Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:00 AM GMT

PDB ID	:	2VKH
Title	:	CRYSTAL STRUCTURE OF THE CATALYTIC DOMAIN OF LETHAL TOXIN FROM CLOSTRIDIUM SORDELLII IN COMPLEX WITH UDP-GLC AND CALCIUM ION
Authors	:	Ziegler, M.O.P.; Jank, T.; Aktories, K.; Schulz, G.E.
Deposited on	:	2007-12-19
Resolution	:	2.30 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:

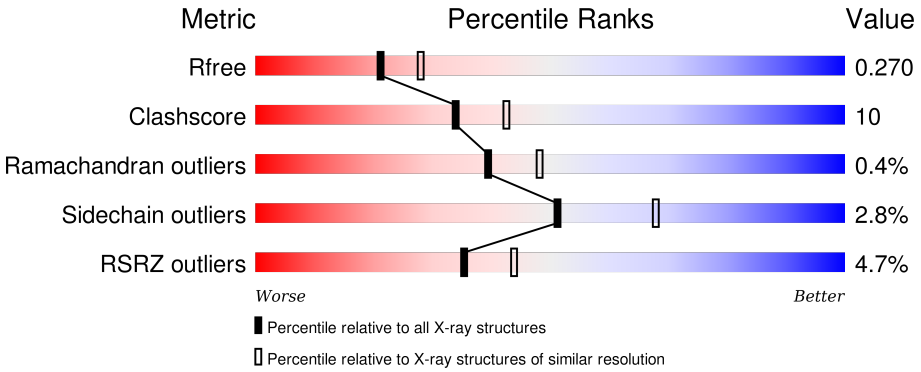
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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% 79% 19%
1	B	546	5% 73% 22%
1	C	546	5% 76% 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13511 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	539	Total	C	N	O	S	0	0	0
			4419	2820	716	867	16			
1	B	533	Total	C	N	O	S	0	0	0
			4374	2792	708	859	15			
1	C	537	Total	C	N	O	S	0	0	0
			4408	2814	714	864	16			

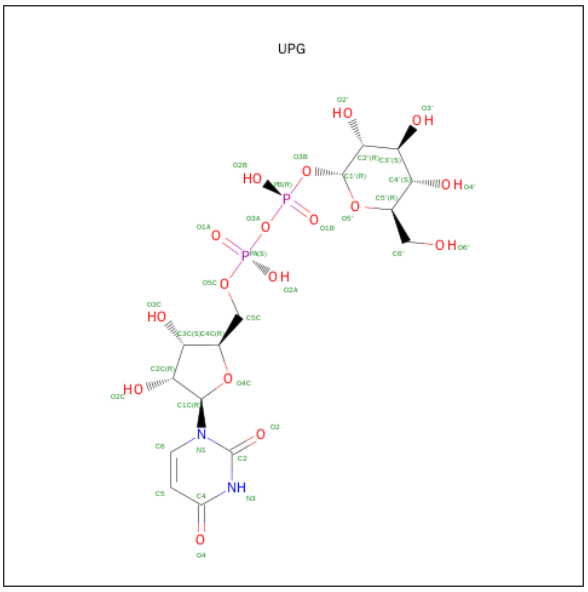
There are 6 discrepancies between the modelled and reference sequences:

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 CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	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.

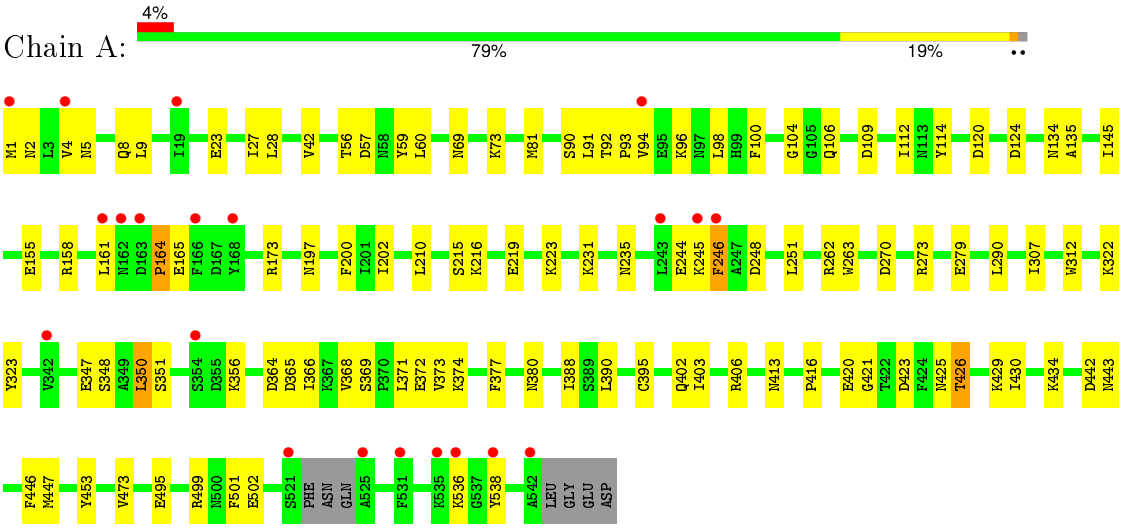
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	60	Total	O	0	0
			60	60		
4	C	75	Total	O	0	0
			75	75		

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.

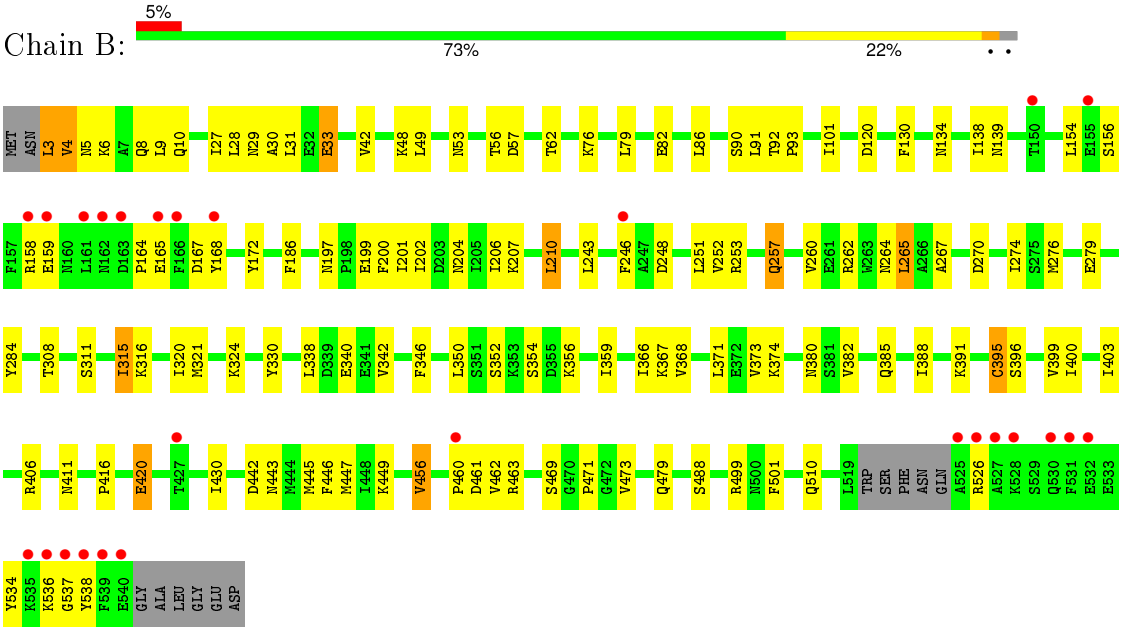
- Molecule 1: CYTOTOXIN L

Chain A:



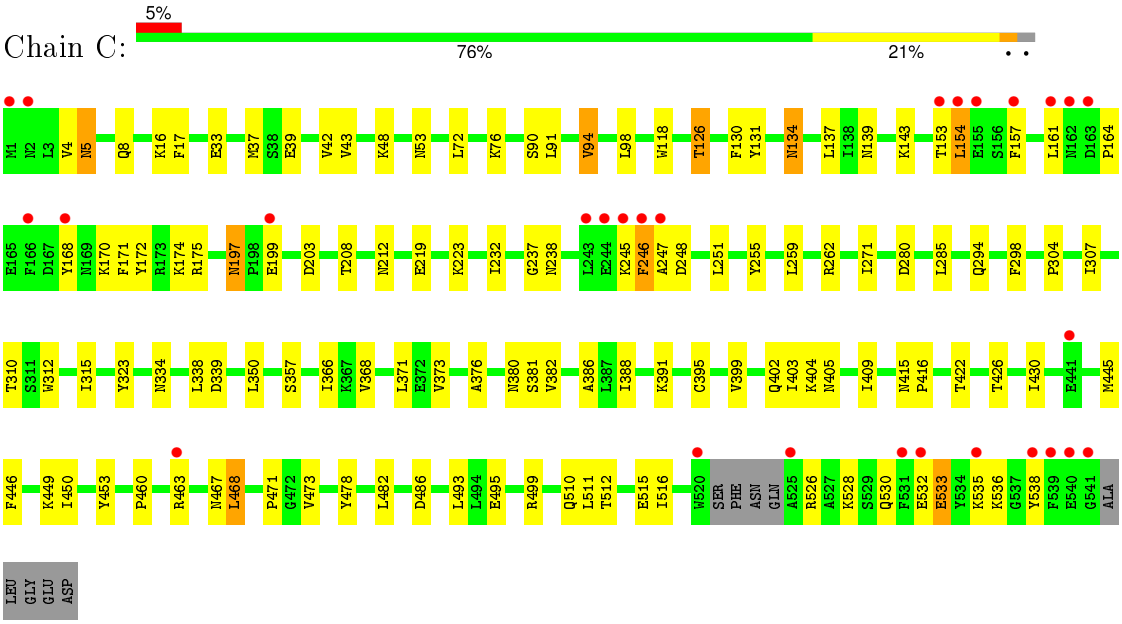
- Molecule 1: CYTOTOXIN L

Chain B:



- Molecule 1: CYTOTOXIN L

Chain C:


5%
76%
21%
M1 N2 L3 V4 N5 Q8 K16 F17 E33 M37 S38 E39 V42 V43 K48 N53 L72 K76 S90 L91 V94 L98 W118 T126 F130 Y131 N134 L137 I138 N139 K143 T153 L154 E155 S156 F157 L161 N162 D163 P164
E165 F166 D167 Y168 N169 K170 F171 Y172 R173 K174 R175 N197 P198 E199 D203 T208 N212 E219 K223 I232 G237 N238 L243 E244 K245 F246 A247 D248 L251 Y255 L259 R262 I271 D280 L285 Q294 F298 P304 I307
T310 S311 W312 I315 Y323 N334 L338 D339 L350 S357 I366 K367 V368 L371 E372 V373 A376 N380 S381 V382 A386 I387 I388 K391 C395 V399 Q402 I403 K404 N405 I409 N415 P416 T422 T426 I430 E441 M445
F446 K449 I450 Y453 P460 R463 N467 L468 P471 G472 V473 Y478 L482 D486 L493 L494 E495 R499 Q510 L511 T512 E515 I516 W520 SER PHE ASN GLN A525 R526 A527 K528 S529 Q530 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	57.17Å 188.59Å 203.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	69.17 – 2.30 69.10 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (69.17-2.30) 96.9 (69.10-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.05 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.235 , 0.273 0.232 , 0.270	Depositor DCC
R_{free} test set	2869 reflections (3.09%)	DCC
Wilson B-factor (Å^2)	27.5	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 60.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.37$, $< L^2 > = 0.19$	Xtriage
Outliers	4 of 95620 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13511	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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 25.53 % 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 3.1193e-03.*

[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, CA

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	0.68	0/4500	0.72	0/6072
1	B	0.70	0/4453	0.73	1/6008 (0.0%)
1	C	0.71	0/4489	0.75	1/6057 (0.0%)
All	All	0.70	0/13442	0.73	2/18137 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	3	LEU	CA-CB-CG	5.50	127.96	115.30
1	C	468	LEU	CA-CB-CG	5.02	126.84	115.30

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	4419	0	4381	77	0
1	B	4374	0	4340	102	0
1	C	4408	0	4371	90	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	36	0	22	0	0
3	B	36	0	22	0	0
3	C	36	0	22	0	0
4	A	64	0	0	0	0
4	B	60	0	0	2	0
4	C	75	0	0	6	0
All	All	13511	0	13158	267	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 10.

All (267) 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:B:460:PRO:HG2	1:B:526:ARG:HG2	1.14	1.10
1:C:315:ILE:HD12	1:C:338:LEU:HD11	1.43	1.00
1:C:304:PRO:HG2	1:C:307:ILE:HD12	1.47	0.96
1:A:4:VAL:HG22	1:A:8:GLN:HB2	1.55	0.89
1:B:385:GLN:HE21	1:B:510:GLN:HE21	1.22	0.88
1:B:158:ARG:HG3	1:B:159:GLU:HG2	1.59	0.83
1:B:246:PHE:HA	1:B:279:GLU:HG3	1.63	0.81
1:A:262:ARG:HE	1:A:453:TYR:HE2	1.26	0.81
1:B:460:PRO:CG	1:B:526:ARG:HG2	2.07	0.79
1:C:366:ILE:HG21	1:C:388:ILE:HD13	1.65	0.78
1:B:158:ARG:HG3	1:B:159:GLU:N	2.03	0.73
1:C:373:VAL:HG23	1:C:395:CYS:HB3	1.70	0.73
1:B:373:VAL:HG23	1:B:395:CYS:HB3	1.71	0.73
1:C:4:VAL:HG22	1:C:8:GLN:HB2	1.70	0.72
1:B:120:ASP:OD2	1:B:356:LYS:NZ	2.22	0.72
1:A:402:GLN:CB	1:A:473:VAL:HG13	2.20	0.71
1:B:42:VAL:HG21	1:B:90:SER:CB	2.19	0.71
1:C:126:THR:HG22	4:C:2011:HOH:O	1.90	0.70
1:A:403:ILE:HG13	1:A:473:VAL:HG11	1.73	0.70
1:C:4:VAL:CG2	1:C:8:GLN:HB3	2.22	0.70
1:C:42:VAL:HG21	1:C:90:SER:CB	2.22	0.69
1:A:406:ARG:HG2	1:A:446:PHE:CE1	2.27	0.69
1:A:402:GLN:HB2	1:A:473:VAL:HG13	1.75	0.69
1:A:5:ASN:HB2	1:A:8:GLN:HG3	1.75	0.67
1:C:4:VAL:CG2	1:C:8:GLN:CB	2.73	0.67
1:B:253:ARG:NH2	4:B:2028:HOH:O	2.24	0.67
1:B:42:VAL:HG21	1:B:90:SER:HB3	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:385:GLN:NE2	1:B:510:GLN:HE21	1.92	0.66
1:C:154:LEU:HD22	1:C:171:PHE:HE1	1.61	0.66
1:B:134:ASN:ND2	1:B:201:ILE:HG12	2.11	0.66
1:C:42:VAL:HG21	1:C:90:SER:HB3	1.78	0.66
1:C:402:GLN:HB2	1:C:473:VAL:HG13	1.76	0.66
1:C:153:THR:HG21	1:C:175:ARG:HA	1.77	0.65
1:A:1:MET:SD	1:C:422:THR:HG21	2.37	0.64
1:C:94:VAL:HG13	1:C:368:VAL:HG11	1.79	0.64
1:A:4:VAL:CG2	1:A:8:GLN:HB2	2.27	0.63
1:C:208:THR:HG22	1:C:212:ASN:HD22	1.64	0.63
1:C:323:TYR:HB2	1:C:350:LEU:HD23	1.81	0.62
1:B:366:ILE:HD12	1:B:388:ILE:HD13	1.82	0.61
1:A:413:ASN:HD22	1:A:434:LYS:HB3	1.65	0.61
1:A:93:PRO:HA	1:A:366:ILE:O	2.00	0.61
1:A:248:ASP:HB3	1:A:251:LEU:HB2	1.81	0.61
1:A:423:ASP:OD1	1:A:426:THR:HB	2.00	0.61
1:A:421:GLY:HA2	1:A:426:THR:CG2	2.30	0.61
1:C:4:VAL:HG22	1:C:8:GLN:CB	2.31	0.60
1:B:395:CYS:O	1:B:399:VAL:HG23	2.00	0.60
1:B:53:ASN:HD22	1:B:79:LEU:HD12	1.65	0.60
1:A:380:ASN:HD22	1:A:495:GLU:CD	2.05	0.60
1:C:197:ASN:HD22	1:C:199:GLU:H	1.49	0.59
1:C:33:GLU:O	1:C:37:MET:HG3	2.01	0.59
1:B:29:ASN:O	1:B:33:GLU:HG2	2.02	0.59
1:C:298:PHE:CZ	1:C:350:LEU:HD11	2.38	0.59
1:C:391:LYS:HE2	4:C:2039:HOH:O	2.01	0.58
1:B:243:LEU:HB3	1:B:246:PHE:CD2	2.37	0.58
1:A:373:VAL:HG23	1:A:395:CYS:HB3	1.84	0.58
1:B:248:ASP:O	1:B:252:VAL:HG23	2.03	0.58
1:C:53:ASN:ND2	4:C:2007:HOH:O	2.34	0.58
1:B:316:LYS:O	1:B:320:ILE:HG12	2.03	0.58
1:B:396:SER:O	1:B:400:ILE:HG12	2.04	0.57
1:A:106:GLN:HE21	1:A:231:LYS:HD2	1.69	0.57
1:B:197:ASN:HB3	1:B:200:PHE:CD2	2.39	0.57
1:B:42:VAL:HG21	1:B:90:SER:HB2	1.83	0.57
1:A:402:GLN:HB3	1:A:473:VAL:HG13	1.86	0.57
1:A:164:PRO:HG2	1:A:165:GLU:H	1.69	0.57
1:A:1:MET:HB2	1:C:422:THR:CG2	2.35	0.57
1:A:323:TYR:HB2	1:A:350:LEU:HD23	1.86	0.57
1:B:315:ILE:HD11	1:B:346:PHE:CZ	2.40	0.57
1:B:168:TYR:O	1:B:172:TYR:HD1	1.88	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:GLY:HA2	1:A:426:THR:HG21	1.87	0.56
1:C:463:ARG:O	1:C:467:ASN:ND2	2.37	0.56
1:C:139:ASN:O	1:C:143:LYS:HG3	2.05	0.56
1:C:4:VAL:HG23	1:C:8:GLN:HB3	1.86	0.56
1:C:350:LEU:C	4:C:2051:HOH:O	2.42	0.56
1:B:251:LEU:HD21	1:B:400:ILE:HD12	1.86	0.56
1:B:416:PRO:O	1:B:420:GLU:HG3	2.05	0.56
1:C:532:GLU:O	1:C:535:LYS:HG2	2.05	0.56
1:C:161:LEU:HD11	1:C:535:LYS:HB2	1.86	0.56
1:C:402:GLN:CB	1:C:473:VAL:HG13	2.35	0.56
1:A:307:ILE:HD11	1:A:312:TRP:CE3	2.40	0.56
1:A:94:VAL:HG11	1:A:388:ILE:CG2	2.36	0.56
1:B:93:PRO:HA	1:B:366:ILE:O	2.07	0.55
1:B:257:GLN:HE22	1:B:411:ASN:HD21	1.54	0.55
1:C:42:VAL:HG21	1:C:90:SER:HB2	1.89	0.55
1:A:42:VAL:HG21	1:A:90:SER:CB	2.36	0.55
1:B:371:LEU:O	1:B:395:CYS:HB2	2.06	0.55
1:B:204:ASN:HA	1:B:207:LYS:HE2	1.88	0.55
1:A:366:ILE:HG21	1:A:388:ILE:HD13	1.89	0.55
1:C:312:TRP:CE3	1:C:315:ILE:HD11	2.43	0.54
1:C:208:THR:HG22	1:C:212:ASN:ND2	2.22	0.54
1:B:93:PRO:HD3	1:B:367:LYS:HE3	1.90	0.54
1:B:9:LEU:HD22	1:B:31:LEU:HD22	1.88	0.54
1:B:62:THR:HG22	1:B:62:THR:O	2.08	0.53
1:B:6:LYS:O	1:B:10:GLN:HG3	2.08	0.53
1:A:57:ASP:HA	1:A:60:LEU:HD12	1.89	0.53
1:B:202:ILE:HD13	1:B:260:VAL:CG2	2.39	0.53
1:A:96:LYS:NZ	1:A:124:ASP:OD2	2.35	0.53
1:B:158:ARG:CG	1:B:159:GLU:HG2	2.34	0.53
1:C:460:PRO:HB2	1:C:526:ARG:HG3	1.91	0.53
1:C:153:THR:O	1:C:157:PHE:HD2	1.92	0.52
1:C:294:GLN:NE2	1:C:357:SER:O	2.41	0.52
1:A:231:LYS:O	1:A:235:ASN:ND2	2.36	0.52
1:C:449:LYS:HB3	1:C:467:ASN:ND2	2.25	0.52
1:C:42:VAL:HG12	1:C:371:LEU:HD11	1.91	0.52
1:C:298:PHE:HZ	1:C:350:LEU:HD11	1.75	0.52
1:C:251:LEU:HD22	1:C:271:ILE:HG23	1.91	0.52
1:A:244:GLU:HG3	1:A:245:LYS:H	1.74	0.52
1:C:4:VAL:CG2	1:C:8:GLN:HB2	2.37	0.52
1:B:246:PHE:CD1	1:B:276:MET:CE	2.94	0.51
1:C:153:THR:HG21	1:C:175:ARG:CA	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:VAL:HG13	1:C:368:VAL:CG1	2.39	0.51
1:B:380:ASN:OD1	1:B:499:ARG:NH2	2.42	0.51
1:B:443:ASN:O	1:B:447:MET:HG2	2.11	0.51
1:B:101:ILE:HD12	1:B:284:TYR:CE1	2.46	0.51
1:C:137:LEU:HB2	1:C:203:ASP:OD1	2.10	0.51
1:B:315:ILE:HD11	1:B:346:PHE:CE2	2.46	0.51
1:A:155:GLU:HG3	1:A:158:ARG:HH21	1.76	0.51
1:B:320:ILE:HD13	1:B:350:LEU:HD21	1.92	0.51
1:B:33:GLU:OE2	1:B:48:LYS:NZ	2.45	0.50
1:C:197:ASN:ND2	1:C:199:GLU:H	2.10	0.50
1:C:380:ASN:HD22	1:C:495:GLU:CD	2.14	0.50
1:A:416:PRO:O	1:A:420:GLU:HG2	2.10	0.50
1:A:323:TYR:CE1	1:A:347:GLU:HG3	2.47	0.50
1:B:202:ILE:HD13	1:B:260:VAL:HG21	1.92	0.50
1:A:1:MET:HG2	1:A:81:MET:CE	2.42	0.50
1:B:382:VAL:HG23	1:B:471:PRO:HB3	1.92	0.50
1:B:368:VAL:HG21	1:B:388:ILE:CG2	2.42	0.49
1:B:406:ARG:HG2	1:B:446:PHE:CE1	2.47	0.49
1:B:158:ARG:CG	1:B:159:GLU:N	2.74	0.49
1:C:315:ILE:HG22	1:C:334:ASN:HB2	1.95	0.49
1:B:338:LEU:HD23	1:B:342:VAL:HG12	1.94	0.49
1:B:279:GLU:O	1:B:391:LYS:HE3	2.13	0.49
1:B:251:LEU:CD2	1:B:400:ILE:HD12	2.43	0.49
1:A:42:VAL:HG21	1:A:90:SER:HB2	1.95	0.49
1:B:202:ILE:CD1	1:B:260:VAL:HG21	2.43	0.48
1:B:456:VAL:HG22	1:B:462:VAL:CG1	2.43	0.48
1:A:443:ASN:O	1:A:447:MET:HG2	2.13	0.48
1:C:512:THR:O	1:C:516:ILE:HG12	2.13	0.48
1:B:92:THR:OG1	1:B:93:PRO:HD2	2.12	0.48
1:C:245:LYS:C	1:C:247:ALA:H	2.15	0.48
1:C:245:LYS:C	1:C:247:ALA:N	2.66	0.48
1:B:536:LYS:C	1:B:538:TYR:H	2.16	0.48
1:B:324:LYS:HE3	1:B:359:ILE:HD11	1.95	0.48
1:C:373:VAL:O	1:C:478:TYR:OH	2.29	0.48
1:A:114:TYR:CD1	1:A:290:LEU:HG	2.48	0.48
1:C:131:TYR:CD1	1:C:232:ILE:HG12	2.48	0.48
1:C:154:LEU:HD22	1:C:171:PHE:CE1	2.46	0.48
1:B:57:ASP:OD1	1:B:76:LYS:NZ	2.37	0.48
1:B:206:ILE:HG22	1:B:210:LEU:CD2	2.43	0.48
1:A:262:ARG:NE	1:A:453:TYR:HE2	2.05	0.48
1:B:479:GLN:HG2	1:B:488:SER:OG	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:MET:HG3	1:B:330:TYR:CG	2.48	0.48
1:A:23:GLU:O	1:A:27:ILE:HG12	2.14	0.47
1:B:456:VAL:HG22	1:B:462:VAL:HG11	1.96	0.47
1:B:274:ILE:HG23	1:B:400:ILE:CD1	2.44	0.47
1:A:109:ASP:OD1	1:A:231:LYS:NZ	2.34	0.47
1:A:219:GLU:HG2	1:A:223:LYS:NZ	2.29	0.47
1:B:368:VAL:HG21	1:B:388:ILE:HG22	1.96	0.47
1:C:37:MET:SD	1:C:48:LYS:HG2	2.54	0.47
1:A:42:VAL:HG21	1:A:90:SER:HB3	1.97	0.47
1:B:399:VAL:HG13	1:B:473:VAL:CG1	2.44	0.47
1:C:262:ARG:HG3	1:C:453:TYR:OH	2.14	0.47
1:A:59:TYR:C	1:A:59:TYR:CD2	2.87	0.47
1:A:322:LYS:HD3	1:A:323:TYR:CZ	2.50	0.47
1:B:168:TYR:O	1:B:172:TYR:CD1	2.68	0.47
1:C:510:GLN:O	1:C:515:GLU:HG2	2.15	0.47
1:B:246:PHE:CE1	1:B:276:MET:CE	2.99	0.46
1:B:284:TYR:C	1:B:284:TYR:CD2	2.87	0.46
1:A:155:GLU:CG	1:A:158:ARG:HH21	2.28	0.46
1:C:405:ASN:O	1:C:409:ILE:HG12	2.14	0.46
1:C:232:ILE:HG13	1:C:237:GLY:HA3	1.97	0.46
1:C:219:GLU:O	1:C:223:LYS:HG3	2.14	0.46
1:B:154:LEU:HD11	1:B:534:TYR:HB3	1.98	0.46
1:C:4:VAL:HG23	1:C:8:GLN:CB	2.44	0.46
1:A:158:ARG:O	1:A:161:LEU:HD13	2.15	0.46
1:B:49:LEU:HD11	1:B:82:GLU:HG3	1.98	0.46
1:C:536:LYS:C	1:C:538:TYR:H	2.19	0.46
1:C:399:VAL:HG13	1:C:473:VAL:HG12	1.97	0.46
1:A:246:PHE:CB	1:A:279:GLU:HG2	2.46	0.46
1:C:280:ASP:OD1	4:C:2041:HOH:O	2.21	0.45
1:A:270:ASP:O	1:A:273:ARG:HG2	2.16	0.45
1:A:197:ASN:O	1:A:200:PHE:HB2	2.17	0.45
1:B:186:PHE:HE2	1:B:260:VAL:O	2.00	0.45
1:C:403:ILE:HG13	1:C:473:VAL:HG11	1.99	0.45
1:C:445:MET:O	1:C:449:LYS:HD2	2.17	0.45
1:A:245:LYS:HD3	1:A:279:GLU:OE2	2.16	0.45
1:C:304:PRO:HG2	1:C:307:ILE:CD1	2.32	0.45
1:A:368:VAL:HG13	1:A:390:LEU:HG	1.98	0.45
1:A:426:THR:O	1:A:430:ILE:HG12	2.17	0.45
1:B:399:VAL:O	1:B:403:ILE:HG13	2.17	0.45
1:C:446:PHE:O	1:C:450:ILE:HB	2.16	0.45
1:A:94:VAL:HG12	1:A:368:VAL:CG1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:TYR:CE2	1:C:259:LEU:HD22	2.51	0.44
1:A:499:ARG:O	1:A:502:GLU:HG2	2.18	0.44
1:B:5:ASN:OD1	1:B:8:GLN:HG3	2.17	0.44
1:B:463:ARG:HA	1:B:463:ARG:HD3	1.79	0.44
1:C:371:LEU:O	1:C:395:CYS:HB2	2.17	0.44
1:B:270:ASP:HB3	1:B:469:SER:HB2	1.99	0.44
1:A:27:ILE:HD11	1:A:56:THR:HA	2.00	0.44
1:A:98:LEU:HD22	1:A:100:PHE:CE1	2.52	0.44
1:B:445:MET:CE	1:B:449:LYS:HE3	2.47	0.44
1:B:138:ILE:HG21	1:B:265:LEU:HD11	1.99	0.44
1:B:460:PRO:O	1:B:461:ASP:HB2	2.16	0.44
1:B:420:GLU:O	1:B:430:ILE:HD12	2.17	0.44
1:B:27:ILE:HD11	1:B:56:THR:HA	1.99	0.44
1:B:320:ILE:CD1	1:B:350:LEU:HD21	2.48	0.44
1:A:536:LYS:C	1:A:538:TYR:H	2.21	0.44
1:B:264:ASN:ND2	1:B:267:ALA:HB2	2.33	0.44
1:B:536:LYS:O	1:B:538:TYR:N	2.51	0.44
1:B:206:ILE:CG2	1:B:210:LEU:CD2	2.96	0.44
1:C:511:LEU:HD23	1:C:511:LEU:HA	1.81	0.43
1:A:9:LEU:HD23	1:A:28:LEU:HD23	2.00	0.43
1:C:134:ASN:N	1:C:134:ASN:HD22	2.17	0.43
1:A:374:LYS:HA	1:A:501:PHE:O	2.18	0.43
1:C:5:ASN:ND2	1:C:8:GLN:HG3	2.34	0.43
1:A:421:GLY:CA	1:A:426:THR:HG22	2.49	0.43
1:B:130:PHE:CZ	1:B:276:MET:HE2	2.54	0.43
1:B:315:ILE:HD13	1:B:338:LEU:HD21	2.00	0.43
1:A:377:PHE:CE1	1:A:502:GLU:HB3	2.53	0.43
1:C:168:TYR:CE1	1:C:528:LYS:HD2	2.53	0.43
1:B:308:THR:HG23	4:B:2033:HOH:O	2.18	0.43
1:C:72:LEU:O	1:C:76:LYS:HG3	2.19	0.43
1:B:311:SER:O	1:B:315:ILE:HG23	2.19	0.43
1:A:210:LEU:HB3	1:A:216:LYS:HB2	2.00	0.43
1:A:104:GLY:HA2	1:A:135:ALA:O	2.18	0.43
1:A:145:ILE:HG13	1:A:263:TRP:CH2	2.54	0.43
1:B:139:ASN:HD22	1:B:139:ASN:HA	1.72	0.43
1:A:120:ASP:OD2	1:A:356:LYS:NZ	2.47	0.43
1:B:274:ILE:HG23	1:B:400:ILE:HD13	2.01	0.42
1:C:5:ASN:HD21	1:C:8:GLN:HG3	1.84	0.42
1:C:170:LYS:HE2	1:C:174:LYS:HD2	2.00	0.42
1:A:425:ASN:O	1:A:429:LYS:HG2	2.19	0.42
1:C:404:LYS:HE2	1:C:404:LYS:HB2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:415:ASN:HB2	1:C:416:PRO:HD3	2.00	0.42
1:C:382:VAL:HG23	1:C:471:PRO:HB3	2.00	0.42
1:A:134:ASN:O	1:A:202:ILE:HB	2.20	0.42
1:C:482:LEU:HD12	1:C:493:LEU:HD11	2.01	0.42
1:A:1:MET:HG2	1:A:81:MET:HE2	2.01	0.42
1:C:426:THR:O	1:C:430:ILE:HG12	2.19	0.42
1:C:530:GLN:HA	1:C:533:GLU:HB2	2.02	0.42
1:C:248:ASP:OD1	4:C:2032:HOH:O	2.22	0.42
1:A:164:PRO:CG	1:A:165:GLU:H	2.32	0.42
1:C:495:GLU:OE2	1:C:499:ARG:NH2	2.51	0.42
1:B:246:PHE:CE1	1:B:276:MET:HE1	2.55	0.41
1:A:364:ASP:HB3	1:A:365:ASP:H	1.41	0.41
1:A:369:SER:HB3	1:A:372:GLU:HG2	2.02	0.41
1:B:197:ASN:OD1	1:B:199:GLU:HB2	2.20	0.41
1:A:421:GLY:CA	1:A:426:THR:CG2	2.99	0.41
1:B:246:PHE:HA	1:B:279:GLU:CG	2.43	0.41
1:B:91:LEU:HB3	1:B:367:LYS:HB3	2.03	0.41
1:A:69:ASN:O	1:A:73:LYS:HG2	2.21	0.41
1:B:30:ALA:O	1:B:48:LYS:HE3	2.20	0.41
1:B:262:ARG:HA	1:B:262:ARG:HD3	1.89	0.41
1:B:158:ARG:HE	1:B:158:ARG:HB2	1.67	0.40
1:A:1:MET:HG2	1:A:81:MET:HE1	2.03	0.40
1:A:112:ILE:HD12	1:A:231:LYS:NZ	2.36	0.40
1:A:219:GLU:HG2	1:A:223:LYS:HZ2	1.86	0.40
1:C:16:LYS:HE3	1:C:17:PHE:CZ	2.57	0.40
1:B:246:PHE:CE1	1:B:276:MET:HE3	2.56	0.40
1:A:92:THR:OG1	1:A:93:PRO:HD2	2.21	0.40
1:B:6:LYS:HE3	1:B:28:LEU:HB3	2.04	0.40
1:C:168:TYR:O	1:C:172:TYR:HD1	2.04	0.40
1:B:374:LYS:HA	1:B:501:PHE:O	2.21	0.40
1:B:165:GLU:C	1:B:167:ASP:H	2.25	0.40
1:C:118:TRP:CE2	1:C:285:LEU:HD13	2.56	0.40
1:B:3:LEU:HG	1:B:4:VAL:H	1.86	0.40
1:C:376:ALA:HB2	1:C:386:ALA:HB3	2.04	0.40
1:C:130:PHE:HA	1:C:238:ASN:O	2.21	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	535/546 (98%)	505 (94%)	29 (5%)	1 (0%)	52	64
1	B	529/546 (97%)	500 (94%)	26 (5%)	3 (1%)	30	36
1	C	533/546 (98%)	502 (94%)	29 (5%)	2 (0%)	39	48
All	All	1597/1638 (98%)	1507 (94%)	84 (5%)	6 (0%)	39	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	164	PRO
1	A	164	PRO
1	B	164	PRO
1	C	246	PHE
1	B	537	GLY
1	B	456	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	499/505 (99%)	488 (98%)	11 (2%)	60	77
1	B	495/505 (98%)	481 (97%)	14 (3%)	51	68
1	C	498/505 (99%)	481 (97%)	17 (3%)	44	59
All	All	1492/1515 (98%)	1450 (97%)	42 (3%)	51	68

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

Mol	Chain	Res	Type
1	A	2	ASN
1	A	91	LEU
1	A	173	ARG
1	A	215	SER
1	A	246	PHE
1	A	348	SER
1	A	350	LEU
1	A	351	SER
1	A	371	LEU
1	A	426	THR
1	A	442	ASP
1	B	4	VAL
1	B	33	GLU
1	B	86	LEU
1	B	156	SER
1	B	210	LEU
1	B	257	GLN
1	B	265	LEU
1	B	315	ILE
1	B	340	GLU
1	B	352	SER
1	B	354	SER
1	B	395	CYS
1	B	420	GLU
1	B	442	ASP
1	C	5	ASN
1	C	39	GLU
1	C	43	VAL
1	C	91	LEU
1	C	94	VAL
1	C	98	LEU
1	C	126	THR
1	C	134	ASN
1	C	154	LEU
1	C	197	ASN
1	C	246	PHE
1	C	310	THR
1	C	339	ASP
1	C	381	SER
1	C	468	LEU
1	C	486	ASP
1	C	533	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	20	GLN
1	A	106	GLN
1	A	113	ASN
1	A	160	ASN
1	A	185	HIS
1	A	343	GLN
1	A	385	GLN
1	A	413	ASN
1	A	415	ASN
1	A	467	ASN
1	A	492	HIS
1	A	510	GLN
1	A	530	GLN
1	B	10	GLN
1	B	53	ASN
1	B	88	ASN
1	B	139	ASN
1	B	257	GLN
1	B	343	GLN
1	B	415	ASN
1	B	467	ASN
1	B	510	GLN
1	C	10	GLN
1	C	69	ASN
1	C	106	GLN
1	C	116	ASN
1	C	134	ASN
1	C	151	ASN
1	C	193	GLN
1	C	197	ASN
1	C	212	ASN
1	C	238	ASN
1	C	242	ASN
1	C	385	GLN
1	C	415	ASN
1	C	467	ASN
1	C	492	HIS
1	C	510	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 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	0.66	0	43,58,58	1.62	7 (16%)
3	UPG	B	1544	2	29,38,38	1.32	4 (13%)	43,58,58	1.67	6 (13%)
3	UPG	C	1544	2	29,38,38	0.82	1 (3%)	43,58,58	1.81	9 (20%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1544	UPG	C6-N1	-3.33	1.31	1.35
3	B	1544	UPG	PA-O2A	-2.20	1.45	1.54
3	B	1544	UPG	PB-O2B	-2.18	1.45	1.54
3	B	1544	UPG	O4C-C4C	-2.14	1.40	1.45
3	C	1544	UPG	O4C-C1C	3.15	1.45	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1544	UPG	PB-O3A-PA	-3.65	122.47	132.73
3	B	1544	UPG	PB-O3A-PA	-3.48	122.94	132.73
3	C	1544	UPG	PB-O3A-PA	-2.80	124.88	132.73
3	A	1544	UPG	O5'-C1'-C2'	-2.67	104.80	110.28
3	B	1544	UPG	O3'-C3'-C4'	-2.66	104.34	110.34
3	C	1544	UPG	O6'-C6'-C5'	-2.43	103.31	111.33
3	C	1544	UPG	O5'-C1'-O3B	-2.40	108.19	111.36
3	C	1544	UPG	C6-N1-C2	-2.09	117.89	121.28
3	C	1544	UPG	O4'-C4'-C3'	-2.03	105.77	110.34
3	C	1544	UPG	O4C-C1C-N1	2.14	112.60	108.08
3	A	1544	UPG	O3B-C1'-C2'	2.15	112.40	108.39
3	A	1544	UPG	C1'-O5'-C5'	2.26	118.13	113.75
3	A	1544	UPG	O5'-C5'-C4'	2.36	114.11	109.68
3	B	1544	UPG	O5'-C5'-C6'	2.45	112.55	106.36
3	A	1544	UPG	O4C-C1C-N1	2.70	113.78	108.08
3	C	1544	UPG	C3'-C4'-C5'	2.85	115.16	110.20
3	B	1544	UPG	O5'-C5'-C4'	3.10	115.50	109.68
3	C	1544	UPG	O5'-C5'-C4'	3.72	116.67	109.68
3	B	1544	UPG	C1'-O5'-C5'	3.79	121.10	113.75
3	B	1544	UPG	C4-N3-C2	6.09	120.17	114.14
3	A	1544	UPG	C4-N3-C2	6.92	121.00	114.14
3	C	1544	UPG	C4-N3-C2	7.80	121.87	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	539/546 (98%)	0.41	21 (3%)	43	52	18, 33, 59, 75	0
1	B	533/546 (97%)	0.49	26 (4%)	33	42	18, 32, 69, 95	0
1	C	537/546 (98%)	0.49	28 (5%)	31	39	18, 31, 61, 81	0
All	All	1609/1638 (98%)	0.46	75 (4%)	35	44	18, 32, 61, 95	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	247	ALA	12.1
1	B	161	LEU	9.2
1	B	538	TYR	8.7
1	B	535	LYS	7.7
1	C	525	ALA	7.6
1	B	246	PHE	7.5
1	B	525	ALA	7.4
1	B	158	ARG	6.3
1	A	161	LEU	5.9
1	C	243	LEU	5.8
1	B	537	GLY	5.6
1	C	168	TYR	5.6
1	B	540	GLU	5.5
1	C	161	LEU	5.4
1	B	168	TYR	5.3
1	B	539	PHE	5.2
1	B	166	PHE	4.9
1	C	539	PHE	4.9
1	A	163	ASP	4.9
1	A	521	SER	4.8
1	C	541	GLY	4.4
1	A	542	ALA	4.3
1	B	530	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	531	PHE	4.2
1	C	166	PHE	4.2
1	B	531	PHE	4.2
1	C	246	PHE	4.1
1	C	538	TYR	4.0
1	B	163	ASP	3.9
1	C	162	ASN	3.7
1	C	199	GLU	3.7
1	A	19	ILE	3.6
1	C	520	TRP	3.6
1	B	165	GLU	3.5
1	B	527	ALA	3.5
1	B	528	LYS	3.5
1	A	246	PHE	3.5
1	B	159	GLU	3.3
1	A	168	TYR	3.3
1	A	1	MET	3.3
1	C	1	MET	3.2
1	B	427	THR	3.2
1	C	540	GLU	3.2
1	A	538	TYR	3.1
1	C	163	ASP	3.1
1	A	162	ASN	3.1
1	B	526	ARG	3.1
1	B	162	ASN	3.0
1	A	535	LYS	2.9
1	A	4	VAL	2.9
1	C	244	GLU	2.8
1	C	245	LYS	2.7
1	C	535	LYS	2.7
1	C	155	GLU	2.6
1	C	532	GLU	2.6
1	C	157	PHE	2.6
1	C	531	PHE	2.6
1	A	536	LYS	2.4
1	A	166	PHE	2.4
1	B	155	GLU	2.3
1	A	342	VAL	2.3
1	B	536	LYS	2.3
1	C	463	ARG	2.2
1	B	150	THR	2.2
1	C	154	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	441	GLU	2.2
1	B	532	GLU	2.1
1	C	2	ASN	2.1
1	A	245	LYS	2.1
1	A	354	SER	2.1
1	A	525	ALA	2.1
1	B	460	PRO	2.0
1	A	94	VAL	2.0
1	C	153	THR	2.0
1	A	243	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no 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	0.95	0.14	-0.73	21,33,44,51	0
3	UPG	A	1544	36/36	0.98	0.12	-1.55	21,33,44,52	0
3	UPG	C	1544	36/36	0.97	0.11	-2.38	18,29,40,46	0
2	CA	A	1543	1/1	0.99	0.07	-3.36	27,27,27,27	0
2	CA	C	1543	1/1	0.99	0.08	-	29,29,29,29	0
2	CA	B	1543	1/1	0.99	0.06	-	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.