



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:00 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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

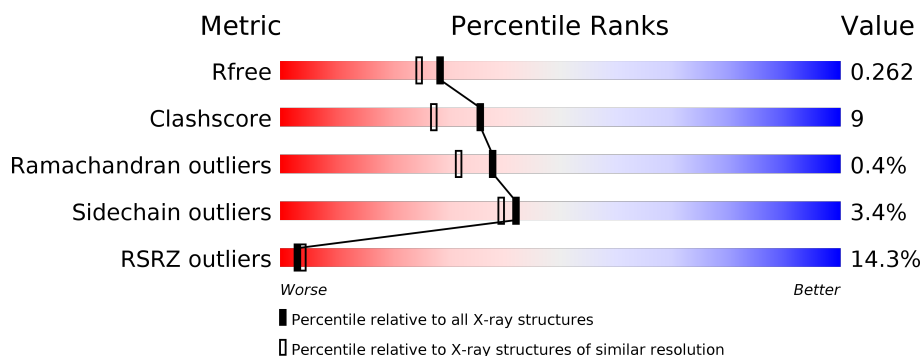
1 Overall quality at a glance

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}	100719	1915 (2.16-2.12)
Clashscore	112137	2047 (2.16-2.12)
Ramachandran outliers	110173	2020 (2.16-2.12)
Sidechain outliers	110143	2019 (2.16-2.12)
RSRZ outliers	101464	1921 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>11%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div></div> </div> <div></div> </div>
1	B	253	<div> <div>14%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div></div> </div> <div></div> </div>
1	C	253	<div> <div>13%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div></div> </div> <div></div> </div>
1	D	253	<div> <div>15%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div></div> </div> <div></div> </div>
1	E	253	<div> <div>11%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div></div> </div> <div></div> </div>
1	F	253	<div> <div>19%</div> <div> <div></div> <div>74%</div> <div>24%</div> <div></div> </div> <div></div> </div>

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	X
5	PEG	D	302	-	-	X	-

2 Entry composition [i](#)

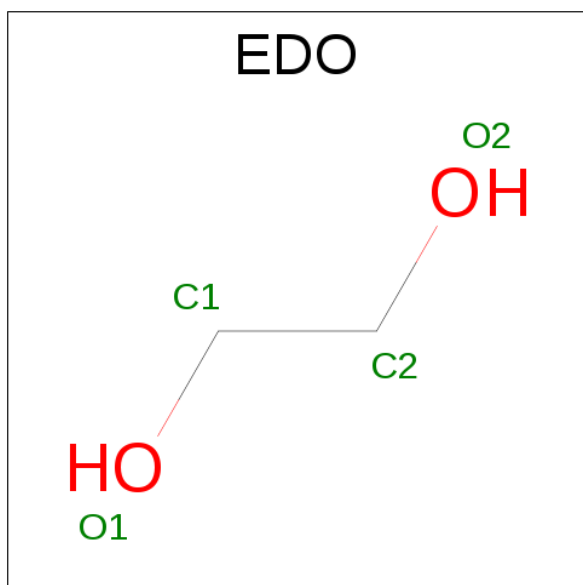
There are 8 unique types of molecules in this entry. The entry contains 11998 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

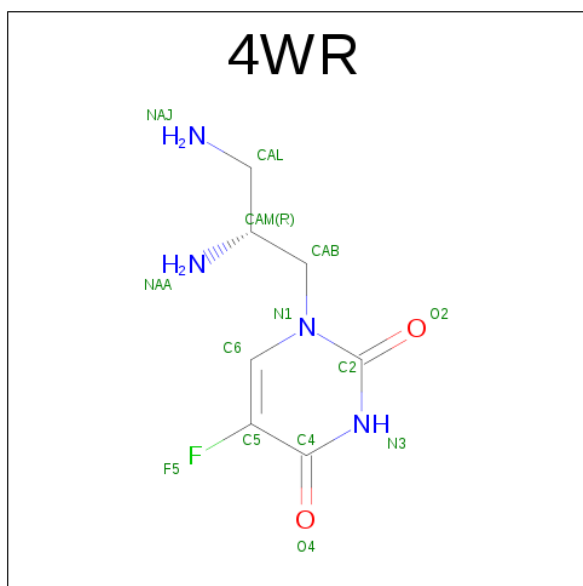
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	2	0
			1840	1154	321	352	13			
1	B	245	Total	C	N	O	S	0	4	0
			1848	1158	318	357	15			
1	C	251	Total	C	N	O	S	0	6	0
			1920	1204	336	366	14			
1	D	242	Total	C	N	O	S	0	8	0
			1866	1169	330	354	13			
1	E	246	Total	C	N	O	S	0	4	0
	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

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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: C₇H₁₁FN₄O₂).



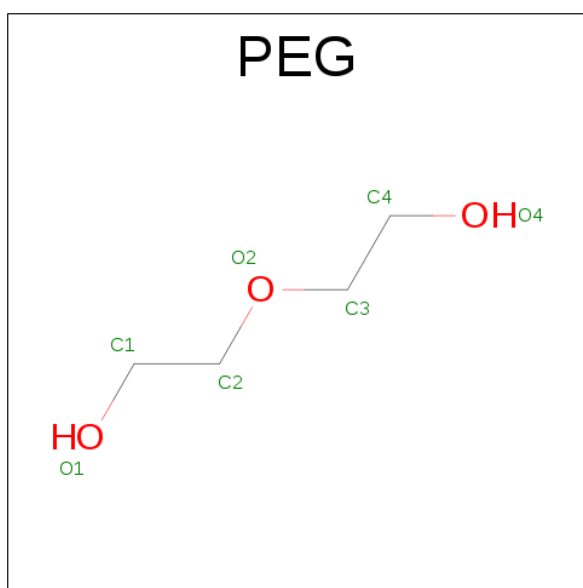
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C F N O 14 7 1 4 2	0	0
3	D	1	Total C F N O 14 7 1 4 2	0	1

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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		

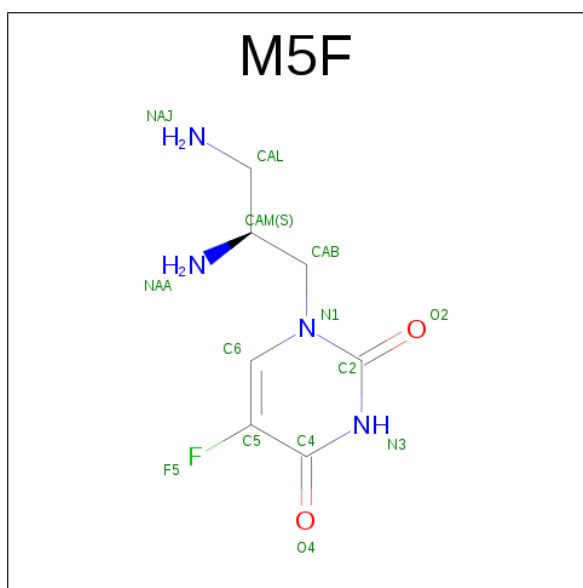
- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

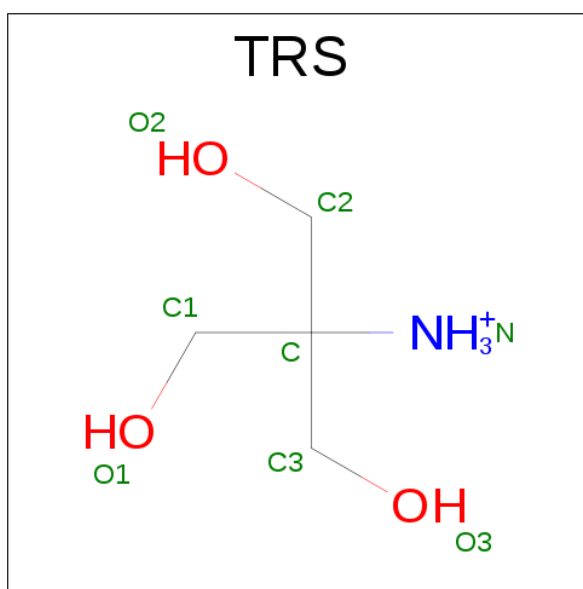
- Molecule 6 is 1-[(2S)-2,3-diaminopropyl]-5-fluoropyrimidine-2,4(1H,3H)-dione (three-letter

code: M5F) (formula: C₇H₁₁FN₄O₂).



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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



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

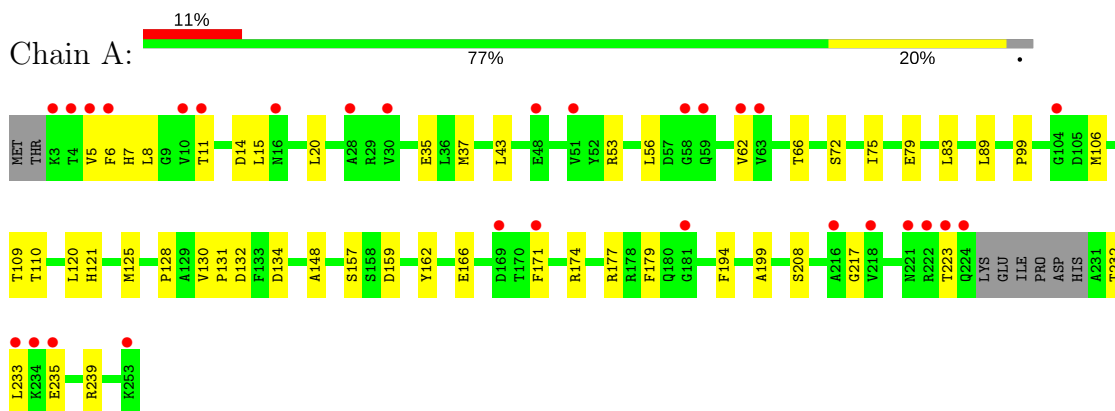
- Molecule 8 is water.

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		

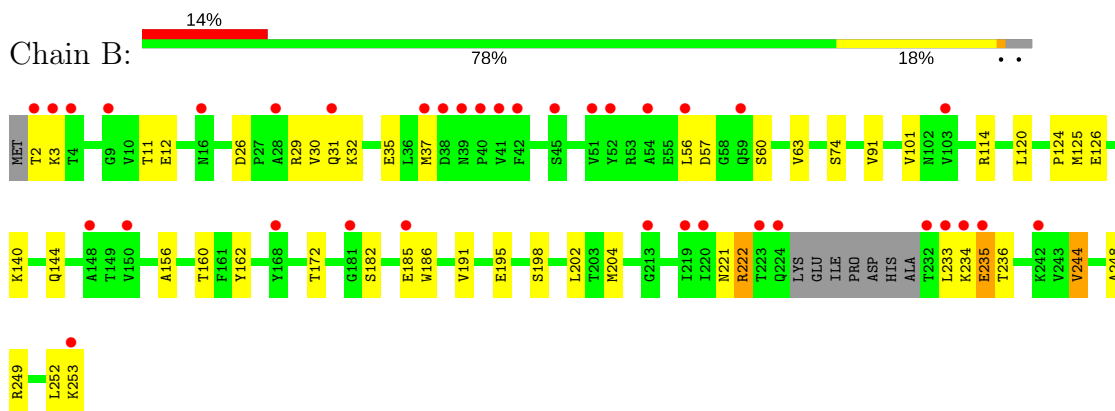
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

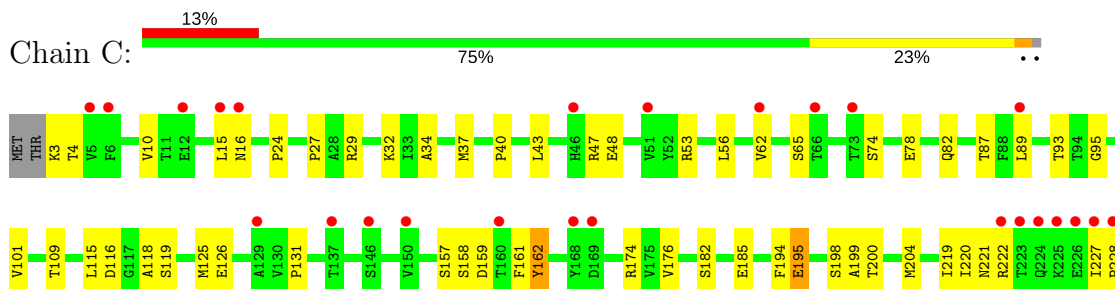
• Molecule 1: Uridine phosphorylase

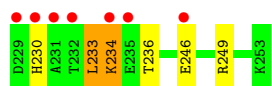


• Molecule 1: Uridine phosphorylase

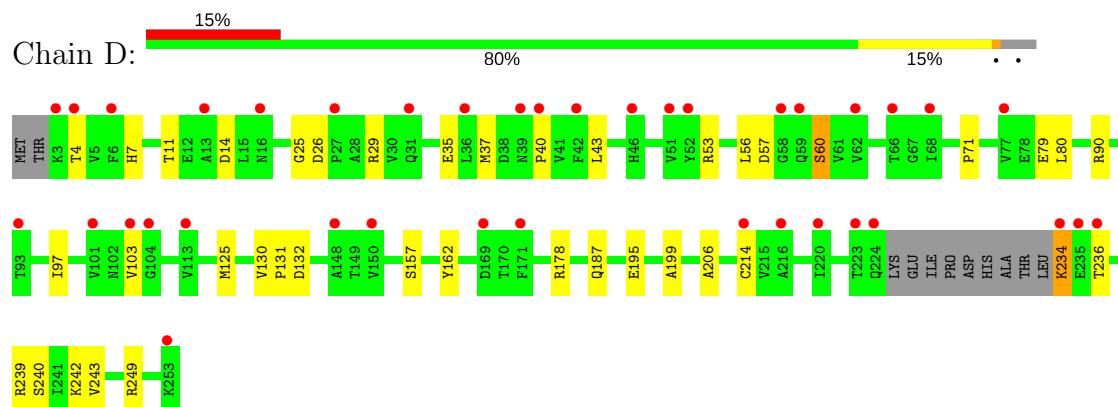


• Molecule 1: Uridine phosphorylase

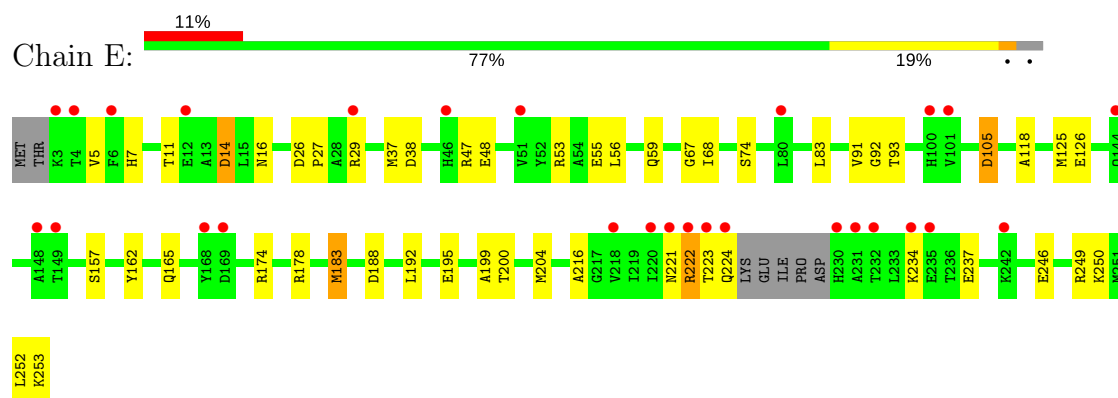




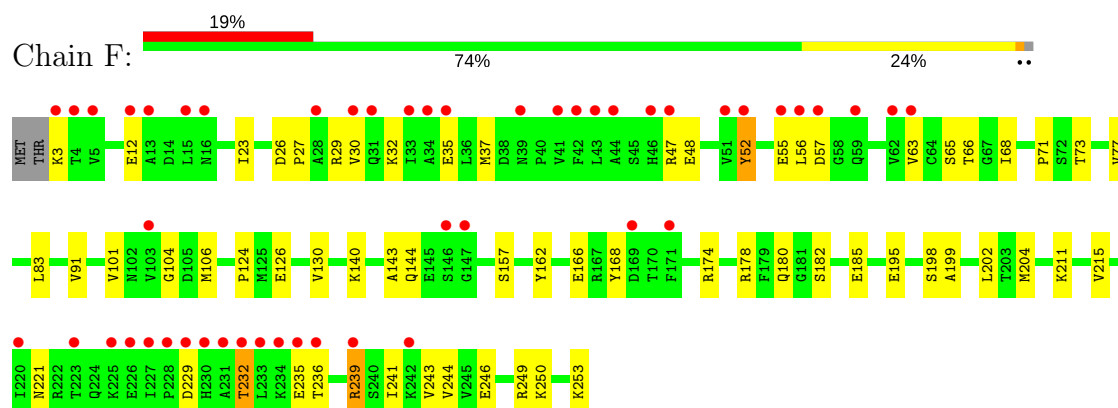
● Molecule 1: Uridine phosphorylase



● Molecule 1: Uridine phosphorylase



● Molecule 1: Uridine phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 2.13Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.208 , 0.262 0.208 , 0.262	Depositor DCC
R_{free} test set	2151 reflections (3.02%)	DCC
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11998	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage'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.*

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: GOL, EDO, 4WR, M5F, 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	0.45	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 [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	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

Continued on next page...

Continued from previous page...

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:HH11	1:D:29[B]:ARG:HA	1.63	0.64

Continued on next page...

Continued from previous page...

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:NZ	1:E:253:LYS:HA	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

Continued on next page...

Continued from previous page...

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:N	1:E:14:ASP:OD1	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:120:LEU:HD21	1:A:125:MET:CE	2.44	0.47
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: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

Continued on next page...

Continued from previous page...

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:H5	3:B:302:4WR:O2	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:118:ALA:HB3	1:C:200:THR:OG1	2.17	0.45
1:C:101:VAL:O	1:C:221:ASN:ND2	2.49	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:219:ILE:O	1:C:228:PRO:HG2	2.18	0.44
1:C:29:ARG:HH11	1:C:32:LYS:NZ	2.11	0.44
1:A:166:GLU:HG3	1:A:179:PHE:O	2.18	0.44
1:A:5:VAL:HG21	1:A:83:LEU:HG	2.00	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

Continued on next page...

Continued from previous page...

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:194:PHE:HB2	1:C:222[B]:ARG:HH22	1.81	0.43
1:C:174[B]:ARG:HD2	1:E:188:ASP:HB3	2.00	0.43
1:B:235:GLU:HG2	1:B:235:GLU:H	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:233:LEU:HB3	1:C:234:LYS:NZ	2.34	0.43
1:C:87:THR:HG22	1:C:89:LEU:CD1	2.49	0.43
1:B:198:SER:O	1:B:202:LEU:HG	2.19	0.43
1:C:234:LYS:HG2	1:C:234:LYS:H	1.51	0.43
1:B:182:SER:HA	1:B:185:GLU:OE1	2.19	0.43
1:C:16:ASN:ND2	1:C:16:ASN:O	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:182:SER:HA	1:C:185:GLU:OE1	2.19	0.42
1:C:27:PRO:HG3	1:C:48:GLU:O	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:HB3	1:D:239:ARG:HE	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:166:GLU:HG2	1:F:168:TYR:CE2	2.54	0.42
1:F:26:ASP:HA	1:F:27:PRO:HD2	1.83	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:HA	1:D:80:LEU:HD23	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

Continued on next page...

Continued from previous page...

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:HE3	1:C:3:LYS:HB2	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:HB3	1:F:211:LYS:HE3	1.83	0.41
1:F:229:ASP:N	1:F:229:ASP:OD1	2.54	0.41
1:E:192:LEU:HD23	1:E:192:LEU:HA	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:234:LYS:CD	1:D:236:THR:H	2.34	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:125:MET:HG3	1:E:125:MET:HG3	2.03	0.41
1:D:43:LEU:HD11	1:D:53[B]:ARG:HB2	2.02	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:156:ALA:HB2	1:B:191:VAL:HG11	2.03	0.40
1:B:74:SER:HA	1:B:204[B]:MET:HE1	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%)	38	32
1	B	245/253 (97%)	243 (99%)	1 (0%)	1 (0%)	38	32
1	C	255/253 (101%)	250 (98%)	4 (2%)	1 (0%)	38	32
1	D	246/253 (97%)	241 (98%)	4 (2%)	1 (0%)	38	32
1	E	246/253 (97%)	237 (96%)	8 (3%)	1 (0%)	38	32
1	F	256/253 (101%)	245 (96%)	10 (4%)	1 (0%)	38	32
All	All	1491/1518 (98%)	1452 (97%)	33 (2%)	6 (0%)	38	32

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 ⓘ

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%)	46	44
1	B	200/203 (98%)	194 (97%)	6 (3%)	46	44
1	C	207/203 (102%)	200 (97%)	7 (3%)	42	39
1	D	201/203 (99%)	195 (97%)	6 (3%)	46	44
1	E	200/203 (98%)	193 (96%)	7 (4%)	41	38
1	F	208/203 (102%)	198 (95%)	10 (5%)	30	25
All	All	1213/1218 (100%)	1171 (96%)	42 (4%)	42	38

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

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

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	EDO	A	301	-	3,3,3	0.48	0	2,2,2	0.27	0
2	EDO	A	302	-	3,3,3	0.43	0	2,2,2	0.39	0
2	EDO	B	301	-	3,3,3	0.59	0	2,2,2	0.30	0
3	4WR	B	302	-	10,14,14	2.09	5 (50%)	7,19,19	3.35	4 (57%)
2	EDO	C	301	-	3,3,3	0.47	0	2,2,2	0.24	0
2	EDO	C	302	-	3,3,3	0.46	0	2,2,2	0.34	0
4	GOL	D	301	-	5,5,5	0.37	0	5,5,5	0.45	0
5	PEG	D	302	-	6,6,6	0.41	0	5,5,5	0.57	0
6	M5F	D	303[B]	-	10,14,14	3.24	8 (80%)	7,19,19	3.01	2 (28%)
3	4WR	D	304[A]	-	10,14,14	2.20	5 (50%)	7,19,19	2.85	2 (28%)
4	GOL	E	301	-	5,5,5	0.34	0	5,5,5	0.43	0
2	EDO	E	302	-	3,3,3	0.42	0	2,2,2	0.46	0
2	EDO	E	303	-	3,3,3	0.48	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	TRS	F	301	-	7,7,7	0.32	0	9,9,9	0.31	0
6	M5F	F	302	-	10,14,14	3.13	8 (80%)	7,19,19	2.96	2 (28%)

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	301	-	-	0/1/1/1	0/0/0/0
2	EDO	A	302	-	-	0/1/1/1	0/0/0/0
2	EDO	B	301	-	-	0/1/1/1	0/0/0/0
3	4WR	B	302	-	-	0/5/6/6	0/1/1/1
2	EDO	C	301	-	-	0/1/1/1	0/0/0/0
2	EDO	C	302	-	-	0/1/1/1	0/0/0/0
4	GOL	D	301	-	-	0/4/4/4	0/0/0/0
5	PEG	D	302	-	-	0/4/4/4	0/0/0/0
6	M5F	D	303[B]	-	-	0/5/6/6	0/1/1/1
3	4WR	D	304[A]	-	-	0/5/6/6	0/1/1/1
4	GOL	E	301	-	-	0/4/4/4	0/0/0/0
2	EDO	E	302	-	-	0/1/1/1	0/0/0/0
2	EDO	E	303	-	-	0/1/1/1	0/0/0/0
7	TRS	F	301	-	-	0/9/9/9	0/0/0/0
6	M5F	F	302	-	-	0/5/6/6	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	303[B]	M5F	F5-C5	-4.25	1.28	1.35
6	D	303[B]	M5F	C2-N3	-3.83	1.30	1.38
6	D	303[B]	M5F	C4-C5	-3.82	1.33	1.38
6	F	302	M5F	F5-C5	-3.74	1.29	1.35
6	F	302	M5F	C2-N3	-3.67	1.30	1.38
3	D	304[A]	4WR	C2-N3	-3.37	1.31	1.38
3	B	302	4WR	C2-N3	-3.21	1.31	1.38
6	F	302	M5F	CAL-NAJ	-3.06	1.39	1.47
6	D	303[B]	M5F	CAL-NAJ	-3.00	1.40	1.47
6	F	302	M5F	C4-C5	-2.58	1.35	1.38
3	D	304[A]	4WR	CAB-N1	-2.34	1.46	1.48
3	B	302	4WR	CAB-N1	-2.26	1.46	1.48
6	D	303[B]	M5F	C6-N1	-2.20	1.30	1.36
6	F	302	M5F	C6-N1	-2.09	1.30	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	4WR	CAL-NAJ	-2.05	1.42	1.47
3	D	304[A]	4WR	CAL-NAJ	-2.00	1.42	1.47
6	D	303[B]	M5F	CAB-N1	2.04	1.50	1.48
6	F	302	M5F	CAB-N1	2.09	1.50	1.48
3	B	302	4WR	C4-C5	2.11	1.41	1.38
6	D	303[B]	M5F	C4-N3	2.49	1.37	1.33
6	F	302	M5F	C4-N3	2.67	1.37	1.33
3	D	304[A]	4WR	C4-C5	3.05	1.42	1.38
3	D	304[A]	4WR	O4-C4	3.29	1.32	1.24
3	B	302	4WR	O4-C4	3.44	1.33	1.24
6	D	303[B]	M5F	O4-C4	5.63	1.38	1.24
6	F	302	M5F	O4-C4	6.08	1.39	1.24

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	302	M5F	C5-C4-N3	-3.30	118.90	122.39
3	D	304[A]	4WR	C5-C4-N3	-3.16	119.06	122.39
6	D	303[B]	M5F	C5-C4-N3	-3.15	119.06	122.39
3	B	302	4WR	C5-C4-N3	-2.38	119.88	122.39
3	B	302	4WR	CAB-CAM-CAL	2.07	112.82	109.82
3	B	302	4WR	CAB-N1-C6	2.15	122.43	118.59
3	D	304[A]	4WR	C4-N3-C2	6.52	120.86	115.16
6	F	302	M5F	C4-N3-C2	6.73	121.05	115.16
6	D	303[B]	M5F	C4-N3-C2	7.09	121.36	115.16
3	B	302	4WR	C4-N3-C2	7.77	121.95	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 22 short contacts:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	302	M5F	2	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	245/253 (96%)	0.86	29 (11%) 5 7	9, 20, 37, 55	0
1	B	245/253 (96%)	0.96	36 (14%) 3 4	11, 21, 39, 57	0
1	C	251/253 (99%)	1.04	32 (12%) 4 6	9, 19, 41, 72	0
1	D	242/253 (95%)	1.09	38 (15%) 2 3	11, 21, 39, 53	0
1	E	246/253 (97%)	0.84	27 (10%) 6 8	11, 20, 37, 57	0
1	F	251/253 (99%)	1.13	49 (19%) 1 2	10, 22, 44, 70	0
All	All	1480/1518 (97%)	0.99	211 (14%) 3 4	9, 20, 40, 72	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	227	ILE	12.0
1	C	228	PRO	11.9
1	B	232	THR	11.5
1	F	230	HIS	8.8
1	C	231	ALA	8.2
1	C	225	LYS	7.1
1	E	230	HIS	6.6
1	A	223	THR	6.4
1	E	231	ALA	6.1
1	C	169	ASP	5.6
1	C	230	HIS	5.6
1	F	233	LEU	5.6
1	F	228	PRO	5.5
1	D	253	LYS	5.5
1	F	52[A]	TYR	5.1
1	C	46	HIS	4.9
1	F	232	THR	4.8
1	C	224	GLN	4.7
1	E	220	ILE	4.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	229	ASP	4.6
1	F	231	ALA	4.5
1	F	34	ALA	4.4
1	C	16	ASN	4.4
1	C	5	VAL	4.3
1	B	223	THR	4.3
1	D	6	PHE	4.2
1	D	51	VAL	4.2
1	D	40	PRO	4.2
1	A	224	GLN	4.2
1	F	16	ASN	4.2
1	C	226	GLU	4.1
1	C	229	ASP	4.1
1	D	224	GLN	4.1
1	F	43	LEU	4.1
1	A	4	THR	4.1
1	C	227	ILE	4.0
1	D	4	THR	3.9
1	D	171	PHE	3.9
1	B	168	TYR	3.9
1	F	220	ILE	3.9
1	A	6	PHE	3.8
1	E	234	LYS	3.8
1	D	42	PHE	3.7
1	F	3	LYS	3.7
1	F	12	GLU	3.7
1	B	41	VAL	3.6
1	A	3	LYS	3.6
1	B	59	GLN	3.5
1	E	4	THR	3.4
1	B	42	PHE	3.4
1	F	147	GLY	3.4
1	D	16	ASN	3.4
1	D	52	TYR	3.3
1	D	66	THR	3.3
1	F	234	LYS	3.3
1	F	4	THR	3.3
1	F	226	GLU	3.3
1	B	9	GLY	3.3
1	A	253	LYS	3.3
1	E	235	GLU	3.3
1	F	103	VAL	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	31	GLN	3.2
1	D	3	LYS	3.2
1	E	6	PHE	3.2
1	D	169	ASP	3.2
1	D	58	GLY	3.1
1	C	232	THR	3.1
1	B	37	MET	3.1
1	D	62	VAL	3.1
1	D	27	PRO	3.1
1	E	224	GLN	3.1
1	F	169	ASP	3.1
1	A	16	ASN	3.1
1	B	4	THR	3.1
1	F	42	PHE	3.1
1	B	103	VAL	3.1
1	F	46	HIS	3.0
1	A	11	THR	3.0
1	D	223	THR	3.0
1	B	148	ALA	3.0
1	F	13	ALA	3.0
1	D	103	VAL	3.0
1	B	2	THR	3.0
1	B	224	GLN	3.0
1	A	235	GLU	2.9
1	E	80	LEU	2.9
1	F	236	THR	2.9
1	E	12	GLU	2.9
1	A	5	VAL	2.8
1	F	39	ASN	2.8
1	C	235	GLU	2.8
1	B	31	GLN	2.8
1	C	168	TYR	2.8
1	A	62	VAL	2.7
1	E	3	LYS	2.7
1	F	225	LYS	2.7
1	B	28	ALA	2.7
1	C	6	PHE	2.7
1	A	59	GLN	2.7
1	F	62	VAL	2.7
1	C	146	SER	2.7
1	D	216	ALA	2.7
1	D	36	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	16	ASN	2.6
1	E	223	THR	2.6
1	D	46[A]	HIS	2.6
1	E	168	TYR	2.6
1	E	222[A]	ARG	2.6
1	A	216	ALA	2.6
1	A	221	ASN	2.6
1	B	51	VAL	2.6
1	F	33	ILE	2.6
1	B	39	ASN	2.6
1	A	28	ALA	2.6
1	A	30	VAL	2.6
1	C	62	VAL	2.6
1	E	51	VAL	2.6
1	D	235	GLU	2.6
1	D	150	VAL	2.5
1	F	63	VAL	2.5
1	A	10	VAL	2.5
1	F	5	VAL	2.5
1	E	232	THR	2.5
1	A	233	LEU	2.5
1	B	185	GLU	2.5
1	F	15	LEU	2.5
1	F	44	ALA	2.5
1	C	234	LYS	2.5
1	F	146	SER	2.5
1	D	13	ALA	2.5
1	C	73	THR	2.5
1	E	242[A]	LYS	2.5
1	C	129	ALA	2.5
1	D	148	ALA	2.5
1	B	52	TYR	2.4
1	B	219	ILE	2.4
1	C	89	LEU	2.4
1	F	35[A]	GLU	2.4
1	B	181	GLY	2.4
1	A	48	GLU	2.4
1	E	221	ASN	2.4
1	F	171	PHE	2.4
1	B	150	VAL	2.4
1	D	101	VAL	2.4
1	E	101	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	160	THR	2.4
1	A	222[A]	ARG	2.4
1	A	171	PHE	2.4
1	E	169	ASP	2.4
1	A	63	VAL	2.4
1	A	218	VAL	2.3
1	C	222[A]	ARG	2.3
1	F	28	ALA	2.3
1	A	181	GLY	2.3
1	D	93[A]	THR	2.3
1	A	169	ASP	2.3
1	B	235	GLU	2.3
1	A	234	LYS	2.3
1	B	56	LEU	2.3
1	C	51	VAL	2.3
1	F	51	VAL	2.3
1	D	39	ASN	2.3
1	B	40	PRO	2.3
1	B	253	LYS	2.3
1	A	58	GLY	2.3
1	F	235	GLU	2.3
1	D	234	LYS	2.3
1	F	47	ARG	2.3
1	C	246[A]	GLU	2.3
1	E	148	ALA	2.2
1	B	38	ASP	2.2
1	F	55	GLU	2.2
1	F	59	GLN	2.2
1	D	68	ILE	2.2
1	B	54	ALA	2.2
1	F	239	ARG	2.2
1	D	214	CYS	2.2
1	F	57	ASP	2.2
1	D	31	GLN	2.2
1	E	144	GLN	2.2
1	C	15	LEU	2.2
1	B	45	SER	2.2
1	B	234	LYS	2.2
1	C	66	THR	2.2
1	D	236	THR	2.2
1	E	149	THR	2.2
1	B	233	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	59	GLN	2.2
1	D	104	GLY	2.2
1	F	223	THR	2.2
1	D	220	ILE	2.1
1	D	113	VAL	2.1
1	F	30	VAL	2.1
1	C	137	THR	2.1
1	C	223	THR	2.1
1	E	46	HIS	2.1
1	E	100	HIS	2.1
1	A	51	VAL	2.1
1	C	150	VAL	2.1
1	F	242	LYS	2.1
1	F	56[A]	LEU	2.0
1	C	12	GLU	2.0
1	E	29[A]	ARG	2.0
1	B	242	LYS	2.0
1	B	220	ILE	2.0
1	B	3	LYS	2.0
1	A	104	GLY	2.0
1	B	213	GLY	2.0
1	D	77	VAL	2.0
1	E	218	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	D	301	6/6	0.73	0.30	2.06	29,29,38,40	0
3	4WR	B	302	14/14	0.76	0.26	1.68	15,22,32,34	14
3	4WR	D	304[A]	14/14	0.76	0.24	1.30	21,24,29,29	14
6	M5F	F	302	14/14	0.78	0.22	0.89	17,26,36,39	14
6	M5F	D	303[B]	14/14	0.79	0.22	0.70	21,24,29,29	14
2	EDO	E	302	4/4	0.83	0.24	0.65	25,28,34,35	0
2	EDO	C	301	4/4	0.82	0.20	0.07	28,28,35,37	0
2	EDO	E	303	4/4	0.91	0.15	-0.28	19,19,26,29	0
2	EDO	A	301	4/4	0.94	0.13	-0.36	12,17,28,35	0
5	PEG	D	302	7/7	0.88	0.15	-0.46	10,17,29,29	0
2	EDO	C	302	4/4	0.86	0.14	-1.10	24,27,31,31	0
7	TRS	F	301	8/8	0.61	0.45	-	44,49,57,58	0
4	GOL	E	301	6/6	0.86	0.19	-	27,34,38,40	0
2	EDO	B	301	4/4	0.85	0.22	-	14,20,23,46	0
2	EDO	A	302	4/4	0.87	0.25	-	20,21,26,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.