Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:00 AM GMT

PDB ID	:	2VKD
Title	:	CRYSTAL STRUCTURE OF THE CATALYTIC DOMAIN OF LETHAL TOXIN FROM CLOSTRIDIUM SORDELLII IN COMPLEX WITH UDP-GLC AND MANGANESE ION
Authors	:	Ziegler, M.O.P.; Jank, T.; Aktories, K.; Schulz, G.E.
Deposited on	:	2007-12-18
Resolution	:	2.53 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

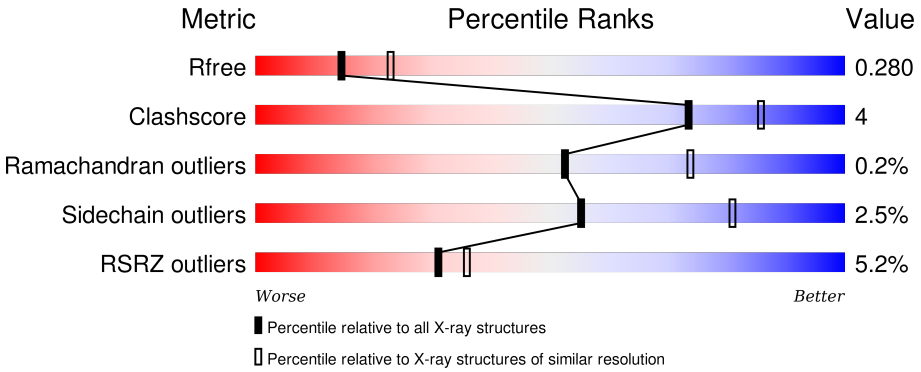
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	91344	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (2.54-2.50)

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 <=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	546	4% 89% 10%
1	B	546	5% 87% 10%
1	C	546	6% 88% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13572 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 CYTOTOXIN L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4447	2838	721	872	16			
1	B	538	Total	C	N	O	S	0	0	0
			4422	2824	716	867	15			
1	C	541	Total	C	N	O	S	0	0	0
			4442	2835	720	871	16			

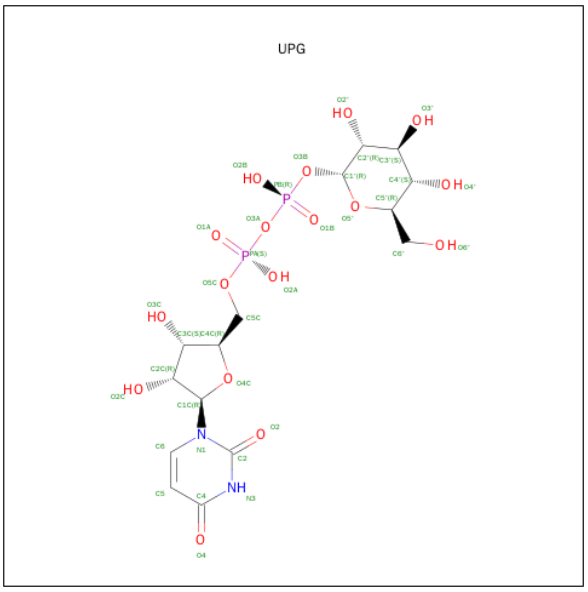
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ALA	VAL	ENGINEERED MUTATION	UNP Q46342
A	289	MET	ILE	ENGINEERED MUTATION	UNP Q46342
B	13	ALA	VAL	ENGINEERED MUTATION	UNP Q46342
B	289	MET	ILE	ENGINEERED MUTATION	UNP Q46342
C	13	ALA	VAL	ENGINEERED MUTATION	UNP Q46342
C	289	MET	ILE	ENGINEERED MUTATION	UNP Q46342

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mn	0	0
			1	1		
2	A	3	Total	Mn	0	0
			3	3		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCOSE (three-letter code: UPG) (formula: $C_{15}H_{24}N_2O_{17}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	B	1	Total	C	N	O	P	0	0
			36	15	2	17	2		
3	C	1	Total	C	N	O	P	0	0
			36	15	2	17	2		

- Molecule 4 is water.

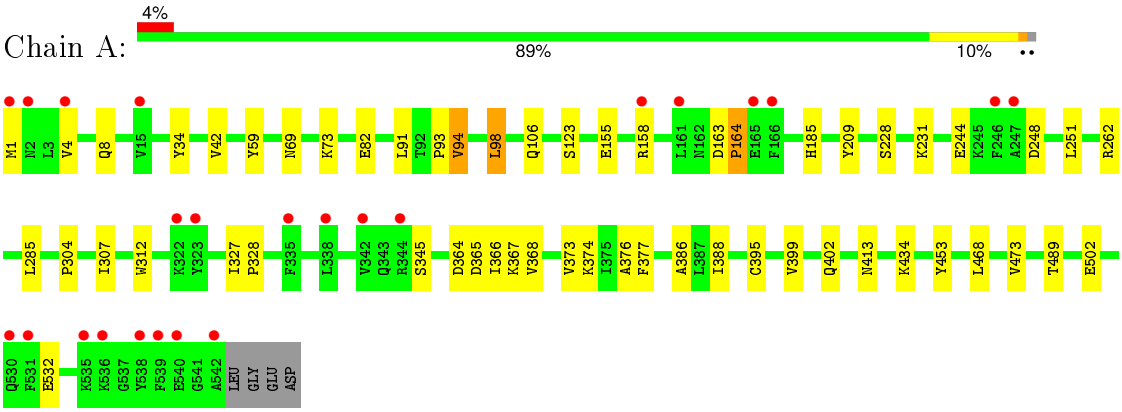
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	47	Total	O	0	0
			47	47		
4	B	57	Total	O	0	0
			57	57		
4	C	44	Total	O	0	0
			44	44		

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 errors 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.

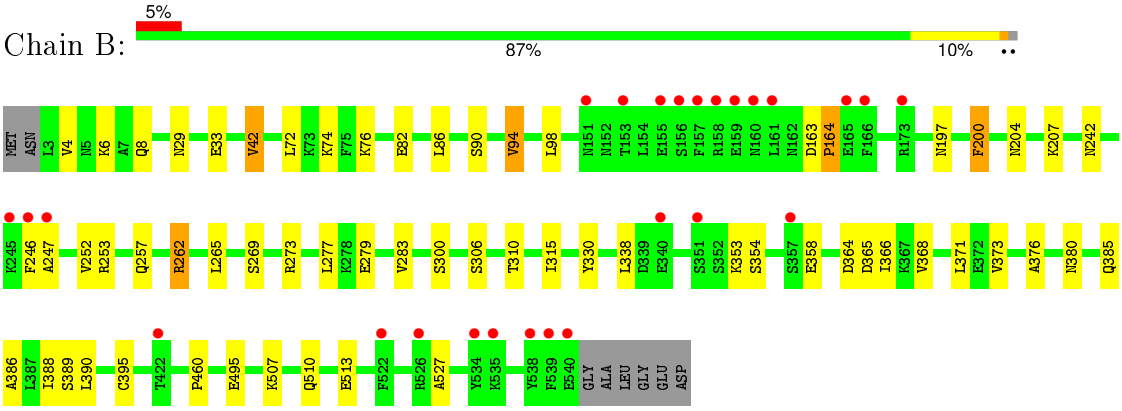
- Molecule 1: CYTOTOXIN L

Chain A:



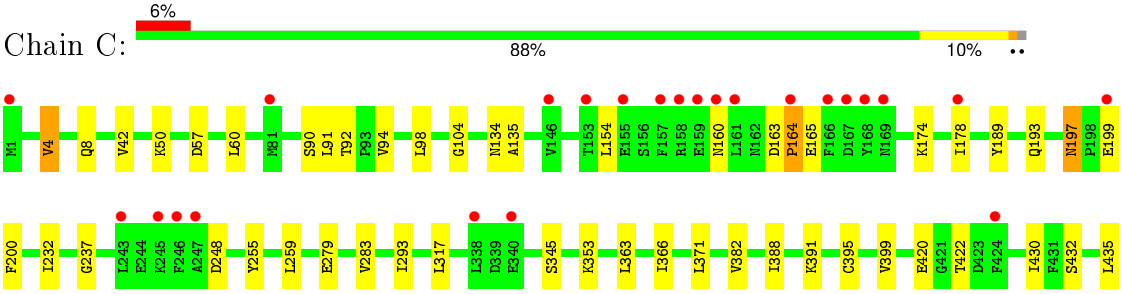
- Molecule 1: CYTOTOXIN L

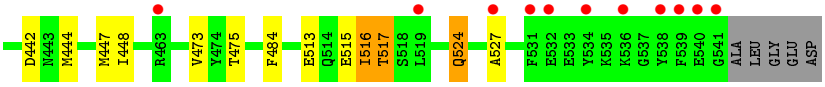
Chain B:



- Molecule 1: CYTOTOXIN L

Chain C:




D442
M443
M444
M447
I448
R463
V473
Y474
T475
F484
E513
Q514
E515
I516
T517
S518
L519
Q524
A527
F531
E532
E533
Y534
K535
K536
G537
Y538
F539
E540
G541
ALA
LEU
GLY
GLU
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.29Å 190.32Å 204.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	90.17 – 2.53 90.05 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.7 (90.17-2.53) 99.7 (90.05-2.53)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.46 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.288 0.239 , 0.280	Depositor DCC
R_{free} test set	3780 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	2 of 75590 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	13572	wwPDB-VP
Average B, all atoms (Å^2)	33.0	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 35.55 % 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 5.7375e-04.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: UPG, MN

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	0.42	0/4530	0.54	0/6114
1	B	0.44	0/4505	0.55	0/6081
1	C	0.43	0/4525	0.54	0/6107
All	All	0.43	0/13560	0.54	0/18302

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	4447	0	4406	34	0
1	B	4422	0	4380	37	0
1	C	4442	0	4401	37	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	36	0	22	0	0
3	B	36	0	22	0	0
3	C	36	0	22	1	0
4	A	47	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	57	0	0	1	0
4	C	44	0	0	1	0
All	All	13572	0	13253	108	0

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

All (108) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ASP:HB2	1:A:164:PRO:HA	1.39	1.03
1:B:262:ARG:HH11	1:B:262:ARG:HG3	1.18	1.02
1:A:106:GLN:HE21	1:A:231:LYS:HD2	1.35	0.91
1:B:262:ARG:NH1	1:B:262:ARG:HG3	1.85	0.89
1:A:4:VAL:HG22	1:A:8:GLN:HB2	1.62	0.81
1:C:366:ILE:HG21	1:C:388:ILE:HD13	1.65	0.78
1:C:163:ASP:HB3	1:C:164:PRO:HA	1.67	0.74
1:C:4:VAL:HG22	1:C:8:GLN:HB3	1.68	0.73
1:A:98:LEU:HD21	1:A:285:LEU:HD12	1.70	0.72
1:A:1:MET:HB2	1:C:422:THR:HG21	1.71	0.71
1:B:262:ARG:HH11	1:B:262:ARG:CG	2.02	0.69
1:C:513:GLU:O	1:C:516:ILE:HG12	1.95	0.67
1:C:42:VAL:HG21	1:C:90:SER:CB	2.27	0.65
1:C:160:ASN:HD22	1:C:164:PRO:HD3	1.60	0.65
1:B:204:ASN:HA	1:B:207:LYS:HE2	1.77	0.65
1:A:4:VAL:HG22	1:A:8:GLN:CB	2.25	0.65
1:A:163:ASP:HB2	1:A:164:PRO:CA	2.22	0.64
1:C:4:VAL:HG22	1:C:8:GLN:CB	2.28	0.64
1:C:371:LEU:O	1:C:395:CYS:HB2	2.00	0.62
1:A:304:PRO:HG2	1:A:307:ILE:HD12	1.81	0.61
1:B:253:ARG:NH2	4:B:2027:HOH:O	2.34	0.60
1:A:373:VAL:HG23	1:A:395:CYS:HB3	1.83	0.60
1:C:524:GLN:HA	1:C:527:ALA:HB3	1.85	0.59
1:C:363:LEU:HD22	1:C:366:ILE:HD11	1.85	0.58
1:C:165:GLU:HA	1:C:165:GLU:OE1	2.04	0.57
1:A:304:PRO:HD2	1:A:312:TRP:CZ3	2.39	0.57
1:B:371:LEU:O	1:B:395:CYS:HB2	2.05	0.56
1:C:42:VAL:HG21	1:C:90:SER:HB2	1.87	0.56
1:A:93:PRO:HA	1:A:366:ILE:O	2.06	0.55
1:B:385:GLN:NE2	1:B:510:GLN:HE21	2.03	0.55
3:C:1544:UPG:H3'	3:C:1544:UPG:H5C2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:HD23	1:B:283:VAL:HB	1.87	0.55
1:A:155:GLU:HB3	1:A:158:ARG:HH21	1.71	0.54
1:C:399:VAL:HG13	1:C:473:VAL:HG12	1.90	0.54
1:B:29:ASN:O	1:B:33:GLU:HG2	2.08	0.54
1:A:185:HIS:HD2	1:A:209:TYR:OH	1.91	0.54
1:A:413:ASN:HD22	1:A:434:LYS:HB3	1.72	0.53
1:B:163:ASP:HB2	1:B:164:PRO:HA	1.91	0.53
1:C:42:VAL:HG21	1:C:90:SER:HB3	1.90	0.53
1:A:366:ILE:HG21	1:A:388:ILE:HD13	1.93	0.50
1:A:399:VAL:HG13	1:A:473:VAL:HG12	1.94	0.49
1:B:380:ASN:ND2	1:B:495:GLU:OE2	2.45	0.49
1:A:91:LEU:HB3	1:A:367:LYS:HB3	1.94	0.49
1:A:262:ARG:HD2	1:A:453:TYR:CE2	2.46	0.49
1:B:373:VAL:HG23	1:B:395:CYS:HB3	1.95	0.49
1:C:420:GLU:HG3	1:C:430:ILE:HD13	1.94	0.48
1:C:255:TYR:CE2	1:C:259:LEU:HD22	2.47	0.48
1:B:273:ARG:O	1:B:277:LEU:HB2	2.13	0.48
1:B:94:VAL:HG23	1:B:366:ILE:HG13	1.95	0.48
1:B:385:GLN:HE21	1:B:510:GLN:HE21	1.62	0.47
1:B:72:LEU:O	1:B:76:LYS:HG3	2.15	0.47
1:A:374:LYS:HB2	1:A:388:ILE:HB	1.96	0.47
1:B:376:ALA:HB2	1:B:386:ALA:HB3	1.96	0.47
1:B:353:LYS:HD2	1:B:358:GLU:HB3	1.97	0.47
1:B:4:VAL:CG2	1:B:8:GLN:HB3	2.45	0.47
1:B:330:TYR:HA	1:B:513:GLU:OE1	2.14	0.47
1:A:248:ASP:HB3	1:A:251:LEU:HB2	1.97	0.46
1:A:69:ASN:O	1:A:73:LYS:HG2	2.14	0.46
1:C:279:GLU:HB3	4:C:2024:HOH:O	2.16	0.46
1:B:373:VAL:HG22	1:B:389:SER:HB2	1.98	0.46
1:C:197:ASN:HB3	1:C:200:PHE:HD2	1.80	0.46
1:C:524:GLN:H	1:C:524:GLN:HG2	1.56	0.46
1:A:163:ASP:CB	1:A:164:PRO:HA	2.26	0.46
1:C:104:GLY:HA2	1:C:135:ALA:O	2.16	0.45
1:A:106:GLN:HG3	1:A:228:SER:HA	1.99	0.45
1:C:399:VAL:HG13	1:C:473:VAL:CG1	2.46	0.45
1:C:197:ASN:HD22	1:C:199:GLU:H	1.64	0.45
1:C:435:LEU:HD22	1:C:447:MET:SD	2.57	0.45
1:B:246:PHE:HA	1:B:279:GLU:HG3	1.98	0.45
1:B:247:ALA:HB1	1:B:252:VAL:HG21	1.99	0.44
1:A:94:VAL:HG13	1:A:368:VAL:CG1	2.47	0.44
1:B:247:ALA:HB1	1:B:252:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ALA:HB2	1:A:386:ALA:HB3	1.98	0.44
1:C:382:VAL:HG21	1:C:475:THR:HG23	1.99	0.44
1:B:265:LEU:O	1:B:269:SER:HB2	2.18	0.44
1:C:524:GLN:HA	1:C:527:ALA:CB	2.48	0.43
1:B:94:VAL:HA	1:B:390:LEU:HD23	2.00	0.43
1:A:395:CYS:O	1:A:399:VAL:HG23	2.18	0.43
1:A:59:TYR:CD2	1:A:59:TYR:C	2.91	0.43
1:A:402:GLN:HB2	1:A:473:VAL:HG13	2.01	0.43
1:B:42:VAL:HG21	1:B:90:SER:HB2	2.00	0.43
1:B:197:ASN:HB3	1:B:200:PHE:CD2	2.54	0.43
1:B:246:PHE:CD1	1:B:279:GLU:HB3	2.54	0.43
1:A:364:ASP:HB3	1:A:365:ASP:H	1.67	0.42
1:A:106:GLN:HE21	1:A:231:LYS:CD	2.17	0.42
1:A:327:ILE:HA	1:A:328:PRO:HD3	1.88	0.42
1:C:232:ILE:HG13	1:C:237:GLY:HA3	2.01	0.42
1:C:444:MET:O	1:C:448:ILE:HG12	2.19	0.42
1:A:34:TYR:OH	1:A:82:GLU:OE2	2.29	0.42
1:B:82:GLU:O	1:B:82:GLU:HG3	2.20	0.42
1:B:366:ILE:HD12	1:B:388:ILE:HD13	2.00	0.42
1:C:164:PRO:HB2	1:C:165:GLU:H	1.61	0.41
1:C:174:LYS:O	1:C:178:ILE:HG12	2.19	0.41
1:B:315:ILE:HD13	1:B:338:LEU:HD11	2.02	0.41
1:B:283:VAL:CG2	1:B:366:ILE:HD11	2.50	0.41
1:C:57:ASP:HA	1:C:60:LEU:HD12	2.02	0.41
1:C:279:GLU:O	1:C:391:LYS:HE2	2.21	0.41
1:A:377:PHE:CE1	1:A:502:GLU:HB3	2.56	0.41
1:C:293:ILE:HD11	1:C:317:LEU:HD23	2.02	0.41
1:B:460:PRO:HB3	1:B:527:ALA:HB2	2.03	0.41
1:B:94:VAL:CG2	1:B:366:ILE:HG13	2.51	0.40
1:A:106:GLN:NE2	1:A:231:LYS:HD2	2.18	0.40
1:C:50:LYS:HA	1:C:484:PHE:CD1	2.56	0.40
1:C:189:TYR:O	1:C:193:GLN:HG2	2.21	0.40
1:B:74:LYS:HA	1:B:74:LYS:HD2	1.72	0.40
1:B:364:ASP:HB3	1:B:365:ASP:H	1.71	0.40
1:C:515:GLU:C	1:C:517:THR:H	2.25	0.40
1:C:98:LEU:HD12	1:C:283:VAL:HB	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	540/546 (99%)	513 (95%)	26 (5%)	1 (0%)	52	74
1	B	536/546 (98%)	507 (95%)	28 (5%)	1 (0%)	52	74
1	C	539/546 (99%)	505 (94%)	32 (6%)	2 (0%)	39	60
All	All	1615/1638 (99%)	1525 (94%)	86 (5%)	4 (0%)	52	74

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	164	PRO
1	B	164	PRO
1	C	164	PRO
1	C	516	ILE

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	502/505 (99%)	493 (98%)	9 (2%)	66	87
1	B	500/505 (99%)	486 (97%)	14 (3%)	51	77
1	C	502/505 (99%)	488 (97%)	14 (3%)	51	77
All	All	1504/1515 (99%)	1467 (98%)	37 (2%)	55	81

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	94	VAL
1	A	98	LEU
1	A	123	SER
1	A	244	GLU
1	A	345	SER
1	A	468	LEU
1	A	489	THR
1	A	532	GLU
1	B	6	LYS
1	B	42	VAL
1	B	86	LEU
1	B	94	VAL
1	B	200	PHE
1	B	242	ASN
1	B	257	GLN
1	B	262	ARG
1	B	300	SER
1	B	306	SER
1	B	310	THR
1	B	354	SER
1	B	368	VAL
1	B	507	LYS
1	C	4	VAL
1	C	91	LEU
1	C	92	THR
1	C	94	VAL
1	C	134	ASN
1	C	154	LEU
1	C	197	ASN
1	C	248	ASP
1	C	345	SER
1	C	353	LYS
1	C	432	SER
1	C	442	ASP
1	C	517	THR
1	C	524	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	113	ASN

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Mol	Chain	Res	Type
1	A	160	ASN
1	A	185	HIS
1	A	238	ASN
1	A	343	GLN
1	A	413	ASN
1	A	415	ASN
1	B	53	ASN
1	B	88	ASN
1	B	89	ASN
1	B	106	GLN
1	B	139	ASN
1	B	257	GLN
1	B	309	ASN
1	B	343	GLN
1	B	385	GLN
1	B	415	ASN
1	B	492	HIS
1	B	523	ASN
1	C	10	GLN
1	C	69	ASN
1	C	134	ASN
1	C	151	ASN
1	C	160	ASN
1	C	197	ASN
1	C	238	ASN
1	C	256	ASN
1	C	302	ASN
1	C	385	GLN
1	C	415	ASN
1	C	467	ASN
1	C	510	GLN
1	C	524	GLN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	UPG	A	1544	2	29,38,38	0.71	1 (3%)	43,58,58	1.70	7 (16%)
3	UPG	B	1544	2	29,38,38	0.68	1 (3%)	43,58,58	1.60	6 (13%)
3	UPG	C	1544	2	29,38,38	0.68	1 (3%)	43,58,58	1.73	7 (16%)

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
3	UPG	A	1544	2	-	0/19/59/59	0/3/3/3
3	UPG	B	1544	2	-	0/19/59/59	0/3/3/3
3	UPG	C	1544	2	-	0/19/59/59	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1544	UPG	O4C-C1C	2.52	1.44	1.41
3	B	1544	UPG	O4C-C1C	2.65	1.44	1.41
3	A	1544	UPG	O4C-C1C	2.72	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1544	UPG	PB-O3A-PA	-3.43	123.11	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1544	UPG	O5'-C1'-O3B	-3.42	106.85	111.36
3	A	1544	UPG	PB-O3A-PA	-3.32	123.39	132.73
3	A	1544	UPG	C6'-C5'-C4'	-3.04	105.52	113.02
3	C	1544	UPG	C6'-C5'-C4'	-2.92	105.81	113.02
3	B	1544	UPG	PB-O3A-PA	-2.65	125.29	132.73
3	B	1544	UPG	O5'-C1'-C2'	-2.38	105.39	110.28
3	A	1544	UPG	O4C-C1C-N1	2.01	112.31	108.08
3	A	1544	UPG	C1'-O5'-C5'	2.27	118.14	113.75
3	B	1544	UPG	O4C-C1C-N1	2.27	112.87	108.08
3	C	1544	UPG	C1'-O5'-C5'	2.43	118.46	113.75
3	C	1544	UPG	C3'-C4'-C5'	3.18	115.74	110.20
3	A	1544	UPG	O5'-C5'-C4'	3.21	115.70	109.68
3	B	1544	UPG	C3'-C4'-C5'	3.35	116.03	110.20
3	B	1544	UPG	O5'-C5'-C4'	3.41	116.09	109.68
3	C	1544	UPG	O5'-C5'-C4'	3.46	116.18	109.68
3	A	1544	UPG	C3'-C4'-C5'	3.61	116.49	110.20
3	C	1544	UPG	C4-N3-C2	6.51	120.59	114.14
3	A	1544	UPG	C4-N3-C2	6.52	120.59	114.14
3	B	1544	UPG	C4-N3-C2	6.96	121.04	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1544	UPG	1	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, 95^{th} 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	542/546 (99%)	0.37	24 (4%)	38	43	12, 29, 59, 87	0
1	B	538/546 (98%)	0.36	26 (4%)	34	39	9, 28, 72, 99	0
1	C	541/546 (99%)	0.46	35 (6%)	22	25	12, 30, 71, 89	0
All	All	1621/1638 (98%)	0.40	85 (5%)	31	36	9, 29, 65, 99	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	9.5
1	C	247	ALA	8.4
1	C	166	PHE	6.6
1	B	539	PHE	6.0
1	B	538	TYR	6.0
1	C	157	PHE	5.7
1	C	161	LEU	5.3
1	B	158	ARG	5.3
1	A	540	GLU	5.3
1	C	243	LEU	5.1
1	B	540	GLU	4.7
1	A	539	PHE	4.7
1	C	540	GLU	4.5
1	A	342	VAL	4.4
1	C	538	TYR	4.4
1	B	246	PHE	4.2
1	C	541	GLY	4.1
1	C	539	PHE	4.1
1	B	173	ARG	3.9
1	B	159	GLU	3.9
1	C	246	PHE	3.8
1	B	161	LEU	3.7
1	A	531	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	538	TYR	3.6
1	C	168	TYR	3.5
1	C	1	MET	3.4
1	A	158	ARG	3.4
1	A	542	ALA	3.3
1	B	166	PHE	3.1
1	C	536	LYS	3.1
1	A	335	PHE	3.0
1	B	153	THR	3.0
1	C	159	GLU	3.0
1	B	156	SER	3.0
1	B	157	PHE	2.9
1	A	323	TYR	2.9
1	B	422	THR	2.9
1	B	245	LYS	2.9
1	C	532	GLU	2.8
1	B	534	TYR	2.8
1	C	158	ARG	2.8
1	B	160	ASN	2.7
1	C	81	MET	2.7
1	C	167	ASP	2.7
1	A	161	LEU	2.7
1	A	530	GLN	2.7
1	C	160	ASN	2.7
1	C	534	TYR	2.7
1	B	155	GLU	2.7
1	B	535	LYS	2.6
1	A	166	PHE	2.6
1	B	165	GLU	2.6
1	B	522	PHE	2.6
1	A	246	PHE	2.6
1	A	338	LEU	2.5
1	C	338	LEU	2.5
1	A	344	ARG	2.4
1	C	527	ALA	2.4
1	C	169	ASN	2.4
1	A	2	ASN	2.4
1	C	164	PRO	2.3
1	A	322	LYS	2.3
1	B	151	ASN	2.3
1	B	351	SER	2.3
1	B	340	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	526	ARG	2.3
1	C	155	GLU	2.3
1	A	4	VAL	2.3
1	C	146	VAL	2.3
1	B	247	ALA	2.2
1	B	357	SER	2.2
1	C	178	ILE	2.2
1	A	247	ALA	2.2
1	C	531	PHE	2.2
1	A	536	LYS	2.2
1	C	153	THR	2.2
1	A	15	VAL	2.1
1	C	519	LEU	2.1
1	C	245	LYS	2.1
1	C	463	ARG	2.1
1	C	340	GLU	2.1
1	C	199	GLU	2.0
1	A	165	GLU	2.0
1	A	535	LYS	2.0
1	C	424	PHE	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, 95^{th} 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(Å^2)	Q<0.9
3	UPG	B	1544	36/36	0.96	0.16	-0.41	31,38,42,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	UPG	C	1544	36/36	0.96	0.15	-0.54	26,31,35,38	0
3	UPG	A	1544	36/36	0.96	0.15	-0.72	30,33,37,38	0
2	MN	A	1543	1/1	0.98	0.12	-1.55	35,35,35,35	0
2	MN	C	1542	1/1	0.99	0.15	-	31,31,31,31	0
2	MN	A	1551	1/1	0.89	0.12	-	56,56,56,56	0
2	MN	A	1552	1/1	0.97	0.09	-	63,63,63,63	0
2	MN	B	1541	1/1	0.97	0.15	-	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.