	1:E:222[B]:ARG:HH12	1.86	0.40
1:F:236:THR:HA	1:F:239:ARG:HB3	2.02	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	243/253 (96%)	236 (97%)	6 (2%)	1 (0%)	34	29
1	B	245/253 (97%)	243 (99%)	1 (0%)	1 (0%)	34	29
1	C	255/253 (101%)	250 (98%)	4 (2%)	1 (0%)	34	29
1	D	246/253 (97%)	241 (98%)	4 (2%)	1 (0%)	34	29
1	E	246/253 (97%)	237 (96%)	8 (3%)	1 (0%)	34	29
1	F	256/253 (101%)	245 (96%)	10 (4%)	1 (0%)	34	29
All	All	1491/1518 (98%)	1452 (97%)	33 (2%)	6 (0%)	34	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	TYR
1	B	162	TYR
1	F	162	TYR
1	C	162	TYR
1	E	162	TYR
1	D	162	TYR

### 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	197/203 (97%)	191 (97%)	6 (3%)	41	39
1	B	200/203 (98%)	194 (97%)	6 (3%)	41	39
1	C	207/203 (102%)	200 (97%)	7 (3%)	37	34
1	D	201/203 (99%)	195 (97%)	6 (3%)	41	39
1	E	200/203 (98%)	193 (96%)	7 (4%)	36	33
1	F	208/203 (102%)	198 (95%)	10 (5%)	25	21
All	All	1213/1218 (100%)	1171 (96%)	42 (4%)	37	33

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	159	ASP
1	A	194	PHE
1	A	232	THR
1	A	233	LEU
1	A	235	GLU
1	B	60	SER
1	B	195	GLU
1	B	222	ARG
1	B	234	LYS
1	B	235	GLU
1	B	244	VAL
1	C	93	THR
1	C	159	ASP
1	C	176	VAL
1	C	195	GLU
1	C	198	SER
1	C	233	LEU
1	C	234	LYS
1	D	4	THR
1	D	60	SER
1	D	195	GLU
1	D	234	LYS
1	D	240	SER
1	D	242	LYS
1	E	14	ASP
1	E	105	ASP
1	E	183	MET
1	E	195	GLU
1	E	222[A]	ARG
1	E	222[B]	ARG
1	E	234	LYS
1	F	48	GLU
1	F	52[A]	TYR
1	F	52[B]	TYR
1	F	55	GLU
1	F	174	ARG
1	F	195	GLU
1	F	204	MET
1	F	232	THR
1	F	239	ARG
1	F	253	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

15 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
7	TRS	F	301	-	7,7,7	0.30	0	9,9,9	0.27	0
2	EDO	B	301	-	3,3,3	0.60	0	2,2,2	0.28	0
3	4WR	B	302	-	12,14,14	2.27	4 (33%)	15,19,19	3.63	9 (60%)
6	M5F	F	302	-	12,14,14	4.60	9 (75%)	15,19,19	3.65	8 (53%)
2	EDO	E	303	-	3,3,3	0.49	0	2,2,2	0.43	0
3	4WR	D	304[A]	-	12,14,14	2.03	2 (16%)	15,19,19	3.56	8 (53%)
4	GOL	E	301	-	5,5,5	0.36	0	5,5,5	0.47	0
2	EDO	A	301	-	3,3,3	0.48	0	2,2,2	0.25	0
4	GOL	D	301	-	5,5,5	0.40	0	5,5,5	0.49	0
2	EDO	C	302	-	3,3,3	0.46	0	2,2,2	0.31	0
2	EDO	E	302	-	3,3,3	0.42	0	2,2,2	0.43	0
6	M5F	D	303[B]	-	12,14,14	4.78	9 (75%)	15,19,19	3.47	8 (53%)
2	EDO	A	302	-	3,3,3	0.43	0	2,2,2	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	D	302	-	6,6,6	0.41	0	5,5,5	0.57	0
2	EDO	C	301	-	3,3,3	0.48	0	2,2,2	0.22	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
7	TRS	F	301	-	-	3/9/9/9	-
2	EDO	B	301	-	-	1/1/1/1	-
3	4WR	B	302	-	-	1/6/6/6	0/1/1/1
6	M5F	F	302	-	-	3/6/6/6	0/1/1/1
2	EDO	E	303	-	-	0/1/1/1	-
3	4WR	D	304[A]	-	-	2/6/6/6	0/1/1/1
4	GOL	E	301	-	-	2/4/4/4	-
2	EDO	A	301	-	-	1/1/1/1	-
4	GOL	D	301	-	-	4/4/4/4	-
2	EDO	C	302	-	-	1/1/1/1	-
2	EDO	E	302	-	-	1/1/1/1	-
6	M5F	D	303[B]	-	-	2/6/6/6	0/1/1/1
2	EDO	A	302	-	-	0/1/1/1	-
5	PEG	D	302	-	-	2/4/4/4	-
2	EDO	C	301	-	-	1/1/1/1	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	302	M5F	O4-C4	8.55	1.39	1.23
6	D	303[B]	M5F	C4-C5	-8.50	1.33	1.44
6	D	303[B]	M5F	O4-C4	7.94	1.38	1.23
6	F	302	M5F	C6-C5	7.59	1.44	1.33
6	D	303[B]	M5F	C6-C5	7.52	1.44	1.33
6	F	302	M5F	C4-C5	-7.27	1.35	1.44
3	B	302	4WR	O4-C4	5.05	1.33	1.23
3	D	304[A]	4WR	O4-C4	4.85	1.32	1.23
6	D	303[B]	M5F	F5-C5	-4.70	1.28	1.35
6	D	303[B]	M5F	C2-N3	-4.15	1.30	1.38
6	F	302	M5F	F5-C5	-4.08	1.29	1.35
6	F	302	M5F	C2-N3	-3.97	1.30	1.38
6	D	303[B]	M5F	O2-C2	3.92	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	303[B]	M5F	C6-N1	-3.69	1.30	1.37
3	D	304[A]	4WR	C2-N3	-3.63	1.31	1.38
6	F	302	M5F	C6-N1	-3.53	1.30	1.37
6	F	302	M5F	O2-C2	3.46	1.29	1.23
3	B	302	4WR	C2-N3	-3.46	1.31	1.38
6	F	302	M5F	CAB-N1	2.88	1.50	1.47
6	D	303[B]	M5F	CAB-N1	2.84	1.50	1.47
3	B	302	4WR	C4-C5	-2.60	1.41	1.44
3	B	302	4WR	C6-C5	2.47	1.36	1.33
6	F	302	M5F	CAL-NAJ	-2.06	1.39	1.48
6	D	303[B]	M5F	CAL-NAJ	-2.03	1.40	1.48

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	4WR	C5-C4-N3	7.44	119.88	112.56
6	D	303[B]	M5F	C5-C4-N3	6.61	119.06	112.56
3	D	304[A]	4WR	C5-C4-N3	6.60	119.06	112.56
6	F	302	M5F	N3-C2-N1	6.58	120.88	114.86
3	D	304[A]	4WR	N3-C2-N1	6.57	120.87	114.86
6	F	302	M5F	C5-C4-N3	6.45	118.90	112.56
3	B	302	4WR	O4-C4-C5	-6.29	120.05	125.72
6	D	303[B]	M5F	N3-C2-N1	6.26	120.59	114.86
6	D	303[B]	M5F	O4-C4-C5	-6.01	120.30	125.72
3	B	302	4WR	N3-C2-N1	5.46	119.86	114.86
6	F	302	M5F	O4-C4-C5	-5.23	121.00	125.72
3	D	304[A]	4WR	O4-C4-C5	-5.09	121.12	125.72
3	D	304[A]	4WR	C4-N3-C2	-5.01	120.86	127.35
6	F	302	M5F	C4-N3-C2	-4.87	121.05	127.35
6	F	302	M5F	O2-C2-N1	-4.69	118.73	122.85
6	D	303[B]	M5F	C4-N3-C2	-4.63	121.36	127.35
6	F	302	M5F	F5-C5-C4	4.55	120.61	116.40
3	D	304[A]	4WR	F5-C5-C4	4.36	120.44	116.40
3	B	302	4WR	C4-N3-C2	-4.17	121.95	127.35
3	B	302	4WR	C6-C5-C4	-3.98	118.89	122.60
3	B	302	4WR	CAB-N1-C6	3.50	122.43	119.93
3	B	302	4WR	F5-C5-C6	3.50	124.11	120.97
3	D	304[A]	4WR	O2-C2-N1	-3.49	119.79	122.85
3	D	304[A]	4WR	C6-C5-C4	-3.28	119.54	122.60
6	D	303[B]	M5F	F5-C5-C4	3.22	119.38	116.40
6	D	303[B]	M5F	O2-C2-N1	-3.20	120.04	122.85
6	F	302	M5F	C6-C5-C4	-3.06	119.74	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	303[B]	M5F	C6-C5-C4	-3.05	119.75	122.60
6	F	302	M5F	C5-C6-N1	-2.99	117.83	120.72
6	D	303[B]	M5F	C5-C6-N1	-2.51	118.29	120.72
3	B	302	4WR	C5-C6-N1	-2.46	118.34	120.72
3	D	304[A]	4WR	C5-C6-N1	-2.39	118.41	120.72
3	B	302	4WR	CAB-N1-C2	-2.03	116.46	118.53

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	4WR	NAJ-CAL-CAM-CAB
3	D	304[A]	4WR	NAJ-CAL-CAM-CAB
4	D	301	GOL	O1-C1-C2-C3
4	D	301	GOL	O2-C2-C3-O3
6	D	303[B]	M5F	N1-CAB-CAM-CAL
6	F	302	M5F	N1-CAB-CAM-CAL
7	F	301	TRS	C1-C-C3-O3
7	F	301	TRS	C2-C-C3-O3
7	F	301	TRS	N-C-C3-O3
6	F	302	M5F	NAJ-CAL-CAM-NAA
4	D	301	GOL	C1-C2-C3-O3
4	E	301	GOL	O1-C1-C2-C3
4	D	301	GOL	O1-C1-C2-O2
2	B	301	EDO	O1-C1-C2-O2
2	E	302	EDO	O1-C1-C2-O2
5	D	302	PEG	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
3	D	304[A]	4WR	NAJ-CAL-CAM-NAA
6	D	303[B]	M5F	N1-CAB-CAM-NAA
6	F	302	M5F	N1-CAB-CAM-NAA
2	C	301	EDO	O1-C1-C2-O2
5	D	302	PEG	C1-C2-O2-C3
2	C	302	EDO	O1-C1-C2-O2
4	E	301	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	4WR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	302	M5F	2	0
2	E	303	EDO	2	0
3	D	304[A]	4WR	1	0
4	D	301	GOL	4	0
6	D	303[B]	M5F	2	0
2	A	302	EDO	1	0
5	D	302	PEG	5	0
2	C	301	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	245/253 (96%)	0.89	30 (12%) 4 5	9, 20, 37, 55	0
1	B	245/253 (96%)	1.01	39 (15%) 1 2	10, 21, 39, 57	0
1	C	251/253 (99%)	1.06	32 (12%) 3 4	9, 19, 41, 72	0
1	D	242/253 (95%)	1.11	41 (16%) 1 1	11, 21, 39, 53	0
1	E	246/253 (97%)	0.87	27 (10%) 5 7	11, 20, 37, 57	0
1	F	251/253 (99%)	1.16	50 (19%) 1 1	10, 22, 44, 70	0
All	All	1480/1518 (97%)	1.02	219 (14%) 2 3	9, 20, 40, 72	0

All (219) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	228	PRO	12.6
1	B	232	THR	12.1
1	F	227	ILE	11.4
1	F	230	HIS	9.3
1	C	231	ALA	9.3
1	C	225	LYS	6.8
1	A	223	THR	6.4
1	D	253	LYS	6.1
1	E	231	ALA	6.0
1	E	230	HIS	5.9
1	C	230	HIS	5.9
1	F	233	LEU	5.6
1	E	220	ILE	5.5
1	F	52[A]	TYR	5.4
1	F	228	PRO	5.2
1	C	46	HIS	5.1
1	C	169	ASP	5.1
1	C	226	GLU	4.9
1	C	5	VAL	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	224	GLN	4.7
1	F	34	ALA	4.6
1	C	16	ASN	4.6
1	F	232	THR	4.5
1	F	229	ASP	4.5
1	D	51	VAL	4.4
1	D	6	PHE	4.4
1	A	3	LYS	4.3
1	F	231	ALA	4.3
1	B	223	THR	4.3
1	F	220	ILE	4.3
1	F	16	ASN	4.3
1	C	229	ASP	4.1
1	C	224	GLN	4.1
1	F	147	GLY	4.1
1	F	3	LYS	4.0
1	F	43	LEU	4.0
1	D	4	THR	4.0
1	B	59	GLN	3.9
1	A	4	THR	3.8
1	F	234	LYS	3.8
1	B	168	TYR	3.8
1	D	224	GLN	3.8
1	A	6	PHE	3.8
1	D	52	TYR	3.7
1	D	40	PRO	3.7
1	E	234	LYS	3.7
1	D	171	PHE	3.7
1	A	5	VAL	3.7
1	F	12	GLU	3.6
1	B	41	VAL	3.6
1	B	42	PHE	3.6
1	E	6	PHE	3.6
1	A	16	ASN	3.5
1	F	169	ASP	3.5
1	D	66	THR	3.5
1	F	31	GLN	3.5
1	D	3	LYS	3.4
1	E	4	THR	3.4
1	F	226	GLU	3.3
1	B	2	THR	3.3
1	C	227	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	169	ASP	3.3
1	F	4	THR	3.3
1	D	42	PHE	3.3
1	B	148	ALA	3.3
1	B	4	THR	3.3
1	D	62	VAL	3.3
1	B	9	GLY	3.2
1	A	11	THR	3.2
1	B	28	ALA	3.2
1	D	58	GLY	3.2
1	F	13	ALA	3.1
1	F	42	PHE	3.1
1	C	232	THR	3.1
1	F	39	ASN	3.1
1	B	51	VAL	3.1
1	B	37	MET	3.1
1	E	168	TYR	3.1
1	C	168	TYR	3.1
1	B	31	GLN	3.0
1	D	27	PRO	3.0
1	F	103	VAL	3.0
1	F	225	LYS	3.0
1	E	224	GLN	3.0
1	D	103	VAL	3.0
1	A	235	GLU	3.0
1	D	16	ASN	3.0
1	A	253	LYS	3.0
1	B	40	PRO	3.0
1	C	146	SER	3.0
1	B	224	GLN	3.0
1	D	223	THR	2.9
1	F	33	ILE	2.9
1	A	233	LEU	2.9
1	C	51	VAL	2.9
1	E	232	THR	2.9
1	A	30	VAL	2.9
1	E	235	GLU	2.9
1	A	28	ALA	2.8
1	E	80	LEU	2.8
1	F	62	VAL	2.8
1	C	6	PHE	2.8
1	E	51	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	3	LYS	2.7
1	F	44	ALA	2.7
1	B	103	VAL	2.7
1	D	216	ALA	2.7
1	C	137	THR	2.7
1	D	68	ILE	2.7
1	B	39	ASN	2.7
1	F	236	THR	2.7
1	F	59	GLN	2.7
1	E	222[A]	ARG	2.7
1	D	36	LEU	2.7
1	C	235	GLU	2.6
1	A	59	GLN	2.6
1	A	216	ALA	2.6
1	F	28	ALA	2.6
1	C	66	THR	2.6
1	F	35[A]	GLU	2.6
1	A	104	GLY	2.6
1	A	222[A]	ARG	2.6
1	B	16	ASN	2.6
1	F	235	GLU	2.6
1	C	62	VAL	2.5
1	D	59	GLN	2.5
1	B	33	ILE	2.5
1	F	15	LEU	2.5
1	A	221	ASN	2.5
1	D	101	VAL	2.5
1	B	185	GLU	2.5
1	B	253	LYS	2.5
1	D	13	ALA	2.5
1	E	101	VAL	2.5
1	F	51	VAL	2.5
1	B	219	ILE	2.5
1	C	222[A]	ARG	2.5
1	F	171	PHE	2.5
1	C	246[A]	GLU	2.5
1	F	55	GLU	2.5
1	D	61	VAL	2.5
1	F	46	HIS	2.5
1	C	129	ALA	2.5
1	D	31	GLN	2.4
1	A	62	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	150	VAL	2.4
1	E	169	ASP	2.4
1	B	61	VAL	2.4
1	B	52	TYR	2.4
1	E	223	THR	2.4
1	E	12	GLU	2.4
1	B	54	ALA	2.4
1	F	146	SER	2.4
1	A	58	GLY	2.4
1	B	56	LEU	2.4
1	D	235	GLU	2.4
1	A	218	VAL	2.4
1	D	150	VAL	2.4
1	F	5	VAL	2.4
1	B	45	SER	2.4
1	F	239	ARG	2.4
1	B	6	PHE	2.4
1	A	63	VAL	2.4
1	F	63	VAL	2.4
1	E	242[A]	LYS	2.4
1	F	223	THR	2.4
1	D	46[A]	HIS	2.3
1	D	104	GLY	2.3
1	C	234	LYS	2.3
1	D	234	LYS	2.3
1	C	15	LEU	2.3
1	C	150	VAL	2.3
1	C	73	THR	2.3
1	F	56[A]	LEU	2.2
1	B	235	GLU	2.2
1	A	168	TYR	2.2
1	C	171	PHE	2.2
1	F	47	ARG	2.2
1	B	234	LYS	2.2
1	E	171	PHE	2.2
1	D	214	CYS	2.2
1	E	100	HIS	2.2
1	E	66	THR	2.2
1	A	169	ASP	2.2
1	E	43	LEU	2.2
1	A	51	VAL	2.2
1	E	29[A]	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	89	LEU	2.1
1	D	113	VAL	2.1
1	C	223	THR	2.1
1	F	29[A]	ARG	2.1
1	A	234	LYS	2.1
1	C	4	THR	2.1
1	D	148	ALA	2.1
1	A	171	PHE	2.1
1	D	14	ASP	2.1
1	B	181	GLY	2.1
1	A	22	ILE	2.1
1	A	240	SER	2.1
1	D	39	ASN	2.1
1	F	30	VAL	2.1
1	A	48	GLU	2.0
1	B	220	ILE	2.0
1	B	34	ALA	2.0
1	E	46	HIS	2.0
1	E	221	ASN	2.0
1	B	242	LYS	2.0
1	F	242	LYS	2.0
1	F	68	ILE	2.0
1	E	148	ALA	2.0
1	B	35	GLU	2.0
1	B	3	LYS	2.0
1	D	60	SER	2.0
1	B	233	LEU	2.0
1	D	93[A]	THR	2.0
1	D	38	ASP	2.0
1	D	91	VAL	2.0
1	D	173	GLY	2.0
1	F	41	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
7	TRS	F	301	8/8	0.59	0.45	44,49,57,58	0
4	GOL	D	301	6/6	0.70	0.28	29,29,38,40	0
3	4WR	D	304[A]	14/14	0.75	0.24	21,24,29,29	14
3	4WR	B	302	14/14	0.77	0.27	15,22,32,34	14
6	M5F	D	303[B]	14/14	0.78	0.22	21,24,29,29	14
6	M5F	F	302	14/14	0.79	0.23	17,26,36,39	14
2	EDO	B	301	4/4	0.83	0.22	14,20,23,46	0
2	EDO	C	301	4/4	0.83	0.20	28,28,35,37	0
2	EDO	E	302	4/4	0.84	0.24	25,28,34,35	0
4	GOL	E	301	6/6	0.86	0.18	27,34,38,40	0
2	EDO	A	302	4/4	0.86	0.29	20,21,26,38	0
2	EDO	C	302	4/4	0.87	0.12	24,27,31,31	0
5	PEG	D	302	7/7	0.89	0.15	10,17,29,29	0
2	EDO	E	303	4/4	0.89	0.16	19,19,26,29	0
2	EDO	A	301	4/4	0.94	0.15	12,17,28,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.